

# Algorithm NCL for constrained optimization

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## Abstract

Standard optimization solvers have difficulty if too many constraints are essentially active at a solution. For example, problems of the form

$$\min f(x) \quad \text{st} \quad c(x) \geq 0 \quad (m \text{ constraints and } n \text{ variables})$$

may have more than  $n$  constraints active at a solution. Such problems arise in the modeling of tax policy (with perhaps millions of constraints and thousands of variables).

Algorithm NCL solves a sequence of about 10 subproblems with regularized constraints  $c(x) + r \geq 0$  and an augmented Lagrangian objective  $f(x) - y_k^T r + \frac{1}{2} \rho_k r^T r$  that drives the extra variables  $r$  to zero. Interior methods are able to warm start each subproblem. Assuming second derivatives are available, NCL expands the use of interior methods for large-scale optimization.

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# Optimization

UCO

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} \quad \phi(x)$$

- $\phi(x)$  is a smooth nonlinear function
- $\nabla \phi(x)$  known: Quasi-Newton method
- $\nabla^2 \phi(x)$  known: Newton's method

NCO

$$\begin{aligned} &\underset{x \in \mathbb{R}^n}{\text{minimize}} \quad \phi(x) \\ &\text{subject to} \quad c(x) = 0 \end{aligned}$$

- $c(x) \in \mathbb{R}^m$  is a vector of smooth nonlinear functions

# Constrained Optimization

NCO

$$\begin{aligned} & \underset{x \in \mathbb{R}^n}{\text{minimize}} && \phi(x) \\ & \text{subject to} && c(x) = 0 \end{aligned}$$

## Penalty function

$$P(x, \rho_k) = \phi(x) + \frac{1}{2} \rho_k \|c(x)\|^2$$

- Penalty parameter  $\rho_k \rightarrow \infty$

## Augmented Lagrangian

$$L(x, y_k, \rho_k) = \phi(x) - y_k^T c(x) + \frac{1}{2} \rho_k \|c(x)\|^2$$

- Lagrange multiplier estimate  $y_k$        $\rho_k$  can remain finite

# A general optimization problem

## A general optimization problem

NLP

$$\begin{aligned} & \underset{x \in \mathbb{R}^n}{\text{minimize}} && \phi(x) \\ & \text{subject to} && c(x) = 0, \quad \ell \leq x \leq u \end{aligned}$$

- $c(x) = 0$  includes linear constraints  $Ax = b$
- Bounds on the variables  $x$

LANCELOT (1992) solves large-scale optimization problems of this form

- Inequalities  $\bar{\ell} \leq c(x) \leq \bar{u}$  are equalities with more variables and bounds:

NLP

$$\begin{aligned} & \underset{x, s}{\text{minimize}} && \phi(x) \\ & \text{subject to} && c(x) - s = 0, \quad \begin{pmatrix} \ell \\ \bar{\ell} \end{pmatrix} \leq \begin{pmatrix} x \\ s \end{pmatrix} \leq \begin{pmatrix} u \\ \bar{u} \end{pmatrix} \end{aligned}$$

# LANCELOT's BCL algorithm for general NLP

Conn, Gould & Toint (1992)

# LANCELOT

$$\min \phi(x) \quad \text{st} \quad c(x) = 0, \quad \ell \leq x \leq u$$

BCL subproblems (Bound-Constrained augmented Lagrangian):

$$\begin{array}{ll} \text{BC}_k & \underset{x}{\text{minimize}} \quad \phi(x) - y_k^T c(x) + \frac{1}{2} \rho_k \|c(x)\|^2 \\ & \text{subject to} \quad \ell \leq x \leq u \end{array}$$

Loop:

solve $\text{BC}_k$ to get $x_k^*$	decreasing opttol $\omega_k$
if $\ c(x_k^*)\  \leq \eta_k$ , $y_{k+1} \leftarrow y_k - \rho_k c(x_k^*)$	decreasing featol $\eta_k$
else $\rho_{k+1} \leftarrow 10\rho_k$	



# Our optimization problem

## Our NLP problem

NLP	$\begin{aligned} & \underset{x \in \mathbb{R}^n}{\text{minimize}} && \phi(x) \\ & \text{subject to} && c(x) \geq 0, \quad \ell \leq x \leq u \end{aligned}$
-----	---

- $\phi(x)$  is a smooth nonlinear function
- $c(x) \in \mathbb{R}^m$  is a vector of smooth nonlinear functions
- General bounds
- Many inequalities  $c(x) \geq 0$  might not satisfy LICQ at  $x^*$

Example:  $m = 571,000$ ,  $n = 1500$   
10,000 constraints essentially active:  $c_i(x^*) \leq 10^{-6}$

**BCL**

**LCL**

**NCL**

**Sequence of subproblems minimizing  
X-constrained (augmented) Lagrangian**

<b>BCL</b>	LANCELOT	Conn, Gould & Toint (1992)
<b>LCL</b>	linearized constraints	Robinson (1972)
	MINOS	Murtagh and S (1982)
<b>sLCL</b>	KNOSSOS	Friedlander (2002)
<b>NCL</b>	New form of <b>BCL!</b>	Today's talk
	AMPL loop + IPOPT	

