SPARSE MATRICES IN OPTIMIZATION

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Abstract

We review some of the standard matrix problems in numerical optimization, and the software tools that are available: LUSOL, LUMOD, MA27, MA47, MA48, etc. Direct methods are important because many similar systems have to be solved.

We then focus on some recent attempts to use Cholesky factorization on "quasi-definite" matrices of the form

$$K = \begin{pmatrix} H & A^T \\ A & -G \end{pmatrix} \quad \text{and} \quad K = \begin{pmatrix} H_0 + \gamma^2 I & A^T \\ A & -\delta^2 I \end{pmatrix},$$

where H and G are positive definite. Thus, $PKP^T = LDL^T$ with D diagonal but indefinite. Regularization $\gamma^2 = \delta^2 = 10^{-8}$ seems to give stability without seriously altering the problem.

For constrained least-squares problems, a few iterations of SYMMLQ or QMR might suffice, with preconditioners $L|D|L^T$ and LDL^T respectively.

References

[1] G. H. Golub and C. F. Van Loan (1979). Unsymmetric positive definite linear systems. *LAA*, 28, 85–98.

[2] R. J. Vanderbei (1994). Symmetric quasi-definite matrices. *SIOPT*, to appear. (Ultimately *SIAM J. Optim.*, 5(1):100-113, 1995.)

[3] P. E. Gill, M. A. Saunders and J. R. Shinnerl (1994). On the stability of Cholesky factorization for symmetric quasi-definite systems, *SIMAX*, to appear. (Ultimately *SIAM J. Matrix Anal. Appl.*, 17(1):35-46, 1996.)

Sparse Updates

LUSOL (Stanford)

- Markowitz $A = LU$ plus Bartels-Golub.
- Rectangular A, general rank-one updates.

MA48 (RAL)

- New sparse LU package.
- No updates.

LUMOD (Stanford)

- Dense $LC = U$.
- C square. Add, drop and replace rows and cols.
- L square, U triangular.

Bisschop and Meeraus (1977)

- Showed how to combine things like MA48 + LUMOD.
- See Gill, et al. (1984). Sparse matrix methods in optimization, *SISSC*, 5, 562–589.

LUMOD: $LC = U$
Updating a Sparse Dense Factorization

Conceptually

- Similar to $QC = R$.
- Easy to implement with 2-D Fortran arrays.
- Arithmetic is all *row* operations.

Row-wise storage

L square, U triangular, both in 1-D arrays:

$$L = \begin{pmatrix} 1 & 2 & 3 & . & . \\ 6 & 7 & 8 & . & . \\ 11 & 12 & 13 & . & . \\ . & . & . & . & . \\ . & . & . & . & . \end{pmatrix}, \qquad U = \begin{pmatrix} 1 & 2 & 3 & . & . \\ & 6 & 7 & . & . \\ & & 10 & . & . \\ & & & . & . \\ & & & & . \end{pmatrix}.$$

Diagonal U_{ii} is in $\mathtt{U}(k)$, $k = (i-1) * \mathtt{maxmod} + (3-i) * i/2$.

Future Sparse LU Packages

It helps to know if L or U is well-conditioned.

Barrier Methods for LP

min	$c^T x$
subject to	$Ax = b, \quad l \le x \le u$

$$\boxed{\quad A \quad} \approx 10000 \times 50000$$

Augmented systems

$$K = \begin{pmatrix} H & A^T \\ A & \end{pmatrix}, \qquad H \ge 0, \text{ diagonal}$$

- Most authors: reduce to $AD^2A^T \quad (H = D^{-2})$.
- Fourer and Mehrotra (1991): Markowitz LBL^T on

$$\bar{K} = \begin{pmatrix} \alpha I & DA^T \\ AD & \end{pmatrix}.$$

- Turner (1990): MA27 on K and $\bar{K}$.
- Gill, Murray, Ponceleón and Saunders (1991): MA27 on K.

