Large-Scale Linear Algebra and Its Role in Optimization

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Abstract

Numerical optimization has always needed reliable numerical linear algebra. Some worries go away when we use quad-precision floating-point (as is now possible with the GCC and Intel compilers). quad-MINOS has proved useful in systems biology for optimizing multiscale metabolic networks, and in computer experimental design for optimizing the IMSPE function with finite-difference gradients (confirming the existence of twin points). Recently quad-MINOS gave a surprising solution to the optimal control problem spring200.

Quad versions of SNOPT and PDCO have been developed in f90 and C++ respectively. Changing a single line of source code leads to double-SNOPT or quad-SNOPT. The C++ PDCO can switch from double to quad at runtime.

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Award U01GM102098
Pre-history
Simplex via Cholesky

\[ B = LQ, \quad Q \text{ not kept, replace one col of } B \]

\[
LL^T \leftarrow LL^T + vv^T - ww^T
\]

or
\[
LL^T - ww^T + vv^T
\]

- Gill and Murray (1973) A numerically stable form of the simplex method
- Saunders (1972) Large-scale Linear Programming using the Cholesky Factorization

Perhaps a modern version is possible via \( LL^T \) or \( QR \):

  Supernodal Sparse Cholesky Factorization and Update/Downdate
- Davis (2011) Algorithm 915, SuiteSparseQR
  Multifrontal multithreaded rank-revealing sparse QR factorization
LU is more sparse than LQ

Early linear programming systems assumed $B$ is close to triangular.

- **Hellerman and Rarick (1971, 1972)** The (partitioned) preassigned pivot procedure $P^3$, $P^4$
- **Saunders (1976)** The complexity of LU updating in the simplex method, MINOS

$$
B = \begin{bmatrix}
\times & \times & \times & \times & \times & \times \\
\times & \times & \times & \times & \times & \times \\
\times & \times & \times & \times & \times & \times \\
\times & \times & \times & \times & \times & \times \\
\times & \times & \times & \times & \times & \times \\
\times & \times & \times & \times & \times & \times
\end{bmatrix}
$$
Markowitz LU is more sparse than $P^4$

Early 1980s: Rob Burchett, General Electric
Basis matrices were close to symmetric

Optimal Power Flow problem
Not good for $P^4$

Sparse LU with Markowitz merit function

- Duff and Reid (1977) Fortran subroutines for sparse unsymmetric linear equations, MA28
- Gill, Murray, S, & Wright (1987) Maintaining LU factors of a general sparse matrix, LUSOL

LUSOL does the linear algebra for MINOS, SQOPT, SNOPT, MILES, PATH, lp_solve
McDonnell Douglas

Huntington Beach, CA

SQP methods

NPSOL, SNOPT
Aerospace Applications of NPSOL and SNOPT

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

A reusable, single-stage-to-orbit-and-return space transportation system

Delta Clipper's robust vehicle design, streamlined ground turnaround, and autonomous flight operations are the keys to reliable, low-cost routine space transportation.
OTIS

DC-Y Landing Maneuver

Retract air brakes at

2800 ft
420 mph
Control engineer
Feasible solution
1 year

2000 x 1200 NLP
NPSOL
Optimal solution
50% of fuel saved

Linear Algebra and Optimization
DC-Y landing, 2nd OTIS/NPSOL optimization

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

Optimum starting altitude = 1400ft(!)

Come back Alan Shephard!
DC-X flying model
1/3 scale = 40ft tall

- 1993-95: DC-X made 8 flights
  Flight 8: demonstrated turnaround maneuver; hard landing damaged aeroshell

- 1996: DC-XA made 4 flights
  Flight 3: demonstrated 26-hour turnaround
  Flight 4: landing strut failed to extend; tipped over and exploded

- 1997: McDonnell Douglas merges with Boeing
  Huntington Beach campus becomes part of Boeing
  Philip continued 5-to-8 days for several years (till Rocky Nelson retired)
McDonnell Douglas motivation

The aerospace problems kept getting bigger

SQP needs Hessian $H$ for QP subproblems and null-space operator $Z$ for constraints

**NPSOL**
- dense quasi-Newton $H = R^T R$
- dense $Z$ from $J^T = QR$

**SNOPT**
- limited-memory $H$
- $Z$ from sparse $B = LU$ (reduced-gradient method)
- **SQIC** can switch from $B = LU$ to block-LU updates of $K$
Block-LU updates
Block-LU updates