# Algorithm NCL for general NLP

## NCL subproblems

NLP

minimize  $\phi(x)$   
 $x, s$

subject to  $c(x) = 0, \quad \ell \leq x \leq u$

## NCL subproblems

NLP

$$\begin{aligned} & \underset{x, s}{\text{minimize}} && \phi(x) \\ & \text{subject to} && c(x) = 0, \quad \ell \leq x \leq u \end{aligned}$$

LANCELOT-type subproblems:

$$\begin{aligned} \text{BC}_k & \underset{x, s}{\text{minimize}} && L(x, y_k, \rho_k) = \phi(x) - y_k^T c(x) + \frac{1}{2} \rho_k \|c(x)\|^2 \\ & \text{subject to} && \ell \leq x \leq u \end{aligned}$$

## NCL subproblems

NLP

$$\begin{aligned} & \underset{x, s}{\text{minimize}} && \phi(x) \\ & \text{subject to} && c(x) = 0, \quad \ell \leq x \leq u \end{aligned}$$

LANCELOT-type subproblems:

$$\begin{aligned} \text{BC}_k & \underset{x, s}{\text{minimize}} && L(x, y_k, \rho_k) = \phi(x) - y_k^T c(x) + \frac{1}{2} \rho_k \|c(x)\|^2 \\ & \text{subject to} && \ell \leq x \leq u \end{aligned}$$

Introduce  $r = -c(x)$ :

$$\begin{aligned} \text{NC}_k & \underset{x, r}{\text{minimize}} && \phi(x) + y_k^T r + \frac{1}{2} \rho_k \|r\|^2 \\ & \text{subject to} && c(x) + r = 0, \quad \ell \leq x \leq u \end{aligned}$$

Free vars  $r$  make the nonlinear constraints independent and feasible IPOPT is happy!



## NCL subproblems

NLP

$$\begin{aligned} & \underset{x, s}{\text{minimize}} && \phi(x) \\ & \text{subject to} && c(x) = 0, \quad \ell \leq x \leq u \end{aligned}$$

NC<sub>k</sub>

$$\begin{aligned} & \underset{x, r}{\text{minimize}} && \phi(x) + y_k^T r + \frac{1}{2} \rho_k \|r\|^2 \\ & \text{subject to} && c(x) + r = 0, \quad \ell \leq x \leq u \end{aligned}$$

Free vars  $r$  make the nonlinear constraints independent and feasible IPOPT is happy!

## NCL subproblems for our problem

NLP

$$\begin{aligned} & \underset{x, s}{\text{minimize}} && \phi(x) \\ & \text{subject to} && c(x) \geq 0, \quad \ell \leq x \leq u \end{aligned}$$

NC<sub>k</sub>

$$\begin{aligned} & \underset{x, r}{\text{minimize}} && \phi(x) + y_k^T r + \frac{1}{2} \rho_k \|r\|^2 \\ & \text{subject to} && c(x) + r \geq 0, \quad \ell \leq x \leq u \end{aligned}$$

Free vars  $r$  make the nonlinear constraints independent and feasible IPOPT is happy!

# Optimal Taxation Policy

# Optimal income taxation with multidimensional taxpayer types

Kenneth L. Judd and Che-Lin Su

Manuscript, Dec 2011



## Optimal tax policy

TAX	maximize <sub>c,y</sub>	$\sum_i \lambda_i U^i(c_i, y_i)$	
	subject to	$U^i(c_i, y_i) - U^i(c_j, y_j) \geq 0$	for all $i, j$
		$\lambda^T(y - c) \geq 0$	
		$c, y \geq 0,$	

where  $c_i$  and  $y_i$  are the consumption and income of taxpayer  $i$ , and  $\lambda$  is a vector of positive weights. The utility functions  $U^i(c_i, y_i)$  are each of the form

$$U(c, y) = \frac{(c - \alpha)^{1-1/\gamma}}{1 - 1/\gamma} - \psi \frac{(y/w)^{1/\eta+1}}{1/\eta + 1},$$

where  $w$  is the wage rate and  $\alpha, \gamma, \psi, \eta$  are taxpayer heterogeneities.

