Optimization Research at SOL
A review of the last 30 years

Michael SAUNDERS
Systems Optimization Laboratory
Dept of Management Science and Engineering
Stanford University
Stanford, CA 94305-4026, USA
saunders@stanford.edu

Mathematisches Forschungsinstitut Oberwolfach
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Abstract

QPSOL, LSSOL, NPSOL, QPOPT, MINOS, SQOPT, SNOPT, Knossos, PDCO, SpaseLoc, SYMMLQ, MINRES, LSQR, LUSOL

These are optimization packages developed at SOL during the last 30 years by Gill, Murray, Saunders, and Wright, with much input from coauthors Paige, Murtagh, Friedlander, and Jin.

We give a personal history of the development of these codes. For example, LUSOL is the engine for most of the large-scale solvers (MINOS, SQOPT, SNOPT, Knossos), as well as for ZIP, MILES, PATH, lp_solve.
Nonlinear Optimization

\[ \begin{align*}
\text{minimize} & \quad \phi(x) \\
\text{subject to} & \quad \ell \leq \begin{pmatrix} x \\ c(x) \\ Ax \end{pmatrix} \leq u
\end{align*} \]

\( \phi(x) \) nonlinear objective function

\( c(x) \) nonlinear constraint functions \( \in \mathbb{R}^m \)

\( A \) sparse matrix

\( \ell, u \) bounds

Assume functions are \textbf{smooth} with known \textbf{gradients}
MINOS

General sparse NLP

- 1975: Bruce Murtagh and MS NZ and SOL
- Sparse linear constraints, nonlinear obj
  Reduced-Gradient method (active set)
  LP + unconstrained optimization
  (Simplex + quasi-Newton)
- 1979: Sparse nonlinear constraints
  UNSW and SOL, extended Robinson 1972
- Assume functions and gradients are cheap
  GAMS and AMPL
QPSOL

Dense QP

- 1978: Gill & Murray
  1984: G, M, Saunders & Wright
- Dense linear constraints, indefinite QP obj $x^T H x$
- Orthogonal factors $A_k Q = (L \ 0)$, $Q = (Y \ Z)$
- Dense reduced Hessian $Z^T H Z = R^T R$

\[
\begin{align*}
Z &= \begin{bmatrix}
\vdots \\
0
\end{bmatrix} \\
R &= \begin{bmatrix}
0 \\
\vdots
\end{bmatrix}
\end{align*}
\]

- Only $\otimes$ needs care when $Z, R$ get bigger
QPOPT

Dense LP and QP (G, M, & S 1995)

- Objective = $c^T x + \frac{1}{2} x^T G^T G x$
  or $c^T x + \frac{1}{2} x^T H x$
- Positive definite, Semidefinite or Indefinite
- Dense linear constraints
- Later version of QPSOL (f77)
LSSOL

Dense Constrained Least Squares

\[ \min \left\| X x - b \right\|^2 \quad \text{s.t.} \quad l \leq \begin{pmatrix} x \\ Ax \end{pmatrix} \leq u \]

- 1971: Josef Stoer

- Orthogonal factors
  \[ PxQ = \]
  \[ A_kQ = \]

- The only method that avoids forming \( X^T X \)
- We don’t know how for sparse \( X \)
Lagrangians

\[
\begin{array}{l}
\text{NP} & \min \; \phi(x) \\
\text{s.t.} & c(x) = 0 \\
\end{array}
\]

**Penalty Function**

\[
\min \; \phi(x) + \frac{1}{2} \rho_k \|c(x)\|^2
\]

**Augmented Lagrangian**

\[
\min \; \phi(x) - y_k^T c(x) + \frac{1}{2} \rho_k \|c(x)\|^2
\]

**Lagrangian in a Subspace**

\[
\min \; \phi(x) - y_k^T c(x) + \frac{1}{2} \rho_k \|c(x)\|^2 \\
\text{s.t. linearized constraints}
\]
NP
\[ \min \phi(x) \]
\[ \text{s.t. } c(x) = 0, \quad \ell \leq x \leq u \]

BC\(_k\)
\[ \min \phi(x) - y_k^T c(x) + \frac{1}{2}\rho_k \|c(x)\|^2 \]
\[ \text{s.t. } \ell \leq x \leq u \]

