Optimization Algorithms and Software at SOL

Michael Saunders
SOL and ICME, Stanford University

Computational Linear Algebra and Optimization for the Digital Economy

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Abstract

When a colleague knocks on your door with a mathematical problem, great joy ensues on both sides if you happen to have numerical software that can solve the problem. This is a reason for writing “general-purpose software”.

If the software is downloadable, similar happiness ensues when it gets used for unexpected applications. You learn about such cases if your software includes bugs(!) or Google does its usual precise search.

The Systems Optimization Laboratory (SOL) was founded by George Dantzig and Richard Cottle at Stanford University in 1974 to encourage algorithm and software development in traditional Operations Research areas. Dantzig’s group built increasingly challenging linear models of the US Economy (the PILOT linear programs), while Alan Manne continued to expand his nonlinear economic models (which began before large-scale optimization software existed). These spurred the development of MINOS at SOL (by the speaker and fellow New Zealander Bruce Murtagh) in parallel with Arne Drud’s development of CONOPT at the World Bank and then in Denmark.
In the 1980s, the SOL “Gang of 4” (Gill, Murray, Saunders, and Wright) developed “dense” solvers LSSOL, QPSOL, and NPSOL. After Philip Gill moved to UC San Diego, NPSOL became increasingly important for trajectory optimization at McDonnell-Douglas (now Boeing). This spurred the development of the large-scale optimizers SQOPT and SNOPT.

Many years later, MINOS, CONOPT, and SNOPT remain heavily used solvers within the GAMS and AMPL algebraic modeling systems (and on the NEOS server), and LUSOL remains the reliable “engine” for basis handling in MINOS, SQOPT, SNOPT, and other solvers such as PATH and lp_solve. A unique feature of LUSOL is its Threshold Rook Pivoting option for estimating the rank of a rectangular sparse matrix.

Other solvers developed at SOL include MINRES, MINRES-QLP, LSQR, LSMR, and PDCO. We review the mechanics of the solvers and some unexpected applications that they’ve been put to work on. We conclude with even more unexpected aspects of optimization reported by radio and TV audiences in New Zealand.
1. SOL
2. Solvers for $Ax \approx b$
3. Applications of linear solvers
4. Rank of stoichiometric matrices
5. Solvers for optimization
6. Applications of optimization solvers
7. Aerospace
8. AC
9. Optimization in NZ
SOL

Systems Optimization Laboratory
Stanford University
SOL

- Founded 1974 by George Dantzig and Richard Cottle
- Dantzig, Alan Manne: economic models (linear & nonlinear)
- Gill, Murray, Saunders, Wright: Software for optimization
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George Dantzig

Gene Golub
SOL

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Recent collaborators:

- Chris Paige (McGill), Sou-Cheng Choi (Chicago)
- David Fong (ICME and Facebook)
- Xiangrui Meng (ICME and LinkedIn)
- Jason Lee, Yuekai Sun (ICME)
- Ding Ma, Nick Henderson, Santiago Akle (ICME)

Recent collaborators:

- MINRES-QLP
- LSMR
- LSRN
- PNOPT
- LUSOL, PDCO

Funding:

- ONR, AFOSR, ARO, DOE, NSF, AHPCRC, . . . ,
- DOE DE-FG02-09ER25917, NIH U01-GM102098
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- Philip Gill, Elizabeth Wong (UC San Diego)
- Ronan Fleming, Ines Thiele (UCSD, Iceland, Luxembourg)

Optimization software
- MINRES-QLP
- LSMR
- LSRN
- PNOPT
- LUSOL, PDCO
- NPSOL, QPOPT, SQOPT, SNOPT, SQIC

Funding: ONR, AFOSR, ARO, DOE, NSF, AHPCRC, . . . , DOE DE-FG02-09ER25917, NIH U01-GM102098
Sparse linear equations $Ax = b$
and least squares problems $Ax \approx b$
Sparse direct methods for $Ax = b$ and $Ax \approx b$

- $A = LDU$
- $A = QR$
- Many sparse solvers

LUSOL (Stanford)
SPQR (Tim Davis, UFL)
HSL Library (RAL, UK)
Iain Duff, John Reid, Jennifer Scott, ... 

LUSOL, SPQR, MA27, MA47, MA57, MA67, MA77, ... offer rank-revealing capability for sparse matrices when used with suitable tolerances
Iterative solvers for $Ax \approx b$
Iterative methods for $Ax \approx b$

$A$ may be a sparse matrix
or an operator for computing $Av$ and/or $A^Tw$

$A$ maybe Hermitian or complex
$A$ may have any rank

- Symmetric $Ax = b$
  \[ A = \begin{bmatrix} 
  \end{bmatrix} \]
  MINRES-QLP

- min $\|Ax - b\|$
  \[ A = \begin{bmatrix} 
  \end{bmatrix} \text{ or } \begin{bmatrix} 
  \end{bmatrix} \text{ or } \begin{bmatrix} 
  \end{bmatrix} \]
  LSQR, LSMR

