Markov Chain Based Algorithms for the Hamiltonian Cycle Problem

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To Giang and Trixie, the two most important women in my life.

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Summary

In this thesis, we continue an innovative line of research in which the Hamiltonian cycle problem (HCP) is embedded in a Markov decision process. This embedding leads to optimisation problems that we attempt to solve using methods that take advantage of the special structure from both HCP and Markov decision processes theory. Since this approach was first suggested in 1992, a number of new theoretical results and optimisation models have been developed for HCP. However, the development of numerical procedures, based on this approach, that actually find Hamiltonian cycles has lagged the rapid development of new theory. The present thesis seeks to redress this imbalance by progressing a number of new algorithmic approaches that take advantage of the Markov decision processes perspective. We present the results in three chapters, each describing a different approach to solving HCP.

In Chapter 2, we detail a method of constructing and intelligently searching a logical branching tree to find a Hamiltonian cycle, or to determine that one does not exist. The benefit of the algorithm, compared to standard branch and bound methods, is that the growth of the tree is significantly slower due to particular checks and fathoming routines. We propose five branching strategies and present numerical results to compare their effectiveness. We then augment the original model with additional constraints that further reduce the growth of the tree, and compare the performance between the original and augmented methods. Finally, we adapt the Markov decision process embedding and these additional constraints to a mixed integer programming method that succeeds in solving large graphs, and compare its performance to some well known mixed integer programming formulations of HCP. We include Hamiltonian solutions to four large non-regular graphs, specifically a

250-node, 500-node, 1000-node and 2000-node graph, obtained by this method.

In Chapter 3, we introduce an interior point method designed to solve an optimisation program that is equivalent to HCP. The chapter is divided into two halves. In the first half, comprised of Sections 3.1 – 3.5, we present an algorithm that implements a variant of the interior point method designed for HCP. This algorithm uses a series of component algorithms designed to take maximum advantage of the significant amount of sparsity inherent in HCP. We present numerical results that demonstrate how reliably Hamiltonian solutions were found, and how much computational power was required. We also propose a conjecture about the existence of a unique strictly interior stationary point in the optimisation program. We further conjecture about the possible use of this stationary point in solving the graph isomorphism problem. In the second half, comprised of Sections 3.6 – 3.7, we investigate an efficient method of calculating derivatives of the objective function in the optimisation program by use of a sparse LU decomposition. Finally, we present an algorithm to compute these derivatives, intended for use in the interior point method presented in Section 3.3, with complexity equal to that of the original sparse LU decomposition.

In Chapter 4, we analyse a polytope, the extreme points of which include all Hamiltonian solutions. We investigate the behaviour induced by perturbation and discount parameters influencing the equations that define this polytope. We then show that the Hamiltonian solution vectors contain entries that are polynomials in these parameters. These polynomials define curves and surfaces, and their exact form is derived by considering the determinant of a matrix of a particular structure, but arbitrary size. We formulate two polynomially solvable feasibility problems that are feasible for all Hamiltonian solutions, but difficult to satisfy by other solutions. We then conjecture that these feasibility programs can identify the majority of non-Hamiltonian graphs, and supply experimental results that support this conjecture.

Throughout this thesis we demonstrate the flexibility and power offered by the embedding of HCP in a Markov decision process. Unlike most graph theory-based solvers, we make few assumptions about the structure of graphs and this allows us to solve a wide variety of graphs. It is worth noting that all models discussed in this thesis have been implemented in the modeling language MATLAB (version 7.4.0.336), with a CPLEX interface used as a linear solver when necessary. Consequently, the running times for these models are not indicative of their full potential. Nonetheless, for each algorithm we provide running times for several test graphs to demonstrate the change in running times for different sized graphs. The sole exception is the mixed integer programming model in Chapter 2.9, which is coded entirely in IBM ILOG OPL-CPLEX, an extremely efficient language for solving these types of models. That this mixed integer programming model is able to solve such large graphs is a testament to the potential offered by the Markov decision process embedding. We expect that subsequent implementations in compiled languages will result in significant improvements in speed and memory management for the other models given in this thesis.

Declaration

I declare that this thesis presents work carried out by myself and does not incorporate without acknowledgment any material previously submitted for a degree or diploma in any university; that to the best of my knowledge it does not contain any materials previously published or written by another person except where due reference is made in the text; and that all substantive contributions by others to the work presented, including jointly authored publications, is clearly acknowledged.

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Publications

This thesis is written under the supervision of Professor Jerzy A. Filar (JF) at University of South Australia, and Professor Walter Murray (WM) at Stanford University.

Chapter 1:

- Section 1.1 contains a conjecture jointly proposed by JF and Giang Nguyen (University of South Australia) that has been submitted to Discussiones Mathematicae Graph Theory.

Chapter 2:

- Sections 2.1–2.7 describe joint work with JF, Vladimir Ejov (University of South Australia) and Giang Nguyen (University of South Australia). A shortened version of these section are included in a manuscript, which was published in Mathematics of Operations Research Volume 34(3) in 2009.
- Section 2.8 describe joint work with JF and Ali Eshragh (University of South Australia). Part of this section is included in a manuscript, which has been accepted by Annals of Operations Research in 2009.

Chapter 3:

- Sections 3.6–3.7 describe joint work with JF and WM. A shortened version of these sections are included in a manuscript, that is under revision for The Gazette in 2010.

Acknowledgements

With the cessation of four years effort, I arrive at the final, and perhaps most difficult, task of acknowledging all of the family, friends, colleagues and fellow researchers that have been instrumental in keeping me sane throughout my time as a postgraduate student. The love and support I have received during these past four years from so many has been instrumental to the completion of this thesis.

Before I get started, I must acknowledge the funding that has allowed me to undertake such enjoyable and fulfilling research. During my four years as a postgraduate student, I have worked under ARC Discovery Grants DP0666632 and DP0984470. I have been supported by the CSIRO-ANZIAM Student Support Scheme which has allowed me to attend the Annual Conference of ANZIAM in 2008, 2009 and 2010. I have received an APA Scholarship from the Australian Government, and a Completion Scholarship from University of South Australia. Needless to say, four years of research does not occur without significant financial assistance and I am extremely appreciative of this necessary support.

First and foremost, I would like to express my eternal gratitude to my supervisors Professor Jerzy Filar and Professor Walter Murray. Their enthusiasm for their craft is unsurpassed and has been a source of great inspiration to me. Their patience, understanding, kindness, and genuine friendship has made researching under their supervision an immensely enjoyable ride, and has seen them extract from me my best work. Between late night phone calls, all-day meetings and car rides to the airport, Jerzy and Walter have repeatedly gone above and beyond the call of duty to help me navigate the bumps in the road, and I am certain that I would not be writing these acknowledgements if not for their tireless efforts. Prior to starting my postgraduate degree, I asked a mentor of mine for the secret of a successful Ph.D thesis. “Select the correct supervisors,” he told me, “and everything else will fall into place.” I am pleased to say that he was correct.

While not my supervisor in an official capacity, Associate Professor Vladimir Ejov has felt like one in every other sense. His mathematical insight has been invaluable in all chapters of this thesis, and his joyful love for this problem, not to mention life itself, has been infectious. Our research team was so much richer for Vladimir’s participation. There is a saying, “the best people make those around them stand taller.” There can be no doubt that Vladimir is, by this and many other definitions, a wonderful person and a brilliant researcher.

Mr. Ali Eshragh entered our research team a year after I did, and immediately made an impact with his knowledge, creativity, and wide range of mathematical skills. I have bounced so many ideas off Ali in the past three years that it is difficult to keep track of who brought them up first. Some of my most enjoyable experiences in the past three years have occurred while sitting at a computer with Ali working on MATLAB code, or while standing in front of a whiteboard looking over equations together.

My love for mathematics can be traced back to three individual teachers, without whose influence I would never have pursued this postgraduate research. Mrs. Jenny Dickson, Mrs. Marilyn Hoey, and Mr. Len Colgan were mathematics teachers of mine during my formative years of study, who planted a seed in me that grew into a rich appreciation of the beauty of mathematics. I cannot imagine what direction my life could have taken if not for their inspiration and guidance.

The staff here in the School of Mathematics and Statistics have been fantastic. The two heads of school, Associate Professor David Panton and Professor Stanley Miklavcic, have always ensured that things have run smoothly for me during the seven years I have spent as a student in our school. The administrative staff in Mrs. Maureen Cotton, Mrs. Anja van Vliet, Mrs. Ingrid van Paridon, Mrs. Pamela Phillips, Mrs. Alison Cameron and Ms. Janelle Brown handled my daily requests for assistance with an efficiency and a smile that has been greatly appreciated. Our information technologist, Mr. Richard Rawinski, has been called on time and time again to help with computer issues. Richard, I am so sorry for all of the computer parts I have destroyed during the past four years.

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It is impossible to describe fully the influence my family has had on me, both as a researcher and as a person, but I will attempt to do so nonetheless. As far back as my memory stretches, I have enjoyed the full belief and confidence of my mother and father, who have always given me every opportunity to achieve as highly as possible. Their boundless love, genuine friendship, constant support and nurture, and undying interest in everything I am doing has made me into the man I am today. I hope this thesis makes you proud. My sister Kathryn has shared the journey through childhood with me, and I am proud to say has also begun her own journey in postgraduate research. Her friendship has been a treasured part of my life.

Last, but certainly not least, is Dr. Giang Nguyen, my fiancee. As a colleague, a friend, and a partner, Giang has been without peer in my life, and to say that this thesis would not exist without her influence is a massive understatement. Her unbelievable patience in helping me edit my thesis, her gentle reminders to get back to work when I was getting sidetracked, and her ability to find answers to questions that I cannot find anywhere else have been invaluable. Her support of me has been second to none. Thank you so much Giang, for everything.

Notation

Throughout this thesis, much symbolic notation is used. For easy reference, a summary of the most commonly used symbols is given in the table below.

$\mathbb{A}$	Adjacency matrix
$\mathcal{A}(i)$	Set of nodes that can be reached in one step from node i
$\mathcal{B}(i)$	Set of nodes that can go to node i in one step
$\mathbf{e}$	Column vector with all elements equal to 1
$\mathbf{e}_i$	Column vector with a 1 in position i, and 0s elsewhere
$\mathcal{DS}$	Set of doubly-stochastic policies
E	Set of arcs in a graph
$f(\mathbf{x})$	Determinant objective function defined as $f(\mathbf{x}) := -\det(I - P(\mathbf{x}) + \frac{1}{N}J)$
$F(\mathbf{x})$	Augmented objective function defined as $F(\mathbf{x}) := f(\mathbf{x}) + \mu\mathcal{L}(\mathbf{x})$
$\mathbf{g}(\mathbf{x})$	Gradient vector of $F(\mathbf{x})$
$H(\mathbf{x})$	Hessian matrix of $F(\mathbf{x})$
I	Identity matrix
J	Square matrix with all elements equal to 1
$\mathcal{L}(\mathbf{x})$	Logarithmic barrier terms defined as $\mathcal{L}(\mathbf{x}) := \sum_{i=1}^{N} \sum_{j\in\mathcal{A}(i)} \ln(x_{ij})$
$\mathcal{M}$	Markov decision process
M^{ij}	Any matrix M with row i and column j deleted
N	Number of nodes in a graph
$P(\mathbf{x})$	Probability transition matrix, containing elements x_{ij}
$\mathbf{r}$	Reward vector in a Markov decision process
$\mathbf{v}$	Value vector in a Markov decision process
V	Set of nodes in a graph
$\mathbf{x}$	Vector containing elements x_{ij} for all $(i,j) \in \Gamma$
x_{ij}	Probability of transition to node j from node i
β	Discount parameter that lies in [0,1)
Γ	Graph
δ_{ij}	The Kronecker delta, equal to 1 if $i = j$, and 0 otherwise
ζ	Policy in a Markov decision process
η	Initial state probability distribution vector
ν	Perturbation parameter used to perturb $P(\mathbf{x})$

Table 1: Notation used in this thesis.

Chapter 1

Introduction and Background

1.1 Hamiltonian cycle problem

The *Hamiltonian cycle problem* (HCP) is an important graph theory problem that features prominently in complexity theory because it is *NP-complete*[1] [31]. HCP has also gained recognition because two special cases: the *Knight's tour* and the *Icosian game*, were solved by famous mathematicians Euler and Hamilton, respectively. Finally, HCP is closely related to the even more famous Traveling salesman problem[2].

The definition of HCP is the following: given a graph Γ containing N nodes, determine whether any simple cycles of length N exist in the graph. These simple cycles of length N are known as *Hamiltonian cycles.* If Γ contains at least one Hamiltonian cycle (HC), we say that Γ is a *Hamiltonian graph.* Otherwise, we say that Γ is a *non-Hamiltonian graph.*

It is well known (e.g., see Robinson and Wormald [50]) that almost all regular graphs are Hamiltonian. It is also well known (e.g., see Woodall [56]) that all sufficiently dense graphs are Hamiltonian, and so in this thesis we primarily consider sparse

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[1] For more information about NP-completeness, the reader is referred to Garey and Johnson [30].

[2] For more information about the Traveling salesman problem, the reader is referred to Lawler et al. [42] pp. 361–401.

graphs. For Hamiltonian graphs, a constructive solution to HCP is to explicitly find a Hamiltonian cycle. Many heuristics have been designed that attempt to find a single Hamiltonian cycle as quickly as possible, solving the HCP quickly in most cases. For non-Hamiltonian graphs, however, no Hamiltonian cycles exist and the heuristics fail.

In this thesis we consider three types of graphs:

(1) Hamiltonian graphs, which contain one or more Hamiltonian cycles.

(2) Bridge (or 1-connected) graphs, which are non-Hamiltonian, but can be detected in polynomial time

(3) Non-bridge non-Hamiltonian (NHNB) graphs, which is the set of all graphs that are neither Hamiltonian nor 1-connected.

Since we can quickly detect bridge graphs, it is (1) and (3) in the above that we are primarily interested in identifying. To give an indication as to the rarity of NHNB graphs, we consider the more restrictive set of cubic graphs, that is, graphs in which each node has precisely three arcs coming in and going out. Even over this seemingly restrictive set of graphs, HCP is still an NP-complete problem [31]. It was conjectured in [26] that as the size N of the graph tends to infinity, the ratio between the number of bridge graphs of size N compared to the entire set of cubic non-Hamiltonian graphs of size N tends to 1. This trend can be seen in Table 1.1. Note that the number of cubic graphs of sizes 40 and 50 was too large to test exhaustively, so a million cubic graphs of those two sizes were randomly generated to be tested.

Given the result in [50] stating that most regular graphs are Hamiltonian, and the conjecture in [26] that most of the relatively few remaining non-Hamiltonian graphs are the easily identified bridge graphs, it seems reasonable to expect that an algorithm which can find a Hamiltonian cycle quickly (after first checking if the graph is a bridge graph) if one exists will work well on the large majority of cubic (and possibly other) graphs.

There has been a wealth of optimisation problems published that attempt to solve

Graph size N	Number of Cubic Graphs	Number of Cubic Non-H Graphs	Number of Cubic Bridge Graphs	Ratio of Bridge/Non-H
10	19	2	1	0.5000
12	85	5	4	0.8000
14	509	35	29	0.8286
16	4060	219	186	0.8493
18	41301	1666	1435	0.8613
20	510489	14498	12671	0.8740
22	7319447	148790	131820	0.8859
24	117940535	1768732	1590900	0.8995
40	1000000*	912	855	0.9375
50	1000000*	549	530	0.9650

Table 1.1: Ratio of cubic graphs over cubic non-Hamiltonian graphs.

HCP, or more commonly the Traveling salesman problem (TSP), which can be formulated as a problem of finding the Hamiltonian cycle of minimum weight in a weighted graph. Classically, the approach to the discrete optimisation problems generally associated with HCP and TSP (as well as other such graph theory problems) has been to solve a linear programming relaxation, followed by heuristics that prevent the formation of sub-cycles (e.g., see Lawler et al [42]). The TSP has been a problem of interest in combinatorial optimisation for much longer than researchers have been fascinated by NP-completeness and has been explored by a large number of researchers, notably by Dantzig et al. [10] and Johnson et al. [38]. Alternative methods for solving TSP and HCP have also been explored such as the use of distributed algorithms (e.g., see Dorigo et al. [13]), Simulated Annealing (e.g., see Kirkpatrick et al. [41]), and more recently a hybrid simulation-optimisation method using the cross-entropy method was applied specifically to HCP with promising results in Eshragh et al. [22].

However, in this thesis we continue a line of work initiated by Filar and Krass [27], that attempts to exploit the properties and tools prevalent in Markov decision processes (MDPs) to solve HCP, by embedding the latter in a *Markov decision process.* This initial approach has been continued by several authors, including but not limited to Feinberg [23, 24], Andramonov et al. [2], Filar and Lasserre [28], Ejov et al. [14, 15, 16, 17, 18, 19, 20, 21] and Borkar et al. [7, 8]. While the rapid growth of this line of research is encouraging, we observe that with the notable exceptions of Andramonov et al. [2], Filar and Lasserre [28] and Ejov et al [15], all the remaining developments have been theoretical. In this thesis, we introduce numerical procedures that take advantage, in some cases for the first time, of the numerous theoretical results that have been published to date. We hope that the promise displayed by these algorithms will encourage further development of algorithms that take advantage of the MDP embedding.

1.2 Embedding of HCP in a Markov decision process

We construct the embedding as follows. Consider a directed graph Γ, containing the set of nodes V, with $|V| = N$, and the set of arcs E. We begin by associating the graph Γ with a Markov decision process $\mathcal{M}$ as follows.

(1) The state space S of $\mathcal{M}$ is equivalent to the set of nodes V in Γ. Clearly, $S = \{1, 2, \ldots, N\}$.

(2) The action space $\mathcal{A}$ of $\mathcal{M}$ is equivalent to the set of arcs E in Γ. Then, $\mathcal{A} = \{(i, a) : i, a \in S \text{ and } (i, a) \in E\}$. We refer to $\mathcal{A}(i)$ as the set of states reachable by actions of the form (i, a). In these cases, we say that $a \in \mathcal{A}(i)$, or equivalently, $(i, a) \in \mathcal{A}$.

(3) We define $\{p(j|i, a) := \delta_{aj} : (i, j) \in \mathcal{A}\}$ as the set of degenerate one-step transition probabilities. The above can be interpreted as the probability of reaching node j in one step by traversing arc (i, a). The Kronecker delta δ_{aj} arises because node j cannot be reached immediately by arc (i, a) unless $a = j$. In the cases when $(i, j) \notin \mathcal{A}$, we define $p(j|i, a) := 0$.

A *stationary policy* ζ in $\mathcal{M}$ is a set of N probability vectors, $\zeta(1)$, $\zeta(2)$, …, $\zeta(N)$. For each node i, $\zeta(i) = (\zeta(i,1), \zeta(i,2), \ldots, \zeta(i,N))$, where $\zeta(i,a)$ is the probability of selecting action a when in state i. In the context of HCP, $\zeta(i,a)$ is the probability of traversing arc (i,a) when node i is reached. At every state, an action must be selected, and therefore $\sum_{a=1}^{N} \zeta(i,a) = 1$. Strictly speaking, $\zeta(i,a)$ should be defined only on $(i,a) \in \mathcal{A}(i)$, but without loss of generality we shall assume that if an arc $(i,a) \notin \mathcal{A}(i)$, then $\zeta(i,a) := 0$. It is then convenient to equivalently represent the stationary policy ζ as an $N \times N$ matrix with entries $\zeta(i,a)$. We refer to the set of all stationary policies as $\mathcal{F}$.

Any stationary policy $\zeta \in \mathcal{F}$ induces a probability transition matrix

$$P(\zeta) \quad = \quad [p(j|i,\zeta)]_{i,j=1}^{N,N}\,,$$

where for all $i, j \in S$,

$$p(j|i,\zeta) \quad := \quad \sum_{a=1}^{N} p(j|i,a)\zeta(i,a).$$

Then, we observe that a stationary policy is one which induces a nonnegative probability transition matrix $P(\zeta)$ with row sums of 1. For this reason, stationary policies are sometimes referred to as stochastic policies.

A *doubly stochastic policy* $\zeta \in \mathcal{F}$ is a stationary policy in which the probability transition matrix $P(\zeta)$ induced also has column sums of 1. We refer to the set of all doubly stochastic policies as $\mathcal{DS}$. As each doubly-stochastic policy is, by definition, stationary, it follows that $\mathcal{DS} \subseteq \mathcal{F}$.

A *deterministic policy* is a stationary policy where $\zeta(i,a) \in \{0,1\}$ for all i and a, that is, at each node a particular arc is always selected by the deterministic policy. For convenience of notation, if $\zeta(i,a) = 1$, we say that $\zeta(i) = a$ in these situations. We refer to the set of all deterministic policies as $\mathcal{D}$. Note that the probability transition matrix $P(\zeta)$ induced by a deterministic policy can also be thought of as a spanning directed subgraph (or subdigraph) Γ_ζ that contains precisely N arcs, with one arc emanating from each node.

Consider a policy that selects arcs that form a Hamiltonian cycle. Such a policy is called a *Hamiltonian policy.* Hamiltonian policies are both doubly stochastic and deterministic, as for any Hamiltonian cycle there is precisely one arc going in and one arc coming out of every node in the graph. Clearly, if $\zeta \notin \mathcal{DS} \bigcap \mathcal{D}$, then ζ is not a Hamiltonian policy. However, the converse is not true. If $\zeta \in \mathcal{DS} \bigcap \mathcal{D}$, then the subgraph Γ_ζ induced is either a Hamiltonian cycle in Γ, or a union of disjoint cycles in Γ, the lengths of which sum to N.

We demonstrate the above in the following example.

Example 1.2.1 *Consider the cubic 6-node graph* Γ_6 *(also known as the envelope graph) shown in Figure 1.1.*

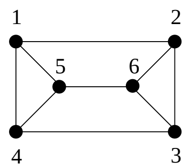


Figure 1.1: The envelope graph.

One Hamiltonian cycle in this graph is $1 \to 2 \to 6 \to 3 \to 4 \to 5 \to 1$. *This Hamiltonian cycle corresponds to a Hamiltonian policy* $\zeta_{HC} \in \mathcal{DS} \bigcap \mathcal{D}$ *such that* $\zeta_{HC}(1) = 2$, $\zeta_{HC}(2) = 6$, $\zeta_{HC}(3) = 4$, $\zeta_{HC}(4) = 5$, $\zeta_{HC}(5) = 1$, $\zeta_{HC}(6) = 3$. *This policy induces a probability transition matrix*

$$P(\zeta_{HC}) = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix}.$$

Note that $P(\zeta_{HC})$ *can also be thought of as the adjacency matrix for a spanning subdigraph* $\Gamma_{HC} = \{(1,2),(2,6),(3,4),(4,5),(5,1),(6,3)\} \subset \Gamma_6$.

Consider another deterministic policy ζ_{SC} *such that* $\zeta_{SC}(1) = 2$, $\zeta_{SC}(2) = 1$, $\zeta_{SC}(3) =$

6, $\zeta_{SC}(4) = 3$, $\zeta_{SC}(5) = 4$, $\zeta_{SC}(6) = 5$, *which induces the probability transition matrix*

$$P(\zeta_{SC}) \quad = \quad \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}.$$

Again, we note that $P(\zeta_{SC})$ *can be thought of as the adjacency matrix for a subdigraph* $\Gamma_{SC} = \{(1,2),(2,1),(3,6),(4,3),(5,4),(6,5)\}$, *which contains two subcycles of lengths 2 and 4 respectively. Both* ζ_{HC} *and* ζ_{SC} *are examples of deterministic, doubly-stochastic policies.*

We can take convex combinations of deterministic policies to obtain randomised policies. For example, consider a randomised policy $\zeta_R = \frac{3}{4}\zeta_{HC} + \frac{1}{4}\zeta_{SC}$. *This policy induces the following probability transition matrix:*

$$P(\zeta_R) = \frac{3}{4}P(\zeta_{HC}) + \frac{1}{4}P(\zeta_{SC}) \quad = \quad \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ \frac{1}{4} & 0 & 0 & 0 & 0 & \frac{3}{4} \\ 0 & 0 & 0 & \frac{3}{4} & 0 & \frac{1}{4} \\ 0 & 0 & \frac{1}{4} & 0 & \frac{3}{4} & 0 \\ \frac{3}{4} & 0 & 0 & \frac{1}{4} & 0 & 0 \\ 0 & 0 & \frac{3}{4} & 0 & \frac{1}{4} & 0 \end{bmatrix}.$$

One inherent difficulty with this MDP embedding is that some (but not all) policies have a multi-chain ergodic structure, which can introduce technical difficulties in the associated methods of analysis. To help avoid this issue, one common technique is to force the MDP to be *completely ergodic*, that is, one in which every stationary policy induces a Markov chain containing only a single, exhaustive, ergodic class. We achieve this through the use of the following *symmetric linear perturbation* of the form

$$p_\nu(j|i,a) \quad := \quad \begin{cases} 1 - \dfrac{(N-1)}{N}\nu, & \text{if } a = j \in \Gamma, \\ \dfrac{\nu}{N}, & \text{otherwise,} \end{cases} \tag{1.1}$$

for all $(i,j) \in \Gamma$, $i,j \in \mathcal{S}$. This perturbation ensures that all policies $\zeta \in \mathcal{F}$ induce a Markov chain with a completely ergodic probability transition matrix $P_\nu(\zeta)$ whose dominant terms (for small ν) correspond to the non-zero entries in the unperturbed probability transition matrix $P(\zeta)$ that the same policy ζ induces in Γ.

Example 1.2.2 *Continuing from Example 1.2.1, consider the probability transition matrices $P_\nu(\zeta_{HC})$ and $P_\nu(\zeta_{SC})$ of the perturbed Markov chains induced by policies ζ_{HC} and ζ_{SC} respectively:*

$$P_\nu(\zeta_{HC}) \quad = \quad \begin{bmatrix} \frac{\nu}{6} & 1-\frac{5\nu}{6} & \frac{\nu}{6} & \frac{\nu}{6} & \frac{\nu}{6} & \frac{\nu}{6} \\ \frac{\nu}{6} & \frac{\nu}{6} & \frac{\nu}{6} & \frac{\nu}{6} & \frac{\nu}{6} & 1-\frac{5\nu}{6} \\ \frac{\nu}{6} & \frac{\nu}{6} & \frac{\nu}{6} & 1-\frac{5\nu}{6} & \frac{\nu}{6} & \frac{\nu}{6} \\ \frac{\nu}{6} & \frac{\nu}{6} & \frac{\nu}{6} & \frac{\nu}{6} & 1-\frac{5\nu}{6} & \frac{\nu}{6} \\ 1-\frac{5\nu}{6} & \frac{\nu}{6} & \frac{\nu}{6} & \frac{\nu}{6} & \frac{\nu}{6} & \frac{\nu}{6} \\ \frac{\nu}{6} & \frac{\nu}{6} & 1-\frac{5\nu}{6} & \frac{\nu}{6} & \frac{\nu}{6} & \frac{\nu}{6} \end{bmatrix},$$

$$P_\nu(\zeta_{SC}) \quad = \quad \begin{bmatrix} \frac{\nu}{6} & 1-\frac{5\nu}{6} & \frac{\nu}{6} & \frac{\nu}{6} & \frac{\nu}{6} & \frac{\nu}{6} \\ 1-\frac{5\nu}{6} & \frac{\nu}{6} & \frac{\nu}{6} & \frac{\nu}{6} & \frac{\nu}{6} & \frac{\nu}{6} \\ \frac{\nu}{6} & \frac{\nu}{6} & \frac{\nu}{6} & \frac{\nu}{6} & \frac{\nu}{6} & 1-\frac{5\nu}{6} \\ \frac{\nu}{6} & \frac{\nu}{6} & 1-\frac{5\nu}{6} & \frac{\nu}{6} & \frac{\nu}{6} & \frac{\nu}{6} \\ \frac{\nu}{6} & \frac{\nu}{6} & \frac{\nu}{6} & 1-\frac{5\nu}{6} & \frac{\nu}{6} & \frac{\nu}{6} \\ \frac{\nu}{6} & \frac{\nu}{6} & \frac{\nu}{6} & \frac{\nu}{6} & 1-\frac{5\nu}{6} & \frac{\nu}{6} \end{bmatrix}.$$

Remark 1.2.3 *Note that this perturbation ensures a single ergodic class and no transient states. While this is desirable theoretically, it also has the effect of eliminating the inherent sparsity present in the unperturbed probability transition matrices that can be exploited when algorithms are developed.*

The symmetric linear perturbation (1.1) is used in [7] and [8] where a perturbation is required that does not destroy double-stochasticity in a probability transition matrix.

For each stationary policy $\zeta \in \mathcal{F}$ and its corresponding probability transition matrix $P(\zeta)$, there is an associated *stationary distribution matrix* $P^*(\zeta)$, also known as the *limit Cesaro-sum matrix*, defined as

$$P^*(\zeta) \quad := \quad \lim_{T \to \infty} \frac{1}{T+1} \sum_{t=0}^{T} P^t(\zeta), \quad P^0(\zeta) = I,$$

where I is an $N \times N$ identity matrix. It is a well known property (e.g., see Blackwell [4]) that $P^*(\zeta)$ satisfies the following identity

$$P(\zeta)P^*(\zeta) = P^*(\zeta)P(\zeta) = P^*(\zeta)P^*(\zeta) = P^*(\zeta). \tag{1.2}$$

If the Markov chain corresponding to $P(\zeta)$ contains only a single ergodic class and no transient states (for example, when perturbed using (1.1)), it is also known that $P^*(\zeta)$ is a nonnegative, stochastic matrix where all rows are identical. We refer to this row as $\pi(\zeta)$, which is known as the *stationary distribution* of this Markov chain. From (1.2), we find $\pi(\zeta)$ by solving the following linear system of equations

$$\pi(\zeta)P(\zeta) = \pi(\zeta), \quad \pi(\zeta)\mathbf{e} = \mathbf{e}, \quad \pi(\zeta) \geq 0, \tag{1.3}$$

where $\mathbf{e} = \begin{bmatrix} 1 & 1 & \dots & 1 \end{bmatrix}^T$. It is known that this system always has a unique solution for $P(\zeta)$ arising from completely ergodic Markov chains (e.g., see Kemeny and Snell [40] p. 100, theorem 5.1.2).

If the probability transition matrix of a completely ergodic Markov chain is doubly-stochastic, it follows from the uniqueness of the solution of (1.3) that

$$\pi(\zeta) \quad = \quad \begin{bmatrix} \frac{1}{N} & \frac{1}{N} & \dots & \frac{1}{N} \end{bmatrix}.$$

Hence, for $\zeta \in \mathcal{DS}$, we observe that $P^*(\zeta) = \frac{1}{N}J$, where J is an $N \times N$ matrix with a unity in every entry.

We next define the *fundamental matrix*

$$G(\zeta) := (I - P(\zeta) + P^*(\zeta))^{-1} \quad = \quad \lim_{\beta \to 1^-} \sum_{t=0}^{\infty} \beta^t (P(\zeta) - P^*(\zeta))^t.$$

The entries of the fundamental matrix are related to moments of first hitting times of node 1. These relationships were exploited in [7] to show that if we use the symmetric linear perturbation 1.1, and constrain the probability transition matrices to be doubly-stochastic, then the HCP can be converted to the problem of minimising the top-left element $g_{11}(\zeta)$ of $G_\nu(\zeta) := \left(I - P_\nu(\zeta) + \frac{1}{N}J\right)^{-1}$, when $\nu > 0$ and sufficiently small. That is, for small positive ν it is sufficient to solve the optimisation problem

$$\begin{aligned}
&\min g_{11}(\zeta) \\
&\text{s.t.} \\
&P_\nu(\zeta)\mathbf{e} = \mathbf{e}, \\
&\mathbf{e}^T P_\nu(\zeta) = \mathbf{e}^T, \\
&[p_\nu(\zeta)]_{ij} \geq 0.
\end{aligned} \tag{1.4}$$

Note that constraints above merely ensure that $\zeta \in \mathcal{DS}$. In [14] it is proven that the objective function in the above optimisation problem can be converted to a problem of maximising the determinant of $(G(\zeta))^{-1} = \left(I - P(\zeta) + \frac{1}{N}J\right)$, after which the symmetric linear perturbation is no longer required. Maximising this determinant function is the subject of Chapter 3 of this thesis.

Another important matrix in Markov decision processes is the resolvent-like matrix

$$R^\zeta(\beta,\nu) := [I - \beta P_\nu(\zeta)]^{-1} \quad = \quad \lim_{T\to\infty} \sum_{t=0}^{T} \beta^t P_\nu^t(\zeta),$$

where the parameter $\beta \in [0, 1)$ is known as the discount factor. Note that the domain of β ensures that the sum above converges, and therefore both the limit and the inverse exist.

Classically, in MDP problems there is a reward (or a cost) denoted by $r(i, a)$ associated with each action a taken in state i. When the actions chosen are prescribed by a policy $\zeta \in \mathcal{F}$, the expected reward achieved each time state i is reached is given by

$$r(i,\zeta) \; := \; \sum_{a=1}^{N} r(i,a)\zeta(i,a), \quad i \in \mathcal{S}.$$

Then, the (single-stage) *expected reward vector* (or expected cost vector) $\mathbf{r}(\zeta)$ is the vector that contains $r(i,\zeta)$ for each state, that is

$$\mathbf{r}(\zeta) \; := \; \begin{bmatrix} r(1,\zeta) & r(2,\zeta) & \ldots & r(N,\zeta) \end{bmatrix}^T.$$

We define the *discounted Markov decision process* $\mathcal{M}_\beta$ where the performance of a policy ζ is defined by the *value vector*

$$\begin{aligned} \mathbf{v}^\beta(\zeta) \; &:= \; \left[I - \beta P_\nu(\zeta)\right]^{-1}\mathbf{r}(\zeta) \\ &= \; \sum_{t=0}^{\infty} \beta^t P_\nu^t(\zeta)\mathbf{r}(\zeta). \end{aligned} \tag{1.5}$$

We also define the value starting from state i as

$$v^\beta(\mathbf{e}_i^T,\zeta) := \mathbf{e}_i^T\mathbf{v}^\beta(\zeta) \;\; = \;\; \mathbf{e}_i^T\left[I - \beta P_\nu(\zeta)\right]^{-1}\mathbf{r}(\zeta). \tag{1.6}$$

The interpretation of β in a discounted Markov decision process is that it is the rate at which rewards depreciate with time. For a discounted Markov decision process, this implies that a preferred policy is one that achieves the largest reward in short time. Typically, an optimisation problem associated with the discounted Markov decision process is of the form

$$\max_{\zeta \in \mathcal{F}} \mathbf{v}^\beta(\zeta). \tag{1.7}$$

This problem has been extensively researched and, for most problems, completely solved. For further reading on this topic the reader is referred to [4] and [48] pp. 142–266. Note that in (1.7), the maximum is achieved componentwise, at each initial state.

In the context of HCP, we use the reward vector $\mathbf{r}(\zeta)$ only to distinguish between visiting the home node (which we define as node 1 for simplicity) and visiting all other nodes. In this case we define $r(i,\zeta) := 0$ for all $i \geq 2$, and $r(1,\zeta) := 1$. That is, in our context, for all $\zeta \in \mathcal{F}$, the reward vector is defined as

$$\mathbf{r}(\zeta) = \mathbf{e}_1 = \begin{bmatrix} 1 & 0 & \dots & 0 \end{bmatrix}^T. \tag{1.8}$$

Note that the above convention applies regardless of whether the symmetric linear perturbation is used or not.

The embedding of the Hamiltonian cycle problem into the framework of a discounted Markov decision process offers us an opportunity to work inside the space of the *(discounted) occupational measures* induced by stationary policies. The latter has been studied extensively (e.g., see Kallenberg [39] pp. 35–94, Puterman [48] pp. 142–276, Borkar [6] pp. 31–41, Filar and Vrieze [29] pp. 23–31). Consider the polyhedral set $X(\beta,\nu)$ defined by the constraints

(1) $\displaystyle\sum_{i=1}^{N} \sum_{a\in\mathcal{A}(i)} \left[\delta_{ij} - \beta p_\nu(j|i,a)\right] x_{ia} = \eta_j, \quad j = 1,\dots,N,$

(2) $x_{ia} \geq 0, \quad (i,a) \in \Gamma.$

Remark 1.2.4 *To the above constraints, we write $j = 1,\dots,N$ and $(i,a) \in \Gamma$ rather than $j \in V$ and $(i,a) \in E$. Since N and Γ is generally specified, but E and V are only implied, this keeps the notation compact. We adopt this standard for the remainder of the thesis.*

In the above, $\eta = [\eta_1, \eta_2, \dots, \eta_N]$ is the *initial state probability distribution vector.* To begin with we assume that $\eta_j > 0$ for every j. It is well known (e.g., see Filar and Vrieze [29] p. 45) that with every stationary policy $\zeta \in \mathcal{F}$ we can associate $\mathbf{x}(\zeta) \in X(\beta,\nu)$. We achieve this by defining a map $M : \mathcal{F} \to X(\beta,\nu)$

$$x_{ia}(\zeta) = \eta\left[I - \beta P(\zeta)\right]^{-1} \mathbf{e}_i \zeta(i,a), \quad \zeta \in \mathcal{F},$$

for each $(i,a) \in \Gamma$. We interpret the quantity $x_{ia}(\zeta)$ as the *discounted occupational measure $x(\zeta)$ of the state-action pair (i,a)* induced by the policy ζ. This interpretation is consistent with the interpretation of $x_i(\zeta) := \sum_{a\in\mathcal{A}(i)} x_{ia}(\zeta)$ as the *discounted occupational measure $x(\zeta)$ of the state/node i.*

Next we define a map $\hat{M} : X(\beta, \nu) \to \mathcal{F}$ by

$$\zeta_x(i, a) \quad = \quad \frac{x_{ia}}{x_i}, \tag{1.9}$$

for every $i = 1, \ldots, N$ and $a \in \mathcal{A}(i)$. The following result can be found in [48] pp. 224–227, [29] p. 45, and [1] pp. 27–36.

Lemma 1.2.5 *(1) The set $X(\beta, \nu) = \{x(\zeta) | \zeta \in \mathcal{F}\}$.*

(2) The map $\hat{M} = M^{-1}$. Hence

$$M\left(\hat{M}(x)\right) = x \quad \text{ and } \quad \hat{M}\left(M(\zeta)\right) = \zeta,$$

for every $x \in X(\beta, \nu)$, and every $\zeta \in \mathcal{F}$.

(3) If x is an extreme point of $X(\beta, \nu)$, then

$$\zeta_x = \hat{M}(x) \in \mathcal{D}.$$

(4) If $\zeta \in \mathcal{D}$ is a Hamiltonian cycle, then $x(\zeta)$ is an extreme point of $X(\beta, \nu)$.

In Feinberg [23] the following, important, result is proved for the case where ν is set equal to zero. Note that, by convention, we will refer to $X(\beta, 0)$ as

$$X(\beta) := X(\beta, 0). \tag{1.10}$$

Theorem 1.2.6 *Consider a graph Γ. The following statements are equivalent:*

(1) A policy ζ is deterministic and corresponds to a Hamiltonian cycle in Γ.

(2) A policy ζ is stationary and corresponds to a Hamiltonian cycle in Γ.

(3) A policy ζ is deterministic and $v^{\beta}(\mathbf{e}_1, \zeta) = \frac{1}{1-\beta^N}$ for at least one $\beta \in (0, 1)$.

(4) A policy ζ is stationary and $v^{\beta}(\mathbf{e}_1, \zeta) = \frac{1}{1-\beta^N}$ for $2N - 1$ distinct discount factors $\beta_k \in (0, 1), \quad k = 1, 2, \ldots, 2N - 1$.

The combination of Lemma 1.2.5 and Theorem 1.2.6 leads naturally to a number of mathematical programming formulations of HCP that are described in Feinberg [23]. We describe a branch and fix method in Chapter 2 of this thesis that takes advantage of the above and results proved in [16]. The branch and fix method is followed by a mixed integer programming method that succeeds in using the above results to solve large graphs. In Chapter 4 we investigate the behaviour of Hamiltonian policies as β and ν approach limiting values.

Chapter 2

Algorithms in the Space of Occupational Measures

In this chapter we present two methods: the *branch and fix method*, and the *Wedged-MIP heuristic*. Both methods take advantage of the Markov decision process embedding outlined in Chapter 1. The branch and fix method is implemented in MATLAB and results are given that demonstrate the potential of this model. The Wedged-MIP heuristic is implemented in IBM ILOG OPL-CPLEX and succeeds in solving large graphs, including two of the large test problems given on the TSPLIB website maintained by University of Heidelberg [49]. Both of these methods operate in the space of discounted occupational measures, but similar methods could be developed for the space of limiting average occupational measures.

2.1 Preliminaries

In this chapter, we continue the exploitation of the properties of the space of discounted occupational measures in the Markov decision process $\mathcal{M}$, associated with a graph Γ, as outlined in Chapter 1. In particular, we apply the non-standard branch and bound method of Filar and Lasserre [28] to Feinberg's embedding of the HCP in a discounted Markov decision process [23] (rather than the limiting average

Markov decision process used previously). This embedding has the benefit that the discount parameter does not destroy sparsity of the coefficient matrices to nearly the same extent as did the perturbation parameter ε, used in [28] to replace the underlying probability transitions $p(j|i,a)$ of $\mathcal{M}$ by the linearly perturbed transitions $p^{\varepsilon}(j|i,a)$. We refer to the method that arises from this embedding as the branch and fix method[1].

We show that in the present application, the aforementioned space of discounted occupational measures is synonymous with a polytope $X(\beta)$ defined by only $N+1$ equality constraints and nonnegativity constraints. Using the results in [16] and [45] about the structure of extreme points of $X(\beta)$, we predict that Hamiltonian cycles will be found far earlier, and the resulting *logical branch and fix tree* will have fewer branches than that for more common polytopes. The logical branch and fix tree (which we also call the *logical B&F tree*) that arises from the branch and fix method is a rooted tree. The root of the logical B&F tree corresponds to the original graph Γ, and each branch corresponds to a certain fixing of arcs in Γ. Then, a branch forms a pathway from the root of the logical B&F tree to a leaf. These leaves correspond to particular subdigraphs of Γ, which may or may not contain Hamiltonian cycles. At the maximum depth of the logical B&F tree, each leaf corresponds to a subdigraph for which there is exactly one arc emanating from every node. We refer to subdigraphs of this type as *spanning 1-out-regular subdigraphs* of Γ. Leaves at a shallower level correspond to subdigraphs for which there are multiple arcs emanating from at least one node.

The set of all spanning 1-out-regular subdigraphs has a 1:1 correspondence with the set of all deterministic policies in Γ. Even for graphs with bounded out-degree, this represents a set with non-polynomial cardinality. Cubic graphs, for example, have 3^N distinct deterministic policies. Hence, it is desirable to be able to fathom branches early, and consequently restrict the number of leaves in the logical B&F tree. The special structure of the extreme points of $X(\beta)$ usually enables us to identify a

[1]Since the speed of convergence depends more on arc fixing features than on bounds, the name "branch and fix" (or B&F) method is more appropriate than "branch and bound".

Hamiltonian cycle before obtaining a spanning 1-out-regular subdigraph, limiting the depth of the logical B&F tree. We achieve significant improvements by introducing into the branch fix method additional feasibility constraints as bounds, and logical checks that allow us to fathom branches early. This further limits the depth of the logical B&F tree. The resulting method is guaranteed to solve HCP in finitely many iterations. While the worst case may involve examination of exponentially many branches, empirically we show that the number of branches required to find a Hamiltonian cycle is generally reduced to a tiny fraction of the total number of deterministic policies. For example, a 24-node Hamiltonian cubic graph has $3^{24} \approx 3 \times 10^{11}$ possible choices for deterministic policies, but the algorithm finds a Hamiltonian cycle by examining only 28 branches. We observe that Hamiltonian graphs perform better than non-Hamiltonian graphs, as they typically have many Hamiltonian cycles spread throughout the logical B&F tree, and only one needs to be found. However, even in non-Hamiltonian graphs we demonstrate that the algorithm performs well. For instance, a 28-node non-Hamiltonian cubic graph has $3^{28} \approx 2 \times 10^{13}$ possible choices for deterministic policies, but the algorithm terminates after investigating only 11708 branches. This example highlights the ability of B&F method to fathom branches early, allowing us to ignore, in this case, 99.99999995% of the potential branches.

In addition to the basic branch and fix method, we develop and compare several branching methods for traversing the logical B&F tree that may find Hamiltonian cycles quicker in certain graphs, and propose additional constraints that can find infeasibility at an earlier depth in the logical B&F tree. We provide experimental results demonstrating the significant improvement achieved by these additions. We also demonstrate that $X(\beta)$ can be a useful polytope in many other optimisation algorithms. In particular we use $X(\beta)$, along with the additional constraints, in a mixed integer programming model that can solve extremely large graphs using commercially available software such as CPLEX. Finally, we present solutions of four large non-regular graphs, with 250, 500, 1000 and 2000 nodes respectively, which are obtained by this model.

2.2 A formulation of HCP by means of a discounted MDP

The fact that HCP can be embedded in a Markov decision process, as outlined in Chapter 1, was demonstrated in [27] and [23]. However, in [27], the long-run average MDP was, used whereas in [23], the discounted MDP was exploited to solve HCP for the first time.

For a given graph Γ, we define its *adjacency matrix* $\mathbb{A}$ as

$$[\mathbb{A}]_{ia} = \begin{cases} 1, & \text{if } (i,a) \in \Gamma, \\ 0, & \text{otherwise.} \end{cases}$$

We now formally introduce the *transition probabilities* for Γ defined by

$$p(j|i,a) := \begin{cases} 1, & \text{if } a = j, (i,a) \in \Gamma, \\ 0, & \text{otherwise.} \end{cases}$$

Here, $p(j|i,a)$ represents the probability of moving from i to j by choosing the action/arc (i,a), such that

$$\sum_{j=1}^{N} p(j|i,a) = 1, \quad \text{for all } (i,a) \in \mathcal{A}. \tag{2.1}$$

Recall from Chapter 1 that a stationary policy ζ contains entries

$$\zeta_{ia} = \begin{cases} \text{probability of action } a \text{ in state } i, & a \in \mathcal{A}(i), \\ 0, & a \notin \mathcal{A}(i), \end{cases}$$

and from (1.5)–(1.8) that the performance of ζ, starting from state i, is given by the value vector whose i-th entry is

$$v_\beta(\mathbf{e}_i^T, \zeta) = \mathbf{e}_i^T (I - \beta P(\zeta))^{-1} \mathbf{e}_1. \tag{2.2}$$

The *space of occupational measures*, $X(\beta) := \{\mathbf{x}(\zeta) | \zeta \in \mathcal{F}\}$ (induced by stationary policies) consists of vectors $\mathbf{x}(\zeta)$ whose entries are the *discounted occupational measures of the state-action pairs* $(i,a) \in \mathcal{A}(i)$ defined by

$$x_{ia}(\zeta) := \eta[(I - \beta P(\zeta))^{-1}]\mathbf{e}_i \zeta_{ia}, \tag{2.3}$$

where $\eta = [\eta_1, \quad \ldots, \quad \eta_N]$ denotes an arbitrary (but fixed) initial state distribution. Note that in (2.2), $\eta = \mathbf{e}_i^T$.

In what follows, we consider a specially structured initial distribution. Namely, for $\mu \in \left(0, \frac{1}{N}\right)$ we define

$$\eta_i = \begin{cases} 1-(N-1)\mu, & \text{if } i = 1, \\ \mu, & \text{otherwise.} \end{cases} \tag{2.4}$$

We define the *occupational measure of the state i* as the aggregate

$$x_i(\zeta) := \sum_{a \in \mathcal{A}(i)} x_{ia}(\zeta) = \eta[I - \beta P(\zeta)]^{-1}\mathbf{e}_i, \tag{2.5}$$

where the second equality follows from (2.3), and the fact that $\sum\limits_{a \in \mathcal{A}(i)} \zeta_{ia} = 1$. In particular,

$$x_1(\zeta) := \sum_{a \in \mathcal{A}(1)} x_{1a}(\zeta) = \eta[I - \beta P(\zeta)]^{-1}\mathbf{e}_1 = v_\beta(\eta, \zeta). \tag{2.6}$$

The construction of $\mathbf{x}$ in (2.3) defines a map M of the policy space $\mathcal{F}$ into $\mathbb{R}^{|E|}$ by

$$M(\zeta) := \mathbf{x}(\zeta).$$

Recall from Lemma 1.2.5 that, for $\eta > 0$, the map M is invertible and its inverse M^{-1} is defined by

$$M^{-1}(\mathbf{x})[i,a] = \zeta_{\mathbf{x}}(i,a) := \frac{x_{ia}}{x_i}. \tag{2.7}$$

It is also known that the extreme points of $X(\beta)$ are in one-to-one correspondence with deterministic policies of Γ. However, this important property is lost when entries of η are permitted to take on zero values. We now recall (see Filar and Vrieze [29] pp. 45–46) the partition of the space $\mathcal{D}$ of deterministic strategies that is based on the spanning 1-out-regular subdigraphs they trace out in Γ. In particular, note that with each $\zeta \in \mathcal{D}$, we associate a subdigraph Γ_ζ of Γ defined by

$$\text{arc } (i,a) \in \Gamma_\zeta \iff \zeta(i) = a.$$

We denote a simple cycle of length k and beginning at 1 by a set of arcs

$$c_k^1 = \{(i_0 = 1, i_1), (i_1, i_2), \ldots, (i_{k-1}, i_k = 1)\}, \quad k = 0, 1, \ldots, N-1.$$

Thus, c_N^1 is a Hamiltonian cycle. Note that, by convention, we say that the initial arc in a Hamiltonian cycle $(1, i_1)$ is the 0-th arc in the Hamiltonian cycle. If Γ_ζ contains a cycle c_k^1, we write $\Gamma_\zeta \supset c_k^1$. Let

$$C_k^1 := \left\{\zeta \in \mathcal{D} | \quad \Gamma_\zeta \supset c_k^1\right\}, \qquad \text{for all } k = 2, 3, \ldots, N,$$

namely, the set of deterministic policies in Γ that trace out a simple cycle of length k beginning at node 1. Thus, $\bigcup_{k=2}^N C_k^1$ contains all deterministic policies in Γ that define a cycle containing node 1. We refer to the policies in the union $\bigcup_{k=2}^{N-1} C_k^1$ as *short cycles* (see Figure 2.1). Denote the complement of $\bigcup_{k=2}^N C_k^1$ in $\mathcal{D}$ by $\mathcal{N}_c$. Then $\mathcal{N}_c$ contains policies that start at the home node 1, and the node where the strategy for the first time repeats itself is different from node 1. We call such policies *noose cycles* (see Figure 2.2). Note that the home node is a transient state in a Markov chain induced by a noose cycle policy.

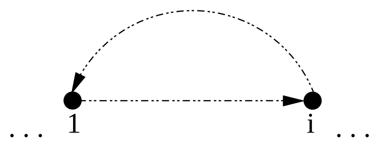


Figure 2.1: A short cycle.

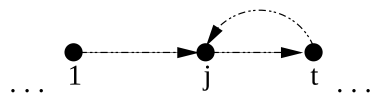


Figure 2.2: A noose cycle.

2.3 Structure of 1-randomised policies

Much of the analysis in this chapter depends on the following proposition; which was proved for $\mu = 0$ in Feinberg [23].

Proposition 2.3.1 *Let $\beta \in [0, 1)$, $\mu \in [0, \frac{1}{N})$, and $\zeta \in \mathcal{F}$. The following two properties hold.*

(1) If the initial state distribution η is given by

$$\eta_i = \begin{cases} 1-(N-1)\mu, & \text{if } i = 1, \\ \mu, & \text{otherwise,} \end{cases}$$

then if ζ is a Hamiltonian policy,

$$v_\beta(\eta,\zeta) = \frac{(1-(N-1)\mu)(1-\beta)+\mu(\beta-\beta^N)}{(1-\beta)(1-\beta^N)}.$$

(2) If $\zeta \in \mathcal{D}$, and $v_\beta(\eta,\zeta)$ is as in part (1), then ζ is a Hamiltonian policy.

Proof. For $\mu = 0$, the first part is established in Feinberg [23], and for $\mu \in (0, \frac{1}{N})$, this part is merely an extension of the case when $\mu = 0$. The second part also follows by the same argument as the analogous result in [23] and [45]. □

Then, for any Hamiltonian policy $\zeta \in \mathcal{F}$, it follows from (2.6) and Proposition 2.3.1 that

$$\begin{aligned} \sum_{a\in\mathcal{A}(1)} x_{1a}(\zeta) &= v_\beta(\eta,\zeta) \\ &= \frac{(1-(N-1)\mu)(1-\beta)+\mu(\beta-\beta^N)}{(1-\beta)(1-\beta^N)}. \end{aligned}$$

The above suggests that Hamiltonian cycles can be sought among the extreme points of the following subset $\bar{X}(\beta)$ of the discounted occupation measure space $X(\beta)$ that is defined by the linear constraints:

$$\sum_{i=1}^{N}\sum_{a\in\mathcal{A}(i)} (\delta_{ij} - \beta p(j|i,a))\, x_{ia} = \eta_j, \quad j = 1,\dots,N, \tag{2.8}$$

$$\sum_{a\in\mathcal{A}(1)} x_{1a} = \frac{(1-(N-1)\mu)(1-\beta)+\mu(\beta-\beta^N)}{(1-\beta)(1-\beta^N)}, \tag{2.9}$$

$$x_{ia} \geq 0, \quad (i,a)\in\Gamma. \tag{2.10}$$

Recall from part (1) of Lemma 1.2.5 that, with $\nu = 0$, $X(\beta) = \{\mathbf{x}|\ \mathbf{x}$ satisfies the constraints (2.8) and (2.10)$\}$. From Lemma 1.2.5 part (iii) we know that (when $\mu > 0$) every extreme point of $X(\beta)$ corresponds to a deterministic policy via the transformations M and M^{-1} introduced earlier. Hence, these extreme points contain exactly N positive entries, one for each node. However, the additional equality constraint (2.9) in $\bar{X}(\beta)$ may introduce one more positive entry in its extreme points. This can be seen as follows. Let $\mathbf{x}_e$ be an extreme point of $\bar{X}(\beta)$. It is clear that if x_e contains exactly N positive entries, then by part (iii) of Lemma 1.2.5, $\zeta = M^{-1}(\mathbf{x}_e)$ is a Hamiltonian policy. However, if $\mathbf{x}_e$ contains $N+1$ positive entries, then $\zeta = M^{-1}(\mathbf{x}_e)$ is a *1-randomised policy* where randomisation occurs only in one state/node, which we call the *splitting node*, and on only two actions/arcs. This terminology is introduced in [25], and the exact structure of these 1-randomised policies is described in [16] and [45].

Specifically, it is shown that each 1-randomised policy that is an extreme point of $\bar{X}(\beta)$ is a convex combination of a short cycle policy ζ_{SC}, and a noose cycle policy ζ_{NC}, that differ only at a single node, and hence the randomisation occurs only at that single node. That is, $\zeta = \alpha\zeta_{SC} + (1-\alpha)\zeta_{NC}$. Only a particular value of α (which is called the *splitting probability*) satisfies (2.8)–(2.10).

We summarise the above findings in the following theorem, which is stated and proved in [16] and [45].

Theorem 2.3.2 *For some $\mu_0 \in (0, \frac{1}{N})$ and for any $\mu \in [0, \mu_0)$, we define the initial state distribution as $\eta = [1-(N-1)\mu, \quad \mu, \quad \ldots, \quad \mu]$. Let an extreme point $\mathbf{x} \in \bar{X}(\beta)$ induce a 1-randomised policy ζ_α via the transformation $M^{-1}(\mathbf{x})$, for some $\alpha \in (0,1)$, and ζ_1, ζ_2 be two deterministic policies which share the same action at all nodes except the splitting node i, such that $\zeta_\alpha = \alpha\zeta_1 + (1-\alpha)\zeta_2$. The following two properties hold.*

(1) One of the policies $\{\zeta_1, \zeta_2\}$ is a short cycle policy, and the other one is a noose cycle policy.

(2) For every such pair $\zeta_1 \in \bigcup_{k=2}^{N-1} C_k^1$ and $\zeta_2 \in \mathcal{N}_c$, there is only one particular value of α such that $\mathbf{x}(\zeta_\alpha)$ is an extreme point of $\bar{X}_\beta$. When $\mu = 0$, this special value of α is given by one of two possible forms[2], depending on one of only

[2]In [16] and [45], the formula for α was also given for $\mu > 0$, but as this is not used in the present thesis, we do not include that result.

two cases that may arise. In particular, we define the first repeated node in ζ_2 as node j. Without loss of generality we assume that the simple cycle in ζ_1 containing node 1 is of length k, and the simple cycle in ζ_2 is of length m. If node j is contained in the simple cycle in ζ_1, then

$$\alpha = \frac{\beta^N - \beta^{N+m}}{\beta^k - \beta^{N+m}},$$

otherwise,

$$\alpha = \frac{\beta^N}{\beta^k}.$$

Theorem 2.3.2 shows that 1-randomised policies satisfying (2.8)–(2.10) have a very special structure. We hope that this particular structure will be relatively rare, therefore increasing the likelihood that an intelligent search of the extreme points of (2.8)–(2.10) may find a Hamiltonian extreme point rather than a 1-randomised policy.

2.4 Branch and fix method

In this section we describe first the branch and fix method, and next some of the techniques used in the branch and fix method to help limit the size of the logical branching tree.

2.4.1 Outline of branch and fix method

In view of the fact that it is only 1-randomised policies that prevent standard simplex methods from finding a Hamiltonian cycle, it has been recognised for some time that branch and bound type methods can be used to eliminate the possibility of arriving at these undesirable extreme points (e.g., see [28]). However, the method reported in [28] uses an embedding in a long-run average MDP, with a perturbation of transition probabilities that introduces a small parameter in most of the $p(j|i,a)$ coefficients of variables in linear constraints (2.8), thereby leading to loss of sparsity.

Furthermore, the method in [28] was never implemented fully, or tested beyond a few simple examples.

Theorem 2.3.2 indicates that 1-randomised policies induced by extreme points of $\bar{X}(\beta)$ are less prevalent than might have been conjectured, since they cannot be made of convex combinations of just any two deterministic policies. This provides motivation for testing algorithmic approaches based on successive elimination of arcs that could be used to construct these convex combinations.

Note that, since our goal is to find an extreme point $\mathbf{x}_e \in \bar{X}(\beta)$ such that

$$\zeta = M^{-1}(\mathbf{x}_e) \in \mathcal{D},$$

we have a number of degrees of freedom in designing an algorithm. In particular, different linear objective functions can be chosen at each stage of the algorithm, the parameter $\beta \in (0,1)$ can be adjusted, and $\mu \in (0, 1/N)$ can be chosen small but not so small as to cause numerical difficulties. The latter parameter needs to be positive to ensure that M^{-1} is well-defined. In the experiments reported here, we choose μ to be $1/N^2$.

The branch and fix (B&F) method is as follows. We solve a sequence of linear programs - two at each branching point of the logical B&F tree - with the generic structure:

$$\begin{gathered}\min L(\mathbf{x}) \\ \text{s.t.} \\ \mathbf{x} \in \bar{X}(\beta), \\ \text{additional constraints, if any, on arcs fixed earlier.}\end{gathered} \tag{2.11}$$

Step 1 - Initiation. We solve the original LP (2.11) without any additional constraints and with some choice of an objective function $L(\mathbf{x})$. We obtain an optimal basic feasible solution $\mathbf{x}_0$. We then find $\zeta_0 := M^{-1}(\mathbf{x}_0)$. If $\zeta_0 \in \mathcal{D}$; we stop, the policy ζ_0 identifies a Hamiltonian cycle. Otherwise ζ_0 is a 1-randomised policy.

Step 2 - Branching. We use the 1-randomised policy ζ_0 to identify the splitting node i, and two arcs (i, j_1) and (i, j_2) corresponding to the single randomisation in

ζ_0. If there are d arcs $\{(i, a_1), \ldots, (i, a_d)\}$ emanating from node i, we construct d subdigraphs: $\Gamma_1, \Gamma_2, \ldots, \Gamma_d$, where in Γ_k the arc (i, a_k) is the only arc emanating from node i. These graphs are identical to the original graph Γ at all other nodes. Note that in this process we, by default, fix an arc in each Γ_k.

Step 3 - Fixing. In many subdigraphs, the fixing of one arc implies that other arcs can also be fixed[3], without a possibility of unintentionally eliminating a Hamiltonian cycle containing already fixed arcs that contain a Hamiltonian cycle in the current subdigraph. Four checks for determining additional arcs that can be fixed are described in Subsection 2.4.3. Once we identify these arcs, we fix them at this step.

Step 4 - Iteration. We solve a second LP (described in Subsection 2.4.2 that checks if (2.9) can still be satisfied with the current fixing of arcs. If so, we repeat Step 1 with the LP (2.11) constructed for the graph at the current branching point of the logical B&F tree, with additional constraints are derived shortly, that is (2.13) and (2.14). Note that this branching point may correspond to $\Gamma_1, \Gamma_2, \ldots, \Gamma_d$, or to a sub-graph constructed from one of these with the help of additional arc fixing[4].

If ζ is a Hamiltonian policy, $\mathbf{x} = M(\zeta)$, and $\mu = 0$, then we can easily check that $\mathbf{x}$ satisfies (2.8)–(2.10) ifs

$$x_{i_k i_{k+1}} = \sum_a x_{i_k a} = \frac{\beta^k}{1-\beta^N}, \quad k = 0, \ldots, N-1, \tag{2.12}$$

where (i_k, i_{k+1}) is the k^{th} arc on the Hamiltonian cycle traced out by ζ. This immediately suggests lower and upper bounds on sums of the $\mathbf{x}$ variables corresponding to arcs emanating from the heads of fixed arcs. This is because if $i_{k+1} \neq 1$

$$\sum_{a \in \mathcal{A}(i_{k+1})} x_{i_{k+1} a} - \beta x_{i_k i_{k+1}} = 0.$$

[3]This frequently happens in the case of cubic graphs that supplied many of our test examples. For instance, see Figure 2.3 in Subsection 2.4.3.

[4]As is typical with branching methods, decisions guiding which branch to select first are important and open to alternative heuristics. We investigate five possible branching methods in Section 2.7.

If $i_{k+1} = 1$, then we have

$$-\beta^N \sum_{a \in \mathcal{A}(1)} x_{1a} + \beta x_{i_{N-1},1} = 0.$$

For $\mu > 0$ analogous (but somewhat more complex) expressions for the preceding sums can be derived and the above relationship between these sums at successive nodes on the Hamiltonian cycle is simply:

$$\sum_{a \in \mathcal{A}(i_{k+1})} x_{i_{k+1}a} - \beta x_{i_k i_{k+1}} = \mu. \tag{2.13}$$

If the fixed arc is the final arc $(i_N, 1)$, we have:

$$-\beta^N \sum_{a \in \mathcal{A}(1)} x_{1a} + \beta x_{i_{N-1},1} = \frac{\mu\beta(1-\beta^{N-1})}{1-\beta}. \tag{2.14}$$

We derive equation (2.13) by simply inspecting the form of (2.8). For (2.14), we know from (2.8) that

$$\sum_{a \in \mathcal{A}(1)} x_{1a} - \beta x_{i_{N-1},1} \quad = \quad 1 - (N-1)\mu,$$

and therefore

$$\beta x_{i_{N-1},1} \quad = \quad \sum_{a \in \mathcal{A}(1)} x_{1a} - 1 + (N-1)\mu. \tag{2.15}$$

Then, we substitute (2.15) into the left hand side of (2.14) to obtain

$$-\beta^N \sum_{a \in \mathcal{A}(1)} x_{1a} + \beta x_{i_{N-1},1} \quad = \quad (1-\beta^N) \sum_{a \in \mathcal{A}(1)} x_{1a} - 1 + (N-1)\mu. \tag{2.16}$$

Finally, we substitute (2.9) into (2.16) to obtain

$$\begin{aligned} -\beta^N \sum_{a \in \mathcal{A}(1)} x_{1a} + \beta x_{i_{N-1},1} &= (1-\beta^N)\frac{(1-(N-1)\mu)(1-\beta) + \mu(\beta-\beta^N)}{(1-\beta)(1-\beta^N)} - 1 + (N-1)\mu, \\ &= \frac{\mu\beta(1-\beta^{N-1})}{1-\beta}, \end{aligned}$$

which coincides with (2.14).

2.4.2 Structure of LP (2.11)

At the initiation step, we solve a feasibility problem of satisfying constraints (2.8), (2.9) and (2.10). This allows us to determine which node to begin branching on.

At every branching point of the logical B&F tree other than the root, we solve an additional LP that attempts to determine if we need to continue exploring the current branch. As the algorithm evolves along successive branching points of the logical B&F tree, we have additional information about which arcs have been fixed, and this consequently permits us to perform tests check the possibility of finding a Hamiltonian cycle that incorporates these fixed arcs. If we determine that it is impossible, we fathom that branching point of the logical B&F tree and no further exploration of that branch is required.

For instance, suppose that all fixed arcs belong to a set $\mathcal{U}$. Let the objective function of a second LP[5] be

$$L(\mathbf{x}) \quad = \sum_{a \in \mathcal{A}(1)} x_{1a}, \tag{2.17}$$

and minimise (2.17) subject to constraints (2.8) and (2.10) together with equations (2.13) and (2.14) providing additional constraints for each arc in $\mathcal{U}$. If the minimum $L^*(\mathbf{x})$ fails to reach the level defined by the right hand side of the now omitted constraint (2.9) of $\bar{X}(\beta)$, or if the constraints are infeasible, then no Hamiltonian cycle exists that uses all the arcs of $\mathcal{U}$, and we fathom the current branching point of the logical B&F tree. Otherwise, we solve the LP (2.11) with the objective function[6]

$$L(\mathbf{x}) = \sum_{(i,j) \in \mathcal{U}} \left[\sum_{a \in \mathcal{A}(j)} x_{ja} - \beta \sum_{a \in \mathcal{A}(i)} x_{ia} \right],$$

[5]Note that, although we call (2.17) the Second LP, it is the first LP solved in all iterations other than the initial iteration. Since it is not solved first in the initial iteration, we refer to (2.17) as the Second LP.

[6]For simplicity, we are assuming here that $\mathcal{U}$ does not contain an arc going into node 1. If such an arc were in $\mathcal{U}$, this objective would have one term consistent with the left hand side of equation (2.14).

and with no additional constraints beyond those in $\bar{X}(\beta)$. This LP will either find a Hamiltonian cycle, or it will lead to an extreme point $\mathbf{x}'_e$ such that $\zeta' = M^{-1}(\mathbf{x}'_e)$ is a new 1-randomised policy.

2.4.3 Arc fixing checks

There are a number of logical checks that enable us to fix additional arcs once a decision is taken to fix one particular arc. This is best illustrated with the help of an example. Note that these checks are in the spirit of well-known rules for constructing Hamiltonian cycles (see, for instance, Section 8.2 of [53]).

Consider the simple 6-node cubic envelope graph (see Figure 1.1). The figure below shows the kind of logical additional arc fixing that can arise.

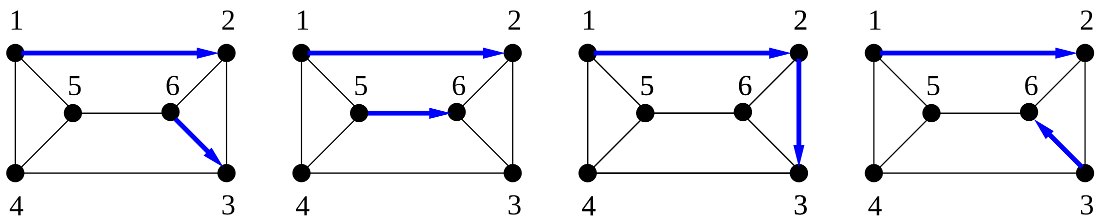


Figure 2.3: Various arc fixing situations.

Check 1: Consider the left-most graph in Figure 2.3. The only fixed arcs are $(1, 2)$ and $(6, 3)$. Since the only arcs that can go to node 5 are $(1, 5)$, $(4, 5)$ and $(6, 5)$, we may also fix arc $(4, 5)$ as nodes 1 and 6 already have fixed arcs going elsewhere. In this case, we say that arc $(4, 5)$ is *free*, whereas arcs $(1, 5)$ and $(6, 5)$ are *not free*. In general, if only one free arc enters a node, it must be fixed.

Check 2: Consider the second graph from the left in Figure 2.3. The only fixed arcs are $(1, 2)$ and $(5, 6)$. The only arcs going to node 5 are $(1, 5)$, $(4, 5)$ and $(6, 5)$. We cannot choose $(6, 5)$ as this will create a subcycle of length 2, and node 1 already has a fixed arc going elsewhere, so we must fix arc $(4, 5)$. In general, if there are only two free arcs, and one will create a subcycle, we must fix the other one.

Check 3: Consider the third graph from the left in Figure 2.3. The only fixed arcs are $(1, 2)$ and $(2, 3)$. Since the only arcs that can come from node 6 are $(6, 2)$,

$(6,3)$ and $(6,5)$, we must fix arc $(6,5)$ as nodes 2 and 3 already have arcs going into them. In this case, we say that arcs $(6,3)$ and $(6,5)$ are *blocked*, whereas arc $(6,2)$ is *unblocked*. In general, if there is only one unblocked arc emanating from a node, the arc must be fixed.

Check 4: Consider the right-most graph in Figure 2.3. The only fixed arcs are $(1,2)$ and $(3,6)$. The only arcs that can come from node 6 are $(6,2)$, $(6,3)$ and $(6,5)$. We cannot choose $(6,2)$ because node 2 already has an incoming arc, and we cannot choose $(6,3)$ as this will create a sub-cycle, so we must fix arc $(6,5)$. In general, if there are two unblocked arcs emanating from a node, and one will create a subcycle, we must fix the other one.

The branch and bound method given in [28] always finds a Hamiltonian cycle if any exist. While the branch and fix method presented here is in the same spirit as the method in [28], we include a finite convergence proof for the sake of completeness.

Theorem 2.4.1 *The branch and fix method converges in finitely many steps. In particular, the following two statements hold.*

(1) If Γ is Hamiltonian, the algorithm finds a Hamiltonian cycle in Γ.

(2) If Γ is non-Hamiltonian, the algorithm terminates after fathoming all the constructed branches of the logical B&F tree.

Proof. The algorithm begins with the original graph Γ. At each stage of the algorithm, a splitting node is identified and branches are created for all arcs emanating from that node. As we consider every arc for this node, it is not possible that the branching process can eliminate the possibility of finding a Hamiltonian cycle if one exists as we will explore every possibility from this node. It then suffices to confirm that none of the checking, bounding, or fixing steps in the branch and fix method can eliminate the possibility of finding a Hamiltonian cycle.

Recall that constraints (2.9), (2.13) and (2.14) are shown to be satisfied by all Hamiltonian cycles. Then, for a particular branching point, if the minimum value of

(2.17) constrained by (2.8), (2.10), (2.13) and (2.14) cannot achieve the value given in (2.9), or if the constraints are infeasible, there cannot be any Hamiltonian cycles remaining in the subdigraph. Therefore, fathoming the branch due to the Second LP in Subsection 2.4.2 cannot eliminate any Hamiltonian cycles.

Checks 1–4 above are designed to ensure that at least one arc goes into and comes out of each node (while preventing the formation of subcycles) by fixing an arc or arcs in situations where any other choice will violate this requirement. Since this is a requirement for all Hamiltonian cycles, it follows that arc fixing performed in Subsection 2.4.3 cannot eliminate any Hamiltonian cycles.

The branch and fix method continues to search the tree until either a Hamiltonian cycle is found, or all the constructed branches are fathomed. Since none of the steps in the branch and fix method can eliminate the chance of finding a Hamiltonian cycle, we are guaranteed to find one of the Hamiltonian cycles in Γ. If all branches of the logical B&F tree have been fathomed without finding any Hamiltonian cycles, we can conclude that Γ is non-Hamiltonian. □

Note that while the branch and fix method only finds a single Hamiltonian cycle, it is possible to find all Hamiltonian cycles by simply recording each Hamiltonian cycle when they are is found, and then continuing to search the branch and fix tree rather than terminating.

Corollary 2.4.2 *The logical B&F tree has a maximum depth of N.*

Proof. Since at each branching point of B&F we branch on all arcs emanating from a node, it follows that once an arc (i, j) is fixed, no other arcs can be fixed emanating from node i. Then, at each level of the branch and fix tree, a different node is branched on. After N levels, all nodes will have exactly one arc fixed, and either a Hamiltonian cycle will be found, or the relevant LP will be infeasible and we will fathom that branch. □

In practice, the arc fixing checks will ensure that we never reach this maximum depth as we will certainly fix multiple arcs at branching points corresponding to subdigraphs where few unfixed arcs remain.

2.5 An algorithm that implements the branch and fix method

In Section 2.4, we describe the branch and fix method for HCP and prove its convergence. Here, we present a recursive algorithm that implements the method in pseudocode format, with separate component algorithms for the arc fixing checks, and for solving the second LP. Note that the input variable *fixed arcs* is initially input as an empty vector, as no arcs are fixed at the commencement of the algorithm. Note that the output term Hamiltonian cycle may either be a Hamiltonian cycle found by the branch and fix method, or a message that no Hamiltonian cycle was found.

```
Input: Γ, β, fixed arcs
Output: HC

begin
    N ← Size(Γ)
    μ ← 1/N^2
    function value ← Algorithm 2.2: Second LP algorithm(Γ, β, fixed arcs)
    if infeasibility is found or function value > ((1 − (N − 1)μ)(1 − β) + μ(β − β^N)) / ((1 − β)(1 − β^N))
        return no HC found
    end
    X̄(β) ← constraints (2.8)–(2.10)
    for Each arc in fixed arcs
        if Arc goes into node 1
            X̄(β) ← Add constraint (2.14)
        else
            X̄(β) ← Add constraint (2.13)
        end
    end
    x ← Solve the LP (2.11) with constraints X̄(β)
    if infeasibility is found
        return no HC found
    elseif a HC is found
        return HC
    end
    splitting node ← Identify which node has 2 non-zero entries in x
    d ← Number of arcs emanating from splitting node
    for i from 1 to d
        Γ_d ← Γ with the d-th arc from splitting node fixed
        (Γ_d, new fixed arcs) ← Algorithm 2.3: Checking algorithm(Γ_d, fixed arcs)
        HC ← Algorithm 2.1: Branch and fix algorithm(Γ_d, β, new fixed arcs)
        if a HC is found
            return HC
        end
    end
    if a HC is found
        return HC
    else
        return no HC found
    end
end
```

Algorithm 2.1: Branch and fix algorithm.

```
Input: Γ, β, fixed arcs
Output: function value

begin
    L(x) ← Sum of all arcs (1, j) emanating from node 1
    X(β) ← constraints (2.8) and (2.10)
    for each arc in fixed arcs
        if arc goes into node 1
            X(β) ← Add constraint (2.14)
        else
            X(β) ← Add constraint (2.13)
        end
    end
    (x,function value) ← Solve the LP min L(x) subject to X(β)
end
```

Algorithm 2.2: Second LP algorithm.

```
Input: Γ, fixed arcs
Output: Γ, fixed arcs

begin
    N ← Size(Γ)
    for i from 1 to N
        if only one arc (j, i) is free to go into node i
            fixed arcs ← Add arc (j, i) to fixed arcs if it is not already in fixed arcs
        end

        if two arcs (j, i), (k, i), j ≠ k are free to go into node i and arc (i, k) is in fixed arcs
            fixed arcs ← Add arc (j, i) to fixed arcs if it is not already in fixed arcs
        end

        if only one arc (i, j) that emanates from node i is unblocked
            fixed arcs ← Add arc (i, j) to fixed arcs if it is not already in fixed arcs
        end

        if two arcs (i, j), (i, k), j ≠ k that emanate from node i are unblocked, and arc (k, i) is in fixed arcs
            fixed arcs ← Add arc (i, j) to fixed arcs if it is not already in fixed arcs
        end
    end
end
```

Algorithm 2.3: Checking algorithm.

2.6 Numerical results

We implemented Algorithms 2.1 – 2.2 in MATLAB (version 7.4.0.336) and used CPLEX (version 11.0.0) to solve all the linear programming sub-problems. The algorithm was tested on a range of small to medium size graphs. The results are encouraging. The number of branches required to solve each of these problems is only a tiny fraction of the number of deterministic policies. It is clear that non-Hamiltonian graphs require more branches to solve than Hamiltonian graphs of the same size. This is because in a Hamiltonian graph, as soon as a Hamiltonian cycle is found, the algorithm terminates. As there is no Hamiltonian cycle in a non-Hamiltonian graph, the algorithm only terminates after exhaustively searching the logical B&F tree.

A sample of results is seen in Tables 2.1 and 2.2, including a comparison between the number of branches examined and the maximum possible number of branches (deterministic policies), and the running time in seconds. The Dodecahedron, Petersen, and Coxeter graphs, and the Knight's Tour problem are well-known in the literature (see [35] p. 12 for the first two, p. 225 for the third, and [5] p. 241 for the last). The 24-node graph is a randomly chosen cubic 24-node graph. In the first column of Table 2.2, we refer to sets of cubic graphs with the prescribed number of nodes. In the second column of Table 2.2, we report the average number of branches examined by the branch and fix method with the average taken over all graphs in the corresponding class. We also report the minimum and maximum branches examined over the set of graphs, and the average running time taken to solve the graphs in the corresponding class. We consider all of the 10 node cubic graphs, of which there are 17 Hamiltonian and 2 non-Hamiltonian graphs, and all of the 12 node cubic graphs, of which there are 80 Hamiltonian and 5 non-Hamiltonian graphs. We randomly generate 50 cubic graphs of size $N = 20, 30, 40$ and 50. All of the randomly generated graphs are Hamiltonian. See [44] for a reference on generating cubic graphs. Every test is run with β set to 0.99, and μ set to $\frac{1}{N^2}$.

Note that with this basic implementation of B&F we were not able to obtain a

Hamiltonian solution for the 8×8 Knight's Tour problem after twelve hours. In Section 2.8, however, we introduce new constraints that allow us solve this problem in little more than a minute.

Graph	**Branches**	**Upper bound**	**Time (secs)**
Dodecahedron: Ham, $N = 20$, arcs $= 60$	75	3.4868×10^{9}	2.98
Ham, $N = 24$, arcs $= 72$	28	2.8243×10^{11}	1.02
8×8 Knight's Tour: Ham, $N = 64$, arcs $= 336$	failed	9.1654×10^{43}	> 12 hrs
Petersen: non-Ham, $N = 10$, arcs $= 30$	53	5.9049×10^{4}	0.99
Coxeter: non-Ham, $N = 28$, arcs $= 84$	11589	2.2877×10^{13}	593.40

Table 2.1: Preliminary results for the branch and fix method.

Type of graphs	**Average branches**	**Minimum branches**	**Maximum branches**	**Average time (secs)**
Hamiltonian, N = 10	2.1	1	4	0.08
Hamiltonian, N = 12	3.4	1	10	0.14
Non-Hamiltonian, N = 10	32.5	12	53	0.61
Non-Hamiltonian, N = 12	25.6	11	80	0.53
50 graphs, N = 20	29.5	1	141	1.08
50 graphs, N = 30	216.5	3	1057	10.41
50 graphs, N = 40	2595.6	52	10536	160.09
50 graphs, N = 50	40316.7	324	232812	2171.46

Table 2.2: Performance of the branch and fix method over cubic graphs.

Example 2.6.1 *We conclude this section with a detailed solution of the simple 6-node envelope graph, shown in Figure 2.4, that is solved using the above implementation of B&F method, given in Section 2.5, with* $\beta = 0.99$, $\mu = \frac{1}{36}$.

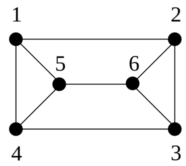


Figure 2.4: The envelope graph.

We start by solving the following feasibility problem:

$$\begin{aligned}
x_{12} + x_{14} + x_{15} - \beta x_{21} - \beta x_{41} - \beta x_{51} &= 1 - 5\mu, \\
x_{21} + x_{23} + x_{26} - \beta x_{12} - \beta x_{32} - \beta x_{62} &= \mu, \\
x_{32} + x_{34} + x_{36} - \beta x_{23} - \beta x_{43} - \beta x_{63} &= \mu, \\
x_{41} + x_{43} + x_{45} - \beta x_{14} - \beta x_{34} - \beta x_{54} &= \mu, \\
x_{51} + x_{54} + x_{56} - \beta x_{15} - \beta x_{45} - \beta x_{65} &= \mu, \\
x_{62} + x_{63} + x_{65} - \beta x_{26} - \beta x_{36} - \beta x_{56} &= \mu, \\
x_{12} + x_{14} + x_{15} &= \frac{(1-5\mu)(1-\beta) + \mu(\beta - \beta^6)}{(1-\beta)(1-\beta^6)}, \\
x_{ia} &\geq 0, \quad \textit{for all } (i,a) \in \Gamma.
\end{aligned}$$

The first iteration produces a 1-randomised policy where the randomisation occurs at node 4. The logical B&F tree then splits into three choices: to fix arc (4,1), (4,3) or (4,5). The algorithm first branches on fixing arc (4,1).

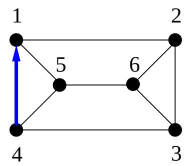


Figure 2.5: Branching on arc $(4, 1)$.

As the algorithm uses a depth first search, the arcs (4,3) and (4,5) will not be fixed unless the algorithm fathoms the (4,1) branch without having found a Hamiltonian cycle. Note that fixing the arc (4,1) is equivalent to eliminating arcs (4,3) and (4,5) in the remainder of this branch of the logical B&F tree. In addition, arcs (1,4), (2,1) and (5,1) can also be eliminated because they cannot be present together with arc (4,1) in a Hamiltonian cycle.

At the second iteration we solve two LPs. We first solve the Second LP, to check the feasibility of the graph remaining after the above round of fixing (and eliminating) of arcs:

$$\min x_{12} + x_{15}$$

$$s.t.$$

$$\begin{aligned}
x_{12} + x_{15} - \beta x_{41} &= 1 - 5\mu, \\
x_{23} + x_{26} - \beta x_{12} - \beta x_{32} - \beta x_{62} &= \mu, \\
x_{32} + x_{34} + x_{36} - \beta x_{23} - \beta x_{63} &= \mu, \\
x_{41} - \beta x_{34} - \beta x_{54} &= \mu, \\
x_{54} + x_{56} - \beta x_{15} - \beta x_{65} &= \mu, \\
x_{62} + x_{63} + x_{65} - \beta x_{26} - \beta x_{36} - \beta x_{56} &= \mu, \\
-\beta^6 x_{12} - \beta^6 x_{15} + \beta x_{41} &= \frac{\mu(\beta - \beta^6)}{1 - \beta}, \\
x_{ia} &\geq 0, \quad \textit{for all } (i, a) \in \Gamma.
\end{aligned}$$

Note that the last equality constraint above comes from (2.14) because the fixed arc (4,1) returns to the home node. The optimal objective function returned is equal to the right hand side of the omitted constraint (2.9), so we cannot fathom this branch, at this stage. Hence, we also solve the updated LP (2.11):

$$\min -\beta^6 x_{12} - \beta^6 x_{15} + \beta x_{41}$$

$$s.t.$$

$$\begin{aligned}
x_{12} + x_{15} - \beta x_{41} &= 1 - 5\mu, \\
x_{23} + x_{26} - \beta x_{12} - \beta x_{32} - \beta x_{62} &= \mu, \\
x_{32} + x_{34} + x_{36} - \beta x_{23} - \beta x_{63} &= \mu, \\
x_{41} - \beta x_{34} - \beta x_{54} &= \mu, \\
x_{54} + x_{56} - \beta x_{15} - \beta x_{65} &= \mu, \\
x_{62} + x_{63} + x_{65} - \beta x_{26} - \beta x_{36} - \beta x_{56} &= \mu, \\
x_{12} + x_{15} &= \frac{(1 - 5\mu)(1 - \beta) + \mu(\beta - \beta^6)}{(1 - \beta)(1 - \beta^6)}, \\
x_{ia} &\geq 0, \quad \textit{for all } (i, a) \in \Gamma.
\end{aligned}$$

The second iteration produces a 1-randomised policy where the randomisation occurs at node 3. The logical B&F tree then splits into three choices: to fix arc (3,2), (3,4) or (3,6). The algorithm first selects the arc (3,2) to continue the branch. The graph at this stage is shown in Figure 2.6.

