Numerical Optimization at SOL

ICME Seminar (CME 500)

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with help from

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Abstract

Some well known software packages have been developed at SOL during the last 30 years. They include algorithms for sparse linear equations (SYMMLQ, MINRES, LSQR, LUSOL) and various optimization solvers (MINOS, NPSOL, QPOPT, SQOPT, SNOPT, PDCO, SpaseLoc). We give a personal history of these codes and some of their scientific applications, including optimal trajectories for aircraft, spacecraft, and autonomous vehicles.

Nonlinear Optimization

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

$$\text{subject to} \quad \ell \le \begin{pmatrix} x \\ c(x) \\ Ax \end{pmatrix} \le u$$

$\phi(x)$	nonlinear objective function
$c_i(x)$	nonlinear constraint functions
A	sparse matrix
ℓ, u	bounds

Assume functions are **smooth** with known **gradients**

Iterative Solvers for $Ax = b$

Symmetric $Ax = b$

A may be a **sparse matrix**
or an **operator** for forming products Av

Solver	A	
CG	positive definite	Hestenes & Stiefel 1952
SYMMLQ	indefinite	Paige & Saunders 1975
MINRES	indefinite	" " " "
MINRES-QLP	indefinite or singular	Sou-Cheng Choi's thesis 2006
		$\min \|Ax - b\|^2$

All based on the **Lanczos process**
for reducing A to tridiagonal form

The Lanczos process for A, b

$\beta_1 = \|b\| \qquad v_1 = b/\beta_1 \qquad\qquad \beta_1 v_1 = b$

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$p_1 = A v_1 \qquad \alpha_1 = p_1^T v_1 \qquad \beta_2 v_2 = p_1 - \alpha_1 v_1$

$p_2 = A v_2 \qquad \alpha_2 = p_2^T v_2 \qquad \beta_3 v_3 = p_2 - \alpha_2 v_2 - \beta_2 v_1$

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Generates

$$V_k = \begin{bmatrix} v_1 & \cdots & v_k \end{bmatrix}, \qquad H_k = \begin{bmatrix} \alpha_1 & \beta_2 & & \\ \beta_2 & \alpha_2 & \beta_3 & \\ & \ddots & \ddots & \ddots \\ & & \beta_k & \alpha_k \\ & & & \beta_{k+1} \end{bmatrix}$$

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such that $$AV_k = V_{k+1} H_k$$

Using Lanczos for $Ax = b$

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Let $x_k = V_k y_k$ for some y_k (we want $Ax_k \approx b$)

$$Ax_k = V_{k+1} H_k y_k$$

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Remember that v_1 is a multiple of b

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CG, SYMMLQ, MINRES, MINRES-QLP make $H_k y_k \approx \begin{bmatrix} \times \\ 0 \\ \vdots \\ 0 \end{bmatrix}$

in various ways (Cholesky, LQ, QR, QLP on H_k)

Applications

CG	$\min \phi(x)$	$H\Delta x = -g(x)$
SYMMLQ	KKT systems	$\begin{pmatrix} H & A^T \\ A & \end{pmatrix} \begin{pmatrix} \Delta x \\ \Delta y \end{pmatrix} = \begin{pmatrix} -g \\ 0 \end{pmatrix}$
MINRES	KKT systems	for those who like $\|r_k\|$ decreasing
MINRES-QLP	indefinite	added reliability
	singular	$\min \|Ax - b\|$

Unsymmetric or rectangular $Ax \approx b$

Lanczos on

$$\begin{pmatrix} \gamma I & A \\ A^T & \delta I \end{pmatrix}, \qquad \begin{pmatrix} b \\ 0 \end{pmatrix}$$

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gives the **Golub-Kahan process** for reducing A to bidiagonal form:

$$AV_k = U_{k+1} B_k \qquad B_k = \begin{bmatrix} \alpha_1 & & & \\ \beta_2 & \alpha_2 & & \\ & \ddots & \ddots & \\ & & \beta_k & \alpha_k \\ & & & \beta_{k+1} \end{bmatrix} \qquad \text{(for all } \gamma, \delta)$$

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Used in LSQR for $\min \|Ax - b\|^2$ (Paige & Saunders 1982)

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QR factorization to solve $\min \|B_k y_k - \beta_1 e_1\|^2$