- Tall skinny min $\|Ax - b\|$
  \[ A = \begin{bmatrix} 
  \end{bmatrix} \text{ (real)} \]
  LSRN
LSQR, LSMR for min $\|Ax - b\|$

Golub-Kahan process generates

\[
U_k = \begin{bmatrix}
u_1 & u_2 & \ldots & u_k
\end{bmatrix}
\]

\[
V_k = \begin{bmatrix}
v_1 & v_2 & \ldots & v_k
\end{bmatrix}
\]

using products $Av_j, A^Tu_j$

$k$th approximation $x_k = V_k y_k$ for some $y_k$

Choose $y_k$ to minimize something
LSQR, LSMR for \( \min \| Ax - b \| \)

**Golub-Kahan process** generates

\[
U_k = \begin{bmatrix} u_1 & u_2 & \ldots & u_k \end{bmatrix} \\
V_k = \begin{bmatrix} v_1 & v_2 & \ldots & v_k \end{bmatrix}
\]

using products \( Av_j, A^T u_j \)

\( k \)th approximation

\( x_k = V_k y_k \) for some \( y_k \)

Choose \( y_k \) to minimize something

<table>
<thead>
<tr>
<th>Solver</th>
<th>Objective</th>
<th>Residual</th>
</tr>
</thead>
<tbody>
<tr>
<td>LSQR</td>
<td>( \min | r_k | )</td>
<td>( r_k = b - Ax_k )</td>
</tr>
<tr>
<td>LSMR</td>
<td>( \min | A^T r_k | )</td>
<td>residual for ( A^T Ax = A^T b )</td>
</tr>
</tbody>
</table>

For LS problems, LSQR, LSMR stop when

\[
\frac{\| A^T r_k \|}{\| r_k \|} \leq \alpha \| A \|
\]

(this is the Stewart backward error)
\[ \log_{10} \left( \frac{\|A^T r_k\|}{\|r_k\|} \right) \] (typical)  
LSMR can stop sooner
SG, MINRES for posdef $Ax = b$

**Lanczos process** generates  

$$V_k = \begin{bmatrix} v_1 & v_2 & \ldots & v_k \end{bmatrix}$$

using **products** $Av_j$

**$k$th approximation**  

$$x_k = V_k y_k \text{ for some } y_k$$

Choose $y_k$ to minimize something
CG, MINRES for posdef $Ax = b$

**Lanczos process** generates

$$V_k = \begin{bmatrix} v_1 & v_2 & \ldots & v_k \end{bmatrix}$$

using products $Av_j$

$k$th approximation

$$x_k = V_k y_k \text{ for some } y_k$$

Choose $y_k$ to minimize something

**CG** \[ \min \|x - x_k\|_A \text{ energy norm of error} \]

**MINRES** \[ \min \|r_k\| \]

They stop when

$$\frac{\|r_k\|}{\alpha \|A\| \|x_k\| + \beta \|b\|} \leq 1 \text{ (backward error argument)}$$
CG, MINRES for posdef $Ax = b$

Lanczos process generates

$$V_k = [v_1 \ v_2 \ \ldots \ v_k]$$

using products $Av_j$

$k$th approximation

$$x_k = V_k y_k \text{ for some } y_k$$

Choose $y_k$ to minimize something

*CG* \quad $\min \|x - x_k\|_A$ \quad energy norm of error

*MINRES* \quad $\min \|r_k\|$

They stop when

$$\frac{\|r_k\|}{\alpha \|A\| \|x_k\| + \beta \|b\|} \leq 1 \quad \text{(backward error argument)}$$

For posdef $A$, $\|x_k\| \nearrow$ for both methods *(Steihaug 1983, Fong 2011)*

Hence, backward error $\searrow$ for MINRES (but not for CG)
SOL Solvers ($Ax \approx b$) Applications ($Ax \approx b$) rank($S$) Solvers (optimization) Applications (optimization)

Aerospace AC NZ

$$\log_{10} \frac{\|r_k\|}{\|x_k\|} \text{ for } A \succ 0$$

MINRES can stop sooner

- Name:Schenk_AFE_af_shell8, Dim:504855x504855, nnz:17579155, id=11
- Name:Cannizzo_sts4098, Dim:4098x4098, nnz:72356, id=13
- Name:Simon_raefsky4, Dim:19779x19779, nnz:1316789, id=7
- Name:BenElechi_BenElechi1, Dim:245874x245874, nnz:13150496, id=22
Stoichiometric matrices in systems biology

Sparse matrices $S$

Rows: Chemical species

Cols: Chemical reactions
S for models 1, 2, 3, 4 (all similar)
S for Models 5, 6, 7, 8 (all similar)
Model 9 (Recon1)

nz = 14300
Model 10 (ThMa = Thermotoga maritima)
Model 11 (GlcAer)
$S$ for models 9, 10, 11
Rank of stoichiometric matrices

