Algorithm NCL

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Abstract

Optimization problems $\min \phi(x)$ st $c(x) \geq 0$ may have LICQ difficulties. We extend the BCL and LCL approaches of LANCELOT and MINOS to Algorithm NCL, whose subproblems optimize an augmented Lagrangian subject to constraints that satisfy LICQ:

$$\min_{x,r} \ \phi(x) + y_k^T r + \frac{1}{2}\rho_k \|r\|^2 \quad \text{st} \quad c(x) + r \geq 0.$$

The variables r lead to many superbasic variables with active-set solvers like MINOS and SNOPT, but are easily accommodated by interior methods. We illustrate with Taxation Policy problems modeled in AMPL. Algorithm NCL converges in about 10 major iterations (independent of problem size), and IPOPT is able to warm-start each major iteration.

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The NLP problem

The NLP problem

NCO
$$\begin{array}{ll} \underset{x\in\mathbb{R}^n}{\text{minimize}} & \phi(x) \\ \text{subject to} & c(x) \ge 0, \quad Ax \ge b, \quad \ell \le x \le u \end{array}$$

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

Example: $m = 571,000$, $n = 1500$, $A: 1 \times n$
10,000 constraints essentially active: $c_i(x^*) \le 10^{-6}$

BCL

LCL

NCL

Sequence of subproblems minimizing X-constrained (augmented) Lagrangian

BCL LANCELOT (1992)

LCL Robinson (1972)
MINOS (1982)
sLCL KNOSSOS (2002)

NCL Ma, Judd, Orban & S (2017)
Different implementation of **BCL**!
(AMPL loop + IPOPT)

LANCELOT's BCL algorithm for general NLP

LANCELOT

Equality constraints:

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

BCL subproblems:

$$\text{BC}_k \qquad \underset{x}{\text{minimize}} \quad L(x, y_k, \rho_k) = \phi(x) - y_k^T c(x) + \tfrac{1}{2}\rho_k \|c(x)\|^2$$
$$\text{subject to} \quad \ell \le x \le u$$

y_k estimates dual variables, ρ_k penalty parameter

Loop:

- solve BC_k to get x_k^* — decreasing optiol ω_k
- if $\|c(x_k^*)\| \le \eta_k$, $y_{k+1} \leftarrow y_k - \rho_k c(x_k^*)$ — decreasing featol η_k
  else $\rho_{k+1} \leftarrow 10\rho_k$

Algorithm NCL
for general NLP

NCL subproblems

$c(x) \geq 0$ as equalities:

$$\text{NCO}' \quad \underset{x,s}{\text{minimize}} \ \ \phi(x) \quad \text{subject to} \ \ c(x) - s = 0, \quad Ax \geq b, \quad \ell \leq x \leq u, \quad s \geq 0$$

NCL subproblems

$c(x) \geq 0$ as equalities:

$$\text{NCO}' \quad \underset{x,s}{\text{minimize}} \quad \phi(x) \quad \text{subject to} \quad c(x) - s = 0, \quad Ax \geq b, \quad \ell \leq x \leq u, \quad s \geq 0$$

LANCELOT subproblems:

$$\text{BC}_k{}' \quad \underset{x,s}{\text{minimize}} \quad L(x, y_k, \rho_k) = \phi(x) - y_k^T(c(x) - s) + \tfrac{1}{2}\rho_k \|c(x) - s\|^2 \quad \text{subject to} \quad Ax \geq b, \quad \ell \leq x \leq u, \quad s \geq 0$$

NCL subproblems

$c(x) \geq 0$ as equalities:

$$\text{NCO}' \quad \underset{x,s}{\text{minimize}} \quad \phi(x)$$
$$\text{subject to} \quad c(x) - s = 0, \quad Ax \geq b, \quad \ell \leq x \leq u, \quad s \geq 0$$

LANCELOT subproblems:

$$\text{BC}_k{}' \quad \underset{x,s}{\text{minimize}} \quad L(x, y_k, \rho_k) = \phi(x) - y_k^T(c(x) - s) + \tfrac{1}{2}\rho_k \left\|c(x) - s\right\|^2$$
$$\text{subject to} \quad Ax \geq b, \quad \ell \leq x \leq u, \quad s \geq 0$$

Introduce $r = -(c(x) - s)$:

$$\text{NC}_k \quad \underset{x,r}{\text{minimize}} \quad \phi(x) + y_k^T r + \tfrac{1}{2}\rho_k \left\|r\right\|^2$$
$$\text{subject to} \quad c(x) + r \geq 0, \quad Ax \geq b, \quad \ell \leq x \leq u$$

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

Optimal Tax Policy

Optimal tax policy

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

where c_i and y_i are the consumption and income of taxpayer i, and λ 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 α, γ, ψ and η 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	$= 5$
nb	elasticities of labor supply	$= 3$
nc	basic need types	$= 3$
nd	levels of distaste for work	$= 2$
ne	elasticities of demand for consumption	$= 2$
$T =$	$na \times nb \times nc \times nd \times ne$	$= 180$
$m =$	$T(T-1)$ nonlinear constraints	$= 32220$
$n =$	$2T$ variables	$= 360$