Features

Estimates of $\|r_k\|$, $\|x_k\|$, $\|A\|$, $\text{cond}(A)$

Stopping rules

$$\frac{\|r_k\|}{\|A\|\|x_k\| + \|b\|} \le \texttt{tol} \qquad \text{or} \qquad \frac{\|A^T r_k\|}{\|A\|\|r_k\|} \le \texttt{tol}$$

Not just $\|r_k\|/\|b\| \le \texttt{tol}$ $(r_k = b - Ax_k)$

LSQR Applications

$\min \|Ax - b\|$

Oil exploration (Schlumberger), $A \approx 20\text{M} \times 1\text{M}$, complex

LSQR could keep all the world's computers busy

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$\min \|Ax - b\|^2 + \lambda \|x\|_1$
MRI (Stanford), geophysics (UBC), $A \approx 1\text{M} \times 20\text{M}$

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Inside PDCO

Constraint matrix A may be an **operator**

LUSOL: Sparse direct solver

LUSOL

Maintaining LU factors of a general sparse matrix A

Gill, Murray, Saunders & Wright 1987

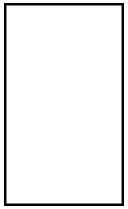
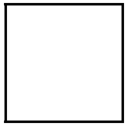
Features

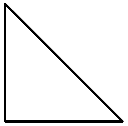
Square or rectangular A	for basis selection, preconditioning
Rank-revealing LU	for "basis repair"
Stable updates	Bartels-Golub-Reid style

Code contributors

F77	Saunders (1986–present)
	following Duff, Reid, Zlatev, Suhl and Suhl
MATLAB Fmex	Michael O'Sullivan (1999–present)
C (for lp_solve)	Kjell Eikland (2004–present)
MATLAB Cmex	Yin Zhang (2005–present)

LUSOL

$A =$  or  or  $= LU$

FACTOR $[L, U, \mathsf{p}, \mathsf{q}] = \text{luSOL}(A)$ $L(\mathsf{p},\mathsf{p}) =$ 

L well-conditioned

UPDATE Add, replace, delete a column $L \leftarrow LM_1M_2\ldots$

Add, replace, delete a row M_j well-conditioned

Add a rank-one matrix

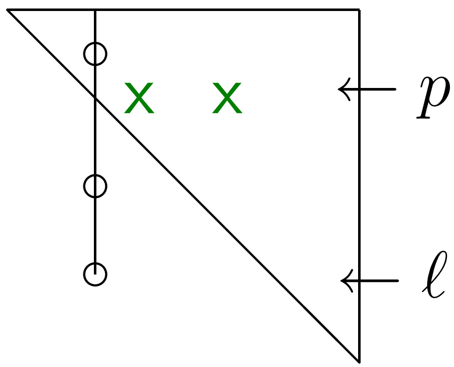
SOLVE $Lx = y,\ L^Tx = y,\ Ux = y,\ U^Tx = y,\ Ax = y,\ A^Tx = y$

MULTIPLY $x = Ly,\ x = L^Ty,\ x = Uy,\ x = U^Ty,\ x = Ay,\ x = A^Ty$

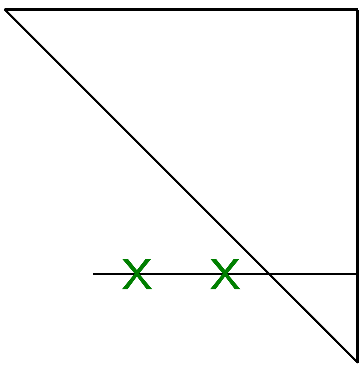
LUSOL's Bartels-Golub updates

à la Reid 1976, 1982, 2004 LA05, LA15

$U' =$



$U'' \equiv P^T U' P =$



- Avoid Hessenberg matrix
- Use **cyclic permutation** P
- Eliminate x using $M_j = \begin{pmatrix} 1 & \\ \mu & 1 \end{pmatrix}$ or $\begin{pmatrix} 1 & \\ \mu & 1 \end{pmatrix} \begin{pmatrix} & 1 \\ 1 & \end{pmatrix}$

LP and QP

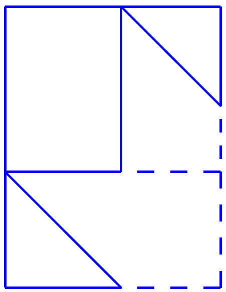
LSSOL

Dense Constrained Least Squares

$$\min \ \|Xx - b\|^2 \quad \text{st} \quad l \le \begin{pmatrix} x \\ Ax \end{pmatrix} \le u$$