## Optimal tax policy

More precisely,

$$U^{i,j,k,g,h}(c_{p,q,r,s,t}, y_{p,q,r,s,t}) = \frac{(c_{p,q,r,s,t} - \alpha_k)^{1-1/\gamma_h}}{1 - 1/\gamma_h} - \psi_g \frac{(y_{p,q,r,s,t}/w_i)^{1/\eta_j+1}}{1/\eta_j + 1},$$

where  $(i, j, k, g, h)$  and  $(p, q, r, s, t)$  run over 5 dimensions:

*na* wage types  $w$  = 5

*nb* elasticities of labor supply  $\eta$  = 3

*nc* basic need types  $\alpha$  = 3

*nd* levels of distaste for work  $\psi$  = 2

*ne* elasticities of demand for consumption  $\gamma$  = 2

$T = na \times nb \times nc \times nd \times ne = 180$

$m = T(T - 1)$  nonlinear constraints = 32220

$n = 2T$  variables = 360

## AMPL model

$$\begin{array}{ll}
 \text{TAX} & \text{maximize}_{c,y} \quad \sum_i \lambda_i U^i(c_i, y_i) \\
 & \text{subject to} \quad U^i(c_i, y_i) - U^i(c_j, y_j) \geq 0 \quad \text{for all } i, j \\
 & \quad \quad \quad \lambda^T (y - c) \geq 0 \\
 & \quad \quad \quad c, y \geq 0,
 \end{array}$$

Incentive{(i,j,k,g,h) in T, (p,q,r,s,t) in T:

!(i=p and j=q and k=r and g=s and h=t)}:

(c[i,j,k,g,h] - alpha[k])^(1-1/gamma[h]) / (1-1/gamma[h])

- psi[g]\*(y[i,j,k,g,h]/w[i])^mu1[j] / mu1[j]

- (c[p,q,r,s,t] - alpha[k])^(1-1/gamma[h]) / (1-1/gamma[h])

+ psi[g]\*(y[p,q,r,s,t]/w[i])^mu1[j] / mu1[j]

>= 0;

Technology:

sum{(i,j,k,g,h) in T} lambda[i,j,k,g,h]\*(y[i,j,k,g,h] - c[i,j,k,g,h]) >= 0;

## Piecewise-smooth extension

```

Incentive{(i,j,k,g,h) in T, (p,q,r,s,t) in T:
    !(i=p and j=q and k=r and g=s and h=t)}:
  (if c[i,j,k,g,h] - alpha[k] >= epsilon then
    (c[i,j,k,g,h] - alpha[k])^(1-1/gamma[h]) / (1-1/gamma[h])
    - psi[g]*(y[i,j,k,g,h]/w[i])^mu1[j] / mu1[j]
  else
    - 0.5/gamma[h] *epsilon^(-1/gamma[h]-1)*(c[i,j,k,g,h] - alpha[k])^2
    + (1+1/gamma[h])*epsilon^(-1/gamma[h])*(c[i,j,k,g,h] - alpha[k])
    + (1/(1-1/gamma[h]) - 1 - 0.5/gamma[h])*epsilon^(1-1/gamma[h])
    - psi[g]*(y[i,j,k,g,h]/w[i])^mu1[j] / mu1[j]
  )
- (if c[p,q,r,s,t] - alpha[k] >= epsilon then
  ...
) >= 0;

```



# SNOPT on problem TAX

$na, nb, nc, nd, ne = 5, 3, 3, 2, 2$     $m = 32220$     $n = 360$

	Total	Normal	Free	Fixed	Bounded
Rows	32222	32221	1	0	0
Columns	360	0	0	0	360
No. of matrix elements			129600	Density	1.117
Biggest			1.0000E+00	(excluding fixed columns,	
Smallest			0.0000E+00	free rows, and RHS)	
Nonlinear constraints	32220	Linear constraints	2		
Nonlinear variables	360	Linear variables	0		
Jacobian variables	360	Objective variables	360		
Total constraints	32222	Total variables	360		

# SNOPT on problem TAX

Major	Minors	Step	nCon	Feasible	Optimal	MeritFunction	nS	condHz	Penalty			
0	866		1	(3.7E-15)	4.9E-04	4.1745522E+02	4	4.1E+08	1.0E+04	_	r	t
1	503	2.7E-02	6	(3.6E-15)	6.5E-02	4.1746922E+02	24	3.2E+05	1.0E+04	_n	r	t
2	134	1.0E-01	11	(1.4E-07)	2.7E-05	4.1755749E+02	8	2.6E+09	1.8E+06	_s		
3	313	9.8E-02	16	(1.4E-07)	8.9E-05	4.1764438E+02	43	1.0E+07	1.8E+06	_		
4	153	2.8E-02	21	(5.5E-08)	1.8E-04	4.1767129E+02	35	2.2E+04	1.8E+06	_		
5	103	2.2E-02	26	(5.4E-08)	9.5E-04	4.1769616E+02	34	6.7E+07	1.8E+06	_		
6	87	2.1E-02	31	(5.3E-08)	1.2E-03	4.1772079E+02	32	1.6E+08	1.8E+06	_		
7	161	7.3E-03	35	(5.2E-08)	9.7E-04	4.1772930E+02	31	2.4E+05	1.8E+06	_		
8	64	7.3E-03	39	(5.2E-08)	1.1E-03	4.1773783E+02	33	9.7E+05	1.8E+06	_		
9	83	7.2E-03	43	(5.2E-08)	1.2E-03	4.1774637E+02	37	1.9E+07	1.8E+06	_		
10	72	7.2E-03	47	(5.1E-08)	9.9E-04	4.1775484E+02	31	1.3E+08	1.8E+06	_		
99	154	7.2E-03	459	(1.0E-08)	2.7E-05	4.1839776E+02	32	7.9E+06	1.8E+06	_		
100	343	7.2E-03	463	(1.0E-08)	4.9E-03	4.1839867E+02	50	4.3E+07	1.8E+06	_		R
106	413	7.3E-03	496	(1.0E-08)	1.8E-05	4.1840397E+02	17	5.0E+07	1.8E+06	_		
107	630	7.2E-03	500	(1.0E-08)	1.4E-01	1.5496435E+06	6	1.0E+12	1.8E+06	_		it