Regularized LP

$$\begin{array}{ll} \text{minimize} & c^T x + \frac{1}{2}\|\gamma x\|^2 + \frac{1}{2}\|p\|^2 \\ \text{subject to} & Ax + \delta p = b, \quad l \le x \le u \end{array}$$

Augmented systems

$$K = \begin{pmatrix} H_0 + \gamma^2 I & A^T \\ A & -\delta^2 I \end{pmatrix}, \qquad H_0 \ge 0, \ \text{diagonal}$$

PDQ1 Version 1.0

- Gill, Murray, Ponceleón and Saunders (1991).
- Apply MA27 (Duff and Reid, 1982) to K or "reduced" K.
- Help MA27 by pivoting on some of H first.
- `Htol` $= 10^{-6}$, `factol` $= 0.01$, $\gamma, \delta = 10^{-5}$.
- γ, δ have little effect on fill-in.
- Has seemed too slow compared to Cholesky on AD^2A^T.

Quasi-definite Systems

Vanderbei (1991)

A matrix is *Symmetric Quasi-Definite* (SQD) if a symmetric permutation has the form

$$K = \begin{pmatrix} H & A^T \\ A & -G \end{pmatrix},$$

with H and G symmetric positive definite.

Theorem

If K is SQD, "Cholesky" factors $PKP^T = LDL^T$ exist for all permutations P.

LOQO

- Vanderbei (1992): LOQO User's Manual.
- Indefinite Cholesky on augmented-type system.
- Choose SQD principal submatrix (delay zero diagonals).
- Remaining matrix becomes SQD.
- In general, multi-tiered ordering.
- Cancellation can give $D_{jj} = 0$. Change to $\sqrt{\epsilon}$!

SQD Theory

Observation (1993)

$$K\begin{pmatrix} I & \\ & -I \end{pmatrix} = \begin{pmatrix} H & -A^T \\ A & G \end{pmatrix},$$

Unsymmetric but *Positive Definite*

Golub and Van Loan (1979)

- If A is positive definite, $A = LU$ exists without permutations.
- If T and S are symmetric and skew-symmetric parts, LU is stable if $\|ST^{-1}S\|/\|A\|$ is "small".

Gill, Saunders and Shinnerl (1994)

$$\text{“}A\text{”} = \begin{pmatrix} H & -A^T \\ A & \delta^2 I \end{pmatrix}, \qquad ST^{-1}S = -\begin{pmatrix} \frac{1}{\delta^2}A^TA & \\ & AH^{-1}A^T \end{pmatrix}$$

- $\|ST^{-1}S\| = \max\{\frac{1}{\delta^2}, \frac{1}{\gamma^2}\}$.
- For $Kd = r$ with $\gamma = \delta$: $\quad \text{cond}(K) \approx \frac{1}{\delta^2}\kappa_2(K)$.

Barrier Method for LP

$$K = \begin{pmatrix} H & A^T \\ A & -\delta^2 I \end{pmatrix}, \qquad H = H_0 + \gamma^2 I, \quad \text{diagonal}$$

The Scene

- 20 to 40 iterations.
- Two systems $Kd = r$ each iteration.
- With γ, δ zero, $\text{cond}(H), \text{ cond}(K) \to \infty$.
- With γ, δ small, $\text{cond}(H), \text{ cond}(K)$ still grow large.

PDQ1

- "Dangerous" pivots tols initially (small `Htol`, `factol`).
- Guard against instability:

$$\text{Require} \quad \|r - Kd\|/\|r\| \le 10^{-5}.$$

- Iterative refinement if necessary.
- Tighter pivot tols if necessary.

Choices: Scaling of K

$$K = \begin{pmatrix} H & A^T \\ A & \end{pmatrix}, \qquad H \text{ diagonal}$$

Ill-conditioned H

- Some $H_{jj} \to \infty$; some $H_{jj} \to 0$.
- $\|A\| \approx 1$.
- Change to $\bar{K} = SKS$, for some $S = \operatorname{diag}(D, I)$.

Choices

- Fourer and Mehrotra; Turner:

  $$D = H^{-1/2}, \qquad \bar{K} = \begin{pmatrix} \alpha I & DA^T \\ AD & \end{pmatrix}.$$

  MA27 Factor more sparse, but $\|AD\| \to \infty$ seems risky.

- PDQ1:

  $$\text{Use } \max\{\operatorname{diag}(H), 1\}, \qquad \bar{K} = \begin{pmatrix} \bar{H} & DA^T \\ AD & \end{pmatrix}.$$

  Scale down big diagonals of H, so $\|\bar{H}\| = 1$, $\|AD\| \approx 1$.
  Require $\|\bar{r} - \bar{K}\bar{d}\| / \|\bar{r}\| \le 10^{-5}$.

