HyKKT: A Hybrid Direct and Iterative Method for Solving KKT Linear Systems

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ECP
EXASCALE COMPUTING PROJECT

General Sparse NLPs

Sparse NLP formulation supports sparse optimization problems, requires Hessians of objective and constraints in addition to gradients

$$
\begin{array}{lcll}
 & \min\limits_{x\in\mathbb{R}^n} & f(x) & \\
 & \text{s.t.} & c(x) = c_E & [y] \\
[y_{d,l}] & & d_l \le d(x) \le d_u & [y_{d,u}] \\
[z_l] & & x_l \le x \le x_u & [z_u]
\end{array}
$$

- Assume gradients and sparse Hessians are available
- Quantities insides brackets are Lagrange multipliers for the constraints
- For infinite bounds, multiplier is 0

Model Requirements

D1 objective and constraint functions $f(x)$, $c(x)$, $d(x)$

D2 first derivatives: $\nabla f(x)$, $J_c(x) = \nabla c(x)$, $J_d(x) = \nabla d(x)$

D3 Hessian of the Lagrangian

$$\nabla^2 L(x) = \nabla^2 f(x) + \sum_i y_{c,i} \nabla^2 c_i(x) + \sum_i y_{d,i} \nabla^2 d_i(x)$$

D4 simple bounds x_l and x_u, inequality bounds d_l and d_u, and rhs c_E of equality constraints

Motivation

- Out of the box GPU solvers do not work well on these problems
- KLU + cuSolver works but is proprietary, only works on NVIDIA GPUs
- Want a solver that allows substantial speedup on GPUs
- Using a Cholesky solver instead of LBL^T would allow parallelization and GPU utilization, but the problem is indefinite

Test case	Size	NNZ	MA57 reference CPU only	SuperLU (ECP – LBNL)		STRUMPACK (ECP – LBNL)		KLU + cuSolver (NVIDIA)		SSIDS (STFC, UK Gov.)	
				CPU	GPU	CPU	GPU	CPU	GPU	CPU	GPU
10k-bus	238,072	1,111,991	0.54s	4.06s	4.95s	2.82s	3.71s	0.81s	0.25s*	2.40s	4.76s
70k-bus	1,640,411	7,671,693	5.30s	30.46s	35.58s	24.4s	26.8s	13.26s	3.26s*	32.25s	197.66s

* *Total computational cost of symbolic factorization amortized over 5 solves, i.e. assumed 1 symbolic factorization can be reused over 5 optimization solver iterations.*

K. Świrydowicz et al. (2021) Linear solvers for power grid optimization problems: a review of GPU-accelerated linear solvers

Problem Setup

Interior method, used to solve KKT systems, generates series of linear systems $K_k \Delta x_k = r_k$:

$$\begin{bmatrix} H + D_x & 0 & J_c^T & J_d^T \\ 0 & D_s & 0 & -I \\ J_c & 0 & 0 & 0 \\ J_d & -I & 0 & 0 \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta s \\ \Delta y \\ \Delta y_d \end{bmatrix} = \begin{bmatrix} \tilde{r}_x \\ r_s \\ r_{yc} \\ r_{yd} \end{bmatrix}$$

- J_c and J_d - sparse Jacobians for equality and inequality constraints
- H - sparse Hessian matrix
- Diagonal D_x arises from primal variables x in log-barrier function
- Diagonal D_s arises from slack variables s in log-barrier function

Simplifying the Problem

Eliminating $\Delta s = J_d \Delta x - r_{yd}$ and $\Delta y_d = D_s \Delta s - r_d$ gives

$$\begin{bmatrix} \widetilde{H} & J_c^T \\ J_c & 0 \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta y \end{bmatrix} = \begin{bmatrix} r_x \\ r_{yc} \end{bmatrix}, \qquad \widetilde{H} \equiv H + D_x + J_d^T D_s J_d,$$

where $r_x = \tilde{r}_x + J_d^T (D_s r_{yd} + r_d)$. Gaussian elimination with pivot $\begin{bmatrix} D_s & -I \\ -I & \end{bmatrix}$.