## SNOPT on problem TAX

Major	Minors	Step	nCon	Feasible	Optimal	MeritFunction	nS	condHz	Penalty		
108	503	5.1E-02	503	(1.0E-08)	3.7E-02	1.2973689E+06	12	2.2E+04	1.8E+06	_	m
109	1805	4.0E-01	506	1.3E-05	7.5E-01	2.3393279E+05	9	4.8E+04	1.8E+06	_	m it
110	16517	2.0E-01	509	1.1E-05	1.0E+00	2.6854996E+05	2	7.5E+03	1.8E+06	_	it
117	175544	1.0E+00	526	1.0E-04	1.0E+00	1.0282166E+09	13	7.6E+07	1.8E+06	_	mr it
118	1681	1.0E+00	528	3.0E-04	1.0E+00	1.7677788E+10	23	1.7E+09	2.9E+06	_	smr it
119	919	1.0E+00	530	2.0E-05	2.4E-02	8.1274014E+07	39	1.1E+06	3.0E+07	_	sm t
194	30811	1.0E+00	795	8.6E-01	9.7E-01	2.8330244E+21	2	1.8E+01	3.5E+13	_	n it
195	1819	1.1E-04	800	8.6E-01	1.0E+00	2.6326936E+22	3	1.4E+02	1.1E+15	_	n R it
195	3314		800	8.6E-01	1.0E+00	2.8661156E+22			1.0E+04	_	n r it
195	4439		800	8.6E-01	9.9E-01	2.8661156E+22			1.0E+04	_	n r it
SNOPTB EXIT 40 -- terminated after numerical difficulties											
SNOPTB INFO 41 -- current point cannot be improved											

## IPOPT on problem TAX

$$na, nb, nc, nd, ne = 5, 3, 3, 2, 2 \quad m = 32220 \quad n = 360$$

This is Ipopt version 3.12.4, running with linear solver mumps.

NOTE: Other linear solvers might be more efficient (see Ipopt documentation).

Number of nonzeros in inequality constraint Jacobian.: 129240

Number of nonzeros in Lagrangian Hessian.....: 360

Total number of variables.....: 360

variables with only lower bounds: 360

Total number of inequality constraints.....: 32221

inequality constraints with only lower bounds: 32221

## IPOPT on problem TAX

iter	objective	inf_pr	inf_du	lg(mu)	d	lg(rg)	alpha_du	alpha_pr	ls
0	-4.1745522e+02	0.00e+00	2.52e+00	-1.0	0.00e+00	-	0.00e+00	0.00e+00	0
1	-4.1734473e+02	6.18e-03	7.36e+00	-1.0	1.34e+00	-	7.69e-01	2.05e-01f	1
2	-4.1682694e+02	4.93e-03	1.78e+01	-1.0	5.48e+00	-	2.23e-01	1.34e-01f	1
3	-4.1656532e+02	4.60e-03	1.66e+02	-1.0	6.95e+00	-	3.06e-01	5.29e-02f	1
4	-4.1553526e+02	3.69e-03	2.13e+02	-1.0	9.40e+00	-	2.38e-01	1.60e-01f	1
5	-4.1470856e+02	3.45e-03	2.96e+02	-1.0	1.14e+01	-	1.65e-01	1.17e-01f	1
6	-4.1433731e+02	3.72e-03	9.79e+02	-1.0	1.30e+01	-	1.73e-01	5.83e-02f	1
7	-4.1433774e+02	3.53e-03	5.22e+03	-1.0	2.47e-02	2.0	5.60e-01	5.64e-02h	1
8	-4.1433988e+02	3.09e-03	5.10e+04	-1.0	3.46e-01	1.5	1.00e+00	1.24e-01h	1
9	-4.1434074e+02	2.15e-03	2.87e+04	-1.0	3.40e-01	1.0	5.03e-01	3.01e-01h	1
10	-4.1428766e+02	1.22e-03	1.50e+04	-1.0	3.01e-01	0.6	4.75e-01	5.39e-01h	1
11	-4.1429091e+02	1.05e-03	1.27e+04	-1.0	2.21e-01	1.0	3.87e-01	1.24e-01h	1
77	-4.0990702e+02	0.00e+00	4.57e-02	-1.0	6.32e-03	-	1.00e+00	1.00e+00h	1
78	-4.0995159e+02	0.00e+00	5.00e+04	-2.5	4.68e+00	-	9.27e-01	1.00e+00f	1