- 1971: Josef Stoer
- 1986: LSSOL: Gill, Hammarling, Murray, Saunders & Wright
- Orthogonal factors

$$PXQ = \qquad A_kQ =$$



- The only method that avoids forming X^TX
- We don't know how for sparse X

QPOPT

Dense LP, QP (Gill, Murray, Saunders, Wright 1978, 1984, 1995)

$$\min \; c^T x + \tfrac{1}{2} x^T H x \quad \text{st} \quad l \le \begin{pmatrix} x \\ Ax \end{pmatrix} \le u$$

- User routine computes Hx for given x $\qquad$ H may be **indefinite**
- Orthogonal factors $\quad A_k Q = (L \;\; 0), \quad Q = (Y \;\; Z)$
- Dense reduced Hessian $\quad Z^T H Z = R^T R$

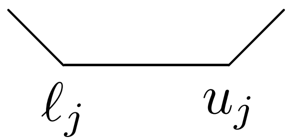
- Only ⊗ needs care when Z, R get bigger

SQOPT

Sparse LP, QP **(G, M, & S 1997)**

$$\min\ c^T x + \tfrac{1}{2}(x - x_0)^T H (x - x_0) \quad \text{st} \quad l \le \begin{pmatrix} x \\ Ax \end{pmatrix} \le u$$

- User routine computes Hx H **semidefinite**
- Allows elastic bounds on variables and constraints



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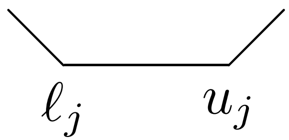

Applications

In SNOPT $\quad H = D + \sum v_j v_j^T - w_j w_j^T \quad$ (Limited-memory quasi-Newton)

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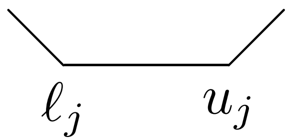

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In SNOPT $\quad H = D + \sum v_j v_j^T - w_j w_j^T \quad$ (Limited-memory quasi-Newton)

In Fused Lasso (Tibshirani, S et al 2004) $\quad Hx = X^T(Xx) \quad$ (not ideal)

$$\min_{\beta}\ \|X\beta - y\|^2 \ \text{ st } \ \sum |\beta_j| \le s_1 \ \text{ and } \ \sum |\beta_j - \beta_{j-1}| \le s_2$$

Constraints on $\|\beta\|_1$ and $\|L\beta\|_1 \Rightarrow$ many $\beta_j = 0$ and $\beta_j = \beta_{j-1}$

Primal-Dual IPM for (Separable) Convex Opt

MATLAB **(Saunders 1997–2006, Kim, Tenenblat)**

- Nominal problem

$$\begin{array}{ll} \min & \phi(x) \\ \text{st} & Ax = b, \qquad \ell \le x \le u \end{array}$$

- Regularized problem

$$\begin{array}{ll} \min & \phi(x) + \frac{1}{2}\|D_1 x\|^2 + \frac{1}{2}\|r\|^2 \\ \text{st} & Ax + D_2 r = b, \qquad \ell \le x \le u \end{array}$$

$\nabla^2\phi(x)$, $D_1 \succeq 0$, $D_2 \succ 0$, all diagonal $\qquad$ A can be an operator

PDCO Applications

- Basis Pursuit (Chen, Donoho, & S 2001)

$$\min \lambda \|x\|_1 + \tfrac{1}{2}\|Ax - b\|^2$$

cf LARS (Hastie et al), Homotopy (Osborne et al 1999, Donoho & Tsaig 2006)

- Image reconstruction (Kim thesis, 2002)

$$\text{Non-negative least squares:} \quad \min \|Ax - b\|^2 \ \text{ st } \ x \geq 0$$

- Maximum entropy (S & Tomlin, 2003)

$$\min \sum x_j \log x_j \ \text{ st } \ Ax = b, \ x \geq 0$$

- Zoom strategy for warm-starting interior methods
(S & Tenenblat, 2006)