- We need to perform Ruiz Scaling on $\widetilde{H}$ and J_c so we can judge the sizes of the entries in the blocks

C. Petra et al. (2009) A computational study of the use of an optimization-based method for simulating large multibody systems
D. Ruiz (2001) A scaling algorithm to equilibrate both rows and columns norms in matrices

Schur Complement System

The KKT system is equivalent to

$$\begin{bmatrix} H_\gamma & J_c^T \\ J_c & 0 \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta y \end{bmatrix} = \begin{bmatrix} \widehat{r}_x \\ r_{yc} \end{bmatrix}, \qquad H_\gamma = \widetilde{H} + \gamma J_c^T J_c, \qquad \widehat{r}_x = r_x + \gamma J_c^T r_{yc}$$

- $\gamma > 0$ makes the system more SPD (increases the eigenvalues)
- If H_γ or whole system are poorly conditioned, only option may be to ignore the block structure and use an LBL^T factorization
- Sparse Cholesky on H_γ and CG on its Schur complement S:

$$S\Delta y = J_c H_\gamma^{-1} \widehat{r}_x - r_{yc}, \qquad S = J_c H_\gamma^{-1} J_c^T$$

$$H_\gamma \Delta x = \widehat{r}_x - J_c^T \Delta y$$

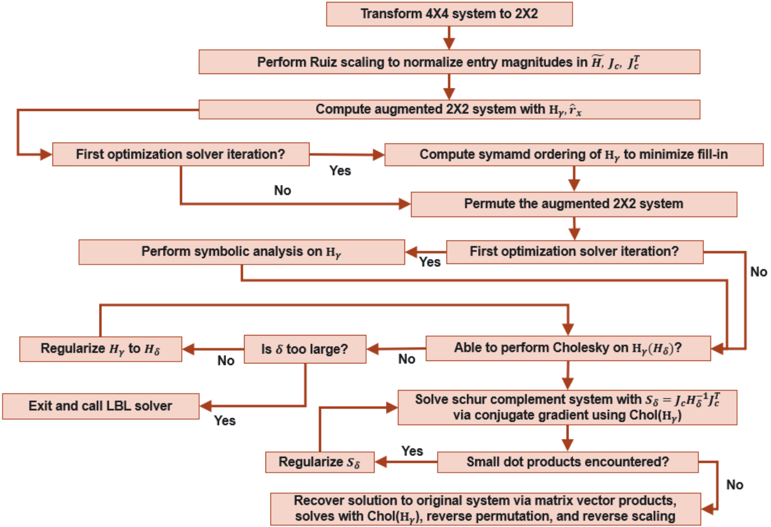
G. H. Golub and C. Greif (2003) On solving block-structured indefinite linear systems

Convergence Theorems

Reminder: $\widetilde{H} \equiv H + D_x + J_d^T D_s J_d, \qquad H_\gamma = \widetilde{H} + \gamma J_c^T J_c$

- For large γ and full-rank J_c, $\widetilde{H}$ is PD on null(J_c) iff H_γ is uniformly PD (required at optimization problem solution).
- HyKKT provides descent direction to interior method (for large γ)
- If $\widetilde{H}$ is positive definite on null$(J_c^T J_c)$, $\exists\gamma_{\text{max}}$ such that for $\gamma \geq \gamma_{\text{max}}$, $\kappa(H_\gamma)$ increases linearly with γ.
- For large enough γ and $C \equiv 1/\gamma \left(J_c \widetilde{H}^{-1} J_c^T\right)^{-1}$, $S_\gamma \equiv \gamma S = \gamma J_c H_\gamma^{-1} J_c^T = \sum_{k=0}^{\infty} (-1)^k C^k = I - C + O\left(\frac{1}{\gamma^2}\right) = I + O\left(\frac{1}{\gamma}\right)$.