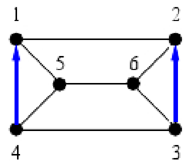


Figure 2.6: Branching on arc $(3, 2)$ after fixing arc $(4, 1)$.

Examining remaining nodes with multiple (non-fixed) arcs and exploiting Checks 1–4 we immediately see that arcs (2,6) and (1,5) must be fixed by Check 4. Once these arcs are fixed, arcs (5,4) and (6,3) are also fixed by Check 4. At this stage, every node has a fixed arc but we have not obtained a Hamiltonian cycle, and hence we fathom the branch.

Travelling back up the tree, the algorithm next selects the arc (3,4) to branch on. The graph at this stage is shown in Figure 2.7.

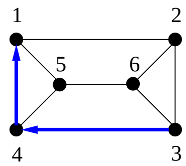


Figure 2.7: Second branching on arc $(3, 4)$.

Examining remaining nodes with multiple (non-fixed) arcs and exploiting Checks 1–4, we immediately see that arc (5,6) must be fixed by Check 3. Once this arc is fixed, arc (2,3) is also fixed by Check 3. Next, arc (6,2) is fixed by Check 4 and, finally, arc (1,5) is fixed by Check 3. At this stage, every node has a fixed arc. Since these fixed arcs correspond to the Hamiltonian cycle $1 \rightarrow 5 \rightarrow 6 \rightarrow 2 \rightarrow 3 \rightarrow 4 \rightarrow 1$, *the algorithm terminates. The Hamiltonian cycle is shown in Figure 2.8. The whole logical B&F tree is illustrated in Figure 2.9.*

Note that, even in this simple example, in the worst case $3^6 = 729$ branches could

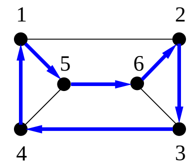


Figure 2.8: Hamiltonian cycle found by B&F method.

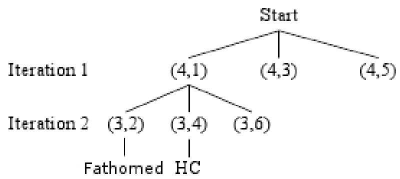


Figure 2.9: The logical B&F tree for the envelope graph.

have been generated. However, our algorithm was able to find a Hamiltonian cycle after examining only two.

2.7 Branching methods

One of the standard questions when using a branching algorithm is which method of branching to use. One of the major benefits of the branch and fix method is that the checks and the second LP (2.17) often allow us to fathom a branching point relatively early, so depth-first searching is used. However, the horizontal ordering of the branch tree is, by default, determined by nothing more than the initial ordering of the nodes. For a non-Hamiltonian graph, this ordering makes no difference as the breadth of the entire tree will need to be traversed to determine that no Hamiltonian cycles exist. However, for a Hamiltonian graph, it is possible that a relabelling of the graph would result in the branch and fix method finding a Hamiltonian cycle sooner.

While it seems impossible to predict, in advance, which relabelling of nodes will find a Hamiltonian cycle the quickest, it is possible that the structure of the 1-randomised policy found at each branching point can provide information about which branch should be traversed first. Each 1-randomised policy with splitting node i contains two non-zero values x_{ij} and x_{ik}, $j \neq k$. Without loss of generality, assume that $x_{ij} \leq x_{ik}$. We propose five branching methods:

1) Default branching (or node order): the branches are traversed in the order of the numerical labels of the nodes.
2) First branch on fixing (i, j), then (i, k) and then traverse the rest of the branches in node order.
3) First branch on fixing (i, k), then (i, j) and then traverse the rest of the branches in node order.
4) All branches are traversed in node order other than those corresponding to fixing (i, j) or (i, k). The last two branches traversed are (i, j) and then (i, k).
5) First branch on fixing (i, k), then traverse the rest of the branches other than the branch corresponding to fixing (i, j) in node order, and finally branch on fixing (i, j).

We tested these five branching methods on the same sets of 50 randomly generated Hamiltonian cubic graphs as those generated for Table 2.2. In Table 2.3, we give the average number of branches examined by B&F for each branching method.

Branching method	**20 node graphs**	**30 node graphs**	**40 node graphs**	**50 node graphs**
1	29.48	216.54	2595.58	40316.68
2	33.28	261.24	2227.24	43646.92
3	24.58	172.30	1624.50	17468.26
4	38.68	285.26	2834.44	53719.96
5	34.04	345.44	3228.44	76159.30

Table 2.3: Average number of branches examined by the five branching methods over sets of Hamiltonian cubic graphs.

From the results shown in Table 2.3 it appears that branching method 3 is the best performing method for cubic graphs. Note that the sets of cubic graphs were produced by GENREG [44] which uses a particular ordering strategy, which may account for the success of branching method 3.

2.8 Wedge constraints

Recall that constraints (2.8)–(2.10) that define $\bar{X}(\beta)$ depend upon parameters β and μ. While the use of β is necessary in the framework of a discounted MDP, the selection of μ as a small, positive parameter is used only to ensure that the mapping $\zeta_x(i,a) = x_{ia}/x_i$ (see (1.9)) is well-defined. Without setting $\mu > 0$, it is possible that x_i could be equal to 0. To illustrate this, recall constraint (2.8)

$$\sum_{i=1}^{N} \sum_{a\in\mathcal{A}(i)} \left(\delta_{ij} - \beta p(j|i,a)\right) x_{ia} \quad = \quad \eta_j, \quad j = 1,\ldots,N,$$

where

$$\eta_j = \begin{cases} 1-(N-1)\mu, & \text{if } i = 1, \\ \mu, & \text{otherwise.} \end{cases}$$

Rearranging constraint (2.8), we obtain

$$\sum_{a\in\mathcal{A}(j)} x_{ja} = \beta \sum_{i=1}^{N} \sum_{a\in\mathcal{A}(i)} p(j|i,a)x_{ia} + \eta_j, \quad j = 1,\ldots,N.$$

Since we cannot ensure that $\sum\limits_{i=1}^{N} \sum\limits_{a\in\mathcal{A}(i)} p(j|i,a)x_{ia} \neq 0$ for all j, we select $\mu > 0$ to ensure that $x_j = \sum\limits_{a\in\mathcal{A}(j)} x_{ja} > 0$. However, an additional set of constraints, first published in [22], can achieve the same goal while allowing us to set $\mu = 0$ by constraining x_j away from 0. We call these constraints *wedge constraints*. The wedge constraints are comprised of the following two sets of inequalities:

$$\sum_{a\in\mathcal{A}(i)} x_{ia} \quad \leq \quad \frac{\beta}{1-\beta^N}, \quad i = 2,\ldots,N, \tag{2.18}$$

$$\sum_{a\in\mathcal{A}(i)} x_{ia} \quad \geq \quad \frac{\beta^{N-1}}{1-\beta^N}, \quad i = 2,\ldots,N. \tag{2.19}$$

The rationale behind the wedge constraints is that, in the case when $\mu = 0$, we know from (2.12) that all Hamiltonian solutions to (2.8)–(2.10) take the form

$$x_{ia} \quad = \quad \begin{cases} \frac{\beta^k}{1-\beta^N}, & (i,a) \text{ is the } k\text{-th arc on the HC,} \\ 0, & \text{otherwise.} \end{cases} \tag{2.20}$$

In every Hamiltonian cycle h, exactly one arc emanates from each node. Let (i, h_i) be the arc emanating from node i in hs. Then,

$$\sum_{a \in \mathcal{A}(i)} x_{ia} = x_{ih_i}. \tag{2.21}$$

Recall that we define the home node of a graph as node 1. Then, the initial (0-th) arc in any Hamiltonian cycle is arc $(1, a)$, for some $a \in \mathcal{A}(1)$, and therefore from (2.20) we obtain

$$\sum_{a \in \mathcal{A}(1)} x_{1a} = \frac{1}{1-\beta^N}.$$

This constraint is already given in (2.9) if we set $\mu = 0$. For all other nodes, however, constraints of this type will partially capture a new property of Hamiltonian solutions that is expressed in (2.20). Substituting (2.21) into (2.20), for all nodes other than the home node, we obtain wedge constraints (2.18)–(2.19).

Recall that in a cubic graph, there are exactly three arcs, say (i, a), (i, b) and (i, c), from a given node i. Thus, in 3-dimensions, the corresponding constraints (2.18)–(2.19) have the shape indicated in Figure 2.10 that looks like a slice of a pyramid. The resulting wedge-like shaped inspires the name "wedge constraints".

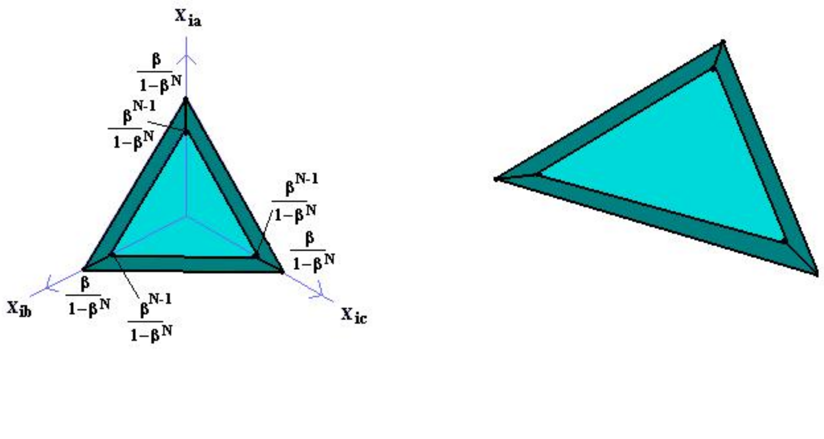


Figure 2.10: Wedge constraints for a node in a cubic graph.

We can add wedge constraints (2.18)–(2.19) to the constraint set (2.8)–(2.10), setting $\mu = 0$ in the latter. However, adding wedge constraints destroys the 1-randomised structure of non-Hamiltonian solutions that exist for the extreme points of the feasible region specified by (2.8)–(2.10), introducing many new extreme points to the feasible region. Since this is undesirable, we only use wedge constraints when solving the second LP (2.17), in an attempt to determine that a branch can be fathomed earlier than is the case without the wedge constraints.

The model incorporating the wedge constraints is

$$\begin{aligned}
\sum_{i=1}^{N} \sum_{a \in \mathcal{A}(i)} (\delta_{ij} - \beta p(j|i,a))\, x_{ia} &= \delta_{1j}, \quad j = 1, \ldots, N, && (2.22)\\
x_{ia} &\geq 0, \quad (i,a) \in \Gamma, && (2.23)\\
\sum_{a \in \mathcal{A}(i)} x_{ia} &\leq \frac{\beta}{1-\beta^N}, \quad i = 2, \ldots, N, && (2.24)\\
\sum_{a \in \mathcal{A}(i)} x_{ia} &\geq \frac{\beta^{N-1}}{1-\beta^N}, \quad i = 2, \ldots, N, && (2.25)
\end{aligned}$$

which replaces constraints (2.8) and (2.10) in the second LP (2.17). Everything else in the branch and fix method is identical to that described in Section 2.4.

We ran this model on the same selection of graphs as those in Section 2.6, to compare its performance to that of the original branch and fix method. There was a significant decrease in the number of branches examined, and consequently, also the running time of the model. A sample of results is seen in Tables 2.4 – 2.6, where we solve the same graphs as those in Tables 2.1 – 2.3. Every test is run with β set to 0.99, and μ set to $\frac{1}{N^2}$.

In Table 2.4, we compare the number of branches examined by B&F for five graphs to the maximum possible number of branches (deterministic policies), and show the running time in seconds.

In Table 2.5, we solve several sets of cubic graphs, and report the average number of branches examined by B&F over each set. We also report the minimum and maximum branches examined over each set, and the average running time. As in Table 2.2, we consider all of the 10 node cubic graphs, of which there are 17 Hamiltonian and 2 non-Hamiltonian graphs, and all of the 12 node cubic graphs, of which there are 80 Hamiltonian and 5 non-Hamiltonian graphs. For each of the sets of larger cubic graphs, we use the same graphs as were randomly generated for Table 2.2.

Graph	Branches	Upper bound	Time (secs)
Dodecahedron: Ham, $N = 20$, arcs = 60	43	3.4868×10^9	1.71
Ham, $N = 24$, arcs = 72	5	2.8243×10^{11}	0.39
8×8 Knight's Tour: Ham, $N = 64$, arcs = 336	220	9.1654×10^{43}	78.46
Petersen: non-Ham, $N = 10$, arcs = 30	53	5.9049×10^4	1.17
Coxeter: non-Ham, $N = 28$, arcs = 84	5126	2.2877×10^{13}	262.28

Table 2.4: Preliminary results for the branch and fix method with wedge constraints included.

Type of graphs	Average branches	Minimum branches	Maximum branches	Average time (secs)
Hamiltonian, N = 10	2.1	1	4	0.09
Hamiltonian, N = 12	3.0	1	10	0.14
Non-Hamiltonian, N = 10	32.5	12	53	0.70
Non-Hamiltonian, N = 12	23.2	11	72	0.50
50 graphs, N = 20	14.6	1	75	0.65
50 graphs, N = 30	41.7	2	182	2.56
50 graphs, N = 40	209.2	7	1264	18.11
50 graphs, N = 50	584.4	8	2522	67.99

Table 2.5: Performance of the branch and fix method with wedge constraints included over cubic graphs.

In Table 2.6, we report the average number of branches examined by B&F for the same set of randomly cubic graphs shown in Table 2.5, for all five branching methods.

We note with interest that the model with wedge constraints included performs well when we select branching method 5, which was the worst performing branching method in the model without wedge constraints. Being that branching method 3 also performs well, it appears that branching first on arc (i, k) is an efficient strategy for graphs generated by GENREG when we include wedge constraints.

In [2], the first numerical procedure taking advantage of the MDP embedding was

Branching method	**20 node graphs**	**30 node graphs**	**40 node graphs**	**50 node graphs**
1	14.60	41.66	209.18	584.40
2	14.76	49.94	164.74	636.88
3	11.86	38	145.54	603.24
4	17.28	50.32	152.50	632.08
5	15.32	39.42	123.72	356.32

Table 2.6: Average number of branches examined by the five branching methods with wedge constraints included over sets of Hamiltonian cubic graphs.

used to solve graphs of similar sizes to those listed in Tables 2.4 and 2.5. The model given in [2] is solved using the MIP solver in CPLEX. The present model outperforms the model in [2] in terms of the number of branches examined in the cases displayed in Tables 2.4 and 2.5. In particular, the number of branches examined to solve each graph was much reduced in the branch and fix method when compared to similar sized graphs in [2]. In particular, to solve the 8×8 Knight's tour graph, between 2000 and 40000 branches were examined in the model given in [2] (depending on the selection of parameters in CPLEX), but only 220 were required in the branch and fix method with wedge constraints included. This significant improvement highlights first the progress made in this line of research over the last decade, and second the advantages obtained by the use of wedge constraints. We seek to take further advantage of the wedge constraints in a new mixed integer programming formulation, the Wedged-MIP heuristic, which we describe in the next section.

2.9 The Wedged-MIP heuristic

The discussion in the preceding section naturally leads us to consider the polytope $Y(\beta)$ defined by the following seven sets of linear constraints:

$$\sum_{i=1}^{N} \sum_{a \in \mathcal{A}(i)} \left(\delta_{ij} - \beta p(j|i,a)\right) y_{ia} \quad = \quad \delta_{1j}(1-\beta^N), \quad j = 1, \ldots, N, \tag{2.26}$$

$$
\begin{aligned}
\sum_{a \in \mathcal{A}(1)} y_{1a} &= 1, && (2.27)\\
y_{ia} &\geq 0, \quad (i,a) \in \Gamma, && (2.28)\\
\sum_{j \in \mathcal{A}(i)} y_{ij} &\geq \beta^{N-1}, \quad i \geq 2, && (2.29)\\
\sum_{j \in \mathcal{A}(i)} y_{ij} &\leq \beta, \quad i \geq 2, && (2.30)\\
y_{ij} + y_{ji} &\leq 1, \quad (i,j) \in \Gamma, (j,k) \in \Gamma, && (2.31)\\
y_{ij} + y_{jk} + y_{ki} &\leq 2, \quad (i,j) \in \Gamma, (j,k) \in \Gamma, (k,i) \in \Gamma. && (2.32)
\end{aligned}
$$

Remark 2.9.1 *(1) Note that the variables y_{ia}, which define $Y(\beta)$, are obtained from the variables x_{ia} that define $X(\beta)$ by the transformation*

$$y_{ia} = (1-\beta^N)x_{ia}, \quad (i,a) \in \Gamma.$$

(2) In view of (1), constraints (2.26)–(2.28) are merely constraints (2.8)–(2.10) normalised by the multiplier $(1-\beta^N)$, and with $\mu = 0$. Furthermore, constraints (2.29)–(2.30) are similarly normalised wedge constraints.

(3) Note that normalising (2.20) in the same way implies that if $\mathbf{y} \in Y(\beta)$ corresponds to a Hamiltonian cycle, then

$$y_{ia} \in \{0, 1, \beta, \beta^2, \ldots, \beta^{N-1}\}, \quad (i,a) \in \Gamma.$$

Thus, for β sufficiently near 1 all positive entries of a Hamiltonian solution $\mathbf{y}$ are also either 1 (if $i = 1$), or close to 1. Therefore, if $\mathbf{y} \in Y(\beta)$ is any feasible point with only one positive entry y_{ia} for all $a \in \mathcal{A}(i)$, for each i, then constraints (2.29)–(2.30) ensure that all those positive entries have values near 1. Furthermore, constraints (2.31)–(2.32) ensure that at most one such large entry is permitted on any potential 2-cycle, and at most two such large entries are permitted on any potential 3-cycle.

(4) In view of (3), it is reasonable that we should be searching for a feasible point $\mathbf{y} \in Y(\beta)$ that has only a single positive entry y_{ia} for all $a \in \mathcal{A}(i)$ and for each i.

We make the last point of the above remark precise in the following proposition that is analogous to a result proved in [9] for an embedding of HCP in a long-run average

MDP. Since it forms the theoretical basis of our most powerful heuristic, we supply a formal proof below.

Proposition 2.9.2 *Given any graph Γ and its embedding in a discounted Markov decision process $\mathcal{M}$, consider the polytope $Y(\beta)$ defined by (2.26)–(2.32) for $\beta \in [0,1)$ and sufficiently near 1. The following statements are equivalent:*

(1) The point $\hat{\mathbf{y}} \in Y(\beta)$ is Hamiltonian in the sense that the positive entries $\hat{y}_{ia}$ of $\hat{\mathbf{y}}$ correspond to arcs (i,a) defining a Hamiltonian cycle in Γ.

(2) The point $\hat{\mathbf{y}} \in Y(\beta)$ is a global minimiser of the nonlinear program

$$\begin{aligned} \min \sum_{i=1}^{N} \sum_{a \in \mathcal{A}(i)} \sum_{b \in \mathcal{A}(i), b \neq a} & y_{ia} y_{ib} \\ s.t. & \\ \mathbf{y} \in Y(\beta), & \end{aligned} \tag{2.33}$$

which gives the objective function value of 0 in (2.33).

(3) The point $\hat{\mathbf{y}} \in Y(\beta)$ satisfies the additional set of nonlinear constraints

$$y_{ia} y_{ib} \;=\; 0, \quad i = 1, \ldots, N, \quad a, b \in \mathcal{A}(i), \quad a \neq b, \tag{2.34}$$

Proof. By the nonnegativity of $\hat{\mathbf{y}} \in Y(\beta)$ it immediately follows that part (2) and part (3) are equivalent.

From (2.20) and part (3) of Remark 2.9.1 we note that if $\hat{\mathbf{y}}$ is Hamiltonian, it implies part (3). Furthermore, if $\hat{\mathbf{y}}$ is a global minimiser of (2.33), constraints (2.29) ensure that it must have at least one positive entry corresponding to some arc $a \in \mathcal{A}(i)$ for each $i = 1, \ldots, N$. Since $\hat{y}_{ia}\hat{y}_{ib} = 0$ for all $a \neq b$, $i = 1, \ldots, N$, we conclude that $\hat{\mathbf{y}}$ has exactly one positive entry $\hat{y}_{ia}$, for each i. We then define $\hat{\mathbf{x}} \in X(\beta)$ by $\hat{x}_{ia} = \frac{1}{1-\beta^N}\hat{y}_{ia}$ for all $(i,a) \in \Gamma$, and use (2.20) to construct the policy $\hat{\zeta} = M^{-1}(\hat{\mathbf{x}})$. It is clear that $\hat{\zeta} \in \mathcal{D}$, and hence $\hat{\mathbf{x}}$ is Hamiltonian by part (iii) of Theorem 1.2.6. Since positive entries of $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ coincide, $\hat{\mathbf{y}}$ is also Hamiltonian, so part (3) implies part (1), completing the proof. $\square$

Corollary 2.9.3 *If $Y(\beta) = \emptyset$, the empty set, then the graph Γ is non-Hamiltonian. If $Y(\beta) \neq \emptyset$, the set of Hamiltonian solutions $Y_H(\beta) \subset Y(\beta)$ is in one-to-one correspondence with Hamiltonian cycles of Γ, and satisfies*

$$Y_H(\beta) \;\; := \;\; Y(\beta)\bigcap\{\mathbf{y} \mid (2.34) \text{ } holds\}.$$

Proof. By construction, if Γ is Hamiltonian, then there exists a policy $\hat{\zeta} \in \mathcal{D}$ tracing out a Hamiltonian cycle in Γ. Let $\hat{\mathbf{x}} = M(\hat{\zeta})$ using (2.3) with $\eta = \mathbf{e}_1^T$, and define $\hat{\mathbf{y}} := (1 - \beta^N)\hat{\mathbf{x}}$. Clearly, $\hat{\mathbf{y}} \in Y(\beta)$, so $Y(\beta) \neq \emptyset$. From Proposition 2.9.2 it follows that $\hat{\mathbf{y}}$ satisfies (2.34). Conversely, only points in $Y_H(\beta)$ define Hamiltonian solutions in $Y(\beta)$. $\square$

For symmetric graphs, in which arc $(i, a) \in \Gamma$ if and only if arc $(a, i) \in \Gamma$, we further improve the wedge constraints (2.29)–(2.30) by considering the shortest path between the home node and each other node in the graph. We define $\ell(i, j)$ to be the length of the shortest path between nodes i and j in Γ.

Lemma 2.9.4 *Any Hamiltonian solution to (2.26)–(2.28) satisfies the following constraints:*

$$\sum_{a\in\mathcal{A}(i)} y_{ia} \;\; \leq \;\; \beta^{\ell(1,i)}, \quad i = 2, \ldots, N \tag{2.35}$$
$$\sum_{a\in\mathcal{A}(i)} y_{ia} \;\; \geq \;\; \beta^{N-\ell(1,i)}, \quad i = 2, \ldots, N. \tag{2.36}$$

Proof. From (2.20), and part (3) of Remark 2.9.1, we know that for a Hamiltonian cycle in which the k-th arc is the arc (i, a), the corresponding variable $y_{ia} = \beta^k$, and all other $y_{ib} = 0$, $b \neq a$. Therefore,

$$\sum_{a\in\mathcal{A}(i)} y_{ia} \;\; = \;\; \beta^k. \tag{2.37}$$

Then, since it takes at least $\ell(1, i)$ arcs to reach node i from the home node 1, we immediately obtain that $k \geq \ell(1, i)$, and therefore

$$\sum_{a\in\mathcal{A}(i)} y_{ia} \;\; \leq \;\; \beta^{\ell(1,i)},$$

which coincides with (2.35). Then, since Γ is an undirected graph, we know that $\ell(i,1) = \ell(1,i)$. Therefore, we obtain that $k \leq N - \ell(1,i)$, and therefore

$$\sum_{a \in \mathcal{A}(i)} y_{ia} \geq \beta^{N-\ell(1,i)},$$

which coincides with (2.36). □

Given the above, we reformulate HCP as a mixed integer programming feasibility problem, which we call the *Wedged-MIP heuristic*, as follows:

$$\begin{aligned}
\sum_{i=1}^{N} \sum_{a \in \mathcal{A}(i)} (\delta_{ij} - \beta p(j|i,a))\, y_{ia} &= \delta_{1j}(1-\beta^N), \quad j = 1, \ldots, N, && (2.38)\\
\sum_{a \in \mathcal{A}(1)} y_{1a} &= 1, && (2.39)\\
y_{ia} &\geq 0, \quad (i,a) \in \Gamma, && (2.40)\\
\sum_{j \in \mathcal{A}(i)} y_{ij} &\geq \beta^{N-\ell(1,i)}, \quad i \geq 2, && (2.41)\\
\sum_{j \in \mathcal{A}(i)} y_{ij} &\leq \beta^{\ell(1,i)}, \quad i \geq 2, && (2.42)\\
y_{ij} + y_{ji} &\leq 1, \quad (i,j) \in \Gamma, (j,i) \in \Gamma, && (2.43)\\
y_{ij} + y_{jk} + y_{ki} &\leq 2, \quad (i,j) \in \Gamma, (j,k) \in \Gamma, (k,i) \in \Gamma, && (2.44)\\
y_{ia} y_{ib} &= 0, \quad i = 1, \ldots, N, a, b \in \mathcal{A}(i), a \neq b. && (2.45)
\end{aligned}$$

We solve the above formulation in IBM ILOG OPL-CPLEX 5.1. One of the benefits of the IBM ILOG OPL-CPLEX solver is that constraints (2.45) may be submitted in a format usually not acceptable in CPLEX and the IBM ILOG OPL-CPLEX CP Optimizer will interpret them in a way most suitable for CPLEX. We allow these constraints to be submitted in one of two different ways, left up to the user's choice. We define the operator $==$ as follows,

$$(a == b) \quad := \quad \begin{cases} 1, & a = b, \\ 0, & a \neq b, \end{cases}$$

and the operator $!=$ as follows,

$$(a \mathrel{!}= b) \quad := \quad \begin{cases} 0, & a = b, \\ 1, & a \neq b, \end{cases}$$

and d_i as the number of arcs emanating from node i. Then, we submit constraints (2.45) to IBM ILOG OPL-CPLEX constraints in either one of the forms

$$\sum_{a \in \mathcal{A}(i)} (y_{ia} == 0) \quad = \quad d_i - 1, \quad i = 1, \ldots, N, \tag{2.46}$$

or

$$\sum_{a \in \mathcal{A}(i)} (y_{ia} \mathrel{!}= 0) \quad = \quad 1, \quad i = 1, \ldots, N. \tag{2.47}$$

Even though (2.46) and (2.47) are theoretically identical when added to (2.38)–(2.44), their interpretation by IBM ILOG OPL-CPLEX produces different solutions, with different running times. Neither choice solved graphs consistently faster than the other, so if one failed to find a solution quickly, the other was tried instead.

Using this model we are able to efficiently obtain Hamiltonian solutions for many large graphs, using a Pentium 3.4GHz with 4GB RAM.

Graph	**Nodes**	**Arcs**	**Choice of β**	**Running time (hh:mm:ss)**
8×8 Knight's tour	64	336	0.99999	00:00:02
Perturbed Horton	94	282	0.99999	00:00:02
12×12 Knight's tour	144	880	0.99999	00:00:03
250-node	250	1128	0.99999	00:00:16
20×20 Knight's tour	400	2736	0.99999	00:20:57
500-node	500	3046	0.99999	00:10:01
1000-node	1000	3996	0.999999	00:30:46
2000-node	2000	7992	0.999999	10:24:05

Table 2.7: Running times for Wedged-MIP heuristic.

Note that the perturbed Horton graph given here is a 94-node cubic graph that, unlike the original Horton graph (96-node cubic graph [55]), is Hamiltonian. The

250 and 500 node graphs are both non-regular graphs that were randomly generated for testing purposes, while the 1000 and 2000 node graphs come from the TSPLIB website, maintained by University of Heidelberg [49].

To conclude this section, we present a visual representation of a solution to the 250-node graph found by the above method. In Figures 2.11, the nodes are drawn as blue dots clockwise in an ellipse, with node 1 at the top, and the arcs between the nodes are inside the ellipse. The arcs in the Hamiltonian cycle found by the Wedged-MIP heuristic are highlighted red, and all other arcs are shown in blue. While it is very difficult to make out much detail from Figure 2.11, it serves as a good illustration of the complexity involved in problems of this size. The adjacency lists for the 250-node, 500-node, 1000-node and 2000-node graphs, as well as the solutions found by the Wedged-MIP heuristic for these four graphs, are given in Appendix A.6.

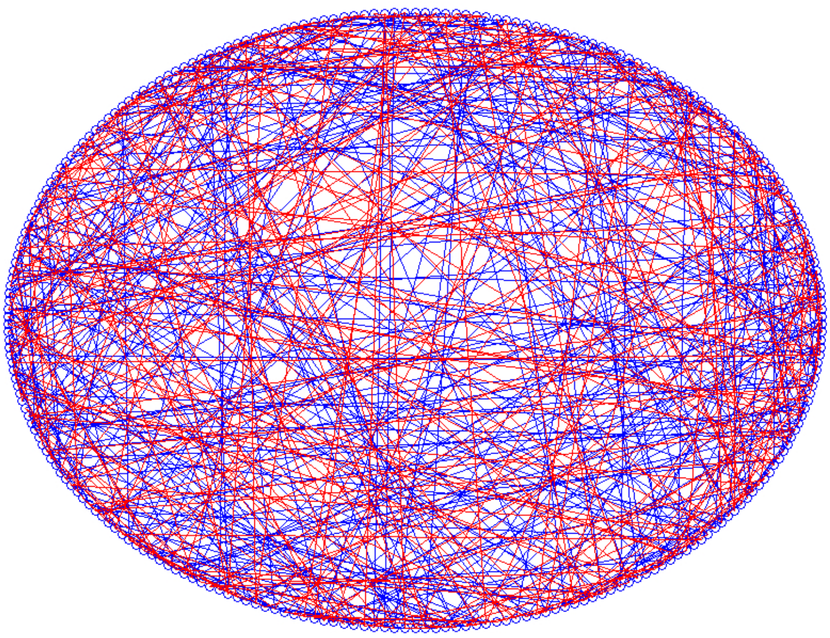


Figure 2.11: Solution to 250-node graph (Hamiltonian cycle in red).

2.10 Comparisons between Wedged-MIP heuristic and other TSP formulations

The Wedged-MIP heuristic is the best-performing method described in this thesis. Since we solve the Wedged-MIP heuristic in OPL-CPLEX, we investigate two other, well-known, MIP formulations, and also solve them in CPLEX for the same set of graphs as in Table 2.7, as well as three, randomly generated, cubic Hamiltonian graphs of sizes 12, 24 and 38, as a benchmark test. The two other formulations are the modified single commodity flow model [32] and the third stage dependent model [54]. These two formulations have been selected because they were the best performing methods of each type (commodity flow and stage dependent respectively) reported in [47].

Both the modified single commodity flow and the third stage dependent models were designed to solve the traveling salesman problem, and so they contain distances c_{ij} for each arc $(i, j) \in \Gamma$. Since we only want to solve HCP with these formulations, we set

$$c_{ij} \quad := \quad \begin{cases} 1, & (i,j) \in \Gamma, \\ 0, & (i,j) \notin \Gamma. \end{cases}$$

The modified single commodity flow model (MSCF) is formulated with decision variables x_{ij} and y_{ij} as follows:

$$\min \sum_{(i,j)\in\Gamma} c_{ij} x_{ij}$$
$$\text{s.t.}$$
$$\begin{aligned} \sum_{j\in\mathcal{A}(i)} x_{ij} &= 1, \quad i = 1,\dots,N, \\ \sum_{i\in\mathcal{B}(j)} x_{ij} &= 1, \quad j = 1,\dots,N, \\ \sum_{j\in\mathcal{A}(1)} y_{1j} &= N-1, \\ \sum_{i\in\mathcal{B}(j)} y_{ij} - \sum_{k\in\mathcal{A}(j)} y_{jk} &= 1, \quad j = 2,\dots,N, \end{aligned}$$

$$
\begin{aligned}
y_{1j} &\leq (N-1)x_{1j}, \quad j \in \mathcal{A}(1) \in \Gamma, \\
y_{ij} &\leq (N-2)x_{ij}, \quad i = 2,\dots,N, \quad j \in \mathcal{A}(i), \\
x_{ij} &\in \{0,1\}, \\
y_{ij} &\geq 0.
\end{aligned}
$$

The third stage dependent model (TSD) is formulated with decision variables x_{ij} and y^t_{ij}, t $= 1,\dots,N$, as follows:

$$
\min \sum_{(i,j)\in\Gamma} c_{ij}x_{ij}
$$
$$
\text{s.t.}
$$
$$
\begin{aligned}
\sum_{j\in\mathcal{A}(i)} x_{ij} &= 1, \quad i = 1,\dots,N, \\
\sum_{i\in\mathcal{B}(j)} x_{ij} &= 1, \quad j = 1,\dots,N, \\
x_{ij} - \sum_{t=1}^{N} y^t_{ij} &= 0, \quad (i,j) \in \Gamma, \\
\sum_{t=1}^{N}\sum_{j\in\mathcal{A}(i)} y^t_{ij} &= 1, \quad i = 1,\dots,N, \\
\sum_{t=1}^{N}\sum_{i\in\mathcal{B}(j)} y^t_{ij} &= 1, \quad j = 1,\dots,N, \\
\sum_{(i,j)\in\Gamma} y^t_{ij} &= 1, \quad t = 1,\dots,N, \\
\sum_{j\in\mathcal{A}(1)} y^1_{1j} &= 1, \\
\sum_{i\in\mathcal{B}(1)} y^N_{i1} &= 1, \\
\sum_{j\in\mathcal{A}(i)} y^t_{ij} - \sum_{k\in\mathcal{B}(i)} y^{t-1}_{ki} &= 0, \quad i = 1,\dots,N, \quad t = 2,\dots,N.
\end{aligned}
$$

We ran these two models on the same graphs as shown in Table 2.7, as well as three additional, randomly generated, cubic Hamiltonian graphs of sizes 12, 24 and 38. The running times, along with the Wedged-MIP heuristic running times, are shown in Table 2.8. For each graph tested other than the 1000-node graph and 2000-node graph, we ran MCSF and TSD for 24 hours, and if no solution had been obtained we terminated the execution. For the 1000-node and 2000-node graphs, we allowed 168 hours (1 week) before terminating.

Graph	**Nodes**	**Wedged-MIP heuristic**	**MCSF**	**TSD**
12-node cubic	12	00:00:01	00:00:01	00:00:01
24-node cubic	24	00:00:01	00:00:01	00:00:02
38-node cubic	38	00:00:01	00:00:01	00:21:04
8×8 Knight's tour	64	00:00:02	00:00:01	$>$ 24 hours
Perturbed Horton	94	00:00:02	00:03:04	$>$ 24 hours
12×12 Knight's tour	144	00:00:03	00:01:12	$>$ 24 hours
250-node	250	00:00:16	00:29:42	$>$ 24 hours
20×20 Knight's tour	400	00:20:57	17:35:57	$>$ 24 hours
500-node	500	00:10:01	$>$ 24 hours	$>$ 24 hours
1000-node	1000	00:30:46	$>$ 1 week	$>$ 1 week
2000-node	2000	10:24:05	$>$ 1 week	$>$ 1 week

Table 2.8: Running times (hh:mm:ss) for Wedged-MIP heuristic, MCSF and TSD.

Chapter 3

Interior Point Method

3.1 Interior point method

In this chapter we investigate an optimisation program that is shown in [14] to be equivalent to the HCP. We attempt to solve this program by using an *interior point method*. Specifically, we design each component of an interior point method that we call the *determinant interior point algorithm* (DIPA) in order to take advantage of the sparsity present in difficult graphs. This represents a significant saving in computation time and memory requirements. We also include additional techniques, such as rounding off variables that converge to their boundary values, that are not available in general implementations of interior point method models but are applicable to HCP. For further reading about techniques that can be used in numerical optimisation methods, see Gill et al. [33].

Interior point methods are now standard and described in detail in many books (e.g., see Nocedal and Wright [46] and den Hertog [11]). Hence, we outline only the basic steps that are essential to follow our adaptation of such a method to one particular formulation of HCP. We note that another version of HCP was tackled by interior point methods in [15] with encouraging preliminary results. However, our approach is entirely different. While the method in [15] operates in the space of occupational measures (see the discussions in Chapters 1 and 2) with a symmetric linear perturbation and a quadratic objective function, the method we describe in this chapter contains a simpler set of constraints, with a determinant objective function augmented with a sum of logarithmic barrier terms. The particular structure and features of this formulation provide motivation for designing a custom interior point method solver that behaves differently to standard interior point methods. In particular, while finding directions of negative curvature can speed up convergence in standard algorithms, in DIPA they become critical to finding a solution. We demonstrate in this chapter that descent directions found by Newton's method often give equal weighting to two arcs emanating from a single node, which prevents progress towards a Hamiltonian solution. Hence, we need directions of negative curvature to avoid this issue.

Computing this objective function value and its derivatives at each iteration of DIPA takes up the overwhelming majority of computation time. Therefore, we present a method of computing these values at a much improved rate in Sections 3.6 and 3.7. We also present numerical results to demonstrate the promise of DIPA.

3.1.1 Interior point method for a problem with inequality constraints

Consider a constrained optimisation problem of the form:

$$\begin{gathered} \min f(\mathbf{x}) \\ \text{s.t.} \\ h_i(\mathbf{x}) \geq 0, \quad i = 1, 2, \ldots, m, \end{gathered} \tag{3.1}$$

that has a solution $\mathbf{x}^* \in \mathbb{R}^n$. We assume that the feasible region Ω has a nonempty interior denoted by $\mathrm{Int}(\Omega)$. That is, there exists $\mathbf{x}$ such that $h_i(\mathbf{x}) > 0$ for all $i = 1, 2, \ldots, m$. We also assume that $f(\mathbf{x})$ and $h_i(\mathbf{x})$, for $i = 1, 2, \ldots, m$, are continuous and possess derivatives up to order 2. This problem is often solved by use of an interior point method. One method of doing so is to consider a parametrised, auxilliary objective function of the form

$$F(\mathbf{x}) \quad = \quad f(\mathbf{x}) - \mu \sum_{i=1}^{m} \ln(h_i(\mathbf{x})), \quad \text{for some } \mu > 0, \tag{3.2}$$

and an associated, essentially unconstrained, auxilliary optimisation problem

$$\min\{F(\mathbf{x}) | \mathbf{x} \in \mathrm{Int}(\Omega)\}. \tag{3.3}$$

The auxiliary objective function $F(\mathbf{x})$ contains, for each of the inequality constraints, a logarithm term which ensures that $F(\mathbf{x}) \uparrow \infty$ as $h_i(\mathbf{x}) \downarrow 0$. This sum of logarithm terms ensures that any minimiser of $F(\mathbf{x})$ strictly satisfies the inequality constraints in (3.1) for $\mu > 0$ and sufficiently large. If we choose μ large enough that $F(x)$ is strictly convex, then its unique global minimiser $\mathbf{x}^*(\mu)$ is well-defined. In well behaved cases, it is standard to expect that $\lim\limits_{\mu \downarrow 0} \mathbf{x}^*(\mu)$ exists and constitutes a global minimum to (3.1). In our implementation, we select $\mu^{k+1} = 0.9\mu^k$. This is an arbitrary choice, but generally performs well. A different multiplier besides 0.9 could be used, or left as input parameter.

We define a sequence $\{\mu^k\}_{k=0}^{\infty}$ such that $\mu^k > 0$ for all k, and $\{\mu^k\} \to 0$. We associate with this sequence a set of auxiliary objective functions $F_k(\mathbf{x}) = f(\mathbf{x}) - \mu^k \sum\limits_{i=1}^{m} \ln(h_i(\mathbf{x}))$, which has a sequence of minimisers $\{\mathbf{x}^k\}$. It is well known (e.g., see den Hertog [11] pp 49–65) that if $f(\mathbf{x})$ is convex and $h_i(\mathbf{x})$ are all concave, for $i = 1, 2, \ldots, m$, then $\mathbf{x}^k \to \mathbf{x}^*$. Note that while in our application $f(\mathbf{x})$ is non-convex, it is still reasonable to expect an interior point method such as the above to perform well as a heuristic.

An interior point method has two main iterations: the *inner iteration*, where the minimiser $\mathbf{x}^k$ of a particular $F_k(\mathbf{x})$ is calculated (at least approximately), and the *outer iteration*, where the new barrier parameter μ^k is chosen and the new auxiliary objective function $F_k(\mathbf{x})$ is constructed.

The inner iteration can be performed using any optimisation solver, but a common method is to calculate the gradient $\mathbf{g}(\mathbf{x})$ and Hessian $H(\mathbf{x})$ of $F(\mathbf{x})$, namely,

$$\mathbf{g}(\mathbf{x}) = \left\{\frac{\partial F(\mathbf{x})}{\partial x_i}\right\}_{i=1}^{|\mathbf{x}|}, \tag{3.4}$$

$$H(\mathbf{x}) = \left\{\frac{\partial^2 F(\mathbf{x})}{\partial x_i \partial x_j}\right\}_{i,j=1}^{|\mathbf{x}|,|\mathbf{x}|}, \tag{3.5}$$

and use a second-order approximation to find the Newton step $\mathbf{d} = -H^{-1}\mathbf{g}$. Then, if we have a current point $\mathbf{x}^k$, we find the next point $\mathbf{x}^{k+1}$:

$$\mathbf{x}^{k+1} = \mathbf{x}^k + \alpha\mathbf{d}, \tag{3.6}$$

where α is a step size selected to ensure that $\mathbf{x}^{k+1}$ is feasible, and that the new objective function value $F(\mathbf{x}^{k+1}) < F(\mathbf{x}^k)$. One method of choosing α is to first compute α_0, the maximum step size that can be taken while ensuring that $\mathbf{x}^{k+1}$ does not violate the inequality constraints in (3.1). Then, we select $\alpha = 0.99\alpha_0$, and check if $F(\mathbf{x}^{k+1}) < F(\mathbf{x})$. If so, we take this step and the next iteration begins. If not, we halve the value of α and check again to see if the objective function has improved. If not, we continue halving α until it does.

If we choose μ^{k+1} in such a way that it is close the previous μ^k, the new solution $\mathbf{x}^{k+1}$ may also be expected to be close to the previous solution $\mathbf{x}^k$. Since $\mathbf{x}^k$ is used as the starting point for the $(k+1)$-th inner iteration, its close proximity to $\mathbf{x}^{k+1}$ may allow us to take advantage of the quadratic convergence of the Newton steps taken in (3.6).

3.1.2 Interior point method for a problem with linear equality constraints and inequality constraints.

Linear equality constraints can be added to (3.1) to form a new optimisation problem:

$$\begin{gathered}\min f(\mathbf{x})\\ \text{s.t.}\end{gathered} \tag{3.7}$$

$$h_i(\mathbf{x}) \geq 0,$$
$$W\mathbf{x} = \mathbf{b}.$$

Once we have obtained an initial interior point satisfying the constraints in (3.7), it is possible to essentially convert the minimisation problem (3.7) to the minimisation problem (3.1) by working in the null space of the equality constraints $W\mathbf{x} = \mathbf{b}$.

We define $F(\mathbf{x})$ in the same way as (3.2). Then, we represent the null space of the linear equality constraints by a matrix Z such that $WZ = 0$, and the columns of Z are linearly independent. Then, given the current feasible point $\mathbf{x}^k$, we find a search direction $\mathbf{d}$ in the null space Z, by solving for $\mathbf{d}$ and $\overline{\mathbf{y}}$ the system

$$H(\mathbf{x}^k)\mathbf{d} = W^T\overline{\mathbf{y}} - \mathbf{g}(\mathbf{x}^k), \tag{3.8}$$
$$W\mathbf{d} = \mathbf{0}, \tag{3.9}$$

where $\mathbf{g}(\mathbf{x})$ and $H(\mathbf{x})$ are the gradient and Hessian of $F(\mathbf{x})$ respectively, evaluated at $\mathbf{x}^k$. Solutions to (3.8)–(3.9) are of the form

$$\mathbf{d} = Z\mathbf{u}, \tag{3.10}$$
$$H(\mathbf{x}^k)Z\mathbf{u} = W^T\overline{\mathbf{y}} - \mathbf{g}(\mathbf{x}^k), \tag{3.11}$$

for some $\mathbf{u}$. Multiplying (3.11) by Z^T we obtain

$$Z^TH(\mathbf{x}^k)Z\mathbf{u} = -Z^T\mathbf{g}(\mathbf{x}^k).$$

We then observe that $\mathbf{u} = -(Z^TH(\mathbf{x}^k)Z)^{-1}Z^T\mathbf{g}(\mathbf{x}^k)$, and therefore

$$\mathbf{d} = -Z(Z^TH(\mathbf{x}^k)Z)^{-1}Z^T\mathbf{g}(\mathbf{x}^k). \tag{3.12}$$

By taking suitable sized steps in the direction $\mathbf{d}$, we ensure that no $\mathbf{x}^{k+1} = \mathbf{x}^k + \alpha\mathbf{d}$ violates the equality constraints as long as the initial $\mathbf{x}^0$ is chosen feasible.

In practice, it is very rare that $\mathbf{d}$ is calculated as above, as the calculation of $(Z^TH(\mathbf{x}^k)Z)^{-1}$ is expensive, and must be recalculated at each new point $\mathbf{x}^k$. Instead, $\mathbf{u}$ is found by solving the following linear equation system:

$$Z^TH(\mathbf{x}^k)Z\mathbf{u} = -Z^T\mathbf{g}(\mathbf{x}^k). \tag{3.13}$$

We refer to $Z^T\mathbf{g}(\mathbf{x})$ and $Z^T H(\mathbf{x})Z$ as the *reduced gradient* and *reduced Hessian*, respectively. Now, we can quickly calculate $d = Z\mathbf{u}$. Any linear equation solver can be used to solve (3.13) but two common algorithms used are the *conjugate-gradient algorithm* (CG) and a variation of CG, the *Lanczos algorithm* (see Nocedal and Wright [46] pp. 100–133 for an excellent introduction to CG). The conjugate-gradient algorithm is an efficient method when $Z^T H(\mathbf{x})Z$ is a large, symmetric, positive-definite matrix, which is the case if $F(\mathbf{x})$ is convex.

In the case where $F(\mathbf{x})$ is not convex, the Lanczos algorithm, which approximates eigenvectors of large, symmetric matrices, is used to find eigenvectors associated with negative eigenvalues of $Z^T H(\mathbf{x})Z$. These eigenvectors are then used as directions of negative curvature.

If no descent direction is found and $Z^T H(\mathbf{x})Z$ is positive definite, then the interior point method has converged to a local minimum. For convex problems, this is a global minimum, but this is not the case in general.

As in the case with problems constrained only by inequality constraints, we have to select an α to ensure that $\mathbf{x}^{k+1} := \mathbf{x}^k + \alpha\mathbf{d}$ remains feasible. We select α in the same way as described in Subsection 3.1.1.

3.2 Determinant interior point method for HCP

In this section, we describe the determinant interior point algorithm (DIPA) that solves HCP. To achieve this, we define decision variables x_{ij}, for each arc $(i, j) \in \Gamma$. Despite the double subscript, we choose to represent these variables in a decision vector $\mathbf{x}$, with each entry corresponding to an arc in Γ. For the complete 4-node graph (without self-loops), for example, the decision vector is

$$\mathbf{x} = \begin{bmatrix} x_{12} & x_{13} & x_{14} & x_{21} & x_{23} & x_{24} & x_{31} & x_{32} & x_{34} & x_{41} & x_{42} & x_{43} \end{bmatrix}^T.$$

We then define $P(\mathbf{x})$, the probability transition matrix that contains the decision variables x_{ij}, in matrix format where the (i,j)-th entry $p_{ij}(\mathbf{x})$ is defined as

$$p_{ij}(\mathbf{x}) \ := \ \begin{cases} x_{ij}, & (i,j) \in \Gamma, \\ 0, & \text{otherwise.} \end{cases} \tag{3.14}$$

Recall that $\mathcal{A}(i)$ is the set of all nodes reachable in one step from node i, and $\mathcal{B}(i)$ is the set of all nodes that can reach node i in one step. We then define $\mathcal{DS}_{\mathbf{x}}$ to be the set of all $\mathbf{x}$ that satisfy the following constraints:

$$x_{ij} \ \geq \ 0, \quad (i,j) \in \Gamma, \tag{3.15}$$

$$\sum_{j \in \mathcal{A}(i)} x_{ij} \ = \ 1, \quad i = 1, \ldots, N, \tag{3.16}$$

$$\sum_{i \in \mathcal{B}(j)} x_{ij} \ = \ 1, \quad j = 1, \ldots, N. \tag{3.17}$$

We refer to constraints (3.15)–(3.17) as the *doubly-stochastic constraints*, which are used to ensure that both the row sums and column sums of $P(\mathbf{x})$ are 1, and that all entries of $P(\mathbf{x})$ are nonnegative. Next, we define the objective function,

$$f(\mathbf{x}) \ = \ -\det(I - P(\mathbf{x}) + \frac{1}{N}J), \tag{3.18}$$

where J is an $N \times N$ matrix where every entry is unity. In [14], the authors prove the following theorem.

Theorem 3.2.1 *The Hamiltonian cycle problem is equivalent to the optimisation problem*

$$\min\{f(\mathbf{x}) | \mathbf{x} \in \mathcal{DS}_{\mathbf{x}}\}. \tag{3.19}$$

If $\mathbf{x}^*$ is the global solution to (3.19) and $f(\mathbf{x}^*) = -N$, then the solution $\mathbf{x}^*$ corresponds to a Hamiltonian cycle in the graph Γ. Conversely, if $f(\mathbf{x}^*) > -N$, the graph is non-Hamiltonian.

The constraints (3.15) are the only inequality constraints we demand of $\mathbf{x} \in \mathcal{DS}_{\mathbf{x}}$, and so from (3.2), the auxiliary objective function is

$$F(\mathbf{x}) \ = \ -\det(I - P(\mathbf{x}) + \frac{1}{N}J) - \mu \sum_{(i,j) \in \Gamma} \ln(x_{ij}). \tag{3.20}$$

We take advantage of the special structure of our formulation (the $\mathcal{DS}_{\mathbf{x}}$ constraints and the determinant function) to develop a particular implementation of the interior point method. After obtaining an initial point and choosing initial parameters, at each iteration of DIPA we perform the following steps:

(1) Calculate $F(\mathbf{x}^k)$, and its gradient $\mathbf{g}(\mathbf{x}^k)$ and Hessian $H(\mathbf{x}^k)$, at $\mathbf{x}^k$ (Algorithm 3.4).

(2) Calculate the reduced gradient $Z^T\mathbf{g}(\mathbf{x}^k)$ and reduced Hessian $Z^TH(\mathbf{x}^k)Z$ (Algorithm 3.5).

(3) Find a direction vector $\mathbf{d}$ (using either conjugate-gradient or Lanczos) and a step size α to determine the new point $\mathbf{x}^{k+1} = \mathbf{x}^k + \alpha\mathbf{d}$ (Algorithms 3.6 – 3.8).

(4) If any variables x_{ij} have converged very close to 0 or 1, fix them to these values and alter the values of the remaining variables slightly to retain feasibility (Algorithms 3.11 – 3.13).

(5) We check if $\mathbf{x}^{k+1}$ corresponds to a Hamiltonian cycle after rounding the variables to 0 or 1. If so, we stop and return the Hamiltonian cycle. Otherwise, we repeat steps (1)–(5) again (Algorithm 3.15).

We perform each of these steps by use of several component algorithms described throughout Section 3.2. In Section 3.3 the main algorithm is given that calls the component algorithms.

3.2.1 Function evaluations and computing directions

We denote the constraint matrix that describes constraints (3.16)–(3.17) by $\overline{W}$, which has the following structure

$$\overline{W} = \begin{bmatrix} W_1 \\ \hdashline W_2 \end{bmatrix}, \tag{3.21}$$

where each column in W_1 and W_2 has exactly one non-zero entry, and the non-zero entry is 1.

We know that $\overline{W}$ is always rank deficient by at least 1. An intuitive explanation for this is that once we have constrained all row sums of $P(\mathbf{x})$ to be 1, it follows that the sum of all the entries of $P(\mathbf{x})$ is N. Then, if we also constrain $N-1$ column sums of $P(\mathbf{x})$ to be 1, the remaining column sum is predetermined to be 1, and therefore the final column sum constraint is redundant.

We find a full rank constraint matrix W by removing the required number of linearly dependant rows from $\overline{W}$. In general, finding a full row-rank subset of constraints is a difficult operation which requires factoring the matrix. In the large majority of cases, however, the matrix is only rank deficient by 1, and so any row can be removed. Then, certain columns of W will contain only a single unit, whereas other columns will all contain two units. We now wish to find the null space Z of the full rank constraints matrix W.

To find Z, we first perform row and column permutations on W to find W^* that has following structure:

$$W^* \quad = \quad \left[\, L \,\vdots\, B \,\right], \tag{3.22}$$

where L is a lower triangular matrix. In this structure, each column of B contains exactly two units, as every column that only contains one unit is inside L. Note that L may (and usually does) contain one or more columns that have two units.

Each column permutation we perform to obtain W^* is also performed on an index set $\mathcal{I}$, where the cardinality of $\mathcal{I}$ is equal to columns(W), the number of columns in W. Initially, $\mathcal{I} = \begin{bmatrix} 1, & \ldots, & \text{columns}(W) \end{bmatrix}$. Once we have performed these column permutations, $\mathcal{I}$ maps the original ordering of the columns to the new ordering. We determine the $\left[\, L \,\vdots\, B \,\right]$ structure of W^* and the index set $\mathcal{I}$ by applying the following algorithm.

Input: $\overline{W}, N$
Output: $L, B, \mathcal{I}$

begin
  count $\leftarrow$ 0
  rows $\leftarrow$ rank($\overline{W}$)
  $W \leftarrow \overline{W}$ *with rows removed to make W full rank*
  cols $\leftarrow$ columns(W)
  $r \leftarrow$ rows - count
  $\mathcal{I} \leftarrow \{1, \ldots, \text{cols}\}$
  while $r > 0$
    C $\leftarrow$ *Identify a set of columns* $\{c_1, \ldots, c_k\}$ *such that* $\sum_{i=1}^{r} w_{ic_j} = 1, \quad \forall j = 1, \ldots, k$
      and $w_{ic_j} w_{ic_k} = 0, \quad \forall i = 1, \ldots, r, \quad j \neq k$
    for i **from** 1 **to** k
      count $\leftarrow$ count + 1
      $\mathcal{I} \leftarrow \left[\begin{array}{cccccc} \mathcal{I}_1 & \ldots & \mathcal{I}_{count-1} & \mathcal{I}_i & \mathcal{I}_{count} & \ldots \end{array} \right]$ *(Moving $\mathcal{I}_i$ into position* count*)*
      $W \leftarrow W(\mathcal{I})$ *(Moving column c_i to column* count*)*
      $W \leftarrow$ *reorder the rows to get a 1 in positive* $(r - i + 1, \text{count})$
    end
    $r \leftarrow$ rows - count
  end
  $\mathcal{I} \leftarrow$ *Reverse the order of the first* rows *entries in* $\mathcal{I}$
  $W \leftarrow W(\mathcal{I})$ *(Reverse the order of the first* rows *columns in* $\overline{W}$*)*
  $L \leftarrow W(1 : \text{rows}, 1 : \text{rows})$
  $B \leftarrow W(1 : \text{rows}, \text{rows}{+}1 : \text{cols})$
end

Algorithm 3.1: Reordering W algorithm.

Remark 3.2.2 *Note that in practice, the above algorithm returns L and B not as full matrices but in sparse form. For large graphs with few arcs adjacent to each node, this represents a significant saving of computational time and storage space. However, for simplicity of notation in subsequent algorithms, we treat L and B as whole matrices for the remainder of this section.*

Example 3.2.3 *Consider the complete 4-node graph, as shown in Figure 3.1.*

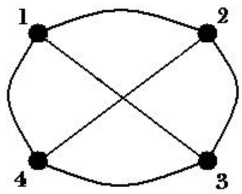


Figure 3.1: The complete 4-node graph.

Then, $\overline{W}$ has the following form:

$$\overline{W} \quad = \quad \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix}. \tag{3.23}$$

In this example, $\overline{W}$ is rank deficient by exactly 1, so we delete the first row to obtain

$$W \quad = \quad \begin{bmatrix} 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix}. \tag{3.24}$$

Now, we begin execution of Algorithm 3.1, with $r = 7$, rows $= 7$, cols $= 12$ and count $= 0$. Initially, $\mathcal{I} = \{1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12\}$. Since the first three columns each contain only a single unit, each in different rows, we select $C = \{1, 2, 3\}$. These columns are already in the required positions, and so we do not need to move them. By swapping rows 5, 6 and 7 to become rows 7, 6 and 5 respectively, we complete the first iteration of the algorithm. At this stage, count $= 3$, $r = 4$, and $\mathcal{I}$ is unchanged *as we have performed no column permutations thus far. Now* W *has become* W_2*:*

$$W_2 \quad = \quad \begin{bmatrix} 0&0&0&1&1&1&0&0&0&0&0&0 \\ 0&0&0&0&0&0&1&1&1&0&0&0 \\ 0&0&0&0&0&0&0&0&0&1&1&1 \\ 0&0&0&1&0&0&1&0&0&1&0&0 \\ 0&0&1&0&0&1&0&0&1&0&0&0 \\ 0&1&0&0&1&0&0&0&0&0&0&1 \\ 1&0&0&0&0&0&0&1&0&0&1&0 \end{bmatrix}.$$

Next, it can be seen that columns 5, 6, 8, 9, 11 and 12 of W_2 *have a single unit in the first* $r = 4$ *rows. However, not all of these columns can be chosen as some pairs of columns (for example, columns 5 and 6) have their single unit in the same row. One possible selection of columns is* $C = \{5, 8, 11\}$*, which we choose. Performing row and column permutations, we move columns 5, 8 and 11 to columns 4, 5 and 6 respectively, and move rows 1, 2 and 3 to rows 4, 3 and 2 respectively. The second iteration of the algorithm is now complete. At this stage, count* $= 6$*,* $r = 1$ *and* $\mathcal{I} = \{1, 2, 3, 5, 8, 11, 4, 6, 7, 9, 10, 12\}$*. Now* W_2 *has become* W_3*:*

$$W_3 \quad = \quad \begin{bmatrix} 0&0&0&0&0&0&1&0&1&0&1&0 \\ 0&0&0&0&0&1&0&0&0&0&1&1 \\ 0&0&0&0&1&0&0&0&1&1&0&0 \\ 0&0&0&1&0&0&1&1&0&0&0&0 \\ 0&0&1&0&0&0&0&1&0&1&0&0 \\ 0&1&0&1&0&0&0&0&0&0&0&1 \\ 1&0&0&0&1&1&0&0&0&0&0&0 \end{bmatrix}.$$

In the final stage of the algorithm, we see that columns 7, 9 and 11 contain a single unit in the first 1 row, and all three columns have their unit in that same row. We select $C = \{7\}$*. No row or column permutations are required as the unit is already in the correct position. Therefore, the third iteration is now complete, with count* $= 7$*,* $r = 0$*, and* $\mathcal{I}$ *is unchanged from the previous stage as no additional column permutations were performed. The final stage is now complete and the while loop is exited.*

Finally, we reverse the order of the first 7 columns to obtain

$$W^* = \left[L \,\vdots\, B\right] = \left[\begin{array}{ccccccc:ccccc} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \end{array}\right], \tag{3.25}$$

and therefore, $\mathcal{I} = \{4, 11, 8, 5, 3, 2, 1, 6, 7, 9, 10, 12\}$.

We can now perform calculations with the null space matrix Z quickly by considering Z^*, the null space for W^* found above. In block-matrix form, the null space for W^* is $Z^* = \left[\begin{array}{c} -L^{-1}B \\ \hdashline I \end{array}\right]$, since $W^*Z^* = -LL^{-1}B + B = 0$. Note that Z^* is equivalent to Z, but with the rows permuted according to $\mathcal{I}$.

Then, we calculate the matrix multiplication ZM for any appropriately sized matrix M simply by calculating Z^*M and then reordering the rows using $\mathcal{I}$. First, we multiply Z^* by M to obtain

$$Z^*M = \left[\begin{array}{c} -L^{-1}BM \\ \hdashline M \end{array}\right]. \tag{3.26}$$

We define $M_1 = L^{-1}BM$, and $\mathbf{m}_i := L^{-1}BM\mathbf{e}_i$. Then, we find M_1 by calculating each $\mathbf{m}_i$. We achieve the latter by solving the following linear system of equations, for each i, for which the left hand side is already in reduced row echelon form where all non-zeros entries are 1:

$$L\mathbf{m}_i = BM\mathbf{e}_i. \tag{3.27}$$

As B contains only units and zeros, we calculate BM simply and efficiently by adding the relevant rows of M. Finally, we reorder the rows of Z^*M to find ZM such that row $\mathcal{I}(j)$ of ZM is row j of Z^*M.

We outline this process in the following algorithm.

Input: $L, B, \mathcal{I}, M$

Output: ZM

begin

```
BM ← zeros(rows(B),cols(M))
for i from 1 to rows(B)
    for j from 1 to cols(B)
        if B(i,j) = 1
            for k from 1 to cols(B)
                BM(i,k) ← BM(i,k) + M(j,k)
            end
        end
    end
end

for i from 1 to cols(M)
    M_1(1 : rows(B), i) ← Linear solver(L, BM(:, i))
end
```

$Z^*M \leftarrow \begin{bmatrix} -M_1 \\ M \end{bmatrix}$

$ZM(\mathcal{I}, :) \leftarrow Z^*M$ *(rearranging Z^*M)*

end

Algorithm 3.2: Algorithm for sparse multiplication ZM.

Example 3.2.4 *Consider the following matrix M, which is arbitrarily chosen for this example:*

$$M = \begin{bmatrix} 1 & -2 & 0 & 3 \\ 4 & -6 & 1 & 2 \\ -2 & 3 & 0 & 4 \\ 1 & 0 & 0 & 3 \\ -1 & 8 & 2 & 5 \end{bmatrix}, \tag{3.28}$$

with Z defined as the null space of W in the previous example (see (3.24)). Then, Z^*M has the following form

$$Z^*M = \begin{bmatrix} -M_1 \\ \hdashline M \end{bmatrix}. \tag{3.29}$$

In order to calculate M_1*, we must first calculate* BM*. Recall from (3.25) that*

$$B = \begin{bmatrix} 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}. \tag{3.30}$$

Then, we calculate the rows in BM *by simply adding the relevant rows of* M *corresponding to units in each row of* B*. For instance, we calculate the first row of* BM *by adding the 2nd and 4th rows of* M*.*

$$BM = \begin{bmatrix} 5 & -6 & 1 & 5 \\ 0 & 8 & 2 & 8 \\ 2 & -3 & 1 & 6 \\ 1 & -2 & 0 & 3 \\ -1 & 1 & 0 & 7 \\ -1 & 8 & 2 & 5 \\ 0 & 0 & 0 & 0 \end{bmatrix}.$$

We then find $\mathbf{m}_1$*,* $\mathbf{m}_2$*,* $\mathbf{m}_3$ *and* $\mathbf{m}_4$ *by solving*

$$L\mathbf{m}_1 = \begin{bmatrix} 5 & 0 & 2 & 1 & -1 & -1 & 0 \end{bmatrix}^T, \tag{3.31}$$

$$L\mathbf{m}_2 = \begin{bmatrix} -6 & 8 & -3 & -2 & 1 & 8 & 0 \end{bmatrix}^T, \tag{3.32}$$

$$L\mathbf{m}_3 = \begin{bmatrix} 1 & 2 & 1 & 0 & 0 & 2 & 0 \end{bmatrix}^T, \tag{3.33}$$

$$L\mathbf{m}_4 = \begin{bmatrix} 5 & 8 & 6 & 3 & 7 & 5 & 0 \end{bmatrix}^T. \tag{3.34}$$

Recall from (3.25) that

$$L = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Hence we solve the four systems (3.31)–(3.34) recursively to obtain

$$\mathbf{m}_1 = \begin{bmatrix} 5 & 0 & 2 & -4 & -1 & 3 & -2 \end{bmatrix}^T, \quad (3.35)$$

$$\mathbf{m}_2 = \begin{bmatrix} -6 & 8 & -3 & 4 & 1 & 4 & -5 \end{bmatrix}^T, \quad (3.36)$$

$$\mathbf{m}_3 = \begin{bmatrix} 1 & 2 & 1 & -1 & 0 & 3 & -3 \end{bmatrix}^T, \quad (3.37)$$

$$\mathbf{m}_4 = \begin{bmatrix} 5 & 8 & 6 & -2 & 7 & 7 & -14 \end{bmatrix}^T. \quad (3.38)$$

Substituting (3.35)–(3.38) and (3.28) into (3.29) we obtain Z^*M

$$Z^*M = \left[\begin{array}{cccc} -5 & 6 & -1 & -5 \\ 0 & -8 & -2 & -8 \\ -2 & 3 & -1 & -6 \\ 4 & -4 & 1 & 2 \\ 1 & -1 & 0 & -7 \\ -3 & -4 & -3 & -7 \\ 2 & 5 & 3 & 14 \\ \hdashline 1 & -2 & 0 & 3 \\ 4 & -6 & 1 & 2 \\ -2 & 3 & 0 & 4 \\ 1 & 0 & 0 & 3 \\ -1 & 8 & 2 & 5 \end{array}\right].$$

Finally, using $\mathcal{I} = \{4, 11, 8, 5, 3, 2, 1, 6, 7, 9, 10, 12\}$ *from Example 3.2.3, we reorder the rows of* Z^*M *to obtain*

$$ZM = \begin{bmatrix} 2 & 5 & 3 & 14 \\ -3 & -4 & -3 & -7 \\ 1 & -1 & 0 & -7 \\ -5 & 6 & -1 & -5 \\ 4 & -4 & 1 & 2 \\ 1 & -2 & 0 & 3 \\ 4 & -6 & 1 & 2 \\ -2 & 3 & -1 & -6 \\ -2 & 3 & 0 & 4 \\ 1 & 0 & 0 & 3 \\ 0 & -8 & -2 & -8 \\ -1 & 8 & 2 & 5 \end{bmatrix}.$$

In many situations (for example, when calculating the reduced gradient $Z^T\mathbf{g}$), we require multiplication by Z^T, rather than by Z. Consider the multiplication Z^TM. To perform this multiplication, we derive a separate method. Recall that $Z^* = \left[\begin{array}{c} -L^{-1}B \\ \hdashline I \end{array}\right]$. Then,

$$(Z^*)^T = \left[\begin{array}{c:c} -B^T(L^{-1})^T & I \end{array}\right]. \quad (3.39)$$

Note that, unlike the case of left multiplication by Z^*, the rows of $(Z^*)^T$ are in the correct (original) order, and therefore it is not necessary to reorder the rows of the matrix that we obtain after multiplication by $(Z^*)^T$. However, the columns of $(Z^*)^T$ are in a different order from their original order. To compensate, we reorder the rows of M to match the column order of $(Z^*)^T$. That is, we find

$$M^* \;=\; M(\mathcal{I}, :), \tag{3.40}$$

which means that the j-th row of M^* is equal to the $\mathcal{I}(j)$-th row of M.

Next, we calculate $Z^T M = (Z^*)^T M^*$. To perform this calculation we represent M^* in block form:

$$M^* \;=\; \begin{bmatrix} M_1^* \\ \hdashline M_2^* \end{bmatrix}, \tag{3.41}$$

where M_1^* has as many rows as L. Then, we derive the form of $(Z^*)^T M^*$:

$$(Z^*)^T M^* \;=\; -B^T (L^{-1})^T M_1^* + M_2^*. \tag{3.42}$$

To calculate $-B^T(L^{-1})^T M_1^*$, we first define $Y = (L^{-1})^T M_1^*$ and $\mathbf{y_i} := (L^{-1})^T M_1^* \mathbf{e}_i$. Then, we calculate each $\mathbf{y}_i$ by solving the sparse system of equations

$$L^T \mathbf{y}_i \;=\; M_1^* \mathbf{e}_i, \tag{3.43}$$

for which the left side again is in reduced row echelon form, and all non-zero entries are 1.

After obtaining Y, we find $-B^T Y$ by simply summing the relevant rows of Y (corresponding to the units in each column of B), to calculate each row of $-B^T Y$. This can be substituted into (3.42) to find $(Z^*)^T M^*$.

We outline this process in the following algorithm.

```
Input: L, B, I, M
Output: Z^T M

begin
    M* ← M(I, :)
    M1* ← M*(1 :rows(L), :)
    M2* ← M*(rows(L) + 1 :rows(M*), :)
    Y ← zeros(rows(L),cols(M))

    for i from 1 to cols(M)
        Y(1 : rows(B), i) ← Linear solver(L^T, M1* e_i)
    end

    B^T Y ← zeros(cols(B),cols(M))
    for i from 1 to cols(B)
        for j from 1 to rows(B)
            if B(j, i) = 1
                for k from 1 to cols(M)
                    B^T Y(i, k) ← B^T Y(i, k) + Y(j, k)
                end
            end
        end
    end

    Z^T M = −B^T Y + M2*
end
```

Algorithm 3.3: Algorithm for sparse multiplication $Z^T M$.

In each iteration of DIPA we evaluate the augmented objective function $F(\mathbf{x})$ at least once (and sometimes several times), as well as its gradient vector and Hessian matrix. Recall from (3.20) that for the HCP formulation (3.19), when solving via DIPA, we use the auxiliary objective function

$$F(\mathbf{x}) \quad = \quad -\det(I - P(\mathbf{x}) + \frac{1}{N}J) - \mu \sum_{(i,j)\in\Gamma} \ln(x_{ij}). \tag{3.44}$$

The gradient vector and Hessian matrix for the barrier terms $\mathcal{L}(\mathbf{x}) = -\sum_{(i,j)\in\Gamma} \ln(x_{ij})$ are easy to calculate. However, the determinant function and its derivatives are expensive to calculate directly. In Sections 3.6 and 3.7, we develop an improved method of computing the determinant function and its derivatives. This method takes advantage of the amount of sparsity inherent in the HCP. However, for the sake of completeness of this section, the algorithm outlined in Section 3.7 that evaluates $F(\mathbf{x})$ and its derivatives is given here. Note that this algorithm uses a number of expressions that are defined or derived later in this chapter.

Input: $\mathbf{x}, \Gamma, \mu$
Output: $f^1, \mathbf{g}^1, H^1$

begin
- $P \leftarrow$ *Transform* $\mathbf{x}$ *into matrix form, putting each* x_{ij} *into the appropriate entry of* $P(\mathbf{x})$
- $(L, U) \leftarrow$ LU Decomposition$(I - P)$
- $\hat{L} \leftarrow$ L *with the bottom row replaced by* e_N^T
- $\hat{U} \leftarrow$ U *with the right column replaced by* e_N
- **for** i **from** 1 **to** N
  - $a_i^1 \leftarrow$ LP solver$(\hat{U}^T, \mathbf{e}_i)$
  - $b_i^1 \leftarrow$ LP solver$(\hat{L}, \mathbf{e}_i)$
- **end**
- **for** i **from** 1 **to** N
  - **for** j **from** 1 **to** N
    - $C(i,j) \leftarrow (a_j^1)^T b_i$
  - **end**
- **end**
- $f^1 \leftarrow \prod_{i=1}^{N-1} u_{ii}$
- $\mathbf{g}^1 \leftarrow$ *Calculate each* $g_{ij}^1 = f^1 C(i,j)$
- $H^1 \leftarrow$ *Calculate each* $H^1_{[ij],[k\ell]} = \begin{cases} g^1_{kj}(\mathbf{a}_i^1)^T\mathbf{b}_\ell^1 - g^1_{ij}(\mathbf{a}_k^1)^T\mathbf{b}_\ell^1, & i \neq k \text{ and } j \neq \ell, \\ 0, & \text{otherwise.} \end{cases}$
- $f^1 \leftarrow$ *Subtract the barrier terms* $\mu \sum_{(i,j)\in\Gamma} \ln(x_{ij})$ *from* f
- $\mathbf{g}^1 \leftarrow$ *Subtract the vector containing terms of the form* $\frac{\mu}{x_{ij}}$ *from* $\mathbf{g}^1$
- $H^1 \leftarrow$ *Add the diagonal matrix containing terms of the form* $\frac{\mu}{x_{ij}^2}$ *to* H^1

end

Algorithm 3.4: Function evaluations algorithm.

At each iteration of DIPA we compute a direction $\mathbf{d} := Z\mathbf{u}$, and $\mathbf{u} = -(Z^T HZ)^{-1} Z^T\mathbf{g}$ (see (3.12)). Since we repose the latter as $Z^T HZ\mathbf{u} = -Z^T\mathbf{g}$, we first calculate the reduced gradient $Z^T\mathbf{g}$ and the reduced Hessian $Z^T HZ$ at each iteration. Using the results of Algorithms 3.4 – 3.3, these are efficiently calculated using the following algorithm.

Input: $L, B, \mathcal{I}, \mathbf{g}, H$
Output: reduced gradient, reduced Hessian

begin
  reduced gradient $\leftarrow$ Algorithm 3.3: Algorithm for sparse multiplication $Z^T M(L, B, \mathcal{I}, \mathbf{g})$
  $Z^T H \leftarrow$ Algorithm 3.3: Algorithm for sparse multiplication $Z^T M(L, B, \mathcal{I}, H)$
  $HZ \leftarrow$ Transpose($Z^T H$)
  reduced Hessian $\leftarrow$ Algorithm 3.3: Algorithm for sparse multiplication $Z^T M(L, B, \mathcal{I}, HZ)$
end

Algorithm 3.5: Reduced gradient and Hessian algorithm.

Now, we calculate $\mathbf{d}$ by solving the system of equations

$$Z^T HZ\mathbf{u} = -Z^T\mathbf{g}, \tag{3.45}$$

and mapping the resulting solution $\mathbf{u} = -(Z^T HZ)^{-1}Z^T\mathbf{g}$ into the null space:

$$\mathbf{d} = Z\mathbf{u}. \tag{3.46}$$

We solve the system of equations (3.45) in our implementation by using either the conjugate-gradient (CG) method, or the Lanczos method. The CG method is an efficient method for large, symmetric, positive definite matrices. In our implementation the reduced Hessian $Z^T H(\mathbf{x})Z$ is a symmetric matrix but is not necessarily positive definite, since our original $f(\mathbf{x})$ is not convex. However, for large enough μ, $F(\mathbf{x})$ is convex and we calculate the direction vector $\mathbf{d}$ using the following algorithm.

Input: $L, B, \mathcal{I}, \mathbf{g}, H$
Output: $\mathbf{d}$

begin
  (reduced gradient, reduced Hessian) $\leftarrow$ Algorithm 3.5 : Reduced gradient and Hessian algorithm($L, B, \mathcal{I}, \mathbf{g}, H$)
  $\mathbf{u} \leftarrow$ Conjugate-gradient algorithm(reduced Hessian,−reduced gradient)
  $\mathbf{d} \leftarrow$ Algorithm 3.2: Algorithm for sparse multiplication $ZM(L, B, \mathcal{I}, \mathbf{u})$
end

Algorithm 3.6: Descent direction algorithm.

If $Z^T H(\mathbf{x})Z$ is indefinite, then a direction of negative curvature exists. We can find this direction of negative curvature by using the Lanczos method to approximate the eigenvectors $\mathbf{v_n}$ corresponding to negative eigenvalues λ_n of $Z^T HZ$. Then, we construct a direction of negative curvature by setting

$$\mathbf{u}_{nc} = \sum_n \mathbf{v}_n,$$

and mapping $\mathbf{u}$ into the null space of W to obtain a feasible direction of negative curvature as follows:

$$\mathbf{d}_{nc} = Z\mathbf{u}_{nc}. \tag{3.47}$$

It is worth noting that a direction of negative curvature is not necessarily a descent direction. However, if this is the case we simply travel in the direction $-\mathbf{d}_{nc}$ instead. We calculate (3.47) using the following algorithm.

```
Input: L, B, I, g, H
Output: d_nc

begin
    (reduced gradient, reduced Hessian) ← Algorithm 3.5: Reduced gradient and Hessian algorithm(L, B, I, g, H)
    u_nc ← Lanczos method(reduced Hessian,-reduced gradient)
    d_nc ← Algorithm 3.2: Algorithm for sparse multiplication ZM(L, B, I, u_nc)
    if d_nc is not a descent direction
        d_nc ← −d_nc
    end
end
```

Algorithm 3.7: Negative curvature algorithm.

Using either the descent direction $\mathbf{d}$ (specified by (3.46)) or the direction of negative curvature $\mathbf{d}_{nc}$ (specified by (3.47)), or $-\mathbf{d}_{nc}$, we now take a step that improves the objective function locally. We perform a line search to determine how large a step can be taken that improves the objective function. First, a maximum step size α_0 is calculated such that $\mathbf{x} + \alpha_0\mathbf{d}$ does not violate the nonnegativity constraints (3.15). Then, the following algorithm is executed.

Input: $\mathbf{x}, \Gamma, \mu, \alpha_0, \mathbf{d}$, evaluations
Output: α, evaluations

begin
  $\alpha \leftarrow 0.99\alpha_0$ *(To ensure we move to an interior point)*
  $F_{old} \leftarrow$ Algorithm 3.4: Function evaluation algorithm$(\mathbf{x}, \Gamma, \mu)$
  $F_{new} \leftarrow$ Algorithm 3.4: Function evaluation algorithm$(\mathbf{x} + \alpha\mathbf{d}, \Gamma, \mu)$
  while $F_{new} \geq F_{old}$
  evaluations $\leftarrow$ evaluations + 1
    $\alpha = \frac{\alpha}{2}$
    $F_{new} \leftarrow$ Algorithm 3.4: Function evaluation algorithm$(\mathbf{x} + \alpha\mathbf{d}, \Gamma, \mu)$
  end
end

Algorithm 3.8: Step size algorithm.

Of course, halving α in the above algorithm is a somewhat arbitrary choice, but it is widely used in such step selection heuristics.

If both $\mathbf{d} = \mathbf{0}$ and $Z^T HZ$ is positive definite, and a Hamiltonian cycle has not been found, then DIPA has converged to a local minimum. In this case, DIPA has failed to find a Hamiltonian cycle, but as we cannot be certain that none exists, we return an inconclusive result.

3.2.2 Initial selections and contracting graphs

In the initial stage of the algorithm, we only consider the barrier terms $\mathcal{L}(\mathbf{x}) = -\sum_{(i,j)\in\Gamma} \ln(x_{ij})$ in the objective function, ignoring $f(\mathbf{x})$ until we minimise $\mathcal{L}(\mathbf{x})$. This is a convex function, so we can easily find the global minimum $\mathbf{x}^*_{\mathcal{L}}$, which is the analytic centre of a polytope defined by the set of constraints (3.15)–(3.17). This process is outlined in the following algorithm.

Input: $L, B, \mathcal{I}, \mathbf{x}$

Output: $\mathbf{x}^*_{\mathcal{L}}$

begin
- **for** i **from** 1 **to** N
  - **for** j **from** 1 **to** N
    - **if** $(i,j) \in \Gamma$
      - $g_{ij} \leftarrow -\frac{1}{x_{ij}}$
      - $H_{ij,ij} \leftarrow \frac{1}{x_{ij}^2}$
    - **end**
  - **end**
- **end**
- reduced gradient $\leftarrow$ Algorithm 3.3: Algorithm for sparse multiplication $Z^T M(L, B, \mathcal{I}, \mathbf{g})$
- **while** norm(reduced gradient) $> \varepsilon$
  - $\mathbf{d} \leftarrow$ Algorithm 3.6: Descent direction algorithm$(L, B, \mathcal{I}, \mathbf{g}, H)$
  - $\mathbf{x} \leftarrow \mathbf{x} + \mathbf{d}$
  - **for** i **from** 1 **to** N
    - **for** j **from** 1 **to** N
      - **if** $(i,j) \in \Gamma$
        - $g_{ij} \leftarrow -\frac{1}{x_{ij}}$
        - $H_{ij,ij} \leftarrow \frac{1}{x_{ij}^2}$
      - **end**
    - **end**
  - **end**
  - reduced gradient $\leftarrow$ Algorithm 3.3: Algorithm for sparse multiplication $Z^T M(L, B, \mathcal{I}, \mathbf{g})$
- **end**
- $\mathbf{x}^*_{\mathcal{L}} \leftarrow \mathbf{x}$

end

Algorithm 3.9: Barrier point algorithm.

Remark 3.2.5 *Experimentally, we have observed that if* $[x^*_{\mathcal{L}}]_{ia} = [x^*_{\mathcal{L}}]_{ib}$*, for* $a \neq b$*, (for example, this is true for all arcs* (i,a) *and* (i,b) *for regular graphs), then it is common that descent directions maintain this equality for some arcs. In this case, we say that these descent directions have failed to* break the tie *between arcs* (i,a) *and* (i,b)*. There may be several ties needing to be broken in a graph. In our experiments we have found that directions of negative curvature break these ties. For this reason, directions of negative curvature become critical in DIPA, and we seek to take advantage of them as soon as possible. This is achieved by choosing the value of the barrier parameter* μ *small enough that negative curvature either exists, or will exist after only a small number of iterations.*

We define $H_D(\mathbf{x})$ as the Hessian of $f(\mathbf{x})$. Then, we consider the eigenvalues and eigenvectors of $Z^T H_D(\mathbf{x}^*_{\mathcal{L}})Z$, the reduced Hessian of $f(\mathbf{x})$ evaluated at $\mathbf{x}^*_{\mathcal{L}}$. Let λ_{min} be the most negative of these eigenvalues and $\mathbf{v}_{min}$ be an eigenvector associated with λ_{min}. Then, $\mathbf{u}_{min} = Z\mathbf{v}_{min}$ is a direction of negative curvature for $f(\mathbf{x})$ at $\mathbf{x} = \mathbf{x}^*_{\mathcal{L}}$.

Since this negative curvature will be nonzero, then for small enough μ, $\mathbf{u}_{min}$ will also be a direction of negative curvature in the augmented function $F(\mathbf{x})$. Defining $H_{\mathcal{L}}(\mathbf{x})$ to be the Hessian of the barrier terms $\mathcal{L}(\mathbf{x})$, we find μ by solving

$$\lambda_{min} + \mu \mathbf{u}^T_{min} H_{\mathcal{L}}(\mathbf{x}^*_{\mathcal{L}})\mathbf{u}_{min} \quad = \quad \gamma\lambda_{min}, \tag{3.48}$$

where the parameter γ allows us to control how much negative curvature we desire. The solution of this equation is

$$\mu \quad = \quad \frac{(1-\gamma)(-\lambda_{min})}{\mathbf{u}^T_{min} H_{\mathcal{L}}(\mathbf{x}^*_{\mathcal{L}})\mathbf{u}_{min}}. \tag{3.49}$$

Note that $H_{\mathcal{L}}(x)$ is a diagonal matrix where each diagonal entry is of the form x_{ij}^{-2}. Then,

$$\mathbf{u}^T_{min} H_{\mathcal{L}}(\mathbf{x}^*_{\mathcal{L}})\mathbf{u}_{min} \quad = \quad \sum_{(i,j)\in\Gamma} \left(\frac{[u_{min}]_{ij}}{[x^*_{\mathcal{L}}]_{ij}} \right)^2 .$$

Note also that this expression is clearly positive and hence $\mu > 0$.

The convexity of $\mathcal{L}(\mathbf{x})$ implies that we cannot achieve more negative curvature in $F(\mathbf{x})$ than is present in $f(\mathbf{x})$. We also cannot achieve the same level unless $\mu := 0$. For this reason, we select γ less than 1. However, it is possible for γ to be negative, which produces positive curvature in $F(\mathbf{x})$. Experimentally we have observed that starting with a small amount of positive curvature is often desirable (so that we can take advantage of descent directions for a small number of iterations before switching to directions of negative curvature) so a small, negative value of γ is often chosen. Once we calculate μ, we begin the main outer iteration with the prescribed amount of positive or negative curvature present. We outline this process in the following algorithm.