**BCL Method**

- Solve subproblem BC\(_k\)
- Update dual variables: \( y_{k+1} = y_k - \rho_k c(x_k^*) \)
- Juggle \( \rho_k \) and repeat
NPSOL

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

• Dense SQP method
  QP subproblems solved by LSSOL

• Search direction $(\Delta x, \Delta y)$
  $\text{QP}_k \min \text{ quadratic approx’n to Lagrangian}$
  $\text{s.t. linearized constraints}$

• Merit function
  Linesearch on augmented Lagrangian:
  $$\min_{\alpha} L(x_k + \alpha \Delta x, y_k + \alpha \Delta y, \rho_k)$$
SQOPT
Sparse QP \text{(G, M, \\ & S 1997)}

\begin{itemize}
\item Semidefinite QP obj \((x - x_0)^TH(x - x_0)\)
\item User routine computes \(Hx\) for given \(x\)
\item Allows elastic bounds on variables and constraints \(\ell_j \leq x_j \leq u_j\)
\end{itemize}

Application 1: Inside SNOPT

\begin{itemize}
\item \(H = D + \sum v_jv_j^T - w_jw_j^T\) (Limited-memory quasi-Newton)
\end{itemize}

Application 1: Fused Lasso \text{(Tibshirani, S et al. 2004)}

\[
\min_{\beta} \|X\beta - y\|^2 \quad \text{s.t.} \quad \sum |\beta_j| \leq s_1 \quad \text{and} \quad \sum |\beta_j - \beta_{j-1}| \leq s_2
\]

\begin{itemize}
\item \(Hx = X^T(Xx)\) \quad (not ideal)
\item Constraints on \(\|\beta\|_1\) and \(\|M\beta\|_1\) \Rightarrow many \(\beta_j = 0\) and \(\beta_j = \beta_{j-1}\)
\end{itemize}
SNOPT

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

- Sparse SQP method
  QP subproblems solved by SQOPT

- Search direction \((\Delta x, \Delta y)\)
  \(\text{QP}_k \min \text{ limited-memory approx'n to Lagrangian}
  \text{s.t. linearized constraints}

- Merit function
  Linesearch on augmented Lagrangian:
  \[
  \min_{\alpha} L(x_k + \alpha \Delta x, y_k + \alpha \Delta y, \rho_k)
  \]
Infeasible Problems

or infeasible subproblems

SNOPT’s solution – modify the original problem:

\[ \min \phi(x) + \sigma \|c(x)\|_1 \]

\[
\begin{array}{ll}
\text{NP}(\sigma) & \min \phi(x) + \sigma e^T(v + w) \\
\text{s.t.} & c(x) + v - w = 0, \quad v, w \geq 0
\end{array}
\]

Implemented by elastic bounds on QP slacks
SNOPT paper
revised for SIAM Review 2005

• **LUSOL**: Threshold Rook Pivoting for **Basis Repair**
• **SYMMLQ** on $Z^T H Z d = -Z^T g_{QP}$ 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
Stabilizing MINOS

Michael Friedlander’s thesis 2002
Minimizing the Augmented Lagrangian

\[ L(x, y, \rho) = \phi(x) - y^T c(x) + \frac{1}{2} \rho \| c(x) \|^2 \]

**BCL (LANCELOT)**

\[
\begin{align*}
\text{minimize} & \quad L(x, y_k, \rho_k) \\
\text{s.t.} & \quad \ell \leq x \leq u
\end{align*}
\]

Globally convergent

**LCL (MINOS)**

\[
\begin{align*}
\text{minimize} & \quad L(x, y_k, \rho_k) \\
\text{s.t.} & \quad \text{linearized } c \\
& \quad \ell \leq x \leq u
\end{align*}
\]

Quadratically convergent
An Elastic LC Subproblem

\[
\min \quad \text{aug Lagrangian} \\
\text{subj to} \\
\text{bounds}
\]

\[
\begin{align*}
\text{minimize} \quad & \phi(x) - y_k^T c(x) + \frac{1}{2} \rho_k \|c(x)\|^2 \\
\text{s.t.} \quad & \ell \leq x \leq u
\end{align*}
\]
An Elastic LC Subproblem

\begin{align*}
\text{min} & \quad \text{aug Lagrangian} \\
\text{subj to} & \quad \text{linearized } c \\
\text{bounds} & \\
\text{minimize} & \quad \phi(x) - y_k^T c(x) + \frac{1}{2} \rho_k \| c(x) \|^2 \\
\text{s.t.} & \quad c_k(x) = 0, \quad \ell \leq x \leq u
\end{align*}
An Elastic LC Subproblem