HyKKT Workflow



Preliminary Results With Solver Prototype

- **RR** for $Ax = b$: $\frac{\|Ax-b\|}{\|b\|}$
- **BE**: $\frac{\|Ax-b\|}{\|A\|\|x\|+\|b\|}$, with $\|A\|_\infty \approx \|A\|$
- 5/6 matrix series (NLPs at different iterations of interior method) solved efficiently and accurately (other needed $O(1)$ regularization)
- BE consistently $< 10^{-8}$
- Average CG iterations < 20.
- δ_{min} in the range 10^{-8} down to 10^{-10} is reasonable for any $\gamma \leq 10^8$
- (1) refers to the 4×4 system, (2) refers to the 2×2 system

Jonathan Maack and Shrirang Abhyankar (2020) ACOPF sparse linear solver test suite, https://github.com/NREL/opf_matrices

US Eastern Interconnection Grid

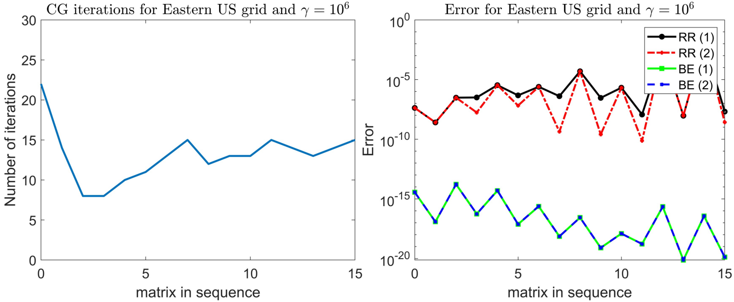


Figure: (Left) CG iterations on S with $\gamma = 10^6$. Mean number of iterations is 13.1. (Right) Various errors for $\gamma = 10^6$. BE $< 10^{-14}$.

Comparison with LBL^T: Factorization Density

Table: Dimensions, number of nonzeros, and factorization densities (average number of nonzeros in the factors per row) for solving full system directly with LBL^Tvia MA57 with pivot tolerance 0.01 (n_L, nnz_L, ρ_L) and solving systems with H_γ with Cholesky (n_C, nnz_C, ρ_C)

Abbreviation	n_L	nnz_L	ρ_L	n_C	nnz_C	ρ_C
Illinois	4.64K	94.7K	**20.4**	2.28K	34.9K	**15.3**
Texas	55.7K	2.95M	**52.9**	25.9K	645K	**24.9**
Western US	238K	10.7M	**44.8**	116K	2.23M	**19.2**
Eastern US	1.64M	85.4M	**52.1**	794K	17.7M	**22.3**

Comparison with LBL^T: Run Time (Preliminary)

Table: Times (in seconds) for solving full system directly on a CPU with LBL^T(via MA57) or HyKKT on a GPU. CG is solved to tolerance of 10^{-12}. All runs are on x86_64 CPUs and A100 GPUs. As the problems grow larger, HyKKT outperforms MA57 by an increasing factor.

Abbreviation	MA57	HyKKT	Relative size	**MA57/HyKKT**
Illinois	$6.24 \cdot 10^{-3}$	$1.01 \cdot 10^{-2}$	1	**0.62**
Texas	$1.00 \cdot 10^{-1}$	$1.04 \cdot 10^{-1}$	10	**1.04**
Western US	$3.38 \cdot 10^{-1}$	$1.46 \cdot 10^{-1}$	50	**2.32**
Eastern US	$3.48 \cdot 10^{0}$	$3.31 \cdot 10^{-1}$	350	**10.5**

Duff (2004)
Chen, Davis, Hager, and Rajamanickam (2008)

Summary

- We designed a linear solver strategy suitable for fine-grain parallelization and deployment on hardware accelerators
- We prove fast CG, holds in practice
- The iterative nature of the solver provides more flexibility to balance trade-offs between accuracy and performance
- Cholesky instead of LBL^T allows for better GPU utilization
- Non-optimized HyKKT outperforms `MA57` by $10x$ on largest problems tested