Conservation analysis for biochemical networks

Need $\text{rank}(S)$ and $\text{nullspace}(S^T)$
**rank(S) by SVD**

**Singular value decomposition** \( S = UDV^T \)

- \( U^TU = I \)  \( V^TV = I \)  \( D \) diagonal  \( \text{rank}(S) = \text{rank}(D) \)
- Ideal for rank-estimation but \( U, V \) are dense

- model 9 (Recon1)  2800 \( \times \)  3700  17 secs
- model 10 (ThMa)  15000 \( \times \)  18000  11 hours
- model 11 (GlcAer)  62000 \( \times \)  77000  \( \infty \)
Singular values of models 1–8

Dense SVD of $S^T$

$\log_{10}(\sigma_i)$
rank($S$) by QR

Householder QR factorization $SP = QR$

- $P = \text{col perm} \quad Q^TQ = I \quad R \text{ triangular} \quad \text{rank}(S) = \text{rank}(R)$
- Nearly as reliable as SVD
- Dense QR used by Vallabhajosyula, Chickarmane, Sauro (2005)
- Sparse QR (SPQR) now available: Davis (2013)

model 9 (Recon1) 2800 $\times$ 3700 0.1 secs
model 10 (ThMa) 15000 $\times$ 18000 2.5 secs
model 11 (GlcAer) 62000 $\times$ 77000 0.2 secs(!)
rank(S) by LUSOL with Threshold Rook Pivoting

\[ P_1SP_2 = LDL^T \]

- \( P_1, P_2 = \text{perms} \quad D \text{ diagonal} \quad \text{rank}(S) \approx \text{rank}(D) \)
- \( L, U \) well-conditioned
- \( L_{ii} = U_{ii} = 1 \)
- \( |L_{ij}| \quad \text{and} \quad |U_{ij}| \leq \text{factol} = 4 \) (or 2 or 1.2, 1.1, \ldots)
- LUSOL: Main engine in sparse linear/nonlinear optimizers MINOS, SQOPT, SNOPT

- model 9 (Recon1) 2800 × 3700 0.1 secs
- model 10 (ThMa) 15000 × 18000 4.0 secs
- model 11 (GlcAer) 62000 × 77000 158 secs
rank($S$) by LUSOL with Threshold Partial Pivoting

\[
P_1 S P_2 = LU
\]

- $P_1, P_2 = \text{perms}$, $U$ trapezoidal, $\text{rank}(S) \approx \text{rank}(U)$
- $L$ well-conditioned

- $L_{ii} = 1$
- $|L_{ij}| \leq \text{factol} = 4$ (or 2 or 1.2, 1.1, ...)

- LUSOL: Main engine in sparse linear/nonlinear optimizers MINOS, SQOPT, SNOPT

- model 9 (Recon1) $2800 \times 3700$ 0.1 secs
- model 10 (ThMa) $15000 \times 18000$ 0.2 secs
- model 11 (GlcAer) $62000 \times 77000$ 0.3 secs
SPQR vs LUSOL with Threshold Rook Pivoting

SPQR: \( S = QR \)

time (secs)

<table>
<thead>
<tr>
<th>model</th>
<th>( m )</th>
<th>( n )</th>
<th>( \text{rank}(S) )</th>
<th>( \text{nnz}(S) )</th>
<th>( \text{nnz}(Q) )</th>
<th>( \text{nnz}(R) )</th>
<th>( \text{SVD} )</th>
<th>( \text{SPQR} )</th>
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</thead>
<tbody>
<tr>
<td>Recon1</td>
<td>2766</td>
<td>3742</td>
<td>2674</td>
<td>14300</td>
<td>2750</td>
<td>21093</td>
<td>17.5</td>
<td>0.1</td>
</tr>
<tr>
<td>ThMa</td>
<td>15024</td>
<td>17582</td>
<td>14983</td>
<td>326035</td>
<td>844096</td>
<td>10595016</td>
<td>11hrs</td>
<td>2.5</td>
</tr>
<tr>
<td>GlcAer</td>
<td>62212</td>
<td>76664</td>
<td>62182</td>
<td>913967</td>
<td>1287</td>
<td>916600</td>
<td>infty</td>
<td>0.2</td>
</tr>
</tbody>
</table>

LUSOL: \( S = LDU \) \( |L_{ij}|, |U_{ij}| \leq 2.0 \)

<table>
<thead>
<tr>
<th>model</th>
<th>( \text{nnz}(L) )</th>
<th>( \text{nnz}(U) )</th>
<th>( \text{time} )</th>
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<tbody>
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<td>16463</td>
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<tr>
<td>ThMa</td>
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<tr>
<td>GlcAer</td>
<td>635571</td>
<td>1810491</td>
<td>186.2</td>
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<tr>
<td>ThMa</td>
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<td>330485</td>
<td>4.0</td>
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<tr>
<td>GlcAer</td>
<td>427456</td>
<td>1584188</td>
<td>157.9</td>
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**SPQR vs LUSOL with Threshold Rook Pivoting**