Choices: Which Matrix to Factor?

$$K = \begin{pmatrix} H & A^T \\ A & -\delta^2 I \end{pmatrix}, \qquad H = H_0 + \gamma^2 I, \text{ diagonal}$$

Assume K is scaled

$$\|H\| \approx 1, \quad \|A\| \approx 1.$$

Choices

- `Htol` $= 10^{30}$ Factorize Full K.
- `Htol` $= 10^{-8}$ Pivot on some of H first ("Reduced K").
- `Htol` $= 0.0$ Pivot on all of H ("Normal Equations").

We prefer second choice.

Choices: Partitioning H and A

$$H \text{ diagonal}, \qquad A = \begin{pmatrix} N & B \end{pmatrix},$$

$$K = \begin{pmatrix} H_N & & N^T \\ & H_B & B^T \\ N & B & -\delta^2 I \end{pmatrix}.$$

Pivot on H_N

MA27 or MA47 see the "reduced KKT system"

$$K_B = \begin{pmatrix} H_B & B^T \\ B & -NH_N^{-1}N^T - \delta^2 I \end{pmatrix}.$$

Conventional logic from sparse LU

Make sure H_N is "big" (diag $\geq$ `Htol`),
N is "sparse" (<10 nonzeros per column).

Choices

- Originally: `Htol` $= 10^{-6}$, $\gamma^2, \delta^2 = 10^{-10}$.
  Needs new Analyze when partition changes.
- Now: `Htol` $= 10^{-8}$, $\gamma^2, \delta^2 = 10^{-8}$.
  Usually just one Analyze.

MA27 versus MA47

MA27

- Analyze: Good.
- Factor: Initially good, but increasingly dense.

MA47

- First seemed disappointing.
- Analyze: 20%–50% more nonzeros.
- Factor: same increase in nonzeros.
- Sometimes a little faster.

MA47 Tree Amalgamation

- Decreases indirect addressing (but more ops).
- Two nodes are merged only if both involve less than k eliminations.
- Default $k = 8$.
- Compare with $k = 2$.
- `factol` $= 0.01$ magnifies the effect.

MA47, Amalgamation of Tree Nodes

KKT matrix:	LP problem	PILOTJA
	Dimension	2900
	Entries	15000
	Negative eigs	940
factol:	CNTL(1)	0.01
Tree amalg:	ICNTL(6)	8 and 2

	MA27		MA47 (8)		MA47 (2)	
	Analyze		Analyze		Analyze	
	63000		100000		70000	
itn	Factor	ntwo	Factor	ntwo	Factor	ntwo
1	66000	122	101000	393	72000	116
2	67	124	102	396	73	118
3	68	126	103	394	74	113
4	69	131	104	389	75	116
5	70	141	106	392	76	124
10	83	212	119	431	90	190
15	90	250	126	441	95	217
20	109	341	140	468	114	279
25	130	579	157	595	133	524
26	133	670	159	667	135	616
27	137000	705	162000	704	136000	668

		MA27 Time	MA47 (8) Time	MA47 (2) Time
Analyze	1	1.00	0.92	1.01
Factor	27	31.88	38.19	38.52
Solve	54	1.64	2.44	1.96
Total secs		37.30	44.26	44.22

DEC Alpha 3000/400 133MHz OpenVMS Fortran real*8
25-Jun-1994 $disk1:[MIKE.PDQ1.OPT]icntl6.pilotja

MA47, Amalgamation of Tree Nodes

```
KKT matrix:  LP problem         GROW22
             Dimension            1400
             Entries              6000
             Negative eigs         450

factol:      CNTL(1)              0.01
Tree amalg:  ICNTL(6)         8  and  2
```

	MA27		MA47 (8)		MA47 (2)	
	Analyze		Analyze		Analyze	
	20400		37000		26000	
itn	Factor	ntwo	Factor	ntwo	Factor	ntwo
1	20400	1	37000	45	26000	1
2	23	0	37	47	28	0
3	31	32	40	71	33	74
4	37	35	42	106	37	111
5	46	86	51	80	43	85
10	72	204	91	155	108	125
15	87	385	118	325	120	253
16	84	403	191	353	133	268
17	84	423	146	402	169	379
18	83500	437	219000	393	195000	385

		Time	Time	Time
Analyze	1	0.26	0.27	0.27
Factor	18	11.39	26.26	45.04
Solve	40	0.83	1.11	1.06
Total secs		13.51	28.64	47.42

```
DEC Alpha 3000/400   133MHz   OpenVMS   Fortran    real*8
28-Jun-1994          $disk1:[MIKE.PDQ1.OPT]icntl6.grow22
```

Progress At Last!