## IPOPT on problem TAX

```

iter    objective    inf_pr    inf_du lg(mu)  ||d||  lg(rg) alpha_du alpha_pr  ls
  88 -4.1227845e+02  0.00e+00  4.45e-03  -2.5  2.55e+00   -   1.00e+00  1.00e+00h  1
  89 -4.1320008e+02  2.97e-03  8.22e+02  -3.8  6.90e+01   -   2.57e-01  4.28e-01f  1
 160 -4.1641067e+02  0.00e+00  1.50e-03  -3.8  1.25e-01   -   1.00e+00  1.00e+00f  1
 161 -4.1646520e+02  8.99e-06  9.47e+00  -5.7  4.36e+00   -   2.62e-01  2.63e-01f  1
 384 -4.1702347e+02  4.14e-07  3.89e+09  -5.7  4.11e-03   0.6  2.59e-01  1.15e-01f  1
 385r-4.1702347e+02  4.14e-07  1.00e+03  -5.4  0.00e+00   4.6  0.00e+00  2.07e-07R  2
 419r-4.1580769e+02  0.00e+00  9.69e-06  -5.4  2.10e-02   -   1.00e+00  1.00e+00h  1
 420r-4.1589722e+02  9.33e-07  2.86e+02  -8.1  1.29e+01   -   1.62e-01  3.97e-01f  1
 449r-4.1630403e+02  1.13e-05  2.79e-05  -8.1  2.92e-01   -   1.00e+00  9.77e-01h  1

```

(scaled)

(unscaled)

```

Objective.....: -4.1630466137535933e+02  -4.1630466137535933e+02
Dual infeasibility.....:  1.1130803588695777e+00  1.1130803588695777e+00
Constraint violation....:  0.0000000000000000e+00  0.0000000000000000e+00
Complementarity.....:  1.3412941119075164e-08  1.3412941119075164e-08
Total CPU secs in IPOPT (w/o function evaluations) = 151.4
Total CPU secs in NLP function evaluations = 65.6

```

# LANCELOT on problem TAX

$na, nb, nc, nd, ne = 5, 3, 3, 2, 2$     $m = 32220$     $n = 360$

k	rhok	etak	omegak	Obj	itns	CGit	TRradius	active
1	1.0e+1	1.0e-1	1.0e-1	-417.455	18	12000	4.1e-01	2831
2	1.0e+1	1.2e-2	1.0e-2	-421.606	39	9000	1.6e-01	2568
3	1.0e+2	7.9e-2	1.0e-2	-421.011	23	11000	2.4e-01	1662
4	1.0e+2	1.3e-3	1.0e-4	-420.188	282	104000	8.6e-02	1444
5	1.0e+3	6.3e-2	1.0e-3	-419.967	134	64000	5.7e-02	1004
6	1.0e+3	1.3e-4	1.0e-6	-419.819	198	156000	3.1e-02	901
7	1.0e+4	5.0e-2	1.0e-4	-419.741	300	308000	3.1e-12	710
8	1.0e+4	1.3e-5	1.0e-6	-419.698	327	623000	5.5e-04	709
9	1.0e+5	4.0e-2	1.0e-5	-419.682	253	724000	4.7e-03	653
10	1.0e+5	1.3e-6	1.0e-6	-419.676	154	1031000	4.2e-11	663
11	1.0e+6	3.2e-2	1.0e-6	...				

1970 iterations, 8 hours CPU on NEOS

# AMPL implementation of NCL



# pTax5Dnclipopt.run

```
reset;  model pTax5Dinitial.run;

reset;  model pTax5Dncl.mod;
        data pTax5Dncl.dat;
        data; var include p5Dinitial.dat;

model;  option solver ipopt;
        option show_stats 1;
        option ipopt_options 'dual_inf_tol=1e-6   max_iter=5000';
```

## pTax5Dnclipopt.run

```
option opt2 $ipopt_options ' warm_start_init_point=yes';

for {K in 1..kmax}
{
  if K == 2 then {option ipopt_options $opt2 ' mu_init=1e-4'};
  if K == 4 then {option ipopt_options $opt2 ' mu_init=1e-5'};
  if K == 6 then {option ipopt_options $opt2 ' mu_init=1e-6'};
  if K == 8 then {option ipopt_options $opt2 ' mu_init=1e-7'};
  if K ==10 then {option ipopt_options $opt2 ' mu_init=1e-8'};

  solve;

  let rmax := max({(i,j,k,g,h) in T, (p,q,r,s,t) in T:
    !(i=p and j=q and k=r and g=s and h=t)} R[i,j,k,g,h,p,q,r,s,t]);
  let rmin := ...
  let rnorm := max(abs(rmax), abs(rmin)); # ||r||_inf
  if rnorm <= rtol then { printf "Stopping: rnorm is small\n"; break; }
```