PDCO on Web Traffic entropy problem

A is a 51000×662000 network matrix, $\text{nnz}(A) = 2$ million

Itn	mu	step	Pinf	Dinf	Cinf	Objective	center	atol	LSQR	Inexact
0			2.5	1.1	-6.7	-1.3403720e+01	1.0			
1	-5.0	0.267	2.4	1.1	-5.1	-1.3321172e+01	242.0	-3.0	5	0.001
2	-5.1	0.195	2.3	1.0	-5.3	-1.3220658e+01	36.9	-3.0	5	0.001
3	-5.2	0.431	2.1	0.9	-5.2	-1.2942743e+01	122.9	-3.0	5	0.001
4	-5.5	0.466	1.9	0.7	-5.3	-1.2711643e+01	41.8	-3.0	6	0.001
5	-5.7	0.671	1.4	0.2	-5.5	-1.2492935e+01	71.8	-3.0	9	0.001
6	-6.0	1.000	-0.0	-0.8	-5.8	-1.2367004e+01	2.7	-3.0	10	0.001
7	-6.0	1.000	-0.1	-2.3	-6.0	-1.2368200e+01	1.1	-3.0	9	0.002
8	-6.0	1.000	-1.1	-4.7	-6.0	-1.2367636e+01	1.0	-3.0	2	0.009
9	-6.0	1.000	-1.3	-5.7	-6.0	-1.2367655e+01	1.0	-3.0	7	0.015
10	-6.0	1.000	-2.5	-7.6	-6.0	-1.2367607e+01	1.0	-3.0	2	0.004
11	-6.0	1.000	-3.7	-8.6	-6.0	-1.2367609e+01	1.0	-3.5	8	0.004
12	-6.0	1.000	-5.9	-11.0	-6.0	-1.2367609e+01	1.0	-4.7	11	0.000

PDitns = 12 LSQRitns = 79 time = 101.4 (MATLAB)
22.4 (C++)

Nonlinear constraints

Lagrangians

NP	min	$\phi(x)$
	st	$c(x) = 0$

Penalty Function

$$\min \ \phi(x) \qquad\qquad + \tfrac{1}{2}\rho_k \|c(x)\|^2$$

Augmented Lagrangian

$$\min \ \phi(x) - {y_k}^T c(x) + \tfrac{1}{2}\rho_k \|c(x)\|^2$$

Lagrangian in a Subspace

$$\min \ \phi(x) - {y_k}^T c(x) + \tfrac{1}{2}\rho_k \|c(x)\|^2$$

st linearized constraints

NPSOL

Dense NLP (G, M, S & W 1986)

- Dense SQP method

  QP subproblems solved by LSSOL

- Search direction $(\Delta x, \Delta y)$

  QP_k $\quad \min$ quadratic approx'n to Lagrangian

  $\quad\quad$ st $\quad$ linearized constraints

- Merit function

  Linesearch on augmented Lagrangian:

$$\min_{\alpha} \; L(x_k + \alpha\Delta x, \;\; y_k + \alpha\Delta y, \;\; \rho_k)$$

Aerospace Applications

NPSOL

- Philip Gill (UCSD)
  Rocky Nelson (McDonnell-Douglas and Boeing)
- F-4 Phantom minimum time-to-climb
- DC-X minimum-fuel landing maneuver

NPSOL, SNOPT

- David Saunders (Eloret at NASA Ames Research Center)
- HSCT supersonic airliner
- Future shuttle no-ditch trajectory optimization
- Shape of Crew Exploration Vehicle heat shield

General sparse NLP

- 1975: Bruce Murtagh and MS
  NZ and SOL
- Sparse linear constraints, nonlinear objective
  Reduced-gradient method (an active-set method)
  LP + unconstrained optimization (simplex + quasi-Newton)
- 1983: Sparse nonlinear constraints
  Sydney and SOL, extended Robinson's method 1972

- Assume functions and gradients are **cheap**
- Still widely used in GAMS and AMPL

SNOPT

Sparse NLP (G, M, & S 2003; SIAM Review SIGEST 2005)

- Sparse SQP method
  QP subproblems solved by SQOPT

- Search direction $(\Delta x, \Delta y)$

  QP$_k$ $\quad \min \quad$ limited-memory approx'n to Lagrangian
  $\quad\quad\quad$ st $\quad$ linearized constraints