Input: $L, B, \mathcal{I}, \mathbf{x}^*_{\mathcal{L}}, \Gamma, \gamma$
Output: μ

begin
  $\mu_{\mathbf{0}} \leftarrow$ *Vector the same size as* $\mathbf{x}^*_{\mathcal{L}}$ *with* 0 *in every position*
  $(F, \mathbf{g}, H) \leftarrow$ Algorithm 3.4: Function evaluations algorithm$(\mathbf{x}^*_{\mathcal{L}}, \Gamma, \mu_{\mathbf{0}})$
  (reduced gradient, reduced Hessian) $\leftarrow$ Algorithm 3.5: Reduced gradient and Hessian algorithm$(L, B, \mathcal{I}, \mathbf{g}, H)$
  $(\lambda_{min}, u_{min}) \leftarrow$ Eigenvalues(reduced Hessian)
  μ value $\leftarrow 0$
  for i **from** 1 **to** N
    for j **from** 1 **to** N
      if $(i, j) \in \Gamma)$
        μ value $\leftarrow \mu$ value $+ \left(\frac{[u_{min}]_{ij}}{[x^*_{\mathcal{L}}]_{ij}}\right)^2$
      end
    end
  end
  μ value $\leftarrow (\mu$ value$)(1-\gamma)(-\lambda_{min})$
  $\mu \leftarrow$ *Vector the same size as* $\mathbf{x}^*_{\mathcal{L}}$ *with* μ value *in every position*
end

Algorithm 3.10: Initial μ algorithm.

If at any stage, some of the x_{ij} variables approach their extremal values (0 or 1), we fix these values and remove the variables from the program. This process takes two forms: *deletion* and *deflation*, that is, setting x_{ij} to 0 and 1, respectively.

Remark 3.2.6 *Note that we use the term deflation because in practice the process of fixing* $x_{ij} := 1$ *results in two nodes being combined to become a single node, reducing the total number of nodes in the graph by 1.*

Deletion is the process of removing one arc from the graph, when the variable corresponding to that arc has a near-zero value. By default, we define 0.02 as being near-zero, but this can be altered or set as an input parameter. We set such a variable to 0, and remove that arc from the graph. Deletion is a simple process which we outline in the following algorithm.

Input: $\mathbf{x}, \Gamma, \mu, i, j$
Output: $\mathbf{x}, \Gamma, \mu$

begin
  index $\leftarrow$ *Identify which element of* $\mathbf{x}$ *corresponds to arc* (i, j)
  $\mathbf{x} \leftarrow$ *Delete element* index *from* $\mathbf{x}$
  $\mu \leftarrow$ *Delete element* index *from* μ
  $\Gamma(i, j) \leftarrow 0$
end

Algorithm 3.11: Deletion algorithm.

Deflation is the process of removing one node from the graph, by combining two nodes together. If a variable x_{ij} is close to 1, we combine nodes i and j by removing node i from the graph. Then, we redirect any arcs (k, i) that previously went into node i to become (k, j), unless this creates a self-loop arc. By default, we define 0.9 as being close to 1, but this can be altered or set as an input parameter.

During deflation, we not only fix one variable (x_{ij}) to have the value 1, but also fix several other variables to have the value 0. Namely, we fix all variables corresponding to arcs (i, k) for $k \neq j$, (k, j) for $k \neq i$, and (j, i) to have the value 0, for all k.

Consequently, we say that the deflation of node i has forced the deletion of the above arcs. We outline this process in the following algorithm.

```
Input: x, Γ, μ, N, i, j, deflations
Output: x, Γ, μ, N, deflations

begin
    (x, Γ, μ) ← Algorithm 3.11: Deletion algorithm(x, Γ, μ, i, j)
    for k from 1 to N
        if Γ(i, k) = 1
            if k ≠ j
                (x, Γ, μ) ← Algorithm 3.11: Deletion algorithm(x, μ, Γ, i, k)
            end
        end
        if Γ(k, j) = 1
            if k ≠ i
                (x, Γ, μ) ← Algorithm 3.11: Deletion algorithm(x, Γ, μ, k, j)
            end
        end
    end
    if (i, j) ∈ Γ
        (x, Γ, μ) ← Algorithm 3.11: Deletion algorithm(x, Γ, μ, j, i)
    end
    N ← N − 1
    Γ ← delete node i from Γ
    deflations ← deflations + 1
    Store the information about the deflated arc in memory
end
```

Algorithm 3.12: Deflation algorithm.

Note that whenever we perform a deflation, we store the information about the deflated arc in memory. This is done so we can reconstruct the original graph once a Hamiltonian cycle is found.

Whenever deletion or deflation is performed, the values of some variables change, and the resultant, smaller dimensional, $\mathbf{x}$ no longer satisfies equality constraints (3.16)–(3.17). Define $\mathbf{s} := \mathbf{e} - \overline{W}\mathbf{x}$ to be the error introduced by Algorithms 3.11 – 3.12. Note that $\mathbf{s}$ is a nonnegative vector in the case of both deletion and deflation. Then, we find a new $\mathbf{x}'$ such that $\mathbf{x}' \in \mathcal{DS}_{\mathbf{x}}$, and $|\mathbf{x}' - \mathbf{x}| < \varepsilon$, where the size of ε depends on how close to 0 or 1 we require a variable to become before we undertake deletion or deflation. The interpretation of $\mathbf{x}'$ is that it is a point that satisfies constraints (3.15)–(3.17) that is as close as possible to the point we obtained after deleting or deflating.

We calculate such a vector $\mathbf{x}'$ by solving a linear program in decision variables $(\mathbf{x}, \gamma)$, where γ is a scalar variable. First, we define x_{min} as the smallest value in $\mathbf{x}$, not including variables corresponding to arcs that have been deleted. Then, we solve

$$\min_{\mathbf{x}',\gamma} \gamma \tag{3.50}$$

$$\text{s.t.}$$

$$\overline{W}\mathbf{x}' + \gamma\mathbf{s} = \mathbf{e}, \tag{3.51}$$

$$\mathbf{x}' \geq \frac{x_{min}}{2}\mathbf{e}, \tag{3.52}$$

$$\gamma \geq 0, \tag{3.53}$$

which gives $\mathbf{x}' \in \mathcal{DS}_{\mathbf{x}}$ when γ is minimised to 0. Of course, many $\mathbf{x}' \in \mathcal{DS}_{\mathbf{x}}$ satisfy the above constraints. However, if we use the Simplex algorithm to solve the LP and provide the previous $\mathbf{x}$ as the starting point, a nearby feasible point is usually found. We include the lower bound (3.52) on the values of $\mathbf{x}'$ because, otherwise, the Simplex algorithm attempts to set many variables to 0, which is undesirable as we wish to remain interior. It is possible that for a particular graph, we may not be able to find a point that satisfies the above constraints, because some variables may need to be 0 or a value very close to 0. In these cases, the LP terminates with a positive objective function value. Then, we relax the lower bound on $\mathbf{x}$ and solve the LP again, continuing this process until we obtain a solution where $\gamma = 0$.

If we cannot minimise γ to 0 without setting $x_{ij} = 0$ for some i and j, then we delete the arcs corresponding to these variables, as they cannot be present in a Hamiltonian cycle (or any $\mathcal{DS}_{\mathbf{x}}$ point) containing the currently fixed arcs.

We outline this method in the following algorithm.

Input: $\mathbf{x}, \Gamma, \mu, W$
Output: $\mathbf{x}, \Gamma, \mu$

begin
  $x_{min} \leftarrow \min(\mathbf{x})$
  $\mathbf{s} \leftarrow \mathbf{e} - W\mathbf{x}$
  $\gamma \leftarrow 1$
  $\text{count} \leftarrow 0$
  while $\gamma > 0$ **and** $\text{count} < 10$
    $\text{count} \leftarrow \text{count} + 1$
    $(\mathbf{x}, \gamma) \leftarrow$ *Solve the LP* (3.50)–(3.53) *with* (3.52) *replaced by* $\mathbf{x} \geq \dfrac{x_{min}}{\text{count}+1}\mathbf{e}$
  end
  if $\gamma > 0$
    $(\mathbf{x}, \gamma) \leftarrow$ *Solve the LP* (3.50)–(3.53) *with* (3.52) *replaced by* $\mathbf{x} \geq 0$
    if *any* $x_{ij} = 0$
      $(\mathbf{x}, \Gamma, \mu) \leftarrow$ Algorithm 3.11: Deletion algorithm$(\mathbf{x}, \Gamma, \mu, i, j)$
    end
  end
end

Algorithm 3.13: Scaling algorithm.

To start executing Algorithm 3.9, we first require a feasible, interior point $\mathbf{x}_0$ that satisfies constraints (3.15)–(3.17). If Γ is a k-regular graph, that is, there are exactly k arcs incident to every node, then we can easily construct an initial point by defining $\mathbf{x}_0 := \begin{bmatrix} \frac{1}{k} & \dots & \frac{1}{k} \end{bmatrix}^T$.

However, for irregular graphs, an initial starting point is more difficult to calculate. To obtain $\mathbf{x}_0$ in these cases, we first define an obviously infeasible point, $\mathbf{x}_{-1} := \begin{bmatrix} \frac{1}{d} & \dots & \frac{1}{d} \end{bmatrix}^T$, for some d larger than the maximum degree of any node in the graph. In our implementation, we define $d :=$ maximum degree $+1$. We then use Algorithm 3.13 to find a nearby $\mathcal{DS}_{\mathbf{x}}$ point to use as $\mathbf{x}_0$. We outline this method in the following algorithm.

Input: $\Gamma, \overline{W}$

Output: $\mathbf{x}_0, \Gamma$

begin

$d \leftarrow$ *Find the maximum degree of* Γ

$\mathbf{x}_{-1} \leftarrow \begin{bmatrix} \frac{1}{d+1} & \cdots & \frac{1}{d+1} \end{bmatrix}^T$

$\mu_0 \leftarrow$ *Vector the same size as* $\mathbf{x}_{-1}$ *with* N *in every position*

$(\mathbf{x}_0, \Gamma, \mu) \leftarrow$ Algorithm 3.13: Scaling algorithm$(\mathbf{x}_{-1}, \mu_0, \Gamma, \overline{W})$

end

Algorithm 3.14: Initial point algorithm.

Note that Γ is output from Algorithm 3.14, because it is possible that no $\mathcal{DS}_{\mathbf{x}}$ points exists where all $x_{ij} > 0$. In these cases, some arcs are deleted from the original graph Γ.

We have no guarantee that the initial point $\mathbf{x}_0$ obtained from Algorithm 3.14 will be near the centroid of the $\mathcal{DS}_{\mathbf{x}}$ polytope. However, this does not adversely effect the result of DIPA, as the first step is to minimise the barrier term $\mathcal{L}(\mathbf{x})$. Since the barrier terms are convex, any interior point will be a sufficient starting point to find the barrier point $\mathbf{x}^*_{\mathcal{L}}$. By virtue of the $\mathcal{L}(\mathbf{x})$ objective function, $\mathbf{x}^*_{\mathcal{L}}$ is typically far away from the boundaries of $\mathcal{DS}_{\mathbf{x}}$.

At each iteration, we temporarily round the values of all variables to either 0 or 1 to see if they correspond to a Hamiltonian solution. If so, the algorithm ends and we return the Hamiltonian cycle. Note that if any deflations have been performed during the algorithm, the Hamiltonian cycle we return will be for the deflated graph. If this has happened, the information about the deflated arcs is recalled and we rebuild the original graph so that a Hamiltonian cycle in the original graph can be obtained.

The benefit of rounding at each iteration is that DIPA needs only obtain $\mathbf{x}^*$ in the neighbourhood of a Hamiltonian solution. Without rounding, we would require DIPA to converge to an extreme point of $\mathcal{DS}_{\mathbf{x}}$, where $F(\mathbf{x})$ is undefined.

We outline one simple method of rounding in the following algorithm.

```
Input: x, Γ, N
Output: HC

begin
    for count = 1 to N
        (i, j) ← Find the largest x_ij not already fixed to 1 or 0
        x_ij ← 1
        x_ji ← 0
        for k = 1 to N
            if k ≠ i
                x_kj ← 0
            end
            if k ≠ j
                x_ik ← 0
            end
        end
    end
    if the resulting matrix is a HC
        return the HC
    else
        return no HC found
    end
end
```

Algorithm 3.15: Rounding algorithm.

Obviously, we could use other, more sophisticated, rounding methods which may allow us to identify a Hamiltonian cycle earlier. One potential improvement of this method would be to solve a heuristic at the completion of each iteration, using the current point $\mathbf{x}$, that tries to find a nearby Hamiltonian cycle. Combining an algorithm with a heuristic solved at each iteration was considered in [22], with promising results.

3.3 Algorithm that implements DIPA

We now present the main determinant interior point algorithm, that uses all the previous component algorithms.

Input: Γ, γ
Output: HC, deflations, iterations, evaluations

begin
    (deflations, iterations, evaluations) $\leftarrow 0$
    $N \leftarrow$ *Number of nodes in* Γ
    $\overline{W} \leftarrow$ *Constraints* (3.16)–(3.17)
    $(L, B, \mathcal{I}) \leftarrow$ Algorithm 3.1: Reordering W algorithm$(\overline{W}, N)$
    $(\mathbf{x}, \Gamma) \leftarrow$ Algorithm 3.14: Initial point algorithm$(\Gamma, \overline{W})$
    $\mathbf{x} \leftarrow$ Algorithm 3.9: Barrier point algorithm$(L, B, \mathcal{I}, \mathbf{x})$
    $\mu \leftarrow$ Algorithm 3.10: Initial μ algorithm$(L, B, \mathcal{I}, \mathbf{x}, \Gamma, \gamma)$
    while *a HC has not been found and* $\mathbf{x}$ *has not converged*
        deflations $\leftarrow$ deflations + 1
        $(f, \mathbf{g}, H) \leftarrow$ Algorithm 3.4: Function evaluations algorithm$(\mathbf{x}, \Gamma, \mu)$
        if *negative curvature exists*
            $\mathbf{d}_{nc} \leftarrow$ Algorithm 3.7: Negative curvature algorithm$(L, B, \mathcal{I}, \mathbf{g}, H)$
        else
            $\mathbf{d} \leftarrow$ Algorithm 3.6: Descent direction algorithm$(L, B, \mathcal{I}, \mathbf{g}, H)$
        end
        $\alpha_0 \leftarrow$ *Maximum value such that* $\mathbf{x} + \alpha_0 \mathbf{d}$ *is a nonnegative vector*
        (α,evaluations) $\leftarrow$ Algorithm 3.8: Step size algorithm($\mathbf{x}, \Gamma, \mu, \alpha_0, \mathbf{d}$,evaluations)
        $x \leftarrow x + \alpha d$
        if *any* $x_{ij} > 0.9$
            ($\mathbf{x}, \Gamma, \mu, N$,deflations) $\leftarrow$ Algorithm 3.12: Deflation algorithm($\mathbf{x}, \Gamma, \mu, N, i, j$,deflations)
        end
        if *any* $x_{ij} < 0.02$
            $(\mathbf{x}, \Gamma, \mu) \leftarrow$ Algorithm 3.11: Deletion algorithm$(\mathbf{x}, \Gamma, \mu, i, j)$
        end
        if *any Deflations or Deletions were performed*
            $(\mathbf{x}, \mu, \Gamma) \leftarrow$ Algorithm 3.13: Scaling algorithm$(\mathbf{x}, \Gamma, \mu, \overline{W})$
        end
        HC $\leftarrow$ Algorithm 3.15: Rounding algorithm$(\mathbf{x}, \Gamma, \mu)$ *to see if a HC has been found.*
        if $\mathbf{x}$ *has converged, but a HC has not been found*
            $\mu \leftarrow 0.9\mu$
        end **end**
    if *a HC was found*
        Rebuild the original graph if necessary
        return *the HC in the original graph*
    else
        return *no HC found*
    end
end

Algorithm 3.16: DIPA.

We implemented Algorithm 3.16: DIPA in MATLAB and tested several sets of

Hamiltonian graphs. The results of these tests are outlined in Table 3.1. Each test set contains 50 randomly generated Hamiltonian graphs of a certain size where each node has degree between 3 and 5. For each test set, we give the number of graphs (out of the 50 generated) in which Algorithm 3.16: DIPA succeeds in finding a Hamiltonian cycle, the average number of iterations performed, the average number of deflations performed, the average number of function evaluations required during Algorithm 3.8 over the course of execution, and the average running time for each graph. Note that since we implemented DIPA in MATLAB, the running times are not competitive when compared to other similar models implemented in compiled language. However, we provide the running times here to demonstrate how they grow as N increases.

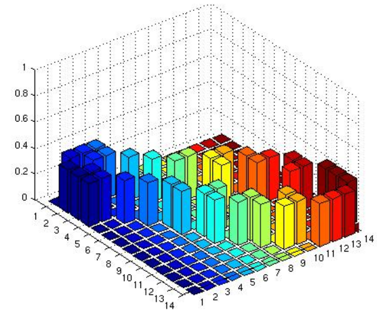
Graph size	**Number solved**	**Average iterations**	**Average deflations**	**Average evaluations**	**Average run time (secs)**
N = 20	48	20.42	9.5	20.76	1.55
N = 40	40	86.98	27.8	87.08	12.05
N = 60	30	198.72	42.62	201.32	54.77
N = 80	33	372.76	65.04	372.84	196.26

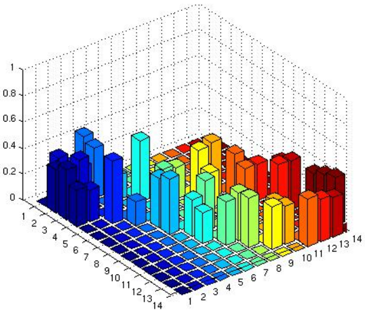
Table 3.1: Results obtained from solving sets of graphs with DIPA.

Example 3.3.1 *We ran Algorithm 3.16: DIPA on a 14-node cubic graph, specifically the graph with the following adjacency matrix:*

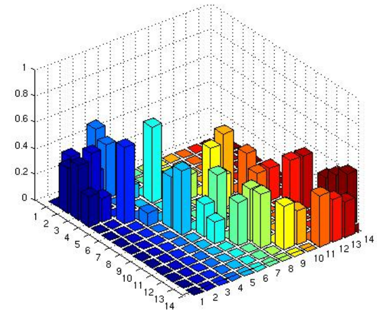
$$\mathbb{A}_{14} = \begin{bmatrix} 0&1&1&1&0&0&0&0&0&0&0&0&0&0 \\ 1&0&1&1&0&0&0&0&0&0&0&0&0&0 \\ 1&1&0&0&1&0&0&0&0&0&0&0&0&0 \\ 1&1&0&0&0&1&0&0&0&0&0&0&0&0 \\ 0&0&1&0&0&0&1&1&0&0&0&0&0&0 \\ 0&0&0&1&0&0&0&0&1&1&0&0&0&0 \\ 0&0&0&0&1&0&0&0&1&0&1&0&0&0 \\ 0&0&0&0&1&0&0&0&0&0&1&1&0&0 \\ 0&0&0&0&0&1&1&0&0&0&0&0&1&0 \\ 0&0&0&0&0&1&0&0&0&0&0&1&1&0 \\ 0&0&0&0&0&0&1&1&0&0&0&0&0&1 \\ 0&0&0&0&0&0&0&1&0&1&0&0&0&1 \\ 0&0&0&0&0&0&0&0&1&1&0&0&0&1 \\ 0&0&0&0&0&0&0&0&0&0&1&1&1&0 \end{bmatrix}.$$

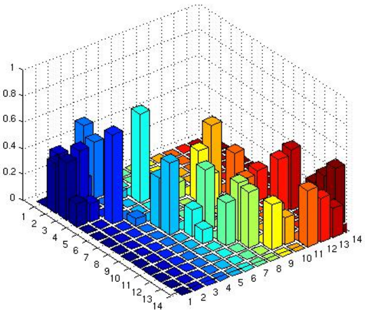
A Hamiltonian cycle was found by DIPA after 8 iterations. The probability assigned to each arc is displayed in the following plots.



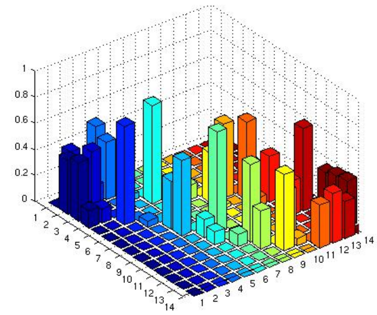


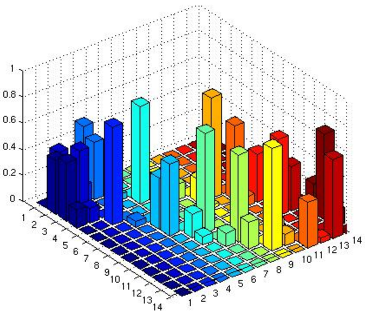
Iteration 1 *Iteration 2*



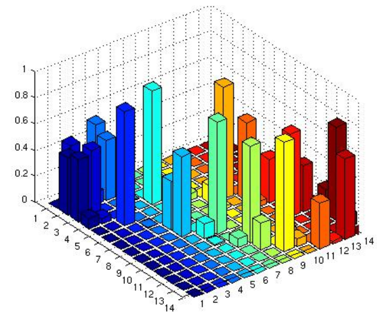


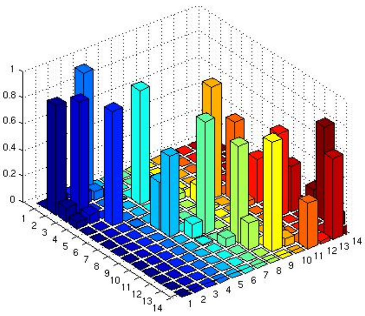
Iteration 3 *Iteration 4*



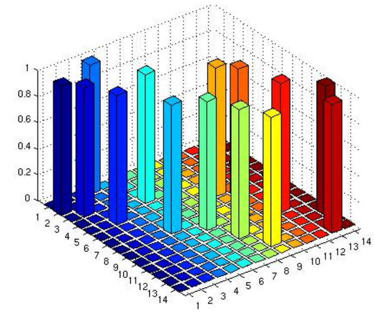


Iteration 5 *Iteration 6*





Iteration 7 *Iteration 8*



Final Hamiltonian cycle

Note that at iteration 1, $P(\mathbf{x})$ assigned equal probabilities to all 42 arcs, but at iteration 8, one arc from each node contains the large majority of the probability. The rounding process at the completion of iteration 8 assigns these arcs to a Hamiltonian cycle $1 \to 4 \to 6 \to 10 \to 12 \to 14 \to 13 \to 9 \to 7 \to 11 \to 8 \to 5 \to 3 \to 2 \to 1$.

Example 3.3.2 *We ran Algorithm 3.16: DIPA on a 16-node cubic graph, specifically the graph with the following adjacency matrix*

$$\mathbb{A}_{16} = \begin{bmatrix} 0&1&1&1&0&0&0&0&0&0&0&0&0&0&0&0 \\ 1&0&1&0&1&0&0&0&0&0&0&0&0&0&0&0 \\ 1&1&0&0&0&1&0&0&0&0&0&0&0&0&0&0 \\ 1&0&0&0&1&0&1&0&0&0&0&0&0&0&0&0 \\ 0&1&0&1&0&0&1&0&0&0&0&0&0&0&0&0 \\ 0&0&1&0&0&0&0&1&1&0&0&0&0&0&0&0 \\ 0&0&0&1&1&0&0&0&0&1&0&0&0&0&0&0 \\ 0&0&0&0&0&1&0&0&1&1&0&0&0&0&0&0 \\ 0&0&0&0&0&1&0&1&0&0&1&0&0&0&0&0 \\ 0&0&0&0&0&0&1&1&0&0&0&1&0&0&0&0 \\ 0&0&0&0&0&0&0&0&1&0&0&0&1&1&0&0 \\ 0&0&0&0&0&0&0&0&0&1&0&0&0&0&1&1 \\ 0&0&0&0&0&0&0&0&0&0&1&0&0&0&1&1 \\ 0&0&0&0&0&0&0&0&0&0&1&0&0&0&1&1 \\ 0&0&0&0&0&0&0&0&0&0&0&1&1&1&0&0 \\ 0&0&0&0&0&0&0&0&0&0&0&1&1&1&0&0 \end{bmatrix}.$$

A Hamiltonian cycle was found by DIPA after nine iterations. The probability assigned to each arc is displayed in the following table over all nine iterations. To make the convergence of the variables easier to see, when a variable has converged to either 0 or 1 we drop the decimal places, and boldface the integer.

After 9 iterations, Algorithm 3.15 found the Hamiltonian cycle

$$1 \to 4 \to 5 \to 7 \to 10 \to 12 \to 15 \to 13 \to 16 \to 14 \to 11 \to 9 \to 8 \to 6 \to 3 \to 2 \to 1.$$

Arc	Iter 1	Iter 2	Iter 3	Iter 4	Iter 5	Iter 6	Iter 7	Iter 8	Iter 9	HC
1 − 2	0.3333	0.2750	0.2210	0.1550	0.0250	0	0	0	0	0
1 − 3	0.3333	0.0720	0.0420	0.0310	0.0250	0	0	0	0	0
1 − 4	0.3333	0.6530	0.7370	0.8140	0.9500	1	1	1	1	1
2 − 1	0.3333	0.3400	0.3600	0.4060	0.5330	0.6660	0.7900	0.8250	0.8860	1
2 − 3	0.3333	0.2340	0.1830	0.1140	0.0110	0	0	0	0	0
2 − 5	0.3333	0.4250	0.4570	0.4800	0.4550	0.3340	0.2100	0.1750	0.1140	0
3 − 1	0.3333	0.4360	0.4360	0.4130	0.3130	0.3340	0.2100	0.1750	0.1140	0
3 − 2	0.3333	0.4510	0.5100	0.5810	0.6820	0.6660	0.7900	0.8250	0.8860	1
3 − 6	0.3333	0.1130	0.0540	0.0070	0.0050	0	0	0	0	0
4 − 1	0.3333	0.2230	0.2040	0.1810	0.1540	0	0	0	0	0
4 − 5	0.3333	0.3470	0.3720	0.4040	0.5310	0.6660	0.7900	0.8250	0.8860	1
4 − 7	0.3333	0.4300	0.4240	0.4140	0.3160	0.3340	0.2100	0.1750	0.1140	0
5 − 2	0.3333	0.2740	0.2700	0.2640	0.2930	0.3340	0.2100	0.1750	0.1140	0
5 − 4	0.3333	0.2990	0.2320	0.1580	0.0260	0	0	0	0	0
5 − 7	0.3333	0.4270	0.4990	0.5780	0.6810	0.6660	0.7900	0.8250	0.8860	1
6 − 3	0.3333	0.6940	0.7750	0.8550	0.9640	1	1	1	1	1
6 − 8	0.3333	0.2370	0.2180	0.1400	0.0320	0	0	0	0	0
6 − 9	0.3333	0.0690	0.0070	0.0060	0.0040	0	0	0	0	0
7 − 4	0.3333	0.0480	0.0310	0.0280	0.0230	0	0	0	0	0
7 − 5	0.3333	0.2270	0.1710	0.1160	0.0140	0	0	0	0	0
7 − 10	0.3333	0.7250	0.7980	0.8560	0.9630	1	1	1	1	1
8 − 6	0.3333	0.4280	0.4800	0.5600	0.7360	0.8140	0.9770	1	1	1
8 − 9	0.3333	0.3290	0.3300	0.3040	0.2310	0.1860	0.0230	0	0	0
8 − 10	0.3333	0.2420	0.1900	0.1360	0.0340	0	0	0	0	0
9 − 6	0.3333	0.4590	0.4660	0.4340	0.2600	0.1860	0.0230	0	0	0
9 − 8	0.3333	0.5080	0.5230	0.5580	0.7370	0.8140	0.9770	1	1	1
9 − 11	0.3333	0.0330	0.0120	0.0080	0.0040	0	0	0	0	0
10 − 7	0.3333	0.1430	0.0770	0.0080	0.0040	0	0	0	0	0
10 − 8	0.3333	0.2560	0.2600	0.3020	0.2310	0.1860	0.0230	0	0	0
10 − 12	0.3333	0.6010	0.6630	0.6900	0.7650	0.8140	0.9770	1	1	1
11 − 9	0.3333	0.6010	0.6630	0.6900	0.7650	0.8140	0.9770	1	1	1
11 − 13	0.3333	0.2650	0.2520	0.2420	0.2090	0.1660	0.0170	0	0	0
11 − 14	0.3333	0.1340	0.0850	0.0680	0.0260	0.0200	0.0060	0	0	0
12 − 10	0.3333	0.0330	0.0120	0.0080	0.0040	0	0	0	0	0
12 − 15	0.3333	0.4100	0.4090	0.4010	0.3090	0.3000	0.3830	0.4570	0.5860	1
12 − 16	0.3333	0.5570	0.5790	0.5910	0.6870	0.7000	0.6170	0.5430	0.4140	0
13 − 11	0.3333	0.4760	0.4830	0.4770	0.4470	0.4510	0.4550	0.4370	0.4060	0
13 − 15	0.3333	0.2960	0.2960	0.2980	0.3030	0.2960	0.1990	0.1100	0.0110	0
13 − 16	0.3333	0.2280	0.2220	0.2250	0.2510	0.2520	0.3460	0.4530	0.5830	1
14 − 11	0.3333	0.4900	0.5060	0.5150	0.5490	0.5490	0.5450	0.5630	0.5940	1
14 − 15	0.3333	0.2940	0.2950	0.3010	0.3880	0.4040	0.4170	0.4330	0.4030	0
14 − 16	0.3333	0.2150	0.1990	0.1840	0.0620	0.0480	0.0380	0.0040	0.0030	0
15 − 12	0.3333	0.2070	0.1800	0.1750	0.1990	0.1820	0.0200	0	0	0
15 − 13	0.3333	0.3670	0.3740	0.3810	0.4390	0.4700	0.6150	0.7310	0.8360	1
15 − 14	0.3333	0.4260	0.4460	0.4440	0.3620	0.3480	0.3650	0.2690	0.1640	0
16 − 12	0.3333	0.1920	0.1560	0.1350	0.0360	0.0040	0.0030	0	0	0
16 − 13	0.3333	0.3680	0.3740	0.3770	0.3530	0.3640	0.3690	0.2690	0.1640	0
16 − 14	0.3333	0.4400	0.4690	0.4880	0.6120	0.6320	0.6290	0.7310	0.8360	1

Table 3.2: Variable values obtained from solving a 16-node graph with Algorithm 3.16: DIPA.

3.4 Variations of DIPA

We obtained the numerical results shown in Table 3.1 using Algorithm 3.16: DIPA. However, we tested other variations of this algorithm that were either abandoned in favour of other choices, or left as non-standard options that can be used if desired. We describe these variations below.

3.4.1 Orthonormal null space

We use the null space Z in Algorithms 3.2 – 3.3 because of the efficiency offered by its sparse structure, and non-zero entries of only ± 1. However, one disadvantage of this null space is that the columns of Z are not orthogonal. While the condition number of $Z^T Z$ was not large for the experiments we ran, it is possible that the lack of orthogonality could lead to scaling issues in certain problems.

We found an orthonormal basis of the null space Z (using MATLAB's `null` command), and performed calculations involving Z in a non-sparse fashion to compare the results with those obtained by the non-orthogonal basis of the null space. In many cases we observed that the orthonormal basis of the null space introduced symmetry into the directions taken in DIPA. This is undesirable, as it implies that DIPA has not made a decision about which node to tend towards, and often leads to DIPA exhibiting jamming, where from many nodes two variables have identical values, and the others converge to 0 and are deleted. However, in some (rare) cases the orthonormal basis of the null space enables us to find a solution when the algorithm that used the non-orthonormal basis of the null space fails.

3.4.2 Stochastic constraints

In [14] it is shown that the optimisation problem $\min\{-\det(I - P(\mathbf{x}) + \frac{1}{N}J)\}$ is optimised at a Hamiltonian $\mathbf{x}$ not only over the constraint set $\mathbf{x} \in \mathcal{DS}_{\mathbf{x}}$, but also the more general superset of stochastic constraints, $\mathbf{x} \in \mathcal{S}_{\mathbf{x}}$. This set of constraints is identical to $\mathcal{DS}_{\mathbf{x}}$ but without equality constraints (3.17) that ensure unit column sums. That is, $\mathcal{S}_{\mathbf{x}}$ is the set of all $\mathbf{x}$ that satisfy the following constraints

$$\begin{aligned} x_{ij} &\geq 0, \quad (i,j) \in \Gamma, & (3.54)\\ \sum_{j \in \mathcal{A}(i)} x_{ij} &= 1, \quad i = 1, \ldots, N. & (3.55) \end{aligned}$$

The equality constraints (3.55) correspond to a constraints matrix W_S with the structure

$$W_S = \begin{bmatrix} 1 & \cdots & 1 & & & & & & \\ & & & 1 & \cdots & 1 & & & \\ & & & & & & \ddots & & \\ & & & & & & & \ddots & \\ & & & & & & 1 & \cdots & 1 \end{bmatrix}.$$

Then, we can find a sparse null space for W_S much more easily than for (3.16)–(3.17). To find the null space for W_S, we move the first column of the i-th block of 1's, to column i, for all $i = 1, \ldots, N$ to form W_S^*, which has the following form:

$$W_S^* = \left[I \,\vdots\, B \right]. \tag{3.56}$$

We store the new column order in an index set $\mathcal{I}_S$. Then, the null space of W_S^* is simply $Z_S^* := \begin{bmatrix} -B \\ \hdashline I \end{bmatrix}$. Finally, we find Z_S by defining $Z_S(\mathcal{I}_S) := Z_S^*$, that is, reordering the rows of Z_S^* such that row $\mathcal{I}_S(j)$ of Z_S is the same as row j of Z_S^*. This process is outlined in the algorithm below.

Input: W_S, Γ
Output: Z_S

begin
  rows $\leftarrow$ Rows(Γ)
  cols $\leftarrow$ Columns(Γ)
  $\mathcal{I}_S \leftarrow \begin{bmatrix} 1 & 2 & \dots & \text{cols} \end{bmatrix}$
  for i **from** 1 **to** rows
    Identify column j where the first 1 appears in row i
    $W_S \leftarrow$ *Insert column j in place of column i, shifting the rest forward one column*
    $\mathcal{I}_S \leftarrow$ *Insert element j in place of position i, shifting the rest forward one position*
  end
  $B \leftarrow W_S$(1:rows,rows+1:cols)
  $Z_S^* \leftarrow \begin{bmatrix} -B \\ \hdashline I \end{bmatrix}$
  $Z_S(\mathcal{I}_S) \leftarrow Z_S^*$
end

Algorithm 3.17: Stochastic null space algorithm.

When using stochastic constraints $\mathcal{S}_{\mathbf{x}}$ instead of $\mathcal{DS}_{\mathbf{x}}$ constraints, we can also use an easier scaling algorithm that simply normalises each row of the probability transition matrix $P(\mathbf{x})$ (see 3.14). However, despite the simpler null space which permits quicker calculations, and the simpler scaling algorithm, we found that DIPA performed far worse in most nontrivial cases when we used the stochastic constraints instead of the doubly-stochastic constraints. We propose that this is due to the fact that $\mathcal{S}$ is, typically, a much larger domain than $\mathcal{DS}_{\mathbf{x}}$ and could contain many more local minima.

3.4.3 Diagonal scaling

We use Algorithm 3.13 after deflations and deletions are performed to find a feasible point in the vicinity of the now infeasible $\mathbf{x}$. We also use Algorithm 3.13 to find an initial feasible point. One other well-known method of finding such a feasible point, given an infeasible $\mathbf{x}$, is the method of diagonal scaling known as Sinkhorn's algorithm [52].

To use Sinkhorn's algorithm on the infeasible $\mathbf{x}$, we consider the equivalent probability transition matrix $P(\mathbf{x})$ (see (3.14)). Then we normalise each row, followed by normalising each column. We achieve this by pre-multiplying and post-multiplying $P(\mathbf{x})$ by diagonal matrices of the following form, where r_i is the i-th row sum of $P(\mathbf{x})$, and c_j is the j-th column sum of $P(\mathbf{x})$

$$\begin{aligned} D_1 &= \begin{bmatrix} c_1 & & & & \\ & c_2 & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & c_N \end{bmatrix}, \\ D_2 &= \begin{bmatrix} r_1 & & & & \\ & r_2 & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & r_N \end{bmatrix}. \end{aligned} \tag{3.57}$$

Thus, we update $P(\mathbf{x})$ by calculating $P(\mathbf{x}) = D_1 P(\mathbf{x}) D_2$. The resulting $P(\mathbf{x})$ is less infeasible than the original $P(\mathbf{x})$.

We repeat this process as many times as necessary. It is known [3] that using this process ensures that $P(\mathbf{x})$ converges to a probability transition matrix in $\mathcal{DS}_{\mathbf{x}}$, and experimentally we found that this process converged quickly in most cases. Overall, however, we found the linear solver method used in Algorithm 3.13 to be more reliable and efficient, and hence we chose not to use diagonal scaling.

3.5 The unique saddle-point conjecture

In early implementations of DIPA, we only used descent directions. For each graph tested, we started from many randomly generated starting points, and in each case DIPA converged either to a point on the boundary of the feasible region, or more commonly, to a particular strictly interior stationary (saddle) point.

We repeated this experiment on many cubic graphs and some larger non-regular graphs, and in each case it appeared that there was a unique interior stationary point for each graph. These experimental findings led to the following, still open, conjecture. Recall that for any graph Γ the nonlinear program (3.19) has the following form

$$\min\{-\det(I - P(\mathbf{x}) + \tfrac{1}{N}J)\}$$
$$\text{s.t.}$$
$$x_{ij} \geq 0, \quad (i,j) \in \Gamma,$$
$$\sum_{j \in \mathcal{A}(i)} x_{ij} = 1, \quad i = 1, \ldots, N,$$
$$\sum_{i \in \mathcal{B}(j)} x_{ij} = 1, \quad j = 1, \ldots, N.$$

Conjecture 3.5.1 *The nonlinear program (3.19) has exactly one strictly interior stationary point, and it is a saddle point. We call this point $\mathbf{x}^M$, or equivalently $P^M := P(\mathbf{x}^M)$.*

If Conjecture 3.5.1 is true, it implies that, for all graphs Γ, there are no strictly interior local minima in (3.19). Then, given any strictly interior starting point $\mathbf{x}^0$, DIPA as described in Algorithm 3.16: DIPA is guaranteed to converge to a boundary point.

For a small percentage of cubic graphs tested, we found that $P^M = \frac{1}{3}\mathbb{A}$ (recall that $\mathbb{A}$ is the adjacency matrix of Γ). For example, this is the case for 5 of the 85 cubic 12-node graphs. This poses a problem since, for these rare cubic graphs, the barrier point $P(\mathbf{x}^*_{\mathcal{L}})$, which we use as the starting point of the main iterations in Algorithm 3.16: DIPA, is $\frac{1}{3}\mathbb{A}$, which is the interior stationary point P^M. In general, it is considered unusual for the starting point to also be a stationary point. In the case when $P(\mathbf{x}^*_{\mathcal{L}}) = P^M$, Algorithm 3.6 gives $\mathbf{d} = \mathbf{0}$, and consequently we require Algorithm 3.7 to move away from the stationary point.

We calculated P^M for every cubic graph up to size 20, and for 500 randomly generated non-regular graphs of random sizes less than 100. In each case, we found that P^M is a symmetric matrix in $\mathcal{DS}_{\mathbf{x}}$, and almost always contains non-zero values in the interval [0.20.45]. In some small graphs we can find P^M explicitly.

Example 3.5.2 *In the 6-node cubic graph* Γ_6 *defined by the following adjacency matrix*

$$\mathbb{A}_6 = \begin{bmatrix} 0 & 1 & 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 & 1 & 0 \end{bmatrix}, \tag{3.58}$$

we can find P_6^M *exactly:*

$$P_6^M = \begin{bmatrix} 0 & \frac{2\sqrt{6}-3}{5} & 0 & \frac{4-\sqrt{6}}{5} & \frac{4-\sqrt{6}}{5} & 0 \\ \frac{2\sqrt{6}-3}{5} & 0 & \frac{4-\sqrt{6}}{5} & 0 & 0 & \frac{4-\sqrt{6}}{5} \\ 0 & \frac{4-\sqrt{6}}{5} & 0 & \frac{2\sqrt{6}-3}{5} & 0 & \frac{4-\sqrt{6}}{5} \\ \frac{4-\sqrt{6}}{5} & 0 & \frac{2\sqrt{6}-3}{5} & 0 & \frac{4-\sqrt{6}}{5} & 0 \\ \frac{4-\sqrt{6}}{5} & 0 & 0 & \frac{4-\sqrt{6}}{5} & 0 & \frac{2\sqrt{6}-3}{5} \\ 0 & \frac{4-\sqrt{6}}{5} & \frac{4-\sqrt{6}}{5} & 0 & \frac{2\sqrt{6}-3}{5} & 0 \end{bmatrix}. \tag{3.59}$$

We also performed experiments on all cubic graphs up to size 20 to see if the entries in P^M were invariant when we relabeled the nodes of the graphs. In every example tested it was found that the entries of P^M were indeed invariant. This finding leads us to speculate that the P^M point may be able to solve the famous graph isomorphism problem [51], if the following (open) Conjecture 3.5.3 is true. Two graphs Γ_1 and Γ_2, with adjacency matrices $\mathbb{A}_1$ and $\mathbb{A}_2$ respectively, are *isomorphic* if a permutation matrix Π can be found such that $\mathbb{A}_1 = \Pi^{-1}\mathbb{A}_2\Pi$. That is, if one graph can be shown to be the relabeling of the other. The graph isomorphism problem can then be stated simply: given two graphs Γ_1 and Γ_2, determine if the graphs are isomorphic.

Conjecture 3.5.3 *Consider two cubic graphs* Γ_1 *and* Γ_2*, their associated adjacency matrices* $\mathbb{A}_1$ *and* $\mathbb{A}_2$*, and the associated strictly interior stationary points* P_1^M *and* P_2^M*. Let* $H_1(P_1^M)$ *and* $H_2(P_2^M)$ *be the Hessians of* $f(\mathbf{x})$ *at each of these points, respectively. Let* Λ_1 *and* Λ_2 *be diagonal matrices with eigenvalues of* $H_1(P_1^M)$ *and* $H_2(P_2^M)$ *in their diagonals, respectively. Then,* $\Lambda_1 = \Lambda_2$ *if and only if* $\mathbb{A}_1 = \Pi^{-1}\mathbb{A}_2\Pi$ *for some permutation matrix* Π*. That is, the spectra are equal if and only if* Γ_1 *is an isomorphism of* Γ_2*.*

We have numerically verified Conjecture 3.5.3 for all cubic graphs up to and including size $N = 18$. This set includes a total of 45,982 graphs. We tested the conjecture by finding the spectra of the Hessian evaluated at P^M for each graph and comparing them to see if any were the same. We found no counterexamples for any of the tested graphs. For 1000 randomly selected cubic graphs up to size 20, we also considered random permutations of these graphs. We compared the spectra of these relabeled graphs to that of their original graphs to confirm that the spectra were the same, and again, no counterexample was found. Finally, we obtained a list of all cospectral pairs of cubic graphs with 20 nodes, that is, pairs of graphs for which the spectra of their adjacency matrices are equal. There are 5195 such cubic 20-node cospectral pairs. Since these cospectral pairs are indistinguishable by their spectra, we tested the above conjecture on these pairs, and found that it held for all cubic 20-node cospectral pairs.

While we only give Conjecture 3.5.3 for cubic graphs (as the bulk of our experiments have been carried out on cubic graphs), there is no experimental evidence as of yet that the conjecture does not hold for other graphs as well. We generated many non-regular graphs of sizes up to $N = 100$, and tested them using the above method, and again no counterexample was found.

The importance of Conjecture 3.5.3 is that the graph isomorphism problem was listed in Garey and Johnson [30] p. 285 as one of only twelve problems to belong to the NP set of problems that was not known at the time to be NP-complete. To this day, it is one of only two of those twelve problems whose complexity remains unknown, even if we restrict the problem to cubic graphs. If Conjectures 3.5.1 and 3.5.3 are proved, we immediately obtain that the graph isomorphism problem is equivalent to solving two Karush-Kuhn-Tucker (KKT) systems for (3.19), one for each graph. That is, the graph isomorphism problem for cubic graphs is equivalent to the problem of solving two systems of $O(N)$ algebraic equations with maximum degree N, and $3N$ nonnegativity constraints. If Conjecture 3.5.3 is proved for all graphs, then we can make similar claims about the graph isomorphism problem for all graphs.

Experimentally, we found that by selecting an initial (infeasible) point $\mathbf{x}_0 = \mathbf{e}$, and using the MATLAB function fsolve to solve the KKT system without any nonnegativity constraints, the outputted solution was always P^M in all graphs we tested. The function fsolve uses a Gauss-Newton method (see [12] pp 269 – 312). A future direction of research will be to determine if this method always finds P^M, and to design an adaptation of the Gauss-Newton methods specifically to find P^M.

3.6 LU decomposition

3.6.1 Introduction

Recall the definitions of $P(\mathbf{x})$, $\mathcal{DS}_{\mathbf{x}}$ and $f(P(\mathbf{x}))$ from (3.14)–(3.18). That is, $P(\mathbf{x})$ is composed of elements p_{ij} such that

$$p_{ij}(\mathbf{x}) \quad := \quad \begin{cases} x_{ij}, & (i,j) \in \Gamma, \\ 0, & \text{otherwise}, \end{cases} \tag{3.60}$$

$\mathcal{DS}_{\mathbf{x}}$ is the set of all $\mathbf{x}$ that satisfy

$$x_{ij} \geq 0, \quad (i,j) \in \Gamma, \tag{3.61}$$

$$\sum_{j \in \mathcal{A}(i)} x_{ij} = 1, \quad i = 1, \ldots, N, \tag{3.62}$$

$$\sum_{i \in \mathcal{B}(j)} x_{ij} = 1, \quad j = 1, \ldots, N, \tag{3.63}$$

and $f(P(\mathbf{x}))$ is defined as

$$f(\mathbf{x}) \quad = \quad -\det(I - P(\mathbf{x}) + \frac{1}{N}J). \tag{3.64}$$

We then define $A(P(\mathbf{x}))$ such that $f(P(\mathbf{x})) = -\det(A(P(\mathbf{x})))$. That is,

$$A(P(\mathbf{x})) \quad = \quad I - P(\mathbf{x}) + \frac{1}{N}\mathbf{e}\mathbf{e}^T. \tag{3.65}$$

In Sections 3.2 – 3.4, we outline an interior point method that attempts to solve the optimisation problem $\{min f(P(\mathbf{x})) | \mathbf{x} \in \mathcal{DS}_{\mathbf{x}}\}$. In our interior point method, a second-order approximation to the objective function $f(P(\mathbf{x}))$ is required at each iteration. This approximation requires us to evaluate the objective function value, the gradient and the Hessian at each iteration. Evaluating these directly is a slow process, as the Hessian matrix of $f(P(\mathbf{x}))$ is dense, and each element of the Hessian matrix is itself a determinant.

An efficient method of calculating the determinant of a matrix G is to perform an LU decomposition to find $G = LU$ and then calculate $\det(G) = \det(L)\det(U)$. Generally, for a determinant objective function, we need to calculate each element in the Hessian matrix by performing a separate LU decomposition. However, this requires $O(N^4)$ individual LU decompositions. In this section we demonstrate how the objective function value, the gradient vector and the Hessian matrix, required in Algorithm 3.16: DIPA, are evaluated using only a single LU decomposition of the negative generator matrix $G(\mathbf{x}) = I - P(\mathbf{x})$. For ease of notation, and when no confusion can arise, we drop the dependency on $\mathbf{x}$ in $P(\mathbf{x})$ for the remainder of this chapter.

In [36] it is proven that such an LU decomposition exists (without requiring prior permutations) for any generator matrix where P is doubly-stochastic and contains only a single ergodic class. For connected graphs, these conditions are satisfied for all doubly-stochastic P in the interior of $\mathcal{DS}_{\mathbf{x}}$, which makes up the entire domain of points that can be reached by Algorithm 3.16: DIPA. We note that P^H corresponding to a Hamiltonian cycle is also doubly-stochastic and has a single ergodic class. However, such a P^H is an extreme point of $\mathcal{DS}_{\mathbf{x}}$ and is only approached - but never attained - by the sequence of points generated by Algorithm 3.16: DIPA.

The process of evaluating the second-order approximation is the most time-consuming part of the inner-step iteration in Algorithm 3.16: DIPA. Therefore, an improvement in the calculation time of the objective function value, gradient and Hessian leads to a similar improvement in DIPA.

3.6.2 Product forms of $A(P)$ and $\det(A(P))$

To calculate the objective function $f(P)$, its gradient and Hessian, we begin by performing an LU decomposition to obtain

$$LU \quad = \quad G = I - P. \tag{3.66}$$

By construction of L and U we know that $\det(L) = 1$ (eg, see Golub and Van Loan [34] p. 97). As the method we describe in this section is used in the implementation of DIPA, described in Sections 3.2 – 3.4, we assume for the remainder of this chapter that $P \in \mathrm{Int}\,(\mathcal{DS}_{\mathbf{x}})$. This assumption ensures that the policy corresponding to P has a single ergodic class. Therefore, G has exactly one zero eigenvalue, which along with the nonsingularity of L implies that U has exactly one eigenvalue of zero. Since U is upper triangular and has its eigenvalues on its diagonal entries, it follows from the standard implementation of the LU-decomposition algorithm (e.g., see Golub and Van Loan [34] pp. 96–97) that $u_{NN} = 0$. Then, we know that

$$A(P) \quad = \quad I - P + \frac{1}{N}\mathbf{e}\mathbf{e}^T = LU + \frac{1}{N}\mathbf{e}\mathbf{e}^T. \tag{3.67}$$

We factorise this expression so as to calculate $\det(A)$ by finding the product of determinants of the factors. In particular, the following result is proved in this subsection:

$$\det(A(P)) \quad = \quad N \prod_{i=1}^{N-1} u_{ii}, \tag{3.68}$$

where u_{ii} is the i-th diagonal entry of U.

The outline of the derivation of (3.68) is as follows.

(1) We express A(P) as the product of three nonsingular factors.

(2) We show that two of these factors have a determinant of 1.

(3) We show that the third factor shares all but one eigenvalue with U, with the single different eigenvalue being N (rather than 0).

(4) We express the determinant as a product of the first $N-1$ diagonal elements of U, and N.

First, we express $A(P)$ as a product of L and another factor. Let $\mathbf{v}$ be an $N \times 1$ vector, and $\bar{U}$ be an $N \times N$ matrix, such that

$$L\mathbf{v} = \mathbf{e}, \quad \text{and} \qquad \bar{U} := U + \mathbf{v}\mathbf{e}_N^T, \tag{3.69}$$

where $\mathbf{e}_N^T = \begin{bmatrix} 0 & \cdots & 0 & 1 \end{bmatrix}$. Since L is nonsingular, $\mathbf{v}$ exists and is unique, and therefore $\bar{U}$ is well-defined. Note that with the exception of the last column (that coincides with $\mathbf{v}$), all other columns of $\mathbf{v}\mathbf{e}_N^T$ are identically equal to the $\mathbf{0}$ vector.

Hence, suppressing (the fixed) argument P in $A(P)$, and exploiting (3.67) and (3.69) we write

$$\begin{aligned} A &= (I-P) + \frac{1}{N}\mathbf{e}\mathbf{e}^T \\ &= LU + \frac{1}{N}L\mathbf{v}\mathbf{e}^T \\ &= L(U + \frac{1}{N}\mathbf{v}\mathbf{e}^T) \\ &= L(\bar{U} + \mathbf{v}[\frac{1}{N}\mathbf{e}^T - \mathbf{e}_N^T]). \end{aligned} \tag{3.70}$$

Since U is upper-triangular, and the addition of $\mathbf{v}\mathbf{e}_N^T$ alters only the rightmost column of U, it follows that $\bar{U}$ is also upper-triangular. Therefore

$$\det \bar{U} = \prod_{i=1}^{N} \bar{u}_{ii} = \left(\prod_{i=1}^{N-1} u_{ii} \right) \bar{u}_{NN}. \tag{3.71}$$

Since $u_{NN} = 0$, we know that $\bar{u}_{NN} = \mathbf{e}_N^T \left(\mathbf{v}\mathbf{e}_N^T\right) \mathbf{e}_N = \mathbf{e}_N^T\mathbf{v}\left(\mathbf{e}_N^T\mathbf{e}_N\right) = \mathbf{e}_N^T\mathbf{v}$, which is the bottom-right element of $\mathbf{v}\mathbf{e}_N^T$.

Lemma 3.6.1 *For any $P \in Int(\mathcal{DS}_\mathbf{x})$, both $(I - P + \mathbf{e}\mathbf{e}_N^T)$ and $\bar{U}$ are nonsingular.*

Proof. Note that

$$L\bar{U} = LU + L\mathbf{v}\mathbf{e}_N^T = I - P + \mathbf{e}\mathbf{e}_N^T, \tag{3.72}$$

and hence

$$\bar{U} \;=\; L^{-1}\left(I - P + \mathbf{e}\mathbf{e}_N^T\right). \tag{3.73}$$

We know that $\det\left(L^{-1}\right) = 1$, so if $\left(I - P + \mathbf{e}\mathbf{e}_N^T\right)$ is nonsingular then $\bar{U}$ will be nonsingular as well. We show that this is the case for an irreducible P.

Suppose that $\left(I - P + \mathbf{e}\mathbf{e}_N^T\right)$ is singular. Then there exists $\alpha = \left[\begin{array}{ccc} \alpha_1, & \dots, & \alpha_N \end{array}\right]^T \neq \mathbf{0}^T$ such that $\left(I - P + \mathbf{e}\mathbf{e}_N^T\right)\alpha = \mathbf{0}$. Therefore

$$(I - P)\alpha + \alpha_N \mathbf{e} \;=\; \mathbf{0}, \tag{3.74}$$

where α_N is the N-th (and final) entry of α. There are then two possibilities: either $\alpha_N \neq 0$ or $\alpha_N = 0$. First, we consider the case where $\alpha_N \neq 0$. We then divide (3.74) by $-\alpha_N$ to obtain

$$(I - P)\bar{\alpha} = \mathbf{e}, \tag{3.75}$$

where $\bar{\alpha} = \dfrac{-\alpha}{\alpha_N}$. Then, because P is irreducible, there exists $\pi^T > 0$, such that $\sum\limits_{j=1}^{N} \pi_j = 1$ and $\pi^T = \pi^T P$. Multiplying (3.75) on the left by π^T we obtain

$$\pi^T (I - P)\bar{\alpha} \;=\; \pi^T \mathbf{e},$$

and therefore, $0 = 1$. This is a contradiction, so $\alpha_N = 0$. Substituting this into (3.74) yields

$$P\alpha = \alpha. \tag{3.76}$$

Therefore, α is an eigenvector of P, corresponding to eigenvalue $\lambda = 1$, but by the irreducibility of P, we know that the multiplicity of eigenvalue $\lambda = 1$ is 1. Since we also know that $P\mathbf{e} = \mathbf{e}$, this implies that $\alpha = c\mathbf{e}$ for some constant c.

But $\alpha_N = 0$, so $\alpha = \mathbf{0}$, which is not a valid eigenvector, and therefore this is a contradiction as well. Hence $\left(I - P + \mathbf{e}\mathbf{e}_N^T\right)$ is nonsingular, as required. Then, from (3.73) and the above, we also see that $\det \bar{U} \neq 0$, which concludes the proof. □

Lemma 3.6.2 *For any $P \in Int(\mathcal{DS}_{\mathbf{x}})$, the bottom-right element of the matrix $\mathbf{v}\mathbf{e}_N^T$ is N. That is, $\mathbf{e}_N^T\mathbf{v} = N$.*

Proof. As $\bar{U}^{-1}$ exists, it follows from (3.73) that

$$L = \left(I - P + \mathbf{e}\mathbf{e}_N^T\right)\bar{U}^{-1},$$

and therefore,

$$\begin{aligned}\mathbf{e}^T L &= \mathbf{e}^T \left(I - P + \mathbf{e}\mathbf{e}_N^T\right)\bar{U}^{-1} \\ &= \mathbf{e}^T (I-P)\bar{U}^{-1} + \mathbf{e}^T\mathbf{e}\mathbf{e}_N^T\bar{U}^{-1}.\end{aligned}$$

From the column-sum $\mathcal{DS}_{\mathbf{x}}$ constraint (3.63) we know that $\mathbf{e}^T(I-P) = \mathbf{0}^T$. Therefore,

$$\mathbf{e}^T L = N\mathbf{e}_N^T\bar{U}^{-1}.$$

Since $\bar{U}$ is upper-triangular, $\bar{U}^{-1}$ is also upper-triangular and therefore

$$\mathbf{e}^T L = N\tilde{u}_{NN}\mathbf{e}_N^T, \tag{3.77}$$

where $\tilde{u}_{NN}$ is the bottom-right entry of $\bar{U}^{-1}$.

Then, because L is lower-triangular, $\mathbf{e}^T L\mathbf{e}_N = 1$. Thus, from (3.77), we see that

$$\begin{aligned}1 = \mathbf{e}^T L\mathbf{e}_N &= N\tilde{u}_{NN}\mathbf{e}_N^T\mathbf{e}_N \\ &= N\tilde{u}_{NN}, \end{aligned}\tag{3.78}$$

and therefore,

$$\tilde{u}_{NN} = \frac{1}{N}. \tag{3.79}$$

Substituting (3.79) into (3.77), we obtain $\mathbf{e}^T L = \mathbf{e}_N^T$, and multiplying both sides by $\mathbf{v}$ and recalling that $L\mathbf{v} = \mathbf{e}$, we obtain

$$N = \mathbf{e}_N^T\mathbf{v}.$$

Therefore, the bottom-right element of $\mathbf{v}\mathbf{e}_N^T$ is N, and since the bottom-right element of U is 0, we can then deduce from the definition of $\bar{U}$ (3.69) that its bottom-right element is N. □

Next, we define $\mathbf{w}$ to be the unique solution to the system

$$\bar{U}^T \mathbf{w} \;=\; \frac{1}{N}\mathbf{e} - \mathbf{e}_N, \tag{3.80}$$

which is well-defined by Lemma 3.6.1. Then, from (3.70)

$$\begin{aligned} A &= L\left(\bar{U} + \mathbf{v}\left[\frac{1}{N}\mathbf{e}^T - \mathbf{e}_N^T\right]\right) \\ &= L\left(\bar{U} + \mathbf{v}\mathbf{w}^T\bar{U}\right) \\ &= L\left(I + \mathbf{v}\mathbf{w}^T\right)\bar{U}. \end{aligned} \tag{3.81}$$

We take the determinant of (3.81) to obtain

$$\det(A) \;=\; \det(L)\det(I + \mathbf{v}\mathbf{w}^T)\det(\bar{U}). \tag{3.82}$$

Note that, for any vectors $\mathbf{c}$ and $\mathbf{d}$,

$$\det(I + \mathbf{c}\mathbf{d}^T) \;=\; 1 + \mathbf{d}^T\mathbf{c}. \tag{3.83}$$

This is because $\mathbf{c}\mathbf{d}^T$ has one eigenvalue $\mathbf{d}^T\mathbf{c}$ of multiplicity 1 and an eigenvalue 0 of multiplicity $N-1$. Consequently,

$$\det(I + \mathbf{v}\mathbf{w}^T) \;=\; 1 + \mathbf{w}^T\mathbf{v}, \tag{3.84}$$

which we substitute into expression (3.82) above.

Lemma 3.6.3 *For any $P \in \mathcal{DS}_{\mathbf{x}}$, the inner-product $\mathbf{w}^T\mathbf{v}$, where $\mathbf{w}$ and $\mathbf{v}$ are defined by (3.80) and (3.69) respectively, satisfies*

$$\mathbf{w}^T\mathbf{v} \;=\; 0.$$

Proof. We know that both L and $\bar{U}$ are non-singular, so we find $\mathbf{w}^T$ and $\mathbf{v}$ directly. In particular, from their respective definitions (3.80) and (3.69),

$$\mathbf{w}^T \;=\; \left(\frac{1}{N}\mathbf{e}^T - \mathbf{e}_N^T\right)(\bar{U})^{-1}, \tag{3.85}$$

$$\mathbf{v} \;=\; L^{-1}\mathbf{e}. \tag{3.86}$$

Then, from (3.85)–(3.86) and (3.72), we obtain

$$\begin{aligned}
\mathbf{w}^T\mathbf{v} &= \left(\frac{1}{N}\mathbf{e}^T - \mathbf{e}_N^T\right)(\bar{U})^{-1}L^{-1}\mathbf{e} \\
&= \left(\frac{1}{N}\mathbf{e}^T - \mathbf{e}_N^T\right)(L\bar{U})^{-1}\mathbf{e} \\
&= \left(\frac{1}{N}\mathbf{e}^T - \mathbf{e}_N^T\right)(I - P + \mathbf{e}\mathbf{e}_N^T)^{-1}\mathbf{e}. \qquad (3.87)
\end{aligned}$$

Since I, P and $\mathbf{e}\mathbf{e_N}^T$ are all stochastic matrices, we know that $I - P + \mathbf{e}\mathbf{e}_N^T$ has row sums of 1 as well. Hence, its inverse also has row sums equal to 1, that is,

$$(I - P + \mathbf{e}\mathbf{e}_N^T)^{-1}\mathbf{e} \;=\; \mathbf{e}. \qquad (3.88)$$

Substituting (3.88) into (3.87), we obtain

$$\mathbf{w}^T\mathbf{v} = \left(\frac{1}{N}\mathbf{e}^T - \mathbf{e}_N^T\right)\mathbf{e} = 0.$$

which concludes the proof. □

We now derive the main theorem of this subsection.

Theorem 3.6.4 *For any $P \in Int(\mathcal{DS}_{\mathbf{x}})$ and $I - P = LU$, where L and U form the LU-decomposition,*

$$\det(A(P)) \;=\; N\left(\prod_{i=1}^{N-1} u_{ii}\right).$$

Proof. From (3.82), (3.84) and Lemma 3.6.3 we know that

$$\det(A(P)) \;=\; \det(L)(1+0)\det(\bar{U}).$$

From the construction of LU decomposition we know that $\det(L) = 1$, so

$$\det(A(P)) \;=\; \det(\bar{U}).$$

From (3.71) and Lemma 3.6.2 we now see that

$$\det(A(P)) \;=\; \det(\bar{U}) = N\left(\prod_{i=1}^{N-1} u_{ii}\right).$$

This concludes the proof. □

Remark 3.6.5 *Note that finding* $\mathbf{v}$ *and* $\mathbf{w}$ *is a simple process because* L *and* $\bar{U}^T$ *are lower-triangular matrices, so we can solve the systems of linear equations in (3.80) and (3.69) directly. Note also that in DIPA, we are not interested in calculating* $\det(A(P))$*, but rather* $f(P) = -\det(A(P))$*.*

3.6.3 Finding the gradient *g(P)*

Next we use the LU decomposition found in Subsection 3.6.2 to find the gradient of $f(P) = -\det(A(P))$. Note that since variables of $f(P)$ are entries x_{ij} of the probability transition matrix $P(\mathbf{x})$, we derive an expression for $g_{ij}(P) := \frac{\partial f(P)}{\partial x_{ij}}$ for each x_{ij} such that $(i,j) \in \Gamma$.

Consider vectors $\mathbf{a}_j$ and $\mathbf{b}_i$ satisfying the equations $\bar{U}^T\mathbf{a}_j = \mathbf{e}_j$ and $L\mathbf{b}_i = \mathbf{e}_i$. Then, we define $Q := I - \mathbf{v}\mathbf{w}^T$, where $\mathbf{v}$ and $\mathbf{w}^T$ are as in (3.85)–(3.86). We prove the following result in this subsection:

$$g_{ij}(P) = \det(A(P))(\mathbf{a}_j^T Q\mathbf{b}_i), \tag{3.89}$$

where $g_{ij}(P)$ is the element of the gradient vector corresponding to the arc $(i,j) \in \Gamma$.

The outline of the derivation of (3.89) is as follows.

(1) We represent each element $g_{ij}(P)$ of the gradient vector as a cofactor of $A(P)$.

(2) We construct an elementary matrix that transforms matrix $A(P)$ into a matrix with determinant equal to the above cofactor of $A(P)$.

(3) We then express the element $g_{ij}(P)$ of the gradient vector as the product of $\det(A(P))$ and the determinant of the elementary matrix, the latter of which is shown to be equal to $\mathbf{a}_j^T Q\mathbf{b}_i$.

For any matrix $V = (v_{ij})_{i,j=1}^{N,N}$ it is well-known (e.g., see May [43]) that $\dfrac{\partial \det(V)}{\partial v_{ij}} = (-1)^{i+j}\det(V^{ij})$, where V^{ij} is the (i,j)-th minor of V. That is, $\dfrac{\partial \det(V)}{\partial v_{ij}}$ is the (i,j)-th cofactor of V. Since the (i,j)-th entry of $A(P)$ is simply $a_{ij} = \delta_{ij} - x_{ij} + \frac{1}{N}$, it now follows that

$$g_{ij}(P) = \frac{\partial f(P)}{\partial x_{ij}} = \frac{\partial \left[-\det A(P)\right]}{\partial a_{ij}} \frac{da_{ij}}{dx_{ij}} = (-1)^{i+j} \det\left(A^{ij}(P)\right). \tag{3.90}$$

Rather than finding the cofactor, however, we calculate (3.90) by finding the determinant of A where row i has been replaced with $\mathbf{e}_j^T$. Since A is a full-rank matrix, it is possible to perform row operations to achieve this. Suppose A is composed of rows $\mathbf{r}_1^T$, $\mathbf{r}_2^T$, ..., $\mathbf{r}_N^T$. Then, we perform the following row operation:

$$\mathbf{r}_i^T \quad \rightarrow \quad \alpha_j(1)\mathbf{r}_1^T + \alpha_j(2)\mathbf{r}_2^T + \ldots + \alpha_j(N)\mathbf{r}_N^T, \tag{3.91}$$

where $\alpha_j(i)$ is the i-th element of vector α_j and $A^T\alpha_j = \mathbf{e}_j$.

In this case, from (3.81), $A^T = \bar{U}^T(I + \mathbf{w}\mathbf{v}^T)L^T$. Since A is nonsingular when $P \in \mathrm{Int}(\mathcal{DS}_{\mathbf{x}})$, α_j can be found directly:

$$\begin{aligned} \alpha_j &= \left(A^T\right)^{-1}\mathbf{e}_j \\ &= \left[\bar{U}^T(I + \mathbf{w}\mathbf{v}^T)L^T\right]^{-1}\mathbf{e}_j \\ &= (L^T)^{-1}(I + \mathbf{w}\mathbf{v}^T)^{-1}(\bar{U}^T)^{-1}\mathbf{e}_j. \end{aligned} \tag{3.92}$$

Lemma 3.6.6 *For any $P \in \mathcal{DS}_{\mathbf{x}}$,*

$$\left(I + \mathbf{w}\mathbf{v}^T\right)^{-1} \quad = \quad I - \mathbf{w}\mathbf{v}^T.$$

Proof. Consider

$$\begin{aligned} (I + \mathbf{w}\mathbf{v}^T)(I - \mathbf{w}\mathbf{v}^T) &= I - \mathbf{w}\mathbf{v}^T + \mathbf{w}\mathbf{v}^T - \mathbf{w}\mathbf{v}^T\mathbf{w}\mathbf{v}^T \\ &= I - \mathbf{w}\mathbf{v}^T\mathbf{w}\mathbf{v}^T \\ &= I, \text{ because } \mathbf{v}^T\mathbf{w} = \mathbf{w}^T\mathbf{v} = 0, \qquad \text{from Lemma 3.6.3.} \end{aligned}$$

Therefore, $\left(I + \mathbf{w}\mathbf{v}^T\right)^{-1} = \left(I - \mathbf{w}\mathbf{v}^T\right)$. □

Taking the above result and substituting into (3.92), we obtain

$$\alpha_j \quad = \quad (L^T)^{-1}(I - \mathbf{w}\mathbf{v}^T)(\bar{U}^T)^{-1}\mathbf{e}_j. \tag{3.93}$$

Next, we define an elementary matrix E_{ij} by

$$E_{ij} \quad := \quad I - \mathbf{e}_i\mathbf{e}_i^T + \mathbf{e}_i\alpha_j^T, \tag{3.94}$$

and note that it performs the desired row operation (3.91) on A because

$$E_{ij}A \quad = \quad A - \mathbf{e}_i\mathbf{r}_i^T + \mathbf{e}_i\mathbf{e}_j^T,$$

in effect replacing the i-th row of A with $\mathbf{e}_j^T$. Therefore,

$$\begin{aligned} g_{ij}(P) &= (-1)^{i+j}\det\left(A^{ij}\right) \\ &= \det(E_{ij}A) \\ &= \det(E_{ij})\det(A). \end{aligned} \tag{3.95}$$

From (3.94), we rewrite $E_{ij} = I - \mathbf{e}_i(\mathbf{e}_i - \alpha_j)^T$. Then, from (3.83) we obtain

$$\begin{aligned} \det(E_{ij}) &= 1 - (\mathbf{e}_i - \alpha_j)^T\mathbf{e}_i \\ &= 1 - \mathbf{e}_i^T\mathbf{e}_i + \alpha_j^T\mathbf{e}_i \\ &= 1 - 1 + \alpha_j^T\mathbf{e}_i \\ &= \alpha_j^T\mathbf{e}_i. \end{aligned} \tag{3.96}$$

Substituting (3.93) into (3.96) we obtain

$$\det(E_{ij}) \quad = \quad \mathbf{e}_j^T(\bar{U})^{-1}(I - \mathbf{v}\mathbf{w}^T)(L)^{-1}\mathbf{e}_i. \tag{3.97}$$

For convenience we define $Q := I - \mathbf{v}\mathbf{w}^T$. Then

$$\det(E_{ij}) \quad = \quad \mathbf{a}_j^T Q\mathbf{b}_i, \quad \text{where } \bar{U}^T\mathbf{a}_j = \mathbf{e}_j \text{ and } L\mathbf{b}_i = \mathbf{e}_i. \tag{3.98}$$

We now derive the main result of this subsection.

Proposition 3.6.7 *For any $P \in Int(\mathcal{DS}_\mathbf{x})$ and $I - P = LU$, where L and U form the LU-decomposition; the general gradient element of $f(P)$ is given by*

$$g_{ij}(P) = \frac{\partial f(P)}{\partial x_{ij}} \quad = \quad \det(A(P))(\mathbf{a}_j^T Q\mathbf{b}_i). \tag{3.99}$$

Proof. Substituting (3.98) into (3.95) immediately yields the result. □

Remark 3.6.8 *Note that we can calculate all* $\mathbf{a}_j$ *and* $\mathbf{b}_i$ *in advance, by solving the systems of linear equations in (3.98), again in reduced row echelon form. Then, for the sake of efficiency we first calculate*

$$\hat{\mathbf{q}}_j^T \ := \ \mathbf{a}_j^T Q, \quad j = 1, \ldots, N, \tag{3.100}$$

and then calculate

$$\hat{q}_{ij} \ := \ \hat{\mathbf{q}}_j^T \mathbf{b}_i, \quad i = 1, \ldots, N, \quad j = 1, \ldots, N. \tag{3.101}$$

This allows us to rewrite the formula for $g_{ij}(P)$ *as*

$$g_{ij}(P) = -f(P)\hat{q}_{ij}.$$

3.6.4 Finding the Hessian matrix *H(P)*

Here, we show that the LU decomposition found in Subsection 3.6.2 can also be used to calculate the Hessian of $f(P)$ more efficiently. Consider g_{ij} and $\hat{q}_{ij}$ as defined in (3.99) and (3.101) respectively. We prove the following result in this subsection:

$$H_{[ij],[k\ell]}(P) := \frac{\partial^2 f(P)}{\partial x_{ij} \partial x_{k\ell}} = g_{kj}\hat{q}_{i\ell} - g_{ij}\hat{q}_{k\ell},$$

where $H_{[ij],[k\ell]}$ is the general element of the Hessian matrix corresponding to arcs (i,j) and $(k,\ell) \in \Gamma$.

The outline of the derivation is as follows.

(1) We represent each element $H_{[ij],[k\ell]}(P)$ of the Hessian matrix as a cofactor of a minor of $A(P)$.

(2) We construct a second elementary matrix that in conjunction with E_{ij} (see (3.94)) transforms matrix $A(P)$ into one with a determinant equivalent to the (k,ℓ)-th cofactor of $A^{ij}(P)$.

(3) We then show that the general element of the Hessian matrix is the product of $\det(A(P))$ and the determinants of the two elementary matrices.

(4) Using results obtained from finding $\mathbf{g}(P)$ in Subsection 3.6.3, we obtain these values immediately.

We define $A^{[ij],[k\ell]}$ to be the matrix A with rows i, k and columns j, ℓ removed. An argument similar to that for $g_{ij}(P)$ in the previous subsection can be made that finding

$$H_{[ij],[k\ell]}(P) = \frac{\partial^2 f(P)}{\partial x_{ij} \partial x_{k\ell}} = (-1)^{(i+j+k+\ell+1)} \det(A^{[ij],[k\ell]}),\ i \neq k,\ j \neq \ell, \tag{3.102}$$

is equivalent to finding the negative determinant of A with the ith and kth rows changed to $\mathbf{e}_j^T$ and $\mathbf{e}_\ell^T$ respectively. That is,

$$\begin{aligned} \frac{\partial^2 f(P)}{\partial x_{ij} \partial x_{k\ell}} &= -\det(\hat{E}_{k\ell} E_{ij} A(P)) \\ &= -\det(\hat{E}_{k\ell}) \det(E_{ij}) \det(A(P)), \end{aligned} \tag{3.103}$$

where $\hat{E}_{k\ell}$ is an additional row operation constructed to change row k of $E_{ij}A$ into $\mathbf{e}_\ell^T$. Note that if $i = k$ or $j = \ell$, the matrix $A^{[ij],[k\ell]}$ is no longer square and the determinant no longer exists. If this occurs, we define $H_{[ij],[k\ell]} := 0$. If both $i = k$ and $j = \ell$, we also define $H_{[ij],[k\ell]} := 0$, as the determinant is linear in each element of $A(P)$.

Consider $E_{ij}A$ composed of rows $\hat{\mathbf{r}}_1^T$, $\hat{\mathbf{r}}_2^T$, …, $\hat{\mathbf{r}}_N^T$. Then, we perform the following row operation:

$$\hat{\mathbf{r}}_k \quad \rightarrow \quad \gamma_\ell(1)\hat{\mathbf{r}}_1 + \gamma_\ell(2)\hat{\mathbf{r}}_2 + \ldots + \gamma_\ell(N)\hat{\mathbf{r}}_N, \tag{3.104}$$

where $(E_{ij}A)^T \gamma_\ell = \mathbf{e}_\ell$. Then, similarly to (3.92), we directly find γ:

$$\gamma_\ell \quad = \quad (E_{ij}^T)^{-1}(L^T)^{-1}(I - \mathbf{w}\mathbf{v}^T)(\overline{U}^T)^{-1}\mathbf{e}_\ell. \tag{3.105}$$

Next, in a similar fashion to (3.94), we construct an elementary matrix $\hat{E}_{k\ell}$

$$\begin{aligned} \hat{E}_{k\ell} &= I - \mathbf{e}_k\mathbf{e}_k^T + \mathbf{e}_k\gamma^T \\ &= I - \mathbf{e}_k(\mathbf{e}_k^T - \gamma^T). \end{aligned} \tag{3.106}$$

Then, we evaluate $\det(\hat{E}_{k\ell})$:

$$\begin{aligned}\det(\hat{E}_{k\ell}) &= 1-(\mathbf{e}_k^T-\gamma^T)\mathbf{e}_k\\ &= 1-1+\gamma^T\mathbf{e}_k\\ &= \mathbf{e}_\ell^T(\bar{U})^{-1}QL^{-1}(E_{ij})^{-1}\mathbf{e}_k.\end{aligned}\tag{3.107}$$

Recall from (3.94) that $E_{ij}=I-\mathbf{e}_i(\mathbf{e}_i^T-\alpha_j^T)$. We now find the inverse of this matrix. It is a known result that $(I-\mathbf{c}\mathbf{d}^T)^{-1}=(I+\frac{1}{1-\mathbf{d}^T\mathbf{c}}\mathbf{c}\mathbf{d}^T)$ for any vectors $\mathbf{c}$, $\mathbf{d}$ such that $\mathbf{d}^T\mathbf{c}\neq 1$. This is easy to see by considering

$$\begin{aligned}\left(I-\mathbf{c}\mathbf{d}^T\right)\left(I+\frac{1}{1-\mathbf{d}^T\mathbf{c}}\mathbf{c}\mathbf{d}^T\right) &= I+\frac{1}{1-\mathbf{d}^T\mathbf{c}}\mathbf{c}\mathbf{d}^T-\mathbf{c}\mathbf{d}^T-\frac{1}{1-\mathbf{d}^T\mathbf{c}}\mathbf{c}\mathbf{d}^T\mathbf{c}\mathbf{d}^T\\ &= I+\frac{1-(1-\mathbf{d}^T\mathbf{c})-\mathbf{d}^T\mathbf{c}}{1-\mathbf{d}^T\mathbf{c}}\mathbf{c}\mathbf{d}^T\\ &= I.\end{aligned}$$

In our case, $\mathbf{c}=\mathbf{e}_i$ and $\mathbf{d}=\mathbf{e}_i-\alpha_j$. Hence

$$\begin{aligned}(E_{ij})^{-1} &= I+\frac{1}{1-(\mathbf{e}_i^T-\alpha_j^T)\mathbf{e}_i}\mathbf{e}_i(\mathbf{e}_i^T-\alpha_j^T)\\ &= I+\frac{1}{\alpha_j^T\mathbf{e}_i}\mathbf{e}_i(\mathbf{e}_i^T-\alpha_j^T).\end{aligned}\tag{3.108}$$

Recall from (3.95) that $g_{ij}=\det(A)\det(E_{ij})$, and from (3.96) that $\det(E_{ij})=\alpha_j^T\mathbf{e}_i$. Note that in our case $\mathbf{d}^T\mathbf{c}\neq 1$ because $\alpha_j^T\mathbf{e}_i=\det(E_{ij})\neq 0$, and therefore (3.108) holds. Then,

$$\alpha_j^T\mathbf{e}_i = \frac{g_{ij}}{\det(A)}.\tag{3.109}$$

Substituting (3.109) into (3.108) we obtain

$$(E_{ij})^{-1} = I+\frac{\det(A)}{g_{ij}}\mathbf{e}_i(\mathbf{e}_i^T-\alpha_j^T),\tag{3.110}$$

and further substituting (3.110) into (3.107), we obtain

$$\begin{aligned}\det(\hat{E}_{k\ell}) &= \mathbf{e}_\ell^T\left(\bar{U}\right)^{-1}QL^{-1}\left(I+\frac{\det(A)}{g_{ij}}\mathbf{e}_i(\mathbf{e}_i^T-\alpha_j^T)\right)\mathbf{e}_k\\ &= \mathbf{e}_\ell^T(\bar{U})^{-1}QL^{-1}\left(\mathbf{e}_k+\frac{\det(A)}{g_{ij}}\mathbf{e}_i\mathbf{e}_i^T\mathbf{e}_k-\frac{\det(A)}{g_{ij}}\mathbf{e}_i\alpha_j^T\mathbf{e}_k\right).\end{aligned}\tag{3.111}$$

Note that since $i \neq k$, $\mathbf{e}_i\mathbf{e}_i^T\mathbf{e}_k = \mathbf{0}$, and from (3.109), $\alpha_j^T\mathbf{e}_k = \dfrac{g_{kj}}{\det(A)}$. Hence, from (3.111) and (3.98) we obtain

$$\begin{aligned}\det(\hat{E}_{k\ell}) &= \mathbf{e}_\ell^T(\bar{U})^{-1}QL^{-1}(\mathbf{e}_k - \frac{g_{kj}}{g_{ij}}\mathbf{e}_i) \\ &= \mathbf{a}_\ell^T Q(\mathbf{b}_k - \frac{g_{kj}}{g_{ij}}\mathbf{b}_i). \end{aligned} \tag{3.112}$$

We now derive the main result of this subsection.

Proposition 3.6.9 *For any $P \in Int(\mathcal{DS}_\mathbf{x})$ and $I - P = LU$, where L and U form the LU-decomposition, the general element of the Hessian of $f(P)$ is given by*

$$H_{[ij],[k\ell]} = g_{kj}\hat{q}_{i\ell} - g_{ij}\hat{q}_{k\ell},$$

where $\hat{q}_{i\ell}$ and $\hat{q}_{k\ell}$ are as in (3.101).

Proof. From (3.103) and (3.95), we can see that $H_{[ij],[k\ell]} = -\det(\hat{E}_{k\ell})g_{ij}$. Then, from (3.112), $\det(\hat{E}_{k\ell}) = \mathbf{a}_\ell^T Q(\mathbf{b}_k - \dfrac{g_{kj}}{g_{ij}}\mathbf{b}_i)$ and so $H_{[ij],[k\ell]} = -\mathbf{a}_\ell^T Q(\mathbf{b}_k g_{ij} - \mathbf{b}_i g_{kj})$.

In order to improve computation time, we take advantage of the fact that we evaluate every $\hat{q}_{ij}$ while calculating the gradient to rewrite the second order partial derivatives of $f(P)$ as

$$\begin{aligned}H_{[ij],[k\ell]} &= g_{kj}\mathbf{a}_\ell^T Q\mathbf{b}_i - g_{ij}\mathbf{a}_\ell^T Q\mathbf{b}_k \\ &= g_{kj}\hat{q}_{i\ell} - g_{ij}\hat{q}_{k\ell}. \end{aligned} \tag{3.113}$$

This concludes the proof. □

Remark 3.6.10 *Note that in practice, we do not calculate some g_{kj}'s when calculating $\mathbf{g}(P)$ as an arc (k,j) need not exist in the graph. In these cases we find g_{jk} using the gradient formula, $g_{jk} = -f(P)(\hat{q}_{jk})$, which remains valid despite arc (k,j) not appearing in the graph.*

3.6.5 Leading principal minor

It is, perhaps, interesting that instead of using the objective function $f(P) = -\det\left(I - P + \frac{1}{N}\mathbf{e}\mathbf{e}^T\right)$, it is also possible to use $f^1(P) := -\det(G^{NN}(P))$, the negative determinant of the leading principal minor of $I-P$. The following, somewhat surprising, result justifies this claim.

Theorem 3.6.11 *For any* $P \in Int(\mathcal{DS}_{\mathbf{x}})$,

(1) $f^1(P) = \frac{1}{N} f(P) = -\frac{1}{N} \det\left(I - P + \frac{1}{N}\mathbf{e}\mathbf{e}^T\right)$.