# pTax5Dnclipopt.run

```

if  $\|r_k^*\| \leq \eta_k$ ,  $y_{k+1} \leftarrow y_k + \rho_k r_k^*$ 

if rnorm <= etak then # update dual estimate dk; save new solution
{let {(i,j,k,g,h) in T, (p,q,r,s,t) in T:
    !(i=p and j=q and k=r and g=s and h=t)}
    dk[i,j,k,g,h,p,q,r,s,t] :=
    dk[i,j,k,g,h,p,q,r,s,t] + rhok*R[i,j,k,g,h,p,q,r,s,t];
let {(i,j,k,g,h) in T} ck[i,j,k,g,h] := c[i,j,k,g,h];
let {(i,j,k,g,h) in T} yk[i,j,k,g,h] := y[i,j,k,g,h];

if etak == etamin then { printf "Stopping: etak = etamin\n"; break; }
let etak := max(etak*etafac, etamin);
}

```

# pTax5Dnclipopt.run

```
else       $\rho_{k+1} \leftarrow 10\rho_k$ 

else      # keep previous solution; increase rhok
{ let {(i,j,k,g,h) in T} c[i,j,k,g,h] := ck[i,j,k,g,h];
  let {(i,j,k,g,h) in T} y[i,j,k,g,h] := yk[i,j,k,g,h];

  if rhok == rhomax then { printf "Stopping: rhok = rhomax\n"; break; }
  let rhok := min(rhok*rhofac, rhomax);
}
} # end main loop
```

# Numerical results

# NCL/IPOPT on problem TAX

$na, nb, nc, nd, ne = 5, 3, 3, 2, 2$     $m = 32220$     $n = 360$

$k$	$\rho_k$	$\eta_k$	$\ r_k^*\ _\infty$	$\phi(x_k^*)$	$\mu\_init$	Itns	Time
1	$10^2$	$10^{-2}$	7.0e-03	-4.2038075e+02	$10^{-1}$	95	41.1
2	$10^2$	$10^{-3}$	4.1e-03	-4.2002898e+02	$10^{-4}$	17	7.2
3	$10^3$	$10^{-3}$	1.3e-03	-4.1986069e+02	$10^{-4}$	20	8.1
4	$10^4$	$10^{-3}$	4.4e-04	-4.1972958e+02	$10^{-4}$	48	25.0
5	$10^4$	$10^{-4}$	2.2e-04	-4.1968646e+02	$10^{-4}$	43	20.5
6	$10^5$	$10^{-4}$	9.8e-05	-4.1967560e+02	$10^{-4}$	64	32.9
7	$10^5$	$10^{-5}$	6.6e-05	-4.1967177e+02	$10^{-4}$	57	26.8
8	$10^6$	$10^{-5}$	4.2e-06	-4.1967150e+02	$10^{-4}$	87	46.2
9	$10^6$	$10^{-6}$	9.4e-07	-4.1967138e+02	$10^{-4}$	96	53.6

527 iterations, 5 mins CPU

# NCL/IPOPT on problem TAX

$na, nb, nc, nd, ne = 5, 3, 3, 2, 2$     $m = 32220$     $n = 360$

$k$	$\rho_k$	$\eta_k$	$\ r_k^*\ _\infty$	$\phi(x_k^*)$	$\mu\_init$	ltns	Time
1	$10^2$	$10^{-2}$	7.0e-03	-4.2038075e+02	$10^{-1}$	95	40.8
2	$10^2$	$10^{-3}$	4.1e-03	-4.2002898e+02	$10^{-4}$	17	7.0
3	$10^3$	$10^{-3}$	1.3e-03	-4.1986069e+02	$10^{-4}$	20	8.5
4	$10^4$	$10^{-3}$	4.4e-04	-4.1972958e+02	$10^{-5}$	57	32.6
5	$10^4$	$10^{-4}$	2.2e-04	-4.1968646e+02	$10^{-5}$	29	14.6
6	$10^5$	$10^{-4}$	9.8e-05	-4.1967560e+02	$10^{-6}$	36	18.7
7	$10^5$	$10^{-5}$	3.9e-05	-4.1967205e+02	$10^{-6}$	35	19.7
8	$10^6$	$10^{-5}$	4.2e-06	-4.1967150e+02	$10^{-7}$	18	7.7
9	$10^6$	$10^{-6}$	9.4e-07	-4.1967138e+02	$10^{-7}$	15	6.8

322 iterations, 3 mins CPU

# NCL/IPOPT on problem TAX

$$na, nb, nc, nd, ne = 5, 3, 3, 2, 2 \quad m = 32220 \quad n = 360$$

Constraints within tol of being active:  $c_i(x) \leq tol$

<i>tol</i>	<i>count</i>	<i>count/n</i>
$10^{-10}$	548	1.5
$10^{-9}$	550	1.5
$10^{-8}$	591	1.6
$10^{-7}$	890	2.5
→ $10^{-6}$	1104	3.1 ←
$10^{-5}$	1225	3.4
$10^{-4}$	1301	3.6
$10^{-3}$	1655	4.6
$10^{-2}$	3483	9.7
$10^{-1}$	10280	28.6

