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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Pre-history

Simplex via Cholesky

$B = LQ$, Q not kept, replace one col of B

$$LL^T \leftarrow LL^T + vv^T - ww^T$$
$$\text{or } LL^T - ww^T + vv^T$$

- 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:

- Chen, Davis, Hager and Rajamanickam (2008) — Algorithm 887, CHOLMOD
  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

$$B = \begin{bmatrix} x & & & & & & & \\ & x & & & & & & \\ & x & x & * & & & & * \\ & x & x & x & & & & * \\ & & & x & x & & * & * \\ x & & & & x & x & * & * \\ & & x & x & x & x & x & \\ x & & & & x & x & x & x \end{bmatrix}$$

Markowitz LU is more sparse than P^4

Early 1980s: Rob Burchett, General Electric — Optimal Power Flow problem
Basis matrices were close to symmetric — Not good for P^4

Sparse LU with Markowitz merit function

- Duff and Reid (1977) — Fortran subroutines for sparse unsymmetric linear equations, MA28
- Reid (1982) — A sparsity-exploiting variant of the Bartels-Golub decomposition, LA05 LA15
- 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

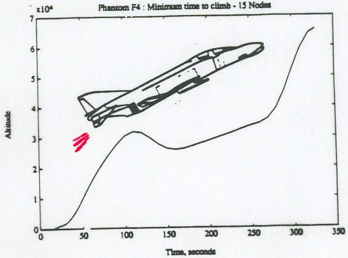
Huntington Beach, CA

SQP methods

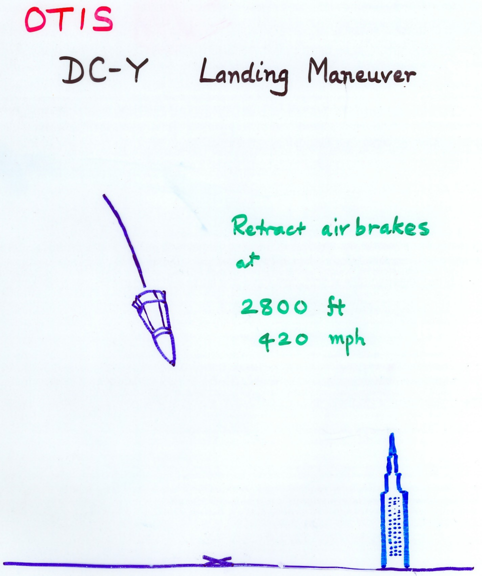
NPSOL, SNOPT

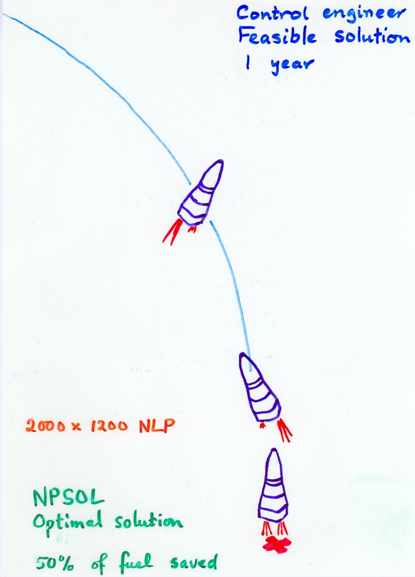
Aerospace Applications of NPSOL and SNOPT

OTIS #1



DC-Y single-stage-to-orbit


OTIS
DC-Y Landing Maneuver
Retract air brakes
at
2800 ft
420 mph


Control engineer
Feasible solution
1 year
2000 × 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: 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
- Gill, Murray, S, and Wright (1984) Sparse matrix methods in optimization
- 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
- Gill and Wong (2015) Methods for convex and general quadratic programming, SQIC

$B_0 = L_0 U_0$ LUSOL, BG updates

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

$K_0 = L_0 U_0$ LUSOL, MA57, MA97 SuperLU, UMFPACK

$$K_k \equiv \begin{pmatrix} K_0 & V_k \\ V_k^T & D_k \end{pmatrix}$$

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

Double MINOS	Quad MINOS
`real(8)`	`real(16)`
`eps = 2.22e-16`	`eps = 1.93e-34`
Hardware	Software