AMPL model

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

```
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

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

	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

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

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

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

```
for {K in 1..kmax}
{  if K == 2 then {option ipopt_options $ipopt_options
                              ' warm_start_init_point=yes    mu_init=1e-4'};
   if K == 4 then {option ipopt_options $ipopt_options ' mu_init=1e-5'};
   if K == 6 then {option ipopt_options $ipopt_options ' mu_init=1e-6'};
   if K == 8 then {option ipopt_options $ipopt_options ' mu_init=1e-7'};
   if K ==10 then {option ipopt_options $ipopt_options ' 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 $\|r_k^*\| \le \eta_k$, $y_{k+1} \leftarrow y_k + \rho_k r_k^*$

```
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

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

k	ρ_k	η_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

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

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

	tol	*count*	*count*/*n*	
	10^{-10}	548	1.5	
	10^{-9}	550	1.5	
	10^{-8}	591	1.6	
	10^{-7}	890	2.5	
$\rightarrow$	10^{-6}	1104	3.1	$\leftarrow$ About $3n$ active constraints
	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	

NCL/IPOPT bigger example

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

k	ρ_k	η_k	$\|r_k^*\|_\infty$	$\phi(x_k^*)$	mu_init	Itns	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: $c_i(x) \le tol$

	tol	*count*	*count/n*	
	10^{-10}	3888	2.6	
	10^{-9}	3941	2.6	
	10^{-8}	4430	2.9	
	10^{-7}	7158	4.7	
$\rightarrow$	10^{-6}	10074	6.6	$\leftarrow$ $\approx 6.6n$ 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, NCL

na = increasing $\quad nb = 3 \quad nc = 3 \quad nd = 2 \quad ne = 2$

			IPOPT		KNITRO		NCL/IPOPT	
na	m	n	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*	∞!	2769	4117	727	1679
17	373933	1224			2598	11447	1021	6347
21	570780	1512					1761	17218

*duals diverge
∞ MUMPS needs more mem
! Loop

A future possibility
AMPL + IPM + 2nd derivatives

KNOSSOS via AMPL + IPM?

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

$$\text{ELC}_k \qquad \underset{x}{\text{minimize}} \quad L(x, y_k, \rho_k) + \sigma_k \, \|\bar{c}_k(x)\|_1 \qquad \text{subject to} \quad \ell \le x \le u$$

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

KNOSSOS via AMPL + IPM?

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

$$\text{ELC}''_k \qquad \underset{x,v,w}{\text{minimize}} \quad M_k(x,v,w) + \sigma_k e^T(v+w) \qquad \text{subject to} \quad \bar{c}_k(x) + v - w = 0, \quad \ell \le x \le u, \quad v, w \ge 0$$

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

Special thanks

- LANCELOT: Andy, Nick, Philippe
- AMPL: Bob Fourer, Dave Gay
- IPOPT: Larry Biegler, Andreas Wächter
- Katya and all the Workshop Committee
- Yuja Wang, youtube
- Coauthors: Ken Judd, Dominique Orban
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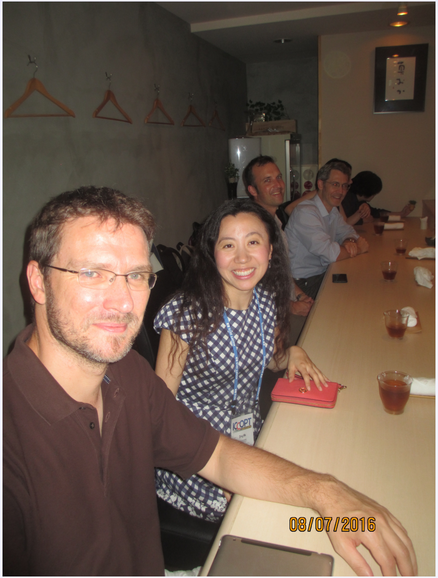
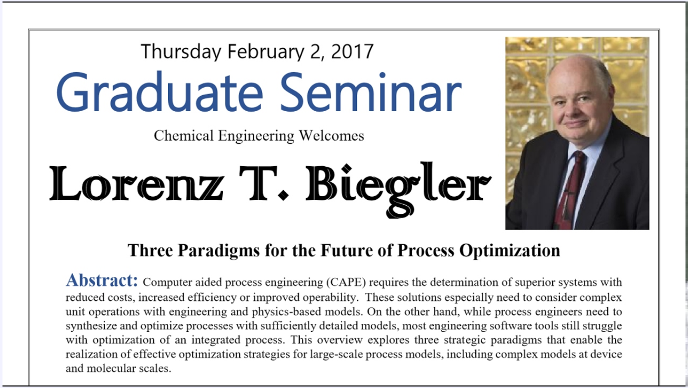


Oman Jan 2017

Mehi Al-Baali + Lancelot

Dave and Bob — AMPL!

Larry and Andreas — IPOPT!



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.


01/04/2016