- Bisschop and Meeraus (1977) Matrix augmentation and partitioning in updating the basis inverse
- Eldersveld and S (1992) A block-LU update for large-scale linear programming, MINOS/SC
- Huynh (2008) A large-scale QP solver based on block-LU updates of the KKT system, QPBLU
- Maes (2010) Maintaining LU factors of a general sparse matrix, QPBLUR
- Wong (2011) Active-set methods for quadratic programming, icQP
- Gill and Wong (2014) Software for large-scale quadratic programming, SQIC

\[
B_0 = L_0 U_0 \quad \text{LUSOL, BG updates}

B_k \equiv \begin{pmatrix} B_0 & V_k \\ E_k & \end{pmatrix} \quad \text{not implemented}

K_0 = L_0 U_0 \quad \text{LUSOL, MA57, MA97}

K_k \equiv \begin{pmatrix} K_0 & V_k \\ V_k^T & D_k \end{pmatrix} \quad \text{SuperLU, UMFPACK}
\]
Quad Precision
“Carrying somewhat more precision in the arithmetic than twice the precision carried in the data and available for the result will vastly reduce embarrassment due to roundoff-induced anomalies.”

“Default evaluation in Quad is the humane option.”

— William Kahan, 2011
### Double MINOS  Quad MINOS

<p>| | |</p>
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<tr>
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#### Hardware

We use this humane approach to Quad implementation

#### Software

2 source codes  2 programs
snopt9 = Double or Quad SQOPT, SNOPT

snPrecision.f90

module snModulePrecision
    integer(4), parameter :: ip = 4, rp = 8 ! double
    ! integer(4), parameter :: ip = 8, rp = 16 ! quad
end module snModulePrecision

module sn50lp

use snModulePrecision, only : ip, rp
subroutine s5solveLP ( x, y )
real(rp), intent(inout) :: x(nb), y(nb)

1 source code 2 programs
DQQ procedure
for multiscale LP and NLP

Developed for systems biology models of metabolism
Ding Ma, Laurence Yang, S, et al. (2017) Reliable and efficient solution of genome-scale models of Metabolism and macromolecular Expression
Double and Quad MINOS
Meszaros “problematic” LP test set

<table>
<thead>
<tr>
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<th>Itns</th>
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\(Pinf, Dinf = \log_{10} \text{Primal/Dual infeasibilities}\)
Systems biology multiscale LP modes

<table>
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Final $P_{\text{inf}}/\|x^*\|_\infty$ and $D_{\text{inf}}/\|y^*\|_\infty$ are $O(10^{-30})$
Quad NLP

Metabolic models and macromolecular expression (ME models)

Laurence Yang, UC San Diego
**Quadratic convergence of major iterations (Robinson 1972)**

quadMINOS 5.6  (Nov 2014)

Begin tinyME-NLP  cold start NLP with mu = mu0
Itn  304  -- linear constraints satisfied.
Calling funcon.  mu = 0.800000000000000000000000000000004
nnCon, nnJac, neJac  1073  1755  2681
funcon sets 2681 out of 2681 constraint gradients.
funobj sets 1 out of 1 objective gradients.

<table>
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<th>minor</th>
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<td>1.0E+01</td>
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</table>

EXIT -- optimal solution found 13.5 secs
Quasi-Newton optimization with finite-difference gradients
Design of computer experiments

Selden Crary, indie-physicist, 2015

\[ n = 11 \text{ points } (x_i, y_i) \text{ on } [-1, 1] \text{ square (one twin-point)} \]

\[[d, n, p, \theta_1, \theta_2] = [2, 11, 2, 0.128, 0.069]\]
Design of computer experiments
Selden Crary, physicist, 2015

**IMSPE-optimal designs (integrated mean-squared prediction error)**

\[
\min \ 1 - \text{trace}(B^{-1}A)
\]

\( A \) and \( B \): symmetric matrices of order \( n + 1 \)

\( B \) increasingly ill-conditioned if points approach each other

**2D, Gaussian covariance parameters \( \sigma, \theta_1, \theta_2 \)**

\[
A \propto \int_{-1}^{1} \int_{-1}^{1} \begin{bmatrix} 1 \\ \nu \end{bmatrix} \begin{bmatrix} 1 & \nu^T \end{bmatrix} \, dx \, dy
\]

\[
B = \begin{bmatrix} 0 & 1^T \\ 1 & V \end{bmatrix}
\]

\( \nu_i \) functions of \( \exp(\cdot) \) and \( \text{erf}(\cdot) \),

\[
V_{ij} = \sigma^2 e^{-\theta_1 (x_i - x_j)^2 - \theta_2 (y_i - y_j)^2}
\]
C∞ a.e.