- Merit function
  Linesearch on augmented Lagrangian:

$$\min_{\alpha} \quad L(x_k + \alpha\Delta x, \quad y_k + \alpha\Delta y, \quad \rho_k)$$

Infeasible Problems

or infeasible subproblems

SNOPT's solution – modify the original problem:

$$\min \ \phi(x) + \sigma \|c(x)\|_1$$

NP(σ)	min	$\phi(x) + \sigma e^T(v + w)$
	st	$c(x) + v - w = 0, \qquad v, w \geq 0$

Implemented by elastic bounds on QP slacks

SNOPT paper

revised for SIAM Review 2005

- LUSOL: Threshold Rook Pivoting for Basis Repair
- SYMMLQ on $Z^T H Z d = -Z^T g_{\mathrm{QP}}$ when many superbasics
- 1000 CUTEr and COPS 3.0 test problems
- Up to 40,000 constraints and variables
- Up to 20,000 superbasics (degrees of freedom)
- 900 problems solved successfully

Localization of Wireless Sensor Networks

MATLAB **(Holly Jin's thesis 2005, SIAM J. Opt 2006)**

$$
\begin{aligned}
&\text{minimize} \quad \text{some norm of } \alpha_{ij} \\
&\|x_i - x_j\|^2 + \alpha_{ij} \quad = \quad d_{ij}^2 \quad (\text{some } i,j) \\
&\|x_i - x_j\|^2 \quad \geq \quad r_{ij}^2 \quad (\text{most } i,j) \\
&x_k \quad = \quad a_k \quad (\text{a few } k) \text{ anchors}
\end{aligned}
$$

d_{ij} noisy distance data

r_{ij} radio ranges

$x_i \in R^2$ or R^3

a_k known positions of anchors

x_i sensors' positions (to be estimated)

Localization of Wireless Sensor Networks

- Biswas and Ye (2003a): SDP relaxation DSDP 2.0
  50 nodes: a few seconds
  200 nodes: too much time and storage

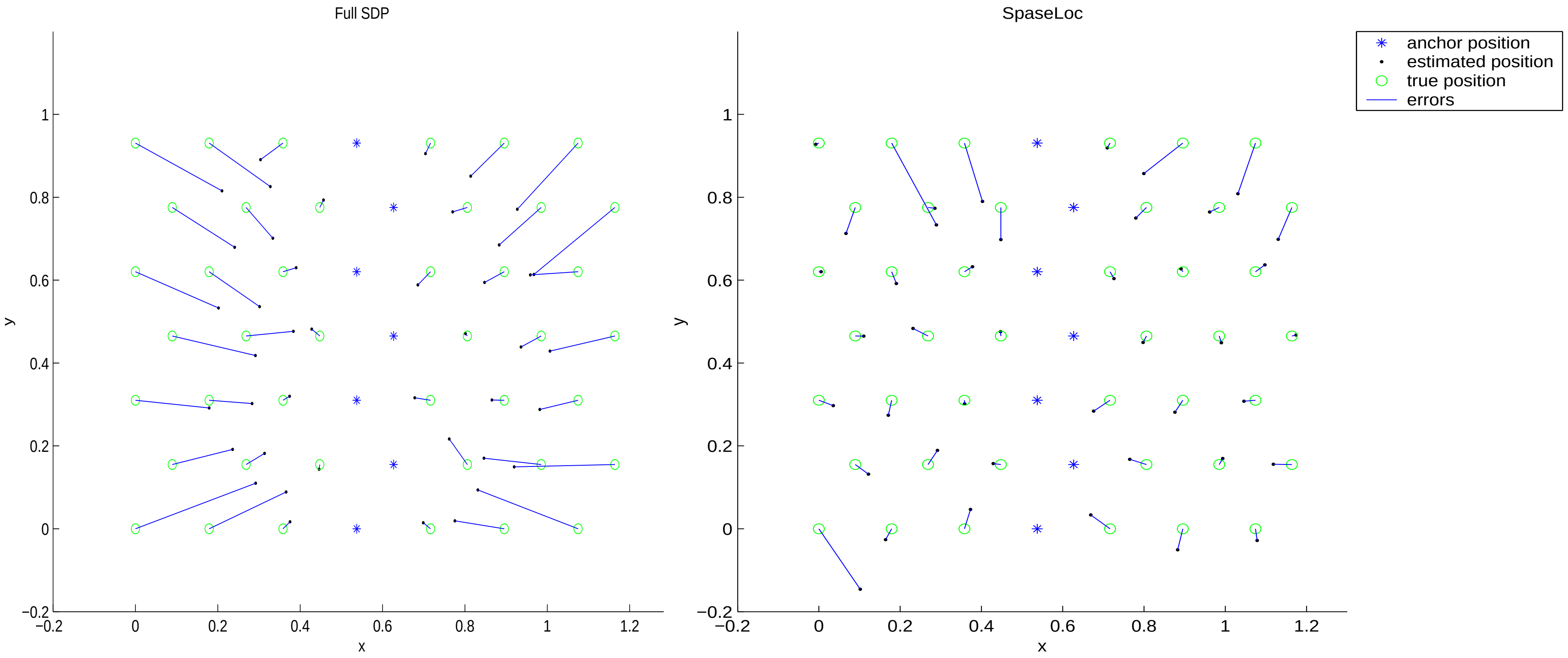
- Biswas and Ye (2003b): Parallel SDP subproblems DSDP 2.0
  4000 nodes: 2 mins