(2) If the graph is Hamiltonian, then

$$\min_{P \in \mathcal{DS}_{\mathbf{x}}} f^1(P) = -1. \tag{3.114}$$

Proof. First, we show part (1) $f^1(P) = \frac{1}{N} f(P)$. To find $f^1(P)$, we construct $LU = I - P$ as before, and define $\hat{L}$, $\hat{U}$ as:

$$\hat{L} = \begin{bmatrix} \mathbf{e}_1^T L \\ \vdots \\ \mathbf{e}_{N-1}^T L \\ \mathbf{e}_N^T \end{bmatrix}, \quad \hat{U} = \begin{bmatrix} U\mathbf{e}_1 & \cdots & U\mathbf{e}_{N-1} & \mathbf{e}_N \end{bmatrix}. \tag{3.115}$$

That is, $\hat{L}$ is the same as L with the last row replaced by $\mathbf{e}_N^T$, and $\hat{U}$ is the same as U with the last column replaced with $\mathbf{e}_N$. Then consider

$$\begin{aligned} \hat{L}\hat{U} &= \begin{bmatrix} \mathbf{e}_1^T L \\ \vdots \\ \mathbf{e}_{N-1}^T L \\ \mathbf{e}_N^T \end{bmatrix} \begin{bmatrix} U\mathbf{e}_1 & \cdots & U\mathbf{e}_{N-1} & \mathbf{e}_N \end{bmatrix} \\ &= \begin{bmatrix} \mathbf{e}_1^T LU\mathbf{e}_1 & \ddots & \mathbf{e}_1^T LU\mathbf{e}_{N-1} & \mathbf{e}_1^T L\mathbf{e}_N \\ \vdots & \ddots & \vdots & \vdots \\ \mathbf{e}_{N-1}^T LU\mathbf{e}_1 & \cdots & \mathbf{e}_{N-1}^T LU\mathbf{e}_{N-1} & \mathbf{e}_{N-1}^T L\mathbf{e}_N \\ \mathbf{e}_N^T U\mathbf{e}_1 & \cdots & \mathbf{e}_N^T U\mathbf{e}_{N-1} & \mathbf{e}_N^T \mathbf{e}_N \end{bmatrix}. \end{aligned}$$

Since L is lower-triangular, $\mathbf{e}_i^T L\mathbf{e}_N = 0$ for all $i \neq N$. Likewise, since U is upper-triangular, $\mathbf{e}_N^T U\mathbf{e}_j = 0$ for all $j \neq N$. Therefore the above matrix simplifies to

$$\hat{L}\hat{U} = \begin{bmatrix} \mathbf{e}_1^T LU\mathbf{e}_1 & \cdots & \mathbf{e}_1^T LU\mathbf{e}_{N-1} & 0 \\ \vdots & \ddots & \vdots & \vdots \\ \mathbf{e}_{N-1}^T LU\mathbf{e}_1 & \cdots & \mathbf{e}_{N-1}^T LU\mathbf{e}_{N-1} & 0 \\ 0 & \cdots & 0 & 1 \end{bmatrix},$$

which is the same as LU with the bottom row and rightmost column removed, and a 1 placed in the bottom-right element. Therefore, $\det(\hat{L}\hat{U}) = \det(G^{NN}(P))$, and consequently

$$f^1(P) \quad = \quad -\det(\hat{L})\det(\hat{U}). \tag{3.116}$$

Note that $\hat{L}$ and $\hat{U}$ are triangular matrices, so

$$\det\left(\hat{L}\right) = \prod_{i=1}^{N} \hat{l}_{ii}, \qquad \text{and} \qquad \det\left(\hat{U}\right) = \prod_{i=1}^{N} \hat{u}_{ii}.$$

However, only the last diagonal elements of $\hat{L}$ and $\hat{U}$ are different from L and $\bar{U}$ (see (3.69)) respectively, so

$$\det\left(\hat{L}\right) = \hat{l}_{NN} \prod_{i=1}^{N-1} l_{ii}, \qquad \text{and} \qquad \det\left(\hat{U}\right) = \hat{u}_{NN} \prod_{i=1}^{N-1} \bar{u}_{ii}. \tag{3.117}$$

Now, since $\hat{l}_{NN} = l_{NN} = 1$, we have

$$\det\left(\hat{L}\right) = \det\left(L\right) = 1. \tag{3.118}$$

We also have $\hat{u}_{NN} = 1$, but by Lemma 3.6.2, $\bar{u}_{NN} = N$ and hence

$$\det\left(\hat{U}\right) = \frac{1}{N}\det\left(\bar{U}\right). \tag{3.119}$$

Therefore, substituting (3.118) and (3.119) into (3.116) we obtain

$$\begin{aligned} f^1(P) \quad &= \quad -\det\left(\hat{L}\right)\det\left(\hat{U}\right) \\ &= \quad -\frac{1}{N}\det\left(\bar{U}\right) \\ &= \quad -\frac{1}{N}\det\left(I - P + \frac{1}{N}\mathbf{e}\mathbf{e}^T\right) = \frac{1}{N}f(P). \end{aligned}$$

Therefore, part (1) is proved.

The proof of part (2) of Theorem 3.6.11 follows directly from the fact that $\min\limits_{P\in\mathcal{DS}_{\mathbf{x}}} f(P) = -N$ (proved in [14]), and part (1). □

Remark 3.6.12 *Using the leading principal minor has the advantage that the rank-one modification* $\frac{1}{N}\mathbf{e}\mathbf{e}^T$ *is not required, which makes calculating the gradient and the Hessian even simpler, as well as more numerically stable than described in Subsection 3.6.3 and Subsection 3.6.4 respectively. The derivation of the gradient and Hessian formulae for the negative derivative of the leading prinpical minor follows the same process as that for the determinant function, except that the matrix* $Q = I - \mathbf{v}\mathbf{w}^T$ *is not required.*

The formulae for $f^1(A(P))$, $\mathbf{g}^1(P)$ and $H^1(P)$ then reduce to

$$f^1 = -\prod_{i=1}^{N-1} u_{ii}, \tag{3.120}$$

$$g^1_{ij} = -f^1(P)(\mathbf{a}^1_j)^T\mathbf{b}^1_i, \tag{3.121}$$

$$H^1_{[i,j],[k,\ell]} = g^1_{kj}(\mathbf{a}^1_i)^T\mathbf{b}^1_\ell - g^1_{ij}(\mathbf{a}^1_k)^T\mathbf{b}^1_\ell, \tag{3.122}$$

where

$$\hat{L}\mathbf{b}^1_i = \mathbf{e}_i, \tag{3.123}$$

$$\hat{U}^T\mathbf{a}^1_j = \mathbf{e}_j. \tag{3.124}$$

Remark 3.6.13 *In practice, we use the negative derivative of the leading principal minor in Algorithm 3.16: DIPA than the determinant, for three reasons. First, it is more efficient to calculate, second, its maximum value is the same for every graph, and third, as is shown in Subsection 3.7.1, it is more numerically stable than the determinant. This eliminates the need to scale any parameters by the size of the graph. When* $f^1(P)$ *is used in lieu of* $f(P)$ *the corresponding gradient vector and Hessian matrix are denoted by* $g^1(P)$ *and* $H^1(P)$*, respectively.*

3.7 LU decomposition-based evaluation algorithm

The algorithm for computing $f^1(P)$, $g^1(P)$, $H^1(P)$ is given in Algorithm 3.4, but is repeated here in a simpler, less structured format for the sake of completion. We also include the complexity of each step of the algorithm.

Input: P

Output: $f^1(P), g^1(P), H^1(P)$

begin | **Complexity**

1) Perform LU decomposition to find $LU = I - P$. — $O(N^3)$

2) Calculate $\hat{L}$ and $\hat{U}$, using (3.115). — $O(N)$

3) Calculate each $(\mathbf{a}_j^1)^T$ and $\mathbf{b}_i^1$, using (3.123) and (3.124). — $O(N^3)$

4) Calculate each $(\mathbf{a}_j^1)^T \mathbf{b}_i^1$. — $O(N^3)$

5) Calculate $f^1(P) = -\prod_{i=1}^{N-1} u_{ii}$. — $O(N)$

6) Calculate each $g_{ij}^1(P) = -f^1(P)(\mathbf{a}_j^1)^T \mathbf{b}_i^1$. — $O(N^2)$

7) Calculate each $H^1_{[ij],[k\ell]}(P) = \begin{cases} g_{kj}^1 (\mathbf{a}_i^1)^T \mathbf{b}_\ell^1 - g_{ij}^1 (\mathbf{a}_k^1)^T \mathbf{b}_\ell^1, & i \neq k \text{ and } j \neq \ell, \\ 0, & \text{otherwise.} \end{cases}$ — $O(N^4)$

end

Algorithm 3.18: Function evaluations algorithm (simplified).

The complexity of the above algorithm is $O(N^4)$. The $O(N^4)$ bound is because there are $O(N^4)$ elements in the Hessian. Each element of the Hessian is calculated in $O(1)$ time, because they simply involve scalar multiplication where all of the scalars have already been calculated in earlier steps, that is, the gradient terms in step 6, and each $(\mathbf{a}_i^1)^T \mathbf{b}_l^1$ in step 4.

This bound is considerably better than the $O(N^7)$ bound that applies if we simply perform an LU decomposition for each element in the Hessian and gradient.

These complexity bounds are calculated assuming that Γ is a dense matrix. For sparse matrices containing $O(N)$ arcs, the above algorithm has complexity $O(N^3)$, compared to $O(N^5)$ when performing an LU decomposition for each element in the Hessian and gradient. This $O(N^3)$ complexity is the same complexity as the original LU decomposition itself, so finding the Hessian and gradient in a sparse graph by Algorithm 3.4 has the same complexity as computing the objective function value.

Example 3.7.1 *Consider the six-node cubic graph* Γ_6 *introduced earlier (see (3.58)).*

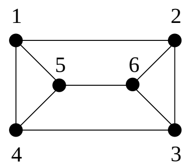


Figure 3.2: The envelope graph Γ_6.

The adjacency matrix of Γ_6 *is*

$$\begin{bmatrix} 0 & 1 & 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 & 1 & 0 \end{bmatrix}.$$

Consider a point $\mathbf{x}$ *such that,*

$$P(\mathbf{x}) = \begin{bmatrix} 0 & \frac{2}{3} & 0 & \frac{1}{6} & \frac{1}{6} & 0 \\ \frac{2}{3} & 0 & \frac{1}{6} & 0 & 0 & \frac{1}{6} \\ 0 & \frac{1}{6} & 0 & \frac{2}{3} & 0 & \frac{1}{6} \\ \frac{1}{6} & 0 & \frac{2}{3} & 0 & \frac{1}{6} & 0 \\ \frac{1}{6} & 0 & 0 & \frac{1}{6} & 0 & \frac{2}{3} \\ 0 & \frac{1}{6} & \frac{1}{6} & 0 & \frac{2}{3} & 0 \end{bmatrix},$$

which is in the interior of $\mathcal{DS}_{\mathbf{x}}$.

Performing the LU decomposition of $I - P$ *using MATLAB's* `lu` *routine we obtain matrices* L *and* U

$$L = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ -0.6667 & 1 & 0 & 0 & 0 & 0 \\ 0 & -0.3000 & 1 & 0 & 0 & 0 \\ -0.1667 & -0.2000 & -0.7368 & 1 & 0 & 0 \\ -0.1667 & -0.2000 & -0.0351 & -0.5556 & 1 & 0 \\ 0 & -0.3000 & -0.2281 & -0.4444 & -1.0000 & 1 \end{bmatrix},$$

$$U = \begin{bmatrix} 1 & -0.6667 & 0 & -0.1667 & -0.1667 & 0 \\ 0 & 0.5556 & -0.1667 & -0.1111 & -0.1111 & -0.1667 \\ 0 & 0 & 0.9500 & -0.7000 & -0.0333 & -0.2167 \\ 0 & 0 & 0 & 0.4342 & -0.2412 & -0.1930 \\ 0 & 0 & 0 & 0 & 0.8148 & -0.8148 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

Consequently, $\hat{L} = \begin{bmatrix} L^T\mathbf{e}_1 & \cdots & L^T\mathbf{e}_{N-1} & \mathbf{e}_N \end{bmatrix}^T$ *and* $\hat{U} = \begin{bmatrix} U\mathbf{e}_1 & \cdots & U\mathbf{e}_{N-1} & \mathbf{e}_N \end{bmatrix}$ *are simply*

$$\hat{L} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ -0.6667 & 1 & 0 & 0 & 0 & 0 \\ 0 & -0.3000 & 1 & 0 & 0 & 0 \\ -0.1667 & -0.2000 & -0.7368 & 1 & 0 & 0 \\ -0.1667 & -0.2000 & -0.0351 & -0.5556 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix},$$

$$\hat{U} = \begin{bmatrix} 1 & -0.6667 & 0 & -0.1667 & -0.1667 & 0 \\ 0 & 0.5556 & -0.1667 & -0.1111 & -0.1111 & 0 \\ 0 & 0 & 0.9500 & -0.7000 & -0.0333 & 0 \\ 0 & 0 & 0 & 0.4342 & -0.2412 & 0 \\ 0 & 0 & 0 & 0 & 0.8148 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

For all i, j*, we calculate the* $\mathbf{a}_j^1$ *and* $\mathbf{b}_i^1$ *vectors using (3.123) and (3.124). Namely,*

$$\mathbf{a}_1^1 = \begin{bmatrix} 1 \\ 0.3750 \\ 0.1429 \\ 0.6 \\ 1.2 \\ 0 \end{bmatrix}, \mathbf{a}_2^1 = \begin{bmatrix} 0 \\ 1.1250 \\ 0.4286 \\ 0.4 \\ 0.6 \\ 0 \end{bmatrix}, \mathbf{a}_3^1 = \begin{bmatrix} 0 \\ 0 \\ 1.1429 \\ 0.6 \\ 0.6 \\ 0 \end{bmatrix}, \mathbf{a}_4^1 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1.4 \\ 1.2 \\ 0 \end{bmatrix}, \mathbf{a}_5^1 = \begin{bmatrix} 0 \\ 0.3750 \\ 0.1429 \\ 0.6 \\ 1.2 \\ 0 \end{bmatrix}, \mathbf{a}_6^1 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{bmatrix},$$

$$\mathbf{b}_1^1 = \begin{bmatrix} 1 \\ 0.3333 \\ 0.1250 \\ 0.4286 \\ 0.6667 \\ 0 \end{bmatrix}, \mathbf{b}_2^1 = \begin{bmatrix} 0 \\ 1 \\ 0.375 \\ 0.2857 \\ 0.3333 \\ 0 \end{bmatrix}, \mathbf{b}_3^1 = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0.4286 \\ 0.3333 \\ 0 \end{bmatrix}, \mathbf{b}_4^1 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0.6667 \\ 0 \end{bmatrix}, \mathbf{b}_5^1 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \mathbf{b}_6^1 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}.$$

We can now represent each $(\mathbf{a}_j^1)^T\mathbf{b}_i^1$ *as the* ij*-th element of the matrix*

$$\left[(\mathbf{a}_j^1)^T(\mathbf{b}_i^1)\right]_{i,j=1}^{N,N} = \begin{bmatrix} 2.2 & 1 & 0.8 & 1.4 & 1.2 & 0 \\ 1 & 1.6 & 0.8 & 0.8 & 0.6 & 0 \\ 0.8 & 0.8 & 1.6 & 1 & 0.6 & 0 \\ 1.4 & 0.8 & 1 & 2.2 & 1.2 & 0 \\ 1.2 & 0.6 & 0.7 & 1.2 & 1.8 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Then, $f^1(P) = \prod_{i=1}^{N-1} \hat{u}_{ii} \approx -0.3086$. *Note that we can directly verify the preceding by confirming that* $\det(A(P)) \approx 1.8516 = -6(f^1(P))$.

The gradient vector is then found using (3.121). Note that we are only interested in the gradient elements for the eighteen arcs in the graph; this yields, to three decimal places:

$$g^1(P) \approx \begin{bmatrix} 0.309 & 0.432 & 0.370 & 0.309 & 0.247 & 0 & 0.247 & 0.309 & 0 & 0.432 & 0.309 & 0.370 & 0.370 & 0.370 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

Finally, the Hessian is be found using (3.122), given here to two decimal places:

$$H^1(P) \approx \begin{bmatrix}
0 & 0 & 0 & 0.78 & 0.15 & 0 & 0 & 0.04 & 0 & 0.11 & -0.11 & -0.07 & 0.04 & -0.11 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0.11 & -0.15 & 0 & -0.04 & 0 & 0 & 0.89 & 0.11 & 0.30 & 0.30 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0.04 & -0.15 & 0 & -0.11 & -0.11 & 0 & 0.30 & -0.07 & 0 & 0.78 & 0.33 & 0 & 0 & 0 & 0 \\
0.78 & 0.11 & 0.04 & 0 & 0 & 0 & 0.15 & -0.11 & 0 & 0 & 0.04 & -0.11 & 0 & -0.07 & 0 & 0 & 0 & 0 \\
0.15 & -0.15 & -0.145 & 0 & 0 & 0 & 0.59 & 0.15 & 0 & -0.04 & 0 & -0.11 & -0.11 & -0.15 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -0.04 & -0.11 & 0.15 & 0.59 & 0 & 0 & 0 & 0 & -0.15 & 0.15 & -0.15 & -0.15 & -0.11 & 0 & 0 & 0 & 0 \\
0.04 & 0 & -0.11 & -0.11 & 0.15 & 0 & 0 & 0 & 0 & 0.11 & 0.78 & 0.04 & -0.07 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0.11 & 0.89 & 0.30 & 0 & -0.04 & 0 & -0.15 & 0.11 & 0 & 0 & 0 & 0 & 0 & 0.30 & 0 & 0 & 0 & 0 \\
-0.11 & 0.11 & -0.07 & 0.04 & 0 & 0 & 0.15 & 0.78 & 0 & 0 & 0 & 0 & -0.11 & 0.04 & 0 & 0 & 0 & 0 \\
-0.07 & 0.30 & 0 & -0.11 & -0.11 & 0 & -0.15 & 0.04 & 0 & 0 & 0 & 0 & 0.33 & 0.78 & 0 & 0 & 0 & 0 \\
0.04 & 0.30 & 0.78 & 0 & -0.11 & 0 & -0.15 & -0.07 & 0 & 0 & -0.11 & 0.33 & 0 & 0 & 0 & 0 & 0 & 0 \\
-0.11 & 0 & 0.33 & -0.07 & -0.15 & 0 & -0.11 & 0 & 0 & 0.30 & 0.04 & 0.78 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}.$$

3.7.1 Sensitivity

In all of the derivations in this chapter we assume that $P(\mathbf{x})$ is doubly-stochastic. However, when a numerical method such as DIPA is executed on a computer, small inaccuracies may be introduced. It is important to analyse the sensitivity of the formulae derived thus far to ensure that they will still perform adequately in a computer implementation of DIPA.

Recall from (3.82) that $\det(A) = \det(L)\det(I + \mathbf{v}\mathbf{w}^T)\det(\bar{U})$. Here, L and $\bar{U}$ can still be found as the LU Decomposition does not require $P(\mathbf{x})$ to be doubly-stochastic. However, where Lemma 3.6.3 proves that $\det(I + \mathbf{v}\mathbf{w}^T) = 1$ for doubly-stochastic $P(\mathbf{x})$, the result no longer holds if, numerically, $P(\mathbf{x})$ is not precisely doubly-stochastic.

Assume that we have obtained $P(\mathbf{x})$ such that $P(\mathbf{x})\mathbf{e} = \mathbf{e} - \mathbf{s}$, for some nonnegative error vector $\mathbf{s}$. Then, from (3.84), (3.85), (3.86) and (3.72) we have

$$\det(I + \mathbf{v}\mathbf{w}^T) = 1 + \left(\frac{1}{N}\mathbf{e}^T - \mathbf{e}_N^T\right)\left(I - P(\mathbf{x}) + \mathbf{e}\mathbf{e}_N^T\right)^{-1}\mathbf{e}. \tag{3.125}$$

Now, $\left[I - P(\mathbf{x}) + \mathbf{e}\mathbf{e}_N^T\right]\mathbf{e} = \mathbf{e} + \mathbf{s}$. Therefore, $\left(I - P(\mathbf{x}) + \mathbf{e}\mathbf{e}_N^T\right)^{-1}\mathbf{e} = \mathbf{e} - \left(I - P(\mathbf{x}) + \mathbf{e}\mathbf{e}_N^T\right)^{-1}\mathbf{s}$. Substituting this into (3.125) we find

$$\det(I + \mathbf{v}\mathbf{w}^T) = 1 - \left(\frac{1}{N}\mathbf{e}^T - \mathbf{e}_N^T\right)\left(I - P(\mathbf{x}) + \mathbf{e}\mathbf{e}_N^T\right)^{-1}\mathbf{s}. \tag{3.126}$$

We observe that the additional error introduced into the determinant value is of the same order as the error in the numerically obtained $P(\mathbf{x})$, and will grow or shrink at the same rate as the error is controlled.

It is worth noting that for the principal minor, the $\det(I+\mathbf{v}\mathbf{w}^T)$ term is not required, and therefore no additional inaccuracy will be introduced for the principal minor when $P(\mathbf{x})$ is not precisely doubly-stochastic.

For the gradient, the equation given in (3.97) is no longer accurate either, as it assumes that $(I + \mathbf{v}\mathbf{w}^T)^{-1} = I - \mathbf{v}\mathbf{w}^T$ which is not the case when $P(\mathbf{x})$ is not precisely doubly-stochastic.

The additional error introduced is found by considering

$$\begin{aligned}\left(I + \mathbf{v}\mathbf{w}^T\right)^{-1} - \left(I - \mathbf{v}\mathbf{w}^T\right) &= \left(I + \mathbf{v}\mathbf{w}^T\right)^{-1}\left[I - \left(I + \mathbf{v}\mathbf{w}^T\right)\left(I - \mathbf{v}\mathbf{w}^T\right)\right] \\ &= \left(I + \mathbf{v}\mathbf{w}^T\right)^{-1}\left(\mathbf{v}\mathbf{w}^T\mathbf{v}\mathbf{w}^T\right). \end{aligned} \tag{3.127}$$

Then, substituting (3.85), (3.86) and (3.72) into (3.127) we obtain

$$\left(I + \mathbf{v}\mathbf{w}^T\right)^{-1} - \left(I - \mathbf{v}\mathbf{w}^T\right) = \left(I + \mathbf{v}\mathbf{w}^T\right)^{-1}\mathbf{v}\left[\left(\frac{1}{N}\mathbf{e}^T - \mathbf{e}_N^T\right)\left(I - P(\mathbf{x}) + \mathbf{e}\mathbf{e}_N^T\right)^{-1}\mathbf{s}\right]\mathbf{w}^T.$$

Note that the term inside the square brackets is a scalar, and so we can move it to the front to obtain

$$\left(I + \mathbf{v}\mathbf{w}^T\right)^{-1} - \left(I - \mathbf{v}\mathbf{w}^T\right) = \left[\left(\frac{1}{N}\mathbf{e}^T - \mathbf{e}_N^T\right)\left(I - P(\mathbf{x}) + \mathbf{e}\mathbf{e}_N^T\right)^{-1}\mathbf{s}\right]\left(I + \mathbf{v}\mathbf{w}^T\right)^{-1}\mathbf{v}\mathbf{w}^T.$$

This additional error is again of the same order as the error in the numerically obtained $P(\mathbf{x})$ and grows or shrinks in accordance with the accuracy of computing $P(\mathbf{x})$. Note that, again, the principal minor form of the problem avoids this issue as the inverse $\left(I + \mathbf{v}\mathbf{w}^T\right)^{-1}$ is not required.

As the elements of the Hessian are simply built out of multiplying terms identical to those used to find the gradient elements, the additional error in the Hessian is also of the same order as the inaccuracy of computing $P(\mathbf{x})$.

These additional inaccuracies provide further evidence as to the merit of selecting the principal minor function over the determinant function.

3.7.2 Experimental results

In Sections 3.6 – 3.7 we demonstrate how the $f(P) = -\det\left(I - P + \frac{1}{N}\mathbf{e}\mathbf{e}^T\right)$ function possesses nice properties that allow us to find its gradient and Hessian efficiently. In practice, we do not actually find $f(P)$ and its derivatives, but rather those of the negative derivative of the leading principal minor $f^1(P)$, for which the same nice features are preserved, but the computation is more efficient and accurate, and the Hessian is sparser. We have implemented this process as part of Algorithm 3.16: DIPA, with some encouraging results.

To conclude, we provide an illustration as to the improvement offered by Algorithm 3.4. The time taken to calculate the Hessian at a randomly selected interior point was calculated for four test graphs, and compared to the time taken to compute each element of the Hessian using MATLAB's `det` function. The results can be seen in Table 3.3.

These encouraging results could be further improved by taking advantage of graph structure to increase the level of sparsity present in the LU decomposition.

Graph	**Time to calculate**	**Using `det` method**
48 nodes, 144 variables	0.1 seconds	362 seconds
94 nodes, 282 variables	0.5 seconds	crashed
144 nodes, 880 variables	0.9 seconds	crashed
1000 nodes, 3996 variables	680 seconds	crashed

Table 3.3: Comparison of Algorithm 3.4 with MATLAB's `det` function.

Chapter 4

Hamiltonian Curves and Surfaces

4.1 Motivation

In this chapter we consider, in considerable detail, the polytope defined in Chapter 2 by linear constraints (2.8)–(2.10). We investigate the behaviour induced on the polytope by the discount parameter β, and later by a perturbation parameter ν. In both cases, we observe that Hamiltonian solutions to the parametrised equations defining the polytopes take the form of vectors whose entries are either 0, or polynomials in these new parameters β and ν. We derive the exact form of these polynomials by considering the determinants of particular matrices. Finally, we introduce new linear feasibility programs by equating coefficients in systems of linear equations characterising the polytopes and show that these new programs are able to identify, by their infeasibility, many non-Hamiltonian graphs.

Every Hamiltonian cycle in an N-node graph Γ induces a doubly stochastic (permutation) matrix whose 1-entries identify precisely the arcs comprising the simple cycle of length N. For instance, if h_s is the standard Hamiltonian graph:

$1 \to 2 \to 3 \to \cdots \to N\text{-}1 \to N \to 1$, the corresponding permutation matrix is

$$P_{h_s} = \begin{pmatrix} & 1 & & & \\ & & 1 & & \\ & & & \ddots & \\ & & & & 1 \\ 1 & & & & \end{pmatrix}.$$

Furthermore, any other Hamiltonian cycle h^* in Γ has the corresponding matrix P_{h^*} that can be obtained from P_{h_s} via a similarity transformation

$$P_{h^*} = \Pi P_{h_s} \Pi^{-1}, \tag{4.1}$$

where Π is some permutation matrix. Thus all Hamiltonian cycles are co-spectral, that is, eigenvalues of P_{h_s} and P_{h^*} are the same. In fact, it is well-known that the spectrum of every P_h consists of the N roots of unity (e.g., see Ejov et al [14]).

Thus the shared properties of matrices P_h contain many of the properties characterising the special characteristics of Hamiltonian cycles. Some of the latter are obvious such as the facts that for any Hamiltonian cycle:

(1) $P_h^N = I$, the identity matrix (since P_h is a clearly circulant matrix).

(2) $P_h^T = P_h^{-1}$, the idempotent property.

(3) P_h is an irreducible matrix with the vector $\frac{1}{N}\mathbf{e}^T = \frac{1}{N}\begin{bmatrix} 1 & \cdots & 1 \end{bmatrix}$ being its unique stationary distribution.

However, a matrix P_h also contains other properties that only become apparent when we consider the associated resolvent matrix[1],

$$R_h(\beta) := [I - \beta P_h]^{-1} = \sum_{n=0}^{\infty} \beta^n P_h^n, \tag{4.2}$$

where $\beta \in [0, 1)$, and $P_h^0 := I$. Note that we exclude $\beta = 1$ because it is an eigenvalue of P_h and hence destroys the convergence of the series (4.2).

[1]Strictly speaking, the resolvent of a square matrix A is defined by $R(z) = [A - zI]^{-1}$, however, in keeping with the conventions of Markov decision processes $R_h(\beta)$ defined above is the more useful matrix.

Interestingly, entries of $R_h(\beta)$ have a simple algebraic form.

Lemma 4.1.1 *Let h be any Hamiltonian cycle in Γ, and P_h be a 0-1 matrix, with 1-entries corresponding exactly to the arcs (i,j) in h. All remaining entries of P_h are equal to 0. Let $d(\beta) := \det(I - \beta P_h)$, $d_{ij}(\beta)$ be the (i,j)-th cofactor of $(I - \beta P_h)$, and $r_{ij}(\beta)$ be the (i,j)-th entry of $R_h(\beta)$. Then*

(1) $d(\beta) = 1 - \beta^N$.

(2) $d_{ij}(\beta) \in \left\{1, \beta, \beta^2, \ldots, \beta^{N-1}\right\}$.

(3) $r_{ij}(\beta) = \dfrac{\beta^k}{1-\beta^N}$, *for some* $k \in \{0, 1, 2, \ldots, N-1\}$.

Proof. First, we show part (1) $d(\beta) = 1 - \beta^N$. From (4.1), we know that

$$\begin{aligned} d(\beta) := \det(I - \beta P_h) &= \det(I - \beta \Pi P_{h_s} \Pi^{-1}) \\ &= \det(\Pi I \Pi^{-1} - \beta \Pi P_{h_s} \Pi^{-1}) \\ &= \det\left[\Pi (I - \beta P_{h_s}) \Pi^{-1}\right] \\ &= \det(I - \beta P_{h_s}). \end{aligned} \tag{4.3}$$

So the determinant $d(\beta)$ is the same for all Hamiltonian cycles, and hence we simply consider the standard Hamiltonian cycle h_s.

Define $D := I - \beta P_{h_s}$. Then, D has the structure

$$D = \begin{bmatrix} 1 & -\beta & & & \\ & 1 & -\beta & & \\ & & \ddots & \ddots & \\ & & & \ddots & -\beta \\ -\beta & & & & 1 \end{bmatrix}. \tag{4.4}$$

We perform the following row operation on the N-th row of D:

$$\mathbf{r}_N^T \to \beta \mathbf{r}_1^T + \beta^2 \mathbf{r}_2^T + \cdots + \beta^{N-1} \mathbf{r}_{N-1}^T + \mathbf{r}_N^T,$$

which changes the N-th row of D to

$$\mathbf{r}_N^T \to \left[\begin{array}{ccccc} 0 & 0 & 0 & \cdots & 1 - \beta^N \end{array}\right]. \tag{4.5}$$

We perform the above row operation by multiplying the matrix on the left by the following elementary matrix E:

$$E = \begin{bmatrix} 1 & & & & & \\ & 1 & & & & \\ & & \ddots & & & \\ & & & \ddots & & \\ & & & & 1 & \\ \beta & \beta^2 & \cdots & \cdots & \beta^{N-1} & 1 \end{bmatrix}. \tag{4.6}$$

Then ED is a triangular matrix with $N-1$ diagonal entries of 1, and one diagonal entry of $1-\beta^N$. Clearly, $\det(E) = 1$, so $\det(D) = \det(ED) = 1-\beta^N$. Therefore, part (1) of Lemma 4.1.1 is proved.

Now, we show part (2) $d_{ij} \in \{1, \beta, \beta^2, \ldots, \beta^{N-1}\}$. We define

$$D_h := I - \beta P_h. \tag{4.7}$$

Consider the matrix D_s^C of cofactors d_{ij}^s of D, such that $d_{ij}^s(\beta)$ is the (i,j)-th cofactor of D, and the matrix D_h^C of cofactors $d_{ij}(\beta)$, such that $d_{ij}(\beta)$ is the (i,j)-th cofactor of D_h. Since $P_h = \Pi P_{h_s} \Pi^{-1}$, it is clear that

$$D_h = \Pi D \Pi^{-1}.$$

We then easily see that

$$D_h^{-1} = \Pi D^{-1} \Pi^{-1},$$

and also, from part (1), that

$$\det(D_h) = \det(D).$$

Then, since an inverse can be thought of as the matrix of cofactors divided by the determinant (e.g., see Horn and Johnson [37] pp. 20–21), we immediately obtain

$$D_h^C = \Pi D_s^C \Pi^{-1}. \tag{4.8}$$

Therefore, the elements in D_h^C are the same as the elements in D_s^C, but in different positions.

Then d_{ij}^s, the (i, j)-th cofactor of D, is

$$d_{ij}^s \;=\; (-1)^{i+j}\det(D^{ij}), \tag{4.9}$$

where D^{ij} is the matrix D with row i and column j removed. Note that both d_{ij}^s and $\det(D^{ij})$ depend on β but for simplicity of notation we drop the dependency. We consider two possibilities - when $i \geq j$ and when $i < j$.

Case 1: $i \geq j$. Then, we observe that D^{ij} has the form:

$$D^{ij} \;=\; \begin{array}{c} \left[\begin{array}{ccccccccccccccc}
1 & -\beta & & & & & & & & & & & & & \\
 & 1 & -\beta & & & & & & & & & & & & \\
 & & \ddots & \ddots & & & & & & & & & & & \\
 & & & \ddots & -\beta & & & & & & & & & & \\
 & & & & 1 & & & & & & & & & & \\
 & \scriptstyle (j-1\times j-1) & & & & -\beta & & & & & & & & & \\
 & & & & & 1 & -\beta & & & & & & & & \\
 & & & & & & 1 & \ddots & & & & & & & \\
 & & & & & & & \ddots & \ddots & & & & & & \\
 & & & & & & & & 1 & -\beta & & & & & \\
 & & & & & & & \scriptstyle (i-j\times i-j) & & & 1 & -\beta & & & \\
 & & & & & & & & & & & 1 & -\beta & & \\
 & & & & & & & & & & & & \ddots & \ddots & \\
 & & & & & & & & & & & & & \ddots & -\beta \\
-\beta & & & & & & & & & & & & & & 1
\end{array}\right] \\ \hspace{18em}\scriptstyle (N-i\times N-i) \end{array}.$$

We now calculate $\det(D^{ij})$. Column i has only a single entry 1, which occurs at the top-left of the third block in position (i, i), so we expand on this entry, deleting row i and column i from D^{ij}. This results in a smaller matrix for which the new column i (which was previously column $i+1$) again has only a single entry. We continue this process until the bottom-right block is entirely depleted (i expansions), which also eliminates the $-\beta$ in the bottom-left position of D^{ij}.

Now, column 1 has only a single entry, and we expand on that column to obtain a smaller matrix that again only has a single entry in column 1. We continue this process until the top-left block is entirely depleted ($j-1$ expansions), leaving only the middle block remaining, which is a lower-triangular matrix with determinant $(-\beta)^{i-j}$. Each entry we expand during the above process is a 1, in a diagonal position (so there is no need to consider the sign of each individual cofactor), and therefore $d_{ij} = (-1)^{i+j}(-\beta)^{i-j} = \beta^{i-j}$.

Case 2: $i < j$. Then, we observe that D^{ij} has the form:

$$D^{ij} \quad = \quad \begin{array}{c}\begin{bmatrix}
1 & -\beta & & & & & & & & & & & & & \\
 & 1 & \ddots & & & & & & & & & & & & \\
 & & \ddots & \ddots & & & & & & & & & & & \\
 & & & 1 & -\beta & & & & & & & & & & \\
 & & \scriptstyle (i-1\times i) & & & 1 & -\beta & & & & & & & & \\
 & & & & & & 1 & -\beta & & & & & & & \\
 & & & & & & & \ddots & \ddots & & & & & & \\
 & & & & & & & & \ddots & -\beta & & & & & \\
 & & & & & & & & & 1 & & & & & \\
 & & & & & & & \scriptstyle (j-i-1\times j-i-1) & & & -\beta & & & & \\
 & & & & & & & & & & 1 & -\beta & & & \\
 & & & & & & & & & & & 1 & -\beta & & \\
 & & & & & & & & & & & & \ddots & \ddots & \\
 & & & & & & & & & & & & & \ddots & -\beta \\
-\beta & & & & & & & & & & & & & & 1
\end{bmatrix} \\ \hfill \scriptstyle (N-j+1\times N-j) \qquad \end{array} .$$

We now calculate $\det(D^{ij})$. Clearly, column i has only a single non-zero entry $-\beta$, which occurs at the bottom-right of the first block in position $(i-1, i)$, so we expand on this entry, deleting row $(i-1)$ and column i from D^{ij}. This results in a smaller matrix for which column $i-1$ has only a single entry, a $-\beta$ in position $(i-2, i-1)$.

We continue this process until the top-left block is depleted ($i-1$ expansions). Next, we expand on column 1 to eliminate the $-\beta$ in the bottom-left position of D^{ij}. This ensures that the rightmost column now has only a single non-zero entry in it, which will be $-\beta$. We expand on this column, which results in a smaller matrix which again has only a single entry, $-\beta$, in the right column. We continue this process until the bottom-right block is depleted ($N-j$ expansions), leaving only the middle block remaining, which is an upper triangular matrix with determinant 1.

Each entry we expand on in the above process is a $-\beta$, but some of the expansions introduce a negative term. All $i-1$ terms in the top-left block are in superdiagonal positions, and therefore each provides a negative term. We expand on the $-\beta$ in the bottom-left of the matrix after $i-1$ rows are eliminated from the matrix (which originally has $N-1$ rows), and so we obtain the negative term $(-1)^{N-1-(i-1)+1} = (-1)^{N-i+1}$ from this expansion. The $(N-j)$ terms we expand on in the bottom-right block are in diagonal positions and do not provide any negative terms. Then, we see that

$$\begin{aligned} d_{ij} &= (-1)^{i+j}(-1)^{i-1}(-1)^{N-i+1}(-\beta)^{i-1}(-\beta)(-\beta)^{N-j} \\ &= (-1)^{N-j+i}(-\beta)^{N-j+i} = \beta^{N-j+i}. \end{aligned}$$

Therefore, we observe that every cofactor of D (and hence $I-\beta P_h$) is β^k for some $k \in \{0,1,2,\ldots,N-1\}$, which completes the proof of part (2) of Lemma 4.1.1.

Then, we recall that an inverse can be thought of as the matrix of cofactors divided by the determinant. Hence, it is immediately obvious from parts (1) and (2) that part (3) holds. □

Corollary 4.1.2 *We assume that $i=1$ is the initial (home) node in the Hamiltonian cycle h and j is the k-th node following the home node in h. By convention, we say that node $i=1$ is the 0-th node after the home node. Then,*

$$d_{j1} = \beta^k \quad \textit{and} \quad r_{1j} = \frac{\beta^k}{1-\beta^N}.$$

Proof. From the proof of Lemma 4.1.1 we see that for the standard Hamiltonian cycle, $d^s_{(k+1),1} = \beta^k$. In the standard Hamiltonian cycle, node $(k+1)$ is the k-th node following the home node.

For a general Hamiltonian cycle h, we know from (4.8) that

$$d_{j1} = d^s_{(k+1),1}. \tag{4.10}$$

Then, from (4.10) and the proofs of parts (1) and (3) in Lemma 4.1.1 we immediately see that

$$r_{1j} = \frac{\beta^k}{1-\beta^N}. \tag{4.11}$$

This completes the proof. $\square$

We recall from Section 2.2 that $\mathcal{A}(i)$ is the set of all nodes reachable in one step from node i, and further define $\mathcal{B}(i)$ to be the set of all nodes that can reach node i in one step. Then, we recall from (1.10) that $X(\beta)$ is a polytope defined by the system of linear constraints

$$\sum_i \sum_a (\delta_{ij} - \beta p_{iaj})\, x_{ia} = \left(1-\beta^N\right) \delta_{ij}, \quad j = 1, \ldots, N, \tag{4.12}$$

$$\sum_{a \in \mathcal{A}(1)} x_{1a} = 1, \tag{4.13}$$

$$x_{ia} \geq 0, \quad i = 1, \ldots, N, \quad a \in \mathcal{A}(i). \tag{4.14}$$

Let $\mathbf{x}(\beta) \in X(\beta)$, then the entries of $\mathbf{x}$ (for simplicity of notation, we drop the dependency on β) are in one-to-one correspondence with arcs (i,a), so that $x_{ia} = [\mathbf{x}]_{ia}$ for all $(i,a) \in \Gamma$. We say that $\mathbf{x}_h \in X(\beta)$ is Hamiltonian if there exists a Hamiltonian cycle h in the graph Γ such that for every $\beta \in (0,1)$,

(1) $[\mathbf{x}_h]_{ia} = 0$ whenever $(i,a) \notin h$, and

(2) $[\mathbf{x}_h]_{ia} > 0$ otherwise.

The importance of Lemma 4.1.1 and Corollary 4.1.2 is that they characterize the Hamiltonian (extreme) points of the polytope above to form a feasible region of various optimisation problems that can solve HCP.

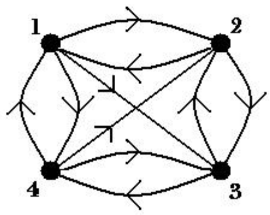


Figure 4.1: A 4-node graph with 10 arcs and two Hamiltonian cycles.

We note that all vectors $\mathbf{x}$ satisfying (4.12) also satisfy the matrix equation

$$W(\beta)\mathbf{x} = \left(1 - \beta^N\right)\mathbf{e}_1, \tag{4.15}$$

where $\mathbf{e_1} = [1, 0, \dots, 0]^T \in \mathbb{R}^N$, $W(\beta)$ is an $N \times m$ matrix (with m denoting the total number of arcs) whose rows are subscripted by j and columns by the pair ia. That is, a typical (j, ia)-entry of $W(\beta)$ is given by

$$w_{j,ia} := [W(\beta)]_{j,ia} \quad = \quad \delta_{ij} - \beta p_{iaj}, \quad j = 1, \dots, N, \quad (i, a) \in \Gamma. \tag{4.16}$$

Example 4.1.3 *Consider the 4-node graph Γ_4 displayed in Figure 4.1.*

It is clear that $\mathcal{A}(1) = \{2, 3, 4\}$, $\mathcal{A}(2) = \{1, 3\}$, $\mathcal{A}(3) = \{2, 4\}$, $\mathcal{A}(4) = \{1, 2, 3\}$. Hence any $\mathbf{x} \in X(\beta)$ is of the form $\mathbf{x}^T = (x_{12}, x_{13}, x_{14}, x_{21}, x_{23}, x_{32}, x_{34}, x_{41}, x_{42}, x_{43})$. Furthermore, $W(\beta)$ is a 4×10 matrix and equation (4.15) becomes

$$\left[\begin{array}{ccc:cc:cc:ccc} 1 & 1 & 1 & -\beta & 0 & 0 & 0 & -\beta & 0 & 0 \\ -\beta & 0 & 0 & 1 & 1 & -\beta & 0 & 0 & -\beta & 0 \\ 0 & -\beta & 0 & 0 & -\beta & 1 & 1 & 0 & 0 & -\beta \\ 0 & 0 & -\beta & 0 & 0 & 0 & -\beta & 1 & 1 & 1 \end{array}\right] \left[\begin{array}{c} x_{12} \\ x_{13} \\ x_{14} \\ \hdashline x_{21} \\ x_{23} \\ \hdashline x_{32} \\ x_{34} \\ \hdashline x_{41} \\ x_{42} \\ x_{43} \end{array}\right] = \left[\begin{array}{c} 1 - \beta^4 \\ 0 \\ 0 \\ 0 \end{array}\right]. \tag{4.17}$$

We define h_1 as the Hamiltonian cycle $1 \to 2 \to 3 \to 4 \to 1$ and h_2 as the reverse cycle $1 \to 4 \to 3 \to 2 \to 1$. Clearly, both h_1 and h_2 are Hamiltonian cycles in Γ_4. Also, we can view them as collections of arcs, namely, $h_1 = \{(1, 2), (2, 3), (3, 4), (4, 1)\}$

and $h_2 = \{(1,4),(4,3),(3,2),(2,1)\}$. *Now, we let* $\mathbf{x}_1^T$ *and* $\mathbf{x}_2^T$ *be two 10-dimensional vectors corresponding to* h_1 *and* h_2 *respectively:*

$$\mathbf{x}_1^T = \left[1\ 0\ 0 \,\vdots\, 0\ \beta \,\vdots\, 0\ \beta^2 \,\vdots\, \beta^3\ 0\ 0\right],$$

and

$$\mathbf{x}_2^T = \left[0\ 0\ 1 \,\vdots\, \beta^3\ 0 \,\vdots\, \beta^2\ 0 \,\vdots\, 0\ 0\ \beta\right].$$

We observe that both $\mathbf{x}_1$ and $\mathbf{x}_2$ in Example 4.1.3 satisfy (4.17), and therefore (4.12). Indeed, they also satisfy (4.13) and (4.14), and their positive entries correspond to linearly independent columns of $W(\beta)$. It follows that $\mathbf{x}_1$ and $\mathbf{x}_2$ are extreme points of $X(\beta)$. They are also (the only) Hamiltonian points in $X(\beta)$ for Γ_4.

Given the above, it seems plausible that all non-zero entries of all Hamiltonian points in $X(\beta)$ lie on exactly N curves $c_k(\beta)$

$$c_k(\beta) = \beta^k, \quad k = 0, 1, \ldots, N-1, \tag{4.18}$$

defined on the interval $(0,1)$. We call these the *canonical Hamiltonian curves* (cHc) of N-node graphs.

Example 4.1.3 (cont.) *For the 4-node graph* Γ_4 *in Example 4.1.3, we display the four canonical Hamiltonian curves in Figure 4.2.*

4.2 Canonical curves and Hamiltonian extreme points

In this section we prove that the characteristics of Hamiltonian points $\mathbf{x}_1$ and $\mathbf{x}_2$ demonstrated in Example 4.1.3 hold in general. Specifically, we show that if $\mathbf{x}_h \in X(\beta)$ is Hamiltonian, then its positive entries, as functions of β, coincide with (4.18). Moreover, the order of the mapping of these entries onto the canonical curves corresponds precisely to the order of arcs on the Hamiltonian cycle h.

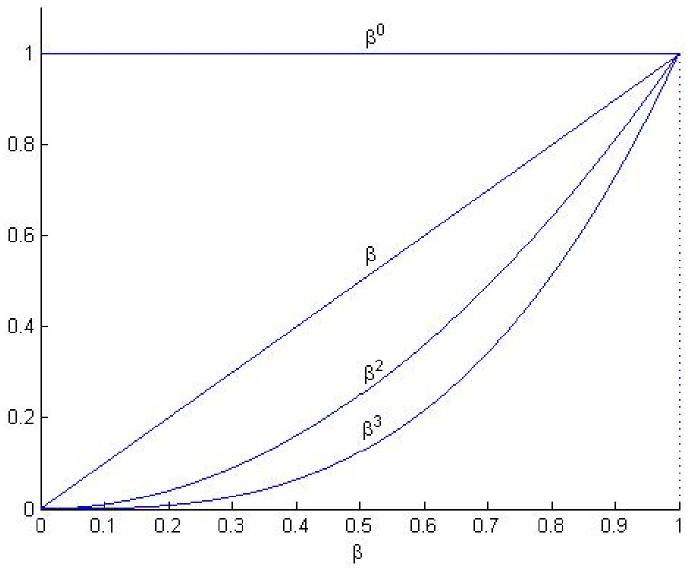


Figure 4.2: The cHc's of 4-node graphs.

In what follows we consider the Hamiltonian cycle

$$h : j_0 = 1 \to j_1 \to j_2 \to \cdots \to j_{N-2} \to j_{N\text{-}1} \to 1 = j_N, \tag{4.19}$$

consisting of the selection of arcs

$$(1, j_1), (j_1, j_2), \ldots, (j_{N-2}, j_{N-1}), (j_{N-1}, 1).$$

Thus j_k is the k-th node in h following the home node $j_0 = 1$, for each $k = 0, 1, \ldots, N-1$. Motivated by Example 4.1.3 we construct a vector $\mathbf{x}_h = \mathbf{x}_h(\beta)$ (with $\beta \in [0, 1)$), according to

$$[\mathbf{x}_h]_{ia} = \begin{cases} 0, & (i,a) \notin h, \\ \beta^k, & (i,a) = (j_k, j_{k+1}), k = 0, 1, 2, \ldots, N-1. \end{cases} \tag{4.20}$$

Theorem 4.2.1 *Recall that $X(\beta)$ is defined by (4.12)–(4.14), h is any Hamiltonian cycle, and that $\mathbf{x}_h$ is constructed as given in (4.20). It follows that*

(1) $\mathbf{x}_h$ is an extreme point of $X(\beta)$.

(2) $[\mathbf{x}_h]_{j_k, j_{k+1}} = c_k(\beta) = d_{j_k,1}, \quad k = 0, 1, \ldots, N-1.$

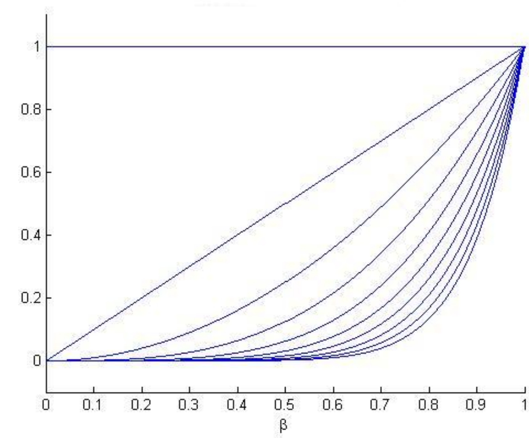


Figure 4.3: The cHc's of 10-node graphs.

Proof. For part (1) we note that, by construction, $\mathbf{x}_h \geq 0$ and $\sum_{a \in A(1)} [\mathbf{x}_h]_{1a} = \beta^0 = 1$. Thus, (4.13) and (4.14) are satisfied. Furthermore, substituting $\mathbf{x}_h$ into the left hand side of (4.12), for $j = 1$, we obtain by (4.20)

$$\begin{aligned}\sum_{a \in \mathcal{A}(1)} [\mathbf{x}_h]_{1a} - \beta \sum_{i \in \mathcal{B}(1)} [\mathbf{x}_h]_{i1} &= [\mathbf{x}_h]_{1j_1} - \beta [\mathbf{x}_h]_{j_{N-1}1} \\ &= \beta^0 - \beta\beta^{N-1} \\ &= 1 - \beta^N,\end{aligned}$$

which coincides with the right hand side of (4.12) for $j = 1$. Now, if $j = j_k$ for $k \geq 1$ and, again, we substitute $\mathbf{x}_h$ into the left hand side of (4.12), then we obtain from (4.20)

$$\begin{aligned}\sum_{a \in A(j_k)} [\mathbf{x}_h]_{j_k a} - \beta \sum_{i \in B(j_k)} [\mathbf{x}_h]_{i j_k} &= [\mathbf{x}_h]_{j_k j_{k+1}} - \beta [\mathbf{x}_h]_{j_{k-1} j_k} \\ &= \beta^k - \beta\beta^{k-1} \\ &= 0,\end{aligned}$$

that coincides with the right hand side of (4.12) for $j \geq 2$. Thus, $\mathbf{x}_h$ satisfies (4.12) as well, and therefore $\mathbf{x} \in X(\beta)$. Next, we define $\overline{\mathbf{x}}_h$ as an N-component vector consisting of only the positive entries in $\mathbf{x}_h$. We then observe that satisfying (4.12) reduces to satisfying

$$(I - \beta P_h)^T \overline{\mathbf{x}}_h = (1 - \beta^N)\mathbf{e}_1, \qquad (4.21)$$

when we suppress columns of $W(\beta)$ that correspond to 0 entries of $\mathbf{x}_h$. Since columns of $(I-\beta P_h)^T$ are linearly independent, $\mathbf{x}_h$ is a basic feasible solution of (4.12) and (4.14) that also satisfies (4.13). It follows that $\mathbf{x}_h$ is an extreme point of $X(\beta)$.

For part (2) it follows from (4.21) that

$$\overline{\mathbf{x}}_h^T = (1-\beta^N)\mathbf{e}_1^T(I-\beta P_h)^{-1} = (1-\beta^N)\mathbf{e}_1^T R_h(\beta). \tag{4.22}$$

The result now follows from Lemma 4.1.1, Corollary 4.1.2, and the adjoint form of $R_h(\beta)$. □

The importance of Theorem 4.2.1 stems from the fact that we now know that the canonical Hamiltonian curves fully describe the relative weights, as functions of β, that a Hamiltonian cycle associates to the arcs it selects. Asymptotically, with the exception of the first arc, all these weights tend to 0 as $\beta \downarrow 0$ and to 1 as $\beta \uparrow 1$. Separation between β^k and β^ℓ when $k > \ell$ may also prove to contain useful information in further analyses.

We represent $\mathbf{x}_h$ in the following form

$$\mathbf{x}_h = \sum_{k=0}^{N-1} \beta^k \mathbf{x}_h^k, \tag{4.23}$$

where each $\mathbf{x}_h^k$ is a vector containing a single unit in the position corresponding to the k-th arc of the Hamiltonian cycle h, and all other entries are zero. Recall that we refer to the initial arc $(1,i)$ of a Hamiltonian cycle as the 0-th arc in that Hamiltonian cycle.

Recall also that the linear equations that defined $X(\beta)$ take the form

$$\begin{aligned} \sum_{i=1}^{N}\sum_{a\in\mathcal{A}(i)} (\delta_{ij}-\beta p_{iaj})\, x_{ia} &= (1-\beta^N)\delta_{1j}, \quad j=1,\dots,N, \\ \sum_{a\in\mathcal{A}(1)} x_{1a} &= 1, \\ x_{ia} &\geq 0, \quad (i,a)\in\Gamma. \end{aligned}$$

We represent the above linear equations in matrix form as $\tilde{W}(\beta)\mathbf{x} = \mathbf{b}$. We then separate $\tilde{W}$ into two matrices W_0 and W_1, which correspond to the expressions without and with β respectively. That is, $\tilde{W} = W_0 + \beta W_1$, where

$$W_0 = \left[\begin{array}{c} \Delta \\ \hline 1 \cdots 1 \; 0 \cdots \cdots 0 \end{array}\right], \qquad W_1 = \left[\begin{array}{c} -P \\ \hline 0 \cdots \cdots \cdots \cdots 0 \end{array}\right], \tag{4.24}$$

where $\Delta := [\delta_{ij}]_{j=1,(i,a)\in\Gamma}^{N}$, and $P = [p_{iaj}]_{j=1,(i,a)\in\Gamma}^{N}$.

Example 4.2.2 *Consider the complete 4-node graph Γ_4^c, defined by the adjacency matrix*

$$\mathbb{A}_4^c = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix}. \tag{4.25}$$

For this graph, $\tilde{W}$ has the form

$$\begin{aligned} \tilde{W}(\beta) &= \left[\begin{array}{ccc|ccc|ccc|ccc} 1 & 1 & 1 & -\beta & 0 & 0 & -\beta & 0 & 0 & -\beta & 0 & 0 \\ -\beta & 0 & 0 & 1 & 1 & 1 & 0 & -\beta & 0 & 0 & -\beta & 0 \\ 0 & -\beta & 0 & 0 & -\beta & 0 & 1 & 1 & 1 & 0 & 0 & -\beta \\ 0 & 0 & -\beta & 0 & 0 & -\beta & 0 & 0 & -\beta & 1 & 1 & 1 \\ \hline 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{array}\right] \\ &= \left[\begin{array}{ccc|ccc|ccc|ccc} 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \\ \hline 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{array}\right] + \beta \left[\begin{array}{ccc|ccc|ccc|ccc} 0 & 0 & 0 & -1 & 0 & 0 & -1 & 0 & 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 & 0 & -1 & 0 & 0 & -1 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{array}\right]. \end{aligned}$$

In a similar fashion, we separate the vector $\mathbf{b}$ into two vectors $\mathbf{b}_0$ and $\mathbf{b}_N$, where $\mathbf{b} = \mathbf{b}_0 + \beta^N \mathbf{b}_N$, by defining

$$\mathbf{b}_0 = \left[\begin{array}{c} 1 \\ 0 \\ \vdots \\ 0 \\ \hline 1 \end{array}\right], \qquad \mathbf{b}_N = \left[\begin{array}{c} -1 \\ 0 \\ \vdots \\ 0 \\ \hline 0 \end{array}\right]. \tag{4.26}$$

Then, we rewrite the constraints of $X(\beta)$ as

$$\begin{aligned} (W_0 + \beta W_1)\mathbf{x} &= \mathbf{b}_0 + \beta^N \mathbf{b}_N, \\ x_{ij} &\geq 0. \end{aligned}$$

Then, from (4.23) we know that any Hamiltonian solution has a particular structure. We can substitute this into the above equality constraints to obtain

$$(W_0 + \beta W_1)\left(\sum_{k=0}^{N-1} \mathbf{x}_h^k \beta^k\right) \quad = \quad \mathbf{b}_0 + \beta^N \mathbf{b}_N,$$

and expanding the above sum we obtain

$$(W_0 + \beta W_1)\left(\mathbf{x}_h^0 + \beta \mathbf{x}_h^1 + \ldots + \beta^{N-1}\mathbf{x}_h^{N-1}\right) \quad = \quad \mathbf{b}_0 + \beta^N \mathbf{b}_N. \tag{4.27}$$

We know from Theorem 4.2.1 that $\mathbf{x}_h$ is feasible (and in particular, extremal) for all choices of $\beta \in [0, 1)$. We take advantage of this fact by expanding the left hand side of (4.27), and equating coefficients of corresponding powers of β to arrive at a new, parameter-free model. To emphasise that we do not know a Hamiltonian cycle in advance, we drop the subscript of h from the $\mathbf{x}^k$ vectors.

$$\begin{aligned}
W_0\mathbf{x}^0 &= \mathbf{b}_0,\\
W_0\mathbf{x}^1 + W_1\mathbf{x}^0 &= \mathbf{0},\\
W_0\mathbf{x}^2 + W_1\mathbf{x}^1 &= \mathbf{0},\\
W_0\mathbf{x}^3 + W_1\mathbf{x}^2 &= \mathbf{0},\\
&\vdots\\
W_0\mathbf{x}^{N-1} + W_1\mathbf{x}^{N-2} &= \mathbf{0},\\
W_1\mathbf{x}^{N-1} &= \mathbf{b}_N.
\end{aligned}$$

The above system of linear equations has the following block structure

$$\begin{bmatrix}
W_0 & & & & \\
W_1 & W_0 & & & \\
 & \ddots & \ddots & & \\
 & & \ddots & \ddots & \\
 & & & \ddots & \ddots \\
 & & & W_1 & W_0 \\
 & & & & W_1
\end{bmatrix}
\begin{bmatrix}
\mathbf{x}^0 \\ \mathbf{x}^1 \\ \vdots \\ \vdots \\ \mathbf{x}^{N-2} \\ \mathbf{x}^{N-1}
\end{bmatrix}
=
\begin{bmatrix}
\mathbf{b}_0 \\ \mathbf{0} \\ \vdots \\ \vdots \\ \vdots \\ \mathbf{0} \\ \mathbf{b}_N
\end{bmatrix}. \tag{4.28}$$

We then add to these parameter free linear equations further constraints on the new $\mathbf{x}^k$ variables. In particular, if each $\mathbf{x}^k$ contains only a single unit and the rest of the entries are non-zero, then $\mathbf{x}^k$ is a Hamiltonian solution. However, this requires integer constraints, so we relax the integer requirement and instead impose the following additional, linear, constraints

$$\sum_{(i,a)\in\Gamma} x_{ia}^k = 1, \qquad k = 0, \ldots, N-1, \tag{4.29}$$

$$x_{ia}^k \geq 0, \qquad k = 0, \ldots, N-1, \quad (i,a) \in \Gamma. \tag{4.30}$$

Our intention for this model is that by requiring the solution to satisfy the original $X(\beta)$ for all values of β as well as the structure specified in (4.23), only Hamiltonian solutions exist. The relaxation of (4.23) to (4.29)–(4.30) admits solutions which do not correspond to Hamiltonian cycles. Nonetheless, it is plausible that for a Hamiltonian graph, an extreme point solution found by an LP solver for the feasibility program made out of constraints (4.28)–(4.30) is more likely to correspond to a Hamiltonian cycle than that for (4.12)–(4.14).

We also hope that for some non-Hamiltonian graphs, the nonexistence of Hamiltonian solutions would imply that there are no feasible solutions to (4.28)–(4.30). Unfortunately, initial testing found no examples of this. However, the separation of the $\mathbf{x}_h$ vector into coefficients of the powers of β offers an additional level of freedom that is not present in the original form of $X(\beta)$, which we now take advantage of. From Theorem 4.2.1, we know that the element (i,a) in $\mathbf{x}_h$ corresponding to the k-th arc of a Hamiltonian cycle is equal to β^k, that is, $[x_h]_{ia} = \beta^k$. In the expanded form of $\mathbf{x}_h$, this implies that $[x^k]_{ia} = 1$.

Consequently, successive arcs belong to the non-zero elements in successive $\mathbf{x}^k$, and hence satisfy the following set of auxilliary constraints

$$\sum_{a\in\mathcal{B}(i)} x_{ai}^k + \sum_{j\neq i}\sum_{b\in\mathcal{A}(j)} x_{jb}^{k+1} = 1, \quad k = 0, \ldots, N-2, \quad i = 1, \ldots, N, \tag{4.31}$$

$$\sum_{a\in\mathcal{B}(1)} x_{a1}^{N-1} + \sum_{j\neq 1}\sum_{b\in\mathcal{A}(j)} x_{1b}^0 = 1. \tag{4.32}$$

The intuition behind these constraints is that exactly one of the following two statements must be true for every node i in every step k:

1) the node i is entered in step k, or

2) a node other than i is departed from in step $k+1$ (or step 0 if $k = N-1$).

We refer to constraints (4.28)–(4.32) the parameter-free LP feasibility model (PFLP). We tested PFLP on many sets of Hamiltonian cubic graphs. In some cases, for Hamiltonian graphs, we found an exact Hamiltonian cycle, but these cases were rare. We also tested PFLP on sets of non-Hamiltonian cubic graphs, and we found that PFLP is an infeasible set of constraints for every cubic bridge graph (all of which are non-Hamiltonian), up to and including size 18. However, for every non-bridge non-Hamiltonian (NHNB) graph considered, up to and including size 18, PFLP is a feasible set of constraints. This experiment led us to the following conjecture.

Conjecture 4.2.3 *The constraints (4.28)–(4.32) form an infeasible polytope for any Γ corresponding to a bridge graph.*

In all of our experiments where a feasible solution is found that does not correspond to the canonical Hamiltonian curves, for each node we observe that the set of variables corresponding to arcs emanating from that node contains multiple non-zero entries whose sum is β^k for some k. We call the curves of this type *fake Hamiltonian curves.* An example of this phenomenon is shown in Figure 4.4.

4.3 Canonical Hamiltonian surfaces

In this section we consider a perturbed probability transition matrix
$P^\nu := (1-\nu)P + \frac{\nu}{N}J$. Clearly, if P is doubly stochastic, then P^ν is doubly stochastic as well for $0 \leq \nu \leq 1$.

In particular, we consider $X(\beta, \nu)$, the more general set of constraints for which $X(\beta)$

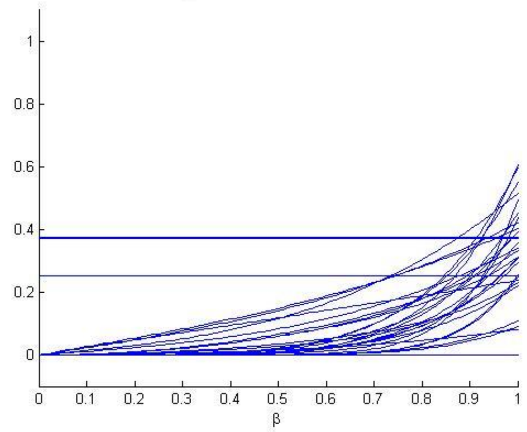


Figure 4.4: A set of 30 fake Hamiltonian curves for a 10-node graph.

is a special case where $\nu = 0$. Let d_{iaj} be defined as

$$d_{iaj} \quad := \quad \begin{cases} \frac{1}{N}, & p_{iaj} = 0, \\ -\frac{N-1}{N}, & p_{iaj} = 1. \end{cases} \tag{4.33}$$

Then, $X(\beta, \nu)$ are defined by the following constraints:

$$\sum_{i=1}^{N} \sum_{a \in \mathcal{A}(i)} \left(\delta_{ij} - \beta(p_{iaj} + \nu d_{iaj})\right) x_{ia} \quad = \quad d^{\nu}(\beta)\delta_{1j}, \quad j = 1, \ldots, N, \tag{4.34}$$

$$\sum_{a \in \mathcal{A}(1)} x_{1a} \quad = \quad 1, \tag{4.35}$$

$$x_{ia} \quad \geq \quad 0, \quad (i, a) \in \Gamma. \tag{4.36}$$

We now derive formulae for the reverse standard Hamiltonian cycle h_R, which is selected in lieu of the standard Hamiltonian cycle h to make some of the proceeding calculations simpler. All of the proceeding formulae can be generalised to generic Hamiltonian cycles via permutation transformations such as that given in (4.1). The eventual result that we prove is that all Hamiltonian solutions to (4.34)–(4.36) take the form

$$[\mathbf{x}^*_{h_R}]_{ia} \quad = \quad \begin{cases} \sum_{k=0}^{N-1} \sum_{\ell=0}^{k} c^r_{k\ell} \beta^k \nu^\ell, & (i, a) = (N - r + 1, N - r) \text{ for some } r, \\ 0, & \text{otherwise,} \end{cases}$$

for certain coefficients $c^r_{k\ell}(\beta)$ that we derive in this section.

Lemma 4.3.1 *Let h_R be the standard reverse Hamiltonian cycle containing arcs $1 \to N \to N$-$1 \to \cdots \to 2 \to 1$, and P_{h_R} be the associated probability transition matrix. We define $P^{\nu}_{h_R} := (1-\nu)P_{h_R} + \frac{\nu}{N}J$, and $M := I - \beta P^{\nu}_{h_R}$. We define $d^{\nu}(\beta) := \det(M)$, and $\lambda := \beta\nu - \beta$. Then*

$$d^{\nu}(\beta) \;=\; (1-\beta)\frac{1-(-\lambda)^N}{1+\lambda}. \tag{4.37}$$

Proof. Consider the matrix M which is of the following form

$$\begin{bmatrix} 1-\frac{1}{N}\beta\nu & -\frac{1}{N}\beta\nu & \cdots & \cdots & -\frac{1}{N}\beta\nu & -\beta(1-\frac{N-1}{N}\nu) \\ -\beta(1-\frac{N-1}{N}\nu) & 1-\frac{1}{N}\beta\nu & -\frac{1}{N}\beta\nu & \cdots & \cdots & -\frac{1}{N}\beta\nu \\ -\frac{1}{N}\beta\nu & -\beta(1-\frac{N-1}{N}\nu) & 1-\frac{1}{N}\beta\nu & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & \ddots & \ddots & -\frac{1}{N}\beta\nu \\ -\frac{1}{N}\beta\nu & \cdots & \cdots & -\frac{1}{N}\beta\nu & -\beta(1-\frac{N-1}{N}\nu) & 1-\frac{1}{N}\beta\nu \end{bmatrix}. \tag{4.38}$$

Finding the determinant of this matrix directly is quite difficult, but an appropriate change of basis makes the matrix sparse, which makes the determinant simpler to calculate. One such basis is

$$B \;=\; I + \mathbf{e}\mathbf{e}_N^T - \mathbf{e}_N\mathbf{e}_N^T, \tag{4.39}$$

whose inverse has the simple form

$$B^{-1} \;=\; I - \mathbf{e}\mathbf{e}_N^T + \mathbf{e}_N\mathbf{e}_N^T. \tag{4.40}$$

We verify (4.40) as follows:

$$\begin{aligned} B(I - \mathbf{e}\mathbf{e}_N^T + \mathbf{e}_N\mathbf{e}_N^T) &= (I + \mathbf{e}\mathbf{e}_N^T - \mathbf{e}_N\mathbf{e}_N^T)(I - \mathbf{e}\mathbf{e}_N^T + \mathbf{e}_N\mathbf{e}_N^T) \\ &= I - \mathbf{e}\mathbf{e}_N^T + \mathbf{e}_N\mathbf{e}_N^T + \mathbf{e}\mathbf{e}_N^T - \mathbf{e}\mathbf{e}_N^T\mathbf{e}\mathbf{e}_N^T + \mathbf{e}\mathbf{e}_N^T\mathbf{e}_N\mathbf{e}_N^T \\ &\qquad -\mathbf{e}_N\mathbf{e}_N^T + \mathbf{e}_N\mathbf{e}_N^T\mathbf{e}\mathbf{e}_N^T - \mathbf{e}_N\mathbf{e}_N^T\mathbf{e}_N\mathbf{e}_N^T \\ &= I - \mathbf{e}\mathbf{e}_N^T + \mathbf{e}_N\mathbf{e}_N^T + \mathbf{e}\mathbf{e}_N^T - \mathbf{e}\mathbf{e}_N^T + \mathbf{e}\mathbf{e}_N^T - \mathbf{e}_N\mathbf{e}_N^T + \mathbf{e}_N\mathbf{e}_N^T - \mathbf{e}_N\mathbf{e}_N^T \\ &= I. \end{aligned}$$

These two matrices have the form

$$B = \begin{bmatrix} 1 & & & & 1 \\ & 1 & & & 1 \\ & & \ddots & & \vdots \\ & & & \ddots & \vdots \\ & & & 1 & 1 \\ & & & & 1 \end{bmatrix}, \quad B^{-1} = \begin{bmatrix} 1 & & & & -1 \\ & 1 & & & -1 \\ & & \ddots & & \vdots \\ & & & \ddots & \vdots \\ & & & 1 & -1 \\ & & & & 1 \end{bmatrix}.$$

For simplicity of notation we define $\gamma_1 := \beta(1-\nu)$ and $\gamma_2 := \frac{\beta\nu}{N}$, so that $M = I - \gamma_1 P_{h_R} - \gamma_2 J$. Note that $\gamma_1 = -\lambda$. Consider $B^{-1}MB$ that corresponds to the change of basis via B:

$$B^{-1}MB \;=\; (I - \mathbf{e}\mathbf{e}_N^T + \mathbf{e}_N\mathbf{e}_N^T)\,[I - \gamma_1 P_{h_R} - \gamma_2 J]\,(I + \mathbf{e}\mathbf{e}_N^T - \mathbf{e}_N\mathbf{e}_N^T).$$

We expand first the two rightmost factors. Recalling that $P_{h_R}\mathbf{e} = \mathbf{e}$, $J\mathbf{e}_N = \mathbf{e}$ and $J\mathbf{e} = (N)\mathbf{e}$, we obtain

$$\begin{aligned} B^{-1}MB \;&=\; (I - \mathbf{e}\mathbf{e}_N^T + \mathbf{e}_N\mathbf{e}_N^T)\left[I + \mathbf{e}\mathbf{e}_N^T - \mathbf{e}_N\mathbf{e}_N^T - \gamma_1 P_{h_R} - \gamma_1 P_{h_R}\mathbf{e}\mathbf{e}_N^T\right. \\ &\qquad \left. + \gamma_1 P_{h_R}\mathbf{e}_N\mathbf{e}_N^T - \gamma_2 J - \gamma_2 J\mathbf{e}\mathbf{e}_N^T + \gamma_2 J\mathbf{e}_N\mathbf{e}_N^T\right] \\ &=\; (I - \mathbf{e}\mathbf{e}_N^T + \mathbf{e}_N\mathbf{e}_N^T)\left[I + \mathbf{e}\mathbf{e}_N^T - \mathbf{e}_N\mathbf{e}_N^T - \gamma_1 P_{h_R} - \gamma_1\mathbf{e}\mathbf{e}_N^T\right. \\ &\qquad \left. + \gamma_1 P_{h_R}\mathbf{e}_N\mathbf{e}_N^T - \gamma_2 J - \gamma_2 N\mathbf{e}\mathbf{e}_N^T + \gamma_2\mathbf{e}\mathbf{e}_N^T\right]. \end{aligned}$$

Gathering like terms we find

$$\begin{aligned} B^{-1}MB \;&=\; (I - \mathbf{e}\mathbf{e}_N^T + \mathbf{e}_N\mathbf{e}_N^T)\left[I + (1 - \gamma_1 - (N-1)\gamma_2)\mathbf{e}\mathbf{e}_N^T - \mathbf{e}_N\mathbf{e}_N^T\right. \\ &\qquad\qquad \left. - \gamma_1 P_{h_R}(I - \mathbf{e}_N\mathbf{e}_N^T) - \gamma_2 J\right]. \end{aligned}$$

Then, expanding the above we obtain

$$\begin{aligned} B^{-1}MB \;&=\; I + (1 - \gamma_1 - (N-1)\gamma_2)\mathbf{e}\mathbf{e}_N^T - \mathbf{e}_N\mathbf{e}_N^T - \gamma_1 P_{h_R}(I - \mathbf{e}_N\mathbf{e}_N^T) - \gamma_2 J \\ &\quad - \mathbf{e}\mathbf{e}_N^T - (1 - \gamma_1 - (N-1)\gamma_2)\mathbf{e}\mathbf{e}_N^T\mathbf{e}\mathbf{e}_N^T + \mathbf{e}\mathbf{e}_N^T\mathbf{e}_N\mathbf{e}_N^T + \gamma_1\mathbf{e}\mathbf{e}_N^T P_{h_R}(I - \mathbf{e}_N\mathbf{e}_N^T) \\ &\quad + \gamma_2\mathbf{e}\mathbf{e}_N^T J + \mathbf{e}_N\mathbf{e}_N^T + (1 - \gamma_1 - (N-1)\gamma_2)\mathbf{e}_N\mathbf{e}_N^T\mathbf{e}\mathbf{e}_N^T - \mathbf{e}_N\mathbf{e}_N^T\mathbf{e}_N\mathbf{e}_N^T \\ &\quad - \gamma_1\mathbf{e}_N\mathbf{e}_N^T P_{h_R}(I - \mathbf{e}_N\mathbf{e}_N^T) - \gamma_2\mathbf{e}_N\mathbf{e}_N^T J. \end{aligned}$$

Noting that $\mathbf{e}_N^T\mathbf{e} = \mathbf{e}_N^T\mathbf{e}_N = 1$, and that $\mathbf{e}\mathbf{e}_N^T J = J$, we see that

$$\begin{aligned} B^{-1}MB &= I + (1-\gamma_1-(N-1)\gamma_2)\mathbf{e}\mathbf{e}_N^T - \mathbf{e}_N\mathbf{e}_N^T - \gamma_1 P_{h_R}(I-\mathbf{e}_N\mathbf{e}_N^T) - \gamma_2 J \\ &\quad -\mathbf{e}\mathbf{e}_N^T - (1-\gamma_1-(N-1)\gamma_2)\mathbf{e}\mathbf{e}_N^T + \mathbf{e}\mathbf{e}_N^T + \gamma_1\mathbf{e}\mathbf{e}_N^T P_{h_R}(I-\mathbf{e}_N\mathbf{e}_N^T) + \gamma_2 J \\ &\quad +\mathbf{e}_N\mathbf{e}_N^T + (1-\gamma_1-(N-1)\gamma_2)\mathbf{e}_N\mathbf{e}_N^T - \mathbf{e}_N\mathbf{e}_N^T - \gamma_1\mathbf{e}_N\mathbf{e}_N^T P_{h_R}(I-\mathbf{e}_N\mathbf{e}_N^T) - \gamma_2\mathbf{e}_N\mathbf{e}^T. \end{aligned}$$

Finally, we collect like terms, note that $\mathbf{e}_N^T P_{h_R} = \mathbf{e}_{N-1}^T$, $P_{h_R}\mathbf{e}_N = \mathbf{e}_1$, and $\mathbf{e}_N^T P_{h_R}\mathbf{e}_N = 0$, and substitute $\gamma_1 = \beta(1-\nu)$ and $\gamma_2 = \frac{\beta\nu}{N}$ back into the equation to obtain

$$\begin{aligned} B^{-1}MB &= I - \mathbf{e}_N\mathbf{e}_N^T - \gamma_1 P_{h_R}(I-\mathbf{e}_N\mathbf{e}_N^T) + \gamma_1\mathbf{e}\mathbf{e}_N^T P_{h_R}(I-\mathbf{e}_N\mathbf{e}_N^T) \\ &\quad +(1-\gamma_1-(N-1)\gamma_2)\mathbf{e}_N\mathbf{e}_N^T - \gamma_1\mathbf{e}_N\mathbf{e}_N^T P_{h_R}(I-\mathbf{e}_N\mathbf{e}_N^T) - \gamma_2\mathbf{e}_N\mathbf{e}^T \\ &= I - (\gamma_1+(N-1)\gamma_2)\mathbf{e}_N\mathbf{e}_N^T - \gamma_1 P_{h_R}(I-\mathbf{e}_N\mathbf{e}_N^T) \\ &\quad +\gamma_1\mathbf{e}\mathbf{e}_N^T P_{h_R} - \gamma_1\mathbf{e}_N\mathbf{e}_N^T P_{h_R} - \gamma_2\mathbf{e}_N\mathbf{e}^T \\ &= I - (\beta - \frac{\beta\nu}{N})\mathbf{e}_N\mathbf{e}_N^T + \lambda\left[P_{h_R} - \mathbf{e}_1\mathbf{e}_N^T - \mathbf{e}\mathbf{e}_{N-1}^T + \mathbf{e}_N\mathbf{e}_{N-1}^T\right] - \frac{\beta\nu}{N}\mathbf{e}_N\mathbf{e}^T. \end{aligned}$$

Thus, the matrix transformation M in the new basis takes the form

$$B^{-1}MB = \begin{bmatrix} 1 & 0 & \cdots & \cdots & \cdots & 0 & -\lambda & 0 \\ \lambda & 1 & 0 & \cdots & \cdots & 0 & -\lambda & 0 \\ 0 & \lambda & 1 & 0 & \cdots & 0 & -\lambda & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots & \vdots & \vdots \\ \vdots & & \ddots & \ddots & \ddots & 0 & \vdots & \vdots \\ 0 & \cdots & \cdots & 0 & \lambda & 1 & -\lambda & 0 \\ 0 & \cdots & \cdots & \cdots & 0 & \lambda & 1-\lambda & 0 \\ -\frac{1}{N}\beta\nu & -\frac{1}{N}\beta\nu & \cdots & \cdots & \cdots & -\frac{1}{N}\beta\nu & \frac{(N-1)\beta\nu}{N} - \beta & 1-\beta \end{bmatrix}. \tag{4.41}$$

To find $d^\nu(\beta) = \det(M) = \det(B^{-1}MB)$, we expand (4.41) on column N. There is only a single non-zero entry in this column, namely $(1-\beta)$, in position (N,N). Performing this expansion, we find

$$\begin{aligned} d^\nu(\beta) &= (-1)^{N+N}(1-\beta)\det([B^{-1}MB]^{N,N}) \\ &= (1-\beta)\det([B^{-1}MB]^{N,N}), \end{aligned} \tag{4.42}$$

where $[B^{-1}MB]^{N,N}$ is (4.41) with row N and column N removed. To find $\det([B^{-1}MB]^{N,N})$, we first multiply $[B^{-1}MB]^{N,N}$, on the right, by an $(N-1)\times(N-1)$ elementary matrix E:

$$E \quad := \quad I + \mathbf{e}\mathbf{e}_{N-1}^T - \mathbf{e}_{N-1}\mathbf{e}_{N-1}^T, \tag{4.43}$$

which has the same structure as the $N \times N$ matrix (4.39). Then, we obtain the following $(N-1)\times(N-1)$ upper-Hessenberg matrix (that is, an upper-triangular matrix that also has non-zeros on its subdiagonal),

$$[B^{-1}MB]^{N,N}E \quad = \quad \begin{bmatrix} 1 & 0 & \cdots & \cdots & 0 & 1-\lambda \\ \lambda & 1 & 0 & \cdots & 0 & 1 \\ 0 & \ddots & \ddots & \ddots & \vdots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 & \vdots \\ \vdots & & \ddots & \ddots & 1 & \vdots \\ 0 & \cdots & \cdots & 0 & \lambda & 1 \end{bmatrix}. \tag{4.44}$$

Note that as $\det(E) = 1$, the determinant of (4.44) is the same as the determinant of $[B^{-1}MB]^{N,N}$. Next, we find $\det([B^{-1}MB]^{N,N}E)$ by performing row operations that convert (4.44) into an upper-triangular matrix. Consider a pair of rows $\mathbf{r}_1^T$ and $\mathbf{r}_2^T$ of the form

$$\begin{bmatrix} \mathbf{r}_1^T \\ \mathbf{r}_2^T \end{bmatrix} = \begin{bmatrix} 0 & \cdots & 0 & 1 & 0 & 0 & \cdots & 0 & \sum_{i=0}^{n}(-\lambda)^i \\ 0 & \cdots & 0 & \lambda & 1 & 0 & \cdots & 0 & 1 \end{bmatrix}, \tag{4.45}$$

which contains an arbitrary (perhaps zero) number of 0 entries at the start of each row. We observe that the first two rows of (4.44) correspond to the pair of rows (4.45) with $n = 1$, and no zero entries at the start of each row. Then, we perform the following row operation

$$\mathbf{r}_2^T \to \mathbf{r}_2^T - \lambda\mathbf{r}_1^T. \tag{4.46}$$

Then, the pair of rows becomes

$$\begin{bmatrix} 0 & \cdots & 0 & 1 & 0 & 0 & \cdots & 0 & \sum_{i=0}^{n}(-\lambda)^i \\ 0 & \cdots & 0 & 0 & 1 & 0 & \cdots & 0 & \sum_{i=0}^{n+1}(-\lambda)^i \end{bmatrix}.$$

After the row operation (4.46), the new second row and the third row of (4.44) also correspond to the pair of rows (4.45), for $n = 2$ and a single zero entry at the start of each row. By induction, we continue this process, performing $N-2$ row operations. We perform these operations by left multiplying by the following elementary matrices E_i

$$E_i \quad := \quad I - \lambda \mathbf{e}_{i+1}\mathbf{e}_i^T, \quad i = 1, \ldots, N-2. \tag{4.47}$$

Clearly, $\det(E_i) = 1$ for all i, so none of these row operations alter the determinant value of (4.44). Then, we obtain the following matrix

$$\left(\prod_{i=1}^{N-2} E_i\right)[B^{-1}MB]^{N,N}E \quad = \quad \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 & \sum\limits_{i=0}^{1}(-\lambda)^i \\ 0 & 1 & 0 & \cdots & 0 & \sum\limits_{i=0}^{2}(-\lambda)^i \\ \vdots & \ddots & \ddots & \ddots & \vdots & \vdots \\ \vdots & & \ddots & \ddots & 0 & \vdots \\ 0 & 0 & 0 & \cdots & 1 & \sum\limits_{i=0}^{N-2}(-\lambda)^i \\ 0 & 0 & 0 & \cdots & 0 & \sum\limits_{i=0}^{N-1}(-\lambda)^i \end{bmatrix}. \tag{4.48}$$

This matrix is upper triangular, and so

$$\det([B^{-1}MB]^{N,N}) = \det\left[\left(\prod_{i=1}^{N-2} E_i\right)[B^{-1}MB]^{N,N}E\right] \quad = \quad \sum_{i=0}^{N-1}(-\lambda)^i. \tag{4.49}$$

Finally, we substitute (4.49) into (4.42), and use the geometric series formula to obtain the value of $d^\nu(\beta)$:

$$\begin{aligned} d^\nu(\beta) \quad &= \quad (1-\beta)\sum_{i=0}^{N-1}(-\lambda)^i \\ &= \quad (1-\beta)\frac{1-(-\lambda)^N}{1+\lambda}, \end{aligned} \tag{4.50}$$

which coincides with (4.37). □

Example 4.3.2 *Consider the standard reverse 8-node Hamiltonian cycle*

$$P_{h_R} \quad = \quad \begin{bmatrix} 0&0&0&0&0&0&0&1\\ 1&0&0&0&0&0&0&0\\ 0&1&0&0&0&0&0&0\\ 0&0&1&0&0&0&0&0\\ 0&0&0&1&0&0&0&0\\ 0&0&0&0&1&0&0&0\\ 0&0&0&0&0&1&0&0\\ 0&0&0&0&0&0&1&0 \end{bmatrix}. \tag{4.51}$$

Then, we construct $M := I - \beta((1-\nu)P_{h_R} + \frac{\nu}{8}J)$

$$M \quad = \quad \begin{bmatrix} 1-\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & \frac{7}{8}\beta\nu-\beta \\ \frac{7}{8}\beta\nu-\beta & 1-\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} \\ -\frac{\beta\nu}{8} & \frac{7}{8}\beta\nu-\beta & 1-\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} \\ -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & \frac{7}{8}\beta\nu-\beta & 1-\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} \\ -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & \frac{7}{8}\beta\nu-\beta & 1-\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} \\ -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & \frac{7}{8}\beta\nu-\beta & 1-\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} \\ -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & \frac{7}{8}\beta\nu-\beta & 1-\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} \\ -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & \frac{7}{8}\beta\nu-\beta & 1-\frac{\beta\nu}{8} \end{bmatrix}.$$

We wish to find $d^\nu(\beta) = \det(M)$*. After the change of basis (4.39), we obtain*

$$B^{-1}MB \quad = \quad \begin{bmatrix} 1&0&0&0&0&0&-\lambda&0\\ \lambda&1&0&0&0&0&-\lambda&0\\ 0&\lambda&1&0&0&0&-\lambda&0\\ 0&0&\lambda&1&0&0&-\lambda&0\\ 0&0&0&\lambda&1&0&-\lambda&0\\ 0&0&0&0&\lambda&1&-\lambda&0\\ 0&0&0&0&0&\lambda&1-\lambda&0\\ -\frac{\beta\nu}{8}&-\frac{\beta\nu}{8}&-\frac{\beta\nu}{8}&-\frac{\beta\nu}{8}&-\frac{\beta\nu}{8}&-\frac{\beta\nu}{8}&\frac{7}{8}\beta\nu-\beta&1-\beta \end{bmatrix}.$$

Then, we expand on the right column to obtain $d^\nu(\beta) = (1-\beta)\det([B^{-1}MB]^{8,8})$*. After multiplying* $[B^{-1}MB]^{8,8}$ *on the right by the elementary matrix* $E = I + \mathbf{e}\mathbf{e}_7^T - \mathbf{e}_7\mathbf{e}_7^T$ *defined in (4.43), we obtain*

$$[B^{-1}MB]^{8,8}E \quad = \quad \begin{bmatrix} 1&0&0&0&0&0&1-\lambda\\ \lambda&1&0&0&0&0&1\\ 0&\lambda&1&0&0&0&1\\ 0&0&\lambda&1&0&0&1\\ 0&0&0&\lambda&1&0&1\\ 0&0&0&0&\lambda&1&1\\ 0&0&0&0&0&\lambda&1 \end{bmatrix}.$$

Finally, we perform six row operations using elementary matrices (4.47) to obtain

$$\left(\prod_{i=2}^{7} E_i\right)[B^{-1}MB]^{8,8}E \;=\; \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 1-\lambda \\ 0 & 1 & 0 & 0 & 0 & 0 & 1-\lambda+\lambda^2 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1-\lambda+\lambda^2-\lambda^3 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1-\lambda+\lambda^2-\lambda^3+\lambda^4 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1-\lambda+\lambda^2-\lambda^3+\lambda^4-\lambda^5 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1-\lambda+\lambda^2-\lambda^3+\lambda^4-\lambda^5+\lambda^6 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1-\lambda+\lambda^2-\lambda^3+\lambda^4-\lambda^5+\lambda^6-\lambda^7 \end{bmatrix}.$$

Clearly, $\det\left(\left(\prod_{i=2}^{7} E_i\right)[B^{-1}MB]^{8,8}E\right) = 1-\lambda+\lambda^2-\lambda^3+\lambda^4-\lambda^5+\lambda^6-\lambda^7$, *and so we obtain the final result*

$$\begin{aligned} d^{\nu}(\beta) &= (1-\beta)(1-\lambda+\lambda^2-\lambda^3+\lambda^4-\lambda^5+\lambda^6-\lambda^7) \\ &= (1-\beta)\left(\frac{1-(-\lambda)^8}{1+\lambda}\right). \end{aligned}$$

Proposition 4.3.3 *For a graph* Γ *with* N *nodes, the determinant* $d^{\nu}(\beta)$ *can be expressed as*

$$d^{\nu}(\beta) \;=\; \sum_{k=0}^{N}\sum_{\ell=0}^{k} c_{k\ell}\beta^k\nu^\ell,$$

for some coefficients $c_{k\ell}$.