“Post”, not pole

Need multistarts

With Maple, Selden has found twin-points, triple-points, … and a new class of rational functions (the Nu class)

Smooth sailing through the black-hole/white-hole event horizon

No string theory

No complex numbers in quantum mechanics

...
Pre-history McDonnell Douglas Block-LU updates Quad Precision DQQ procedure Quad NLP Finite-difference gradients PDCO spring200

IMSPE, 2D, \( n = 11, \theta = (0.128, 0.069) \)

Quad MINOS unconstrained optimization \( \in \mathbb{R}^{22} \) without gradients 6 secs

<table>
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<th>Itn</th>
<th>ph</th>
<th>pp</th>
<th>rg</th>
<th>step</th>
<th>objective</th>
<th>nobj</th>
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</table>

Search exit 7 -- too many functions.

EXIT -- optimal solution found

No. of iterations 239 Objective value 5.0276215358E-06
No. of calls to funobj 7538 Calls with mode=2 (f, known g) 244
Calls for forward differencing 4466 Calls for central differencing 1716
Max Primal infeas 0 0.0E+00 Max Dual infeas 2 1.1E-07

not great ↑
17 points on $[-1, 1]^2$ (two twin-points)

Quad MINOS design refined by Selden via MAPLE

After further downhill searching, both sets of twins are now close, confirming the conjecture of a true double–twin-point design. 20161106
Linear algebra question

\[ A, B \text{ real, symmetric, indefinite, ill-conditioned} \]
\[ \min \text{ IMSPE} = 1 - \text{trace}(B^{-1}A) \]
\[ \text{trace}(B^{-1}A) = \sum \lambda_i \]

- QZ algorithm ignores symmetry but avoids ill-conditioned \( L^{-1} \)
- Will QZ compute real \( \lambda_i \)?

Yuji Nakatsukasa (Oxford) is developing \texttt{qdwhgep.m} for \( Ax = \lambda Bx \) (real, symmetric)

- Congruence transformations are real \( P^TAPy = \lambda P^TBPy \)
- Eigenvalues can be complex conjugate pairs
- \( \text{trace}(B^{-1}A) = \sum \lambda_i \) will be real
PDCO in C++

Ron Estrin, UBC → Stanford
**PDCO in C++**

Matlab PDCO: regularized convex optimization ($D_1, D_2 > 0$, diagonal)

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

- Needed for huge metabolic LP models that are near-block-diagonal
- C++ has **double** and **float128** data-types
- Compiler generates multiple codes
- Switch from **double** to **quad** at run-time

1 source code 1 program
spring200

An optimal control problem
modeling a spring/mass/damper
min \( f(y, z, u) = \frac{1}{2} \sum_{t=0}^{T} z_t^2 \)

\[
y_{t+1} = y_t - 0.01y_t^2 - 0.004z_t + 0.2u_t \\
z_{t+1} = z_t + 0.2y_t \quad t = 0, \ldots, T - 1
\]

\[-1 \leq y_t \leq 0.2 \leq u_t \leq 0.2 \]

\( y_0 = 0 \quad y_T = 0 \quad z_0 = 10 \)

<table>
<thead>
<tr>
<th>Format</th>
<th>Opt tol</th>
<th>Majors</th>
<th>Minors</th>
<th>Superbasics</th>
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quad-MINOS gives an unexpectedly “clean” solution (many variables exactly zero, including control variables \( u_t \))
double-MINOS
quad-MINOS

spring200: Quad MINOS solution and bounds

solution
upper bounds
lower bounds

Linear Algebra and Optimization SIOPT17 Vancouver
PEG: Tireless teacher, author, implementer

- Let’s get things nice and sparkling clear.
- I’ve taught you much, my little droogies.
- It had been a wonderful evening and what I needed now, to give it the perfect ending, was a little of the Ludwig Van.

— Alex, in “Clockwork Orange”

HAPPY ROUND NUMBER droogie!