**SPQR:** \( S^T = QR \)

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<th>n</th>
<th>rank(S')</th>
<th>nnz(S)</th>
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<th>nnz(R)</th>
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**LUSOL:** \( S^T = LDU \) \(|L_{ij}|, |U_{ij}| \leq 2.0\)

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<tr>
<td>Recon1</td>
<td>12832</td>
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<tr>
<td>ThMa</td>
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<td>586.0</td>
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<td>9811</td>
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<td>0.2</td>
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<tr>
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<td>355475</td>
<td>14.8</td>
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<tr>
<td>GlcAer</td>
<td>1823067</td>
<td>711906</td>
<td>791.2</td>
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SPQR vs LUSOL with Threshold Partial Pivoting

SPQR: \[ S = QR \]

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LUSOL: \[ S = LU \]

\[ |L_{ij}|, |U_{ij}| \leq 2.0 \]

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<td>GlcAer</td>
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SPQR vs LUSOL with Threshold Partial Pivoting

\[
\text{SPQR: } S^T = QR \quad \text{time (secs)}
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\[
\text{LUSOL: } S^T = LU \quad |L_{ij}| \leq 2.0
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<tr>
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<td>316889</td>
<td>701139</td>
<td>176.5</td>
</tr>
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</table>
Rank of stoichiometric $S$

Perhaps

$$\text{Sparse LU with TPP} \quad P_1 S P_2 = LU$$

$L$ well-conditioned \quad \text{rank}(S) \approx \text{rank}(U)$

Then

$$\text{Sparse LU with TRP} \quad \tilde{P}_1 U \tilde{P}_2 = \tilde{L} \tilde{D} \tilde{U}$$

$\tilde{L}, \tilde{U}$ well-conditioned \quad \text{rank}(S) \approx \text{rank}(U) \approx \text{rank}(\tilde{D})$
Rank of stoichiometric $S$

Perhaps

$$\text{Sparse LU with TPP} \quad P_1SP_2 = LU$$

$L$ well-conditioned $\quad \text{rank}(S) \approx \text{rank}(U)$

Then

$$\text{Sparse LU with TRP} \quad \bar{P}_1U\bar{P}_2 = \bar{L}\bar{D}\bar{U}$$

$\bar{L}$, $\bar{U}$ well-conditioned $\quad \text{rank}(S) \approx \text{rank}(U) \approx \text{rank}(\bar{D})$

or

$$\text{Sparse LU with TPP} \quad \bar{P}_1U^T\bar{P}_2 = \bar{L}\bar{U}$$

$\bar{L}$ well-conditioned $\quad \text{rank}(S) \approx \text{rank}(U) \approx \text{rank}(\bar{U})$
LSQR

in parallel!
LSQR for tomography

Huang, Dennis, Wang, Chen 2013
A scalable parallel LSQR algorithm for solving large-scale linear system for tomographic problems: a case study in seismic tomography
_procedia computer science_ 18:581–590

\[
\min \|Ax - b\| \quad A = \begin{pmatrix}
261M \times 38M \\
5 \text{ billion nonzeros}
\end{pmatrix}
\]

- 3D structural seismology
- Modest-sized dataset from Los Angeles Basin (ANGF)
- Cray XT5 (Kraken) at Oak Ridge National Lab
- Parallelize \( y \leftarrow Ax + y \) and \( x \leftarrow A^Ty + x \)
- 2400 cores: 10 times faster than PETSc
- 19200 cores: 33 times faster than PETSc
SOL optimization solvers
Optimization solvers (dense)

- **LSSOL (f77):** \[ \min \|Xx - b\|^2 \quad \text{st} \quad \ell \leq \begin{pmatrix} x \\ Ax \end{pmatrix} \leq u \]

  Avoids forming $X^TX$
  We still don’t have a good method for sparse $X$ + constraints

- **QPOPT (f77):** \[ \min \frac{1}{2}x^THx \quad \text{st} \quad \ell \leq \begin{pmatrix} x \\ Ax \end{pmatrix} \leq u \]

  $H$ may be indefinite

- **NPSOL (f77):** \[ \min \phi(x) \quad \text{st} \quad \ell \leq \begin{pmatrix} x \\ Ax \\ c(x) \end{pmatrix} \leq u \]

Philip Gill has recently completed a new **NPSOL** that includes elastic bounds to handle infeasible QP subproblems (like **SQOPT** and **SNOPT**).
Optimization solvers (sparse)

- **MINOS** (f77): Sparse NLP
  No elastic bounds, but still widely used. f90 version half started.