\[
\begin{align*}
\text{min} & \quad \text{aug Lagrangian } + \ell_1 \text{ penalty function} \\
\text{subj to} & \quad \text{linearized } c + \text{ elastic vars, \ bounds} \\
\end{align*}
\]

\[
\begin{align*}
\begin{array}{ll}
\text{minimize} & \phi(x) - y_k^T c(x) + \frac{1}{2} \rho_k \|c(x)\|^2 + \sigma_k e^T (v + w) \\
\text{s.t.} & \bar{c}_k(x) + v - w = 0, \quad v, w \geq 0, \quad \ell \leq x \leq u \\
\end{array}
\end{align*}
\]
An Elastic LC Subproblem

minimize $\phi(x) - y_k^T c(x) + \frac{1}{2} \rho_k \|c(x)\|^2 + \sigma_k e^T (v + w)$

subject to $c_k(x) + v - w = 0$, $v, w \geq 0$, $\ell \leq x \leq u$

\[\Uparrow\]

minimize $\phi(x) - y_k^T c(x) + \frac{1}{2} \rho_k \|c(x)\|^2 + \sigma_k \|\bar{c}_k(x)\|_1$

subject to $\ell \leq x \leq u$
An Elastic LC Subproblem

\[
\begin{align*}
\text{min} & \quad \text{aug Lagrangian} + \ell_1 \text{ penalty function} \\
\text{subj to} & \quad \text{linearized } c + \text{ elastic vars}, \quad \text{bounds}
\end{align*}
\]

\[
\begin{align*}
\text{minimize} & \quad \phi(x) - y_k^T c(x) + \frac{1}{2} \rho_k \|c(x)\|^2 + \sigma_k e^T(v + w) \\
\text{s.t.} & \quad c_k(x) + v - w = 0, \quad v, w \geq 0, \quad \ell \leq x \leq u
\end{align*}
\]

- Subproblems are always feasible
- Multiplier estimates are controlled by \( \|\Delta y_k^*\|_\infty \leq \sigma_k \)
- Eventually, \( x_k^* \) is same as for MINOS subproblem
The Stabilized LCL (sLCL) Method

1. Solve subproblem with optimality tol $\omega_k$

   $$(x_k^*, y_k^*) \leftarrow \text{Elastic LC subproblem} \ (x_k, y_k, \rho_k, \sigma_k)$$

2. If $\|c(x_k^*)\| \leq \eta_k$
   
   Decrease $\rho_k$ (finitely often)
   
   Reset $\sigma_k$ (sufficiently large)
   
   Update $(x_{k+1}, y_{k+1}) \leftarrow (x_k^*, y_k^*)$

   else
   
   Reject $(x_k^*, y_k^*)$
   
   Increase $\rho_k$
   
   Decrease $\sigma_k$

- $\rho_k$ and $\sigma_k$ work together to ensure global convergence
- $\omega_k$ and $\eta_k$ are adjusted dynamically to save work
- cf. Conn, Gould, Sartenaer, & Toint, 1996
Sparse NLP  (Michael Friedlander & S 2004)

Fortran 90

- Dynamic memory
- LC solver “isolated”
- Threadsafe design (LC solver permitting)

LC subproblems

- Solve with MINOS or SNOPT
- Hot start on major itn 2, 3, 4, …
  (keep quasi-Newton Hessian or reduced Hessian)
- Early termination of subproblems
PDCO
Primal-Dual IPM for (Separable) Convex Opt
MATLAB (Saunders 1997–2004)

• Nominal problem

\[
\begin{align*}
\text{CO} & \quad \min \phi(x) \\
\text{s.t.} & \quad Ax = b, \quad \ell \leq x \leq u
\end{align*}
\]

• Regularized problem

\[
\begin{align*}
\text{COR} & \quad \min \phi(x) + \frac{1}{2} \|D_1 x\|^2 + \frac{1}{2} \|r\|^2 \\
\text{s.t.} & \quad Ax + D_2 r = b, \quad \ell \leq x \leq u
\end{align*}
\]

\[\nabla^2 \phi(x), \ D_1 \succeq 0, \ D_2 \succ 0, \ \text{all diagonal} \quad A \text{ can be an operator}\]
PDCO applications