We use this humane approach to Quad implementation

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

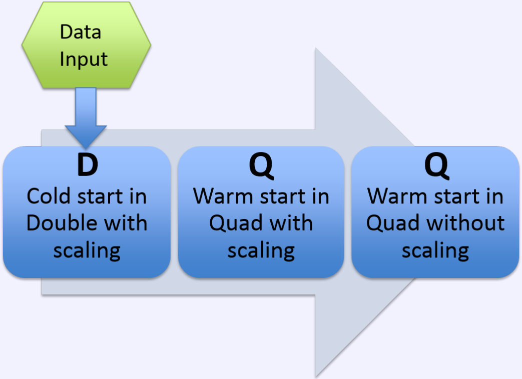
```
use snModulePrecision, only :  ip, rp
subroutine s5solveLP ( x, y )
real(rp), intent(inout) ::  x(nb), y(nb)
```

1 source code	2 programs

DQQ procedure
for multiscale LP and NLP

Developed for systems biology models of metabolism

DQQ procedure



- Ding Ma, Laurence Yang, MS, 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

	Itns	Times	Final objective	Pinf	Dinf
gen1	369502	205.3	−1.6903658594e−08	−06	−12
	246428	9331.3	1.2935699163e−06	−12	−31
	2394	81.6	1.2953925804e−06	−**45**	−**30**
gen2	44073	60.0	3.2927907828e+00	−04	−11
	1599	359.9	3.2927907840e+00	–	−29
	0	10.4	3.2927907840e+00	–	−**32**
gen4	45369	212.4	1.5793970394e−07	−06	−10
	53849	14812.5	2.8932268196e−06	−12	−30
	37	10.4	2.8933064888e−06	−**54**	−**30**
l30	1229326	876.7	9.5266141574e−01	−10	−09
	275287	7507.1	−7.5190273434e−26	−25	−32
	0	0.2	−4.2586876849e−24	−**24**	−**33**

Pinf, Dinf $= \log_{10}$ Primal/Dual infeasibilities

Systems biology multiscale LP modes

	Itns	Times	Final objective	Pinf	Dinf
TMA_ME	12225	37.1	8.0051076669e−07	−06	−05
	685	61.5	8.7036315385e−07	−24	−30
	0	6.7	8.7036315385e−07	**–**	**−31**
GlcAerWT	62856	9707.3	−2.4489880182e+04	+04	−05
	5580	3995.6	−7.0382449681e+05	−07	−26
	4	60.1	−7.0382449681e+05	**−19**	**−21**
GlcAlift	134693	14552.8	−5.1613878666e+05	−03	−01
	3258	1067.1	−7.0434008750e+05	−09	−26
	2	48.1	−7.0434008750e+05	**−20**	**−22**

Final Pinf/ $\|x^*\|_\infty$ and Dinf/ $\|y^*\|_\infty$ are $\mathbf{O(10^{-30})}$

Quad NLP

Metabolic models and macromolecular expression (ME models)

Laurence Yang, UC San Diego

Quadratic convergence of major iterations (Robinson 1972)

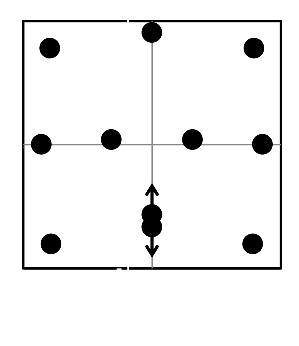
```
quadMINOS  5.6      (Nov 2014)

Begin tinyME-NLP   cold start NLP with mu = mu0
Itn       304 -- linear constraints satisfied.
Calling funcon.  mu =  0.8000000000000000000000000000000000004
nnCon, nnJac, neJac        1073        1755        2681
funcon  sets     2681   out of     2681   constraint gradients.
funobj  sets        1   out of        1   objective  gradients.

Major minor  step     objective  Feasible Optimal   nsb   ncon penalty
    1    304T 0.0E+00  8.00000E-01 6.1E-03 2.1E+03     0       4 1.0E+02
    2    561T 1.0E+00  8.00000E-01 2.6E-14 3.2E-04     0      46 1.0E+02
    3     40T 1.0E+00  8.28869E-01 5.4E-05 3.6E-05     0      87 1.0E+02
    4      7 1.0E+00  8.46923E-01 1.2E-05 2.9E-06     0      96 1.0E+02
    5      0 1.0E+00  8.46948E-01 4.2E-10 2.6E-10     0      97 1.0E+02
    6      0 1.0E+00  8.46948E-01 7.9E-23 1.2E-20     0      98 1.0E+01

EXIT -- optimal solution found                                13.5 secs
```