- **SQOPT, SNOPT** (f77): Sparse convex QP + general NLP
  Elastic bounds, threadsafe, good for expensive functions

- **SNOPT9** (f2003): Gill, S, Wong
  Includes **SQIC** QP solver
  Switches from **SQOPT**’s reduced-gradient method to KKT-factorization +
  block-LU updates for problems with many degrees of freedom

- Change 1 line and recompile ⇒ everything in **quad precision**
  **SNOPT9**’s simplex implementation gives us solutions with
  **astounding accuracy**! Great for systems biologists!
NEOS

Free optimization solvers
via Argonne National Lab
(now Univ of Madison, Wisconsin)
### NEOS Solver Statistics for 1 year

#### 1 Oct 2012 -- 30 Sep 2013

**Total Jobs**: 1,264,001

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### NEOS Solver Statistics for 1 year

**Total Jobs**: 1264001

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DICOPT

MINLP solver

Ignacio Grossman, Carnegie-Mellon
MINLP model

- MS student Rui-Jie Zhou transferring from MS&E to EE, mentioned MINOS had been useful
- 2 papers in *Industrial Engineering and Chemistry Research*
  Zhou, Ji-Juan Li, Hong-Guang Dong, Ignacio Grossmann
- Part I (44 pages) Multiscale state-space superstructure for interplant water-allocation and heat-exchange networks design with direct and indirect integration schemes in fixed flow rate (FF) processes
- Part II (42 pages) Extends to fixed contaminant-load (FC) processes and integration of FF and FC processes
- Nonlinear objective
  1500 linear and nonlinear constraints
  1600 variables (some binary)
  GAMS/DICOPT = MINOS + CPLEX or CONOPT + CPLEX
MINLP model

Figure 1. State-space superstructure for stand-alone WAHEN
MINLP model

Figure 2. Multi-scale state-space superstructure for interplant WAHEN
MINLP model

Figure 3. Optimal interplant HEN configuration in Example 1
MINLP model

Figure 4. Optimal stand-alone WAHEN designs in Case 1 of Example 2
MINLP model

Figure 5. Optimal direct integrated WAHEN design in Case 2 of Example 2
MINLP model

[Diagram of a MINLP model showing various sources, sinks, and flows labeled with quantities and temperatures.]

---

Michael Saunders: Optimization software at SOL
CLAODE, ICMS, Edinburgh Oct 31–Nov 1, 2013 50/101
MINLP model

Lower total annualized cost can be obtained in all examples by solving the corresponding MINLP model
PDCO

Primal-dual interior method
for convex optimization
PDCO (Matlab primal-dual convex optimizer)

Nominally

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

\(\phi(x)\) is convex with known gradient and Hessian

For example, \(\phi(x) = c^T x\) or \(\lambda \|x\|_1\) or \(\sum x_j \log(x_j)\)

\(A\) may be a sparse matrix or an operator for \(Av\) and \(A^Tw\)

Basis Pursuit (BP)
Basis Pursuit denoising (BPDN)  
Chen, Donoho, & S (2001)
PDCO (Matlab primal-dual convex optimizer)

To ensure unique solutions, PDCO solves regularized problems:

$$\begin{align*}
\text{minimize} & \quad \phi(x) + \frac{1}{2} \|D_1 x\|^2 + \frac{1}{2} \|r\|^2 \\
\text{subject to} & \quad Ax + D_2 r = b, \quad \ell \leq x \leq u
\end{align*}$$

where $D_1, D_2$ are diagonal and positive-definite

- $D_1 = \gamma I$, $\gamma = 10^{-3}$ or $10^{-4}$
- $D_2 = \delta I$ for linear programs, $\delta = 10^{-3}$ or $10^{-4}$
- $D_2 = I$ for least squares
- Jacek prefers $D_1, D_2$ semi-definite and dynamic!
PDCO for LP feasibility

Regularized least squares with bounds:

\[
\begin{align*}
\text{minimize} \quad & \frac{1}{2} \| \gamma x \|^2 + \frac{1}{2} \| r \|^2 \\
\text{subject to} \quad & Ax + r = b, \quad \ell \leq x \leq u
\end{align*}
\]

\[\gamma = 10^{-4}\]
\[\text{declare feasible if } \| r \|_{\infty} \leq 10^{-4} \text{ say}\]
Regularized least squares with bounds:

\[
\begin{align*}
\text{minimize} & \quad \frac{1}{2} \| \gamma x \|^2 + \frac{1}{2} \| r \|^2 \\
\text{subject to} & \quad A x + r = b, \quad \ell \leq x \leq u
\end{align*}
\]

\[\gamma = 10^{-4}\]

declare feasible if \( \| r \|_\infty \leq 10^{-4} \) say

Jon Dattorro (2010)

- 10,000 \times 200,000 1.1M nonzeros
  - Solve 200,000 times with different \( b \)
- Gurobi: average 2 mins
- PDCO (Matlab): average 1 min
PDCO applied to FBA

Flux Balance Analysis = LP problem (Palsson 2006)

\[
\begin{align*}
\text{FBA} & \quad \text{minimize} \quad d^T v_e \\
& \quad \text{subject to} \quad S v_f - S v_r + S_e v_e = 0 \\
& \quad v_f, v_r \geq 0, \quad \ell \leq v_e \leq u
\end{align*}
\]

- \( d \) optimizes a biological objective
  
  e.g., maximize replication rate in unicellular organisms

- \( v_e = \text{exchange fluxes} = \text{sources and sinks of chemicals} \)