About  $3n$  active constraints



# NCL/KNITRO on problem TAX

$na, nb, nc, nd, ne = 5, 3, 3, 2, 2$   $m = 32220$   $n = 360$

$k$	$\rho_k$	$\eta_k$	$\ r_k^*\ _\infty$	$\phi(x_k^*)$	mu_init	ltns	Time
1	$10^2$	$10^{-2}$	7.0e-03	-4.2038075e+02	$10^{-1}$	168	34.6
2	$10^2$	$10^{-3}$	4.1e-03	-4.2002898e+02	$10^{-4}$	17	3.3
3	$10^3$	$10^{-3}$	1.3e-03	-4.1986068e+02	$10^{-4}$	87	22.8
4	$10^4$	$10^{-3}$	4.2e-04	-4.1972698e+02	$10^{-5}$	4583	2141.9
5	$10^4$	$10^{-4}$	1.7e-04	-4.1968557e+02	$10^{-5}$	63	13.1
6	$10^5$	$10^{-4}$	1.1e-04	-4.1967201e+02	$10^{-6}$	4482	2884.5
7	$10^6$	$10^{-4}$	1.1e-05	-4.1964566e+02	$10^{-6}$	8754	7944.4
8	$10^6$	$10^{-5}$	1.2e-06	-4.1964629e+02	$10^{-7}$	403	194.9
9	$10^6$	$10^{-6}$	7.9e-06	-4.1964298e+02	$10^{-7}$	355	168.7
10	$10^7$	$10^{-6}$	4.8e-07	-4.1964798e+02	$10^{-8}$	7176	10239.7

26088 iterations, 394 mins CPU

## NCL/IPOPT bigger example

$na, nb, nc, nd, ne = 21, 3, 3, 2, 2$   $m = 570780$   $n = 1512$

$k$	$\rho_k$	$\eta_k$	$\ r_k^*\ _\infty$	$\phi(x_k^*)$	mu_init	ltns	Time
1	$10^2$	$10^{-2}$	5.1e-03	-1.7656816e+03	$10^{-1}$	825	7763.3
2	$10^2$	$10^{-3}$	2.4e-03	-1.7648480e+03	$10^{-4}$	66	472.8
3	$10^3$	$10^{-3}$	1.3e-03	-1.7644006e+03	$10^{-4}$	106	771.3
4	$10^4$	$10^{-3}$	3.8e-04	-1.7639491e+03	$10^{-5}$	132	1347.0
5	$10^4$	$10^{-4}$	3.2e-04	-1.7637742e+03	$10^{-5}$	229	2450.9
6	$10^5$	$10^{-4}$	8.6e-05	-1.7636804e+03	$10^{-6}$	104	1096.9
7	$10^5$	$10^{-5}$	4.9e-05	-1.7636469e+03	$10^{-6}$	143	1633.4
8	$10^6$	$10^{-5}$	1.5e-05	-1.7636252e+03	$10^{-7}$	71	786.1
9	$10^7$	$10^{-5}$	2.8e-06	-1.7636196e+03	$10^{-7}$	67	725.7
10	$10^7$	$10^{-6}$	5.1e-07	-1.7636187e+03	$10^{-8}$	18	171.0

1761 iterations, 5 hours CPU

## NCL/IPOPT bigger example

$$na, nb, nc, nd, ne = 21, 3, 3, 2, 2 \quad m = 570780 \quad n = 1512$$

Constraints within tol of being active:  $c_i(x) \leq tol$

<i>tol</i>	<i>count</i>	<i>count/n</i>
$10^{-10}$	3888	2.6
$10^{-9}$	3941	2.6
$10^{-8}$	4430	2.9
$10^{-7}$	7158	4.7
→ $10^{-6}$	10074	6.6 ← $\approx 6.6n$ active constraints
$10^{-5}$	11451	7.6
$10^{-4}$	13109	8.7
$10^{-3}$	23099	15.3
$10^{-2}$	66361	43.9
$10^{-1}$	202664	134.0

## Comparison of IPOPT, KNITRO (via NEOS), NCL

$na = \text{increasing}$     $nb = 3$     $nc = 3$     $nd = 2$     $ne = 2$

$na$	$m$	$n$	IPOPT		KNITRO		NCL/IPOPT	
			itns	time	itns	time	itns	time
5	32220	360	449	217	168	53	322	146
9	104652	648	> 98*	> 360*	928	825	655	1023
11	156420	792	> 87*	$\infty!$	2769	4117	727	1679
17	373933	1224			2598	11447	1021	6347
21	570780	1512					1761	17218