Quasi-Newton optimization with finite-difference gradients

Design of computer experiments

Selden Crary, indie-physicist, 2015

$n = 11$ points (x_i, y_i) on $[-1, 1]$ square (one twin-point)



[d,n,p,theta1,theta2]=[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 σ, θ_1, θ_2

$$A \propto \int_{-1}^{1}\int_{-1}^{1} \begin{bmatrix} 1 \\ v \end{bmatrix} \begin{bmatrix} 1 & v^T \end{bmatrix} dx\, dy \qquad B = \begin{bmatrix} 0 & \mathbf{1}^T \\ \mathbf{1} & V \end{bmatrix}$$

v_i functions of $\exp(\cdot)$ and $\text{erf}(\cdot)$, $\qquad V_{ij} = \sigma^2 e^{-\theta_1(x_i - x_j)^2 - \theta_2(y_i - y_j)^2}$

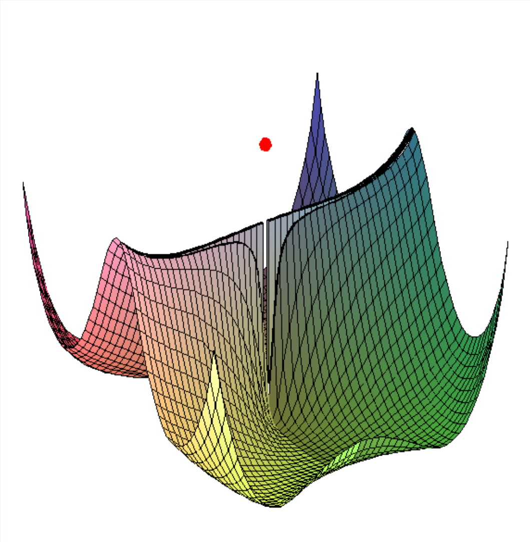
Pagoda plot of IMSPE function

Selden Crary, 2015

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

...