- PDCO works with \( A = \begin{bmatrix} S & -S & S_e \end{bmatrix} \) then \( LL^T = AD^2A^T \)
  
  (sparse Cholesky with \( D \) increasingly ill-conditioned)

- Solution is \( v^* = v^*_f - v^*_r \) and \( v^*_e \)
PDCO applied to Entropy problem

\[ \text{EP} \quad \min_{v_f, v_r} \quad v_f^T (\log v_f + c - e) + v_r^T (\log v_r + c - e) \]
subject to \( S v_f - S v_r = -S_e v_e^* \)
\( v_f, v_r > 0 \)

- \( c = \) any vector, \( e = (1, 1, \ldots, 1)^T \)
- \( v_e^* = \) optimal exchange fluxes from FBA
- Entropy objective function is strictly convex
- Solution \( v_f^*, v_r^* \) is thermodynamically feasible
  (satisfies energy conservation and 2nd law of thermodynamics)

Fleming, Maes, S, Ye, Palsson (2012)
PDCO applied to LR-NMR problems

Laplace Inversion of Low-Resolution NMR Relaxometry Data
Biotech and Environmental Engineering, Ben Gurion Univ, Israel
Determine composition of olive oil, rapeseed oil, biodiesel, ... 

\[ s(t) \approx \int_0^\infty e^{-t/T_2} x(T_2) \, dT_2 \quad x = \text{probability density} \]

Standard method (discretize):

\[
\min_{x \geq 0} \left\| \begin{pmatrix} A & \lambda I \end{pmatrix} x - \begin{pmatrix} s \\ 0 \end{pmatrix} \right\|_2^2
\]

- \( A = \text{discrete Laplace transform (fast operator)} \)
- \( \lambda = \text{Tikhonov regularization} \)
- Could apply PDCO to handle \( x \geq 0 \)
- Distorts solution by broadening peaks
PDCO applied to LR-NMR problems

Laplace inversion via basis pursuit denoising:

\[
\text{BPDN} \quad \begin{array}{ll}
\text{minimize} & \alpha \|x\|_1 + \frac{1}{2} \|\lambda x\|_2^2 + \frac{1}{2} \|r\|_2^2 \\
\text{subject to} & Ax + r = s : y \\
& x \geq 0
\end{array}
\]

- \(A = \text{discrete Laplace transform (fast operator)}\)
- PDCO solves \(\min \left\| \begin{pmatrix} DA^T \\ I \end{pmatrix} \Delta y - \begin{pmatrix} Dw \\ t \end{pmatrix} \right\|\) using LSMR, where posdef diagonal \(D\) becomes increasingly ill-conditioned
- \(\alpha\) helps resolve close adjacent peaks
\[ \alpha = 0 \]

\[ \alpha > 0 \]

Figure 6  Comparison of WinDXP (a)–(d) and PDCO using the universal regularization values for \( a_1 \) and \( a_2 \) (e)–(h) solutions on a real LR-NMR dataset acquired from an oil sample. The results are ordered by descending number of scans (descending SNR).
PDCO applied to LR-NMR problems

- **Berman, Leshem, Etziony, Levi, Parmet, S, Wiesman 2013**
  Novel $^1H$ low field nuclear magnetic resonance applications for the field of biodiesel
  *Biotechnology for Biofuels* 6:55, 20pp

- **Berman, Levi, Parmet, S, Wiesman 2013**
  Laplace inversion of low-resolution NMR relaxometry data using sparse representation methods
PDCO applied to LR-NMR problems

  Novel $^1\text{H}$ low field nuclear magnetic resonance applications for the field of biodiesel
  *Biotechnology for Biofuels* 6:55, 20pp

  Laplace inversion of low-resolution NMR relaxometry data using sparse representation methods

Problem setup (normal numerical people):

$$[U, S, V] = \text{svd}(A);$$
PDCO applied to LR-NMR problems

  Novel $^1H$ low field nuclear magnetic resonance applications for the field of biodiesel
  *Biotechnology for Biofuels* 6:55, 20pp

  Laplace inversion of low-resolution NMR relaxometry data using sparse representation methods

Problem setup (normal numerical people):

$$[U,S,V] = \text{svd}(A);$$

Astounding line of code (one coauthor):

$$[S,V,D] = \text{svd}(A); \quad (!)$$
SQOPT in quad precision
 Flux Balance Analysis (FBA) on Thermotoga maritima

\[
\min c^T v \quad \text{subject to} \quad Sv = 0, \quad \ell \leq v \leq u
\]

S rows and cols \(18210 \times 17535\)
Nonzero \(S_{ij}\) \(33602\)
max and min \(|S_{ij}|\) \(2 \times 10^4\) and \(3 \times 10^{-6}\)

SQOPT in double precision (15 digits)
Feasibility tol \(1e^{-6}\)
Optimality tol \(1e^{-6}\)