\*duals diverge

MUMPS needs more mem

!Loop

## Comparison of IPOPT, KNITRO (on iMAC), NCL

$na = \text{increasing}$     $nb = 3$     $nc = 3$     $nd = 2$     $ne = 2$

$na$	$m$	$n$	IPOPT		KNITRO		NCL/IPOPT	
			itns	time	itns	time	itns	time
5	32220	360	449	217	736	141	322	146
9	104652	648	> 98*	> 360*	862	630	655	1023
11	156420	792	> 87*	$\infty!$	2835	3719	727	1679
17	373933	1224			3856	14746	1021	6347
21	570780	1512					1761	17218

\*duals diverge

MUMPS needs more mem

!Loop

## Other research

- **M. P. Friedlander and D. Orban**, A primal-dual regularized interior-point method for convex quadratic programs. *Math. Prog. Comp.*, 4(1):71–107, 2012.
- **S. Arreckx and D. Orban**, A regularized factorization-free method for equality-constrained optimization, Technical Report GERAD G-2016-65, GERAD, Montréal, QC, Canada, 2016, doi:10.13140/RG.2.2.20368.00007.
- **P. E. Gill, V. Kungurtsev, and D. P. Robinson**, A stabilized SQP method: global convergence, *IMA J. Numer. Anal.*, 37 (2017), 407–443.
- **P. E. Gill, V. Kungurtsev, and D. P. Robinson**, A stabilized SQP method: superlinear convergence, *Math. Program., Ser. A*, 163 (2017), 369–410.
- **O. Hinder and Y. Ye**, A one-phase IPM for nonconvex optimization, Oliver's MS&E PhD thesis (2018).

**A future possibility**  
**AMPL + IPM + 2nd derivatives**

## KNOSSOS via AMPL + IPM?

Stablized LCL (Friedlander and S, 2005) is equivalent to a BCL method:

$$\begin{array}{ll} \text{ELC}_k & \text{minimize}_x \quad L(x, y_k, \rho_k) + \sigma_k \|\bar{c}_k(x)\|_1 \\ & \text{subject to} \quad \ell \leq x \leq u \end{array}$$

- $\bar{c}_k(x) =$  linear approximation to  $c(x)$  at  $x_k$  (MINOS has very big  $\sigma_k$ )



## KNOSSOS via AMPL + IPM?

Stablized LCL (Friedlander and S, 2005) is equivalent to a BCL method:

$$\begin{array}{ll} \text{ELC}_k & \underset{x}{\text{minimize}} \quad L(x, y_k, \rho_k) + \sigma_k \|\bar{c}_k(x)\|_1 \\ & \text{subject to} \quad \ell \leq x \leq u \end{array}$$

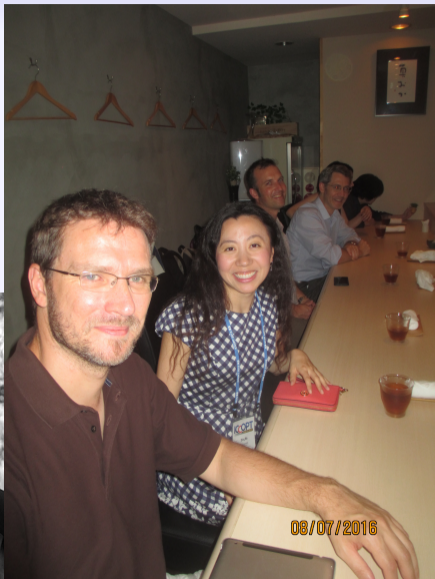
- $\bar{c}_k(x) =$  linear approximation to  $c(x)$  at  $x_k$  (MINOS has very big  $\sigma_k$ )

$$\begin{array}{ll} \text{ELC}_k'' & \underset{x, v, w}{\text{minimize}} \quad M_k(x, v, w) + \sigma_k e^T(v + w) \\ & \text{subject to} \quad \bar{c}_k(x) + v - w = 0, \quad \ell \leq x \leq u, \quad v, w \geq 0 \end{array}$$

- $M_k =$  modified augmented Lagrangian  $d_k(x, v, w) = c(x) - \bar{c}_k(x) - v + w$
- IPOPT, KNITRO, ... won't mind the extra elastic variables  $v, w$

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Ding Ma, Michael Friedlander



# Merida Jan 2016

AMPL: Dave Gay and Bob Fourer



# Oman Jan 2017



# Oman Jan 2017

LANCELOT: Andy Conn, Nick Gould, Philippe Toint




## IPOPT: Larry Biegler and Andreas Wächter

Thursday February 2, 2017

# Graduate Seminar

Chemical Engineering Welcomes

## Lorenz T. Biegler



**Three Paradigms for the Future of Process Optimization**

**Abstract:** Computer aided process engineering (CAPE) requires the determination of superior systems with reduced costs, increased efficiency or improved operability. These solutions especially need to consider complex unit operations with engineering and physics-based models. On the other hand, while process engineers need to synthesize and optimize processes with sufficiently detailed models, most engineering software tools still struggle with optimization of an integrated process. This overview explores three strategic paradigms that enable the realization of effective optimization strategies for large-scale process models, including complex models at device and molecular scales.



## Che-Lin Su