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

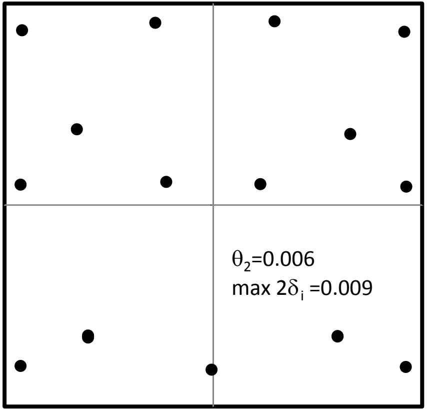
Quad MINOS   unconstrained optimization $\in \mathbb{R}^{22}$ without gradients   6 secs

```
 Itn ph pp      rg      step       objective      nobj  nsb  cond(H)
   1  4  0  3.9E-05  1.0E+03  2.47305090E-05    57   22  4.5E+01
  50  4  1  6.4E-07  6.2E+00  6.01181966E-06  1384   22  2.1E+04
 100  3  1 -7.6E-08  1.1E+00  5.65611811E-06  2726   22  1.4E+05
 150  4  1  8.5E-07  6.0E+00  5.11053080E-06  4102   22  8.2E+03
 200  4  1  2.6E-08  1.1E-01  5.02762155E-06  5464   22  1.0E+07
 239  4  1  1.1E-07  1.5E-06  5.02762154E-06  7478   22  1.0E+10
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 real, symmetric, indefinite, ill-conditioned

min IMSPE $= 1 - \text{trace}(B^{-1}A)$

cf. GEV problem $Ax = \lambda Bx$

$\text{trace}(B^{-1}A) = \sum \lambda_i$

- QZ algorithm ignores symmetry but avoids ill-conditioned B^{-1}
- Will QZ compute real λ_i?

Yuji Nakatsukasa (Oxford) is developing `qdwhgep.m` for $Ax = \lambda Bx$ (real, symmetric)

- Congruence transformations are real $\quad P^T APy = \lambda P^T BPy$
- 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 ($D_1, D_2 \succ 0$, diagonal)

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

- 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

spring200

$$\min \; f(y,z,u) = \frac{1}{2}\sum_{t=0}^{T} z_t^2$$

$$y_{t+1} = y_t - 0.01y_t^2 - 0.004z_t + 0.2u_t$$

$$z_{t+1} = z_t + 0.2y_t \qquad\qquad t = 0,\ldots,T-1$$

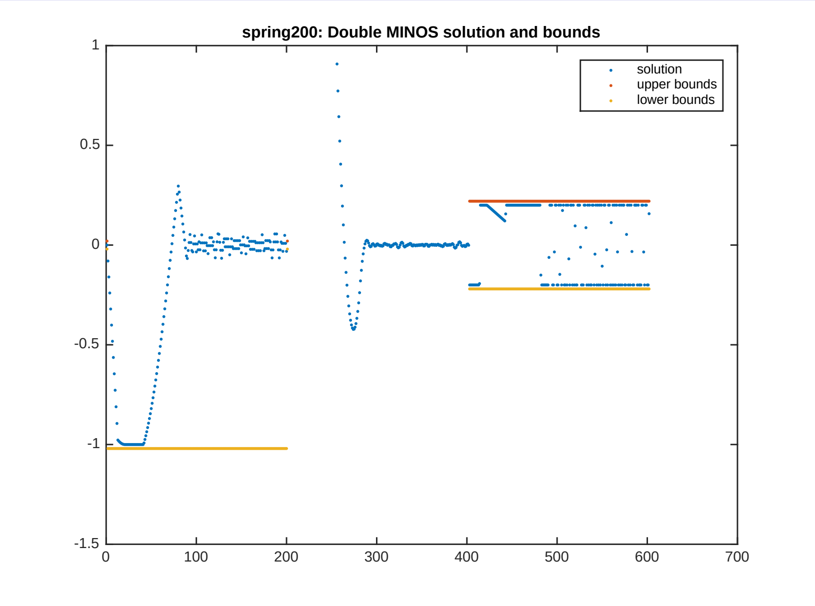
$$-1 \le y_t \qquad -0.2 \le u_t \le 0.2$$

$$y_0 = 0 \qquad y_T = 0 \qquad z_0 = 10$$

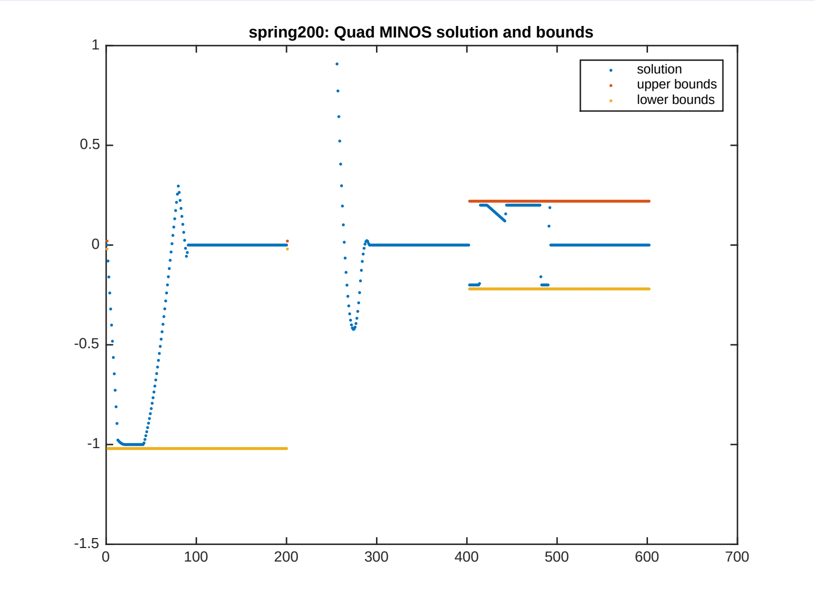
	Opt tol	Majors	Minors	Superbasics	Objective	Time
double	1e-06	13	576	18	1186.3839	0.05
quad	1e-15	31	1282	113	1186.3820	2.75

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
1
0.5
0
-0.5
-1
-1.5
0
100
200
300
400
500
600
700

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!