Fourer and Mehrotra (1993)

Implemented barrier method with their own LBL^T code for augmented systems

$$\bar{K} = \begin{pmatrix} \alpha\beta I & DA^T \\ AD & \end{pmatrix}, \qquad \beta = \|AD\|_\infty.$$

- Markowitz strategy as in MA47.
- Combined Analyze/Factor as in MA28, LUSOL, etc.
- Initially `factol` $= 16^{-6}$, $\alpha = 16^{-2}$.
- Keep pivot order if $\|r - \bar{K}d\|/\|r\| \leq 10^{-5}$.
- Increase `factol` to 16^{-5}, 16^{-4}, $\ldots$, 16^{-1}.
- Decrease α to 16^{-3}, 16^{-4}, $\ldots$.
- Most problems need only 1 or 2 orderings.

Implications for PDQ1 with Regularization

- $16^{-6} = 10^{-7.2}$.
- SQD theory suggests `factol` $= 10^{-30}$ first (LDL^T).
- Stabilize with `factol` $= 10^{-8}, 10^{-7}, 10^{-6}, \ldots$ (LBL^T).
- PDQ1 Version 1.0 (MA27) better with $\gamma^2, \delta^2 = 10^{-6}$.
- PDQ1 Version 2.0 (MA47) happy with $\gamma^2, \delta^2 = 10^{-8}$.

MA27, MA47: LDL^T then LBL^T
Full K, $\gamma^2, \delta^2 = 10^{-8}$

LP Problem	25FV47	Size of Full K	2700
Nonzeros	13400	Negative eigenvalues	821

MA27	No. of calls	Time
A x	154	0.23
A'y	150	0.43
Form KB	30	0.36
Analyze	1	0.69
Factor	30	17.29
Solve	74	1.69
Total		22.33

MA47	No. of calls	Time
A x	98	0.12
A'y	94	0.22
Form KB	23	0.24
Analyze	1	0.58
Factor	23	12.04
Solve	46	1.59
Total		16.06

itn	factol	nz	realA	realB	ntwo
1	1.0E-30	13402	53438	53438	0
2	1.0E-30	13402	53438	53438	0
3	1.0E-30	13402	53438	53438	0
4	1.0E-30	13402	53438	53438	0
5	1.0E-30	13402	53438	53438	0
10	1.0E-30	13402	53438	53438	0
15	1.0E-30	13402	53438	53438	0
16	1.0E-30	13402	53438	53438	0
17	1.0E-30	13402	53438	53438	0
18	1.0E-30	13402	53438	53438	0
18	1.0E-08	13402	53438	54015	96
18	1.0E-07	13402	53438	55482	160
19	1.0E-07	13402	53438	55881	157
20	1.0E-07	13402	53438	56458	152
21	1.0E-07	13402	53438	58523	148
21	1.0E-06	13402	53438	67856	201
21	1.0E-05	13402	53438	80899	282
22	1.0E-05	13402	53438	90809	337
23	1.0E-05	13402	53438	100660	418
23	1.0E-04	13402	53438	108528	537
24	1.0E-04	13402	53438	110520	565
24	1.0E-03	13402	53438	115260	670

17 refinements, starting at itn 13.
4 Backtracks. (Poor search direction until factol = 1.0E-3)

itn	factol	nz	realA	realB	ntwo
1	1.0E-30	13402	90596	90596	0
2	1.0E-30	13402	90596	90596	0
3	1.0E-30	13402	90596	90596	0
4	1.0E-30	13402	90596	90596	0
5	1.0E-30	13402	90596	90596	0
10	1.0E-30	13402	90596	90596	0
15	1.0E-30	13402	90596	90596	0
16	1.0E-30	13402	90596	90596	0
17	1.0E-30	13402	90596	90596	0
18	1.0E-30	13402	90596	90596	0
19	1.0E-30	13402	90596	90596	0
20	1.0E-30	13402	90596	90596	0
21	1.0E-30	13402	90596	90596	0
22	1.0E-30	13402	90596	90596	0
23	1.0E-30	13402	90596	90596	0

No iterative refinement.