• Basis Pursuit (Chen, Donoho, & S, 2001)
• Image reconstruction (Kim thesis, 2002)
• Maximum entropy (S & Tomlin, 2003)
**PDCO on Web Traffic entropy problem**

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

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$\text{PDitns} = 12$, $\text{LSQRitns} = 79$, $\text{time} = 101.4$ (MATLAB)

$\text{time} = 22.4$ (C++)
SpaseLoc

Localization of Wireless Sensor Networks

MATLAB (Holly Jin + Carter, Saunders & Ye, 2004)

minimize  \[ \sum_{(i,j) \in N_1} |\alpha_{ij}| + \sum_{(i,k) \in N_2} |\alpha_{ik}| \]

subject to
\[
\begin{align*}
\|x_i - x_j\|^2 - \alpha_{ij} &= d_{ij}^2, \quad \forall \ (n_{i,j}) \in N_1 \\
\|x_i - a_k\|^2 - \alpha_{ik} &= d_{ik}^2, \quad \forall \ (i, k) \in N_2 \\
\|x_i - x_j\|^2 &\geq r_{ij}^2, \quad \forall \ (i, j) \in \overline{N}_1, \\
\|x_i - a_k\|^2 &\geq r_{ik}^2, \quad \forall \ (i, k) \in \overline{N}_2,
\end{align*}
\]

\(x_i, x_j \in \mathbb{R}^2,\) \quad \(\alpha_{ij}, \alpha_{ik} \in \mathbb{R},\)

\(i < j:\) sensors  \quad k:\) anchors

\(d_{ij}\) noisy distance data  \quad \(a_k\) known positions of anchors

\(r_{ij}\) radio ranges  \quad \(x_i\) sensors’ positions (to be estimated)
Localization of Wireless Sensor Networks

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

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

- SpaseLoc (2004): Sequential SDP subproblems \( \text{DSDP 5.0} \)
  - 4000 nodes: 25 secs

\((\text{DSDP} = \text{SDP solver of Benson and Ye})\)
 Localization errors for full SDP model and **SpaseLoc**
LUSOL

Sparse LU + Updates (like Reid’s LA05)

G, M, S & W 1987
Revised 1989–2004
Part of Mike O’Sullivan’s thesis 2002

• Square or rectangular $A = LU$
• Markowitz strategy for sparsity
• Threshold strategies for stability and detecting rank
  - TPP Threshold Partial Pivoting
  - TRP Threshold Rook Pivoting
  - TCP Threshold Complete Pivoting
    - Rank-revealing
• Bartels-Golub updating
Threshold Pivoting

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Threshold Rook Pivoting is the right compromise for revealing singularity
LUSOL

BFP (Basis Factorization Package)

The engine for

MINOS
ZIP
MILES
PATH
SQOPT

Hence SNOPT and Knossos
lp_solve

Also Basis Repair

Square $B$ — fix singularity
Rectangular $(B \ S)$ — find better $B$
Summary

Key concepts for Nonlinear Optimization

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

Software

- MINOS, SNOPT in GAMS, AMPL, NEOS
- TOMLAB/SOL (Holmström) for MATLAB users
- SNOPT has its own MATLAB interface
- PDCO (MATLAB) \( \min \phi(x) \) s.t. \( Ax = b + \text{bounds} \), \( A \) an operator
- SpaseLoc (MATLAB) Scalable sensor localization
- LUSOL (C version) now in open source system lp_solve
- LUSOL (original F77) will be in COIN-OR
- SYMMLQ, MINRES, LSQR (F77, MATLAB) CG-type iterative solvers
Other SOL Research

• **Uday Shanbhag** (with Walter Murray)
  Stochastic nonlinear programming, equilibrium programming, nonlinear facility location problems

• **Che-Lin Su** (with Dick Cottle)
  MPEC and 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
  ...!!

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 of each accepted clipping receives a $5 Lotto Lucky Dip. The following clippings illustrate some characteristics of optimization problems in the real(?) world.

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.

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)
≥ or ≤?

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.
≥ or ≤?

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.
Stochastic optimization

Life is Uncertain.
Eat Dessert First. (Marie Callender T-shirt)

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.
0 or 1 is sometimes not enough

When Taupo police arrested a Bay of Plenty man for driving over the limit they discovered he was a bigamist

Nelson Mail, 5/04