SQOPT in quad precision (32 digits)
Feasibility tol \(1e^{-15}\)
Optimality tol \(1e^{-15}\)
Flux Balance Analysis (FBA) on Thermotoga maritima

\[
\begin{align*}
& \text{min } c^T v \quad \text{subject to} \quad S v = 0, \quad \ell \leq v \leq u \\
& S \text{ rows and cols } 18210 \times 17535 \\
& \text{Nonzero } S_{ij} \quad 33602 \\
& \text{max and min } |S_{ij}| \quad 2 \times 10^4 \text{ and } 3 \times 10^{-6}
\end{align*}
\]

SQOPT in double precision \hspace{1em} (42 secs)

SQOPT EXIT 10 -- the problem appears to be infeasible

Problem name \hspace{1em} ThMa
No. of iterations \hspace{1em} 18500 \hspace{1em} Objective value \hspace{1em} 8.2286249495E-07
No. of infeasibilities \hspace{1em} 9 \hspace{1em} Sum of infeas \hspace{1em} 1.9606461069E-03
No. of degenerate steps \hspace{1em} 11611 \hspace{1em} Percentage \hspace{1em} 62.76
Max x \hspace{1em} (scaled) \hspace{1em} 3482 \hspace{1em} 8.2E+00 \hspace{1em} Max pi \hspace{1em} (scaled) \hspace{1em} 18210 \hspace{1em} 9.8E-01
Max x \hspace{1em} \hspace{1em} 5134 \hspace{1em} 5.9E+00 \hspace{1em} Max pi \hspace{1em} \hspace{1em} 18210 \hspace{1em} 1.0E+00
Max Prim inf(scaled) \hspace{1em} 32832 \hspace{1em} 1.3E-03 \hspace{1em} Max Dual inf(scaled) \hspace{1em} 16417 \hspace{1em} 1.0E+00
Max Primal infeas \hspace{1em} 32832 \hspace{1em} 5.6E-06 \hspace{1em} Max Dual infeas \hspace{1em} 32669 \hspace{1em} 2.3E+02
Flux Balance Analysis (FBA) on Thermotoga maritima

\[
\min c^T v \quad \text{subject to} \quad Sv = 0, \quad \ell \leq v \leq u
\]

S rows and cols \(18210 \times 17535\)
Nonzero \(S_{ij}\) \(33602\)
max and min \(|S_{ij}|\) \(2 \times 10^4\) and \(3 \times 10^{-6}\)

Restart SQOPT in quad precision \(36\) secs

SQOPT EXIT 0 -- finished successfully

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Flux Balance Analysis (FBA) on GlcAer

\[
\begin{align*}
\min \ c^T v & \quad \text{subject to} \quad Sv = 0, \quad l \leq v \leq u \\
S & \text{rows and cols} \quad 68300 \times 76664 \\
\text{Nonzero } S_{ij} & \quad 926357 \\
\max \text{ and min } |S_{ij}| & \quad 8 \times 10^5 \text{ and } 5 \times 10^{-5}
\end{align*}
\]

**SQOPT in quad precision**

```
SQOPT EXIT 0 -- finished successfully
```

**Problem name**   GlcAer
**No. of iterations**   84685  **Objective value** -7.0382454070E+05
**No. of degenerate steps**  62127  **Percentage** 73.36
**Max x**   61436  6.3E+07  **Max pi** 25539  2.4E+07
**Max Primal infeas**   72623  3.0E-21  **Max Dual infeas** 17817  2.7E-21
Flux Balance Analysis (FBA) on GlcAer

\[ \min c^T v \quad \text{subject to} \quad Sv = 0, \quad \ell \leq v \leq u \]

S rows and cols \( 68300 \times 76664 \)
Nonzero \( S_{ij} \) \( 926357 \)
max and min \( |S_{ij}| \) \( 8 \times 10^5 \) and \( 5 \times 10^{-5} \)

**SQOPT in quad precision**
cold start, with scaling (4642 secs)

SQOPT EXIT 0 -- finished successfully

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Flux Balance Analysis (FBA) on GlcAer

\[ \min c^T v \quad \text{subject to} \quad Sv = 0, \quad \ell \leq v \leq u \]

S rows and cols \(68300 \times 76664\)
Nonzero \(S_{ij}\) \(926357\)
max and min \(|S_{ij}|\) \(8 \times 10^5\) and \(5 \times 10^{-5}\)

SQOPT in quad precision
warm start, no scaling (28 secs)

SQOPT EXIT 0 -- finished successfully

Problem name GlcAer
No. of iterations 1 Objective value \(-7.0382454070E+05\)
No. of degenerate steps 0 Percentage 0.00
Max x 61436 \(6.3E+07\) Max pi 25539 \(2.4E+07\)
Max Primal infeas 141186 \(7.1E-21\) Max Dual infeas 14993 \(8.9E-23\)
Aerospace Applications
NASA Aerospace Applications

- **David Saunders**
  - 1970 Visit Stanford for 1 month (now 43 years)
  - 1973 Serra House, RA, MS (thanks to Gene)
  - 1974–present NASA Ames