Proof. The determinant $d^{\nu}(\beta)$ is of the $N\times N$ matrix M, each element of which contains terms of the form $k_1+k_2\beta+k_3\beta\nu$, for some coefficients k_1,k_2,k_3. Then, we observe that $d^{\nu}(\beta)$ is a bivariate polynomial in β and ν (with maximum degree of $2N$), and that the power of ν cannot exceed the power of β. That is, $d^{\nu}(\beta)$ takes the form $\sum\limits_{k=0}^{N}\sum\limits_{\ell=0}^{k} c_{k\ell}\beta^k\nu^\ell$. □

We find the coefficients $c_{k\ell}$ by calculating

$$c_{k\ell} \;=\; \frac{1}{k!\ell!}\left[\frac{\partial^{k+\ell}d^{\nu}(\beta)}{\partial\beta^k\partial\nu^\ell}\right]_{\beta=0,\nu=0}.$$

In other words, starting with $d^{\nu}(\beta)$, we find the k-th derivative with respect to β, the ℓ-th derivative with respect to ν, divide by $k!\ell!$ and set both $\beta=0$ and $\nu=0$.

Proposition 4.3.4 *The coefficients $c_{k\ell}$ have the values*

$$c_{k\ell} = \begin{cases} (-1)^{\ell}\begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix}, & k \neq N, \\ (-1)^{\ell-1}\begin{pmatrix} N-1 \\ \ell \end{pmatrix}, & k = N, \quad \ell < N, \\ 0, & k = \ell = N. \end{cases} \tag{4.52}$$

Proof. From (4.50) we know that

$$\begin{aligned} d^{\nu}(\beta) &= (1-\beta)\frac{1-(-\lambda)^N}{1+\lambda} = (1-\beta)\left(1+(-\lambda)+(-\lambda)^2+\cdots+(-\lambda)^{N-1}\right) \\ &= \theta_1\theta_2, \end{aligned}$$

where $\theta_1 := (1-\beta)$ and $\theta_2 := \left(1+(-\lambda)+(-\lambda)^2+\ldots+(-\lambda)^{N-1}\right)$.

We first find the k-th derivative of $d^{\nu}(\beta)$ with respect to β. Using the product rule for derivatives, we obtain

$$\frac{\partial^k d^{\nu}(\beta)}{\partial\beta^k} = \sum_{i=0}^{k}\frac{k!}{i!(k-i)!}\frac{\partial^i\theta_1}{\partial\beta^i}\frac{\partial^{k-i}\theta_2}{\partial\beta^{k-i}}.$$

Since θ_1 is a linear function, it is clear that $\frac{\partial^i\theta_1}{\partial\beta^i} = 0$ for all $i \geq 2$, and therefore we ignore most of the terms in this sum. Then,

$$\begin{aligned} \frac{\partial^k d^{\nu}(\beta)}{\partial\beta^k} &= \sum_{i=0}^{1}\frac{k!}{i!(k-i)!}\frac{\partial^i\theta_1}{\partial\beta^i}\frac{\partial^{k-i}\theta_2}{\partial\beta^{k-i}} \\ &= \theta_1\frac{\partial^k\theta_2}{\partial\beta^k} + k\frac{\partial\theta_1}{\partial\beta}\frac{\partial^{k-1}\theta_2}{\partial\beta^{k-1}}. \end{aligned} \tag{4.53}$$

Consider the n-th derivative of θ_2 with respect to β, for any $n \geq 1$. We recall that $\lambda = \beta\nu - \beta$ and therefore $\frac{\partial\lambda}{\partial\beta} = (\nu - 1)$. Consequently,

$$\frac{\partial^n\theta_2}{\partial\beta^n} = (-1)^n(\nu-1)^n\sum_{j=n}^{N-1}\frac{j!}{(j-n)!}(-\lambda)^{j-n}. \tag{4.54}$$

Then, substituting (4.54) into (4.53), we obtain

$$\begin{aligned} \frac{\partial^k d^{\nu}(\beta)}{\partial\beta^k} &= (1-\beta)(-1)^k(\nu-1)^k\sum_{j=k}^{N-1}\frac{j!}{(j-k)!}(-\lambda)^{j-k} \\ &\quad +(k)(-1)(-1)^{k-1}(\nu-1)^{k-1}\sum_{j=k-1}^{N-1}\frac{j!}{(j-k+1)!}(-\lambda)^{j-k+1}. \end{aligned} \tag{4.55}$$

We observe that if $k = N$, the first of the two sums in (4.55) is 0. To accommodate this, we consider two cases - first, when $k < N$, and second when $k = N$.

Case 1: $k < N$. Next, we set $\beta = 0$. Note that this also sets $\lambda = \beta\nu - \beta = 0$, and so the only non-zero terms remaining in the sums (4.55) are those where the power of $(-\lambda)$ is 0. Hence,

$$\begin{aligned}\left[\frac{\partial^k d^\nu(\beta)}{\partial\beta^k}\right]_{\beta=0} &= (-1)^k(\nu-1)^k k! + (-1)^k(\nu-1)^{k-1}k(k-1)! \\ &= (-1)^k k!\left[(\nu-1)^k + (\nu-1)^{k-1}\right]. \end{aligned} \tag{4.56}$$

Next, we find the ℓ-th derivative (for $\ell \le k$) of (4.56) with respect to ν. However, if $\ell = k$, the second term in the square brackets in (4.56) is 0. Hence, we consider the ℓ-th derivative for two cases, one where $\ell < k$ and one where $\ell = k$.

$$\left[\frac{\partial^{k+\ell} d^\nu(\beta)}{\partial\beta^k\partial\nu^\ell}\right]_{\beta=0} = \begin{cases} (-1)^k k!\left[\frac{k!}{(k-\ell)!}(\nu-1)^{k-\ell} + \frac{(k-1)!}{(k-1-\ell)!}(\nu-1)^{k-\ell-1}\right], & \ell < k, \\ \\ (-1)^k k! k!, & \ell = k. \end{cases} \tag{4.57}$$

Setting $\nu = 0$ and dividing by $k!\ell!$ in (4.57), we obtain the coefficient $c_{k\ell}$. We first consider $\ell < k$:

$$\begin{aligned} c_{k\ell} = \frac{1}{k!\ell!}\left[\frac{\partial^{k+\ell} d^\nu(\beta)}{\partial\beta^k\partial\nu^\ell}\right]_{\beta=0,\nu=0} &= (-1)^k\frac{k!}{k!\ell!}\left[\frac{k!}{(k-\ell)!}(-1)^{k-\ell} - \frac{(k-1)!}{(k-1-\ell)!}(-1)^{k-\ell}\right] \\ &= \frac{(-1)^\ell}{\ell!}\left[\frac{(k-1)!}{(k-1-\ell)!}\left(\frac{k}{k-\ell} - 1\right)\right] \\ &= \frac{(-1)^\ell}{\ell!}\frac{(k-1)!}{(k-1-\ell)!}\frac{\ell}{k-\ell} \\ &= \frac{(-1)^\ell(k-1)!}{(\ell-1)!(k-l)!} \\ &= (-1)^\ell\begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix}. \end{aligned} \tag{4.58}$$

Next, we consider $\ell = k$. We set $\nu = 0$ and divide by $k!k!$ to obtain

$$c_{kk} = (-1)^k. \tag{4.59}$$

Note that setting $\ell = k$ in (4.58) yields (4.59), so we simply use the expression (4.58) for all $\ell \le k$. Expression (4.58) coincides with the first case of (4.52).

Case 2: $k = N$. Next, we set $\beta = 0$. Again, note that this sets $\lambda = 0$ and therefore the only term remaining from the sum is when $j = N - 1$.

$$\begin{aligned}\left[\frac{\partial^N d^\nu(\beta)}{\partial \beta^N}\right]_{\beta=0} &= (-1)^N(\nu-1)^{N-1}N(N-1)! \\ &= (-1)^N N!(\nu-1)^{N-1}. \end{aligned} \tag{4.60}$$

Next, we find the ℓ-th derivative of (4.60) with respect to ν. Note that if $\ell = N$, the derivative is precisely 0, which coincides with the third formula in Proposition 4.3.4. If $\ell < N$, we obtain

$$\left[\frac{\partial^{N+\ell} d^\nu(\beta)}{\partial \beta^N \partial \nu^\ell}\right]_{\beta=0} = (-1)^N N! \frac{(N-1)!}{(N-1-\ell)!}(\nu-1)^{N-1-\ell}.$$

Setting $\nu = 0$ and dividing by $N!\ell!$, we obtain the coefficient $c_{N\ell}$

$$\begin{aligned} c_{N\ell} &= \frac{(-1)^N N!}{N!\ell!}\frac{(N-1)!}{(N-1-\ell)!}(-1)^{N-1-\ell} \\ &= \frac{(-1)^{\ell-1}(N-1)!}{\ell!(N-1-\ell)!} \\ &= (-1)^{\ell-1}\begin{pmatrix} N-1 \\ \ell \end{pmatrix}, \end{aligned} \tag{4.61}$$

which coincides with the second formula in Proposition 4.3.4. This concludes the proof. □

Next, we derive a closed form expression for the $(j,1)$-th cofactor of M. This is analogous to the proof of Lemma 4.3.1 but more complicated since the structure of the underlying matrix is more complex. To accommodate the flow of this chapter, we omit some of the more arduous parts of the proof of the following proposition, as well as some special cases. The omitted parts can be found in Appendices A.1 – A.5 as indicated throughout the proof. We follow the proof of the following proposition with an example.

Proposition 4.3.5 *Consider h_R, $P^\nu_{h_R}$ and M as defined in Lemma 4.3.1. We further define $d^\nu_{j1}(\beta)$ as the $(j,1)$-th cofactor of M. Then, for $j = 1$,*

$$d^\nu_{11}(\beta) = \frac{\frac{1}{N}\beta\nu}{(1+\lambda)^2}\left[1 - (-\lambda)^N - N(1+\lambda)\right] + 1, \tag{4.62}$$

and, for $j \geq 2$

$$d^{\nu}_{j1}(\beta) \;=\; \frac{\left(\frac{1}{N}\beta\nu\right)}{(1+\lambda)^2}\left[1-(-\lambda)^N - N(-\lambda)^{N-j+1}(1+\lambda)\right] + (-\lambda)^{N-j+1}. \quad (4.63)$$

In the proceeding proof we only consider the general case where $j \geq 2$. For the proof of Proposition 4.3.5 for the case where $j = 1$, see Appendix A.1.

Proof. Consider M which has the structure shown in (4.38). Then, we define M^{j1} as the matrix M with row j and column 1 removed. Clearly then

$$d^{\nu}_{j1}(\beta) \;=\; (-1)^{j+1}\det(M^{j1}). \quad (4.64)$$

We observe that M^{j1} is an $(N-1)\times(N-1)$ matrix which has the following structure:

$$\left[\begin{array}{cccccccccccc}
-\frac{\beta\nu}{N} & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & -\frac{\beta\nu}{N} & -\beta(1-\frac{N-1}{N}\nu) \\
1-\frac{\beta\nu}{N} & \ddots & & & & & & & & & & -\frac{\beta\nu}{N} \\
-\beta(1-\frac{N-1}{N}\nu) & \ddots & \ddots & & & & & & & & & -\frac{\beta\nu}{N} \\
-\frac{\beta\nu}{N} & \ddots & \ddots & \ddots & & & & & & & & \vdots \\
\vdots & \ddots & \ddots & \ddots & \ddots & & & & & & & \vdots \\
-\frac{\beta\nu}{N} & \cdots & -\frac{\beta\nu}{N} & -\beta(1-\frac{N-1}{N}\nu) & 1-\frac{\beta\nu}{N} & -\frac{\beta\nu}{N} & \cdots & \cdots & \cdots & \cdots & \cdots & -\frac{\beta\nu}{N} \\
\hdashline
-\frac{\beta\nu}{N} & \cdots & \cdots & \cdots & -\frac{\beta\nu}{N} & -\beta(1-\frac{N-1}{N}\nu) & 1-\frac{\beta\nu}{N} & -\frac{\beta\nu}{N} & \cdots & \cdots & \cdots & -\frac{\beta\nu}{N} \\
\vdots & & & & \ddots & \ddots & \ddots & \ddots & \ddots & & & \vdots \\
\vdots & & & & & \ddots & \ddots & \ddots & \ddots & \ddots & & \vdots \\
\vdots & & & & & & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\
\vdots & & & & & & & \ddots & \ddots & \ddots & \ddots & -\frac{\beta\nu}{N} \\
-\frac{\beta\nu}{N} & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & -\frac{\beta\nu}{N} & -\beta(1-\frac{N-1}{N}\nu) & 1-\frac{\beta\nu}{N}
\end{array}\right],$$

where the separation is between rows $j-1$ and j. We define the following elementary matrix

$$E_2 \;=\; I - \mathbf{e}\mathbf{e}_2^T + \mathbf{e}_2\mathbf{e}_2^T. \quad (4.65)$$

Then, the multiplication $E_2 M^{j1}$ subtracts row 2 from every other row in M^{j1}. In general, row 2 contains the entry $(-\frac{\beta\nu}{N})$ in all but the first position, and so these row operations eliminate the majority of non-zero entries in M^{j1}. However, if $j = 2$, this outcome is not achieved, and so we consider the proof of Proposition 4.3.5 separately for the case $j = 2$. For the remainder of this proof, we assume $j \geq 3$. For the proof of Proposition 4.3.5 for $j = 2$, see Appendix A.2.

Performing the multiplication E_2M^{j1}, we obtain an $(N-1) \times (N-1)$ matrix with the following structure:

$$E_2M^{j1} = \left[\begin{array}{ccccccccccc}
-1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & \beta\nu-\beta \\
1-\frac{\beta\nu}{N} & -\frac{\beta\nu}{N} & -\frac{\beta\nu}{N} & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & -\frac{\beta\nu}{N} \\
\beta\nu-\beta-1 & 1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\
-1 & \beta\nu-\beta & 1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\
-1 & 0 & \beta\nu-\beta & 1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots & & & & & \vdots \\
\vdots & \vdots & & \ddots & \ddots & \ddots & \ddots & & & & \vdots \\
\vdots & \vdots & & & \ddots & \ddots & \ddots & \ddots & & & \vdots \\
-1 & 0 & \cdots & \cdots & 0 & \beta\nu-\beta & 1 & 0 & \cdots & \cdots & 0 \\
\hline
-1 & 0 & \cdots & \cdots & \cdots & 0 & \beta\nu-\beta & 1 & 0 & \cdots & 0 \\
\vdots & \vdots & & & & & \ddots & \ddots & \ddots & \ddots & \vdots \\
\vdots & \vdots & & & & & & \ddots & \ddots & \ddots & \vdots \\
\vdots & \vdots & & & & & & & \ddots & \ddots & 0 \\
-1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & \beta\nu-\beta & 1
\end{array}\right],$$

where the separation is between rows $j-1$ and j.

Next, we define E_3, another $(N-1) \times (N-1)$ elementary matrix of the form

$$E_3 := \begin{bmatrix}
1 & 0 & 0 & 0 & \cdots & \cdots & 0 \\
0 & 1 & 0 & 0 & \cdots & \cdots & 0 \\
0 & -1 & 1 & 0 & \cdots & \cdots & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots & & \vdots \\
\vdots & & \ddots & \ddots & \ddots & \ddots & \vdots \\
\vdots & & & \ddots & \ddots & \ddots & 0 \\
0 & \cdots & \cdots & \cdots & 0 & -1 & 1
\end{bmatrix}. \tag{4.66}$$

Then, we multiply E_2M^{j1} on the right by this elementary matrix. For simplicity, we define $Y^{j1} := E_2M^{j1}E_3$. We now find the determinant of Y^{j1}, noting that $\det(E_2) = \det(E_3) = 1$. This yields $\det(M^{j1}) = \det(Y^{j1})$. Recalling that $\lambda = \beta\nu - \beta$, we observe that Y^{j1} is an $(N-1)\times(N-1)$ matrix that has the following structure

$$
Y^{j1} = \left[\begin{array}{ccccccccccc}
-1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda & \lambda \\
1-\frac{\beta\nu}{N} & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & -\frac{\beta\nu}{N} \\
\lambda-1 & 1 & \ddots & & & & & & & & 0 \\
-1 & \lambda-1 & 1 & \ddots & & & & & & & \vdots \\
-1 & -\lambda & \lambda-1 & \ddots & \ddots & & & & & & \vdots \\
-1 & 0 & -\lambda & \ddots & \ddots & \ddots & & & & & \vdots \\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & & & & \vdots \\
\vdots & \vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & & & \vdots \\
-1 & 0 & \cdots & 0 & -\lambda & \lambda-1 & 1 & 0 & \cdots & \cdots & 0 \\
\hdashline
-1 & 0 & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1 & 0 & \cdots & 0 \\
\vdots & \vdots & & & & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\
\vdots & \vdots & & & & & \ddots & \ddots & \ddots & \ddots & \vdots \\
\vdots & \vdots & & & & & & \ddots & \ddots & \ddots & 0 \\
-1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1
\end{array}\right], \quad (4.67)
$$

where the separation is between rows $j-1$ and j.

We calculate $\det(Y^{j1})$ by expanding on the rightmost column. There are three non-zero entries to consider in general, in rows 1, 2 and N. However, we consider the case where $j=N$ separately. In that case, the separation occurs after the last row of Y^{j1}, and the 1 in the bottom-right corner does not appear, so there will be only two non-zero entries in the expansion. However, we demonstrate shortly that the third expression in the general expansion is equal to 0 when $j=N$, so there is no need to consider $j=N$ as a separate case. Note that, since we are considering $j\geq 3$, we can be certain that the two non-zero entries in positions $(1,N-1)$ and $(2,N-1)$ are present.

We expand on these three terms, and obtain three minors by in each case removing column $N-1$ and one of rows 1, 2 and $N-1$. We call these minors N_1, N_2 and N_3 respectively. Then,

$$
\det(Y^{j1}) = (-1)^N(\lambda)\det(N_1) + (-1)^{N+1}(-\frac{\beta\nu}{N})\det(N_2) + \det(N_3), \quad (4.68)
$$

where N_1 is an $(N-2)\times(N-2)$ matrix that has the form

$$
N_1 = \left[\begin{array}{ccccccccccccc}
1-\frac{\beta\nu}{N} & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\
\lambda-1 & 1 & \ddots & & & & & & & & & & \vdots \\
-1 & \lambda-1 & 1 & \ddots & & & & & & & & & \vdots \\
-1 & -\lambda & \lambda-1 & \ddots & \ddots & & & & & & & & \vdots \\
-1 & 0 & -\lambda & \ddots & \ddots & \ddots & & & & & & & \vdots \\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & & & & & & \vdots \\
\vdots & \vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & & & & & \vdots \\
-1 & 0 & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1 & 0 & \cdots & \cdots & \cdots & 0 \\
\hline
-1 & 0 & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1 & 0 & \cdots & 0 \\
\vdots & \vdots & & & & & & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\
\vdots & \vdots & & & & & & & \ddots & \ddots & \ddots & \ddots & 0 \\
\vdots & \vdots & & & & & & & & \ddots & \ddots & \ddots & 1 \\
-1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda & \lambda-1
\end{array}\right], \tag{4.69}
$$

N_2 is an $(N-2)\times(N-2)$ matrix that has the form

$$
N_2 = \left[\begin{array}{ccccccccccccc}
-1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda \\
\lambda-1 & 1 & \ddots & & & & & & & & & & 0 \\
-1 & \lambda-1 & 1 & \ddots & & & & & & & & & \vdots \\
-1 & -\lambda & \lambda-1 & \ddots & \ddots & & & & & & & & \vdots \\
-1 & 0 & -\lambda & \ddots & \ddots & \ddots & & & & & & & \vdots \\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & & & & & & \vdots \\
\vdots & \vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & & & & & \vdots \\
-1 & 0 & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1 & 0 & \cdots & \cdots & \cdots & 0 \\
\hline
-1 & 0 & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1 & 0 & \cdots & 0 \\
\vdots & \vdots & & & & & & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\
\vdots & \vdots & & & & & & & \ddots & \ddots & \ddots & \ddots & 0 \\
\vdots & \vdots & & & & & & & & \ddots & \ddots & \ddots & 1 \\
-1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda & \lambda-1
\end{array}\right], \tag{4.70}
$$

and N_3 is an $(N-2)\times(N-2)$ matrix that has the form

$$N_3 \;=\; \left[\begin{array}{ccccccccccccc}
-1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda \\
1-\frac{\beta\nu}{N} & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\
\lambda-1 & 1 & \ddots & & & & & & & & & & 0 \\
-1 & \lambda-1 & 1 & \ddots & & & & & & & & & \vdots \\
-1 & -\lambda & \lambda-1 & \ddots & \ddots & & & & & & & & \vdots \\
-1 & 0 & -\lambda & \ddots & \ddots & \ddots & & & & & & & \vdots \\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & & & & & & \vdots \\
\vdots & \vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & & & & & \vdots \\
-1 & 0 & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1 & 0 & \cdots & \cdots & \cdots & 0 \\
\hline
-1 & 0 & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1 & 0 & \cdots & 0 \\
\vdots & \vdots & & & & & & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\
\vdots & \vdots & & & & & & & \ddots & \ddots & \ddots & \ddots & 0 \\
-1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1
\end{array}\right]. \tag{4.71}$$

We show (see Lemma A.3.1 in Appendix A.3, Lemma A.4.1 in Appendix A.4 and Lemma A.5.1 in Appendix A.5) that

$$\det(N_1) \;=\; (-1)^{N+j}(1-\frac{\beta\nu}{N})\frac{1-(-\lambda)^{N-j+1}}{1+\lambda}, \tag{4.72}$$

$$\det(N_2) \;=\; (-1)^{N+j}\frac{1}{1+\lambda}\left[(N-1-\lambda)(-\lambda)^{N-j+1}+\frac{(-\lambda)^N-1}{1+\lambda}\right], \tag{4.73}$$

$$\det(N_3) \;=\; (-1)^{j}(1-\frac{\beta\nu}{N})\frac{(-\lambda)-(-\lambda)^{N-j+1}}{1+\lambda}. \tag{4.74}$$

Recall that if $j=N$, the third non-zero in the last column of (4.67) is not present, and minor N_3 is not considered. However, if we substitute $j=N$ in (4.74), we observe that $\det(N_3)=0$. Therefore, we can use (4.74) for all $3\le j\le N$, and hence (4.68) also holds for all $3\le j\le N$.

Substituting (4.72), (4.73) and (4.74) into (4.68), we obtain

$$\begin{aligned}
\det(M^{j1}) \;=\;& (-1)^N(\lambda)(-1)^{N+j}(1-\frac{\beta\nu}{N})\frac{1-(-\lambda)^{N-j+1}}{1+\lambda} \\
&+(-1)^{N+1}(-\frac{\beta\nu}{N})\left((-1)^{N+j}\frac{1}{1+\lambda}\left[(N-1-\lambda)(-\lambda)^{N-j+1}+\frac{(-\lambda)^N-1}{1+\lambda}\right]\right) \\
&+(-1)^{j}(1-\frac{\beta\nu}{N})\frac{(-\lambda)-(-\lambda)^{N-j+1}}{1+\lambda} \\
=\;& (-1)^j\left\{(\lambda)(1-\frac{\beta\nu}{N})\frac{1-(-\lambda)^{N-j+1}}{1+\lambda}\right.
\end{aligned}$$

$$-(-\frac{\beta\nu}{N})\left(\frac{1}{1+\lambda}\left[(N-1-\lambda)(-\lambda)^{N-j+1}+\frac{(-\lambda)^N-1}{1+\lambda}\right]\right)$$
$$+(1-\frac{\beta\nu}{N})\frac{(-\lambda)-(-\lambda)^{N-j+1}}{1+\lambda}\Bigg\}.$$

Factorising all terms containing $(\frac{-1}{N}\beta\nu)$, we obtain

$$\begin{aligned}\det(M^{j1}) &= \frac{(\frac{-1}{N}\beta\nu)(-1)^j}{(1+\lambda)^2}\Big[\lambda(1+\lambda)(1-(-\lambda)^{N-j+1})-(1+\lambda)((N-1-\lambda)(-\lambda)^{N-j+1})\\ &\quad Big.-(-\lambda)^N+1+(1+\lambda)((-\lambda)-(-\lambda)^{N-j+1})\Big]\\ &\quad +(-1)^j\lambda\frac{1-(-\lambda)^{N-j+1}}{1+\lambda}+(-1)^j\frac{(-\lambda)-(-\lambda)^{N-j+1}}{1+\lambda}.\end{aligned}$$

Then, inside the square brackets we factorise all terms containing $(1+\lambda)$ while in the final term we factorise out $-\lambda$ to obtain

$$\begin{aligned}\det(M^{j1}) &= \frac{(\frac{-1}{N}\beta\nu)(-1)^j}{(1+\lambda)^2}\Big[1-(-\lambda)^N+(1+\lambda)\big[\lambda+(-\lambda)^{N-j+2}\\ &\quad -(N-1-\lambda)(-\lambda)^{N-j+1}-\lambda-(-\lambda)^{N-j+1}\big]\Big]\\ &\quad -(-1)^j(-\lambda)\frac{1-(-\lambda)^{N-j+1}}{1+\lambda}+(-1)^j(-\lambda)\frac{1-(-\lambda)^{N-j}}{1+\lambda}.\end{aligned}$$

Finally, we simplify this expression to obtain

$$\begin{aligned}\det(M^{j1}) &= \frac{(\frac{-1}{N}\beta\nu)(-1)^j}{(1+\lambda)^2}\Big[1-(-\lambda)^N-N(1+\lambda)(-\lambda)^{N-j+1}\Big]\\ &\quad -(-1)^j(-\lambda)\frac{1}{1+\lambda}\Big[1-(-\lambda)^{N-j+1}-1+(-\lambda)^{N-j}\Big]\\ &= \frac{(\frac{-1}{N}\beta\nu)(-1)^j}{(1+\lambda)^2}\big[1-(-\lambda)^N-N(1+\lambda)(-\lambda)^{N-j+1}\big]-(-1)^j(-\lambda)^{N-j+1}.\end{aligned}$$

Then, from (4.64), we obtain

$$d^{\nu}_{j1}(\beta) = \frac{(\frac{1}{N}\beta\nu)}{(1+\lambda)^2}\big[1-(-\lambda)^N-N(-\lambda)^{N-j+1}(1+\lambda)\big]+(-\lambda)^{N-j+1},$$

which coincides with (A.2). □

Example 4.3.6 *Consider the 8-node reverse Hamiltonian cycle defined in (4.51).*

Then, we consider M^{51}

$$M^{51} = \left[\begin{array}{ccccccc} -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & \frac{7}{8}\beta\nu-\beta \\ 1-\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} \\ \frac{7}{8}\beta\nu-\beta & 1-\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} \\ -\frac{\beta\nu}{8} & \frac{7}{8}\beta\nu-\beta & 1-\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} \\ \hdashline -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & \frac{7}{8}\beta\nu-\beta & 1-\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} \\ -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & \frac{7}{8}\beta\nu-\beta & 1-\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} \\ -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & -\frac{\beta\nu}{8} & \frac{7}{8}\beta\nu-\beta & 1-\frac{\beta\nu}{8} \end{array}\right].$$

We observe that $d^{\nu}_{51}(\beta) = \det(-1)^{5+1}\det(M^{51}) = \det(M^{51})$. Multiplying M^{51} on the left by the elementary matrix (4.65), we obtain

$$E_2M^{51} = \left[\begin{array}{ccccccc} -1 & 0 & 0 & 0 & 0 & 0 & \lambda \\ 1-\frac{\beta\nu}{8} & 1-\frac{\beta\nu}{8} & 1-\frac{\beta\nu}{8} & 1-\frac{\beta\nu}{8} & 1-\frac{\beta\nu}{8} & 1-\frac{\beta\nu}{8} & 1-\frac{\beta\nu}{8} \\ \lambda-1 & 1 & 0 & 0 & 0 & 0 & 0 \\ -1 & \lambda & 1 & 0 & 0 & 0 & 0 \\ \hdashline -1 & 0 & 0 & \lambda & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 & \lambda & 1 & 0 \\ -1 & 0 & 0 & 0 & 0 & \lambda & 1 \end{array}\right].$$

Then, multiplying on the right by the elementary matrix (4.66), we find

$$Y^{51} = E_2M^{51}E_3 = \left[\begin{array}{ccccccc} -1 & 0 & 0 & 0 & 0 & -\lambda & \lambda \\ 1-\frac{\beta\nu}{8} & 0 & 0 & 0 & 0 & 0 & -\frac{\beta\nu}{8} \\ \lambda-1 & 1 & 0 & 0 & 0 & 0 & 0 \\ -1 & \lambda-1 & 1 & 0 & 0 & 0 & 0 \\ \hdashline -1 & 0 & -\lambda & \lambda-1 & 1 & 0 & 0 \\ -1 & 0 & 0 & -\lambda & \lambda-1 & 1 & 0 \\ -1 & 0 & 0 & 0 & -\lambda & \lambda-1 & 1 \end{array}\right].$$

We expand this matrix on the last (seventh) column to obtain

$$\begin{aligned} d^{\nu}_{51}(\beta) &= (-1)^{1+7}(\lambda)\det(N_1) + (-1)^{2+7}(-\frac{\beta\nu}{8})\det(N_2) + (-1)^{7+7}(1)\det(N_3) \\ &= (\lambda)\det(N_1) + (\frac{\beta\nu}{8})\det(N_2) + \det(N_3), \end{aligned}$$

where

$$N_1 = \left[\begin{array}{cccccc} 1-\frac{\beta\nu}{8} & 0 & 0 & 0 & 0 & 0 \\ \lambda-1 & 1 & 0 & 0 & 0 & 0 \\ -1 & \lambda-1 & 1 & 0 & 0 & 0 \\ \hdashline -1 & 0 & -\lambda & \lambda-1 & 1 & 0 \\ -1 & 0 & 0 & -\lambda & \lambda-1 & 1 \\ -1 & 0 & 0 & 0 & -\lambda & \lambda-1 \end{array}\right],$$

$$N_2 = \left[\begin{array}{cccccc} -1 & 0 & 0 & 0 & 0 & -\lambda \\ \lambda-1 & 1 & 0 & 0 & 0 & 0 \\ -1 & \lambda-1 & 1 & 0 & 0 & 0 \\ \hdashline -1 & 0 & -\lambda & \lambda-1 & 1 & 0 \\ -1 & 0 & 0 & -\lambda & \lambda-1 & 1 \\ -1 & 0 & 0 & 0 & -\lambda & \lambda-1 \end{array}\right],$$

$$N_3 = \left[\begin{array}{cccccc} -1 & 0 & 0 & 0 & 0 & -\lambda \\ 1-\frac{\beta\nu}{8} & 0 & 0 & 0 & 0 & 0 \\ \lambda-1 & 1 & 0 & 0 & 0 & 0 \\ -1 & \lambda-1 & 1 & 0 & 0 & 0 \\ \hdashline -1 & 0 & -\lambda & \lambda-1 & 1 & 0 \\ -1 & 0 & 0 & -\lambda & \lambda-1 & 1 \end{array}\right].$$

We confirm that the determinants of these matrices are agree with (4.72)–(4.74). That is,

$$\begin{aligned}
\det(N_1) &= (-1)^{13}(1-\frac{\beta\nu}{8})(1-\lambda+\lambda^2-\lambda^3) \\
&= (1-\frac{\beta\nu}{8})(\lambda^3-\lambda^2+\lambda-1), \\
\det(N_2) &= (-1)^{13}\frac{1}{1+\lambda}\left[7\lambda^4-\lambda^5+\lambda^7-\lambda^6+\lambda^5-\lambda^4+\lambda^3-\lambda^2+\lambda-1\right] \\
&= \frac{-1}{1+\lambda}\left[(1+\lambda)(\lambda-2\lambda^5+2\lambda^4+4\lambda^3-3\lambda^2+2\lambda-1)\right] \\
&= 1-2\lambda+3\lambda^2-4\lambda^3-2\lambda^4+2\lambda^5-\lambda^6, \\
\det(N_3) &= (-1)^5(1-\frac{\beta\nu}{8})(-\lambda^3+\lambda^2-\lambda) \\
&= (1-\frac{\beta\nu}{8})(\lambda^3-\lambda^2+\lambda).
\end{aligned}$$

Then, we find

$$\begin{aligned}
d_{51}^{\nu}(\beta) &= (\lambda)\det(N_1)+(\frac{\beta\nu}{8})\det(N_2)+\det(N_3) \\
&= \lambda(1-\frac{\beta\nu}{8})(\lambda^3-\lambda^2+\lambda-1) \\
&\quad +(\frac{\beta\nu}{8})(1-2\lambda+3\lambda^2-4\lambda^3-2\lambda^4+2\lambda^5-\lambda^6) \\
&\quad +(1-\frac{\beta\nu}{8})(\lambda^3-\lambda^2+\lambda) \\
&= (\frac{\beta\nu}{8})(-\lambda^6+2\lambda^5-3\lambda^4-4\lambda^3+3\lambda^2-2\lambda+1)+\lambda^4 \\
&= \frac{\left(\frac{\beta\nu}{8}\right)(1+\lambda)^2}{(1+\lambda)^2}(-\lambda^6+2\lambda^5-3\lambda^4-4\lambda^3+3\lambda^2-2\lambda+1)+\lambda^4 \\
&= \frac{\left(\frac{1}{8}\beta\nu\right)}{(1+\lambda)^2}\left[1-\lambda^8-8\lambda^4-8\lambda^5\right]+\lambda^4,
\end{aligned}$$

which coincides with the formula given in (A.2).

Proposition 4.3.7 *For a graph Γ with N nodes, $d^{\nu}_{j1}(\beta)$ can be expressed as*

$$d^{\nu}_{j1}(\beta) \quad = \quad \sum_{k=0}^{N-1} \sum_{\ell=0}^{k} c^j_{k\ell} \beta^k \nu^\ell,$$

for some coefficients $c^j_{k\ell}$.

Proof. This cofactor is a determinant of an $(N-1) \times (N-1)$ matrix where each element only contains terms of the form $k_1 + k_2\beta + k_3\beta\nu$, for some constants k_1, k_2, k_3. Therefore, we observe that $d^{\nu}_{j1}(\beta)$ is a bivariate polynomial of bounded degree, and that the power of ν does not exceed the power of β. That is, $d^{\nu}_{j1}(\beta)$ takes the form $\sum_{k=0}^{N-1} \sum_{\ell=0}^{k} c^j_{k\ell} \beta^k \nu^\ell$, where $c^j_{k\ell}$ are particular coefficients. □

As with $d^{\nu}(\beta)$, these coefficients can be found by computing

$$c^j_{k\ell} \quad = \quad \frac{1}{k!\ell!} \left[\frac{\partial^{k+\ell} d^{\nu}_{j1}(\beta))}{\partial \beta^k \partial \nu^\ell} \right]_{\beta=0,\nu=0}. \tag{4.75}$$

That is, we find the coefficient $c^j_{k\ell}$ by finding the k-th derivative with respect to β, the ℓ-th derivative with respect to ν, dividing by $k!\ell!$ and setting both $\beta = 0$ and $\nu = 0$.

Proposition 4.3.8 *The coefficients $c^j_{k\ell}$ for $j \geq 2$ take the following form for $\ell > 0$,*

$$c^j_{k\ell} = \begin{cases} (-1)^{\ell+1} \frac{k}{N} \begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix}, & k < N-j+1, \\ (-1)^{\ell} \frac{N-\ell}{N} \begin{pmatrix} k \\ \ell \end{pmatrix}, & k = N-j+1, \\ (-1)^{\ell} \frac{N-k}{N} \begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix}, & k > N-j+1, \end{cases} \tag{4.76}$$

and the following form for $\ell = 0$,

$$c^j_{k0} = \begin{cases} 1, & k = N-j+1, \\ 0, & \textit{otherwise}. \end{cases} \tag{4.77}$$

Proof. We first consider the case when $\ell = 0$. Since we do not need to take any derivatives of $d^{\nu}_{j1}(\beta)$ with respect to ν, we set $\nu = 0$ first to obtain $d^{0}_{j1}(\beta)$. Then, from Proposition 4.3.7, $d^{0}_{j1}(\beta)$ is

$$d^{0}_{j1}(\beta) \quad = \quad \beta^{N-j+1}. \tag{4.78}$$

Next, we will take the k-th derivative of (4.78). If $k > N-j+1$, the k-th derivative of (4.78) will be 0. If $k \leq N-j+1$, then the k-th derivative of (4.78) with respect to β is

$$\frac{\partial^k d^{0}_{j1}(\beta)}{\partial \beta^k} \quad = \quad \frac{(N-j+1)!}{(N-j+1-k!}\beta^{N-j+1-k}. \tag{4.79}$$

Then, if we set $\beta = 0$ in (4.79), we obtain

$$\left[\frac{\partial^k d^{0}_{j1}(\beta)}{\partial \beta^k}\right]_{\beta=0} \quad = \quad \begin{cases} (N-j+1)!\,, & k = N-j+1, \\ \quad 0, & \text{otherwise.} \end{cases} \tag{4.80}$$

Then, dividing (4.80) by $k!$, we obtain

$$c^{j}_{k0} \quad = \quad \begin{cases} 1, & k = N-j+1, \\ 0, & \text{otherwise,} \end{cases}$$

which coincides with (4.77).

We next consider the case when $k \geq \ell > 0$. From (A.2), we separate $d^{\nu}_{j1}(\beta)$ into three terms, m^{j1}_1, m^{j1}_2 and m^{j1}_3 as follows:

$$\begin{aligned} d^{\nu}_{j1}(\beta) \quad &= \quad \frac{1}{N}\frac{\beta\nu}{1+\lambda}\frac{1-(-\lambda)^N}{1+\lambda} - \frac{\beta\nu}{1+\lambda}(-\lambda)^{N-j+1} + (-\lambda)^{N-j+1} &\text{(4.81)} \\ &= \quad \frac{1}{N}m^{j1}_1 - m^{j1}_2 + m^{j1}_3. &\text{(4.82)} \end{aligned}$$

The first step is to find the k-th derivatives of m^{j1}_1, m^{j1}_2 and m^{j1}_3 separately, and set $\beta = 0$ in each of them.

We first consider $m^{j1}_1 = \dfrac{\beta\nu}{1+\lambda}\dfrac{1-(-\lambda)^N}{1+\lambda} = \dfrac{\beta\nu}{1+\lambda}\left[1 + (-\lambda) + (-\lambda)^2 + \ldots + (-\lambda)^{N-1}\right]$.

We now calculate $\left[\dfrac{\partial^k m_1^{j1}}{\partial\beta^k}\right]_{\beta=0}$. To achieve this, we split up m_1^{j1} further into m_{11}^{j1} and m_{12}^{j1} such that

$$m_1^{j1} := m_{11}^{j1} m_{12}^{j1},$$

where $m_{11}^{j1} := \dfrac{\beta\nu}{1+\lambda}$ and $m_{12}^{j1} := \left[1 + (-\lambda) + (-\lambda)^2 + \ldots + (-\lambda)^{N-1}\right]$. Then, we calculate

$$\begin{aligned}\frac{\partial^k \det(m_1^{j1})}{\partial\beta^k} &= \sum_{i=0}^{k} \frac{k!}{i!(k-i)!}\frac{\partial^{k-i} m_{11}^{j1}}{\partial\beta^{k-i}}\frac{\partial^i m_{12}^{j1}}{\partial\beta^i} \\ &= \frac{\partial^k m_{11}^{j1}}{\partial\beta^k} m_{12}^{j1} + \sum_{i=1}^{k-1} \frac{k!}{i!(k-i)!}\frac{\partial^{k-i} m_{11}^{j1}}{\partial\beta^{k-i}}\frac{\partial^i m_{12}^{j1}}{\partial\beta^i} + m_{11}^{j1}\frac{\partial^k m_{12}^{j1}}{\partial\beta^k}. \quad (4.83)\end{aligned}$$

Then, setting $\beta = 0$ and noting that $\left[m_{11}^{j1}\right]_{\beta=0} = 0$ and $\left[m_{12}^{j1}\right]_{\beta=0} = 1$, we obtain

$$\left[\frac{\partial^k \det(m_1^{j1})}{\partial\beta^k}\right]_{\beta=0} = \left[\frac{\partial^k m_{11}^{j1}}{\partial\beta^k} + \sum_{i=1}^{k-1} \frac{k!}{i!(k-i)!}\frac{\partial^{k-i} m_{11}^{j1}}{\partial\beta^{k-i}}\frac{\partial^i m_{12}^{j1}}{\partial\beta^i}\right]_{\beta=0}. \quad (4.84)$$

Noting that $\dfrac{\partial\lambda}{\partial\beta} = (\nu - 1)$, we find the first derivative of m_{11}^{j1}:

$$\begin{aligned}\frac{\partial m_{11}^{j1}}{\partial\beta} &= \frac{\nu(1+\lambda) - (\nu-1)\beta\nu}{(1+\lambda)^2} \\ &= \frac{\nu + \nu\lambda - (\beta\nu - \beta)\nu}{(1+\lambda)^2} \\ &= \nu(1+\lambda)^{-2}.\end{aligned}$$

From this point, we observe that in general, the n-th derivative of m_{11}^{j1} (or the $(n-1)$-th derivative of (4.85)) with respect to β is

$$\begin{aligned}\frac{\partial^n m_{11}^{j1}}{\partial\beta^n} &= (-1)^{n-1} n!\nu(\nu-1)^{n-1}(1+\lambda)^{-n-1} \\ &= n!\nu(1-\nu)^{n-1}(1+\lambda)^{-n-1}. \quad (4.85)\end{aligned}$$

Then, setting $\beta = 0$, we obtain

$$\left[\frac{\partial^n m_{11}^{j1}}{\partial\beta^n}\right]_{\beta=0} = n!\nu(1-\nu)^{n-1}. \quad (4.86)$$

Next, we find the n-th derivative of m_{12}^{j1}:

$$\frac{\partial^n m_{12}^{j1}}{\partial\beta^n} = (-1)^n(\nu-1)^n \sum_{j=n}^{N-1} \frac{j!}{(j-n)!}(-\lambda)^{j-n}.$$

Then, setting $\beta = 0$ in the above, we observe that every term in the sum is 0 except for when the power of $(-\lambda)$ is 0, which is when $j = n$. Hence,

$$\left[\frac{\partial^n m_{12}^{j1}}{\partial\beta^n}\right]_{\beta=0} = (1-\nu)^n n!\ . \tag{4.87}$$

We substitute (4.86) and (4.87) into (4.84) to obtain

$$\begin{aligned}\left[\frac{\partial^k m_1^{j1}}{\partial\beta^k}\right]_{\beta=0} &= k!\nu(1-\nu)^{k-1} + \sum_{i=1}^{k-1} \frac{k!}{i!(k-i)!}(k-1)!\nu(1-\nu)^{k-i-1}(1-\nu)^i i! \\ &= k!\nu(1-\nu)^{k-1} + \sum_{i=1}^{k-1} k!\nu(1-\nu)^{k-1}.\end{aligned}$$

Then, we note that the term in the sum does not depend on i. Therefore,

$$\begin{aligned}\left[\frac{\partial^k m_1^{j1}}{\partial\beta^k}\right]_{\beta=0} &= k!\nu(1-\nu)^{k-1} + (k-1)k!\nu(1-\nu)^{k-1} \\ &= kk!\nu(1-\nu)^{k-1}.\end{aligned} \tag{4.88}$$

Next, we consider $m_2^{j1} = \dfrac{\beta\nu}{1+\lambda}(-\lambda)^{N-j+1}$, and find the k-th derivative of m_2^{j1} with respect to β. To achieve this we split up m_2^{j1} into m_{21}^{j1} and m_{22}^{j1} such that

$$m_2^{j1} = m_{21}^{j1} m_{22}^{j1},$$

where $m_{21}^{j1} := \dfrac{\beta\nu}{1+\lambda}$ and $m_{22}^{j1} := (-\lambda)^{N-j+1}$. Then, we calculate

$$\begin{aligned}\frac{\partial^k \det(m_2^{j1})}{\partial\beta^k} &= \sum_{i=0}^{k} \frac{k!}{i!(k-i)!} \frac{\partial^{k-i} m_{21}^{j1}}{\partial\beta^{k-i}} \frac{\partial^i m_{22}^{j1}}{\partial\beta^i} \\ &= \frac{\partial^k m_{21}^{j1}}{\partial\beta^k} m_{22}^{j1} + \sum_{i=1}^{k-1} \frac{k!}{i!(k-i)!} \frac{\partial^{k-i} m_{21}^{j1}}{\partial\beta^{k-i}} \frac{\partial^i m_{22}^{j1}}{\partial\beta^i} + m_{21}^{j1} \frac{\partial^k m_{22}^{j1}}{\partial\beta^k}.\end{aligned} \tag{4.89}$$

Setting $\beta = 0$ in (4.92) and noting that $\left[m_{21}^{j1}\right]_{\beta=0} = \left[m_{22}^{j1}\right]_{\beta=0} = 0$, we obtain

$$\left[\frac{\partial^k \det(m_2^{j1})}{\partial\beta^k}\right]_{\beta=0} = \sum_{i=1}^{k-1} \frac{k!}{i!(k-i)!} \frac{\partial^{k-i} m_{21}^{j1}}{\partial\beta^{k-i}} \frac{\partial^i m_{22}^{j1}}{\partial\beta^i}. \tag{4.90}$$

We first consider m_{21}^{j1}, which we note is identical to m_{11}^{j1}, and so we use (4.86) to find derivatives of m_{21}^{j1}. Next, we consider m_{22}^{j1}. We observe that the n-th derivative of m_{22}^{j1} is 0 if $n > N-j+1$. Otherwise, if $n \leq N-j+1$,

$$\begin{aligned}\frac{\partial^n m_{22}^{j1}}{\partial \beta^n} &= \frac{(-1)^n(N-j+1)!}{(N-j+1-n)!}(-\lambda)^{N-j+1-n}(\nu-1)^n \\ &= \frac{(N-j+1)!}{(N-j+1-n)!}(-\lambda)^{N-j+1-n}(1-\nu)^n.\end{aligned}$$

Then, setting $\beta = 0$, we obtain

$$\left[\frac{\partial^n m_{22}^{j1}}{\partial \beta^n}\right]_{\beta=0} = \begin{cases} (N-j+1)!(1-\nu)^{N-j+1}, & n = N-j+1, \\ \\ 0, & n \neq N-j+1. \end{cases} \tag{4.91}$$

We substitute (4.86) and (4.91) into (4.90) to obtain

$$\left[\frac{\partial^k m_2^{j1}}{\partial \beta^k}\right]_{\beta=0} = \sum_{i=1}^{k-1} \frac{k!}{i!(k-i)!}(k-i)!\nu(1-\nu)^{k-i-1}\frac{\partial^i m_{22}^{j1}}{\partial \beta^i}.$$

We know from (4.91) that all terms in the above sum will be 0 except for when $i = N-j+1$. However, if $k-1 < N-j+1$ (or, since k is integer, $k \leq N-j+1$), then i never reaches this value and all the terms are 0. Hence, the above expression becomes

$$\left[\frac{\partial^k m_2^{j1}}{\partial \beta^k}\right]_{\beta=0} = \begin{cases} k!\nu(1-\nu)^{k-1}, & k > N-j+1, \\ \\ 0, & k \leq N-j+1. \end{cases} \tag{4.92}$$

Finally, we consider $m_3^{j1} = (-\lambda)^{N-j+1}$. We note that m_3^{j1} is identical to m_{22}^{j1}, so we use (4.91) to find derivatives of m_3^{j1}. That is,

$$\left[\frac{\partial^n m_3^{j1}}{\partial \beta^n}\right]_{\beta=0} = \begin{cases} (N-j+1)!(1-\nu)^{N-j+1}, & n = N-j+1, \\ \\ 0, & n \neq N-j+1. \end{cases} \tag{4.93}$$

Substituting (4.88), (4.92) and (4.93) into (4.82) we obtain

$$\left[\frac{\partial^k d_{j1}^{\nu}(\beta)}{\partial \beta^k}\right]_{\beta=0} = \begin{cases} \frac{1}{N}kk!\nu(1-\nu)^{k-1}, & k < N-j+1, \\ \frac{1}{N}kk!\nu(1-\nu)^{k-1} + k!(1-\nu)^k, & k = N-j+1, \\ \frac{1}{N}kk!\nu(1-\nu)^{k-1} - k!\nu(1-\nu)^{k-1}, & k > N-j+1. \end{cases} \tag{4.94}$$

We now consider each case in (4.94) separately.

Case 1: $k < N - j + 1$. Then, we have

$$\begin{aligned}\left[\frac{\partial^k d^{\nu}_{j1}(\beta)}{\partial \beta^k}\right]_{\beta=0} &= \frac{1}{N} k k! \nu (1-\nu)^{k-1} \\ &= \frac{1}{N}(-1)^{k-1} k k! (\nu - 1 + 1)(\nu - 1)^{k-1} \\ &= \frac{kk!}{N}(-1)^{k-1}\left[(\nu-1)^k + (\nu-1)^{k-1}\right]. \end{aligned} \tag{4.95}$$

We now find the ℓ-th derivative with respect to ν of (4.95), for $\ell \leq k$, and set $\nu = 0$. However, if $\ell = k$, then the second term $(\nu - 1)^{k-1}$ in the square bracket above becomes 0 after ℓ derivatives, so we consider two more cases.

Case 1.1: $\ell < k$. Then, we have

$$\left[\frac{\partial^{k+\ell} d^{\nu}_{j1}(\beta))}{\partial \beta^k \nu^\ell}\right]_{\beta=0} = \frac{k(k)!}{N}(-1)^{k-1}\left[\frac{k!}{(k-\ell)!}(\nu-1)^{k-\ell} + \frac{(k-1)!}{(k-1-\ell)!}(\nu-1)^{k-1-\ell}\right].$$

Next, we set $\nu = 0$, and obtain

$$\begin{aligned}\left[\frac{\partial^{k+\ell} d^{\nu}_{j1}(\beta))}{\partial \beta^k \nu^\ell}\right]_{\beta=0,\nu=0} &= \frac{k(k)!}{N}(-1)^{k-1}\left[\frac{k!}{(k-\ell)!}(-1)^{k-\ell} + \frac{(k-1)!}{(k-1-\ell)!}(-1)^{k-1-\ell}\right] \\ &= \frac{k(k)!}{N}(-1)^{\ell+1}\left[\frac{k!}{(k-\ell)!} - \frac{(k-1)!}{(k-1-\ell)!}\right] \\ &= \frac{k(k)!}{N}(-1)^{\ell+1}\left[\frac{(k-1)!}{(k-1-\ell)!}\left(\frac{k}{k-\ell} - 1\right)\right] \\ &= \frac{k(k)!(k-1)!}{N(k-1-\ell)!}(-1)^{\ell+1}\frac{\ell}{k-\ell} \\ &= \frac{k(k)!(k-1)!}{N(k-\ell)!}(-1)^{\ell+1}\ell. \end{aligned} \tag{4.96}$$

Case 1.2: $\ell = k$. Then, the k-th derivative of (4.95) with respect to ν is

$$\left[\frac{\partial^{2k} \det(M^{j1})}{\partial \beta^k \nu^k}\right]_{\beta=0} = (-1)^{k-1}\frac{kk!k!}{N}. \tag{4.97}$$

Since (4.97) does not depend on ν, setting $\nu = 0$ does not change its value. We observe that setting $\ell = k$ in (4.96) yields (4.97), and so we use (4.96) for all $\ell \leq k$.

Finally, to find the coefficient $c^j_{k\ell}$, for $k < N - j + 1$, we divide (4.96) by $k!\ell!$ to obtain

$$\begin{aligned} c^j_{k\ell} &= \frac{k(k)!(k-1)!}{N(k-\ell)!k!\ell!}(-1)^{\ell+1}\ell \\ &= \frac{k(k-1)!}{N(k-\ell)!(\ell-1)!}(-1)^{\ell+1} \\ &= (-1)^{\ell+1}\frac{k}{N}\begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix}. \end{aligned} \tag{4.98}$$

Case 2: $k = N - j + 1$. Then, we have

$$\left[\frac{\partial^k d^\nu_{j1}(\beta)}{\partial \beta^k}\right]_{\beta=0} = \frac{1}{N} k k! \nu (1-\nu)^{k-1} + (k)!(1-\nu)^k.$$

We observe that this expression contains two terms, c_1 and c_2, the first of which is identical to the expression (4.95) in Case 1. We use (4.98) to obtain the coefficient for the first term c_1. Next, we consider the second term c_2,

$$c_2 = (k)!(1-\nu)^k. \tag{4.99}$$

Next, we find the ℓ-th derivative with respect to ν of (4.99), where $\ell \leq k$:

$$\frac{\partial^\ell c_2}{\partial \nu^\ell} = (-1)^\ell \frac{k!k!}{(k-\ell)!}(1-\nu)^{k-\ell}. \tag{4.100}$$

Then, we set $\nu = 0$ in (4.100) to obtain

$$\left[\frac{\partial^\ell c_2}{\partial \nu^\ell}\right]_{\nu=0} = (-1)^\ell \frac{k!k!}{(k-\ell)!}. \tag{4.101}$$

Finally, dividing (4.101) by $k!\ell!$ and adding the result to the coefficient (4.98) found in Case 1, we obtain the coefficient $c^j_{k\ell}$ for $k = N - j + 1$:

$$\begin{aligned} c^j_{k\ell} &= (-1)^\ell \frac{k!k!}{(k-\ell)!k!\ell!} + (-1)^{\ell+1} \frac{k}{N} \left(\begin{array}{c} k-1 \\ \ell-1 \end{array} \right) \\ &= (-1)^\ell \frac{k!}{(k-\ell)!\ell!} + (-1)^{\ell+1} \frac{k(k-1)!}{N(\ell-1)!(k-\ell)!} \\ &= \frac{(-1)^\ell k!}{N(k-\ell)!(\ell-1)!} \left[\frac{N}{\ell} - 1 \right] \\ &= (-1)^\ell \frac{N-\ell}{N} \frac{k!}{\ell!(k-\ell)!} \\ &= (-1)^\ell \frac{N-\ell}{N} \left(\begin{array}{c} k \\ \ell \end{array} \right). \end{aligned} \tag{4.102}$$

Case 3: $k > N - j + 1$. Then, we have

$$\left[\frac{\partial^k d^\nu_{j1}(\beta)}{\partial \beta^k} \right]_{\beta=0} = \frac{1}{N} k k! \nu (1-\nu)^{k-1} - k! \nu (1-\nu)^{k-1}.$$

Similarly to Case 2, we observe that the above expression contains two terms, c_1 and c_3, the first of which is identical to the expression (4.95) in Case 1. We use (4.98) to obtain the coefficient for the first term c_1. Next, we consider the additional term c_3,

$$\begin{aligned} c_3 &= -k! \nu (1-\nu)^{k-1} \\ &= (-1)^k k! \left[(\nu-1)^k + (\nu-1)^{k-1} \right]. \end{aligned} \tag{4.103}$$

Next, we find the ℓ-th derivative of c_3, and set $\nu = 0$. We note that if $\ell = k$, the second term in the square bracket above becomes 0 after ℓ derivatives, and so we consider two separate cases.

Case 3.1: $\ell < k$. Then, we have

$$\frac{\partial^\ell c_3}{\partial \nu^\ell} = (-1)^k k! \left[\frac{k!}{(k-\ell)!} (\nu-1)^{k-\ell} + \frac{(k-1)!}{(k-1-\ell)!} (\nu-1)^{k-1-\ell} \right].$$

Setting $\nu = 0$, we obtain

$$\begin{aligned}
\left[\frac{\partial^\ell c_3}{\partial \nu^\ell}\right]_{\nu=0} &= (-1)^k k! \left[\frac{k!}{(k-\ell)!}(-1)^{k-\ell} + \frac{(k-1)!}{(k-1-\ell)!}(-1)^{k-1-\ell}\right] \\
&= (-1)^\ell k! \left[\frac{(k-1)!}{(k-1-\ell)!}\left(\frac{k}{k-\ell} - 1\right)\right] \\
&= (-1)^\ell \frac{k!(k-1)!}{(k-1-\ell)!}\frac{\ell}{k-\ell} \\
&= (-1)^\ell \frac{k!(k-1)!\ell}{(k-\ell)!}. \qquad (4.104)
\end{aligned}$$

Case 3.2: $\ell = k$. Then, we find the k-th derivative with respect to ν of (4.103):

$$\frac{\partial^\ell c_3}{\partial \nu^k} = (-1)^k k! k! \, . \qquad (4.105)$$

This term does not contain ν, so setting $\nu = 0$ does not change the result. Note that setting $\ell = k$ in (4.104) yields (4.105), and so we use (4.104) for all $\ell \leq k$.

Finally, dividing (4.104) by $k!\ell!$, and adding the result to coefficient (4.98) found in Case 1, we obtain the coefficient $c^j_{k\ell}$ for $k > N - j + 1$:

$$\begin{aligned}
c^j_{k\ell} &= (-1)^\ell \frac{k!(k-1)!\ell}{(k-\ell)!k!\ell!} + (-1)^{\ell+1}\frac{k}{N}\begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix} \\
&= (-1)^\ell \frac{(k-1)!}{(k-\ell)!(\ell-1)!} + (-1)^{\ell+1}\frac{k}{N}\frac{(k-1)!}{(\ell-1)!(k-\ell)!} \\
&= (-1)^\ell \frac{(k-1)!}{(k-\ell)!(\ell-1)!}\left[1 - \frac{k}{N}\right] \\
&= (-1)^\ell \frac{N-k}{N}\begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix}.
\end{aligned}$$

This concludes the proof. $\square$

Now that we have found the coefficients $c^j_{k\ell}$ for the general case when $j \geq 2$, we find the coefficients $c^1_{k\ell}$ for $j = 1$.

Proposition 4.3.9 *The coefficients $c^1_{k\ell}$ have the following form for $\ell > 0$:*

$$c^1_{k\ell} = (-1)^\ell \frac{N-k}{N}\begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix},$$

and they have the following form for $\ell = 0$

$$c^1_{k0} \;=\; \begin{cases} 1, & k = 0, \\ 0, & \textit{otherwise.} \end{cases}$$

Proof. We recall from Proposition 4.3.5 that

$$d^{\nu}_{11}(\beta) \;=\; \frac{\frac{1}{N}\beta\nu}{(1+\lambda)^2}\left[1-(-\lambda)^N - N(1+\lambda)\right] + 1.$$

However, for this proof, we find it convenient to use the more expanded form from (A.11). That is,

$$d^{\nu}_{11}(\beta) \;=\; 1 - \frac{1}{N}\beta\nu\left(\sum_{i=0}^{N-2}(-\lambda)^{N-2-i}(i+1)\right).$$

We now find the coefficients $c^1_{k\ell}$ by calculating

$$c^1_{k\ell} \;=\; \frac{1}{k!\ell!}\left[\frac{\partial^{k+\ell}d^{\nu}_{11}(\beta)}{\partial\beta^k\partial\nu^\ell}\right]_{\beta=0,\nu=0}.$$

Clearly, if $k = \ell = 0$, no derivatives are required and setting $\beta = 0, \nu = 0$ immediately yields $c^1_{00} = 1$, as required.

We rewrite $d^{\nu}_{11}(\beta)$ in the form $d^{\nu}_{11}(\beta) = 1 + m^{11}_1 m^{11}_2$, where

$$\begin{aligned} m^{11}_1 &= -\frac{\beta\nu}{N}, \\ m^{11}_2 &= \sum_{i=0}^{N-2}(-\lambda)^{N-2-i}(i+1). \end{aligned}$$

Then, we find the k-th derivative of $d^{\nu}_{11}(\beta)$ for $k > 0$:

$$\frac{\partial^k d^{\nu}_{11}(\beta)}{\partial\beta^k} \;=\; \sum_{i=0}^{k}\frac{k!}{(k-i)!}\frac{\partial^i m^{11}_1}{\partial\beta^i}\frac{\partial^{k-i}m^{11}_2}{\partial\beta^{k-i}}. \tag{4.106}$$

We observe that $\frac{\partial m^{11}_1}{\partial\beta} = -\frac{\nu}{N}$, and any further derivatives of m^{11}_1 are zero. Substituting this into (4.106) we obtain

$$\frac{\partial^k d^{\nu}_{11}(\beta)}{\partial\beta^k} \;=\; -\frac{\beta\nu}{N}\frac{\partial^k m^{11}_2}{\partial\beta^k} - \frac{k\nu}{N}\frac{\partial^{k-1}m^{11}_2}{\partial\beta^{k-1}}. \tag{4.107}$$

Then, setting $\beta = 0$ in the above we obtain

$$\left[\frac{\partial^k d_{11}^{\nu}(\beta)}{\partial\beta^k}\right]_{\beta=0} = -\frac{k\nu}{N}\left[\frac{\partial^{k-1} m_2^{11}}{\partial\beta^{k-1}}\right]_{\beta=0}. \tag{4.108}$$

Next, we calculate the $(k-1)$-th derivative of m_2^{11} with respect to β, recalling that $\frac{\partial\lambda}{\partial\beta} = (\nu - 1)$:

$$\frac{\partial^{k-1} m_2^{11}}{\partial\beta^{k-1}} = \sum_{i=0}^{N-k-1} \frac{(N-2-i)!}{(N-k-i-1)!}(-\lambda)^{N-k-i-1}(-1)^{k-1}(\nu-1)^{k-1}(i+1). \tag{4.109}$$

Then, setting $\beta = \lambda = 0$ in the above, we obtain

$$\left[\frac{\partial^{k-1} m_2^{11}}{\partial\beta^{k-1}}\right]_{\beta=0} = (k-1)!(-1)^{k-1}(\nu-1)^{k-1}(N-k). \tag{4.110}$$

Substituting (4.110) into (4.108), we find

$$\begin{aligned}\left[\frac{\partial^k d_{11}^{\nu}(\beta)}{\partial\beta^k}\right]_{\beta=0} &= -\frac{N-k}{N}k(k-1)!(-1)^{k-1}(\nu-1)^{k-1}\nu \\ &= -\frac{N-k}{N}k!(-1)^{k-1}\left[(\nu-1)^k + (\nu-1)^{k-1}\right]. \end{aligned} \tag{4.111}$$

If we set $\nu = 0$ in (4.111), we obtain 0. This corresponds to the case where $k > 0$ and $\ell = 0$, and therefore $c_{k0}^1 = 0$ for $k > 0$, which coincides with the required formula. For $\ell > 0$, we find the ℓ-th derivative of (4.111) with respect to ν, and set $\nu = 0$. However, if $\ell = k$, the second term in the square brackets in (4.111) becomes 0 after ℓ derivatives, so we consider two cases.

Case 1: $\ell < k$. We observe that the ℓ-th derivative of (4.111) with respect to ν is

$$\left[\frac{\partial^{k+\ell} d_{11}^{\nu}(\beta)}{\partial\beta^k\partial\nu^\ell}\right]_{\beta=0} = -\frac{(N-k)}{N}k!(-1)^{k-1}\left[\frac{k!}{(k-\ell)!}(\nu-1)^{k-\ell} + \frac{(k-1)!}{(k-\ell-1)!}(\nu-1)^{k-\ell-1}\right].$$

Then, setting $\nu = 0$ in the above we obtain

$$\begin{aligned}\left[\frac{\partial^{k+\ell} d_{11}^{\nu}(\beta)}{\partial\beta^k\partial\nu^\ell}\right]_{\beta=0,\nu=0} &= -\frac{(N-k)}{N}k!(-1)^{k-1}\left[\frac{k!}{(k-\ell)!}(-1)^{k-\ell} + \frac{(k-1)!}{(k-\ell-1)!}(-1)^{k-\ell-1}\right] \\ &= \frac{(N-k)}{N}k!(-1)^{\ell}\left[\frac{k!}{(k-\ell)!} - \frac{(k-1)!}{(k-\ell-1)!}\right] \\ &= \frac{(N-k)}{N}k!(-1)^{\ell}\left[\frac{k!}{(k-\ell)!}\left(1 - \frac{k-\ell}{k}\right)\right] \\ &= \frac{(N-k)}{N}k!(-1)^{\ell}\frac{k!}{(k-\ell)!}\frac{\ell}{k}. \end{aligned} \tag{4.112}$$

Finally, dividing by $k!\ell!$ we obtain

$$
\begin{aligned}
c^1_{k\ell} &= \frac{1}{k!\ell!}\frac{(N-k)}{N}k!(-1)^{\ell}\frac{k!}{(k-\ell)!}\frac{\ell}{k} \\
&= (-1)^{\ell}\frac{(N-k)}{N}\frac{(k-1)!}{(\ell-1)!(k-\ell)!} \\
&= (-1)^{\ell}\frac{(N-k)}{N}\begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix}, \qquad (4.113)
\end{aligned}
$$

which coincides with the desired formula. Now all that remains is to check the case when $\ell = k$.

Case 2: $\ell = k$. We observe that the ℓ-th derivative of (4.111) (which is the same as the k-th derivative) of (4.111) is

$$
\left[\frac{\partial^{2k} d^{\nu}_{11}(\beta)}{\partial\beta^k\partial\nu^k}\right]_{\beta=0} = -\frac{(N-k)}{N}k!(-1)^{k-1}k!\,. \qquad (4.114)
$$

The above expression does not contain ν, so we now simply divide by $k!\ell!$ to obtain

$$
c^1_{kk} = (-1)^k\frac{(N-k)}{N}. \qquad (4.115)
$$

Setting $k = \ell$ in (4.113) yields (4.115), and so we use (4.113) for all $\ell = k > 0$. This concludes the proof. □

Remark 4.3.10 *We note that the formula for $c^1_{k\ell}$ is identical to the third equation (corresponding to the case when $k > N - j + 1$) for $c^r_{k\ell}$ (see Proposition 4.3.8) for $\ell > 0$. However, this is not the case for $\ell = 0$, unless we ensure that $k > 0$.*

Now, using the results of Propositions 4.3.7 – 4.3.9, we see that the following solution vector for the reverse Hamiltonian cycle h_R satisfies $X(\beta,\nu)$:

$$
[\mathbf{x}^*_{h_R}]_{ia} = \begin{cases} \sum_{k=0}^{N-1}\sum_{\ell=0}^{k} c^r_{k\ell}\beta^k\nu^\ell, & (i,a) = (N-r+1, N-r) \text{ for some } r, \\ 0, & \text{otherwise.} \end{cases} \qquad (4.116)
$$

Then, using analogous arguments to those in Theorem 4.2.1, we see that for any Hamiltonian cycle h such that $P_h = \Pi P_{h_R}\Pi^{-1}$, the elements inside $\mathbf{x}^*_h$ are the same as those for $\mathbf{x}^*_{h_R}$, but in different positions.

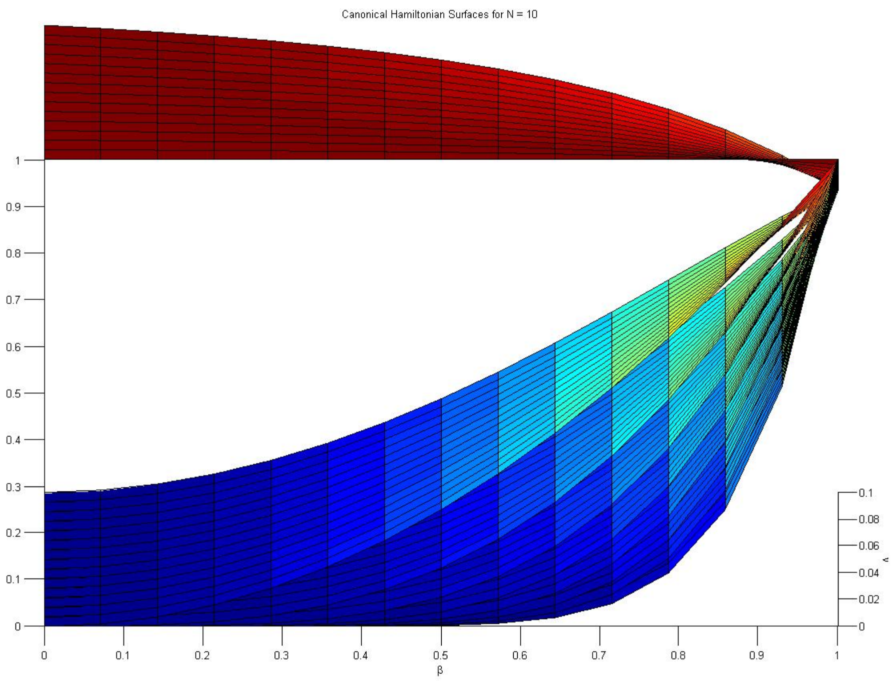


Figure 4.5: Canonical Hamiltonian surfaces for 10-node graphs.

Remark 4.3.11 *Similarly to the canonical Hamiltonian curves shown in Figure 4.3, solutions of the form shown in (4.116) can be represented on a figure as 3-dimensional surfaces in parameters β and ν. We call these surfaces the canonical Hamiltonian surfaces. The canonical Hamiltonian surfaces for 10-node graphs can be seen in Figure 4.5.*

4.4 Auxilliary constraints

Now that we know from (4.118) the form of all Hamiltonian solutions in $X(\beta, \nu)$, in this section we derive constraints that facilitate the search for solutions of that form. We begin by defining N vectors $\mathbf{y}^r$, for $r = 1, \ldots, N$. These vectors correspond to arcs in a Hamiltonian cycle in the following way:

$$y^r_{ia} = \begin{cases} 1, & \text{if arc } (i,a) \text{ is selected as the } (r-1)\text{-th step in the HC,} \\ 0, & \text{otherwise.} \end{cases} \qquad (4.117)$$

For a generic Hamiltonian cycle h we observe that the form of the solution vector is

$$\mathbf{x}^*_h \;=\; \sum_{k=0}^{N-1}\sum_{\ell=0}^{k}\beta^k\nu^\ell\sum_{r=1}^{N} c^r_{k\ell}\mathbf{y}^r. \tag{4.118}$$

We then define new decision vectors $\mathbf{x}^{k\ell}$ such that

$$\mathbf{x}^{k\ell} \;:=\; \sum_{r=1}^{N} c^r_{k\ell}\mathbf{y}^r, \tag{4.119}$$

and search for a solution vector $\mathbf{x}$ of the form

$$\mathbf{x} \;=\; \sum_{k=0}^{N-1}\sum_{\ell=0}^{k}\beta^k\nu^\ell\mathbf{x}^{k\ell}. \tag{4.120}$$

Recall that the polytope $X(\beta,\nu)$ is defined by the following constraints:

$$\begin{aligned}
\sum_{i=1}^{N}\sum_{a\in\mathcal{A}(i)}\left(\delta_{ij}-\beta(p_{iaj}+\nu d_{iaj})\right)x_{ia} &= d^\nu(\beta)\delta_{1j}, \quad j=1,\ldots,N, && (4.121)\\
\sum_{a\in\mathcal{A}(1)} x_{1a} &= 1, && (4.122)\\
x_{ia} &\geq 0, \quad (i,a)\in\Gamma, && (4.123)
\end{aligned}$$

where

$$d_{iaj} \;:=\; \begin{cases} \frac{1}{N}, & p_{iaj}=0,\\ -\frac{N-1}{N}, & p_{iaj}=1.\end{cases} \tag{4.124}$$

Note that if we set $\nu = 0$, the resulting polytope is the special case $X(\beta)$ (see (4.12)–(4.14)). Using analogous arguments to those in Section 4.2, we represent these equations in the matrix form $\tilde{W}(\beta,\nu)\mathbf{x} = \mathbf{b}(\beta,\nu)$, and separate $\tilde{W}$ into the components involving no parameters, those involving only β, and those involving $\beta\nu$. That is, $\tilde{W} = W_{00} + \beta W_{10} + \beta\nu W_{11}$, where

$$W_{00} = \left[\begin{array}{c} \Delta \\ \hdashline 1\cdots 1\; 0\cdots\cdots 0 \end{array}\right], \qquad W_{10} = \left[\begin{array}{c} -P \\ \hdashline 0\cdots\cdots 0 \end{array}\right], \qquad W_{11} = \left[\begin{array}{c} -D \\ \hdashline 0\cdots\cdots 0 \end{array}\right], \tag{4.125}$$

where $D := [d_{iaj}]_{j=1,(i,a)\in\Gamma}^{N}$ (recall that the columns of $\tilde{W}(\beta,\nu)$ are indexed by arcs $(i,a)\in\Gamma$).

Using Proposition 4.3.3, we also separate $\mathbf{b}$ into vectors of the form

$$\mathbf{b}_{00} = \begin{bmatrix} c_{00} \\ 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix}, \quad \mathbf{b}_{k\ell} = \begin{bmatrix} c_{k\ell} \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix}, \quad \text{for all } k = 1, \ldots, N, \quad \ell = 0, \ldots, k.$$

Then, from (4.120), we know the form of all Hamiltonian solutions, and using analogous arguments to those in Section 4.2 we obtain

$$(W_{00} + \beta W_{10} + \beta\nu W_{11}) \sum_{k=0}^{N-1} \sum_{\ell=0}^{k} \beta^k \nu^\ell \mathbf{x}^{k\ell} \;=\; \sum_{k=0}^{N} \sum_{\ell=0}^{k} \beta^k \nu^\ell \mathbf{b}_{k\ell}. \tag{4.126}$$

Expanding (4.126) and equating coefficients of powers of β and ν we obtain

$$\begin{aligned}
W_{00}\mathbf{x}^{00} &= \mathbf{b}_{00}, \\
W_{00}\mathbf{x}^{10} + W_{10}\mathbf{x}^{00} &= \mathbf{b}_{10}, \\
W_{00}\mathbf{x}^{11} + W_{11}\mathbf{x}^{00} &= \mathbf{b}_{11}, \\
W_{00}\mathbf{x}^{20} + W_{10}\mathbf{x}^{10} &= \mathbf{b}_{20}, \\
W_{00}\mathbf{x}^{21} + W_{10}\mathbf{x}^{11} + W_{11}\mathbf{x}^{10} &= \mathbf{b}_{21}, \\
W_{00}\mathbf{x}^{22} + W_{11}\mathbf{x}^{11} &= \mathbf{b}_{22}, \\
W_{00}\mathbf{x}^{30} + W_{10}\mathbf{x}^{20} &= \mathbf{b}_{30}, \\
&\vdots \\
W_{00}\mathbf{x}^{N-1,N-1} + W_{11}\mathbf{x}^{N-2,N-2} &= \mathbf{b}_{N-1,N-1}, \\
W_{10}\mathbf{x}^{N-1,0} &= \mathbf{b}_{N0}, \\
W_{10}\mathbf{x}^{N-1,1} + W_{11}\mathbf{x}^{N-1,0} &= \mathbf{b}_{N1}, \\
&\vdots \\
W_{10}\mathbf{x}^{N-1,N-1} + W_{11}\mathbf{x}^{N-1,N-2} &= \mathbf{b}_{N,N-1}, \\
W_{11}\mathbf{x}^{N-1,N-1} &= \mathbf{b}_{NN}.
\end{aligned}$$

This new, parameter-free, system of equations replaces the parametrised system

$W(\beta,\nu)\mathbf{x} = \mathbf{b}(\beta,\nu)$, and has the following block structure

$$
\left[\begin{array}{cccccccccccc}
W_{00} & & & & & & & & & & & \\
W_{10} & W_{00} & & & & & & & & & & \\
W_{11} & & W_{00} & & & & & & & & & \\
 & W_{10} & & W_{00} & & & & & & & & \\
 & W_{11} & W_{10} & & W_{00} & & & & & & & \\
 & & W_{11} & & & W_{00} & & & & & & \\
 & & & \ddots & & & \ddots & & & & & \\
 & & & & & & & \ddots & & & & \\
 & & & & & & & & \ddots & & & \\
 & & & & & & & & & \ddots & & \\
 & & & & & & & W_{11} & W_{10} & \cdots & W_{00} & \\
 & & & & & & & & W_{11} & & & W_{00} \\
 & & & & & & & & & \ddots & & \vdots \\
 & & & & & & & & & & W_{11} & W_{10} \\
 & & & & & & & & & & & W_{11}
\end{array}\right]
\begin{bmatrix} \mathbf{x}^{00} \\ \mathbf{x}^{10} \\ \mathbf{x}^{11} \\ \mathbf{x}^{20} \\ \mathbf{x}^{21} \\ \mathbf{x}^{22} \\ \mathbf{x}^{30} \\ \vdots \\ \vdots \\ \mathbf{x}^{N-1,N-1} \end{bmatrix}
=
\begin{bmatrix} \mathbf{b}_{00} \\ \mathbf{b}_{10} \\ \mathbf{b}_{11} \\ \mathbf{b}_{20} \\ \mathbf{b}_{21} \\ \mathbf{b}_{22} \\ \mathbf{b}_{30} \\ \mathbf{b}_{31} \\ \mathbf{b}_{32} \\ \mathbf{b}_{33} \\ \vdots \\ \vdots \\ \vdots \\ \mathbf{b}_{N,N-1} \\ \mathbf{b}_{NN} \end{bmatrix}. \tag{4.127}
$$

Example 4.4.1 *Recall the 4-node graph Γ_4 shown in Example 4.1.3 that has the following adjacency matrix $\mathbb{A}_4$:*

$$
\mathbb{A}_4 = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix}.
$$

For this graph, we have

$$
W_{00} = \begin{bmatrix}
1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \\
1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix},
$$

$$
W_{10} = \begin{bmatrix}
0 & 0 & 0 & -1 & 0 & 0 & 0 & -1 & 0 & 0 \\
-1 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 0 \\
0 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & -1 \\
0 & 0 & -1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix},
$$

$$W_{11} = \begin{bmatrix} -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} & \frac{3}{4} & -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} & \frac{3}{4} & -\frac{1}{4} & -\frac{1}{4} \\ \frac{3}{4} & -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} & \frac{3}{4} & -\frac{1}{4} & -\frac{1}{4} & \frac{3}{4} & -\frac{1}{4} \\ -\frac{1}{4} & \frac{3}{4} & -\frac{1}{4} & -\frac{1}{4} & \frac{3}{4} & -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} & \frac{3}{4} \\ -\frac{1}{4} & -\frac{1}{4} & \frac{3}{4} & -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} & \frac{3}{4} & -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

Then, the block structure (4.127) for Γ_4 *is:*

$$\left[\begin{array}{c:c:c:c:c:c:c:c:c:c} W_{00} & & & & & & & & & \\ \hdashline W_{10} & W_{00} & & & & & & & & \\ \hdashline W_{11} & & W_{00} & & & & & & & \\ \hdashline & W_{10} & & W_{00} & & & & & & \\ \hdashline & W_{11} & W_{10} & & W_{00} & & & & & \\ \hdashline & & W_{11} & & & W_{00} & & & & \\ \hdashline & & & W_{10} & & & W_{00} & & & \\ \hdashline & & & W_{11} & W_{10} & & & W_{00} & & \\ \hdashline & & & & W_{11} & W_{10} & & & W_{00} & \\ \hdashline & & & & & W_{11} & & & & W_{00} \\ \hdashline & & & & & & W_{10} & & & \\ \hdashline & & & & & & W_{11} & W_{10} & & \\ \hdashline & & & & & & & W_{11} & W_{10} & \\ \hdashline & & & & & & & & W_{11} & W_{10} \\ \hdashline & & & & & & & & & W_{11} \end{array}\right] \begin{bmatrix} \mathbf{x}^{00} \\ \mathbf{x}^{10} \\ \mathbf{x}^{11} \\ \mathbf{x}^{20} \\ \mathbf{x}^{21} \\ \mathbf{x}^{22} \\ \mathbf{x}^{30} \\ \mathbf{x}^{31} \\ \mathbf{x}^{32} \\ \mathbf{x}^{33} \end{bmatrix} = \begin{bmatrix} \mathbf{b}^{00} \\ \mathbf{b}^{10} \\ \mathbf{b}^{11} \\ \mathbf{b}^{20} \\ \mathbf{b}^{21} \\ \mathbf{b}^{22} \\ \mathbf{b}^{30} \\ \mathbf{b}^{31} \\ \mathbf{b}^{32} \\ \mathbf{b}^{33} \\ \mathbf{b}^{40} \\ \mathbf{b}^{41} \\ \mathbf{b}^{42} \\ \mathbf{b}^{43} \\ \mathbf{b}^{44} \end{bmatrix}.$$

We want solutions of (4.127) to emulate solutions induced by Hamiltonian cycles (if there are any in the graph). Hence, we add to (4.127) constraints on the vectors $\mathbf{x}^{k\ell}$, to try to force them to resemble $\sum\limits_{r=0}^{N-1} c_{k\ell}^r \mathbf{y}^r$ as closely as possible. Since we have exact expressions for each $c_{k\ell}^r$, we could impose constraints of the form

$$\mathbf{x}^{k\ell} = \sum_{r=1}^{N} c_{k\ell}^r \mathbf{y}^r, \tag{4.128}$$

$$\sum_{(i,a)\in\Gamma} y_{ia}^r = 1, \tag{4.129}$$

$$y_{ia}^r \in \{0,1\}. \tag{4.130}$$

However, we do not want to have the set of (binary) integer constraints (4.130), and so we relax these constraints. We now form ten sets of auxilliary constraints which, while not equivalent to (4.128)–(4.130), are designed to be difficult to satisfy while simultaneously satisfying (4.127) without obtaining integer $\mathbf{y}^r$. First, we derive three lemmata about sums of the coefficients $c^r_{k\ell}$.

Lemma 4.4.2 *For all $k = 2, \ldots, N-1$, $r = 1, \ldots, N$, we have*

$$\sum_{\ell=0}^{k} c^r_{k\ell} = 0.$$

Proof. We know from Propositions 4.3.8 and 4.3.9 that coefficients $c^r_{k\ell}$ take one of many forms, depending on the values of r, k and ℓ. If $r \geq 2$, we consider separately the three cases where $r < N-k+1$, $r = N-k+1$ and $r > N-k+1$. In the case where $r = 1$, we know from Remark 4.3.10 that since $k > 0$, the formula for $c^1_{k\ell}$ is the same as the general formula for the case where $r > N-k+1$, which is one of the three cases we are already considering. Therefore, we do not need to consider $r = 1$ separately.

Case 1: $r < N-k+1$. Then, we have

$$\begin{aligned}\sum_{\ell=0}^{k} c^r_{k\ell} &= 0 + \sum_{\ell=1}^{k} (-1)^{\ell+1} \frac{k}{N} \binom{k-1}{\ell-1} \\ &= \frac{k}{N} \sum_{\ell=0}^{k-1} (-1)^{\ell} \binom{k-1}{\ell}.\end{aligned}$$

We observe that $\sum_{\ell=0}^{k-1} (-1)^{\ell} \binom{k-1}{\ell} = 0$. This is because it is equivalent to a binomial expansion of $(1+x)^{k-1}$, setting $x = -1$. Therefore

$$\sum_{\ell=0}^{k} c^r_{k\ell} = (1-1)^{k-1} = 0, \quad \text{since } k \geq 2. \tag{4.131}$$

Case 2: $r = N - k + 1$. Then, we have

$$\begin{aligned}
\sum_{\ell=0}^{k} &= 1 + \sum_{\ell=1}^{k} (-1)^{\ell} \frac{N-\ell}{N} \begin{pmatrix} k \\ \ell \end{pmatrix} \\
&= 1 + \sum_{\ell=1}^{k} (-1)^{\ell} \begin{pmatrix} k \\ \ell \end{pmatrix} + \sum_{\ell=1}^{k} (-1)^{\ell+1} \frac{\ell}{N} \frac{k!}{\ell!(k-\ell)!} \\
&= \sum_{\ell=0}^{k} (-1)^{\ell} \begin{pmatrix} k \\ \ell \end{pmatrix} + \frac{k}{N} \sum_{\ell=1}^{k} (-1)^{\ell+1} \frac{(k-1)!}{(\ell-1)!(k-\ell)!} \\
&= (1-1)^k + \frac{k}{N}(1-1)^{k-1} = 0.
\end{aligned}$$

We are able to deduce the final line using the same argument as in (4.131).