- SpaseLoc (2004): Sequential SDP subproblems DSDP 5.0
  4000 nodes: 25 secs

- SpaseLoc (2006):
  10000 nodes: 2 mins

(DSDP = SDP solver of Benson and Ye)

Full SDP vs. SpaseLoc



Localization errors for full SDP model and SpaseLoc

Two demos by Holly Jin

SpaseLoc Wireless sensor localization

SNOPT CurveSmoother for the Stanford Racing Team

Summary

Key concepts for Nonlinear Optimization

- Stable dense and sparse matrix factorizations
- Minimize augmented Lagrangian in (relaxed) subspace

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- Stable dense and sparse matrix factorizations
- Minimize augmented Lagrangian in (relaxed) subspace

Software

- SYMMLQ, MINRES, MINRES-QLP, LSQR (F77, MATLAB)
- LUSOL (F77) engine for MINOS, SNOPT
- LUSOL (C version) now in open source system lp_solve
- MINOS, SNOPT in GAMS, AMPL, NEOS
- TOMLAB/SOL (Holmström) for MATLAB users
- SNOPT has its own MATLAB interface
- PDCO (MATLAB) $\min\ \phi(x)$ st $Ax = b +$ bounds (A an operator)
- SpaseLoc (MATLAB) Scalable sensor localization

Other SOL Research

- Uday Shanbhag (with Walter Murray)
  Stochastic nonlinear programming, equilibrium programming, nonlinear facility location problems (Tucker Prize 2006)
- Che-Lin Su (with Dick Cottle)
  MPEC, EPEC (math programs with equilibrium constraints)
- Samantha Infeld (with Walter Murray)
  Trajectory optimization for spacecraft
- Yinyu Ye
  Large-scale (dual) SDP
  Wireless sensor network localization
  Other graph realization problems
  . . . !!
- http://www.stanford.edu/group/SOL/dissertations.html

The Lighter Side of Optimization

In New Zealand, the equivalent of the TV guide is called **The Listener**. Every week a Life in New Zealand column publishes clippings describing local events. The first sender receives a $5 Lotto Lucky Dip. The following clippings illustrate some characteristics of optimization problems in the real(?) world.

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Robust solutions

RECOVERY CARE gives you financial protection from specified sudden illness. You get cash if you live . . . and cash if you don't.

No objective function

People have been marrying and bringing up children for centuries now. Nothing has ever come of it. (Evening Post, 1977)

Multiple objectives

"I had the choice of running over my team-mate or going onto the grass, so I ran over my team-mate then ran onto the grass", Rymer recalled later.

Obvious objective

He said the fee was increased from $5 to $20 because some people had complained it was not worth writing a cheque for $5.

Equilibrium condition

"The pedestrian count was not considered high enough to justify an overbridge", Helen Ritchie said. "And if there continues to be people knocked down on the crossing, the number of pedestrians will dwindle."

Constraints

ENTERTAINERS, DANCE BAND, etc. Vocalist wanted for New Wave rock band, must be able to sing.

DRIVING INSTRUCTOR Part-time position. No experience necessary.

HOUSE FOR REMOVAL in excellent order, $800. Do not disturb tenant.

Exactly one feasible solution

MATTHEWS RESTAURANT, open 365 nights. Including Mondays.