MA27, MA47: LDL^T then LBL^T
Full K, $\gamma^2, \delta^2 = 10^{-8}$

LP Problem	PILOTJA	Size of Full K	2900
Nonzeros	15000	Negative eigenvalues	940

MA27	No. of calls	Time
A x	172	0.40
A'y	168	0.58
Form K	31	0.42
Analyze	1	0.99
Factor	31	21.55
Solve	83	1.91
Total		27.94

MA47	No. of calls	Time
A x	120	0.25
A'y	116	0.38
Form K	28	0.33
Analyze	1	0.67
Factor	28	21.13
Solve	57	2.19
Total		26.76

MA27:

itn	factol	nz	realA	realB	ntwo
1	1.0E-30	14996	63013	63013	0
2	1.0E-30	14996	63013	63013	0
3	1.0E-30	14996	63013	63013	0
4	1.0E-30	14996	63013	63013	0
5	1.0E-30	14996	63013	63013	0
10	1.0E-30	14996	63013	63013	0
15	1.0E-30	14996	63013	63013	0
16	1.0E-30	14996	63013	63013	0
17	1.0E-30	14996	63013	63013	0
18	1.0E-30	14996	63013	63013	0
19	1.0E-30	14996	63013	63013	0
19	1.0E-08	14996	63013	63641	86
20	1.0E-08	14996	63013	63701	88
20	1.0E-07	14996	63013	63863	108
21	1.0E-07	14996	63013	63863	107
22	1.0E-07	14996	63013	63935	110
23	1.0E-07	14996	63013	64297	126
24	1.0E-07	14996	63013	65056	140
25	1.0E-07	14996	63013	67695	166
26	1.0E-07	14996	63013	70329	177
26	1.0E-06	14996	63013	75131	249
26	1.0E-05	14996	63013	83075	313
27	1.0E-05	14996	63013	90623	378

24 refinements, starting at itn 4.
1 Backtrack. (Poor search direction
until factol = 1.0E-5)

MA47:

itn	factol	nz	realA	realB	ntwo
1	1.0E-30	14996	101250	101250	0
2	1.0E-30	14996	101250	101250	0
3	1.0E-30	14996	101250	101250	0
4	1.0E-30	14996	101250	101250	0
5	1.0E-30	14996	101250	101250	0
10	1.0E-30	14996	101250	101250	0
15	1.0E-30	14996	101250	101250	0
16	1.0E-30	14996	101250	101250	0
17	1.0E-30	14996	101250	101250	0
18	1.0E-30	14996	101250	101250	0
19	1.0E-30	14996	101250	101250	0
20	1.0E-30	14996	101250	101250	0
21	1.0E-30	14996	101250	101250	0
22	1.0E-30	14996	101250	101250	0
23	1.0E-30	14996	101250	101250	0
24	1.0E-30	14996	101250	101250	0
25	1.0E-30	14996	101250	101250	0
26	1.0E-30	14996	101250	101250	0
26	1.0E-08	14996	101250	102600	301
27	1.0E-08	14996	101250	103638	312

1 iterative refinement.

MA27, MA47: LDL^T then LBL^T
Reduced K, $\gamma^2, \delta^2 = 10^{-8}$

LP Problem	PILOTJA	Size of Reduced K	1300
Nonzeros	17000	Negative eigenvalues	940

MA27	No. of calls	Time	MA47	No. of calls	Time
A x	226	0.54	A x	114	0.31
A'y	222	0.69	A'y	110	0.30
Form K	30	0.49	Form K	27	0.33
Analyze	3	2.59	Analyze	1	0.46
Factor	30	17.67	Factor	27	15.00
Solve	110	1.86	Solve	54	1.40
Total		26.25	Total		19.50

MA27:

itn	factol	nz	realA	realB	ntwo
1	1.0E-30	17163	55321	55321	0
2	1.0E-30	17163	55321	55321	0
3	1.0E-30	17163	55321	55321	0
4	1.0E-30	17163	55321	55321	0
5	1.0E-30	17163	55321	55321	0
10	1.0E-30	17163	55321	55321	0
20	1.0E-30	17163	55321	55321	0
25	1.0E-30	17163	55321	55321	0
26	1.0E-30	17163	55321	55321	0
26	1.0E-08	17163	55321	56308	22
27	1.0E-08	17163	55321	56779	21
27	1.0E-07	17021	56479	68642	110
27	1.0E-06	16901	58392	77186	200

53 refinements, starting at itn 1.