Case 3: $r > N - k + 1$ (or $r = 1$).

$$\begin{aligned}
\sum_{\ell=0}^{k} &= 0 + \sum_{\ell=1}^{k} (-1)^{\ell} \frac{N-k}{N} \begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix} \\
&= -\frac{N-k}{N} \sum_{\ell=0}^{k-1} (-1)^{\ell} \begin{pmatrix} k-1 \\ \ell \end{pmatrix} \\
&= (1-1)^{k-1} = 0.
\end{aligned}$$

This completes the proof of the lemma. □

Lemma 4.4.3 *For all $r = 1, \ldots, N$, we have*

$$\sum_{k=0}^{1} \sum_{\ell=0}^{k} c_{k\ell}^{r} = c_{11}^{r} + c_{10}^{r} + c_{00}^{r} \quad = \quad \frac{1}{N}.$$

Proof. We consider three cases, that is, $r = 1$, $2 \leq r \leq N - 1$ and $r = N$.

Case 1: $r = 1$. Then, from Proposition 4.3.9 we obtain

$$c_{11}^{1} + c_{10}^{1} + c_{00}^{1} = (-1)\frac{N-1}{N} + 0 + 1 = \frac{1-N}{N} + \frac{N}{N} = \frac{1}{N}.$$

Case 2: $2 \leq r \leq N$. Then, from Proposition 4.3.8 we obtain

$$c_{11}^{r} + c_{10}^{r} + c_{00}^{r} = \frac{1}{N} + 0 + 0 = \frac{1}{N}.$$

Case 3: $r = N$. Then, from Proposition 4.3.8 we obtain

$$c_{11}^N + c_{10}^N + c_{00}^N = (-1)\frac{N-1}{N} + 1 + 0 = \frac{1}{N}.$$

Therefore, $\sum_{k=0}^{1}\sum_{\ell=0}^{k} c_{k\ell}^r = \frac{1}{N}$, for all $r = 1, \ldots, N$, which concludes the proof. □

Lemma 4.4.4 *For all $k = 1, \ldots, N-1$, $\ell = 1, \ldots, k$, we have*

$$\sum_{r=1}^{N} c_{k\ell}^r \;=\; (-1)^\ell \begin{pmatrix} k \\ \ell \end{pmatrix}.$$

Proof. Since the formula for $c_{k\ell}^r$ is separate for $r = 1$, we break the sum to obtain

$$\sum_{r=1}^{N} c_{k\ell}^r \;=\; c_{k\ell}^1 + \sum_{r=2}^{N} c_{k\ell}^r.$$

Then, from Propositions 4.3.8 Proposition 4.3.9 we obtain

$$\begin{aligned}
\sum_{r=1}^{N} c_{k\ell}^r \;=\;& (-1)^\ell \frac{N-k}{N}\begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix} + (N-k-1)(-1)^{\ell+1}\frac{k}{N}\begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix} \\
&+(-1)^\ell \frac{N-\ell}{N}\begin{pmatrix} k \\ \ell \end{pmatrix} + (k-1)(-1)^\ell \frac{N-k}{N}\begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix} \\
=\;& \frac{(-1)^\ell}{N}\begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix}\left[-(N-k-1)k + (N-\ell)\frac{k}{\ell} + k(N-k)\right] \\
=\;& \frac{(-1)^\ell}{N}\begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix}\left[k + \frac{Nk}{\ell} - k\right] \\
=\;& (-1)^\ell \begin{pmatrix} k \\ \ell \end{pmatrix}, \qquad (4.132)
\end{aligned}$$

which concludes the proof. □

We now use Lemmata 4.4.2 – 4.4.4 to derive new constraints on $\mathbf{x}^{k\ell}$ that are satisfied by all solutions induced by Hamiltonian cycles.

Remark 4.4.5 *The three lemmata above, and the auxilliary constraints that are derived in the remainder of this chapter, all take advantage of our knowledge of the* *exact form of the coefficients $c^r_{k\ell}$ from Propositions 4.3.8 and 4.3.9. Although those Propositions were given only for the standard reverse Hamiltonian cycle h_R, we note that the set $\left\{ c^1_{k\ell}, \ \ldots, \ c^N_{k\ell} \right\}$ is identical for all Hamiltonian cycles, and it is only the order of the coefficients that changes. None of the auxilliary constraints that we derive depend on r in their final form, and though the ordering of the Hamiltonian cycle is used in some of the proceeding derivations (most notably for the tenth and final set of auxilliary constraints), an analogous argument can be given for any Hamiltonian cycle that arrives at the same set of auxilliary constraints. Hence, the auxilliary constraints that we derive are satisfied for all Hamiltonian cycles that exist in the graph Γ.*

auxilliary constraints set 1: We consider $\sum_{\ell=0}^{k} x^{k\ell}_{ia}$ for all $k \geq 2$, $(i,a) \in \Gamma$. It immediately follows that for any arcs $(i,a) \in \Gamma$,

$$\begin{aligned} \sum_{\ell=0}^{k} x^{k\ell}_{ia} &= \sum_{r=1}^{N} y^r_{ia} \sum_{\ell=0}^{k} c^r_{k\ell} \\ &= 0, \quad \text{from Lemma 4.4.2.} \end{aligned} \tag{4.133}$$

The constraints (4.133) are the first set of auxilliary constraints.

Auxilliary constraints set 2: We consider $\sum_{k=0}^{N-1} \sum_{\ell=0}^{k} x^{k\ell}_{ia}$ for all $(i,a) \in \Gamma$.

$$\begin{aligned} \sum_{k=0}^{N-1} \sum_{\ell=0}^{k} x^{k\ell}_{ia} &= \sum_{r=1}^{N} y^r_{ia} \sum_{k=0}^{N-1} \sum_{\ell=0}^{k} c^r_{k\ell} \\ &= \sum_{r=1}^{N} y^r_{ia} \frac{1}{N}, \text{ from Lemmata 4.4.2 and 4.4.3.} \end{aligned}$$

From (4.117), we know that for any Hamiltonian cycle, each $\mathbf{y}^r$ contains only a single non-zero value, which is a 1. Then, we impose the relaxed 0-1 constraint by requiring

$$0 \leq \sum_{k=0}^{N-1} \sum_{\ell=0}^{k} x^{k\ell}_{ia} \leq \frac{1}{N}, \quad (i,a) \in \Gamma. \tag{4.134}$$

The constraints (4.134) are the second set of auxilliary constraints.

Auxilliary constraints set 3: We consider $\sum\limits_{(i,a)\in\Gamma} x_{ia}^{k\ell}$, for all $k = 1,\dots,N-1$, $\ell = 1,\dots,k$. Then,

$$\begin{aligned}\sum_{(i,a)\in\Gamma} x_{ia}^{k\ell} &= \sum_{r=1}^{N} c_{k\ell}^{r} \sum_{(i,a)\in\Gamma} y_{ia}^{r} \\ &= \sum_{r=1}^{N} c_{k\ell}^{r} \\ &= (-1)^{\ell} \begin{pmatrix} k \\ \ell \end{pmatrix}, \quad \text{from Lemma 4.4.4.} \end{aligned} \tag{4.135}$$

The constraints (4.135) are the third set of auxilliary constraints.

Auxilliary constraints set 4: We consider $\sum\limits_{k=0}^{N-1} \sum\limits_{a\in\mathcal{A}(i)} x_{ia}^{k0}$, for all $i = 1,\dots,N$. Then,

$$\sum_{k=0}^{N-1} \sum_{a\in\mathcal{A}(i)} x_{ia}^{k0} = \sum_{r=1}^{N} \sum_{a\in\mathcal{A}(i)} y_{ia}^{r} \sum_{k=0}^{N-1} c_{k0}^{r}.$$

We recall from Propositions 4.3.8 and 4.3.9 that, for any r, the coefficient $c_{k0}^{r} = 0$ for all but one choice of k, for which $c_{k0}^{r} = 1$. Therefore,

$$\sum_{k=0}^{N-1} \sum_{a\in\mathcal{A}(i)} x_{ia}^{k0} = \sum_{r=1}^{N} \sum_{a\in\mathcal{A}(i)} y_{ia}^{r}.$$

For a Hamiltonian cycle, we know that each node has a single arc emanating from it exactly once, and so for each $i = 1,\dots,N$

$$\sum_{k=0}^{N-1} \sum_{a\in\mathcal{A}(i)} x_{ia}^{k0} = 1. \tag{4.136}$$

The constraints (4.136) are the fourth set of auxilliary constraints.

Auxilliary constraints set 5: We consider $\sum\limits_{k=\ell}^{N-1} c_{k\ell}^{r}$, for $\ell > 0$, $r = 1,\dots,N$. First, we consider the case where $r \geq 2$. Again, while we do not know a Hamiltonian cycle in advance, we know from Proposition 4.3.8 that, if since $r \geq 2$, the above sum gives (we define $m := N - r + 1$ for ease of notation):

$$\begin{aligned}\sum_{k=\ell}^{N-1} c^r_{k\ell} &= \sum_{k=l}^{m-1}(-1)^{\ell+1}\frac{k}{N}\begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix} + (-1)^{\ell}\frac{N-\ell}{N}\begin{pmatrix} m \\ \ell \end{pmatrix} + \sum_{k=m+1}^{N-1}(-1)^{\ell}\frac{N-k}{N}\begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix} \\ &= \sum_{k=\ell}^{m-1}(-1)^{\ell}\frac{N-k}{N}\begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix} + \sum_{k=\ell}^{m-1}(-1)^{\ell+1}\begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix} \\ &\quad +(-1)^{\ell}\frac{N-\ell}{N}\begin{pmatrix} m \\ \ell \end{pmatrix} + \sum_{k=m+1}^{N-1}(-1)^{\ell}\frac{N-k}{N}\begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix}. \end{aligned} \tag{4.137}$$

We consider just the middle two terms for now, which we call t_M. That is,

$$\sum_{k=\ell}^{N-1} c^r_{k\ell} = \sum_{k=\ell}^{m-1}(-1)^{\ell}\frac{N-k}{N}\begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix} + t_M + \sum_{k=m+1}^{N-1}(-1)^{\ell}\frac{N-k}{N}\begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix}, \tag{4.138}$$

where

$$t_M = \sum_{k=\ell}^{m-1}(-1)^{\ell+1}\begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix} + (-1)^{\ell}\frac{N-\ell}{N}\begin{pmatrix} m \\ \ell \end{pmatrix}. \tag{4.139}$$

Then, we consider the Diagonal Sums identity from Pascal's triangle:

$$\sum_{i=r}^{n}\begin{pmatrix} i \\ r \end{pmatrix} = \begin{pmatrix} n+1 \\ r+1 \end{pmatrix}.$$

We select $r = \ell - 1$ and $n = m - 2$, and obtain

$$\sum_{i=\ell-1}^{m-2}\begin{pmatrix} i \\ \ell-1 \end{pmatrix} = \sum_{i=\ell}^{m-1}\begin{pmatrix} i-1 \\ \ell-1 \end{pmatrix} = \begin{pmatrix} m-1 \\ \ell \end{pmatrix} = \begin{pmatrix} m-1 \\ m-1-\ell \end{pmatrix}. \tag{4.140}$$

Then, substituting (4.140) into (4.139) we obtain

$$\begin{aligned} t_M &= (-1)^{\ell+1}\frac{(m-1)!}{(m-1-\ell)!\ell!} - (-1)^{\ell+1}\frac{N-\ell}{N}\frac{m!}{(m-\ell)!\ell!} \\ &= (-1)^{\ell+1}\frac{(m-1)!}{(m-1-\ell)!\ell!}\left[1 - \frac{m}{m-\ell}\frac{N-\ell}{N}\right] \\ &= (-1)^{\ell+1}\frac{(m-1)!}{(m-1-\ell)!\ell!}\left[\frac{Nm - N\ell - Nm + m\ell}{(m-\ell)N}\right] \\ &= \frac{(-1)^{\ell+1}}{N}\frac{(m-1)!}{(m-\ell)!\ell!}\left[(m-N)\ell\right] \end{aligned}$$

$$
\begin{aligned}
&= \frac{(-1)^\ell (N-m)}{N} \frac{(m-1)!}{(m-\ell)!(\ell-1)!} \\
&= \frac{(-1)^\ell (N-m)}{N} \begin{pmatrix} m-1 \\ \ell-1 \end{pmatrix}. \qquad (4.141)
\end{aligned}
$$

Next, we substitute (4.141) into (4.138) to obtain

$$
\begin{aligned}
\sum_{k=\ell}^{N-1} c^r_{k\ell} &= \sum_{k=\ell}^{m-1} (-1)^\ell \frac{N-k}{N} \begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix} + \frac{(-1)^\ell (N-m)}{N} \begin{pmatrix} m-1 \\ \ell-1 \end{pmatrix} \\
&\quad + \sum_{k=m+1}^{N-1} (-1)^\ell \frac{N-k}{N} \begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix} \\
&= \sum_{k=\ell}^{N-1} (-1)^\ell \frac{N-k}{N} \begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix}. \qquad (4.142)
\end{aligned}
$$

Note that if we now consider $r = 1$, (4.142) follows immediately from Proposition 4.3.9, and so we say that (4.142) holds for all $r = 1, \ldots, N$. We make use of this result by considering $\sum_{k=\ell}^{N-1} \sum_{a \in \mathcal{A}(i)} x^{k\ell}_{ia}$ for all $\ell > 0$, $i = 1, \ldots, N$. That is,

$$
\sum_{k=\ell}^{N-1} \sum_{a \in \mathcal{A}(i)} x^{k\ell}_{ia} = \sum_{r=1}^{N} \sum_{a \in \mathcal{A}(i)} y^r_{ia} \sum_{k=\ell}^{N-1} c^r_{k\ell}. \qquad (4.143)
$$

We substitute (4.142) into (4.143) to obtain

$$
\begin{aligned}
\sum_{k=\ell}^{N-1} \sum_{a \in \mathcal{A}(i)} x^{k\ell}_{ia} &= \sum_{k=\ell}^{N-1} (-1)^\ell \frac{N-k}{N} \begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix} \sum_{r=1}^{N} \sum_{a \in \mathcal{A}(i)} y^r_{ia} \\
&= \sum_{k=\ell}^{N-1} (-1)^\ell \frac{N-k}{N} \begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix}, \qquad (4.144)
\end{aligned}
$$

for all $i = 1, \ldots, N$, $\ell = 1, \ldots, N-1$. The constraints (4.144) are the fifth set of auxilliary constraints.

Auxilliary constraints set 6: We consider $\sum_{a \in \mathcal{A}(i)} x^{k\ell}_{ia}$, for all $i = 1, \ldots, N$, $k = 1, \ldots, N$, $\ell = 1, \ldots, k$. Then,

$$
\sum_{a \in \mathcal{A}(i)} x^{k\ell}_{ia} = \sum_{r=1}^{N} c^r_{k\ell} \sum_{a \in \mathcal{A}(i)} y^r_{ia}.
$$

We know that for any Hamiltonian cycle, exactly one of the above y^r_{ia} will be 1 and the rest will be 0, and therefore for all $i = 1, \ldots, N$, $k = 1, \ldots, N-1$, $\ell = 1, \ldots, k$,

$$\sum_{a \in \mathcal{A}(i)} x^{k\ell}_{ia} \quad = \quad c^{r^*}_{k\ell}, \tag{4.145}$$

for some r^*. Since we do not know in advance which value r^* takes, we only achieve lower and upper bounds on $\sum\limits_{a \in \mathcal{A}(i)} x^{k\ell}_{ia}$. From Propositions 4.3.8 and 4.3.9, we define lower bound $b_L(k,\ell)$ and upper bound $b_U(k,\ell)$ of (4.145) as

$$\begin{aligned} b_L(k,\ell) \quad &:= \quad \min\left\{(-1)^{\ell+1}\frac{k}{N}\begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix}, (-1)^{\ell}\frac{N-\ell}{N}\begin{pmatrix} k \\ \ell \end{pmatrix}, (-1)^{\ell}\frac{N-k}{N}\begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix}\right\}, \\ b_U(k,\ell) \quad &:= \quad \max\left\{(-1)^{\ell+1}\frac{k}{N}\begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix}, (-1)^{\ell}\frac{N-\ell}{N}\begin{pmatrix} k \\ \ell \end{pmatrix}, (-1)^{\ell}\frac{N-k}{N}\begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix}\right\}. \end{aligned}$$

Then, substituting the above bounds into (4.145) we obtain

$$\sum_{a \in \mathcal{A}(i)} x^{k\ell}_{ia} \leq b_U(k,\ell), \quad i = 1, \ldots, N, \quad k = 1, \ldots, N-1, \quad \ell = 1, \ldots, k. \tag{4.146}$$

$$\sum_{a \in \mathcal{A}(i)} x^{k\ell}_{ia} \geq b_L(k,\ell), \quad i = 1, \ldots, N, \quad k = 1, \ldots, N-1, \quad \ell = 1, \ldots, k. \tag{4.147}$$

The constraints (4.146)–(4.147) are the sixth set of auxilliary constraints.

Auxilliary constraints set 7: We consider the expression (4.145), but for $\ell = 0$. Then, from Propositions 4.3.8 and 4.3.9, we obtain

$$\sum_{a \in \mathcal{A}(i)} x^{k0}_{ia} \quad = \quad c^r_{k0} = \{0, 1\}.$$

Therefore, relaxing the above, we obtain

$$0 \leq \sum_{a \in \mathcal{A}(i)} x^{k0}_{ia} \leq 1, \quad \ell = 0, \ldots, N, \quad i = 1, \ldots, N. \tag{4.148}$$

The constraints (4.148) form the seventh set of auxilliary constraints.

Auxilliary constraints set 8: We consider next $\sum_{k=0}^{N-1} \sum_{(i,a)\in\Gamma} x_{ia}^{kk}$, then since $\sum_{(i,a)\in\Gamma} y_{ia}^{r} = 1$ for each r, we obtain

$$\begin{aligned}\sum_{k=0}^{N-1} \sum_{(i,a)\in\Gamma} x_{ia}^{kk} &= \sum_{r=1}^{N} \sum_{k=0}^{N-1} c_{kk}^{r} \sum_{(i,a)\in\Gamma} y_{ia}^{r} \\ &= \sum_{r=1}^{N} \sum_{k=0}^{N-1} c_{kk}^{r} \\ &= \sum_{r=1}^{N} c_{00}^{r} + \sum_{k=1}^{N-1} \sum_{r=1}^{N} c_{kk}^{r}.\end{aligned}$$

Recall from Propositions 4.3.8 and 4.3.9 that $c_{00}^{1} = 1$, and $c_{00}^{r} = 0$, for all $r \geq 2$. Then, from (4.135) we obtain

$$\begin{aligned}\sum_{k=0}^{N-1} \sum_{(i,a)\in\Gamma} x_{ia}^{kk} &= 1 + \sum_{k=1}^{N-1} (-1)^{k} \begin{pmatrix} k \\ k \end{pmatrix} \\ &= 1 + \sum_{k=1}^{N-1} (-1)^{k} \\ &= \sum_{k=0}^{N-1} (-1)^{k} \\ &= \frac{1}{2} + \left(-\frac{1}{2}\right)^{N}. \end{aligned} \tag{4.149}$$

The constraint (4.149) forms the eighth set of auxiliary constraints (though in this case, the set contains only a single constraint).

Auxilliary constraints set 9: We consider $\sum_{a\in\mathcal{A}(i)} \sum_{k=0}^{N-1} x_{ia}^{kk}$, for all $i = 1, \ldots, N$. Then

$$\sum_{a\in\mathcal{A}(i)} \sum_{k=0}^{N-1} x_{ia}^{kk} = \sum_{r=1}^{N} \sum_{a\in\mathcal{A}(i)} y_{ia}^{r} \sum_{k=0}^{N-1} c_{kk}^{r}.$$

For each $i = 1, \ldots, N$, exactly one $y_{ia}^{r} = 1$, for some r. Then

$$\sum_{a\in\mathcal{A}(i)} \sum_{k=0}^{N-1} x_{ia}^{kk} = \sum_{k=0}^{N-1} c_{kk}^{r}. \tag{4.150}$$

We first consider the case when $r \geq 2$. Recall from Proposition 4.3.8 that $c_{00}^{r} = 0$, for $r \geq 2$. Substituting this and the results from Proposition 4.3.8 for $\ell = k$ into (4.150) we obtain

$$\sum_{a\in\mathcal{A}(i)}\sum_{k=0}^{N-1} x_{ia}^{kk} = \sum_{k=1}^{N-r}(-1)^{k+1}\frac{k}{N} + (-1)^{N-r+1}\frac{N-(N-r+1)}{N} + \sum_{k=N-r+2}^{N-1}(-1)^{k}\frac{N-k}{N}. \tag{4.151}$$

Next, we consider (4.150) when $r = 1$. Then, from Proposition 4.3.9 we obtain

$$\sum_{a\in\mathcal{A}(i)}\sum_{k=0}^{N-1} x_{ia}^{kk} = 1 + \sum_{k=1}^{N-1}(-1)^{k}\frac{N-k}{N}. \tag{4.152}$$

Now we consider three cases, the first where $r = 1$, the second where $2 \le r \le N-1$, and the third where $r = N$.

Case 1: If $r = 1$, then from (4.152) we have

$$\begin{aligned}\sum_{a\in\mathcal{A}(i)}\sum_{k=0}^{N-1} x_{ia}^{kk} &= 1 + \sum_{k=1}^{N-1}(-1)^{k}\frac{N-k}{N}\\ &= 1 + \sum_{k=1}^{N-1}(-1)^{k} + \frac{1}{N}\sum_{k=1}^{N-1}(-1)^{k+1}k.\end{aligned}$$

Then, if N is odd, the middle term above disappears and the expression reduces to

$$\sum_{a\in\mathcal{A}(i)}\sum_{k=0}^{N-1} x_{ia}^{kk} = 1 + \frac{1}{N}\sum_{k=1}^{N-1}(-1)^{k+1}k. \tag{4.153}$$

Note that

$$\sum_{k=1}^{N-1}(-1)^{k+1}k = [1-2]+[3-4]+\ldots+[(N-2)-(N-1)] = -\left(\frac{N-1}{2}\right). \tag{4.154}$$

Substituting (4.154) into (4.153) we obtain

$$\sum_{a\in\mathcal{A}(i)}\sum_{k=0}^{N-1} x_{ia}^{kk} = 1 - \frac{N-1}{2N} = \frac{1}{2} + \frac{1}{2}N. \tag{4.155}$$

If N is even, using a similar argument we instead obtain

$$\sum_{a\in\mathcal{A}(i)}\sum_{k=0}^{N-1} x_{ia}^{kk} = 1 - 1 + \frac{1}{2} = \frac{1}{2}. \tag{4.156}$$

Case 2: If $2 \leq r \leq N-1$, then from (4.151) we have

$$\begin{aligned}
\sum_{a\in\mathcal{A}(i)}\sum_{k=0}^{N-1} x_{ia}^{kk} &= \sum_{k=1}^{N-r}(-1)^{k+1}\frac{k}{N} + (-1)^{N-r+1}\frac{N-(N-r+1)}{N} + \sum_{k=N-r+2}^{N-1}(-1)^k\frac{N-k}{N} \\
&= \sum_{k=1}^{N-r}(-1)^k\frac{N-k}{N} + \sum_{k=1}^{N-r}(-1)^{k+1} + (-1)^{N-r+1}\frac{N-(N-r+1)}{N} \\
&\quad + \sum_{k=N-r+2}^{N-1}(-1)^k\frac{N-k}{N} \\
&= \sum_{k=1}^{N-1}(-1)^k\frac{N-k}{N} + \sum_{k=1}^{N-r}(-1)^{k+1} \\
&= \sum_{k=1}^{N-1}(-1)^k + \sum_{k=1}^{N-r}(-1)^{k+1} + \frac{1}{N}\sum_{k=1}^{N-1}(-1)^{k+1}k \\
&= \sum_{k=N-r+1}^{N-1}(-1)^k + \frac{1}{N}\sum_{k=1}^{N-1}(-1)^{k+1}k.
\end{aligned}$$

Then, if N is odd (4.151) simplifies to

$$\sum_{a\in\mathcal{A}(i)}\sum_{k=0}^{N-1} x_{ia}^{kk} = \sum_{k=N-r+1}^{N-1}(-1)^k - \frac{N-1}{2N}.$$

We do not know the value of r, so we cannot find the exact value of the above expression. However, we know the final term of the sum will be $+1$ (as $N-1$ is even), and therefore the sum will either be 0 or 1. Thus, we can impose the following bounds:

$$-\frac{1}{2} + \frac{1}{2N} \leq \sum_{a\in\mathcal{A}(i)}\sum_{k=0}^{N-1} x_{ia}^{kk} \leq \frac{1}{2} + \frac{1}{2N}. \tag{4.157}$$

If N is even we instead obtain

$$\sum_{a\in\mathcal{A}(i)}\sum_{k=0}^{N-1} x_{ia}^{kk} = \sum_{k=N-r+1}^{N-1}(-1)^k + \frac{1}{2}.$$

Again, we cannot find the exact value of the above expression, but using analogous arguments as above, we can impose the following bounds

$$-\frac{1}{2} \leq \sum_{a\in\mathcal{A}(i)}\sum_{k=0}^{N-1} x_{ia}^{kk} \leq \frac{1}{2}. \tag{4.158}$$

Case 3: If $r = N$, then from (4.151) we have

$$\begin{aligned}\sum_{a\in\mathcal{A}(i)}\sum_{k=0}^{N-1} x_{ia}^{kk} &= -\left(\frac{N-1}{N}\right)+\sum_{k=2}^{N-1}(-1)^k\frac{N-k}{N}\\ &= \sum_{k=1}^{N-1}(-1)^k+\frac{1}{N}\sum_{k=1}^{N-1}(-1)^{k+1}k.\end{aligned}$$

If N is odd, we obtain

$$\sum_{a\in\mathcal{A}(i)}\sum_{k=0}^{N-1} x_{ia}^{kk} = \frac{1-N}{2N} = -\frac{1}{2}+\frac{1}{2}N. \tag{4.159}$$

If N is even, we obtain

$$\sum_{a\in\mathcal{A}(i)}\sum_{k=0}^{N-1} x_{ia}^{kk} = -\frac{1}{2}. \tag{4.160}$$

Note that the bounds given in (4.157) also encompass the equality constraints (4.155) and (4.159). In addition, the bounds given in (4.158) also encompass the equality constraints (4.156) and (4.160). Then, since we do not know in advance the value of r, we simply consider (4.157) and (4.158) for all $r = 1,\dots,N$. We can further combine (4.157) and (4.158) into a single set of constraints that accommodates any N:

$$-\frac{1}{2}+\frac{1}{4N}-(-1)^N\frac{1}{4N} \le \sum_{a\in\mathcal{A}(i)}\sum_{k=0}^{N-1} x_{ia}^{kk} \le \frac{1}{2}+\frac{1}{4N}-(-1)^N\frac{1}{4N}, \tag{4.161}$$

for $i = 1,\dots,N$. The constraints (4.161) are the ninth set of auxilliary constraints.

Auxilliary constraints set 10: For the final set of auxilliary constraints, we want to replicate the auxilliary constraints (4.31) that causes the one-parameter model in Section 4.2 to be infeasible for bridge graphs. We consider $\sum\limits_{j\neq i}\sum\limits_{a\in\mathcal{A}(j)} x_{ja}^{k0} - \sum\limits_{\ell\neq i} x_{\ell i}^{k-1,0}$, for all $i = 1,\dots,N, k = 2,\dots,N-1$. Then, we know that

$$\sum_{j\neq i}\sum_{a\in\mathcal{A}(j)} x_{ja}^{k0} - \sum_{\ell\neq i} x_{\ell i}^{k-1,0} = \sum_{j\neq i}\sum_{a\in\mathcal{A}(j)}\sum_{r=1}^{N} c_{k0}^r y_{ja}^r - \sum_{\ell\neq i}\sum_{r=1}^{N} c_{k-1,0}^r y_{\ell i}^r.$$

Then, from Proposition 4.3.8, we know that $c^r_{k0} = 1$ when $r = N - k + 1$, and $c^r_{k0} = 0$ for all other r. Likewise, we know that $c^r_{k-1,0} = 1$ when $r = N - k + 2$, and $c^r_{k-1,0} = 0$ for all other r. Note that we need not consider c^1_{k0} or $c^1_{k-1,0}$, as $k > 1$ and therefore from Proposition 4.3.9, $c^1_{k0} = c^1_{k-1,0} = 0$. Hence,

$$\sum_{j\neq i}\sum_{a\in\mathcal{A}(j)} x^{k0}_{ja} - \sum_{\ell\neq i} x^{k-1,0}_{\ell i} \;=\; \sum_{j\neq i}\sum_{a\in\mathcal{A}(j)} y^{N-k+1}_{ja} - \sum_{\ell\neq i} y^{N-k+2}_{\ell i}. \tag{4.162}$$

Remark 4.4.6 *For the standard reverse Hamiltonian cycle, we think of r as the ordering index of the nodes in the Hamiltonian cycle. Then, (4.162) corresponds to constraints (4.31). For any other Hamiltonian cycle, the choices of r in the two sums above are no longer $N - k + 1$ and $N - k + 2$ respectively, but nonetheless they correspond to the order of successive arcs in a Hamiltonian cycle, and therefore still correspond to (4.31).*

Therefore, from (4.31), for all $i = 1, \dots, N$ and $k = 1, \dots, N - 1$, we have

$$\sum_{j\neq i}\sum_{a\in\mathcal{A}(j)} x^{k0}_{ja} - \sum_{\ell\neq i} x^{k-1,0}_{\ell i} \;=\; 1. \tag{4.163}$$

The constraint (4.163) are the tenth and final set of auxilliary constraints.

We combine each of the auxilliary constraints we have derived, with the block constraints (4.127), to form a new, parameter-free LP

$$\begin{aligned}
W_{00}\mathbf{x}^{00} &= \mathbf{b}_{00},\\
W_{00}\mathbf{x}^{10} + W_{10}\mathbf{x}^{00} &= \mathbf{b}_{10},\\
W_{00}\mathbf{x}^{11} + W_{11}\mathbf{x}^{00} &= \mathbf{b}_{11},\\
&\vdots\\
W_{11}\mathbf{x}^{N-1,N-1} &= \mathbf{b}_{NN},\\
\sum_{\ell=0}^{k} x^{k\ell}_{ia} &= 0, \quad k = 2, \dots, N-1, \quad (i,a) \in \Gamma,\\
\sum_{k=0}^{N-1}\sum_{\ell=0}^{k} x^{k\ell}_{ia} &\leq \frac{1}{N}; \quad (i,a) \in \Gamma,\\
\sum_{k=0}^{N-1}\sum_{\ell=0}^{k} x^{k\ell}_{ia} &\geq 0; \quad (i,a) \in \Gamma,
\end{aligned}$$

$$
\begin{aligned}
\sum_{(i,a)\in\Gamma} x_{ia}^{k\ell} &= (-1)^{\ell}\begin{pmatrix} k \\ \ell \end{pmatrix}, \quad 1 \leq \ell \leq k \leq N-1, \\
\sum_{k=0}^{N-1}\sum_{a\in\mathcal{A}(i)} x_{ia}^{k0} &= 1, \quad i = 1,\ldots,N, \\
\sum_{k=\ell}^{N-1}\sum_{a\in\mathcal{A}(i)} x_{ia}^{k\ell} &= \sum_{k=\ell}^{N-1}(-1)^{\ell}\frac{N-k}{N}\begin{pmatrix} k-1 \\ \ell-1 \end{pmatrix}, \quad i = 1,\ldots,N, \quad \ell = 1,\ldots,N-1, \\
\sum_{a\in\mathcal{A}(i)} x_{ia}^{k\ell} &\leq b_U(k,\ell), \quad i = 1,\ldots,N, \quad 1 \leq \ell \leq k \leq N-1, \\
\sum_{a\in\mathcal{A}(i)} x_{ia}^{k\ell} &\geq b_L(k,\ell), \quad i = 1,\ldots,N, \quad 1 \leq \ell \leq k \leq N-1, \\
\sum_{a\in\mathcal{A}(i)} x_{ia}^{k0} &\leq 1, \quad i = 1,\ldots,N, \quad 0 \leq k \leq N-1, \\
\sum_{a\in\mathcal{A}(i)} x_{ia}^{k0} &\geq 0, \quad i = 1,\ldots,N, \quad 0 \leq k \leq N-1, \\
\sum_{k=0}^{N-1}\sum_{(i,a)\in\Gamma} x_{ia}^{kk} &= \frac{1}{2} + \left(-\frac{1}{2}\right)^{N}, \\
\sum_{a\in\mathcal{A}(i)}\sum_{k=0}^{N-1} x_{ia}^{kk} &\leq \frac{1}{2} + \frac{1}{4N} - (-1)^{N}\frac{1}{4N}, \quad i = 1,\ldots,N, \\
\sum_{a\in\mathcal{A}(i)}\sum_{k=0}^{N-1} x_{ia}^{kk} &\geq -\frac{1}{2} + \frac{1}{4N} - (-1)^{N}\frac{1}{4N}, \quad i = 1,\ldots,N, \\
\sum_{j\neq i}\sum_{a\in\mathcal{A}(j)} x_{ja}^{k0} - \sum_{j\neq i} x_{\ell i}^{k-1,0} &= 1, \quad i = 1,\ldots,N, \quad 1 \leq k \leq N.
\end{aligned}
$$

This model attempts to find a solution of the form (4.120). We have implemented this model in MATLAB using a CPLEX interface. Unfortunately, while this model was able to correctly identify all bridge graphs in a similar fashion to Conjecture 4.2.3, it was not able to identify any other non-Hamiltonian graphs and so currently, the additional effort required to solve the above model compared to (4.28)–(4.31) yields no additional results. However, we hope that further refining of the above model will lead to additional non-Hamiltonian graphs being identified. We suggest some improvements are suggested in Section 5.3 that at the time of submission of this thesis are already leading to promising results.

Chapter 5

Conclusions and Future Work

In this thesis we have demonstrated a number of algorithmic developments ensuing from the embedding of the Hamiltonian cycle problem in a discounted Markov decision process. We have discovered new properties of Hamiltonian cycles, revealed by this embedding, and have developed four new algorithmic approaches as a result.

In Chapter 2, we outlined an improved version of the branch and fix method in [28], and demonstrated that this method works well in the space of discounted occupational measures. We used the discount parameter inherited from the discounted Markov decision process embedding to develop wedge constraints that improved the model significantly. We then used a tightened version of the wedge constraints to formulate the Wedged-MIP heuristic that succeeded in solving large graphs.

In Chapter 3, we outlined the interior point method, DIPA, designed to solve the optimisation problem given in [14], that is equivalent to the Hamiltonian cycle problem. We derived formulae that allow us to calculate the derivatives of the objective function much quicker than standard algorithms, and designed DIPA to take advantage of the sparsity inherent in difficult graphs. We conjectured about the existence of a unique strictly interior saddle-point in the optimisation problem formulated in [14], and gave experimental evidence supporting this conjecture.

In Chapter 4, we investigated the form of Hamiltonian solutions of linear equations, derived from the discounted Markov decision process embedding. We derived exact expressions for all Hamiltonian cycles for both unperturbed and perturbed discounted Markov decision process embeddings. Furthermore, we supplied experimental evidence that our understanding of these expressions allows us to formulate new linear feasibility programs that identify (by their infeasibility) the majority of non-Hamiltonian graphs.

All models in this thesis, other than the Wedged-MIP heuristic, have been implemented in MATLAB. The most obvious direction of future research is to implement these models in compiled language, which will lead to an improvement in the running times compared to the results displayed in this thesis. However, we have also raised new questions that are as of yet unanswered, and identified many potentially fruitful directions of further research. These include, but are not limited to, the following.

5.1 Future work arising from Chapter 2

In both the branch and fix method and the Wedged-MIP heuristic, we currently only use constraints that seek a single, directed, Hamiltonian cycle starting from the first node. One possible improvement is to introduce new variables that find the reverse Hamiltonian cycle. Then, by use of some coupling constraints, we can demand that a solution be satisfied in two directions simultaneously. Alternatively (or additionally), we can introduce new variables for each possible home node in the graph. Then, by use of some further coupling constraints, we can demand that a solution be satisfied for N Hamiltonian cycles, all using the same arcs, but each starting at a different node. This will lead to a reduced feasible region.

We can apply the tightened wedge constraints, currently used only in the Wedged-MIP heuristic, to the branch and fix method. These constraints are graph-specific constraints, which will lead to further improvement in the performance of the branch and fix method.

5.2 Future work arising from Chapter 3

An interior point method was developed in [15] that solved a quadratic programming problem, with constraints arising from embedding the Hamiltonian cycle problem in a long-run average Markov decision process. Modifying DIPA to solve an equivalent quadratic programming problem, but with constraints arising from the discounted Markov decision process embedding will allow us to take advantage of knowledge gained from both [15] and this thesis. In particular, the addition of wedge constraints from Chapter 2 will prove fruitful.

The knowledge gained about the LU decomposition of the negative generator matrix for Hamiltonian cycles has led to a new quartic feasibility program that is satisfied only by solutions corresponding to Hamiltonian cycles.

$$
\begin{aligned}
\left(\sum_{k=1}^{N} l_{ik}u_{kj}\right)\left(\sum_{k=1}^{N} l_{ik}u_{kj}+1\right) &= 0, \quad i=1,\ldots,N, \quad j=1,\ldots,N, \quad i\neq j,\\
l_{ik}u_{ki} &= 0, \quad i=k+1,\ldots,N,\\
l_{ii}=u_{ii} &= 1, \quad i=1,\ldots,N-1,\\
l_{NN} &= 1,\\
u_{NN} &= 0,\\
l_{ij}=u_{ji} &= 0, \quad i=1,\ldots,N-1, \quad j=i+1,\ldots,N,\\
-1\leq l_{ji} &\leq 0, \quad i=1,\ldots,N-1, \quad j=i+1,\ldots,N,\\
-1\leq u_{ij} &\leq 0, \quad i=1,\ldots,N-1, \quad j=i+1,\ldots,N,
\end{aligned}
$$

The variables in the above program are from the L and U matrices in the LU decomposition, $LU = I - P$. This formulation of the Hamiltonian cycle problem contains only $N(N-1)$ nonlinear constraints, all of degree 4. Solving this feasibility program will be the subject of future research.

The unique saddle-point conjecture, and its potential use in the graph isomorphism problem are also new directions of research that will be further investigated. In addition to determining if the saddle-point exists and is unique for all graphs, we will investigate methods of identifying the saddle-point quickly.

5.3 Future work arising from Chapter 4

We aim to prove that the two models given in Chapter 4 are infeasible for all bridge graphs, which will verify the experimental results we have obtained so far. The two models can also be extended, in a similar sense to the improvements suggested in Section 5.1, by introducing new variables corresponding to alternative starting nodes. Then, by the use of suitable coupling constraints, we will demand that solutions satisfy the original constraints in both directions, for all possible starting nodes. This more restrictive set of constraints will, hopefully, lead to further non-Hamiltonian graphs being identified by the infeasibility of the new constraints.

Appendix A

Appendices

Recall that Proposition 4.3.5:

Consider h_R, $P^{\nu}_{h_R}$ and M as defined in Lemma 4.3.1. We further define $d^{\nu}_{j1}(\beta)$ as the $(j,1)$-th cofactor of M. Then, for $j = 1$,

$$d^{\nu}_{11}(\beta) \quad = \quad \frac{\frac{1}{N}\beta\nu}{(1+\lambda)^2}\left[1-(-\lambda)^N - N(1+\lambda)\right] + 1, \tag{A.1}$$

and, for $j \geq 2$

$$d^{\nu}_{j1}(\beta) \quad = \quad \frac{\left(\frac{1}{N}\beta\nu\right)}{(1+\lambda)^2}\left[1-(-\lambda)^N - N(-\lambda)^{N-j+1}(1+\lambda)\right] + (-\lambda)^{N-j+1}. \tag{A.2}$$

In Appendices A.1 – A.5, we prove Proposition 4.3.5 for the special cases $j = 1$ and $j = 2$, and we derive closed-form expressions for three determinants that are used in the proof of Proposition 4.3.5. Recall from that proof that we define $\lambda := \beta\nu - \beta$. In Appendix A.6 we provide adjacency lists, and a Hamiltonian solution, for each of four graphs, of sizes 250, 500, 1000 and 2000 respectively.

A.1 Proof of Proposition 4.3.5 for $j = 1$

Recall the form of M as defined in Lemma 4.3.1, and that $d^{\nu}_{11}(\beta)$ is defined as the $(1,1)$-th cofactor of M in Proposition 4.3.5.

Lemma A.1.1

$$d^{\nu}_{11}(\beta) \;=\; \frac{\frac{1}{N}\beta\nu}{(1+\lambda)^2}\left[1-(-\lambda)^N - N(1+\lambda)\right]+1. \tag{A.3}$$

This proof is intended to follow the general proof of Proposition 4.3.5 for $j \geq 2$ and hence utilises some expressions and derivations from that proof. We recommend that the general proof is read first.

Proof. Recall from (4.64) that

$$d^{\nu}_{11}(\beta) \;=\; \det(M^{11}). \tag{A.4}$$

Then, consider the $(N-1)\times(N-1)$ matrix M^{11}, which is the $(1,1)$-th minor of M. This minor has the following structure

$$M^{11} \;=\; \begin{bmatrix} 1-\frac{\beta\nu}{N} & -\frac{\beta\nu}{N} & \cdots & \cdots & \cdots & \cdots & \cdots & -\frac{\beta\nu}{N} \\ -\beta(1-\frac{N-1}{N}\nu) & 1-\frac{\beta\nu}{N} & -\frac{\beta\nu}{N} & \cdots & \cdots & \cdots & \cdots & -\frac{\beta\nu}{N} \\ -\frac{\beta\nu}{N} & -\beta(1-\frac{N-1}{N}\nu) & 1-\frac{\beta\nu}{N} & -\frac{\beta\nu}{N} & \cdots & \cdots & \cdots & -\frac{\beta\nu}{N} \\ \vdots & \ddots & \ddots & \ddots & \ddots & & & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \ddots & & \vdots \\ \vdots & & & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & & & \ddots & \ddots & \ddots & -\frac{\beta\nu}{N} \\ -\frac{\beta\nu}{N} & \cdots & \cdots & \cdots & \cdots & -\frac{\beta\nu}{N} & -\beta(1-\frac{N-1}{N}\nu) & 1-\frac{\beta\nu}{N} \end{bmatrix}. \tag{A.5}$$

We define two elementary matrices, E^1_{11} and E^2_{11}, as the following.

$$\begin{aligned} E^1_{11} &= I - \mathbf{e}\mathbf{e}_1^T + \mathbf{e}_1\mathbf{e}_1^T, \\ E^2_{11} &= \begin{bmatrix} 1 & 0 & \cdots & \cdots & 0 \\ 0 & 1 & \ddots & & \vdots \\ 0 & -1 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & -1 & 1 \end{bmatrix}. \end{aligned} \tag{A.6}$$

Note that these two elementary matrices are equivalent to E_2 and E_3, given in equations (4.65) and (4.66) in the general proof of Proposition 4.3.5.

Then, premultiplying M^{11} by E^1_{11}, postmultiplying the result by E^2_{11}, and recalling that $\lambda := \beta\nu - \beta$, we obtain the $(N-1) \times (N-1)$ matrix Y^{11}

$$Y^{11} := E^1_{11} M^{11} E^2_{11} = \begin{bmatrix} 1-\frac{\beta\nu}{N} & 0 & \cdots & \cdots & \cdots & \cdots & 0 & -\frac{\beta\nu}{N} \\ \lambda-1 & 1 & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ -1 & \lambda-1 & 1 & \ddots & & & & \vdots \\ -1 & \lambda & \lambda-1 & \ddots & \ddots & & & \vdots \\ \vdots & 0 & -\lambda & \ddots & \ddots & \ddots & & \vdots \\ \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & & \ddots & \ddots & \ddots & 1 & 0 \\ -1 & 0 & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1 \end{bmatrix}.$$

Since E^1_{11} and E^2_{11} are triangular matrices with units on their diagonals, we see that

$$\det(M^{11}) = \det(Y^{11}). \tag{A.7}$$

We find $\det(Y^{11})$ by expanding on the last column where there are two non-zero entries, in the first and $(N-1)$-th positions. Expanding on this column, we find two minors M^{11}_1 and M^{11}_2. Then,

$$\det(Y^{11}) = (-1)^N(-\frac{\beta\nu}{N})\det(M^{11}_1) + \det(M^{11}_2). \tag{A.8}$$

The determinant of the second minor, M^{11}_2, is the simplest to evaluate. It is an $(N-2) \times (N-2)$ matrix with the structure

$$M^{11}_2 = \begin{bmatrix} 1-\frac{\beta\nu}{N} & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\ \lambda-1 & 1 & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ -1 & \lambda-1 & 1 & \ddots & & & & \vdots \\ -1 & \lambda & \lambda-1 & \ddots & \ddots & & & \vdots \\ \vdots & 0 & -\lambda & \ddots & \ddots & \ddots & & \vdots \\ \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & & \ddots & \ddots & \ddots & \ddots & 0 \\ -1 & 0 & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1 \end{bmatrix}.$$

M_2^{11} is a lower-triangular matrix, and therefore

$$\det(M_2^{11}) = 1 - \frac{\beta\nu}{N}. \tag{A.9}$$

The other minor, M_1^{11}, is an $(N-2) \times (N-2)$ matrix with the structure

$$M_1^{11} = \begin{bmatrix} \lambda - 1 & 1 & 0 & \cdots & \cdots & \cdots & 0 \\ -1 & \lambda - 1 & \ddots & \ddots & & & \vdots \\ -1 & -\lambda & \ddots & \ddots & \ddots & & \vdots \\ \vdots & 0 & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & \vdots & & \ddots & \ddots & \ddots & 1 \\ -1 & 0 & \cdots & \cdots & 0 & -\lambda & \lambda - 1 \end{bmatrix}.$$

This minor has the same form as a matrix (A.64), that is investigated in the general proof of Proposition 4.3.5, and its determinant is given in (A.68). However, the latter matrix had dimensions $(j-3) \times (j-3)$, rather than $(N-2) \times (N-2)$ for M_1^{11}. Substituting $j = N+1$ into (A.68) we obtain

$$\det(M_1^{11}) = \left[\sum_{i=0}^{N-2} \lambda^{N-2-i}(i+1)(-1)^i\right] + (-1)^{N+1}. \tag{A.10}$$

Substituting (A.9) and (A.10) into (A.8) we find

$$\begin{aligned} \det(Y^{11}) &= (-1)^N(-\frac{\beta\nu}{N})\left(\sum_{i=0}^{N-2} \lambda^{N-2-i}(i+1)(-1)^i\right) + \frac{\beta\nu}{N} + 1 - \frac{\beta\nu}{N} \\ &= 1 - \frac{1}{N}\beta\nu\left(\sum_{i=0}^{N-2}(-\lambda)^{N-2-i}(i+1)\right), \end{aligned}$$

and we substitute the above into (A.7) to obtain

$$\det(M^{11}) = 1 - \frac{1}{N}\beta\nu\left(\sum_{i=0}^{N-2}(-\lambda)^{N-2-i}(i+1)\right). \tag{A.11}$$

Consider the sum in (A.11). We rewrite the sum as

$$\sum_{i=0}^{N-2}(-\lambda)^{N-2-i}(i+1) = N\sum_{i=0}^{N-2}(-\lambda)^i - \sum_{i=0}^{N-2}(-\lambda)^i(i+1).$$

We use the geometric series formula in the first sum above to obtain

$$\sum_{i=0}^{N-2}(-\lambda)^{N-2-i}(i+1) = \frac{N(1-(-\lambda)^{N-1})}{(1+\lambda)} - \sum_{i=0}^{N-2}(-\lambda)^{i}(i+1).$$

Next, we rewrite the remaining sum as a sum of derivatives of $(-\lambda)^{i+1}$ to obtain

$$\begin{aligned}\sum_{i=0}^{N-2}(-\lambda)^{N-2-i}(i+1) &= \frac{N(1-(-\lambda)^{N-1})}{(1+\lambda)} + \sum_{i=0}^{N-2}\frac{\partial(-\lambda)^{i+1}}{\partial\lambda} \\ &= \frac{N(1-(-\lambda)^{N-1})}{(1+\lambda)} + \frac{\partial}{\partial\lambda}\sum_{i=1}^{N-1}(-\lambda)^{i}.\end{aligned}$$

We augment the second sum by the additional term when $i = 0$, for which the derivative is 0, and use the geometric series formula to find

$$\sum_{i=0}^{N-2}(-\lambda)^{N-2-i}(i+1) = \frac{N(1-(-\lambda)^{N-1})}{(1+\lambda)} + \frac{\partial}{\partial\lambda}\left(\frac{1-(-\lambda)^{N}}{1+\lambda}\right).$$

We take the derivative in the above and simply to obtain

$$\begin{aligned}\sum_{i=0}^{N-2}(-\lambda)^{N-2-i}(i+1) &= \frac{N(1-(-\lambda)^{N-1})}{(1+\lambda)} + \frac{(-\lambda)^{N-1}(N)(1+\lambda)-1+(-\lambda)^{N}}{(1+\lambda)^2} \\ &= \frac{N(1-(-\lambda)^{N-1})(1+\lambda)+(-\lambda)^{N-1}(N)(1+\lambda)-1+(-\lambda)^{N}}{(1+\lambda)^2} \\ &= \frac{N+N\lambda-N(-\lambda)^{N-1}+N(-\lambda)^{N}}{(1+\lambda)^2} \\ &\quad + \frac{N(-\lambda)^{N-1}-N(-\lambda)^{N}-1+(-\lambda)^{N}}{(1+\lambda)^2} \\ &= \frac{-1+(-\lambda)^{N}+N(1+\lambda)}{(1+\lambda)^2}. \qquad \text{(A.12)}\end{aligned}$$

Finally, we substitute (A.12) into (A.11) to obtain

$$\det(M^{11}) = \frac{\frac{1}{N}\beta\nu}{(1+\lambda)^2}\left[1-(-\lambda)^{N}-N(1+\lambda)\right]+1. \qquad \text{(A.13)}$$

Substituting (A.13) into (A.4) concludes the proof. □

A.2 Proof of Proposition 4.3.5 for $j = 2$

In this appendix we will prove Proposition 4.3.5 for the special case $j = 2$. Recall the form of M as defined in Lemma 4.3.1, and that we define $\lambda := \beta\nu - \beta$.

Lemma A.2.1

$$d_{21}^{\nu}(\beta) \quad = \quad \frac{(\frac{1}{N}\beta\nu)}{(1+\lambda)^2}\left[1-(-\lambda)^N - N(-\lambda)^{N-1}(1+\lambda)\right] + (-\lambda)^{N-1}.$$

Proof. Recall from (4.64) that

$$d_{21}^{\nu}(\beta) \quad = \quad -\det(M^{21}). \tag{A.14}$$

Then, consider the $(N-1)\times(N-1)$ matrix M^{21}, which is the $(2,1)$-th minor of M. This minor has the following structure

$$M^{21} \quad = \quad \begin{bmatrix} -\frac{\beta\nu}{N} & \cdots & \cdots & \cdots & \cdots & \cdots & -\frac{\beta\nu}{N} & -\beta(1-\frac{N-1}{N}\nu) \\ -\beta(1-\frac{N-1}{N}\nu) & 1-\frac{\beta\nu}{N} & -\frac{\beta\nu}{N} & \cdots & \cdots & \cdots & \cdots & -\frac{\beta\nu}{N} \\ -\frac{\beta\nu}{N} & \ddots & \ddots & \ddots & & & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & & & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \ddots & & \vdots \\ \vdots & & & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & & & \ddots & \ddots & \ddots & -\frac{\beta\nu}{N} \\ -\frac{\beta\nu}{N} & \cdots & \cdots & \cdots & \cdots & -\frac{\beta\nu}{N} & -\beta(1-\frac{N-1}{N}\nu) & 1-\frac{\beta\nu}{N} \end{bmatrix}.$$

First, we shift the last column to the front of the matrix using the following $(N-1)\times(N-1)$ elementary matrix E_1^{21}:

$$E_1^{21} \quad = \quad \begin{bmatrix} & 1 & & & \\ & & 1 & & \\ & & & \ddots & \\ & & & & 1 \\ 1 & & & & \end{bmatrix},$$

which has determinant

$$\det(E_1^{21}) \quad = \quad (-1)^N. \tag{A.15}$$

Next, we use a second elementary matrix E_2^{21} which subtracts the top row from every other row, and multiplies the top row by -1,

$$E_2^{21} \quad = \quad I - \mathbf{e}\mathbf{e}_1^T - \mathbf{e}_1\mathbf{e}_1^T, \tag{A.16}$$

for which $\det(E_2^{21}) = -1$. Multiplying M^{21} on the right by E_1^{21} and on the left by E_2^{21} we obtain a new $(N-1) \times (N-1)$ matrix, which we call Y^{21}:

$$Y^{21} := E_2^{21} M^{21} E_1^{21} \quad = \quad \begin{bmatrix} \beta(1-\frac{N-1}{N}\nu) & \frac{\beta\nu}{N} & \frac{\beta\nu}{N} & \cdots & \cdots & \cdots & \cdots & \frac{\beta\nu}{N} \\ -\lambda & \lambda & 1 & 0 & \cdots & \cdots & \cdots & 0 \\ \vdots & 0 & \lambda & 1 & \ddots & & & \vdots \\ \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & & \vdots \\ \vdots & \vdots & & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & & & \ddots & \ddots & \ddots & 0 \\ -\lambda & \vdots & & & & \ddots & \ddots & 1 \\ -\lambda+1 & 0 & \cdots & \cdots & \cdots & \cdots & 0 & \lambda \end{bmatrix}. \tag{A.17}$$

From (A.15) and (A.16) we see that

$$\det(M^{21}) \quad = \quad (-1)^{N-1} \det(Y^{21}). \tag{A.18}$$

Next, we eliminate the $-\lambda$ terms in the first column of (A.17). Define $\mathbf{c}_k^{21}$ to be the k-th column of Y^{21}. We then find a_1 such that the following column operation

$$\mathbf{c}_1^{21} \rightarrow \mathbf{c}_1^{21} + a_1 \left(\sum_{i=2}^{N-1} \mathbf{c}_i^{21} \right), \tag{A.19}$$

gives a column with zeros in all positions other than the first and last position. We find a_1 by solving

$$-\lambda + a_1(\lambda + 1) \quad = \quad 0,$$

and therefore

$$a_1 \quad = \quad \frac{\lambda}{1+\lambda}. \tag{A.20}$$

This column operation is performed by multiplying Y^{21} on the right by the following elementary matrix E_3^{21}:

$$E_3^{21} \quad = \quad I + \frac{\lambda}{1+\lambda} \mathbf{e}\mathbf{e}_1^T - \frac{\lambda}{1+\lambda} \mathbf{e}_1 \mathbf{e}_1^T, \tag{A.21}$$

for which $\det(E_3^{21}) = 1$. Then $Y^{21}E_3^{21}$, which is the same as Y^{21} except for the first column, has the following structure

$$Y^{21}E_3^{21} = \left[\begin{array}{c:ccccccc} \beta(1-\frac{N-1}{N}\nu)+(N-2)\frac{\lambda}{1+\lambda}\frac{\beta\nu}{N} & \frac{\beta\nu}{N} & \cdots & \cdots & \cdots & \cdots & \cdots & \frac{\beta\nu}{N} \\ 0 & \lambda & 1 & 0 & \cdots & \cdots & \cdots & 0 \\ \vdots & 0 & \ddots & \ddots & \ddots & & & \vdots \\ \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & & \vdots \\ \vdots & \vdots & & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & & & \ddots & \ddots & \ddots & 0 \\ 0 & \vdots & & & & \ddots & \ddots & 1 \\ \frac{1}{1+\lambda} & 0 & \cdots & \cdots & \cdots & \cdots & 0 & \lambda \end{array}\right]. \quad \text{(A.22)}$$

Next, we eliminate all but the first two entries in the first row of (A.22). Define $\mathbf{r}_k^{21}$ to be the k-th row of $Y^{21}E_3^{21}$. We then find a_2 such that the following row operation

$$\mathbf{r}_1^{21} \rightarrow \mathbf{r}_1^{21} + a_2\left(\sum_{i=2}^{N-1}\mathbf{r}_i^{21}\right), \quad \text{(A.23)}$$

gives a row with zeros in all entries other than in the first and second positions. We find a_2 by solving

$$\frac{\beta\nu}{N} + a_2(1+\lambda) = 0,$$

and therefore

$$a_2 = -\frac{\beta\nu}{N(1+\lambda)}. \quad \text{(A.24)}$$

This row operation is performed by multiplying $Y^{21}E_3^{21}$ on the left by the following elementary matrix E_4^{21}:

$$E_4^{21} = I - \frac{\beta\nu}{N(1+\lambda)}\mathbf{e}_1\mathbf{e}^T + \frac{\beta\nu}{N(1+\lambda)}\mathbf{e}_1\mathbf{e}_1^T, \quad \text{(A.25)}$$

for which $\det(E_4^{21}) = 1$. Then, $E_4^{21}Y^{21}E_3^{21}$, which is the same as $Y^{21}E_3^{21}$ except for the first row, has the following structure (where a and b are complicated expression we will derive shortly):

$$E_4^{21} Y^{21} E_3^{21} \quad = \quad \left[\begin{array}{c:cccccccc} a & b & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ \hdashline 0 & \lambda & 1 & \ddots & & & & \vdots \\ \vdots & 0 & \ddots & \ddots & \ddots & & & \vdots \\ \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & & \vdots \\ \vdots & \vdots & & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & & & \ddots & \ddots & \ddots & 0 \\ 0 & \vdots & & & & \ddots & \ddots & 1 \\ \frac{1}{1+\lambda} & 0 & \cdots & \cdots & \cdots & \cdots & 0 & \lambda \end{array}\right]. \qquad (A.26)$$

For simplicity we define $Z^{21} := E_4^{21} Y^{21} E_3^{21}$. As $\det(E_4^{21}) = \det(E_3^{21}) = 1$, then from (A.18) we obtain

$$\det(M^{21}) \quad = \quad (-1)^{N-1} \det(Z^{21}). \qquad (A.27)$$

We find $\det(Z^{21})$ by expanding on the first column, where there are two non-zero terms in positions $(1, 1)$ and $(N - 1, 1)$, and obtain two minors Z_1^{21} and Z_2^{21} respectively. Then,

$$\det(Z^{21}) \quad = \quad a \det(Z_1^{21}) + (-1)^N \frac{1}{1+\lambda} \det(Z_2^{21}). \qquad (A.28)$$

The $(N - 2) \times (N - 2)$ minor Z_1^{21} has the structure

$$Z_1^{21} \quad = \quad \begin{bmatrix} \lambda & 1 & & & \\ & \ddots & \ddots & & \\ & & \ddots & \ddots & \\ & & & \ddots & 1 \\ & & & & \lambda \end{bmatrix}.$$

The above minor is upper-triangular and therefore

$$\det(Z_1^{21}) \quad = \quad \lambda^{N-2}. \qquad (A.29)$$

The $(N-2) \times (N-2)$ minor Z_2^{21} has the structure

$$Z_2^{21} = \begin{bmatrix} b & & & & \\ \lambda & 1 & & & \\ & \ddots & \ddots & & \\ & & \ddots & \ddots & \\ & & & \lambda & 1 \end{bmatrix}. \tag{A.30}$$

The above minor is lower-triangular and therefore

$$\det(Z_2^{21}) = b. \tag{A.31}$$

Substituting (A.29) and (A.31) into (A.28) we obtain

$$\det(Z^{21}) = a\lambda^{N-2} + (-1)^N \frac{b}{1+\lambda}. \tag{A.32}$$

We now derive the expression for a, recalling that it arises from row operation (A.23),

$$\begin{aligned} a &= \beta(1 - \frac{N-1}{N}\nu) + (N-2)\frac{\lambda}{1+\lambda}\frac{\beta\nu}{N} - \frac{\beta\nu}{N(1+\lambda)^2} \\ &= \beta - \beta\nu + \frac{\beta\nu}{N} + \frac{(\frac{1}{N}\beta\nu)}{1+\lambda}\left[(N-2)\lambda - \frac{1}{1+\lambda}\right] \\ &= -\lambda + \frac{(\frac{1}{N}\beta\nu)}{1+\lambda}\left[\lambda + 1 + (N-2)\lambda - \frac{1}{1+\lambda}\right] \\ &= -\lambda + \frac{(\frac{1}{N}\beta\nu)}{(1+\lambda)^2}\left[((N-1)\lambda + 1)(1+\lambda) - 1\right] \\ &= -\lambda + \frac{(\frac{1}{N}\beta\nu)}{(1+\lambda)^2}\left[N\lambda + (N-1)\lambda^2\right]. \end{aligned} \tag{A.33}$$

Similarly, we now derive the expression for b,

$$b = \frac{\beta\nu}{N} - \frac{\beta\nu\lambda}{N(1+\lambda)} = \frac{\beta\nu}{N}\left(1 - \frac{\lambda}{1+\lambda}\right) = \frac{\beta\nu}{N}\left(\frac{1}{1+\lambda}\right). \tag{A.34}$$

Substituting (A.33) and (A.34) into (A.32) we obtain

$$\begin{aligned} \det(Z^{21}) &= -\lambda^{N-1} + \frac{(\frac{1}{N}\beta\nu)}{(1+\lambda)^2}\left[N\lambda^{N-1} + (N-1)\lambda^N\right] + (-1)^N \frac{(\frac{1}{N}\beta\nu)}{(1+\lambda)^2} \\ &= -(-\lambda)^{N-1}(-1)^{N-1} + \frac{(\frac{1}{N}\beta\nu)(-1)^{N-1}}{(1+\lambda)^2}\left[N(-\lambda)^{N-1} - (N-1)(-\lambda)^N\right] \\ &\quad +(-1)^N \frac{(\frac{1}{N}\beta\nu)}{(1+\lambda)^2}. \end{aligned} \tag{A.35}$$

Finally we substitute (A.35) into (A.27) to obtain

$$\begin{aligned}
\det(M^{21}) &= -(-\lambda)^{N-1} + \frac{(\frac{1}{N}\beta\nu)}{(1+\lambda)^2}\left[N(-\lambda)^{N-1}(1+\lambda) + (-\lambda)^N - 1\right] \\
&= -\frac{(\frac{1}{N}\beta\nu)}{(1+\lambda)^2}\left[1 - (-\lambda)^N - N(-\lambda)^{N-1}(1+\lambda)\right] - (-\lambda)^{N-1}. \qquad \text{(A.36)}
\end{aligned}$$

Substituting (A.36) into (A.14) concludes the proof. □

A.3 Derivation of $\det(N_1)$

Recall the form of the $(N-2)\times(N-2)$ minor N_1, as shown in (A.37):

$$N_1 = \left[\begin{array}{cccccccccccccc}
1-\frac{\beta\nu}{N} & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\
\lambda-1 & 1 & \ddots & & & & & & & & & & \vdots \\
-1 & \lambda-1 & 1 & \ddots & & & & & & & & & \vdots \\
-1 & -\lambda & \lambda-1 & \ddots & \ddots & & & & & & & & \vdots \\
-1 & 0 & -\lambda & \ddots & \ddots & \ddots & & & & & & & \vdots \\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & & & & & & \vdots \\
\vdots & \vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & & & & & \vdots \\
-1 & 0 & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1 & 0 & \cdots & \cdots & \cdots & 0 \\
\hdashline
-1 & 0 & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1 & 0 & \cdots & 0 \\
\vdots & \vdots & & & & & & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\
\vdots & \vdots & & & & & & & \ddots & \ddots & \ddots & \ddots & 0 \\
\vdots & \vdots & & & & & & & & \ddots & \ddots & \ddots & 1 \\
-1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda & \lambda-1
\end{array}\right], \qquad \text{(A.37)}$$

where the separation occurs between rows $(j-2)$ and $(j-1)$.

Lemma A.3.1

$$\det(N_1) = (-1)^{N+j}(1-\frac{\beta\nu}{N})\frac{1-(-\lambda)^{N-j+1}}{1+\lambda}. \qquad \text{(A.38)}$$

Proof. To find $\det(N_1)$ we first expand over the first row, where there is only one non-zero term, in position (1,1). Then we obtain a new minor N_{11} of size $(N-3)\times$

$(N-3)$ with the separation between rows $(j-3)$ and $(j-2)$:

$$N_{11} = \left[\begin{array}{ccccccccccccc}
1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\
\lambda-1 & 1 & \ddots & & & & & & & & & & \vdots \\
-\lambda & \lambda-1 & 1 & \ddots & & & & & & & & & \vdots \\
0 & -\lambda & \lambda-1 & \ddots & \ddots & & & & & & & & \vdots \\
0 & 0 & -\lambda & \ddots & \ddots & \ddots & & & & & & & \vdots \\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & & & & & & \vdots \\
\vdots & \vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & & & & & \vdots \\
0 & 0 & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1 & 0 & \cdots & \cdots & \cdots & 0 \\
\hline
0 & 0 & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1 & 0 & \cdots & 0 \\
\vdots & \vdots & & & & & & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\
\vdots & \vdots & & & & & & & \ddots & \ddots & \ddots & \ddots & 0 \\
\vdots & \vdots & & & & & & & & \ddots & \ddots & \ddots & 1 \\
0 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda & \lambda-1
\end{array}\right], \tag{A.39}$$

and we know that

$$\det(N_1) = (1 - \frac{\beta\nu}{N}) \det(N_{11}). \tag{A.40}$$

We notice that N_{11} is lower-Hessenberg (ie lower-triangular, but with non-zeros on the superdiagonal), but all non-zero superdiagonals are in the lower part of the matrix, where they are all 1's. Starting from column $(j-1)$, we perform column operations one at a time to remove each of these 1's, with the intention of transforming N_{11} into a lower-triangular matrix.

Consider a pair of columns of the following form:

$$\begin{bmatrix}
0 & 0 \\
\vdots & \vdots \\
0 & 0 \\
\left(\sum_{i=0}^{n} \lambda^{n-i}(-1)^i\right) & 1 \\
\left(\sum_{i=0}^{n-1} \lambda^{n-i}(-1)^{i+1}\right) & \lambda-1 \\
0 & -\lambda \\
0 & 0 \\
\vdots & \vdots \\
0 & 0
\end{bmatrix}. \tag{A.41}$$

Then consider the column operation required to remove the 1 from the second column $\mathbf{c}_2$ of (A.41):

$$\mathbf{c}_2 \to \left(\sum_{i=0}^{n} \lambda^{n-i}(-1)^i\right) \mathbf{c}_2 - \mathbf{c}_1. \tag{A.42}$$

The column operation (A.42) results in a new pair of columns,

$$\begin{bmatrix} 0 & 0 \\ \vdots & \vdots \\ \left(\sum_{i=0}^{n} \lambda^{n-i}(-1)^i\right) & 0 \\ \left(\sum_{i=0}^{n-1} \lambda^{n-i}(-1)^{i+1}\right) & t_1 \\ 0 & t_2 \\ 0 & 0 \\ \vdots & \vdots \\ 0 & 0 \end{bmatrix},$$

where $t_1 := (\lambda-1)\left(\sum_{i=0}^{n} \lambda^{n-i}(-1)^i\right) - \left(\sum_{i=0}^{n-1} \lambda^{n-i}(-1)^{i+1}\right)$, and $t_2 := (-\lambda)\left(\sum_{i=0}^{n} \lambda^{n-i}(-1)^i\right)$. We now simplify t_1 and t_2. First, for t_1, we have

$$\begin{aligned} t_1 &= (\lambda-1)\left(\sum_{i=0}^{n} \lambda^{n-i}(-1)^i\right) - \left(\sum_{i=0}^{n-1} \lambda^{n-i}(-1)^{i+1}\right) \\ &= (\lambda-1)(-1)^n + \sum_{i=0}^{n-1} \left[(\lambda-1)\lambda^{n-i}(-1)^i + \lambda^{n-i}(-1)^i\right] \\ &= (\lambda-1)(-1)^n + \sum_{i=0}^{n-1} \left[\lambda^{n-i+1}(-1)^i\right] \\ &= \sum_{i=0}^{n+1} \lambda^{(n+1)-i}(-1)^i. \end{aligned} \tag{A.43}$$

Next, for t_2, we have

$$t_2 = \left(\sum_{i=0}^{n} \lambda^{n-i}(-1)^i\right)(-\lambda) = \sum_{i=0}^{(n+1)-1} \lambda^{(n+1)-i}(-1)^{i+1}. \tag{A.44}$$

Then, after the column operation (A.42) is performed, the pair of columns (A.41) becomes

$$\begin{bmatrix} 0 & 0 \\ \vdots & \vdots \\ \left(\sum_{i=0}^{n} \lambda^{n-i}(-1)^{i}\right) & 0 \\ \left(\sum_{i=0}^{n-1} \lambda^{n-i}(-1)^{i+1}\right) & \left(\sum_{i=0}^{n+1} \lambda^{(n+1)-i}(-1)^{i}\right) \\ 0 & \left(\sum_{i=0}^{(n+1)-1} \lambda^{(n+1)-i}(-1)^{i+1}\right) \\ 0 & 0 \\ \vdots & \vdots \\ 0 & 0 \end{bmatrix}.$$

Note that after the column operation, the second column is the same as the first column except shifted one row down, with the index n changing to $(n+1)$.

In N_{11}, columns $(j-2)$ and $(j-1)$ correspond to (A.41) for the case $n = 1$. After performing the column operation (A.42) for $n = 1$, we obtain a new matrix for which columns $(j-1)$ and j correspond to (A.41) for the case $n = 2$. By induction, we continue to perform the column operation (A.42) with increasing values of n on all subsequent pairs of columns, and predict the form of N_{11}^{*}, the resulting matrix after the column operations are complete:

$$N_{11}^{*} = \left[\begin{array}{ccccccccccccc}
1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\
\lambda-1 & 1 & \ddots & & & & & & & & & & \vdots \\
-\lambda & \lambda-1 & 1 & \ddots & & & & & & & & & \vdots \\
0 & -\lambda & \lambda-1 & \ddots & \ddots & & & & & & & & \vdots \\
0 & 0 & -\lambda & \ddots & \ddots & \ddots & & & & & & & \vdots \\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & & & & & & \vdots \\
\vdots & \vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & & & & & \vdots \\
0 & 0 & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1 & 0 & \cdots & \cdots & \cdots & 0 \\
\hdashline
0 & 0 & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 0 & \cdots & \cdots & 0 \\
\vdots & \vdots & & & & & & \ddots & -\lambda & \lambda^2-\lambda+1 & \ddots & & \vdots \\
\vdots & \vdots & & & & & & & \ddots & -\lambda^2+\lambda & \lambda^3-\lambda^2+\lambda-1 & \ddots & \vdots \\
\vdots & \vdots & & & & & & & & \ddots & \ddots & \ddots & 0 \\
0 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & \sum\limits_{i=0}^{N-j-2}(-1)^{i+1}\lambda^{N-j-1-i} & \sum\limits_{i=0}^{N-j}(-1)^{i}\lambda^{N-j-i}
\end{array}\right].$$

We observe that N_{11}^{*} is lower-triangular and its determinant is the product of its diagonal terms. In the upper part of N_{11}^{*} the terms are all 1, but in the lower part the terms all take the form $\sum\limits_{i=0}^{n}\lambda^{n-i}(-1)^{i}$, for $n = 1, \ldots, N-j$.

Each of the column operations performed to obtain N_{11}^{*} is performed by multiplication by elementary matrices of the form:

$$E_4^n = \begin{bmatrix}
1 & & & & & & \\
& \ddots & & & & & \\
& & 1 & -1 & & & \\
& & & \left(\sum\limits_{i=0}^{n}\lambda^{n-i}(-1)^{i}\right) & & & \\
& & & & 1 & & \\
& & & & & \ddots & \\
& & & & & & 1
\end{bmatrix}.$$

Each of these elementary matrices are upper-triangular, and therefore

$$\det(E_4^n) = \left(\sum_{i=0}^{n}\lambda^{n-i}(-1)^{i}\right).$$

Then, we know that by a sequence of matrix multiplications,

$$N_{11}^* = N_{11} \prod_{n=1}^{N-j-1} E_4^n,$$

and therefore

$$\det(N_{11}) = \frac{\det(N_{11}^*)}{\prod_{n=1}^{N-j-1} \det(E_4^n)}. \tag{A.45}$$

Since each $\det(E_4^n)$ coincides with the entry in the $(j-3+n)$-th diagonal position in N_{11}^*, we cancel each of these, leaving only the bottom-right entry of N_{11}^* remaining in (A.45). Hence

$$\det(N_{11}) = \sum_{i=0}^{N-j} (-1)^i \lambda^{N-j-i}. \tag{A.46}$$

Substituting (A.46) into (A.40), we find

$$\begin{aligned} \det(N_1) &= (1 - \frac{\beta\nu}{N}) \left(\sum_{i=0}^{N-j} (-1)^i \lambda^{N-j-i} \right) \\ &= (-1)^{N+j} (1 - \frac{\beta\nu}{N}) \sum_{i=0}^{N-j} (-\lambda)^{N-j-i}. \end{aligned}$$

Then, we use the geometric series formula to obtain

$$\det(N_1) = (-1)^{N+j} (1 - \frac{\beta\nu}{N}) \frac{1 - (-\lambda)^{N-j+1}}{1 + \lambda},$$

which coincides with (A.38). □

Example A.3.2 *Recall from Example 4.3.6 the form of* N_1

$$N_1 = \left[\begin{array}{cccccc} 1 - \frac{\beta\nu}{8} & 0 & 0 & 0 & 0 & 0 \\ \lambda - 1 & 1 & 0 & 0 & 0 & 0 \\ -1 & \lambda - 1 & 1 & 0 & 0 & 0 \\ \hline -1 & 0 & -\lambda & \lambda - 1 & 1 & 0 \\ -1 & 0 & 0 & -\lambda & \lambda - 1 & 1 \\ -1 & 0 & 0 & 0 & -\lambda & \lambda - 1 \end{array} \right].$$

In this example, $N = 8$ and $j = 5$. First we expand over row 1, where there is only one non-zero entry, to obtain the minor N_{11}

$$N_{11} = \left[\begin{array}{ccccc} 1 & 0 & 0 & 0 & 0 \\ \lambda-1 & 1 & 0 & 0 & 0 \\ \hdashline 0 & -\lambda & \lambda-1 & 1 & 0 \\ 0 & 0 & -\lambda & \lambda-1 & 1 \\ 0 & 0 & 0 & -\lambda & \lambda-1 \end{array}\right]. \tag{A.47}$$

Then, $\det(N_1) = (1 - \frac{\beta\nu}{8})\det(N_{11})$*. Now the lower part of N_{11} contains 1's on the superdiagonal so we perform column operations to make N_{11} lower-triangular. First we perform the column operation (A.42) with $n = 1$ on the fourth column c_4:*

$$c_4 \leftarrow (\lambda-1)\, c_4 - c_3.$$

This is done by postmultiplying N_{11} by the elementary matrix E_4^1

$$E_4^1 = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & \lambda-1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Note that $\det(E_4^1) = \lambda - 1$*. We calculate*

$$N_{11}E_4^1 = \left[\begin{array}{ccccc} 1 & 0 & 0 & 0 & 0 \\ \lambda-1 & 1 & 0 & 0 & 0 \\ \hdashline 0 & -\lambda & \lambda-1 & 0 & 0 \\ 0 & 0 & -\lambda & \lambda^2-\lambda+1 & 1 \\ 0 & 0 & 0 & -\lambda^2+\lambda & \lambda-1 \end{array}\right].$$

Next, we perform the column operation (A.42) with $n = 2$ on the fifth column c_5:

$$c_5 \leftarrow \left(\lambda^2 - \lambda + 1\right) c_5 - c_4.$$

This is done by postmultipliying $N_{11}E_4^1$ by the elementary matrix E_4^2

$$E_4^2 = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 & \lambda^2-\lambda+1 \end{bmatrix}.$$

Note that $\det(E_4^2) = \lambda^2 - \lambda + 1$*. We thus arrive at the lower-triangular form N_{11}^**

$$N_{11}^* = N_{11}E_4^1E_4^2 = \left[\begin{array}{ccccc} 1 & 0 & 0 & 0 & 0 \\ \lambda-1 & 1 & 0 & 0 & 0 \\ \hdashline 0 & -\lambda & \lambda-1 & 0 & 0 \\ 0 & 0 & -\lambda & \lambda^2-\lambda+1 & 0 \\ 0 & 0 & 0 & -\lambda^2+\lambda & \lambda^3-\lambda^2+\lambda-1 \end{array}\right].$$

Then, we see

$$\det(N_{11}^*) \quad = \quad (\lambda - 1)\left(\lambda^2 - \lambda + 1\right)\left(\lambda^3 - \lambda^2 + \lambda - 1\right).$$

However, dividing by $\det(E_4^1)$ *and* $\det(E_4^2)$ *we obtain*

$$\det(N_{11}) \quad = \quad \lambda^3 - \lambda^2 + \lambda - 1. \tag{A.48}$$

Finally, we find

$$\begin{aligned}
\det(N_1) &= (1 - \frac{\beta\nu}{8})\left(\lambda^3 - \lambda^2 + \lambda - 1\right) \\
&= -(1 - \frac{\beta\nu}{8})\left((-\lambda)^3 - (-\lambda)^2 + (-\lambda) - 1\right) \\
&= -(1 - \frac{\beta\nu}{8})\frac{1 - (-\lambda)^4}{1 + \lambda}.
\end{aligned}$$

A.4 Derivation of $\det(N_2)$

Recall the form of the $(N-2) \times (N-2)$ minor N_2, as shown in (A.49):

$$N_2 = \left[\begin{array}{ccccccccccccc}
-1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda \\
\lambda-1 & 1 & \ddots & & & & & & & & & & 0 \\
-1 & \lambda-1 & 1 & \ddots & & & & & & & & & \vdots \\
-1 & -\lambda & \lambda-1 & \ddots & \ddots & & & & & & & & \vdots \\
-1 & 0 & -\lambda & \ddots & \ddots & \ddots & & & & & & & \vdots \\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & & & & & & \vdots \\
\vdots & \vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & & & & & \vdots \\
-1 & 0 & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1 & 0 & \cdots & \cdots & \cdots & 0 \\
\hdashline
-1 & 0 & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1 & 0 & \cdots & 0 \\
\vdots & \vdots & & & & & & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\
\vdots & \vdots & & & & & & & \ddots & \ddots & \ddots & \ddots & 0 \\
\vdots & \vdots & & & & & & & & \ddots & \ddots & \ddots & 1 \\
-1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda & \lambda-1
\end{array}\right], \tag{A.49}$$

where the separation occurs between rows $(j-2)$ and $(j-1)$.

Lemma A.4.1

$$\det(N_2) \;=\; (-1)^{N+j}\frac{1}{1+\lambda}\left[(N-1-\lambda)(-\lambda)^{N-j+1}+\frac{(-\lambda)^N-1}{1+\lambda}\right]. \tag{A.50}$$

Proof. To find $\det(N_2)$, we first expand over the first row, where there are only two non-zero terms, in position $(1,1)$ and $(1,N-2)$. Then we obtain two new minors, N_{21} and N_{22} respectively, both of dimensions $(N-3)\times(N-3)$ with the separation occurring between rows $(j-3)$ and $(j-2)$. Therefore,

$$\begin{aligned}\det(N_2) &= (-1)\det(N_{21})+(-1)^{N-1}(-\lambda)\det(N_{22})\\ &= -\det(N_{21})+(-1)^N\lambda\det(N_{22}).\end{aligned} \tag{A.51}$$

Note that N_{21} is the submatrix obtained by removing rows 1 and 2, and columns 1 and $N-1$ from Y^{j1} (see 4.67). This is identical to how N_{11} (see Appendix A.3) is obtained, so $N_{11}=N_{21}$ and therefore

$$\det(N_{21})=\det(N_{11}). \tag{A.52}$$

The minor N_{22} is an $(N-3)\times(N-3)$ matrix that has the following structure:

$$N_{22} = \left[\begin{array}{ccccccccccccc}
\lambda-1 & 1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0\\
-1 & \lambda-1 & 1 & \ddots & & & & & & & & & \vdots\\
-1 & -\lambda & \lambda-1 & \ddots & \ddots & & & & & & & & \vdots\\
-1 & 0 & -\lambda & \ddots & \ddots & \ddots & & & & & & & \vdots\\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & & & & & & \vdots\\
\vdots & \vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & & & & & \vdots\\
-1 & 0 & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1 & 0 & \cdots & \cdots & \cdots & 0\\
\hdashline
-1 & 0 & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1 & 0 & \cdots & 0\\
\vdots & \vdots & & & & & & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots\\
\vdots & \vdots & & & & & & & \ddots & \ddots & \ddots & \ddots & 0\\
\vdots & \vdots & & & & & & & & \ddots & \ddots & \ddots & 1\\
\vdots & \vdots & & & & & & & & & \ddots & \ddots & \lambda-1\\
-1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda
\end{array}\right], \tag{A.53}$$

with the separation occurring between rows $(j-3)$ and $(j-2)$. To find $\det(N_{22})$, a recursive procedure is used. At each step of the procedure, an elementary matrix is constructed that shifts the last row to row $(j-2)$, and shifts rows $(j-2)$ through to the second to last row one row down. The row that is shifted into the $(j-2)$-th row is expanded on, containing two non-zero entries. We calculate the determinant of one of the two resulting minors, and show that the other minor is simply a smaller version of the original matrix. We continue this procedure until the latter is an upper-Hessenberg matrix, whose determinant we then evaluate.