Buying your own business might mean working 24 hours a day. But at least when you're self-employed you can decide which 24.

Peters: Oh, it's not that I don't want to be helpful. But in this case the answer is that I don't want to be helpful. (Listener, 1990)

Sergeant J Johnston said when Hall was stopped by a police patrol the defendant denied being the driver, but after it was pointed out he was the only person in the car he admitted to being the driver.

His companion was in fact a transvestite, X, known variously as X or X.

Bound your variables

By the way, have you ever seen a bird transported without the use of a cage? If you don't use a cage it will fly away and maybe the same could happen to your cat. Mark my words, we have seen it happen.

Redundant constraints

If you are decorating before the baby is born, keep in mind that you may have a boy or a girl.

EAR PIERCING while you wait.

CONCURRENT TERM FOR BIGAMY (NZ Herald, 1990)

Infeasible constraints

I chose to cook myself to be quite sure what was going into the meals.

We apologize to Wellington listeners who may not be receiving this broadcast.

The model 200 is British all the way from its stylish roofline to its French-made Michelin tyres. (NZ Car Magazine)

BALD, 36 yr old, handsome male seeking social times and fun with bald 22 years and upwards female Napier Courier, 28/2/02

$\geq$ or $\leq$?

BUY NOW! At $29.95 these jeans will not last long!

NOT TOO GOOD TO BE TRUE! We can sell your home for much less than you'd expect! (NZ Property Weekly)

The BA 146's landing at Hamilton airport was barely audible above airport background noise, which admittedly included a Boeing 737 idling in the foreground.

Yesterday Mr Palmer said "The Australian reports are not correct that I've seen, although I can't say that I've seen them".

It will be a chance for all women of this parish to get rid of anything that is not worth keeping but is too good to throw away. Don't forget to bring your husbands.

$\geq$ or $\leq$?

The French were often more blatant and more active, particularly prop X and number eight Y, but at least one All Black was seen getting his retaliation in first.

WHAT EVERY TEENAGER SHOULD KNOW — PARENTS ONLY

“Love Under 17” Persons under 18 not admitted.

“Keeping young people in the dark would not stop them having sex—in fact it usually had the opposite effect,” she said.

NELSON, approximately 5 minutes from airport. Golf course adjacent. Sleeps seven all in single beds. Ideal for honeymoons. (Air NZ News, 1978)

Hard or soft constraints

The two have run their farm as equal partners for 10 years, with Jan in charge of grass management, Lindsay looking after fertilizer, and both working in the milk shed. "We used to have our staff meetings in bed. That got more difficult when we employed staff!" (NZ country paper)

Elastic constraints

The Stationary Engine Drivers Union is planning rolling stoppages.

When this happens there are set procedures to be followed and they are established procedures, provided they are followed.

APATHY RAMPANT? Not in Albany—the closing of the electoral rolls saw fully 103.49 percent of the area's eligible voters signed up.

Auckland City ratepayers are to be reminded that they can pay their rates after they die. (Auckland Herald, 1990)

He was remanded in custody to appear again on Tuesday if he is still in the country.

Convergence

"There is a trend to open libraries when people can use them", he says.

Mayor for 15 years, Sir Dove-Myer wants a final three years at the helm "to restore sanity and stability in the affairs of the city".

Applications

(Yachting) It is not particularly dangerous, as it only causes vomiting, hot and cold flushes, diarrhoea, muscle cramping, paralysis, and sometimes death . . . (Boating New Zealand, 1990)

(Ecological models) CAR POLLUTION SOARS IN CHRISTCHURCH—BUT CAUSE REMAINS MYSTERY

Nappies wanted for window cleaning. Must be used.

(Optimal control) Almost half the women seeking fertility investigations at the clinic knew what to do to get pregnant

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(Optimal control) Almost half the women seeking fertility investigations at the clinic knew what to do to get pregnant, but not when to do it.

Integer variables

0 or 1 or 2 . . .

Integer variables

0 or 1 is sometimes not optimal

When Taupo police arrested a Bay of Plenty man
for driving over the limit,
they discovered he was a bigamist. Nelson Mail, 5/04

Always room for improvement

The owner Craig Andrew said the three main qualities for the job were speed, agility and driving skills. “Actually, Merv has none of those, but he’s still the best delivery boy we’ve had”, he said.