MA47:

itn	factol	nz	realA	realB	ntwo
1	1.0E-30	17163	74254	74074	0
2	1.0E-30	17163	74254	74254	0
3	1.0E-30	17163	74254	74254	0
4	1.0E-30	17163	74254	74254	0
5	1.0E-30	17163	74254	74254	0
10	1.0E-30	17163	74254	74254	0
20	1.0E-30	17163	74254	74254	0
25	1.0E-30	17163	74254	74251	0
26	1.0E-30	17163	74254	74248	0
27	1.0E-30	17163	74254	74251	0

No iterative refinement.

PDQ1 with MA47
Full K, Reduced K, Normal Eqns

```
Times for First 53 Netlib LP Problems
(Seconds on DEC Alpha 3000/400)

Regularization:  gamma  = delta  = e-4
MA47 stability:  factol = e-30 initially         (LDL', D indefinite)
                        = e-8, e-7, ... if needed (LBL')
```

	Full K	Reduced K ndense = 10	Normal eqns
AFIRO	.10	.07	.09
ADLITTLE	.20	.17	.16
SC205	.42	.28	.29
SCAGR7	.33	.24	.23
SHARE2B	.29	.23	.20
RECIPE	.44 *	.32 *	.27
VTPBASE	.72	.52	.53
SHARE1B	.60	.43	.43
BORE3D	1.02	.82	.90
SCORPION	.70	.53	.55
CAPRI	1.55	1.27	1.68 *
SCAGR25	1.23	.86	.87
SCTAP1	1.01	.67	.69
BRANDY	1.13	.89	1.08
ISRAEL	1.36	1.00	4.18
ETAMACRO	3.69	2.55	2.55
SCFXM1	1.56	1.14	1.21
GROW7	1.44 *	.99	1.09
BANDM	1.38	1.08	1.14
E226	1.56	1.25	1.18
STANDATA	2.11	1.13	1.16
SCSD1	.73	.32	.34
GFRDPNC	1.87	1.23	1.22
BEACONFD	1.25	1.17	1.76
STAIR	2.93	2.18	3.97
SCRS8	2.74	1.95	1.95
SEBA	2.45	1.57	33.07
SHELL	3.52	2.07	2.09
PILOT4	4.54	3.61	6.22
SCFXM2	3.55	2.52	2.80
SCSD6	1.60	.71	.71
GROW15	3.26 *	2.10	2.54
SHIP04S	3.19	1.45	1.44
FFFFF800	8.28	6.13	6.94

	Full K		Reduced K	Normal eqns
GANGES	5.16		4.22	5.49
SCFXM3	5.30		3.78	4.18
SCTAP2	4.98		3.47	3.53
GROW22	4.71	*	3.08	3.73
SHIP04L	4.98		2.03	1.99
PILOTWE	11.51		7.95	8.08
SIERRA	5.74		3.98	4.05
SHIP08S	4.82		2.35	2.37
SCTAP3	7.09		4.85	4.88
SHIP12S	5.72		3.02	2.97
25FV47	16.22		11.62	10.69
SCSD8	3.20		1.65	1.69
NESM	12.39		8.38	8.91
CZPROB	15.62		6.64	6.55
PILOTJA	27.00	*	19.51	27.25
SHIP08L	9.73		3.87	3.85
SHIP12L	14.04		5.67	5.69
80BAU3B	54.42		33.91	33.81
PILOTS	168.62		160.24	185.39

	Full K	Reduced K	Normal eqns
	86 refines	2 refines	2 refines
*	Recipe : 10, e-8	Recipe: 11, e-8	Capri : 18, e-8
	13, e-7		18, e-7
	Grow7 : 13, e-8		
	Grow15 : 14, e-8		
	Grow22 : 14, e-8		
	Pilotja: 26, e-8		
Total time	9 min 46	7 min 55	9 min 12

PILOTJA					
Dimension		2900		1300	940
Nonzeros		15000		17000	93000
LDL' nonzeros		101000		74000	72000
Analyze time	(1)	0.74		0.44	0.50
Factor time	(28)	21.24	(27)	14.94	20.75
Solve time	(57)	2.21	(54)	1.34	1.18