Consider the elementary matrix E_5^0 of the following form:

$$E_5^0 = \left[\begin{array}{cccc|ccc|c}
1 & & & & & & & \\
& \ddots & & & & & & \\
& & \ddots & & & & & \\
& & & 1 & & & & \\
\hline
& & & & & & & 1 \\
\hline
& & & & 1 & & & \\
& & & & & \ddots & & \\
& & & & & & \ddots & \\
& & & & & & 1 &
\end{array}\right],$$

where E_5^0 is an $(N-3)\times(N-3)$ matrix with the 1 in the last column occurring in row $(j-2)$. Note that the I block on the bottom right is of size $(N-j-1)\times(N-j-1)$. We then define

$$N_{22}^{00} = E_5^0 N_{22}. \tag{A.54}$$

It is easy to see that $\det(E_5^0) = (-1)^{N-3+j-2} = (-1)^{N+j+1}$. Then,

$$\det(N_{22}) = (-1)^{N+j+1} \det(N_{22}^{00}). \tag{A.55}$$

Now we see that the $(N-3)\times(N-3)$ matrix N_{22}^{00} has the structure

$$
N_{22}^{00} = \left[\begin{array}{ccccccccccccc}
\lambda-1 & 1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\
-1 & \lambda-1 & 1 & \ddots & & & & & & & & & \vdots \\
-1 & -\lambda & \lambda-1 & \ddots & \ddots & & & & & & & & \vdots \\
-1 & 0 & -\lambda & \ddots & \ddots & \ddots & & & & & & & \vdots \\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & & & & & & \vdots \\
\vdots & \vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & & & & & \vdots \\
-1 & 0 & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1 & 0 & \cdots & \cdots & \cdots & 0 \\
\hline
-1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda \\
\hline
-1 & 0 & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1 & 0 & \cdots & 0 \\
\vdots & \vdots & & & & & & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\
\vdots & \vdots & & & & & & & \ddots & \ddots & \ddots & \ddots & 0 \\
\vdots & \vdots & & & & & & & & \ddots & \ddots & \ddots & 1 \\
\vdots & \vdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \lambda-1
\end{array}\right].
$$

Next, we calculate $\det(N_{22}^{00})$ by expanding on row $(j-2)$, which contains non-zero terms in only the first and last positions. We name the minor obtained by expanding on the first term N_{22}^{01}, and the minor obtained by expanding on the last term N_{22}^{02}. Then, the expanded determinant is

$$
\det(N_{22}^{00}) \;=\; (-1)^{j}\det(N_{22}^{01}) + (-1)^{N-3+j-2}(-\lambda)\det(N_{22}^{02}). \tag{A.56}
$$

We first consider first the structure of N_{22}^{01}:

$$
N_{22}^{01} = \left[\begin{array}{ccccccccccccc}
1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\
\lambda-1 & 1 & \ddots & & & & & & & & & & \vdots \\
-\lambda & \lambda-1 & 1 & \ddots & & & & & & & & & \vdots \\
0 & -\lambda & \lambda-1 & \ddots & \ddots & & & & & & & & \vdots \\
0 & 0 & -\lambda & \ddots & \ddots & \ddots & & & & & & & \vdots \\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & & & & & & \vdots \\
\vdots & \vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & & & & & \vdots \\
0 & 0 & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1 & 0 & \cdots & \cdots & \cdots & 0 \\
\hline
0 & 0 & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1 & 0 & \cdots & 0 \\
\vdots & \vdots & & & & & & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\
\vdots & \vdots & & & & & & & \ddots & \ddots & \ddots & \ddots & 0 \\
\vdots & \vdots & & & & & & & & \ddots & \ddots & \ddots & 1 \\
0 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda & \lambda-1
\end{array}\right].
$$

Notice that N_{22}^{01} is of identical structure to N_{11} (see (A.39) in Appendix A.3), except that N_{22}^{01} is of size $(N-4)\times(N-4)$, one row and column smaller than N_{11}. Hence, replacing N by $N-1$ in (A.46) from Appendix A.3, we obtain

$$\det(N_{22}^{01}) \;=\; \sum_{i=0}^{N-j-1} (-1)^i \lambda^{N-j-1-i}. \tag{A.57}$$

Next, we consider the structure of N_{22}^{02}:

$$N_{22}^{02} \;=\; \left[\begin{array}{ccccccccccccc}
\lambda-1 & 1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\
-1 & \lambda-1 & 1 & \ddots & & & & & & & & & \vdots \\
-1 & -\lambda & \lambda-1 & \ddots & \ddots & & & & & & & & \vdots \\
-1 & 0 & -\lambda & \ddots & \ddots & \ddots & & & & & & & \vdots \\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & & & & & & \vdots \\
\vdots & \vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & & & & & \vdots \\
-1 & 0 & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1 & 0 & \cdots & \cdots & \cdots & 0 \\
\hline
-1 & 0 & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1 & 0 & \cdots & 0 \\
\vdots & \vdots & & & & & & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\
\vdots & \vdots & & & & & & & \ddots & \ddots & \ddots & \ddots & 0 \\
\vdots & \vdots & & & & & & & & \ddots & \ddots & \ddots & 1 \\
\vdots & \vdots & & & & & & & & & \ddots & \ddots & \lambda-1 \\
-1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda
\end{array}\right].$$

We observe that N_{22}^{02} is of identical structure to N_{22} (see (A.53)), except that N_{22}^{02} is of size $(N-4)\times(N-4)$, one row and column smaller than N_{22}. Define an elementary matrix E_5^1 of size $(N-4)\times(N-4)$, which has the following structure:

$$E_5^1 \;=\; \left[\begin{array}{ccc|ccc|c}
1 & & & & & & \\
& \ddots & & & & & \\
& & \ddots & & & & \\
& & 1 & & & & \\
\hline
& & & & & & 1 \\
\hline
& & & 1 & & & \\
& & & & \ddots & & \\
& & & & & \ddots & \\
& & & & & 1 &
\end{array}\right]. \tag{A.58}$$

Note that this is identical in structure to E_5^0, except the I block on the bottom right is of size $(N-j-2)\times(N-j-2)$. The single 1 in the last column is again in the $(j-2)$-th position.

Next, we define $N_{22}^{10} = E_5^1 N_{22}^{02}$. This matrix has the structure

$$
N_{22}^{10} = \left[\begin{array}{ccccccccccccc}
\lambda-1 & 1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\
-1 & \lambda-1 & 1 & \ddots & & & & & & & & & \vdots \\
-1 & -\lambda & \lambda-1 & \ddots & \ddots & & & & & & & & \vdots \\
-1 & 0 & -\lambda & \ddots & \ddots & \ddots & & & & & & & \vdots \\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & & & & & & \vdots \\
\vdots & \vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & & & & & \vdots \\
-1 & 0 & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1 & 0 & \cdots & \cdots & \cdots & 0 \\
\hdashline
-1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda \\
\hdashline
-1 & 0 & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1 & 0 & \cdots & 0 \\
\vdots & \vdots & & & & & & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\
\vdots & \vdots & & & & & & & \ddots & \ddots & \ddots & \ddots & 0 \\
\vdots & \vdots & & & & & & & & \ddots & \ddots & \ddots & 1 \\
\vdots & \vdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \lambda-1
\end{array}\right].
$$

We now observe that N_{22}^{10} of identical structure to N_{22}^{00}, except of size $(N-4) \times (N-4)$, and we expand again on row $(j-2)$ to obtain new minors N_{22}^{11} and N_{22}^{12}. The same process as before is repeated, noting N_{22}^{11} is of the same structure as the $(N-3) \times (N-3)$ matrix (A.39), and using another elementary matrix E_5^2 to find N_{22}^{20}. We continue this process, at the k-th iteration finding $\det(N_{22}^{k1})$ from (A.46), and constructing $N_{22}^{(k+1),0} = E_5^k N_{22}^{k2}$, until we encounter an iteration where the second minor obtained is lower-Hessenberg with 1's on the superdiagonal. This is definitely the case for the $(N-j-1)$-th iteration, but it may be the case for an earlier iteration depending on the selection of j. However, once a lower-Hessenberg form is reached, further iterations of the type outlined above maintain the lower-Hessenberg form so for the sake of simplicity we assume for the remainder of this proof that $N-j-1$ iterations are performed.

In general we say that for $k = 0, 1, \ldots, N-j-2$,

$$\det(N_{22}^{k0}) = (-1)^j \det(N_{22}^{k1}) + (-1)^{N+j-k-1}(-\lambda)\det(N_{22}^{k2}), \tag{A.59}$$

$$\det(N_{22}^{k1}) = \sum_{i=0}^{N-j-1-k} \lambda^{N-j-1-k-i}(-1)^i, \tag{A.60}$$

$$\det(N_{22}^{k2}) = (-1)^{N+j-k}\det(N_{22}^{k+1,0}). \tag{A.61}$$

Note that by substituting (A.61) into (A.59), we eliminate the need to calculate the former in all but the final iteration. We then obtain a reduced set of recursive equations for $k = 0, 1, \ldots, N - j - 2$,

$$\begin{aligned} \det(N_{22}^{k0}) &= (-1)^j \det(N_{22}^{k1}) + \lambda \det(N_{22}^{k+1,0}), \qquad (A.62)\\ \det(N_{22}^{k1}) &= \sum_{i=0}^{N-j-1-k} \lambda^{N-j-1-k-i}(-1)^i. \qquad (A.63) \end{aligned}$$

When $k = N - j - 1$, the last remaining matrix to consider is $N_{22}^{N-j-1,0}$, which is a matrix of size $(j-3) \times (j-3)$ of the form

$$N_{22}^{N-j-1,0} = \begin{bmatrix} \lambda-1 & 1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\ -1 & \lambda-1 & 1 & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ -1 & -\lambda & \lambda-1 & 1 & 0 & \cdots & \cdots & \cdots & 0 \\ -1 & 0 & -\lambda & \lambda-1 & 1 & 0 & \cdots & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & & \vdots \\ \vdots & \vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & & & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & \vdots & & & & \ddots & \ddots & \ddots & 1 \\ -1 & 0 & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda & \lambda-1 \end{bmatrix}. \qquad (A.64)$$

We use an inductive argument to calculate $\det(N_{22}^{N-j-1,2})$, similar to the argument used in Appendix A.3. That is, we use $j-2$ column operations to transform all of the 1's on the superdiagonals into 0's, and show inductively the form that each column takes as a result. Consider a pair of columns of the form

$$\begin{bmatrix} 0 & 0 \\ \vdots & \vdots \\ 0 & 0 \\ \left(\sum_{i=0}^{n} \lambda^{n-i}(i+1)(-1)^i\right) + (-1)^{n+1} & 1 \\ \left(\sum_{i=0}^{n-1} \lambda^{n-i}(i+1)(-1)^{i+1}\right) + (-1)^{n+1}(\lambda-1) & \lambda-1 \\ (-1)^n & -\lambda \\ (-1)^n & 0 \\ \vdots & \vdots \\ (-1)^n & 0 \end{bmatrix}. \qquad (A.65)$$

Note that for $n = 1$, this pair of columns is equivalent to the first two columns in (A.64). Now consider the column operation required to remove the 1 from the second column $\mathbf{c}_2$

$$\mathbf{c}_2 \rightarrow \left(\left[\sum_{i=0}^{n} \lambda^{n-i}(i+1)(-1)^i \right] + (-1)^{n+1} \right) \mathbf{c}_2 - \mathbf{c}_1. \tag{A.66}$$

This results in a new pair of columns

$$\begin{bmatrix} 0 & 0 \\ \vdots & \vdots \\ 0 & 0 \\ \left(\sum\limits_{i=0}^{n} \lambda^{n-i}(i+1)(-1)^i \right) + (-1)^{n+1} & 0 \\ \left(\sum\limits_{i=0}^{n-1} \lambda^{n-i}(i+1)(-1)^{i+1} \right) + (-1)^{n+1}(\lambda-1) & t_3 \\ (-1)^n & t_4 \\ (-1)^n & (-1)^{n+1} \\ \vdots & \vdots \\ (-1)^n & (-1)^{n+1} \end{bmatrix}, \tag{A.67}$$

where

$$\begin{aligned} t_3 &:= \left(\left[\sum_{i=0}^{n} \lambda^{n-i}(i+1)(-1)^i \right] + (-1)^{n+1} \right) (\lambda - 1) \\ &\quad - \left[\sum_{i=0}^{n-1} \lambda^{n-i}(i+1)(-1)^{i+1} \right] - (-1)^{n+1}(\lambda-1), \\ t_4 &:= \left(\left[\sum_{i=0}^{n} \lambda^{n-i}(i+1)(-1)^i \right] + (-1)^{n+1} \right) (-\lambda) - (-1)^n. \end{aligned}$$

First,, we simplify t_3:

$$\begin{aligned} t_3 &= \left(\left[\sum_{i=0}^{n} \lambda^{n-i}(i+1)(-1)^i \right] + (-1)^{n+1} \right) (\lambda - 1) \\ &\quad - \left[\sum_{i=0}^{n-1} \lambda^{n-i}(i+1)(-1)^{i+1} \right] - (-1)^{n+1}(\lambda-1) \\ &= \left(\left[\sum_{i=0}^{n} \lambda^{n-i}(i+1)(-1)^i \right] \right) (\lambda - 1) - \left[\sum_{i=0}^{n-1} \lambda^{n-i}(i+1)(-1)^{i+1} \right] \\ &= \left(\left[\sum_{i=0}^{n} \lambda^{n-i}(i+1)(-1)^i \right] \right) (\lambda - 1) + \left[\sum_{i=0}^{n} \lambda^{n-i}(i+1)(-1)^i \right] - (n+1)(-1)^n. \end{aligned}$$

Factorising out the sum, we obtain

$$\begin{aligned} t_3 &= \left(\left[\sum_{i=0}^{n} \lambda^{n-i}(i+1)(-1)^i\right]\right)\lambda + (n+2)(-1)^{n+1} + (-1)^{n+2} \\ &= \left(\left[\sum_{i=0}^{n+1} \lambda^{n+1-i}(i+1)(-1)^i\right]\right) + (-1)^{(n+1)+1} \\ &= \left(\left[\sum_{i=0}^{n+1} \lambda^{(n+1)-i}(i+1)(-1)^i\right]\right) + (-1)^{(n+1)+1}. \end{aligned}$$

Next, we simplify t_4:

$$\begin{aligned} t_4 &= \left(\left[\sum_{i=0}^{n} \lambda^{n-i}(i+1)(-1)^i\right] + (-1)^{n+1}\right)(-\lambda) - (-1)^n \\ &= \left[\sum_{i=0}^{(n+1)-1} \lambda^{(n+1)-i}(i+1)(-1)^{i+1}\right] + (-1)^{(n+1)+1}(\lambda-1). \end{aligned}$$

Then, we observe that, after the column operation (A.66), the second column in (A.67) becomes the same as the first but with n replaced by $n+1$ and shifted down one row. Using analogous arguments to those used in Appendix A.3, we find

$$\det(N_{22}^{N-j-1,2}) = \left[\sum_{i=0}^{j-3} \lambda^{j-3-i}(i+1)(-1)^i\right] + (-1)^j. \tag{A.68}$$

Now, recursively substituting (A.68), (A.62), (A.63) into (A.55), we obtain

$$\begin{aligned} \det(N_{22}) &= \sum_{k=1}^{N-j}\sum_{i=0}^{N-j-k} (-1)^{N+j+1+j+i}\lambda^{N-1-j-k-i+k} \\ &\quad + \sum_{i=0}^{j-3}(-1)^{N+j+1+N+j-(N-j-1)+i}(i+1)\lambda^{N-j+j-3-i} \\ &\quad + (-1)^{N+j+1+N+j-(N-j-1)+j}\lambda^{N-j} \\ &= \sum_{k=1}^{N-j}\sum_{i=0}^{N-j-k} (-1)^{N+1+i}\lambda^{N-1-j-i} \\ &\quad + \sum_{i=0}^{j-3}(-1)^{N+j+i}(i+1)\lambda^{N-3-i} + (-1)^N\lambda^{N-j} \\ &= \sum_{i=0}^{N-j-1} (-1)^{N+i+1}(N-j-i)\lambda^{N-j-1-i} \\ &\quad + \sum_{i=0}^{j-3}(-1)^{N+j+i}(i+1)\lambda^{N-3-i} + (-1)^N\lambda^{N-j}. \end{aligned} \tag{A.69}$$

Finally, substituting (A.52) and (A.69) into (A.51), we obtain

$$
\begin{aligned}
\det(N_2) &= -\det(N_{21}) + (-\lambda)(-1)^{N-1}\det(N_{22}) \\
&= \sum_{i=0}^{N-j}(-1)^{i+1}\lambda^{N-j-1} + (-1)^N\left[\sum_{i=0}^{N-j-1}(-1)^{N+i+1}(N-j-i)\lambda^{N-j-1-i}\right. \\
&\quad \left. +\sum_{i=0}^{j-3}(-1)^{N+j+i}(i+1)\lambda^{N-3-i} + (-1)^N\lambda^{N-j}\right] \\
&= \sum_{i=0}^{N-j}(-1)^{i+1}\lambda^{N-j-i} + \sum_{i=0}^{N-j-1}(-1)^{i+1}(N-j-i)\lambda^{N-j-i} \\
&\quad +\sum_{i=0}^{j-3}(-1)^{j+i}(i+1)\lambda^{N-2-i} + \lambda^{N-j+1} \\
&= \sum_{i=0}^{N-j}(-1)^{i+1}(N-j-i+1)\lambda^{N-j-i} \\
&\quad +\sum_{i=0}^{j-3}(-1)^{j+i}(i+1)\lambda^{N-2-i} + \lambda^{N-j+1}.
\end{aligned}
$$

We define p_1 and p_2 as the first two (summation) expressions of the last equation above. That is,

$$
\det(N_2) \;=\; p_1 + p_2 + \lambda^{N-j+1}. \tag{A.70}
$$

Then, we consider the first part p_1 of (A.70):

$$
\begin{aligned}
p_1 &:= \sum_{i=0}^{N-j}(-1)^{i+1}(N-j-i+1)\lambda^{N-j-i} \\
&= (-1)^{N+j+1}\sum_{i=0}^{N-j}(N-j-i+1)(-\lambda)^{N-j-i}.
\end{aligned}
$$

Each term inside the sum has a coefficient one larger than the power of λ. We then rewrite the above as a sum of derivatives of the form

$$
\begin{aligned}
p_1 &= (-1)^{N+j+1}\sum_{i=0}^{N-j}\frac{\partial}{\partial\lambda}(-\lambda)^{N-j+1-i} \\
&= (-1)^{N+j+1}\frac{\partial}{\partial\lambda}\left[\frac{(-\lambda)-(-\lambda)^{N-j+2}}{1+\lambda}\right].
\end{aligned}
$$

Now we take the derivative and simplify to obtain

$$
\begin{aligned}
p_1 &= (-1)^{N+j+1}\left[\frac{\left(-1-(N-j+2)(-\lambda)^{N-j+1}\right)(1+\lambda)-\left((-\lambda)-(-\lambda)^{N-j+2}\right)}{(1+\lambda)^2}\right] \\
&= \frac{(-1)^{N+j}}{(1+\lambda)}\left[\frac{(N-j+2)(-\lambda)^{N-j+1}-(N-j+1)(-\lambda)^{N-j+2}-1}{(1+\lambda)}\right]. \qquad \text{(A.71)}
\end{aligned}
$$

Next, we consider the second part p_2 of (A.70):

$$
\begin{aligned}
p_2 &:= \sum_{i=0}^{j-3}(-1)^{j+i}(i+1)\lambda^{N-2-i} \\
&= (-1)^{N+j}\sum_{i=0}^{j-3}(i+1)(-\lambda)^{N-2-i} \\
&= (-1)^{N+j}\left[(-\lambda)^{N-2}+2(-\lambda)^{N-3}+\cdots+(j-2)(-\lambda)^{N-j+1}\right]. \qquad \text{(A.72)}
\end{aligned}
$$

Then, (A.72) is equivalent to the following

$$
\begin{aligned}
p_2 &= (-1)^{N+j}\left[\frac{\partial}{\partial\alpha}\left[\left(\frac{\alpha}{-\lambda}\right)(-\lambda)^{N-1}+\left(\frac{\alpha}{-\lambda}\right)^2(-\lambda)^{N-1}+\cdots+\left(\frac{\alpha}{-\lambda}\right)^{j-2}(-\lambda)^{N-1}\right]\right]_{\alpha=1} \\
&= (-1)^{N+j}(-\lambda)^{N-1}\left[\frac{\partial}{\partial\alpha}\left[\frac{\left(\frac{\alpha}{-\lambda}\right)-\left(\frac{\alpha}{-\lambda}\right)^{j-1}}{1+\frac{\alpha}{\lambda}}\right]\right]_{\alpha=1} \\
&= (-1)^{N+j}(-\lambda)^{N-1}\left[\frac{\partial}{\partial\alpha}\left[\frac{\alpha(-\lambda)^{j-2}-\alpha^{j-1}}{\lambda+\alpha}\right]\left(\frac{\lambda}{(-\lambda)^{j-1}}\right)\right]_{\alpha=1} \\
&= (-1)^{N+j+1}(-\lambda)^{N-j+1}\left[\frac{\partial}{\partial\alpha}\left[\frac{\alpha(-\lambda)^{j-2}-\alpha^{j-1}}{\lambda+\alpha}\right]\right]_{\alpha=1}.
\end{aligned}
$$

Now we take the derivative, and set $\alpha = 1$ to obtain

$$
\begin{aligned}
p_2 &= (-1)^{N+j}(-\lambda)^{N-j+1}\left[\frac{\left((-\lambda)^{j-2}-(j-1)\alpha^{j-2}\right)(\lambda+\alpha)-\left(\alpha(-\lambda)^{j-2}-\alpha^{j-1}\right)}{(\lambda+\alpha)^2}\right]_{\alpha=1} \\
&= (-1)^{N+j+1}(-\lambda)^{N-j+1}\left[\frac{\left((-\lambda)^{j-2}-(j-1)\right)(\lambda+1)-(-\lambda)^{j-2}+1}{(1+\lambda)^2}\right] \\
&= (-1)^{N+j+1}(-\lambda)^{N-j+1}\left[\frac{(-\lambda)^{j-2}-(-\lambda)^{j-1}-(j-1)(\lambda+1)-(-\lambda)^{j-2}+1}{(1+\lambda)^2}\right] \\
&= \frac{(-1)^{N+j}}{(1+\lambda)}\left[\frac{(-\lambda)^{N}-(j-1)(-\lambda)^{N-j+2}+(j-2)(-\lambda)^{N-j+1}}{(1+\lambda)}\right]. \qquad \text{(A.73)}
\end{aligned}
$$

Substituting (A.71) and (A.73) into (A.70), we obtain

$$\begin{aligned}\det(N_2) &= \frac{(-1)^{N+j}}{(1+\lambda)}\left[\frac{(-\lambda)^N - N(-\lambda)^{N-j+2} + N(-\lambda)^{N-j+1} - 1}{(1+\lambda)} - (1+\lambda)(-\lambda)^{N-j+1}\right]\\ &= \frac{(-1)^{N+j}}{(1+\lambda)}\left[\frac{(-\lambda)^N - 1}{(1+\lambda)} + N(-\lambda)^{N-j+1} - (-\lambda)^{N-j+1} + (-\lambda)^{N-j+2}\right]\\ &= \frac{(-1)^{N+j}}{(1+\lambda)}\left[(-\lambda)^{N-j+1}(N-1-\lambda) + \frac{(-\lambda)^N - 1}{(1+\lambda)}\right],\end{aligned}$$

which coincides with (A.4.1). □

Example A.4.2 *Recall from Example 4.3.6 the form of* N_2

$$N_2 = \left[\begin{array}{cccccc} -1 & 0 & 0 & 0 & 0 & -\lambda \\ \lambda-1 & 1 & 0 & 0 & 0 & 0 \\ -1 & \lambda-1 & 1 & 0 & 0 & 0 \\ \hdashline -1 & 0 & -\lambda & \lambda-1 & 1 & 0 \\ -1 & 0 & 0 & -\lambda & \lambda-1 & 1 \\ -1 & 0 & 0 & 0 & -\lambda & \lambda-1 \end{array}\right].$$

In this example, $N = 8$ *and* $j = 5$*. We start by expanding over the first row to obtain two minors*

$$N_{21} = \left[\begin{array}{ccccc} 1 & 0 & 0 & 0 & 0 \\ \lambda-1 & 1 & 0 & 0 & 0 \\ \hdashline 0 & -\lambda & \lambda-1 & 1 & 0 \\ 0 & 0 & -\lambda & \lambda-1 & 1 \\ 0 & 0 & 0 & -\lambda & \lambda-1 \end{array}\right],$$

$$N_{22} = \left[\begin{array}{ccccc} \lambda-1 & 1 & 0 & 0 & 0 \\ -1 & \lambda-1 & 1 & 0 & 0 \\ \hdashline -1 & 0 & -\lambda & \lambda-1 & 1 \\ -1 & 0 & 0 & -\lambda & \lambda-1 \\ -1 & 0 & 0 & 0 & -\lambda \end{array}\right].$$

Then, we have

$$\det(N_2) = -\det(N_{21}) + \lambda\det(N_{22}).$$

Note that $N_{21} = N_{11}$ *(see (A.47)) and so we know from (A.48)*

$$\det(N_{21}) = \lambda^3 - \lambda^2 + \lambda - 1.$$

Next, we transform N_{22} *into a lower-Hessenberg matrix by (eventually) finding* N_{22}^{22} *(see (A.64)). First, we find*

$$E_5^0 = \left[\begin{array}{cc:cc:c} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ \hdashline 0 & 0 & 0 & 0 & 1 \\ \hdashline 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{array}\right].$$

Clearly, $\det(E_5^0) = 1$*. Then we calculate* N_{22}^{00}*:*

$$N_{22}^{00} = E_5^0 N_{22} \quad = \quad \begin{bmatrix} \lambda-1 & 1 & 0 & 0 & 0 \\ -1 & \lambda-1 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 & -\lambda \\ -1 & 0 & -\lambda & \lambda-1 & 1 \\ -1 & 0 & 0 & -\lambda & \lambda-1 \end{bmatrix}.$$

Then, $\det(N_{22}) = \det(N_{22}^{00})$*. We expand* N_{22}^{00} *over the third row to obtain minors* N_{22}^{01} *and* N_{22}^{02}

$$\begin{aligned} N_{22}^{01} \quad &= \quad \begin{bmatrix} 1 & 0 & 0 & 0 \\ \lambda-1 & 1 & 0 & 0 \\ 0 & -\lambda & \lambda-1 & 1 \\ 0 & 0 & -\lambda & \lambda-1 \end{bmatrix}, \\ N_{22}^{02} \quad &= \quad \begin{bmatrix} \lambda-1 & 1 & 0 & 0 \\ -1 & \lambda-1 & 1 & 0 \\ -1 & 0 & -\lambda & \lambda-1 \\ -1 & 0 & 0 & -\lambda \end{bmatrix}. \end{aligned} \tag{A.74}$$

The expanded determinant is

$$\det(N_{22}^{00}) \quad = \quad (-1)\det(N_{22}^{01}) + (-\lambda)\det(N_{22}^{02}).$$

Note that N_{22}^{01} *is identical in structure to* N_{11} *(see (A.47)), but has one less row and column. Using a similar argument to that used to find* $\det(N_{11})$ *in Appendix A.3, we find*

$$\det(N_{22}^{01}) \quad = \quad \lambda^2 - \lambda + 1.$$

Next, we construct another elementary matrix E_5^1 *(see (A.58)):*

$$E_5^1 \quad = \quad \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}.$$

Clearly, $\det(E_5^1) = -1$*. Then, we can calculate* N_{22}^{10}*:*

$$N_{22}^{10} = E_5^1 N_{22}^{02} \quad = \quad \begin{bmatrix} \lambda-1 & 1 & 0 & 0 \\ -1 & \lambda-1 & 1 & 0 \\ -1 & 0 & 0 & -\lambda \\ -1 & 0 & -\lambda & \lambda-1 \end{bmatrix}.$$

Note that $\det(N_{22}^{02}) = -\det(N_{22}^{10})$. *Again, we expand on the third row to obtain minors* N_{22}^{11} *and* N_{22}^{12}

$$\begin{aligned} N_{22}^{11} &= \left[\begin{array}{ccc} 1 & 0 & 0 \\ \lambda-1 & 1 & 0 \\ \hdashline 0 & -\lambda & \lambda-1 \end{array}\right], \\ N_{22}^{12} &= \left[\begin{array}{ccc} \lambda-1 & 1 & 0 \\ -1 & \lambda-1 & 1 \\ \hdashline -1 & 0 & -\lambda \end{array}\right]. \end{aligned}$$

The expanded determinant is

$$\det(N_{22}^{10}) = (-1)\det(N_{22}^{11}) + (-1)(-\lambda)\det(N_{22}^{12}).$$

We observe that $\det(N_{22}^{11}) = \lambda - 1$. *The final elementary matrix is*

$$E_5^2 = \left[\begin{array}{cc:c} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \hdashline 0 & 0 & 1 \end{array}\right].$$

Clearly $\det(E_5^2) = 1$, *so* $\det(N_{22}^{12}) = \det(N_{22}^{20})$. *Then, we calculate* N_{22}^{20}

$$N_{22}^{20} = E_5^2 N_{22}^{12} = \left[\begin{array}{ccc} \lambda-1 & 1 & 0 \\ -1 & \lambda-1 & 1 \\ \hdashline -1 & 0 & -\lambda \end{array}\right].$$

The expanded determinant is

$$\det(N_{22}^{20}) = (-1)\det(N_{22}^{21}) + (-\lambda)\det(N_{22}^{22}).$$

We expand on the third row to obtain minors N_{22}^{21} *and* N_{22}^{22}

$$\begin{aligned} N_{22}^{21} &= \begin{bmatrix} 1 & 0 \\ \lambda-1 & 1 \end{bmatrix}, \\ N_{22}^{22} &= \begin{bmatrix} \lambda-1 & 1 \\ -1 & \lambda-1 \end{bmatrix}. \end{aligned}$$

Clearly, $\det(N_{22}^{21}) = 1$ *and* $\det(N_{22}^{22}) = \lambda^2 - 2\lambda + 2$.

Summarising the above, we have

(1) $\det(N_{22}^{00}) = -\det(N_{22}^{01}) - \lambda\det(N_{22}^{02})$,

(2) $\det(N_{22}^{01}) = \lambda^2 - \lambda + 1$,

(3) $\det(N_{22}^{02}) = -\det(N_{22}^{10})$,

(4) $\det(N_{22}^{10}) = -\det(N_{22}^{11}) + \lambda \det(N_{22}^{12})$,

(5) $\det(N_{22}^{11}) = \lambda - 1$,

(6) $\det(N_{22}^{12}) = \det(N_{22}^{20})$,

(7) $\det(N_{22}^{20}) = -\det(N_{22}^{21}) - \lambda \det(N_{22}^{22})$,

(8) $\det(N_{22}^{21}) = 1$,

(9) $\det(N_{22}^{22}) = \lambda^2 - 2\lambda + 2$.

Recursively substituting (2)–(9) into (1), as needed, we obtain

$$\det(N_{22}) = \det(N_{22}^{00}) \quad = \quad -\lambda^5 + 2\lambda^4 - 2\lambda^3 - 3\lambda^2 + 2\lambda - 1.$$

Finally, we calculate $\det(N_2)$*:*

$$\begin{aligned}\det(N_2) &= -\det(N_{21}) + \lambda \det(N_{22}) \\ &= -\lambda^3 + \lambda^2 - \lambda + 1 - \lambda^6 + 2\lambda^5 - 2\lambda^4 - 3\lambda^3 + 2\lambda^2 - \lambda \\ &= -\lambda^6 + 2\lambda^5 - 2\lambda^4 - 4\lambda^3 + 3\lambda^2 - 2\lambda + 1. \end{aligned} \tag{A.75}$$

We now confirm that this can be rewritten in the compressed form (A.50),

$$\det(N_2) \quad = \quad \frac{-1}{1+\lambda}\left[(-\lambda)^4(7-\lambda) + \frac{(-\lambda)^8 - 1}{1+\lambda}\right],$$

by expanding the latter and confirming that these two forms coincide

$$\begin{aligned}\det(N_2) &= \frac{-1}{1+\lambda}\left[7\lambda^4 - \lambda^5 - \frac{1-(-\lambda)^8}{1+\lambda}\right] \\ &= \frac{-1}{1+\lambda}\left[7\lambda^4 - \lambda^5 - (1 - \lambda + \lambda^2 - \lambda^3 + \lambda^4 - \lambda^5 + \lambda^6 - \lambda^7)\right] \\ &= \frac{-1}{1+\lambda}\left[\lambda^7 - \lambda^6 + 6\lambda^4 + \lambda^3 - \lambda^2 + \lambda - 1\right].\end{aligned}$$

The expression in the above square brackets can be factorised to obtain

$$\begin{aligned}\det(N_2) &= \frac{-1}{1+\lambda}(1+\lambda)(\lambda^6 - 2\lambda^5 + 2\lambda^4 + 4\lambda^3 - 3\lambda^2 + 2\lambda - 1) \\ &= -\lambda^6 + 2\lambda^5 - 2\lambda^4 - 4\lambda^3 + 3\lambda^2 - 2\lambda + 1,\end{aligned}$$

which agrees with (A.75).

A.5 Derivation of $\det(N_3)$

Recall the form of the $(N-2)\times(N-2)$ minor N_3, as shown in (4.71):

$$N_3 = \left[\begin{array}{ccccccccccccc}
-1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda \\
1-\frac{\beta\nu}{N} & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\
\lambda-1 & 1 & \ddots & & & & & & & & & & 0 \\
-1 & \lambda-1 & 1 & \ddots & & & & & & & & & \vdots \\
-1 & -\lambda & \lambda-1 & \ddots & \ddots & & & & & & & & \vdots \\
-1 & 0 & -\lambda & \ddots & \ddots & \ddots & & & & & & & \vdots \\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & & & & & & \vdots \\
\vdots & \vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & & & & & \vdots \\
-1 & 0 & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1 & 0 & \cdots & \cdots & \cdots & 0 \\
\hline
-1 & 0 & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1 & 0 & \cdots & 0 \\
\vdots & \vdots & & & & & & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\
\vdots & \vdots & & & & & & & \ddots & \ddots & \ddots & \ddots & 0 \\
-1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1
\end{array}\right], \quad (A.76)$$

with the separation occurring between rows $(j-2)$ and $(j-1)$.

Lemma A.5.1

$$\det(N_3) = (-1)^j(1-\frac{\beta\nu}{N})\frac{(-\lambda)-(-\lambda)^{N-j+1}}{1+\lambda}. \quad (A.77)$$

Proof. To find $\det(N_3)$, we expand over the first row, which contains two non-zero entries, in positions $(1,1)$ and $(1,N-2)$. However, expanding on the first entry results in a zero row in the minor and therefore a zero determinant, so we only need to expand on the last entry in the first row. This leaves us with a new first row, that has only a single non-zero entry $(1-\frac{\beta\nu}{N})$. This is expanded on as well to arrive at the following $(N-4)\times(N-4)$ matrix, which we will call N_{31}, with the separation occurring between rows $(j-4)$ and $(j-3)$.

$$N_{31} \;=\; \left[\begin{array}{ccccccccccccc}
1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\
\lambda-1 & 1 & \ddots & & & & & & & & & & \vdots \\
-\lambda & \lambda-1 & 1 & \ddots & & & & & & & & & \vdots \\
0 & -\lambda & \lambda-1 & \ddots & \ddots & & & & & & & & \vdots \\
0 & 0 & -\lambda & \ddots & \ddots & \ddots & & & & & & & \vdots \\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & & & & & & \vdots \\
\vdots & \vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & & & & & \vdots \\
0 & 0 & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1 & 0 & \cdots & \cdots & \cdots & 0 \\
\hdashline
0 & 0 & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda & \lambda-1 & 1 & 0 & \cdots & 0 \\
\vdots & \vdots & & & & & & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\
\vdots & \vdots & & & & & & & \ddots & \ddots & \ddots & \ddots & 0 \\
\vdots & \vdots & & & & & & & & \ddots & \ddots & \ddots & 1 \\
0 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & -\lambda & \lambda-1
\end{array}\right].$$

Then, we observe that

$$\begin{aligned}
\det(N_3) &= \Big[(-1)^{N-1}(-\lambda)\Big]\left[(-1)^2(1-\frac{\beta\nu}{N})\right]\det(N_{31}) \\
&= (-1)^{N-1}(-\lambda)(1-\frac{\beta\nu}{N})\det(N_{31}). \qquad \text{(A.78)}
\end{aligned}$$

We note that N_{31} is identical to N_{22}^{01}, the determinant of which is calculated in Appendix A.4. Therefore, from (A.60), we see that

$$\det(N_{31}) \;=\; \sum_{i=0}^{N-j-1} \lambda^{N-j-1-i}(-1)^i. \qquad \text{(A.79)}$$

Therefore, substituting (A.79) into (A.78) we obtain

$$\begin{aligned}
\det(N_3) &= (-1)^{N-1}(-\lambda)(1-\frac{\beta\nu}{N})\sum_{i=0}^{N-j-1}\lambda^{N-j-1-i}(-1)^i \\
&= (-1)^j(-\lambda)(1-\frac{\beta\nu}{N})\sum_{i=0}^{N-j-1}(-\lambda)^{N-j-1-i} \\
&= (-1)^j(-\lambda)(1-\frac{\beta\nu}{N})\left(\frac{1-(-\lambda)^{N-j}}{1+\lambda}\right) \\
&= (-1)^j(1-\frac{\beta\nu}{N})\frac{(-\lambda)-(-\lambda)^{N-j+1}}{1+\lambda},
\end{aligned}$$

which coincides with (A.77). □

Example A.5.2 *Recall from Example 4.3.6 the form of N_3*

$$N_3 = \left[\begin{array}{cccccc} -1 & 0 & 0 & 0 & 0 & -\lambda \\ 1-\frac{\beta\nu}{8} & 0 & 0 & 0 & 0 & 0 \\ \lambda-1 & 1 & 0 & 0 & 0 & 0 \\ -1 & \lambda-1 & 1 & 0 & 0 & 0 \\ \hdashline -1 & 0 & -\lambda & \lambda-1 & 1 & 0 \\ -1 & 0 & 0 & -\lambda & \lambda-1 & 1 \end{array}\right].$$

Expanding on the first row, we obtain two minors, but the minor obtain from expanding on the $(1,1)$*-th entry of N_3 has the following form*

$$\left[\begin{array}{ccccc} 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ \lambda-1 & 1 & 0 & 0 & 0 \\ \hdashline 0 & -\lambda & \lambda-1 & 1 & 0 \\ 0 & 0 & -\lambda & \lambda-1 & 1 \end{array}\right],$$

and this minor has a zero row and therefore a determinant of zero. So we simply expand on the $(1,6)$*-th entry of N_3 to obtain*

$$\left[\begin{array}{ccccc} 1-\frac{\beta\nu}{8} & 0 & 0 & 0 & 0 \\ \lambda-1 & 1 & 0 & 0 & 0 \\ -1 & \lambda-1 & 1 & 0 & 0 \\ \hdashline -1 & 0 & -\lambda & \lambda-1 & 1 \\ -1 & 0 & 0 & -\lambda & \lambda-1 \end{array}\right]. \tag{A.80}$$

Then, we expand on the first row of (A.80), where only a single non-zero term exists (in position (1,1)) to obtain N_{31}

$$N_{31} = \left[\begin{array}{cccc} 1 & 0 & 0 & 0 \\ \lambda-1 & 1 & 0 & 0 \\ \hdashline 0 & -\lambda & \lambda-1 & 1 \\ 0 & 0 & -\lambda & \lambda-1 \end{array}\right].$$

Note that

$$\det(N_3) = -(-\lambda)(1-\frac{\beta\nu}{8})\det(N_{31}). \tag{A.81}$$

Then, N_{31} is identical to N_{22}^{01} (see (A.74)), and so we immediately see that

$$\det(N_{31}) = \det(N_{22}^{01}) = \lambda^2 - \lambda + 1. \tag{A.82}$$

Finally, substituting (A.82) into (A.81), we obtain

$$\begin{aligned}
\det(N_3) &= -(-\lambda)(1-\frac{\beta\nu}{8})\det(N_{31}) \\
&= -(-\lambda)(1-\frac{\beta\nu}{8})(\lambda^2-\lambda+1) \\
&= -(-\lambda)(1-\frac{\beta\nu}{8})\frac{1-(-\lambda)^3}{1+\lambda} \\
&= -(1-\frac{\beta\nu}{8})\frac{(-\lambda)-(-\lambda)^4}{1+\lambda}.
\end{aligned}$$

A.6 Adjacency lists and solutions for 250, 500, 1000 and 2000-node graph

In this section we give the adjacency lists that define four large graphs that we solve using the Wedged-MIP Heuristic in Section 2.9, and the Hamiltonian solutions that are obtained.

A.6.1 Adjacency list for 250-node graph

1 :	48	96	104	221		
2 :	69	70	84	109	173	176
3 :	104	175	197			
4 :	40	119	181	241		
5 :	8	53	167	180		
6 :	63	102	125	192	208	
7 :	110	128	191			
8 :	5	58	135	149	173	244
9 :	83	91	111			
10 :	107	152	217	239		
11 :	88	156	219			
12 :	88	99	107	184	185	239
13 :	36	38	130	170	192	
14 :	36	134	187			
15 :	70	96	165	192	217	
16 :	92	102	175	180	200	
17 :	36	206	225	226	238	244
18 :	22	103	160	195	247	
19 :	49	56	59	100	136	140
20 :	36	55	114	212		
21 :	65	74	161	203		
22 :	18	116	232	237		
23 :	34	76	105	174		
24 :	113	154	162	204	226	243
25 :	58	183	200	227		
26 :	31	49	69	80		
27 :	49	173	177	233		
28 :	75	90	138	223	227	
29 :	41	87	180	189		
30 :	89	98	239			
31 :	26	111	129	156	219	245
32 :	42	119	126	146	206	
33 :	50	88	92	155		
34 :	23	64	218			
35 :	97	161	240			
36 :	13	14	17	20	185	
37 :	39	90	93	228		
38 :	13	43	79	211	238	
39 :	37	69	79			
40 :	4	76	81	123	188	221
41 :	29	73	91	161	188	
42 :	32	193	230			
43 :	38	46	79	88	194	239
44 :	65	83	209			
45 :	113	139	194	230	232	
46 :	43	123	142	167	215	
47 :	59	62	226			
48 :	1	54	155			
49 :	19	26	27	104	146	194
50 :	33	106	115	121	157	166
51 :	56	137	198	250		
52 :	71	77	153			
53 :	5	86	106	135	149	
54 :	48	147	190			
55 :	20	66	101	178	205	
56 :	19	51	97	130	235	
57 :	68	92	99	173		
58 :	8	25	89	173	233	249
59 :	19	47	76	112	147	195
60 :	71	122	132	150	162	238
61 :	143	171	208			
62 :	47	176	222			
63 :	6	64	100	129	136	
64 :	34	63	73	136	143	
65 :	21	44	168	190	216	237
66 :	55	96	102	117	234	
67 :	106	151	174	197		
68 :	57	183	197	239	248	
69 :	2	26	39	73	184	201
70 :	2	15	91	95	134	
71 :	52	60	110	171	221	
72 :	171	176	194	226		
73 :	41	64	69	134	146	
74 :	21	77	151	190		
75 :	28	121	162	167	195	
76 :	23	40	59	124	196	231
77 :	52	74	89	125	179	242
78 :	80	111	151	163	170	207
79 :	38	39	43	89	175	192
80 :	26	78	87	154	229	247
81 :	40	109	242			
82 :	159	162	223			
83 :	9	44	213			
84 :	2	102	108	236		
85 :	101	141	234			
86 :	53	143	176	200		
87 :	29	80	124	238		
88 :	11	12	33	43	102	
89 :	30	58	77	79	110	112
90 :	28	37	247	249		
91 :	9	41	70	176		
92 :	16	33	57	112	171	216
93 :	37	166	204	213		
94 :	110	191	231			
95 :	70	158	162	179	203	
96 :	1	15	66	137	203	232
97 :	35	56	106	115		
98 :	30	186	188	200	207	
99 :	12	57	100	146	222	
100 :	19	63	99	123		
101 :	55	85	147	222		
102 :	6	16	66	84	88	131
103 :	18	180	212			
104 :	1	3	49	118		
105 :	23	187	198	217		
106 :	50	53	67	97	114	
107 :	10	12	151	154	206	216
108 :	84	182	193	233		
109 :	2	81	150	198		
110 :	7	71	89	94	153	
111 :	9	31	78	216		
112 :	59	89	92	121	163	198
113 :	24	45	211	240		
114 :	20	106	166	186		
115 :	50	97	181	214		
116 :	22	198	207			
117 :	66	219	224			
118 :	104	136	137			
119 :	4	32	160	171	182	209

120 :	148	225	228			
121 :	50	75	112	126	149	165
122 :	60	127	189	223	229	
123 :	40	46	100	139	176	181
124 :	76	87	128	156	215	224
125 :	6	77	235			
126 :	32	121	201	230		
127 :	122	141	142	208	237	248
128 :	7	124	138	218	228	
129 :	31	63	177	182	204	249
130 :	13	56	158	248		
131 :	102	190	248			
132 :	60	152	189	201	224	
133 :	179	200	206			
134 :	14	70	73	164	202	
135 :	8	53	190	214	228	
136 :	19	63	64	118	249	
137 :	51	96	118	207	250	
138 :	28	128	144	183		
139 :	45	123	158			
140 :	19	160	174	231		
141 :	85	127	155			
142 :	46	127	197	234	243	
143 :	61	64	86	157	182	218
144 :	138	157	213			
145 :	221	230	236			
146 :	32	49	73	99	173	232
147 :	54	59	101			
148 :	120	155	177			
149 :	8	53	121	159	210	240
150 :	60	109	245			
151 :	67	74	78	107	169	205
152 :	10	132	171			
153 :	52	110	191	247		
154 :	24	80	107	192	193	
155 :	33	48	141	148	164	
156 :	11	31	124	172	250	
157 :	50	143	144	219	235	
158 :	95	130	139	204		
159 :	82	149	244			
160 :	18	119	140	164	184	229
161 :	21	35	41			
162 :	24	60	75	82	95	
163 :	78	112	168	172	186	188
164 :	134	155	160			
165 :	15	121	167	210	220	249
166 :	50	93	114			
167 :	5	46	75	165	181	238
168 :	65	163	175	203	206	229
169 :	151	182	234			
170 :	13	78	196	201	227	
171 :	61	71	72	92	119	152
172 :	156	163	196	198		
173 :	2	8	27	57	58	146
174 :	23	67	140	201	236	
175 :	3	16	79	168	192	227
176 :	2	62	72	86	91	123
177 :	27	129	148			
178 :	55	186	214	249		
179 :	77	95	133	187	233	
180 :	5	16	29	103		
181 :	4	115	123	167	186	209
182 :	108	119	129	143	169	
183 :	25	68	138	226	233	
184 :	12	69	160	231		
185 :	12	36	232	243		
186 :	98	114	163	178	181	235
187 :	14	105	179	245		
188 :	40	41	98	163	202	242
189 :	29	122	132			
190 :	54	65	74	131	135	219
191 :	7	94	153			
192 :	6	13	15	79	154	175
193 :	42	108	154	199	202	229
194 :	43	45	49	72	242	
195 :	18	59	75			
196 :	76	170	172			
197 :	3	67	68	142	231	
198 :	51	105	109	112	116	172
199 :	193	213	222			
200 :	16	25	86	98	133	206
201 :	69	126	132	170	174	208
202 :	134	188	193	220		
203 :	21	95	96	168	245	
204 :	24	93	129	158		
205 :	55	151	234			
206 :	17	32	107	133	168	200
207 :	78	98	116	137	240	
208 :	6	61	127	201		
209 :	44	119	181	210	250	
210 :	149	165	209	243		
211 :	38	113	223			
212 :	20	103	246			
213 :	83	93	144	199		
214 :	115	135	178	246		
215 :	46	124	225	235		
216 :	65	92	107	111		
217 :	10	15	105			
218 :	34	128	143	237		
219 :	11	31	117	157	190	
220 :	165	202	250			
221 :	1	40	71	145	230	
222 :	62	99	101	199		
223 :	28	82	122	211		
224 :	117	124	132			
225 :	17	120	215			
226 :	17	24	47	72	183	
227 :	25	28	170	175		
228 :	37	120	128	135	241	
229 :	80	122	160	168	193	241
230 :	42	45	126	145	221	
231 :	76	94	140	184	197	
232 :	22	45	96	146	185	239
233 :	27	58	108	179	183	241
234 :	66	85	142	169	205	
235 :	56	125	157	186	215	241
236 :	84	145	174			
237 :	22	65	127	218		
238 :	17	38	60	87	167	246
239 :	10	12	30	43	68	232

240 :	35	113	149	207		
241 :	4	228	229	233	235	
242 :	77	81	188	194		
243 :	24	142	185	210		
244 :	8	17	159			
245 :	31	150	187	203		
246 :	212	214	238			
247 :	18	80	90	153		
248 :	68	127	130	131		
249 :	58	90	129	136	165	178
250 :	51	137	156	209	220	

A.6.2 Hamiltonian cycle for 250-node graph

The Hamiltonian cycle that we found using the Wedged-MIP Heuristic for 250-node graph is shown below. This Hamiltonian cycle is the one shown in Figure 2.11.

$1 \to 104 \to 118 \to 137 \to 250 \to 220 \to 202 \to 134 \to 14 \to 187 \to 105$
$\to 217 \to 15 \to 165 \to 210 \to 149 \to 159 \to 244 \to 8 \to 5 \to 167$
$\to 46 \to 43 \to 38 \to 79 \to 192 \to 154 \to 24 \to 113 \to 211 \to 223$
$\to 82 \to 162 \to 60 \to 71 \to 221 \to 145 \to 236 \to 84 \to 102 \to 131$
$\to 248 \to 127 \to 122 \to 189 \to 29 \to 87 \to 124 \to 215 \to 225 \to 17$
$\to 238 \to 246 \to 212 \to 103 \to 180 \to 16 \to 200 \to 206 \to 133 \to 179$
$\to 95 \to 158 \to 130 \to 56 \to 51 \to 198 \to 116 \to 207 \to 240 \to 35$
$\to 97 \to 115 \to 181 \to 209 \to 44 \to 65 \to 216 \to 92 \to 33 \to 50$
$\to 166 \to 93 \to 204 \to 129 \to 177 \to 148 \to 120 \to 228 \to 241 \to 235$
$\to 125 \to 77 \to 52 \to 153 \to 191 \to 7 \to 110 \to 94 \to 231 \to 184$
$\to 12 \to 88 \to 11 \to 219 \to 190 \to 74 \to 21 \to 161 \to 41 \to 188$
$\to 98 \to 186 \to 178 \to 214 \to 135 \to 53 \to 86 \to 176 \to 62 \to 47$
$\to 226 \to 72 \to 171 \to 152 \to 10 \to 107 \to 151 \to 169 \to 182 \to 108$
$\to 233 \to 27 \to 49 \to 26 \to 80 \to 247 \to 18 \to 195 \to 75 \to 121$
$\to 112 \to 59 \to 19 \to 140 \to 174 \to 23 \to 34 \to 64 \to 136 \to 249$
$\to 58 \to 89 \to 30 \to 239 \to 232 \to 22 \to 237 \to 218 \to 128 \to 138$
$\to 28 \to 90 \to 37 \to 39 \to 69 \to 73 \to 146 \to 173 \to 2 \to 70$
$\to 91 \to 9 \to 83 \to 213 \to 144 \to 157 \to 143 \to 61 \to 208 \to 6$
$\to 63 \to 100 \to 123 \to 139 \to 45 \to 194 \to 242 \to 81 \to 109 \to 150$
$\to 245 \to 203 \to 96 \to 66 \to 117 \to 224 \to 132 \to 201 \to 170 \to 13$

$\rightarrow 36 \rightarrow 185 \rightarrow 243 \rightarrow 142 \rightarrow 234 \rightarrow 205 \rightarrow 55 \rightarrow 20 \rightarrow 114 \rightarrow 106$

$\rightarrow 67 \rightarrow 197 \rightarrow 3 \rightarrow 175 \rightarrow 227 \rightarrow 25 \rightarrow 183 \rightarrow 68 \rightarrow 57 \rightarrow 99$

$\rightarrow 222 \rightarrow 199 \rightarrow 193 \rightarrow 42 \rightarrow 230 \rightarrow 126 \rightarrow 32 \rightarrow 119 \rightarrow 4 \rightarrow 40$

$\rightarrow 76 \rightarrow 196 \rightarrow 172 \rightarrow 156 \rightarrow 31 \rightarrow 111 \rightarrow 78 \rightarrow 163 \rightarrow 168 \rightarrow 229$

$\rightarrow 160 \rightarrow 164 \rightarrow 155 \rightarrow 141 \rightarrow 85 \rightarrow 101 \rightarrow 147 \rightarrow 54 \rightarrow 48 \rightarrow 1$

A.6.3 Adjacency list for 500-node graph

1 :	36	74	124	197	201	222	259	312	325
2 :	7	55	79	232	288	384			
3 :	11	44	166	239	255	357	381	414	482
4 :	15	19	67	305	352	363			
5 :	33	118	154	297	371	399	431	456	481
6 :	43	220	233	275	324	357	365	401	415
7 :	2	71	262						
8 :	76	134	209	260	419	420	447		
9 :	41	94	178	262	279	345	382	407	
10 :	40	246	379	466					
11 :	3	209	292	304					
12 :	53	80	81	153	322	373	416	425	439
13 :	119	237	330	389	470	482			
14 :	98	158	176	343	381	451	477	499	
15 :	4	75	288	372	479				
16 :	239	317	403	430					
17 :	90	198	201	220	245	296	360	395	
18 :	109	262	299	392	394				
19 :	4	27	230	233	338	352	402		
20 :	55	183	213	225	235	331	381		
21 :	163	204	243	456					
22 :	72	175	232	258	325	438			
23 :	144	147	450						
24 :	50	54	248	299	350	390	491		
25 :	31	81	219	290	363	398			
26 :	31	71	163	305	387				
27 :	19	214	265	395	436	451	454	458	493
28 :	46	107	137	167	169	296	370	392	448
29 :	279	334	374	455	493				
30 :	104	132	285	303	403	486			
31 :	25	26	94	100	101	252	356	402	429
32 :	141	362	376						
33 :	5	90	104	105	211	285	473		
34 :	35	61	89	157	256				
35 :	34	50	299						
36 :	1	430	433						
37 :	86	267	400						
38 :	166	298	332	435					
39 :	225	366	375						
40 :	10	178	216	285	336				
41 :	9	171	174	212	326	428	477	490	
42 :	48	49	159	207	255	268	376	413	453
43 :	6	161	239	285	450				
44 :	3	161	269	324	441				
45 :	106	319	396	438	471				
46 :	28	134	257	271	277	327	367	404	
47 :	96	133	299	442					
48 :	42	244	251	252	267	361	417		
49 :	42	53	303	304	406	432	495		
50 :	24	35	244						
51 :	166	366	435						
52 :	70	149	180	183	255	279	373	398	466
53 :	12	49	305	308	355	404			
54 :	24	88	193	197	233	376			
55 :	2	20	135	168	195	248	262	317	348
56 :	86	154	218						
57 :	105	126	145	170	216	226	292	392	482
58 :	125	396	404						
59 :	63	99	134	136	151	247	275	344	464
60 :	195	246	264	296	469	480			
61 :	34	184	216	372	456				
62 :	236	393	452						
63 :	59	67	123	139	148	236	395	398	
64 :	111	267	378	436	443	454	471	481	485
65 :	205	344	392	433					
66 :	122	130	188	235	344	352			
67 :	4	63	118	253	261	303			
68 :	77	89	220	320	363	483			
69 :	160	238	445						
70 :	52	155	202	208	244	280	381	482	
71 :	7	26	191	214	270	325			
72 :	22	100	167	324	326	375	402	427	441
73 :	140	189	238	272	383	404	475		
74 :	1	156	248	258	395	447			
75 :	15	260	276	309	367				
76 :	8	163	368	461					
77 :	68	162	487						
78 :	221	364	379	412	438				
79 :	2	141	202	255	344	376			
80 :	12	130	137	236	350	382	481	484	
81 :	12	25	155	192	266	269	279	398	476
82 :	108	170	288	334	335	384	395	466	
83 :	149	216	252	261	279				
84 :	187	191	201	288	311	316	344	365	
85 :	106	130	223	245	280	294	328	387	487
86 :	37	56	92	114	141	294	307	324	326
87 :	106	243	304	385	452	464			
88 :	54	141	163	254	326	404	416	418	471
89 :	34	68	208	475					
90 :	17	33	328	366	450				
91 :	158	259	340	468	486				
92 :	86	161	194	263	266	352	373	376	
93 :	198	214	328						
94 :	9	31	124	170	193	273	326	410	466
95 :	135	323	428						
96 :	47	156	175	234	290	302	354		
97 :	123	251	422						
98 :	14	270	321	377	405	412	439		
99 :	59	132	152	245	277	367			
100 :	31	72	126	170	187	350	421		
101 :	31	137	152	243	279	388			
102 :	247	336	355						
103 :	195	222	430	465	474	492			
104 :	30	33	134	136	233				
105 :	33	57	117	242	244	274	308	338	
106 :	45	85	87	280					
107 :	28	170	241	362					
108 :	82	298	405	443	471				
109 :	18	278	346	448					
110 :	287	379	385						
111 :	64	180	184	304	316	326	396		
112 :	114	115	341						
113 :	238	248	256	319	391	496			
114 :	86	112	154	252	295	316	383	430	
115 :	112	196	257	307	372	450			
116 :	132	162	187	356	399				
117 :	105	210	255	486					
118 :	5	67	203	209	219	331	402	408	
119 :	13	160	195	248	320	329	459	464	485

120 : 206 273 319 373 484
121 : 156 184 200 207 310 317 441 452 473
122 : 66 201 250
123 : 63 97 158 170 320 478 494 495
124 : 1 94 192 205 236 261 318 336 426
125 : 58 127 135 188 289 306 343 407
126 : 57 100 244 272 305 352
127 : 125 145 174 216 397 470
128 : 446 450 461
129 : 237 397 431
130 : 66 80 85 255 290
131 : 164 228 353
132 : 30 99 116 183 293 328 403
133 : 47 180 351 405 411 447
134 : 8 46 59 104 207 306 307 318
135 : 55 95 125 224 426 441 454
136 : 59 104 189 205 211 225 251 344 351
137 : 28 80 101 179 192 290 309 354
138 : 237 353 365
139 : 63 145 169 176 260 298 306 451 489
140 : 73 199 224 380 426 428 493
141 : 32 79 86 88
142 : 209 264 303 310 371 410 448 489
143 : 154 221 319 362 378 400
144 : 23 193 318 402 478
145 : 57 127 139 169 269 389 433 476
146 : 182 269 292 296 459
147 : 23 308 330 397
148 : 63 217 250
149 : 52 83 302 315 347 351 399
150 : 160 270 340
151 : 59 233 249 279 292 344 368 394 497
152 : 99 101 326
153 : 12 198 369 406
154 : 5 56 114 143
155 : 70 81 208 215 317 355 370 403 408
156 : 74 96 121 217 222 326
157 : 34 162 172 280 424 432
158 : 14 91 123 202 240
159 : 42 322 364 370 427 430 434 464 475
160 : 69 119 150 241 310 361 465
161 : 43 44 92 179 198 270 452 461 466
162 : 77 116 157 179 275 293 312 448 449
163 : 21 26 76 88 369 385 398 429
164 : 131 199 271 321 343
165 : 214 229 293 488
166 : 3 38 51 203 252 350 416 418 454
167 : 28 72 266 349 356 419 485 489
168 : 55 307 348 425
169 : 28 139 145 206 211 242 268 355
170 : 57 82 94 100 107 123 177 181 449
171 : 41 273 299
172 : 157 339 386
173 : 212 281 439 458 475 497 500
174 : 41 127 309 339 420
175 : 22 96 237 274 318 354 483
176 : 14 139 288 297 306 451 463 481
177 : 170 182 303
178 : 9 40 396
179 : 137 161 162 180 214 273
180 : 52 111 133 179 184 204 293 301 306
181 : 170 248 296 391 442 464
182 : 146 177 425
183 : 20 52 132 219 266 318 392
184 : 61 111 121 180 228 323 331 410 444
185 : 228 446 462 470
186 : 275 381 399 420 495 500
187 : 84 100 116 199 261 316 426 444
188 : 66 125 190 257 269 280 303 388 419
189 : 73 136 360 378 407 413 429 484
190 : 188 235 415
191 : 71 84 327 375
192 : 81 124 137 194 219 287 327 354
193 : 54 94 144 225 235 330 359 368 450
194 : 92 192 297 430
195 : 55 60 103 119 282 335
196 : 115 284 488
197 : 1 54 252 260 316 349 443 444 466
198 : 17 93 153 161 378 398 436 479 495
199 : 140 164 187 234 424 473 489
200 : 121 263 348 363 489
201 : 1 17 84 122 284
202 : 70 79 158 226 304 306 308 319 439
203 : 118 166 224 312 389 401 409 492
204 : 21 180 229 266 297 312 393 488
205 : 65 124 136 242 273 290 294 363 377
206 : 120 169 273 274 307
207 : 42 121 134 356
208 : 70 89 155 222 266 316 333 425 473
209 : 8 11 118 142 228 277 320 369 466
210 : 117 250 282 357
211 : 33 136 169 462
212 : 41 173 445 473
213 : 20 234 304 379 492
214 : 27 71 93 165 179 373 488
215 : 155 237 293 315 451 460
216 : 40 57 61 83 127 338 371 422
217 : 148 156 234 345
218 : 56 271 285
219 : 25 118 183 192 291 305 366 410 437
220 : 6 17 68 437 441 494
221 : 78 143 231 465 473 479
222 : 1 103 156 208 387 484
223 : 85 251 377
224 : 135 140 203 231 256 321 450
225 : 20 39 136 193 250 453
226 : 57 202 482
227 : 312 347 378 434
228 : 131 184 185 209 261 360 372 390
229 : 165 204 233 244 264 272
230 : 19 265 295 297
231 : 221 224 301 420 457
232 : 2 22 386 411
233 : 6 19 54 104 151 229 256 262 365
234 : 96 199 213 217
235 : 20 66 190 193 329
236 : 62 63 80 124 268 287 359 394
237 : 13 129 138 175 215 344 353
238 : 69 73 113 313 406 409 467 482
239 : 3 16 43

240 :	158	301	387	427					
241 :	107	160	417						
242 :	105	169	205	300	399	436	478	494	
243 :	21	87	101	249	374				
244 :	48	50	70	105	126	229	405	473	
245 :	17	85	99	266	307	337	444	448	
246 :	10	60	269	427					
247 :	59	102	317	329	377				
248 :	24	55	74	113	119	181	289	422	475
249 :	151	243	277	281	337	461			
250 :	122	148	210	225	314	367	475		
251 :	48	97	136	223	396	452			
252 :	31	48	83	114	166	197	448	489	491
253 :	67	280	328	402	407	426			
254 :	88	270	273	312	329	400	467		
255 :	3	42	52	79	117	130	390	395	
256 :	34	113	224	233	308	322	432		
257 :	46	115	188	362	376				
258 :	22	74	325	350					
259 :	1	91	405						
260 :	8	75	139	197	316	381	466		
261 :	67	83	124	187	228	486			
262 :	7	9	18	55	233	292	418	469	
263 :	92	200	311	323	381	387	407	474	
264 :	60	142	229	322	346	392	441	459	491
265 :	27	230	295						
266 :	81	92	167	183	204	208	245		
267 :	37	48	64	314					
268 :	42	169	236	270	293	315	320	350	463
269 :	44	81	145	146	188	246	275	391	425
270 :	71	98	150	161	254	268	392	420	450
271 :	46	164	218	337					
272 :	73	126	229	371	372	468	500		
273 :	94	120	171	179	205	206	254	315	416
274 :	105	175	206	320	489				
275 :	6	59	162	186	269	361	457	462	
276 :	75	380	407	497					
277 :	46	99	209	249					
278 :	109	398	499						
279 :	9	29	52	81	83	101	151	280	463
280 :	70	85	106	157	188	253	279		
281 :	173	249	374						
282 :	195	210	379	411					
283 :	313	367	371	393	471				
284 :	196	201	289	305	340	465			
285 :	30	33	40	43	218	355	488		
286 :	295	345	409						
287 :	110	192	236	291	342	470			
288 :	2	15	82	84	176	411	474		
289 :	125	248	284	294	386	400	419		
290 :	25	96	130	137	205	357	376	388	460
291 :	219	287	332	337	338	395	402	441	448
292 :	11	57	146	151	262	302	355	365	402
293 :	132	162	165	180	215	268	308	409	
294 :	85	86	205	289	330	421	454		
295 :	114	230	265	286	317	378	393	403	493
296 :	17	28	60	146	181	363	400	473	
297 :	5	176	194	204	230	325	370	444	
298 :	38	108	139	333	338	453			
299 :	18	24	35	47	171				
300 :	242	382	418	432	440	443	463	492	
301 :	180	231	240	396	414				
302 :	96	149	292	339	343	355	448		
303 :	30	49	67	142	177	188	357	416	
304 :	11	49	87	111	202	213	316	405	
305 :	4	26	53	126	219	284	361	486	
306 :	125	134	139	176	180	202	318	430	
307 :	86	115	134	168	206	245	430		
308 :	53	105	147	202	256	293	366	370	402
309 :	75	137	174	315	403	459	463		
310 :	121	142	160	391	449				
311 :	84	263	391						
312 :	1	162	203	204	227	254	374		
313 :	238	283	321	329					
314 :	250	267	379	440	461				
315 :	149	215	268	273	309	329	369	498	
316 :	84	111	114	187	197	208	260	304	477
317 :	16	55	121	155	247	295	350		
318 :	124	134	144	175	183	306	337	397	
319 :	45	113	120	143	202	445	490		
320 :	68	119	123	209	268	274			
321 :	98	164	224	313	364	476			
322 :	12	159	256	264	382	404	418	444	
323 :	95	184	263	479					
324 :	6	44	72	86	436	498			
325 :	1	22	71	258	297	457			
326 :	41	72	86	88	94	111	152	156	476
327 :	46	191	192	332					
328 :	85	90	93	132	253	460			
329 :	119	235	247	254	313	315			
330 :	13	147	193	294					
331 :	20	118	184	415					
332 :	38	291	327	378	404	410	426	435	460
333 :	208	298	460						
334 :	29	82	372	375					
335 :	82	195	411	434	445				
336 :	40	102	124	480					
337 :	245	249	271	291	318	372	422	470	
338 :	19	105	216	291	298	372	390	408	450
339 :	172	174	302	467					
340 :	91	150	284	497					
341 :	112	446	455						
342 :	287	397	430	440	487				
343 :	14	125	164	302	481	487			
344 :	59	65	66	79	84	136	151	237	443
345 :	9	217	286	362					
346 :	109	264	390	414	465				
347 :	149	227	465						
348 :	55	168	200	434					
349 :	167	197	357						
350 :	24	80	100	166	258	268	317	399	454
351 :	133	136	149	474					
352 :	4	19	66	92	126	419	426		
353 :	131	138	237						
354 :	96	137	175	192					
355 :	53	102	155	169	285	292	302	488	
356 :	31	116	167	207	410				
357 :	3	6	210	290	303	349	373	387	
358 :	423	425	426						
359 :	193	236	375	406					

360 : 17 189 228 391
361 : 48 160 275 305 377 418 437 451
362 : 32 107 143 257 345
363 : 4 25 68 200 205 296 411
364 : 78 159 321
365 : 6 84 138 233 292
366 : 39 51 90 219 308 413 467
367 : 46 75 99 250 283 385 394 480 482
368 : 76 151 193 416 460
369 : 153 163 209 315 482 483 499
370 : 28 155 159 297 308 422 437 439 470
371 : 5 142 216 272 283
372 : 15 61 115 228 272 334 337 338
373 : 12 52 92 120 214 357 484
374 : 29 243 281 312 468 478
375 : 39 72 191 334 359 394 480
376 : 32 42 54 79 92 257 290 394 445
377 : 98 205 223 247 361 400 437 460 486
378 : 64 143 189 198 227 295 332 405
379 : 10 78 110 213 282 314 403 437 468
380 : 140 276 452
381 : 3 14 20 70 186 260 263
382 : 9 80 300 322 390 435 457
383 : 73 114 477
384 : 2 82 495
385 : 87 110 163 367 422 454
386 : 172 232 289
387 : 26 85 222 240 263 357 425
388 : 101 188 290 441
389 : 13 145 203 409 414
390 : 24 228 255 338 346 382 476 498
391 : 113 181 269 310 311 360
392 : 18 28 57 65 183 264 270 401 484
393 : 62 204 283 295 415 422 488
394 : 18 151 236 367 375 376 410
395 : 17 27 63 74 82 255 291 423
396 : 45 58 111 178 251 301
397 : 127 129 147 318 342 442 461 479 496
398 : 25 52 63 81 163 198 278 472
399 : 5 116 149 186 242 350 408 495
400 : 37 143 254 289 296 377 486 489 490
401 : 6 203 392
402 : 19 31 72 118 144 253 291 292 308
403 : 16 30 132 155 295 309 379 485
404 : 46 53 58 73 88 322 332 418
405 : 98 108 133 244 259 304 378 423 490
406 : 49 153 238 359 467
407 : 9 125 189 253 263 276 435
408 : 118 155 338 399 423 464 467 493
409 : 203 238 286 293 389
410 : 94 142 184 219 332 356 394 416 423
411 : 133 232 282 288 335 363 480
412 : 78 98 419 469
413 : 42 189 366
414 : 3 301 346 389 443
415 : 6 190 331 393 417 462
416 : 12 88 166 273 303 368 410 441
417 : 48 241 415
418 : 88 166 262 300 322 361 404 463 472
419 : 8 167 188 289 352 412
420 : 8 174 186 231 270
421 : 100 294 446 467
422 : 97 216 248 337 370 385 393 464
423 : 358 395 405 408 410
424 : 157 199 439
425 : 12 168 182 208 269 358 387
426 : 124 135 140 187 253 332 352 358 497
427 : 72 159 240 246 452 459
428 : 41 95 140 499
429 : 31 163 189 475
430 : 16 36 103 114 159 194 306 307 342
431 : 5 129 476
432 : 49 157 256 300 445
433 : 36 65 145
434 : 159 227 335 348
435 : 38 51 332 382 407
436 : 27 64 198 242 324 437 467 495
437 : 219 220 361 370 377 379 436 476
438 : 22 45 78
439 : 12 98 173 202 370 424 496
440 : 300 314 342 461
441 : 44 72 121 135 220 264 291 388 416
442 : 47 181 397 460
443 : 64 108 197 300 344 414
444 : 184 187 197 245 297 322
445 : 69 212 319 335 376 432
446 : 128 185 341 421
447 : 8 74 133 497
448 : 28 109 142 162 245 252 291 302
449 : 162 170 310 487
450 : 23 43 90 115 128 193 224 270 338
451 : 14 27 139 176 215 361 458 485
452 : 62 87 121 161 251 380 427 468 490
453 : 42 225 298
454 : 27 64 135 166 294 350 385
455 : 29 341 493
456 : 5 21 61 496
457 : 231 275 325 382 476
458 : 27 173 451 459 489
459 : 119 146 264 309 427 458 462
460 : 215 290 328 332 333 368 377 442
461 : 76 128 161 249 314 397 440 467
462 : 185 211 275 415 459
463 : 176 268 279 300 309 418
464 : 59 87 119 159 181 408 422
465 : 103 160 221 284 346 347
466 : 10 52 82 94 161 197 209 260
467 : 238 254 339 366 406 408 421 436 461
468 : 91 272 374 379 452
469 : 60 262 412
470 : 13 127 185 287 337 370 495
471 : 45 64 88 108 283
472 : 398 418 492 496
473 : 33 121 199 208 212 221 244 296
474 : 103 263 288 351
475 : 73 89 159 173 248 250 429
476 : 81 145 321 326 390 431 437 457 496
477 : 14 41 316 383
478 : 123 144 242 374 484
479 : 15 198 221 323 397 490

480 :	60	336	367	375	411				
481 :	5	64	80	176	343				
482 :	3	13	57	70	226	238	367	369	
483 :	68	175	369						
484 :	80	120	189	222	373	392	478		
485 :	64	119	167	403	451				
486 :	30	91	117	261	305	377	400		
487 :	77	85	342	343	449				
488 :	165	196	204	214	285	355	393	493	
489 :	139	142	167	199	200	252	274	400	458
490 :	41	319	400	405	452	479			
491 :	24	252	264						
492 :	103	203	213	300	472				
493 :	27	29	140	295	408	455	488		
494 :	123	220	242						
495 :	49	123	186	198	384	399	436	470	
496 :	113	397	439	456	472	476	499		
497 :	151	173	276	340	426	447			
498 :	315	324	390						
499 :	14	278	369	428	496				
500 :	173	186	272						

A.6.4 Hamiltonian cycle for 500-node graph

The Hamiltonian cycle that we found using the Wedged-MIP Heuristic for 500-node graph is shown below. This Hamiltonian cycle is the one shown in Figure A.1.

$1 \to 312 \to 204 \to 229 \to 165 \to 214 \to 93 \to 328 \to 90 \to 366 \to 413$
$\to 189 \to 378 \to 332 \to 327 \to 191 \to 71 \to 7 \to 2 \to 384 \to 495$
$\to 49 \to 304 \to 111 \to 396 \to 58 \to 125 \to 289 \to 419 \to 8 \to 260$
$\to 466 \to 10 \to 40 \to 178 \to 9 \to 407 \to 435 \to 51 \to 166 \to 38$
$\to 298 \to 338 \to 390 \to 498 \to 315 \to 309 \to 75 \to 276 \to 380 \to 140$
$\to 428 \to 95 \to 323 \to 263 \to 200 \to 348 \to 434 \to 227 \to 347 \to 149$
$\to 351 \to 474 \to 103 \to 465 \to 284 \to 196 \to 115 \to 372 \to 228 \to 360$
$\to 391 \to 311 \to 84 \to 288 \to 15 \to 4 \to 352 \to 126 \to 100 \to 421$
$\to 294 \to 330 \to 13 \to 470 \to 185 \to 462 \to 275 \to 6 \to 365 \to 292$
$\to 302 \to 343 \to 481 \to 176 \to 297 \to 444 \to 184 \to 331 \to 415 \to 417$
$\to 241 \to 107 \to 170 \to 57 \to 482 \to 226 \to 202 \to 158 \to 240 \to 427$
$\to 72 \to 167 \to 485 \to 451 \to 361 \to 377 \to 223 \to 85 \to 487 \to 77$
$\to 68 \to 89 \to 475 \to 429 \to 163 \to 369 \to 483 \to 175 \to 354 \to 96$
$\to 234 \to 213 \to 492 \to 472 \to 496 \to 113 \to 248 \to 74 \to 156 \to 222$
$\to 387 \to 26 \to 305 \to 53 \to 308 \to 147 \to 23 \to 144 \to 402 \to 291$
$\to 219 \to 25 \to 398 \to 81 \to 279 \to 52 \to 180 \to 306 \to 430 \to 159$

$\rightarrow 364 \rightarrow 321 \rightarrow 98 \rightarrow 439 \rightarrow 370 \rightarrow 437 \rightarrow 379 \rightarrow 110 \rightarrow 287 \rightarrow 236$

$\rightarrow 62 \rightarrow 452 \rightarrow 490 \rightarrow 479 \rightarrow 221 \rightarrow 78 \rightarrow 412 \rightarrow 469 \rightarrow 262 \rightarrow 18$

$\rightarrow 394 \rightarrow 367 \rightarrow 385 \rightarrow 454 \rightarrow 64 \rightarrow 267 \rightarrow 37 \rightarrow 86 \rightarrow 307 \rightarrow 206$

$\rightarrow 120 \rightarrow 319 \rightarrow 445 \rightarrow 335 \rightarrow 82 \rightarrow 334 \rightarrow 375 \rightarrow 39 \rightarrow 225 \rightarrow 453$

$\rightarrow 42 \rightarrow 48 \rightarrow 251 \rightarrow 136 \rightarrow 211 \rightarrow 169 \rightarrow 139 \rightarrow 145 \rightarrow 389 \rightarrow 409$

$\rightarrow 286 \rightarrow 345 \rightarrow 217 \rightarrow 148 \rightarrow 250 \rightarrow 314 \rightarrow 440 \rightarrow 342 \rightarrow 397 \rightarrow 129$

$\rightarrow 237 \rightarrow 138 \rightarrow 353 \rightarrow 131 \rightarrow 164 \rightarrow 271 \rightarrow 218 \rightarrow 56 \rightarrow 154 \rightarrow 143$

$\rightarrow 362 \rightarrow 257 \rightarrow 46 \rightarrow 134 \rightarrow 104 \rightarrow 30 \rightarrow 285 \rightarrow 355 \rightarrow 488 \rightarrow 493$

$\rightarrow 455 \rightarrow 29 \rightarrow 374 \rightarrow 281 \rightarrow 249 \rightarrow 461 \rightarrow 76 \rightarrow 368 \rightarrow 416 \rightarrow 12$

$\rightarrow 322 \rightarrow 256 \rightarrow 432 \rightarrow 157 \rightarrow 424 \rightarrow 199 \rightarrow 473 \rightarrow 33 \rightarrow 105 \rightarrow 244$

$\rightarrow 405 \rightarrow 259 \rightarrow 91 \rightarrow 468 \rightarrow 272 \rightarrow 500 \rightarrow 173 \rightarrow 212 \rightarrow 41 \rightarrow 174$

$\rightarrow 127 \rightarrow 216 \rightarrow 83 \rightarrow 261 \rightarrow 124 \rightarrow 318 \rightarrow 337 \rightarrow 245 \rightarrow 448 \rightarrow 109$

$\rightarrow 278 \rightarrow 499 \rightarrow 14 \rightarrow 477 \rightarrow 316 \rightarrow 187 \rightarrow 426 \rightarrow 358 \rightarrow 423 \rightarrow 395$

$\rightarrow 255 \rightarrow 79 \rightarrow 141 \rightarrow 32 \rightarrow 376 \rightarrow 290 \rightarrow 388 \rightarrow 101 \rightarrow 31 \rightarrow 252$

$\rightarrow 491 \rightarrow 24 \rightarrow 50 \rightarrow 35 \rightarrow 34 \rightarrow 61 \rightarrow 456 \rightarrow 21 \rightarrow 243 \rightarrow 87$

$\rightarrow 106 \rightarrow 45 \rightarrow 438 \rightarrow 22 \rightarrow 232 \rightarrow 386 \rightarrow 172 \rightarrow 339 \rightarrow 467 \rightarrow 436$

$\rightarrow 324 \rightarrow 44 \rightarrow 269 \rightarrow 246 \rightarrow 60 \rightarrow 195 \rightarrow 282 \rightarrow 210 \rightarrow 117 \rightarrow 486$

$\rightarrow 400 \rightarrow 296 \rightarrow 363 \rightarrow 411 \rightarrow 480 \rightarrow 336 \rightarrow 102 \rightarrow 247 \rightarrow 317 \rightarrow 16$

$\rightarrow 239 \rightarrow 3 \rightarrow 11 \rightarrow 209 \rightarrow 277 \rightarrow 99 \rightarrow 152 \rightarrow 326 \rightarrow 94 \rightarrow 410$

$\rightarrow 356 \rightarrow 207 \rightarrow 121 \rightarrow 310 \rightarrow 449 \rightarrow 162 \rightarrow 116 \rightarrow 399 \rightarrow 408 \rightarrow 118$

$\rightarrow 203 \rightarrow 401 \rightarrow 392 \rightarrow 28 \rightarrow 137 \rightarrow 192 \rightarrow 194 \rightarrow 92 \rightarrow 266 \rightarrow 183$

$\rightarrow 20 \rightarrow 235 \rightarrow 190 \rightarrow 188 \rightarrow 280 \rightarrow 253 \rightarrow 67 \rightarrow 63 \rightarrow 59 \rightarrow 464$

$\rightarrow 181 \rightarrow 442 \rightarrow 460 \rightarrow 333 \rightarrow 208 \rightarrow 425 \rightarrow 168 \rightarrow 55 \rightarrow 135 \rightarrow 224$

$\rightarrow 231 \rightarrow 301 \rightarrow 414 \rightarrow 346 \rightarrow 264 \rightarrow 441 \rightarrow 220 \rightarrow 494 \rightarrow 123 \rightarrow 97$

$\rightarrow 422 \rightarrow 393 \rightarrow 283 \rightarrow 313 \rightarrow 238 \rightarrow 69 \rightarrow 160 \rightarrow 150 \rightarrow 340 \rightarrow 497$

$\rightarrow 447 \rightarrow 133 \rightarrow 47 \rightarrow 299 \rightarrow 171 \rightarrow 273 \rightarrow 179 \rightarrow 161 \rightarrow 43 \rightarrow 450$

$\rightarrow 128 \rightarrow 446 \rightarrow 341 \rightarrow 112 \rightarrow 114 \rightarrow 383 \rightarrow 73 \rightarrow 404 \rightarrow 418 \rightarrow 88$

$\rightarrow 471 \rightarrow 108 \rightarrow 443 \rightarrow 344 \rightarrow 151 \rightarrow 233 \rightarrow 19 \rightarrow 27 \rightarrow 265 \rightarrow 230$

$\rightarrow 295 \rightarrow 403 \rightarrow 132 \rightarrow 293 \rightarrow 215 \rightarrow 155 \rightarrow 70 \rightarrow 381 \rightarrow 186 \rightarrow 420$

$\rightarrow 270 \rightarrow 254 \rightarrow 329 \rightarrow 119 \rightarrow 320 \rightarrow 274 \rightarrow 489 \rightarrow 458 \rightarrow 459 \rightarrow 146$

$\rightarrow 182 \rightarrow 177 \rightarrow 303 \rightarrow 142 \rightarrow 371 \rightarrow 5 \rightarrow 431 \rightarrow 476 \rightarrow 457 \rightarrow 325$

$\rightarrow 258 \rightarrow 350 \rightarrow 268 \rightarrow 463 \rightarrow 300 \rightarrow 382 \rightarrow 80 \rightarrow 130 \rightarrow 66 \rightarrow 122$
$\rightarrow 201 \rightarrow 17 \rightarrow 198 \rightarrow 153 \rightarrow 406 \rightarrow 359 \rightarrow 193 \rightarrow 54 \rightarrow 197 \rightarrow 349$
$\rightarrow 357 \rightarrow 373 \rightarrow 484 \rightarrow 478 \rightarrow 242 \rightarrow 205 \rightarrow 65 \rightarrow 433 \rightarrow 36 \rightarrow 1$

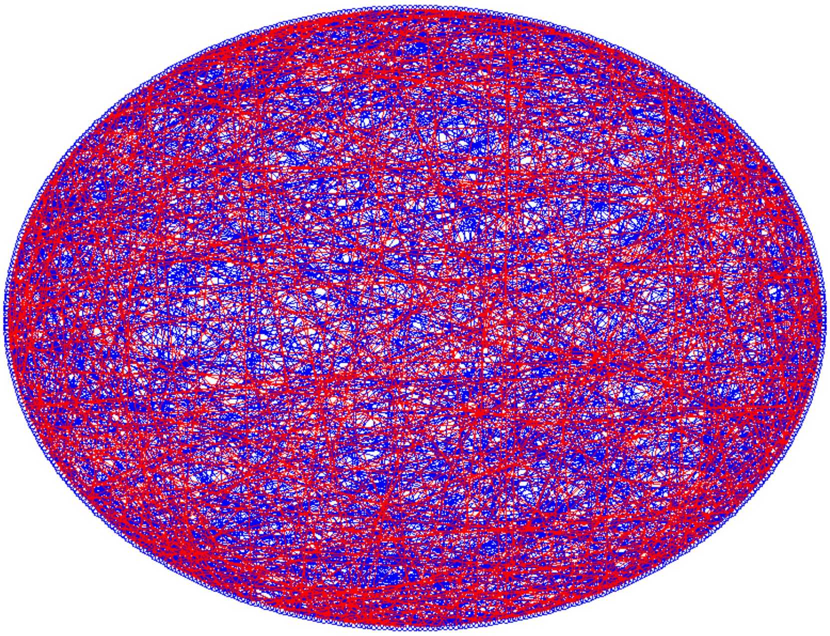


Figure A.1: Solution to 500-node graph (Hamiltonian cycle in red).