- **Projects**
  - **OAW**  Oblique All-Wing supersonic airliner
  - **HSCT**  Supersonic airliner
  - **CTV**   SHARP shuttle design
  - **MSL**   Heat shield for landing Mars rover Curiosity
  - **CEV**   Heat shield for Apollo-type capsule to ISS/moon
OAW oblique all wing airliner
HSCT high speed civil transport
SHARP design (Slender Hypervelocity Aerothermodynamic Research Probes)
Aerothermal performance constraint in (Velocity, Altitude) space, used during trajectory optimization with UHTC materials (Ultra High Temperature Ceramics) to avoid exceeding material limits

- Trajectory optimization with SNOPT
- Could always abort to Kennedy, Boston, Gander, or Shannon
- 4000-mile cross-range capability during reentry

Image credit: David Kinney, NASA Ames Research Center
CEV crew exploration vehicle
McDonnell-Douglas Aerospace Applications

- Philip Gill, Rocky Nelson
  1979–1988 SOL QPSOL, LSSOL, NPSOL
  1988–2007 UC San Diego QPOPT, SQOPT, SNOPT
  McDonnell-Douglas Space Systems, LA (now Boeing)

- Projects
  - F-4 Minimum time-to-climb
  - DC-Y SSTO Minimum-fuel landing maneuver
F-4 minimum time-to-climb

Aerospace Applications

of NPSOL and SNOPT

OTIS #1
DC-Y single-stage-to-orbit
OTIS

DC-Y Landing Maneuver

Retract airbrakes at
2800 ft
420 mph
Control engineer
Feasible solution
1 year

2000 x 1200 NLP

NPSOL
Optimal solution
50% of fuel saved
DC-Y landing, 2nd OTIS/NPSOL optimization

- 1st optimization: starting altitude = 2800ft
- 2nd optimization: starting altitude = variable
- New constraint needed:
DC-Y landing, 2nd OTIS/NPSOL optimization

- 1st optimization: starting altitude = 2800ft
- 2nd optimization: starting altitude = variable
- New constraint needed: Don’t exceed 3g
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Optimum starting altitude = 1400ft(!)
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Optimum starting altitude = 1400ft(!)

Come back Alan Shephard!
Stanford Aerospace Applications

- Ilan Kroo  Stanford Aircraft Aerodynamics and Design Group
  Blended Wing-Body  Transonic airliner
Stanford Aerospace Applications

- **Ilan Kroo**  Stanford Aircraft Aerodynamics and Design Group
  Blended Wing-Body  Transonic airliner

- **Antony Jameson, Juan Alonso**  Aerospace Computing Lab
  MDO  Multidisciplinary Design Optimization
  ASO  Aerodynamic Shape Optimization
Blended wing airliner
Blended wing airliner

Ilan Kroo, Michael Holden, Aero/Astro Dept, Stanford 1999

- Compute control for stable flight of 17ft-span flying model
- Collocation model:
  - minimize wing weight (or move CG as far aft as possible)
  - subject to flutter constraints
- 9000 nonlinear equations
- 9000 state variables, 7 design variables

MINOS 5.5:

- 26 major iterations
- 4000 minor iterations (first 3000 = LP)
- 1500 constraint + Jacobian evaluations
- = 60000 function evaluations
- 3 days on SGI Octane
News Flash, 3 March 2007

- **Mike Ross** Naval Postgraduate School, Monterey
  
  **DIDO**: A package for solving optimal control problems
  Implemented in **MATLAB**
  Calls **TOMLAB/SNOPT** for the optimization

- **GMT 062:19:26**
  The International Space Station was successfully maneuvered using DIDO/TOMLAB/SNOPT
  Found zero propellant solutions (globally optimal)
  Saved NASA $1M fuel cost
America’s Cup Yacht Race

AC 95: NPSOL was used in different ways by both AC95 finalists

- **For Team Dennis Conner**, NPSOL was used with Boeing’s TRANAIR CFD system for optimal hull design of Young America

- **For Team NZ**, Andy Philpott (University of Auckland) used NPSOL to maximize the velocity around the course of 11 potential hull designs. One design appeared significantly faster and was chosen to become Black Magic
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AC 2013 (San Francisco Bay): NZ Herald blog
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- (Score 8–5) Come on whale, where are you?
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- I haven’t had so much fun since the cat died
- ...
- (Score 8–9) In the immortal words, 'bugga'
 Optimization in NZ
In New Zealand, the radio/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.

BALD, 36 yr old, handsome male seeking social times and fun with bald 22 years and upwards female

(NZ Car Magazine)

(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!

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.
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.

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

0 or 1

Sometimes neither is optimal
Binary variables

0 or 1  Sometimes neither is optimal

Integer variables

0 or 1 or 2 . . .
Binary variables

0 or 1
Sometimes neither is optimal

Integer variables

0 or 1 or 2 . . .

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.
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Final thoughts

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that we don’t learn from history

– G. W. F. Hegel
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Special thanks!

Jacek Gondzio
Rachael Tappenden
EPSRC, Maxwell Institute