80BAU3B				
Dimension		14000	2362	2262
Nonzeros		37000	18000	24000
LDL' nonzeros		178000	74000	73000
Analyze time	(1)	1.92	0.61	0.61
Factor time	(38)	28.69	15.16	14.90
Solve time	(76)	8.23	2.24	2.26

Good Old VMS

```
Mike> dfp pilotja.lis;32 ;33
---------------------------------------------------------------------------
File [MIKE.PDQ1.OPT]PILOTJA.LIS;32   | File [MIKE.PDQ1.OPT]PILOTJA.LIS;33
------------------- 20 -------------------------------- 20 ----------------
         Htol              1.0d+30   |          Htol              1.0d-8
------------------- 89 -------------------------------- 89 ----------------
  25 2.1E-09 9.2E-01 8.7E-01 1.6E-09 |   25 2.1E-09 9.2E-01 8.7E-01 1.7E-09
 Residual |r-Kd|/|r|  = 2.3E-05      |   26 2.8E-10 7.6E-01 8.3E-01 2.8E-09
 Refine. New residual = 2.1E-03      |   27 6.6E-11 8.3E-01 8.0E-01 1.4E-10
 factol increased to    1.0E-08      |
  26 2.7E-10 7.5E-01 8.3E-01 3.1E-09 |
  27 6.7E-11 8.3E-01 8.0E-01 1.2E-10 |
------------------- 139 ------------------------------- 136 ---------------
   1 MPS read           1    2.91    |  1 MPS read           1    2.90
   2 A  prod          120    0.18    |  2 A  prod          114    0.26
   3 At prod          116    0.42    |  3 At prod          110    0.42
   4 Form KB           28    0.41    |  4 Form KB           27    0.40
   5 Analyze            1    0.70    |  5 Analyze            1    0.46
   6 Factor            28   21.21    |  6 Factor            27   15.02
   7 Solve             57    2.20    |  7 Solve             54    1.30
                                     |
  19 Solution           1   26.84    | 19 Solution           1   19.67
------------------- 155 ------------------------------- 152 ---------------
 itn  KBsize   factol      nz   realA| itn  KBsize   factol      nz   realA
   1    2896  1.0E-30   14996  101250|  1    1304  1.0E-30   17163   74254
...
  26    2896  1.0E-30   14996  101250| 26    1304  1.0E-30   17163   74254
  26    2896  1.0E-08   14996  101250| 27    1304  1.0E-30   17163   74254
  27    2896  1.0E-08   14996  101250|
---------------------------------------------------------------------------

Number of difference sections found: 4
Number of difference records found: 50

DIFFERENCES /IGNORE=(TRAILING_SPACES)/PARALLEL-
    DKA300:[MIKE.PDQ1.OPT]PILOTJA.LIS;32-
    DKA300:[MIKE.PDQ1.OPT]PILOTJA.LIS;33
```

Robustness Anyone?

```
rm pilotja.lis      del pilotja.lis;
rm pilotja.*        del pilotja.*;
rm pilotja *        del pilotja *;
```

Constrained Least Squares

$$\text{minimize} \quad \|Ax - b\| \quad \text{subject to} \quad Cx = d$$

Regularize

$$\min \quad \left\| D \begin{pmatrix} A \\ C \\ I \end{pmatrix} x - D \begin{pmatrix} b \\ d \\ 0 \end{pmatrix} \right\|, \qquad D = \begin{pmatrix} I & & \\ & \gamma^{-1} I & \\ & & \delta I \end{pmatrix}$$

Augmented System

$$\begin{pmatrix} I & & A \\ & \gamma^2 I & C \\ A^T & C^T & -\delta^2 I \end{pmatrix} \begin{pmatrix} r \\ s \\ x \end{pmatrix} = \begin{pmatrix} b \\ d \\ 0 \end{pmatrix}$$

SQD

GO MA47!

- Assume $\|A\|$, $\|C\| \approx 1$.
- First pivot on $\text{diag}(I, \gamma^2 I)$ if row of A or C has < 10 entries.
- MA47 on remainder.
- Equivalent to LDL^T or LBL^T on full system.
- γ^2, $\delta^2 = 10^{-8}$ should mean 1 Factor, 1 Solve.
- Smaller γ, δ: Precond SYMMLQ with $L|B|L^T$, or QMR with LBL^T.

Thanks to

Golub and Van Loan	positive definite LU
Vanderbei	quasi-definite LDL^T
Duff and Reid	sparse LDL^T and LBL^T