A.6.5 Adjacency list for 1000-node graph

1 :	9	80	190	283	295	354	748	771	783
2 :	7	71	405	714	741	801	888	911	915
3 :	84	108	188	219	260	315	627	984	
4 :	34	60	118	251	296	661	677	724	
5 :	186	333	368	587	658	677	678	988	
6 :	209	240	327	338	456	479	687	710	
7 :	2	158	159	437	568	608	807	989	
8 :	113	364	395	681	682	772	864	902	
9 :	1	12	38	101	110	318	913	956	
10 :	22	142	247	253	279	450	674		
11 :	19	38	104	112	263	477	916		
12 :	9	22	125	270	279	486	700		
13 :	14	22	68	382	549	593	636		
14 :	13	55	200	436	559	599	720		
15 :	83	175	198	314	471	611	831		
16 :	138	176	274	322	341	629	755		
17 :	24	116	307	324	378	642	722		
18 :	75	95	160	500	618	645	866		
19 :	11	174	264	394	456	645	853		
20 :	33	165	353	605	616	651	861		
21 :	45	64	396	424	443	669	701		
22 :	10	12	13	446	453	675	815		
23 :	141	152	169	339	693	717	800		
24 :	17	107	124	483	708	726	727		
25 :	107	249	269	386	460	737	788		
26 :	164	244	246	357	429	744	867		
27 :	127	137	205	324	415	746	876		
28 :	96	129	288	540	589	844	992		
29 :	90	113	234	728	774	845	982		
30 :	73	74	103	257	291	847	930		
31 :	82	105	112	210	388	855	856		
32 :	77	126	130	276	341	924	987		
33 :	20	35	122	149	641	931	981		
34 :	4	50	66	79	207	478			
35 :	33	75	163	216	250	552			
36 :	41	54	140	192	268	632			
37 :	94	97	198	273	275	389			
38 :	9	11	141	161	313	449			
39 :	137	291	310	349	358	378			
40 :	73	145	164	342	359	669			
41 :	36	101	117	194	379	690			
42 :	95	135	232	345	385	803			
43 :	72	75	87	143	445	919			
44 :	274	304	308	343	459	792			
45 :	21	212	411	447	460	512			
46 :	53	215	273	396	468	497			
47 :	49	123	154	458	481	977			
48 :	146	225	314	329	496	935			
49 :	47	220	242	271	497	780			
50 :	34	231	245	415	504	636			
51 :	72	293	296	392	505	732			
52 :	147	155	346	419	506	914			
53 :	46	321	368	412	523	698			
54 :	36	118	404	548	554	683			
55 :	14	274	367	434	568	740			
56 :	61	162	293	391	580	645			
57 :	101	102	144	431	592	912			
58 :	114	250	269	330	606	797			
59 :	62	133	351	420	606	980			

60 :	4	240	397	455	610	958
61 :	56	220	319	570	613	823
62 :	59	293	355	513	617	840
63 :	85	375	436	567	617	628
64 :	21	103	196	297	619	893
65 :	218	301	316	319	628	631
66 :	34	385	488	550	635	695
67 :	110	351	353	614	639	962
68 :	13	416	490	612	643	983
69 :	96	109	170	172	652	691
70 :	193	281	417	564	653	702
71 :	2	127	134	175	653	835
72 :	43	51	122	134	660	731
73 :	30	40	309	327	672	905
74 :	30	95	169	502	681	872
75 :	18	35	43	111	683	945
76 :	120	151	323	508	686	687
77 :	32	106	414	423	690	971
78 :	150	422	686	694	695	750
79 :	34	179	403	569	696	752
80 :	1	279	326	662	699	859
81 :	290	301	370	372	701	763
82 :	31	109	184	239	705	863
83 :	15	238	242	590	719	758
84 :	3	416	626	724	725	738
85 :	63	116	136	294	725	785
86 :	102	117	136	493	731	922
87 :	43	442	467	532	740	784
88 :	104	350	558	563	759	760
89 :	159	256	294	692	760	800
90 :	29	125	641	667	764	918
91 :	222	236	547	767	770	785
92 :	127	427	504	537	773	774
93 :	105	143	388	718	785	904
94 :	37	102	409	481	787	985
95 :	18	42	74	381	795	838
96 :	28	69	382	681	809	920
97 :	37	158	442	662	826	910
98 :	113	131	299	620	842	868
99 :	271	369	402	857	865	914
100 :	135	228	383	821	881	907
101 :	9	41	57	111	656	
102 :	57	86	94	122	519	
103 :	30	64	133	143	934	
104 :	11	88	148	161	193	
105 :	31	93	114	165	312	
106 :	77	132	153	167	325	
107 :	24	25	174	186	624	
108 :	3	166	167	192	517	
109 :	69	82	167	210	276	
110 :	9	67	182	232	301	
111 :	75	101	180	241	252	
112 :	11	31	150	253	512	
113 :	8	29	98	254	773	
114 :	58	105	144	254	708	
115 :	153	206	218	255	440	
116 :	17	85	190	258	263	
117 :	41	86	244	259	408	
118 :	4	54	271	272	300	
119 :	126	182	211	277	565	

120 :	76	126	276	285	491
121 :	158	214	260	286	287
122 :	33	72	102	292	817
123 :	47	128	133	295	302
124 :	24	171	181	297	955
125 :	12	90	303	305	584
126 :	32	119	120	316	685
127 :	27	71	92	320	824
128 :	123	154	173	331	473
129 :	28	178	259	333	849
130 :	32	294	295	343	837
131 :	98	190	303	344	648
132 :	106	169	227	352	525
133 :	59	103	123	352	605
134 :	71	72	284	355	836
135 :	42	100	152	360	820
136 :	85	86	285	376	716
137 :	27	39	250	391	430
138 :	16	261	292	399	536
139 :	156	218	272	420	663
140 :	36	369	417	431	531
141 :	23	38	248	432	869
142 :	10	205	280	435	709
143 :	43	93	103	441	533
144 :	57	114	280	457	574
145 :	40	208	272	463	897
146 :	48	247	422	465	886
147 :	52	261	370	466	622
148 :	104	193	430	470	813
149 :	33	246	342	474	640
150 :	78	112	335	475	915
151 :	76	256	365	476	973
152 :	23	135	426	485	964
153 :	106	115	335	487	488
154 :	47	128	332	499	516
155 :	52	254	379	511	619
156 :	139	265	337	511	936
157 :	285	463	464	513	745
158 :	7	97	121	518	609
159 :	7	89	192	521	801
160 :	18	224	363	526	694
161 :	38	104	318	534	818
162 :	56	398	421	538	868
163 :	35	191	507	541	607
164 :	26	40	383	543	825
165 :	20	105	360	549	878
166 :	108	311	358	560	574
167 :	106	108	109	572	823
168 :	255	256	425	573	711
169 :	23	74	132	577	828
170 :	69	258	289	579	602
171 :	124	278	349	580	972
172 :	69	377	390	581	630
173 :	128	189	306	584	977
174 :	19	107	265	590	957
175 :	15	71	280	591	970
176 :	16	340	341	601	635
177 :	347	418	529	602	879
178 :	129	312	461	607	608
179 :	79	465	558	608	879

180 :	111	350	371	609	627
181 :	124	405	487	611	799
182 :	110	119	262	613	820
183 :	278	348	610	614	806
184 :	82	282	283	619	729
185 :	237	255	604	620	954
186 :	5	107	588	623	723
187 :	257	384	454	623	986
188 :	3	363	624	625	944
189 :	173	277	601	626	627
190 :	1	116	131	629	873
191 :	163	262	366	636	812
192 :	36	108	159	637	765
193 :	70	104	148	644	712
194 :	41	287	296	646	752
195 :	236	275	338	650	651
196 :	64	224	313	653	654
197 :	600	649	654	655	843
198 :	15	37	323	658	670
199 :	226	259	658	659	949
200 :	14	315	365	666	794
201 :	233	278	492	666	699
202 :	304	314	320	670	671
203 :	225	267	672	673	938
204 :	264	305	448	674	895
205 :	27	142	235	676	745
206 :	115	223	534	690	841
207 :	34	329	484	691	692
208 :	145	328	472	700	894
209 :	6	348	620	711	970
210 :	31	109	663	715	968
211 :	119	257	427	717	998
212 :	45	293	425	733	850
213 :	326	439	643	737	885
214 :	121	215	489	739	948
215 :	46	214	545	740	804
216 :	35	306	679	742	766
217 :	221	603	742	743	1000
218 :	65	115	139	747	959
219 :	3	275	366	756	875
220 :	49	61	270	776	976
221 :	217	340	347	781	950
222 :	91	277	712	786	946
223 :	206	286	607	788	789
224 :	160	196	476	791	873
225 :	48	203	707	797	798
226 :	199	495	801	802	890
227 :	132	258	542	802	911
228 :	100	298	373	803	804
229 :	503	594	813	814	899
230 :	266	650	816	817	969
231 :	50	572	796	818	865
232 :	42	110	282	821	837
233 :	201	249	564	829	830
234 :	29	263	280	834	996
235 :	205	395	413	839	937
236 :	91	195	840	841	931
237 :	185	251	331	858	859
238 :	83	249	302	869	908
239 :	82	407	688	875	876

240 :	6	60	401	878	941
241 :	111	380	884	894	906
242 :	49	83	552	896	990
243 :	290	531	719	897	921
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930 :	30	245	246
931 :	33	236	246
932 :	343	574	933
933 :	488	581	932
934 :	103	247	403
935 :	48	446	511
936 :	156	528	937
937 :	235	436	936
938 :	203	395	939
939 :	593	938	940
940 :	433	939	941
941 :	240	940	942
942 :	496	941	943
943 :	560	942	944
944 :	188	943	945
945 :	75	944	946
946 :	222	945	947
947 :	422	485	946
948 :	214	503	594
949 :	199	347	594
950 :	221	416	595
951 :	245	595	952
952 :	414	951	953
953 :	494	596	952
954 :	185	596	955
955 :	124	954	956
956 :	9	955	957
957 :	174	956	958
958 :	60	597	957
959 :	218	597	598

960 :	462	598	961
961 :	497	960	962
962 :	67	961	963
963 :	599	962	964
964 :	152	963	965
965 :	244	964	966
966 :	321	465	965
967 :	558	565	600
968 :	210	600	969
969 :	230	968	970
970 :	175	209	969
971 :	77	248	591
972 :	171	248	592
973 :	151	350	526
974 :	247	365	975
975 :	512	974	976
976 :	220	584	975
977 :	47	173	445
978 :	499	550	601
979 :	374	432	601
980 :	59	538	554
981 :	33	352	602
982 :	29	602	983
983 :	68	982	984
984 :	3	983	985
985 :	94	984	986
986 :	187	985	987
987 :	32	603	986
988 :	5	603	989
989 :	7	988	990
990 :	242	989	991
991 :	481	990	992
992 :	28	991	993
993 :	585	992	994
994 :	428	434	993
995 :	251	413	440
996 :	234	444	997
997 :	299	604	996
998 :	211	599	604
999 :	519	537	577
1000 :	217	456	593

A.6.6 Hamiltonian cycle for 1000-node graph

The Hamiltonian cycle that we found using the Wedged-MIP Heuristic for 1000-node graph is shown below. This Hamiltonian cycle is the one shown in Figure A.2.

$1 \rightarrow 354 \rightarrow 814 \rightarrow 815 \rightarrow 816 \rightarrow 513 \rightarrow 709 \rightarrow 906 \rightarrow 907 \rightarrow 908 \rightarrow 589$
$\rightarrow 909 \rightarrow 552 \rightarrow 807 \rightarrow 808 \rightarrow 553 \rightarrow 383 \rightarrow 414 \rightarrow 952 \rightarrow 951 \rightarrow 595$
$\rightarrow 950 \rightarrow 416 \rightarrow 489 \rightarrow 655 \rightarrow 495 \rightarrow 656 \rightarrow 101 \rightarrow 57 \rightarrow 431 \rightarrow 616$
$\rightarrow 474 \rightarrow 617 \rightarrow 62 \rightarrow 355 \rightarrow 618 \rightarrow 417 \rightarrow 140 \rightarrow 36 \rightarrow 268 \rightarrow 266$
$\rightarrow 307 \rightarrow 308 \rightarrow 309 \rightarrow 901 \rightarrow 408 \rightarrow 424 \rightarrow 704 \rightarrow 705 \rightarrow 82 \rightarrow 863$
$\rightarrow 862 \rightarrow 861 \rightarrow 20 \rightarrow 605 \rightarrow 133 \rightarrow 103 \rightarrow 934 \rightarrow 403 \rightarrow 462 \rightarrow 960$

→ 598 → 730 → 521 → 729 → 184 → 619 → 64 → 297 → 124 → 955
→ 956 → 957 → 174 → 107 → 624 → 288 → 28 → 96 → 809 → 810
→ 811 → 555 → 255 → 185 → 954 → 596 → 953 → 494 → 651 → 195
→ 650 → 649 → 197 → 654 → 196 → 653 → 70 → 702 → 449 → 396
→ 46 → 468 → 720 → 721 → 419 → 498 → 662 → 80 → 859 → 860
→ 483 → 633 → 576 → 876 → 27 → 746 → 534 → 161 → 818 → 231
→ 865 → 573 → 866 → 867 → 26 → 246 → 931 → 33 → 641 → 90
→ 764 → 765 → 303 → 125 → 305 → 306 → 173 → 977 → 47 → 458
→ 579 → 888 → 580 → 171 → 278 → 509 → 698 → 697 → 551 → 792
→ 793 → 794 → 200 → 666 → 500 → 665 → 664 → 499 → 978 → 601
→ 979 → 374 → 366 → 668 → 669 → 40 → 145 → 463 → 157 → 745
→ 744 → 743 → 217 → 603 → 470 → 713 → 515 → 714 → 561 → 828
→ 560 → 827 → 482 → 259 → 117 → 41 → 379 → 406 → 467 → 905
→ 73 → 672 → 671 → 202 → 304 → 667 → 275 → 37 → 273 → 247
→ 974 → 365 → 151 → 76 → 687 → 688 → 239 → 407 → 362 → 367
→ 839 → 501 → 421 → 386 → 295 → 130 → 294 → 757 → 400 → 455
→ 575 → 872 → 476 → 621 → 466 → 405 → 610 → 60 → 958 → 597
→ 959 → 218 → 747 → 748 → 535 → 439 → 213 → 326 → 884 → 883
→ 882 → 371 → 180 → 111 → 241 → 894 → 208 → 700 → 701 → 21
→ 443 → 545 → 769 → 770 → 771 → 546 → 772 → 773 → 113 → 98
→ 620 → 209 → 970 → 175 → 591 → 917 → 918 → 357 → 356 → 919
→ 920 → 921 → 922 → 345 → 346 → 52 → 147 → 370 → 389 → 429
→ 522 → 731 → 72 → 660 → 661 → 442 → 87 → 740 → 215 → 804
→ 805 → 806 → 314 → 15 → 611 → 181 → 799 → 438 → 317 → 315
→ 3 → 627 → 189 → 626 → 381 → 409 → 612 → 68 → 643 → 490
→ 789 → 790 → 791 → 224 → 873 → 190 → 629 → 479 → 887 → 578
→ 457 → 877 → 334 → 333 → 129 → 849 → 848 → 415 → 484 → 642
→ 17 → 722 → 723 → 724 → 84 → 738 → 530 → 737 → 25 → 788
→ 787 → 786 → 502 → 452 → 779 → 520 → 728 → 514 → 425 → 727
→ 453 → 22 → 675 → 539 → 754 → 538 → 753 → 375 → 399 → 138
→ 261 → 262 → 325 → 324 → 881 → 100 → 821 → 822 → 510 → 703

$\rightarrow 491 \rightarrow 646 \rightarrow 647 \rightarrow 344 \rightarrow 131 \rightarrow 648 \rightarrow 387 \rightarrow 423 \rightarrow 507 \rightarrow 689$
$\rightarrow 274 \rightarrow 44 \rightarrow 343 \rightarrow 932 \rightarrow 933 \rightarrow 488 \rightarrow 66 \rightarrow 695 \rightarrow 588 \rightarrow 186$
$\rightarrow 623 \rightarrow 622 \rightarrow 477 \rightarrow 824 \rightarrow 127 \rightarrow 320 \rightarrow 903 \rightarrow 586 \rightarrow 559 \rightarrow 826$
$\rightarrow 97 \rightarrow 910 \rightarrow 590 \rightarrow 911 \rightarrow 2 \rightarrow 915 \rightarrow 562 \rightarrow 829 \rightarrow 233 \rightarrow 830$
$\rightarrow 563 \rightarrow 831 \rightarrow 564 \rightarrow 832 \rightarrow 833 \rightarrow 834 \rightarrow 835 \rightarrow 71 \rightarrow 134 \rightarrow 836$
$\rightarrow 566 \rightarrow 837 \rightarrow 232 \rightarrow 282 \rightarrow 281 \rightarrow 272 \rightarrow 118 \rightarrow 271 \rightarrow 264 \rightarrow 19$
$\rightarrow 853 \rightarrow 854 \rightarrow 855 \rightarrow 532 \rightarrow 741 \rightarrow 742 \rightarrow 216 \rightarrow 35 \rightarrow 75 \rightarrow 683$
$\rightarrow 54 \rightarrow 554 \rightarrow 980 \rightarrow 59 \rightarrow 420 \rightarrow 858 \rightarrow 570 \rightarrow 857 \rightarrow 569 \rightarrow 798$
$\rightarrow 225 \rightarrow 707 \rightarrow 706 \rightarrow 258 \rightarrow 116 \rightarrow 263 \rightarrow 640 \rightarrow 149 \rightarrow 342 \rightarrow 638$
$\rightarrow 637 \rightarrow 192 \rightarrow 159 \rightarrow 801 \rightarrow 226 \rightarrow 802 \rightarrow 227 \rightarrow 132 \rightarrow 106 \rightarrow 153$
$\rightarrow 115 \rightarrow 440 \rightarrow 536 \rightarrow 750 \rightarrow 749 \rightarrow 353 \rightarrow 67 \rightarrow 110 \rightarrow 301 \rightarrow 437$
$\rightarrow 762 \rightarrow 380 \rightarrow 337 \rightarrow 338 \rightarrow 339 \rightarrow 351 \rightarrow 352 \rightarrow 981 \rightarrow 602 \rightarrow 170$
$\rightarrow 289 \rightarrow 290 \rightarrow 81 \rightarrow 763 \rightarrow 543 \rightarrow 164 \rightarrow 825 \rightarrow 323 \rightarrow 322 \rightarrow 16$
$\rightarrow 755 \rightarrow 756 \rightarrow 219 \rightarrow 875 \rightarrow 874 \rightarrow 572 \rightarrow 864 \rightarrow 571 \rightarrow 454 \rightarrow 187$
$\rightarrow 986 \rightarrow 987 \rightarrow 32 \rightarrow 341 \rightarrow 925 \rightarrow 926 \rightarrow 265 \rightarrow 267 \rightarrow 880 \rightarrow 529$
$\rightarrow 736 \rightarrow 735 \rightarrow 390 \rightarrow 172 \rightarrow 630 \rightarrow 631 \rightarrow 632 \rightarrow 481 \rightarrow 94 \rightarrow 985$
$\rightarrow 984 \rightarrow 983 \rightarrow 982 \rightarrow 29 \rightarrow 845 \rightarrow 844 \rightarrow 843 \rightarrow 842 \rightarrow 841 \rightarrow 206$
$\rightarrow 690 \rightarrow 77 \rightarrow 971 \rightarrow 248 \rightarrow 972 \rightarrow 592 \rightarrow 929 \rightarrow 928 \rightarrow 927 \rightarrow 582$
$\rightarrow 460 \rightarrow 708 \rightarrow 24 \rightarrow 726 \rightarrow 518 \rightarrow 725 \rightarrow 85 \rightarrow 785 \rightarrow 91 \rightarrow 236$
$\rightarrow 840 \rightarrow 492 \rightarrow 201 \rightarrow 699 \rightarrow 335 \rightarrow 336 \rightarrow 245 \rightarrow 930 \rightarrow 30 \rightarrow 847$
$\rightarrow 846 \rightarrow 472 \rightarrow 613 \rightarrow 182 \rightarrow 820 \rightarrow 135 \rightarrow 360 \rightarrow 165 \rightarrow 878 \rightarrow 879$
$\rightarrow 179 \rightarrow 465 \rightarrow 966 \rightarrow 321 \rightarrow 53 \rightarrow 368 \rightarrow 625 \rightarrow 188 \rightarrow 363 \rightarrow 160$
$\rightarrow 18 \rightarrow 645 \rightarrow 56 \rightarrow 391 \rightarrow 657 \rightarrow 497 \rightarrow 961 \rightarrow 962 \rightarrow 963 \rightarrow 599$
$\rightarrow 998 \rightarrow 604 \rightarrow 997 \rightarrow 299 \rightarrow 300 \rightarrow 296 \rightarrow 4 \rightarrow 677 \rightarrow 676 \rightarrow 205$
$\rightarrow 142 \rightarrow 435 \rightarrow 644 \rightarrow 193 \rightarrow 148 \rightarrow 813 \rightarrow 812 \rightarrow 505 \rightarrow 684 \rightarrow 504$
$\rightarrow 685 \rightarrow 126 \rightarrow 316 \rightarrow 65 \rightarrow 628 \rightarrow 63 \rightarrow 567 \rightarrow 850 \rightarrow 410 \rightarrow 393$
$\rightarrow 372 \rightarrow 364 \rightarrow 870 \rightarrow 329 \rightarrow 48 \rightarrow 496 \rightarrow 942 \rightarrow 943 \rightarrow 944 \rightarrow 945$
$\rightarrow 946 \rightarrow 222 \rightarrow 712 \rightarrow 711 \rightarrow 168 \rightarrow 256 \rightarrow 475 \rightarrow 150 \rightarrow 112 \rightarrow 512$
$\rightarrow 975 \rightarrow 976 \rightarrow 584 \rightarrow 900 \rightarrow 461 \rightarrow 585 \rightarrow 412 \rightarrow 478 \rightarrow 34 \rightarrow 50$
$\rightarrow 636 \rightarrow 191 \rightarrow 163 \rightarrow 541 \rightarrow 761 \rightarrow 760 \rightarrow 89 \rightarrow 800 \rightarrow 23 \rightarrow 717$
$\rightarrow 211 \rightarrow 257 \rightarrow 696 \rightarrow 79 \rightarrow 752 \rightarrow 194 \rightarrow 287 \rightarrow 328 \rightarrow 327 \rightarrow 893$

$\rightarrow 892 \rightarrow 891 \rightarrow 250 \rightarrow 137 \rightarrow 430 \rightarrow 523 \rightarrow 732 \rightarrow 51 \rightarrow 293 \rightarrow 212$
$\rightarrow 45 \rightarrow 411 \rightarrow 382 \rightarrow 716 \rightarrow 715 \rightarrow 210 \rightarrow 663 \rightarrow 139 \rightarrow 156 \rightarrow 936$
$\rightarrow 528 \rightarrow 436 \rightarrow 937 \rightarrow 235 \rightarrow 395 \rightarrow 448 \rightarrow 204 \rightarrow 895 \rightarrow 896 \rightarrow 242$
$\rightarrow 990 \rightarrow 991 \rightarrow 992 \rightarrow 993 \rightarrow 994 \rightarrow 428 \rightarrow 413 \rightarrow 995 \rightarrow 251 \rightarrow 237$
$\rightarrow 331 \rightarrow 128 \rightarrow 123 \rightarrow 302 \rightarrow 238 \rightarrow 249 \rightarrow 606 \rightarrow 58 \rightarrow 797 \rightarrow 796$
$\rightarrow 795 \rightarrow 95 \rightarrow 838 \rightarrow 369 \rightarrow 99 \rightarrow 914 \rightarrow 451 \rightarrow 398 \rightarrow 162 \rightarrow 868$
$\rightarrow 869 \rightarrow 141 \rightarrow 432 \rightarrow 330 \rightarrow 332 \rightarrow 154 \rightarrow 516 \rightarrow 427 \rightarrow 92 \rightarrow 774$
$\rightarrow 775 \rightarrow 392 \rightarrow 444 \rightarrow 996 \rightarrow 234 \rightarrow 280 \rightarrow 144 \rightarrow 114 \rightarrow 254 \rightarrow 155$
$\rightarrow 511 \rightarrow 935 \rightarrow 446 \rightarrow 394 \rightarrow 678 \rightarrow 679 \rightarrow 680 \rightarrow 503 \rightarrow 948 \rightarrow 214$
$\rightarrow 739 \rightarrow 531 \rightarrow 243 \rightarrow 897 \rightarrow 583 \rightarrow 898 \rightarrow 899 \rightarrow 229 \rightarrow 594 \rightarrow 949$
$\rightarrow 347 \rightarrow 177 \rightarrow 418 \rightarrow 384 \rightarrow 377 \rightarrow 402 \rightarrow 557 \rightarrow 819 \rightarrow 517 \rightarrow 719$
$\rightarrow 83 \rightarrow 758 \rightarrow 759 \rightarrow 540 \rightarrow 916 \rightarrow 378 \rightarrow 404 \rightarrow 464 \rightarrow 710 \rightarrow 6$
$\rightarrow 240 \rightarrow 941 \rightarrow 940 \rightarrow 433 \rightarrow 525 \rightarrow 733 \rightarrow 524 \rightarrow 734 \rightarrow 527 \rightarrow 434$
$\rightarrow 55 \rightarrow 14 \rightarrow 13 \rightarrow 549 \rightarrow 924 \rightarrow 923 \rightarrow 385 \rightarrow 42 \rightarrow 803 \rightarrow 228$
$\rightarrow 298 \rightarrow 751 \rightarrow 537 \rightarrow 999 \rightarrow 519 \rightarrow 102 \rightarrow 122 \rightarrow 292 \rightarrow 291 \rightarrow 39$
$\rightarrow 358 \rightarrow 885 \rightarrow 886 \rightarrow 146 \rightarrow 422 \rightarrow 947 \rightarrow 485 \rightarrow 152 \rightarrow 964 \rightarrow 965$
$\rightarrow 244 \rightarrow 260 \rightarrow 121 \rightarrow 158 \rightarrow 609 \rightarrow 471 \rightarrow 902 \rightarrow 8 \rightarrow 681 \rightarrow 74$
$\rightarrow 169 \rightarrow 577 \rightarrow 456 \rightarrow 1000 \rightarrow 593 \rightarrow 939 \rightarrow 938 \rightarrow 203 \rightarrow 673 \rightarrow 376$
$\rightarrow 401 \rightarrow 768 \rightarrow 311 \rightarrow 310 \rightarrow 544 \rightarrow 767 \rightarrow 766 \rightarrow 508 \rightarrow 691 \rightarrow 207$
$\rightarrow 692 \rightarrow 693 \rightarrow 694 \rightarrow 78 \rightarrow 686 \rightarrow 506 \rightarrow 526 \rightarrow 973 \rightarrow 350 \rightarrow 349$
$\rightarrow 348 \rightarrow 183 \rightarrow 614 \rightarrow 447 \rightarrow 480 \rightarrow 318 \rightarrow 9 \rightarrow 913 \rightarrow 473 \rightarrow 615$
$\rightarrow 253 \rightarrow 252 \rightarrow 286 \rightarrow 223 \rightarrow 607 \rightarrow 178 \rightarrow 608 \rightarrow 7 \rightarrow 989 \rightarrow 988$
$\rightarrow 5 \rightarrow 587 \rightarrow 904 \rightarrow 93 \rightarrow 718 \rightarrow 441 \rightarrow 542 \rightarrow 912 \rightarrow 469 \rightarrow 600$
$\rightarrow 968 \rightarrow 969 \rightarrow 230 \rightarrow 817 \rightarrow 556 \rightarrow 851 \rightarrow 568 \rightarrow 852 \rightarrow 547 \rightarrow 777$
$\rightarrow 776 \rightarrow 220 \rightarrow 49 \rightarrow 780 \rightarrow 781 \rightarrow 221 \rightarrow 340 \rightarrow 176 \rightarrow 635 \rightarrow 634$
$\rightarrow 279 \rightarrow 10 \rightarrow 674 \rightarrow 277 \rightarrow 119 \rightarrow 565 \rightarrow 967 \rightarrow 558 \rightarrow 88 \rightarrow 104$
$\rightarrow 11 \rightarrow 38 \rightarrow 313 \rightarrow 312 \rightarrow 105 \rightarrow 31 \rightarrow 856 \rightarrow 548 \rightarrow 778 \rightarrow 361$
$\rightarrow 359 \rightarrow 670 \rightarrow 198 \rightarrow 658 \rightarrow 199 \rightarrow 659 \rightarrow 459 \rightarrow 581 \rightarrow 889 \rightarrow 890$
$\rightarrow 533 \rightarrow 143 \rightarrow 43 \rightarrow 445 \rightarrow 550 \rightarrow 782 \rightarrow 373 \rightarrow 397 \rightarrow 450 \rightarrow 783$
$\rightarrow 784 \rightarrow 388 \rightarrow 426 \rightarrow 682 \rightarrow 493 \rightarrow 86 \rightarrow 136 \rightarrow 285 \rightarrow 120 \rightarrow 276$
$\rightarrow 109 \rightarrow 69 \rightarrow 652 \rightarrow 269 \rightarrow 270 \rightarrow 12 \rightarrow 486 \rightarrow 639 \rightarrow 487 \rightarrow 871$

$\rightarrow 574 \rightarrow 166 \rightarrow 108 \rightarrow 167 \rightarrow 823 \rightarrow 61 \rightarrow 319 \rightarrow 284 \rightarrow 283 \rightarrow 1$

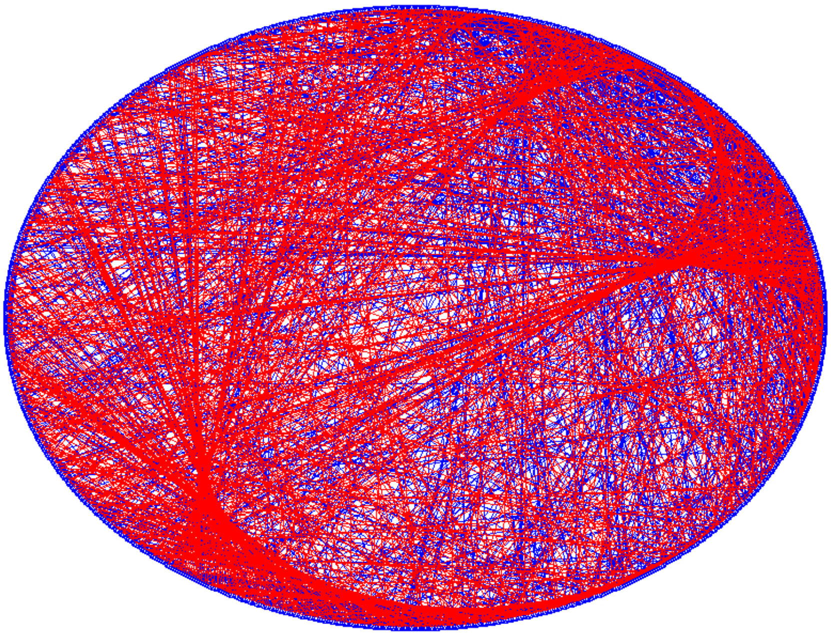

Figure A.2: Solution to 1000-node graph (Hamiltonian cycle in red).

A.6.7 Adjacency list for 2000-node graph

1 :	196	207	224	460	509	581	883	1051	1521
2 :	57	168	231	292	1082	1131	1191	1261	1542
3 :	11	80	184	330	589	1301	1477	1531	1814
4 :	611	978	999	1244	1511	1578	1579	1797	1954
5 :	82	409	533	680	1230	1287	1648	1934	1995
6 :	329	428	451	518	522	581	789	1963	
7 :	20	83	105	505	529	671	893	1367	
8 :	31	182	205	552	746	816	1077	1108	
9 :	24	296	531	613	625	1014	1103	1283	
10 :	12	17	76	156	231	900	1148	1734	
11 :	3	147	465	507	683	733	1228	1686	
12 :	10	77	245	565	638	1056	1393	1751	
13 :	119	188	281	574	582	842	1404	1949	
14 :	147	185	355	377	503	622	1570	1577	
15 :	48	284	325	424	1236	1304	1698	1980	
16 :	19	42	63	253	366	650	1586		
17 :	10	178	325	338	356	657	678		
18 :	98	418	484	578	848	914	995		
19 :	16	72	75	508	737	947	1147		
20 :	7	213	220	537	539	949	1311		
21 :	66	287	579	667	790	988	1788		
22 :	181	187	304	390	1043	1061	1062		
23 :	50	136	140	200	293	1104	1382		
24 :	9	82	513	609	777	1133	1198		
25 :	60	600	745	1015	1017	1152	1961		
26 :	78	375	474	549	604	1171	1314		
27 :	189	288	747	884	968	1181	1625		
28 :	62	145	511	681	1214	1219	1744		
29 :	161	396	967	987	1192	1234	1759		
30 :	31	201	233	400	536	1253	1289		
31 :	8	30	184	265	437	1254	1869		
32 :	36	439	659	890	1083	1308	1921		
33 :	51	262	846	1217	1333	1368	1710		
34 :	54	672	705	802	1250	1409	1809		
35 :	149	210	344	349	1266	1412	1731		
36 :	32	288	380	929	1238	1442	1529		
37 :	67	183	267	380	1058	1453	1819		
38 :	52	64	237	311	620	1473	1834		
39 :	159	185	519	637	702	1479	1562		
40 :	77	780	791	1082	1157	1495	1742		
41 :	252	452	804	941	1132	1554	1563		
42 :	16	584	822	839	1068	1636	1986		
43 :	71	449	511	556	843	1699	1976		
44 :	55	195	422	1322	1373	1714	1715		
45 :	562	871	1262	1316	1465	1806	1879		
46 :	162	279	497	1461	1462	1832	1989		
47 :	74	461	866	1446	1828	1847	1867		
48 :	15	89	493	723	1388	1899	1972		
49 :	572	873	1665	1666	1728	1916	1933		
50 :	23	111	159	197	215	1029			
51 :	33	52	69	208	259	717			
52 :	38	51	230	462	463	1668			
53 :	54	285	337	395	510	1813			
54 :	34	53	314	396	515	1684			
55 :	44	236	319	444	523	1323			
56 :	177	203	460	564	594	1475			
57 :	2	126	181	446	611	1007			
58 :	194	306	324	594	628	753			
59 :	179	466	565	576	634	1332			

60 :	25	585	598	691	696	1439
61 :	99	109	242	256	708	1079
62 :	28	87	331	610	713	1375
63 :	16	76	120	157	717	1102
64 :	38	124	546	688	753	1716
65 :	68	174	278	404	755	1267
66 :	21	211	457	574	773	1259
67 :	37	479	512	514	780	1371
68 :	65	129	187	212	789	1263
69 :	51	545	754	762	791	1073
70 :	213	221	425	796	820	1631
71 :	43	128	177	237	844	1018
72 :	19	155	436	618	845	1947
73 :	74	238	772	786	854	1205
74 :	47	73	258	277	862	1386
75 :	19	331	608	732	867	1315
76 :	10	63	446	652	880	1161
77 :	12	40	189	671	896	1859
78 :	26	155	240	626	915	1296
79 :	295	298	385	669	918	1612
80 :	3	348	614	833	932	1390
81 :	92	221	436	570	933	1328
82 :	5	24	130	251	960	1412
83 :	7	172	742	797	962	1955
84 :	167	520	588	714	994	1394
85 :	545	581	665	788	1012	1426
86 :	242	636	637	767	1016	1638
87 :	62	586	825	1054	1063	1493
88 :	161	517	569	977	1075	1265
89 :	48	193	595	882	1076	1891
90 :	134	300	778	1033	1097	1388
91 :	125	607	1004	1046	1111	1343
92 :	81	261	386	965	1123	1565
93 :	461	533	583	692	1128	1655
94 :	153	295	536	906	1138	1186
95 :	585	586	907	946	1163	1436
96 :	249	683	897	903	1178	1886
97 :	157	277	384	793	1206	1533
98 :	18	294	591	673	1221	1237
99 :	61	253	264	636	1245	1310
100 :	190	245	710	1056	1247	1252
101 :	422	612	835	1233	1248	1970
102 :	417	621	1080	1248	1249	1407
103 :	351	597	850	1049	1254	1372
104 :	147	159	514	877	1258	1990
105 :	7	206	524	711	1268	1420
106 :	322	525	661	787	1269	1845
107 :	530	546	938	1172	1273	1275
108 :	199	209	569	930	1285	1421
109 :	61	320	533	1091	1288	1943
110 :	139	837	870	933	1297	1554
111 :	50	264	728	730	1298	1520
112 :	493	658	948	1282	1299	1739
113 :	642	694	891	1109	1302	1872
114 :	267	761	958	1302	1303	1677
115 :	547	643	997	1010	1303	1987
116 :	640	711	1008	1281	1327	1957
117 :	211	306	629	690	1329	1526
118 :	223	551	629	709	1339	1628
119 :	13	330	590	821	1348	1461

120 :	63	426	518	1092	1357	1358
121 :	174	207	419	525	1358	1380
122 :	541	682	879	955	1375	1903
123 :	158	266	526	1115	1377	1878
124 :	64	920	1251	1287	1378	1757
125 :	91	299	578	980	1381	1476
126 :	57	260	343	874	1395	1456
127 :	176	554	590	1317	1399	1444
128 :	71	704	922	1401	1402	1497
129 :	68	381	663	1251	1410	1452
130 :	82	383	668	1359	1413	1713
131 :	539	579	1018	1073	1417	1770
132 :	628	669	691	1065	1426	1564
133 :	641	652	1254	1335	1438	1736
134 :	90	633	1269	1403	1440	1511
135 :	680	958	1059	1295	1455	1506
136 :	23	535	557	1253	1481	1482
137 :	649	698	1191	1362	1494	1865
138 :	623	925	1325	1374	1497	1816
139 :	110	537	601	914	1508	1900
140 :	23	291	362	733	1518	1866
141 :	208	981	1231	1398	1555	1595
142 :	176	467	910	1577	1581	1760
143 :	225	703	1114	1459	1593	1857
144 :	201	346	516	545	1600	1645
145 :	28	351	645	1220	1608	1884
146 :	229	723	1008	1166	1612	1613
147 :	11	14	104	506	1613	1959
148 :	510	559	1253	1523	1615	1766
149 :	35	566	1306	1615	1616	1683
150 :	327	1090	1391	1392	1618	1653
151 :	332	414	560	1003	1619	1893
152 :	171	344	602	1445	1621	1737
153 :	94	504	816	1185	1622	1812
154 :	664	867	1119	1449	1626	1790
155 :	72	78	540	857	1639	1671
156 :	10	300	650	1372	1641	1837
157 :	63	97	540	1170	1652	1788
158 :	123	309	619	782	1658	1781
159 :	39	50	104	1194	1683	1952
160 :	656	697	764	996	1703	1707
161 :	29	88	492	691	1719	1960
162 :	46	180	1415	1676	1732	1733
163 :	256	747	1468	1736	1737	1882
164 :	250	716	1535	1536	1743	1779
165 :	355	998	1243	1542	1746	1898
166 :	372	515	1125	1764	1765	1935
167 :	84	301	538	1290	1774	1928
168 :	2	702	1754	1771	1778	1838
169 :	185	191	822	1156	1808	1906
170 :	206	895	896	1795	1821	1998
171 :	152	457	665	1546	1835	1984
172 :	83	498	539	1338	1848	1912
173 :	472	1057	1347	1701	1905	1906
174 :	65	121	340	1270	1925	1953
175 :	301	563	807	1216	1966	1998
176 :	127	142	263	275	911	
177 :	56	71	255	279	1261	
178 :	17	195	231	287	1945	
179 :	59	203	205	292	939	

180 :	162	222	306	315	1344
181 :	22	57	193	361	971
182 :	8	214	345	361	387
183 :	37	218	317	397	1521
184 :	3	31	192	401	1550
185 :	14	39	169	408	503
186 :	209	258	260	409	1229
187 :	22	68	295	427	794
188 :	13	192	211	430	912
189 :	27	77	415	455	1702
190 :	100	191	197	471	657
191 :	169	190	239	472	544
192 :	184	188	404	473	703
193 :	89	181	394	506	640
194 :	58	225	500	507	1416
195 :	44	178	477	509	1975
196 :	1	307	484	513	1387
197 :	50	190	305	517	1286
198 :	204	387	422	522	642
199 :	108	269	485	530	708
200 :	23	209	268	531	1210
201 :	30	144	312	534	651
202 :	220	237	283	555	1428
203 :	56	179	519	557	1330
204 :	198	454	542	567	1481
205 :	8	179	555	568	1334
206 :	105	170	572	573	1887
207 :	1	121	379	578	1022
208 :	51	141	482	580	1076
209 :	108	186	200	582	583
210 :	35	412	592	597	721
211 :	66	117	188	599	1866
212 :	68	568	588	599	1849
213 :	20	70	377	602	1432
214 :	182	344	420	604	1548
215 :	50	266	411	616	1101
216 :	345	491	542	624	1331
217 :	238	445	591	644	803
218 :	183	416	645	646	1060
219 :	249	443	577	654	1142
220 :	20	202	623	654	973
221 :	70	81	615	658	1614
222 :	180	318	405	660	1435
223 :	118	508	663	664	814
224 :	1	272	281	667	1626
225 :	143	194	238	670	1458
226 :	389	521	593	670	1652
227 :	288	317	632	673	743
228 :	241	242	580	674	1257
229 :	146	239	556	675	676
230 :	52	579	647	677	1410
231 :	2	10	178	679	1366
232 :	268	368	610	683	1721
233 :	30	332	470	687	1584
234 :	256	517	578	696	1478
235 :	298	441	642	697	865
236 :	55	676	679	699	1927
237 :	38	71	202	700	859
238 :	73	217	225	701	1543
239 :	191	229	447	704	734

240 :	78	398	404	708	1853
241 :	228	274	512	712	1802
242 :	61	86	228	715	1572
243 :	257	316	368	718	1838
244 :	583	603	643	720	735
245 :	12	100	584	722	1997
246 :	371	453	730	739	782
247 :	391	524	590	752	1433
248 :	563	719	725	763	1160
249 :	96	219	269	764	1047
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251 :	82	526	528	783	1389
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253 :	16	99	548	785	787
254 :	458	575	677	786	972
255 :	177	643	644	792	1700
256 :	61	163	234	796	1705
257 :	243	668	770	800	1920
258 :	74	186	543	805	1306
259 :	51	393	442	809	993
260 :	126	186	307	815	1351
261 :	92	414	495	817	889
262 :	33	276	686	820	1332
263 :	176	409	654	824	1756
264 :	99	111	459	826	856
265 :	31	419	551	827	1817
266 :	123	215	574	830	1380
267 :	37	114	467	836	1485
268 :	200	232	326	839	1674
269 :	199	249	274	840	1769
270 :	352	361	461	847	1448
271 :	458	598	748	858	1314
272 :	224	353	490	861	1646
273 :	335	346	399	875	1763
274 :	241	269	534	878	1643
275 :	176	286	719	880	1472
276 :	262	534	552	886	1203
277 :	74	97	655	892	1361
278 :	65	312	365	892	1871
279 :	46	177	555	894	1318
280 :	359	462	620	898	1882
281 :	13	224	632	902	1644
282 :	456	731	781	906	1510
283 :	202	509	527	909	1514
284 :	15	384	690	916	1686
285 :	53	622	873	919	1424
286 :	275	388	587	922	1307
287 :	21	178	866	926	1630
288 :	27	36	227	927	936
289 :	353	706	740	931	1496
290 :	328	658	757	934	1782
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293 :	23	713	724	943	1635
294 :	98	538	792	950	1942
295 :	79	94	187	952	1164
296 :	9	540	639	955	1908
297 :	392	508	915	957	1877
298 :	79	235	613	959	1116
299 :	125	638	855	961	1055
300 :	90	156	813	964	1543
301 :	167	175	596	966	1948
302 :	323	332	350	970	1389
303 :	613	649	775	975	1965
304 :	22	577	695	980	1919
305 :	197	532	842	981	1355
306 :	58	117	180	983	1773
307 :	196	260	624	990	1167
308 :	354	537	547	992	1118
309 :	158	567	923	993	1737
310 :	499	566	573	1001	1675
311 :	38	375	841	1010	1170
312 :	201	278	652	1019	1929
313 :	362	522	774	1020	1314
314 :	54	406	731	1029	1259
315 :	180	423	485	1032	1352
316 :	243	617	766	1034	1137
317 :	183	227	448	1035	1520
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319 :	55	511	979	1052	1324
320 :	109	745	746	1065	1384
321 :	411	756	801	1069	1727
322 :	106	334	338	1072	1539
323 :	302	693	988	1072	1409
324 :	58	478	541	1074	1218
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326 :	268	587	811	1081	1348
327 :	150	700	1041	1086	1777
328 :	290	575	845	1086	1718
329 :	6	507	957	1087	1201
330 :	3	119	996	1089	1673
331 :	62	75	565	1094	1851
332 :	151	233	302	1095	1585
333 :	510	558	593	1096	1155
334 :	322	401	633	1109	1116
335 :	273	484	881	1112	1247
336 :	413	497	631	1114	1274
337 :	53	742	785	1117	1252
338 :	17	322	665	1125	1507
339 :	358	491	506	1129	1849
340 :	174	527	630	1130	1841
341 :	412	576	577	1130	1923
342 :	603	685	727	1134	1404
343 :	126	686	999	1139	1950
344 :	35	152	214	1141	1148
345 :	182	216	541	1144	1836
346 :	144	273	886	1144	1764
347 :	580	605	847	1145	1452
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349 :	35	846	1044	1169	1336
350 :	252	302	438	1184	1388
351 :	103	145	719	1190	1888
352 :	270	709	1124	1197	1290
353 :	272	289	985	1197	1972
354 :	308	505	1180	1205	1821
355 :	14	165	398	1209	1541
356 :	17	714	848	1211	1830
357 :	666	1189	1195	1212	1349
358 :	339	525	526	1217	1501
359 :	280	1006	1071	1223	1837

360 :	544	983	1153	1228	1637
361 :	181	182	270	1248	1262
362 :	140	313	771	1250	1272
363 :	527	767	1246	1255	1379
364 :	611	612	827	1258	1341
365 :	278	637	736	1260	1504
366 :	16	516	1199	1263	1890
367 :	488	516	1025	1264	1968
368 :	232	243	679	1264	1453
369 :	452	535	1159	1265	1294
370 :	522	571	606	1266	1447
371 :	246	729	881	1267	1985
372 :	166	523	1019	1268	1364
373 :	575	712	1051	1268	1588
374 :	405	586	587	1271	1667
375 :	26	311	635	1272	1548
376 :	529	562	612	1274	1454
377 :	14	213	917	1277	1413
378 :	675	752	938	1279	1738
379 :	207	531	660	1284	1795
380 :	36	37	1233	1293	1294
381 :	129	454	1215	1293	1590
382 :	489	727	778	1298	1862
383 :	130	421	455	1300	1579
384 :	97	284	743	1300	1876
385 :	79	653	852	1305	1660
386 :	92	544	807	1307	1804
387 :	182	198	684	1310	1747
388 :	286	956	1084	1312	1939
389 :	226	523	939	1316	1969
390 :	22	410	1275	1318	1437
391 :	247	726	1092	1319	1449
392 :	297	407	1078	1321	1322
393 :	259	676	1280	1326	1364
394 :	193	804	1305	1327	1597
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396 :	29	54	1222	1339	1762
397 :	183	754	1122	1340	1695
398 :	240	355	542	1341	1692
399 :	273	806	1000	1349	1956
400 :	30	573	644	1351	1578
401 :	184	334	421	1357	1605
402 :	638	784	1356	1357	1974
403 :	470	515	860	1361	1952
404 :	65	192	240	1369	1817
405 :	222	374	1023	1379	1400
406 :	314	524	1195	1383	1384
407 :	392	883	904	1385	1551
408 :	185	543	544	1391	1911
409 :	5	186	263	1394	1603
410 :	390	757	772	1395	1438
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412 :	210	341	928	1411	1587
413 :	336	613	935	1412	1498
414 :	151	261	716	1414	1852
415 :	189	741	1356	1425	1854
416 :	218	469	1149	1430	1431
417 :	102	694	1108	1437	1533
418 :	18	647	808	1442	1462
419 :	121	265	596	1448	1816
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421 :	383	401	434	1467	1880
422 :	44	101	198	1469	1470
423 :	315	982	1196	1470	1776
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425 :	70	666	1394	1483	1484
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429 :	755	766	979	1500	1843
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431 :	709	1135	1240	1509	1624
432 :	582	634	1048	1512	1940
433 :	512	853	949	1513	1731
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435 :	648	1151	1155	1530	1531
436 :	72	81	1218	1536	1632
437 :	31	562	625	1543	1749
438 :	350	810	1011	1545	1546
439 :	32	663	1128	1546	1844
440 :	868	1550	1551	1565	1910
441 :	235	1098	1540	1565	1566
442 :	259	1009	1200	1566	1679
443 :	219	947	1362	1569	1758
444 :	55	653	763	1583	1623
445 :	217	518	1542	1594	1785
446 :	57	76	1036	1601	1647
447 :	239	810	863	1604	1723
448 :	317	449	684	1607	1712
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453 :	246	1226	1621	1622	1824
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458 :	254	271	665	1645	1791
459 :	264	799	1471	1649	1650
460 :	1	56	1200	1654	1809
461 :	47	93	270	1656	1720
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466 :	59	659	926	1686	1687
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468 :	675	833	1061	1690	1691
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470 :	233	403	1721	1722	1994
471 :	190	749	1146	1726	1859
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473 :	192	615	1311	1733	1907
474 :	26	699	1405	1741	1761
475 :	606	1176	1744	1745	1971
476 :	489	589	590	1748	1820
477 :	195	1573	1574	1752	1983
478 :	324	543	853	1754	1881
479 :	67	532	1113	1761	1914

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481 :	576	861	1260	1783	1793
482 :	208	682	1784	1785	1842
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484 :	18	196	335	1807	1930
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486 :	614	672	674	1823	1868
487 :	318	693	1721	1825	1839
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489 :	382	476	1158	1835	1836
490 :	272	831	852	1843	1915
491 :	216	339	605	1846	1848
492 :	161	1152	1213	1853	1909
493 :	48	112	1853	1854	1937
494 :	732	768	790	1862	1873
495 :	261	1353	1487	1864	1865
496 :	670	781	1219	1871	1876
497 :	46	336	653	1872	1873
498 :	172	771	1107	1896	1945
499 :	310	507	1818	1918	1919
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501 :	456	1805	1922	1923	1988
502 :	1118	1402	1559	1930	1931
503 :	14	185	838	1984	1985
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725 :	248	724	726	854
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727 :	342	382	728	1246
728 :	111	726	727	1856
729 :	371	687	730	925
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754 :	69	397	758	1524
755 :	65	429	758	762
756 :	321	753	759	1898
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762 :	69	755	763	918
763 :	248	444	762	765
764 :	160	249	765	1611
765 :	678	763	764	1942
766 :	316	429	768	1473
767 :	86	363	769	937
768 :	494	766	769	1037
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770 :	257	769	771	1864
771 :	362	498	770	772
772 :	73	410	771	1944
773 :	66	685	774	1725
774 :	313	773	775	1941
775 :	303	774	776	1724
776 :	250	775	777	1676
777 :	24	776	779	851
778 :	90	382	779	1067
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781 :	282	496	783	1028
782 :	158	246	783	1944
783 :	251	781	782	784
784 :	252	402	783	1722
785 :	253	337	510	1959
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792 :	255	294	793	1291
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794 :	187	793	797	1967
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796 :	70	256	800	901
797 :	83	794	801	1179
798 :	572	795	802	1224
799 :	459	488	803	860
800 :	257	796	805	1256
801 :	321	797	806	1726
802 :	34	798	811	1996
803 :	217	799	812	1951
804 :	41	394	813	1932
805 :	258	800	818	1747
806 :	399	801	818	1764
807 :	175	386	819	1278
808 :	418	746	821	1247
809 :	259	576	823	1307
810 :	438	447	823	1722
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812 :	606	803	825	1958
813 :	300	804	828	1690
814 :	223	318	828	1750
815 :	260	736	829	948
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821 :	119	808	835	1517
822 :	42	169	836	1798
823 :	809	810	838	1184
824 :	263	811	840	1334
825 :	87	812	841	1093
826 :	264	462	843	885
827 :	265	364	849	1110
828 :	813	814	850	1796
829 :	815	816	851	1513
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831 :	490	686	857	1723
832 :	818	819	858	1044
833 :	80	468	862	1021
834 :	820	849	863	1093
835 :	101	821	864	1515
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837 :	110	483	868	1273
838 :	503	823	870	1989
839 :	42	268	871	1834

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858 :	271	832	905	1748	**918** :	79	762	1020	1941
859 :	237	730	908	1177	**919** :	285	865	1021	1276
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880 :	76	275	944	1098	**940** :	291	876	1064	1377
881 :	335	371	945	1955	**941** :	41	877	1066	1383
882 :	89	844	952	1365	**942** :	878	879	1066	1520
883 :	1	407	953	1939	**943** :	292	293	1067	1829
884 :	27	759	954	1631	**944** :	880	1006	1078	1629
885 :	826	916	954	1666	**945** :	745	881	1085	1203
886 :	276	346	956	1552	**946** :	95	1074	1087	1088
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892 :	277	278	969	1403	**952** :	295	882	1101	1765
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898 :	280	853	978	1787	**958** :	114	135	1112	1115
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981 :	141	305	1162	1399
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998 :	165	820	1202	1941
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1967 :	794	1966	1968
1968 :	367	1967	1969
1969 :	389	1968	1970
1970 :	101	1239	1969
1971 :	475	1239	1972
1972 :	48	353	1971
1973 :	985	1177	1974
1974 :	402	1240	1973
1975 :	195	1240	1976
1976 :	43	1241	1975
1977 :	1227	1241	1978
1978 :	1222	1977	1979
1979 :	899	1978	1980
1980 :	15	1979	1981
1981 :	1140	1242	1980
1982 :	921	1242	1243
1983 :	477	1243	1244
1984 :	171	503	1244
1985 :	371	503	1986
1986 :	42	1985	1987
1987 :	115	504	1986
1988 :	501	504	1184
1989 :	46	838	1245
1990 :	104	1245	1991
1991 :	585	1990	1992
1992 :	1127	1246	1991
1993 :	1163	1246	1994
1994 :	470	1993	1995
1995 :	5	1171	1994
1996 :	802	1219	1997
1997 :	245	1996	1998
1998 :	170	175	1997
1999 :	738	1137	
2000 :	1135	1792	

A.6.8 Hamiltonian cycle for 2000-node graph

The Hamiltonian cycle that we found using the Wedged-MIP Heuristic for 2000-node graph is shown below. This Hamiltonian cycle is the one shown in Figure A.3.

1 → 883 → 1939 → 1940 → 863 → 834 → 820 → 998 → 1202 → 1799 → 710
→ 711 → 1800 → 1801 → 1238 → 1964 → 1237 → 1963 → 1962 → 1961 → 1960
→ 789 → 788 → 1714 → 1713 → 130 → 1413 → 1414 → 1415 → 162 → 180
→ 1344 → 1046 → 1840 → 1212 → 357 → 1349 → 399 → 1000 → 1208 → 1828
→ 903 → 887 → 1946 → 1947 → 1948 → 1949 → 1950 → 343 → 686 → 685
→ 773 → 1725 → 701 → 700 → 1726 → 801 → 321 → 411 → 1378 → 1065
→ 1463 → 1462 → 46 → 1461 → 1460 → 1459 → 1098 → 1854 → 493 → 1937
→ 1938 → 904 → 550 → 549 → 1094 → 1500 → 429 → 766 → 316 → 617
→ 1085 → 1437 → 390 → 1275 → 107 → 546 → 64 → 688 → 1519 → 717
→ 63 → 1102 → 953 → 1476 → 1475 → 844 → 882 → 89 → 1891 → 1892
→ 1893 → 151 → 414 → 1852 → 1152 → 1637 → 360 → 544 → 191 → 190
→ 471 → 1859 → 1216 → 1566 → 442 → 1679 → 1678 → 1677 → 895 → 974
→ 1507 → 338 → 665 → 85 → 545 → 1803 → 1804 → 1805 → 501 → 1922
→ 1229 → 186 → 209 → 583 → 1401 → 1400 → 1399 → 981 → 1162 → 1655
→ 1125 → 1538 → 1149 → 1623 → 444 → 55 → 523 → 687 → 233 → 332
→ 1095 → 1370 → 1369 → 404 → 65 → 755 → 762 → 763 → 765 → 678
→ 676 → 236 → 679 → 1659 → 680 → 681 → 732 → 494 → 768 → 1037
→ 1474 → 1101 → 952 → 1765 → 166 → 1935 → 1934 → 1933 → 1231 → 1292
→ 604 → 214 → 182 → 8 → 1108 → 1491 → 428 → 633 → 334 → 1109
→ 1493 → 87 → 825 → 841 → 311 → 1010 → 1549 → 642 → 235 → 697
→ 698 → 1279 → 378 → 938 → 1058 → 37 → 1453 → 368 → 1264 → 1017
→ 1265 → 369 → 452 → 1872 → 113 → 1302 → 1301 → 1028 → 709 → 118
→ 551 → 900 → 991 → 1316 → 389 → 1969 → 1970 → 1239 → 1971 → 1972
→ 353 → 985 → 1168 → 984 → 901 → 796 → 70 → 213 → 602 → 603
→ 342 → 727 → 728 → 1856 → 1196 → 1775 → 1774 → 1195 → 1773 → 306
→ 58 → 594 → 595 → 593 → 333 → 510 → 53 → 54 → 515 → 1258
→ 104 → 1990 → 1245 → 1989 → 838 → 503 → 1985 → 1986 → 1987 → 115

→ 547 → 548 → 1297 → 110 → 933 → 1340 → 629 → 117 → 1526 → 1123
→ 961 → 299 → 1055 → 1169 → 1850 → 1214 → 28 → 1744 → 1189 → 1640
→ 874 → 935 → 1050 → 1553 → 1131 → 2 → 1542 → 165 → 1898 → 1897
→ 1896 → 1895 → 509 → 195 → 1975 → 1976 → 1241 → 1977 → 1227 → 1911
→ 1912 → 172 → 539 → 20 → 949 → 1732 → 1076 → 1421 → 1420 → 105
→ 1268 → 372 → 1364 → 1054 → 1323 → 1322 → 44 → 1715 → 1716 → 1717
→ 1181 → 1729 → 620 → 280 → 1882 → 1883 → 1221 → 98 → 591 → 592
→ 876 → 1319 → 391 → 1449 → 154 → 867 → 1027 → 1300 → 383 → 1579
→ 4 → 999 → 1685 → 690 → 284 → 1686 → 466 → 1687 → 516 → 144
→ 1600 → 1599 → 1598 → 291 → 940 → 1377 → 123 → 526 → 1926 → 1927
→ 1230 → 5 → 533 → 93 → 461 → 1720 → 1182 → 1383 → 406 → 1384
→ 1385 → 407 → 1551 → 1130 → 1552 → 886 → 956 → 388 → 1312 → 1034
→ 967 → 1810 → 1192 → 1763 → 273 → 335 → 1247 → 100 → 245 → 722
→ 721 → 751 → 752 → 1878 → 1879 → 1880 → 421 → 1467 → 1466 → 1465
→ 1464 → 1093 → 1451 → 1450 → 1092 → 1556 → 1557 → 1133 → 1809 → 460
→ 1654 → 1161 → 1831 → 950 → 636 → 99 → 1310 → 925 → 1033 → 1311
→ 473 → 1733 → 1185 → 1734 → 1186 → 1288 → 109 → 1091 → 1448 → 270
→ 352 → 1290 → 1289 → 30 → 1253 → 136 → 1481 → 1480 → 424 → 1479
→ 1478 → 1477 → 3 → 1531 → 1532 → 896 → 77 → 40 → 780 → 1954
→ 1235 → 970 → 1138 → 1578 → 400 → 644 → 217 → 803 → 1951 → 1032
→ 1309 → 856 → 830 → 1326 → 1325 → 1324 → 325 → 15 → 1698 → 989
→ 1174 → 1697 → 1696 → 843 → 826 → 264 → 111 → 1520 → 317 → 1035
→ 726 → 725 → 248 → 719 → 351 → 1888 → 1887 → 1886 → 96 → 683
→ 1661 → 1662 → 664 → 540 → 155 → 1671 → 1670 → 1166 → 983 → 1669
→ 1064 → 1376 → 1063 → 1755 → 1756 → 1190 → 1757 → 1191 → 1758 → 443
→ 219 → 654 → 220 → 973 → 1146 → 1611 → 764 → 249 → 269 → 274
→ 1643 → 1155 → 1642 → 1156 → 908 → 859 → 730 → 729 → 371 → 1267
→ 1266 → 35 → 1731 → 1730 → 472 → 706 → 289 → 740 → 1492 → 931
→ 873 → 1580 → 1139 → 1363 → 947 → 1088 → 1591 → 1592 → 1593 → 143
→ 1857 → 1858 → 1115 → 1505 → 877 → 941 → 41 → 1554 → 1555 → 141
→ 208 → 51 → 69 → 791 → 1574 → 1575 → 1137 → 1999 → 738 → 739

→ 246 → 782 → 158 → 1781 → 1197 → 1780 → 1779 → 968 → 27 → 747
→ 1877 → 749 → 750 → 714 → 84 → 1394 → 409 → 1603 → 1602 → 1601
→ 446 → 1647 → 1158 → 978 → 1648 → 1649 → 1159 → 1909 → 492 → 1853
→ 240 → 708 → 1770 → 131 → 1073 → 1411 → 412 → 210 → 597 → 598
→ 60 → 696 → 1741 → 462 → 1667 → 374 → 586 → 1931 → 1932 → 804
→ 813 → 1690 → 1689 → 1688 → 467 → 267 → 1485 → 1486 → 871 → 839
→ 1834 → 38 → 1473 → 995 → 907 → 1011 → 1472 → 275 → 176 → 263
→ 824 → 840 → 1845 → 1844 → 758 → 754 → 1524 → 932 → 80 → 833
→ 1021 → 1337 → 1044 → 349 → 1336 → 1042 → 929 → 1263 → 68 → 187
→ 22 → 181 → 193 → 506 → 147 → 1613 → 1043 → 1147 → 1614 → 221
→ 615 → 1210 → 1881 → 478 → 1754 → 1753 → 455 → 189 → 1702 → 1703
→ 160 → 656 → 1711 → 1712 → 448 → 1607 → 1606 → 1605 → 401 → 184
→ 1550 → 1129 → 694 → 695 → 1740 → 1739 → 1187 → 1738 → 993 → 259
→ 393 → 1280 → 1281 → 948 → 112 → 1299 → 1026 → 1298 → 382 → 1862
→ 1863 → 1864 → 770 → 769 → 767 → 937 → 875 → 842 → 13 → 1404
→ 1405 → 1406 → 1407 → 1408 → 1409 → 323 → 302 → 1389 → 1390 → 1391
→ 408 → 185 → 39 → 702 → 168 → 1771 → 1772 → 480 → 1287 → 124
→ 1251 → 1013 → 570 → 571 → 370 → 522 → 198 → 422 → 1470 → 1471
→ 459 → 799 → 860 → 403 → 1952 → 1234 → 1953 → 174 → 1925 → 1924
→ 1923 → 341 → 577 → 304 → 1919 → 499 → 1918 → 1917 → 1056 → 1367
→ 7 → 505 → 1822 → 1207 → 992 → 308 → 1118 → 1518 → 1517 → 821
→ 808 → 746 → 320 → 745 → 945 → 881 → 1955 → 83 → 797 → 1179
→ 1708 → 1707 → 1178 → 1706 → 1705 → 256 → 234 → 517 → 88 → 569
→ 641 → 640 → 639 → 296 → 955 → 1236 → 1958 → 812 → 606 → 475
→ 1176 → 1701 → 173 → 1905 → 954 → 1103 → 1482 → 1483 → 425 → 1484
→ 975 → 735 → 737 → 1829 → 943 → 292 → 179 → 939 → 1315 → 753
→ 756 → 759 → 884 → 1631 → 1632 → 436 → 1536 → 1537 → 1164 → 1664
→ 1663 → 601 → 535 → 536 → 1295 → 1296 → 928 → 870 → 1282 → 1283
→ 9 → 1014 → 1306 → 149 → 1683 → 159 → 1194 → 1769 → 1148 → 10
→ 231 → 1366 → 1365 → 980 → 125 → 1381 → 1382 → 1066 → 1913 → 1228
→ 11 → 507 → 329 → 957 → 297 → 508 → 744 → 743 → 227 → 632

→ 1508 → 139 → 537 → 538 → 1167 → 307 → 624 → 626 → 1330 → 203
→ 56 → 564 → 562 → 437 → 625 → 627 → 623 → 622 → 285 → 919
→ 1276 → 587 → 286 → 922 → 1106 → 1875 → 1874 → 1220 → 1873 → 497
→ 336 → 631 → 630 → 340 → 1841 → 1842 → 482 → 682 → 122 → 1375
→ 1062 → 1786 → 1787 → 898 → 853 → 433 → 512 → 67 → 1371 → 1372
→ 103 → 1254 → 31 → 1869 → 1218 → 1868 → 1217 → 358 → 1501 → 1502
→ 971 → 1140 → 1582 → 1583 → 1128 → 439 → 1546 → 438 → 350 → 252
→ 784 → 1722 → 810 → 447 → 1604 → 1145 → 1694 → 1695 → 397 → 183
→ 1521 → 1119 → 1522 → 1120 → 1523 → 1016 → 86 → 242 → 61 → 1079
→ 1833 → 817 → 261 → 92 → 81 → 1328 → 1329 → 563 → 175 → 1966
→ 1965 → 303 → 613 → 413 → 1412 → 82 → 251 → 783 → 781 → 496
→ 1876 → 384 → 97 → 1533 → 417 → 102 → 621 → 1260 → 365 → 637
→ 1792 → 2000 → 1135 → 1567 → 1009 → 914 → 18 → 578 → 207 → 1022
→ 920 → 866 → 1610 → 1609 → 1608 → 449 → 43 → 511 → 1255 → 363
→ 1379 → 405 → 222 → 1435 → 1436 → 95 → 585 → 1991 → 1992 → 1246
→ 1993 → 1163 → 1658 → 675 → 468 → 1691 → 1171 → 1995 → 1994 → 470
→ 1721 → 232 → 610 → 1452 → 129 → 1410 → 1072 → 322 → 1539 → 1540
→ 441 → 1565 → 440 → 1910 → 979 → 319 → 1052 → 1359 → 1360 → 1361
→ 277 → 655 → 1069 → 1396 → 1397 → 1070 → 609 → 608 → 75 → 19
→ 72 → 618 → 619 → 559 → 558 → 561 → 990 → 1327 → 394 → 1597
→ 1144 → 346 → 1764 → 806 → 818 → 832 → 819 → 790 → 21 → 579
→ 986 → 811 → 326 → 1348 → 119 → 590 → 247 → 524 → 1269 → 106
→ 525 → 720 → 244 → 643 → 1561 → 1121 → 960 → 1562 → 1563 → 1134
→ 1564 → 965 → 1127 → 1544 → 1545 → 469 → 416 → 1430 → 1429 → 1428
→ 1427 → 581 → 6 → 518 → 521 → 226 → 1652 → 1653 → 150 → 1392
→ 1224 → 1901 → 1900 → 1899 → 761 → 114 → 1303 → 1029 → 1304 → 1030
→ 1305 → 385 → 653 → 1584 → 616 → 215 → 266 → 574 → 1351 → 260
→ 815 → 736 → 734 → 239 → 704 → 707 → 705 → 1433 → 1082 → 1434
→ 1083 → 1666 → 885 → 916 → 1053 → 1362 → 137 → 1494 → 1495 → 1496
→ 1110 → 827 → 849 → 893 → 1710 → 1709 → 1057 → 1368 → 33 → 262
→ 1332 → 59 → 576 → 481 → 1783 → 1784 → 1200 → 1808 → 169 → 1906

→ 1907 → 1225 → 1908 → 1226 → 453 → 1622 → 153 → 94 → 295 → 79
→ 1612 → 1047 → 1346 → 1345 → 519 → 520 → 560 → 1342 → 1343 → 91
→ 607 → 605 → 347 → 580 → 1077 → 1672 → 1673 → 330 → 996 → 1347
→ 891 → 848 → 356 → 1830 → 1099 → 1469 → 1468 → 163 → 1737 → 309
→ 923 → 1660 → 897 → 852 → 1914 → 479 → 1761 → 474 → 699 → 1742
→ 1188 → 1743 → 164 → 250 → 1270 → 1018 → 1271 → 1019 → 1272 → 375
→ 1548 → 915 → 78 → 26 → 1314 → 271 → 748 → 1682 → 465 → 1398
→ 661 → 659 → 32 → 1921 → 1920 → 257 → 243 → 1838 → 1211 → 1768
→ 1767 → 1142 → 1585 → 1223 → 1894 → 434 → 1530 → 1124 → 1793 → 1794
→ 795 → 798 → 802 → 34 → 1250 → 362 → 313 → 774 → 1941 → 918
→ 1020 → 1273 → 837 → 483 → 1107 → 1490 → 427 → 934 → 1049 → 1353
→ 495 → 1865 → 1866 → 140 → 733 → 741 → 1426 → 132 → 628 → 1443
→ 966 → 1132 → 1902 → 1903 → 1904 → 912 → 188 → 192 → 703 → 1249
→ 855 → 693 → 692 → 612 → 101 → 1248 → 361 → 1262 → 45 → 1806
→ 1807 → 484 → 1930 → 502 → 1402 → 1403 → 134 → 1511 → 1512 → 432
→ 582 → 1431 → 1080 → 1570 → 1571 → 1572 → 997 → 1201 → 1785 → 445
→ 1594 → 1595 → 1596 → 793 → 794 → 1967 → 1968 → 367 → 488 → 1826
→ 1825 → 963 → 888 → 846 → 1386 → 74 → 862 → 1487 → 426 → 1488
→ 1489 → 1084 → 962 → 1126 → 1824 → 1823 → 486 → 614 → 552 → 554
→ 553 → 718 → 1839 → 487 → 318 → 1039 → 927 → 288 → 936 → 959
→ 298 → 1116 → 1510 → 1117 → 1778 → 1777 → 1776 → 1114 → 1504 → 1503
→ 850 → 828 → 814 → 223 → 663 → 1354 → 760 → 757 → 290 → 658
→ 1615 → 148 → 1766 → 1193 → 1870 → 1219 → 1996 → 1997 → 1998 → 170
→ 1795 → 1204 → 911 → 1004 → 1846 → 1847 → 1848 → 491 → 339 → 1849
→ 212 → 588 → 1393 → 1068 → 42 → 584 → 634 → 635 → 1419 → 1418
→ 1075 → 1417 → 1416 → 194 → 500 → 1915 → 1916 → 988 → 1173 → 987
→ 29 → 1759 → 1760 → 142 → 1581 → 972 → 254 → 575 → 373 → 1051
→ 1633 → 1634 → 1635 → 1636 → 1151 → 435 → 648 → 649 → 1573 → 477
→ 1983 → 1243 → 1012 → 1547 → 1122 → 1525 → 847 → 890 → 1447 → 1090
→ 1446 → 47 → 1867 → 742 → 337 → 1252 → 1003 → 1215 → 1851 → 331
→ 62 → 713 → 293 → 724 → 723 → 48 → 1388 → 90 → 1097 → 1457

$\rightarrow$ 1096 $\rightarrow$ 1458 $\rightarrow$ 1081 $\rightarrow$ 1432 $\rightarrow$ 589 $\rightarrow$ 476 $\rightarrow$ 489 $\rightarrow$ 1835 $\rightarrow$ 171 $\rightarrow$ 1984
$\rightarrow$ 1244 $\rightarrow$ 1333 $\rightarrow$ 951 $\rightarrow$ 1100 $\rightarrow$ 1527 $\rightarrow$ 1528 $\rightarrow$ 1529 $\rightarrow$ 36 $\rightarrow$ 1442 $\rightarrow$ 418
$\rightarrow$ 647 $\rightarrow$ 646 $\rightarrow$ 218 $\rightarrow$ 645 $\rightarrow$ 145 $\rightarrow$ 1884 $\rightarrow$ 1885 $\rightarrow$ 906 $\rightarrow$ 994 $\rightarrow$ 1509
$\rightarrow$ 673 $\rightarrow$ 674 $\rightarrow$ 228 $\rightarrow$ 1257 $\rightarrow$ 1256 $\rightarrow$ 800 $\rightarrow$ 805 $\rightarrow$ 258 $\rightarrow$ 543 $\rightarrow$ 566
$\rightarrow$ 310 $\rightarrow$ 1001 $\rightarrow$ 567 $\rightarrow$ 204 $\rightarrow$ 542 $\rightarrow$ 1023 $\rightarrow$ 1285 $\rightarrow$ 108 $\rightarrow$ 930 $\rightarrow$ 872
$\rightarrow$ 1959 $\rightarrow$ 785 $\rightarrow$ 253 $\rightarrow$ 787 $\rightarrow$ 786 $\rightarrow$ 73 $\rightarrow$ 854 $\rightarrow$ 899 $\rightarrow$ 982 $\rightarrow$ 423
$\rightarrow$ 315 $\rightarrow$ 1352 $\rightarrow$ 573 $\rightarrow$ 206 $\rightarrow$ 572 $\rightarrow$ 49 $\rightarrow$ 1665 $\rightarrow$ 671 $\rightarrow$ 672 $\rightarrow$ 1657
$\rightarrow$ 1656 $\rightarrow$ 454 $\rightarrow$ 1625 $\rightarrow$ 1624 $\rightarrow$ 431 $\rightarrow$ 1240 $\rightarrow$ 1974 $\rightarrow$ 1973 $\rightarrow$ 1177 $\rightarrow$ 1704
$\rightarrow$ 1175 $\rightarrow$ 1699 $\rightarrow$ 1700 $\rightarrow$ 255 $\rightarrow$ 177 $\rightarrow$ 1261 $\rightarrow$ 1015 $\rightarrow$ 25 $\rightarrow$ 600 $\rightarrow$ 599
$\rightarrow$ 211 $\rightarrow$ 66 $\rightarrow$ 457 $\rightarrow$ 1644 $\rightarrow$ 281 $\rightarrow$ 902 $\rightarrow$ 1024 $\rightarrow$ 1286 $\rightarrow$ 197 $\rightarrow$ 50
$\rightarrow$ 23 $\rightarrow$ 1104 $\rightarrow$ 504 $\rightarrow$ 1988 $\rightarrow$ 1184 $\rightarrow$ 823 $\rightarrow$ 809 $\rightarrow$ 1307 $\rightarrow$ 386 $\rightarrow$ 807
$\rightarrow$ 1278 $\rightarrow$ 1277 $\rightarrow$ 377 $\rightarrow$ 14 $\rightarrow$ 1577 $\rightarrow$ 651 $\rightarrow$ 201 $\rightarrow$ 534 $\rightarrow$ 276 $\rightarrow$ 1203
$\rightarrow$ 1956 $\rightarrow$ 1957 $\rightarrow$ 116 $\rightarrow$ 1008 $\rightarrow$ 146 $\rightarrow$ 229 $\rightarrow$ 556 $\rightarrow$ 557 $\rightarrow$ 1320 $\rightarrow$ 1321
$\rightarrow$ 392 $\rightarrow$ 1078 $\rightarrow$ 1569 $\rightarrow$ 1136 $\rightarrow$ 969 $\rightarrow$ 892 $\rightarrow$ 278 $\rightarrow$ 1871 $\rightarrow$ 1089 $\rightarrow$ 1445
$\rightarrow$ 1444 $\rightarrow$ 127 $\rightarrow$ 1317 $\rightarrow$ 1002 $\rightarrow$ 910 $\rightarrow$ 1576 $\rightarrow$ 348 $\rightarrow$ 1154 $\rightarrow$ 1641 $\rightarrow$ 156
$\rightarrow$ 1837 $\rightarrow$ 359 $\rightarrow$ 1071 $\rightarrow$ 1836 $\rightarrow$ 345 $\rightarrow$ 216 $\rightarrow$ 1331 $\rightarrow$ 565 $\rightarrow$ 12 $\rightarrow$ 638
$\rightarrow$ 402 $\rightarrow$ 1357 $\rightarrow$ 120 $\rightarrow$ 1358 $\rightarrow$ 121 $\rightarrow$ 1380 $\rightarrow$ 660 $\rightarrow$ 379 $\rightarrow$ 1284 $\rightarrow$ 568
$\rightarrow$ 205 $\rightarrow$ 1334 $\rightarrow$ 1040 $\rightarrow$ 1335 $\rightarrow$ 1041 $\rightarrow$ 327 $\rightarrow$ 1086 $\rightarrow$ 1439 $\rightarrow$ 1440 $\rightarrow$ 1441
$\rightarrow$ 1087 $\rightarrow$ 946 $\rightarrow$ 1074 $\rightarrow$ 324 $\rightarrow$ 541 $\rightarrow$ 878 $\rightarrow$ 942 $\rightarrow$ 879 $\rightarrow$ 689 $\rightarrow$ 531
$\rightarrow$ 200 $\rightarrow$ 268 $\rightarrow$ 1674 $\rightarrow$ 1675 $\rightarrow$ 1676 $\rightarrow$ 776 $\rightarrow$ 775 $\rightarrow$ 1724 $\rightarrow$ 1183 $\rightarrow$ 1723
$\rightarrow$ 831 $\rightarrow$ 857 $\rightarrow$ 1684 $\rightarrow$ 1170 $\rightarrow$ 157 $\rightarrow$ 1788 $\rightarrow$ 1007 $\rightarrow$ 57 $\rightarrow$ 611 $\rightarrow$ 364
$\rightarrow$ 1341 $\rightarrow$ 398 $\rightarrow$ 1692 $\rightarrow$ 1693 $\rightarrow$ 1172 $\rightarrow$ 1143 $\rightarrow$ 1590 $\rightarrow$ 381 $\rightarrow$ 1293 $\rightarrow$ 380
$\rightarrow$ 1294 $\rightarrow$ 684 $\rightarrow$ 387 $\rightarrow$ 1747 $\rightarrow$ 1746 $\rightarrow$ 1745 $\rightarrow$ 1005 $\rightarrow$ 913 $\rightarrow$ 889 $\rightarrow$ 1541
$\rightarrow$ 355 $\rightarrow$ 1209 $\rightarrow$ 1832 $\rightarrow$ 1105 $\rightarrow$ 716 $\rightarrow$ 715 $\rightarrow$ 532 $\rightarrow$ 305 $\rightarrow$ 1355 $\rightarrow$ 1356
$\rightarrow$ 415 $\rightarrow$ 1425 $\rightarrow$ 1424 $\rightarrow$ 1423 $\rightarrow$ 1422 $\rightarrow$ 1031 $\rightarrow$ 1308 $\rightarrow$ 924 $\rightarrow$ 868 $\rightarrow$ 1274
$\rightarrow$ 376 $\rightarrow$ 1454 $\rightarrow$ 420 $\rightarrow$ 1455 $\rightarrow$ 1456 $\rightarrow$ 126 $\rightarrow$ 1395 $\rightarrow$ 410 $\rightarrow$ 1438 $\rightarrow$ 133
$\rightarrow$ 1736 $\rightarrow$ 1735 $\rightarrow$ 816 $\rightarrow$ 829 $\rightarrow$ 1513 $\rightarrow$ 1514 $\rightarrow$ 283 $\rightarrow$ 527 $\rightarrow$ 528 $\rightarrow$ 514
$\rightarrow$ 513 $\rightarrow$ 24 $\rightarrow$ 1198 $\rightarrow$ 1782 $\rightarrow$ 1199 $\rightarrow$ 366 $\rightarrow$ 1890 $\rightarrow$ 1889 $\rightarrow$ 1222 $\rightarrow$ 1978
$\rightarrow$ 1979 $\rightarrow$ 1980 $\rightarrow$ 1981 $\rightarrow$ 1242 $\rightarrow$ 1982 $\rightarrow$ 921 $\rightarrow$ 1025 $\rightarrow$ 1291 $\rightarrow$ 792 $\rightarrow$ 294
$\rightarrow$ 1942 $\rightarrow$ 1233 $\rightarrow$ 1943 $\rightarrow$ 1944 $\rightarrow$ 772 $\rightarrow$ 771 $\rightarrow$ 498 $\rightarrow$ 1945 $\rightarrow$ 178 $\rightarrow$ 17
$\rightarrow$ 657 $\rightarrow$ 1048 $\rightarrow$ 1350 $\rightarrow$ 666 $\rightarrow$ 667 $\rightarrow$ 224 $\rightarrow$ 1626 $\rightarrow$ 1150 $\rightarrow$ 1627 $\rightarrow$ 1628

$\rightarrow 1629 \rightarrow 1630 \rightarrow 287 \rightarrow 926 \rightarrow 1789 \rightarrow 1790 \rightarrow 1791 \rightarrow 458 \rightarrow 1645 \rightarrow 977$
$\rightarrow 1157 \rightarrow 1646 \rightarrow 272 \rightarrow 490 \rightarrow 1843 \rightarrow 1213 \rightarrow 1516 \rightarrow 1515 \rightarrow 835 \rightarrow 864$
$\rightarrow 917 \rightarrow 1180 \rightarrow 1802 \rightarrow 241 \rightarrow 712 \rightarrow 1815 \rightarrow 1816 \rightarrow 138 \rightarrow 1497 \rightarrow 128$
$\rightarrow 71 \rightarrow 237 \rightarrow 202 \rightarrow 555 \rightarrow 1719 \rightarrow 161 \rightarrow 691 \rightarrow 1718 \rightarrow 328 \rightarrow 845$
$\rightarrow 1827 \rightarrow 463 \rightarrow 1558 \rightarrow 1559 \rightarrow 1560 \rightarrow 430 \rightarrow 1506 \rightarrow 135 \rightarrow 958 \rightarrow 1112$
$\rightarrow 1498 \rightarrow 1111 \rightarrow 1499 \rightarrow 1113 \rightarrow 1762 \rightarrow 396 \rightarrow 1339 \rightarrow 1045 \rightarrow 1338 \rightarrow 395$
$\rightarrow 1617 \rightarrow 1618 \rightarrow 1619 \rightarrow 1620 \rightarrow 451 \rightarrow 662 \rightarrow 1621 \rightarrow 152 \rightarrow 344 \rightarrow 1141$
$\rightarrow 1616 \rightarrow 450 \rightarrow 1727 \rightarrow 1728 \rightarrow 905 \rightarrow 858 \rightarrow 1748 \rightarrow 1749 \rightarrow 1750 \rightarrow 1751$
$\rightarrow 1752 \rightarrow 869 \rightarrow 677 \rightarrow 230 \rightarrow 52 \rightarrow 1668 \rightarrow 1165 \rightarrow 1534 \rightarrow 1535 \rightarrow 1036$
$\rightarrow 1313 \rightarrow 964 \rightarrow 300 \rightarrow 1543 \rightarrow 238 \rightarrow 225 \rightarrow 670 \rightarrow 669 \rightarrow 668 \rightarrow 1651$
$\rightarrow 1650 \rightarrow 1160 \rightarrow 1855 \rightarrow 909 \rightarrow 861 \rightarrow 1259 \rightarrow 314 \rightarrow 731 \rightarrow 282 \rightarrow 456$
$\rightarrow 1639 \rightarrow 1638 \rightarrow 1153 \rightarrow 976 \rightarrow 1796 \rightarrow 1797 \rightarrow 1798 \rightarrow 822 \rightarrow 836 \rightarrow 865$
$\rightarrow 1038 \rightarrow 1318 \rightarrow 279 \rightarrow 894 \rightarrow 1589 \rightarrow 1588 \rightarrow 1587 \rightarrow 1586 \rightarrow 16 \rightarrow 650$
$\rightarrow 1059 \rightarrow 1373 \rightarrow 1060 \rightarrow 1374 \rightarrow 1061 \rightarrow 1568 \rightarrow 1006 \rightarrow 944 \rightarrow 880 \rightarrow 76$
$\rightarrow 652 \rightarrow 312 \rightarrow 1929 \rightarrow 1928 \rightarrow 167 \rightarrow 301 \rightarrow 596 \rightarrow 419 \rightarrow 265 \rightarrow 1817$
$\rightarrow 1818 \rightarrow 1819 \rightarrow 1820 \rightarrow 1821 \rightarrow 354 \rightarrow 1205 \rightarrow 1811 \rightarrow 1812 \rightarrow 1813 \rightarrow 1206$
$\rightarrow 1814 \rightarrow 485 \rightarrow 199 \rightarrow 530 \rightarrow 529 \rightarrow 1936 \rightarrow 1232 \rightarrow 1860 \rightarrow 1861 \rightarrow 464$
$\rightarrow 1680 \rightarrow 1681 \rightarrow 851 \rightarrow 777 \rightarrow 779 \rightarrow 778 \rightarrow 1067 \rightarrow 1387 \rightarrow 196 \rightarrow 1$

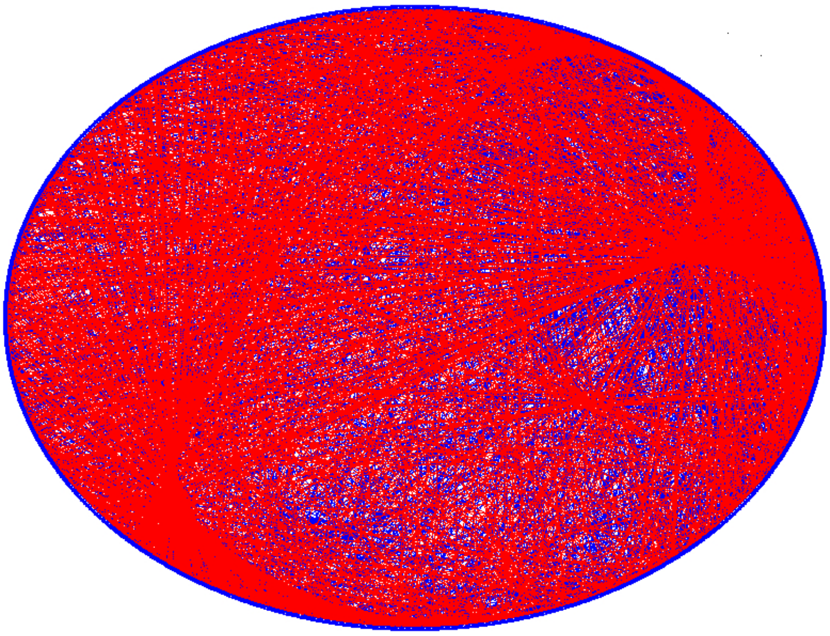

Figure A.3: Solution to 2000-node graph (Hamiltonian cycle in red).

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