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New robust limited-memory incomplete Cholesky preconditioners

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Overview

- Introduction : background and history of *IC* factorizations
- Semi-definite modification schemes : prevent breakdown
- Limited-memory approach
- Numerical experiments on practical problems
- The indefinite case ..... signed *IC* factorizations for KKT systems

Introduction

We want to solve

$$Ax = b$$

where $A \in R^{n \times n}$ is large and sparse.

Direct Methods: Factorize $A = LU$, solve $Ly = b$, $Ux = y$.

Black-box, robust.

Memory-hungry$\Rightarrow$ unsuitable for very large problems.

Iterative Methods: CG, GMRES, BiCGStab, etc.

Matrix-free. Fast? Efficient? .

Non-robust, performance depends on preconditioner.

Introduction

An ideal preconditioner should be:

- cheap to compute
- sparse and fast to apply
- provide sufficient approximation of the algebraic problem
- result in rapidly converging preconditioned iterative method

Key target for library software is robustness

Introduction

Incomplete Cholesky (alert*IC*) factorization

$$A \simeq LL^T$$

Some entries that occur in complete factorization are ignored.

- Long history of incomplete factorizations.
- Early days (late 1950s and 1960s) motivated by finite differences for PDEs. Often for specific problems.
- Real revolution in practical use and growth in popularity came in late 1970s.
- In particular, Meijerink and van der Vorst '77 recognised potential of incomplete factorizations as preconditioners for use with CG and proved existence for M-matrices (later extended to H-matrices).

Introduction

Different variants of incomplete factorizations:

- $IC(\tau)$: Dropping by value (Tuff and Jennings '73)
- $IC(\ell)$: originally exploited finite difference-based structure (small number of sub-diagonals). Generalised to level-based approach to preserve structure (Watts '81)
- $IC(p)$: Limited/prescribed memory: Axelsson, Munksgaard '83; Jones, Plassman '95; Saad '94.

Lots of variations/hybrids that combine approaches.

Introduction: problem of breakdown

- Kershaw '78 locally perturbed zero or negative diagonal entries to prevent breakdown so method more widely applicable. Straightforward but can give large growth and unstable preconditioner.
- Manteuffel '80 proposed global diagonal shift so that $A + \alpha I$ factorized for some $\alpha > 0$. Shift α chosen by trial-and-error but can be effective.
- Alternative approach: positive semi-definite modifications.

Our goals

- Study two positive semi-definite modification schemes:
  - Jennings and Malik '77,'78 (and Ajiz and Jennings '84)
  - Tismenetsky '91 (and Kaporin '98)

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- Propose memory-efficient variant of Tismenetsky approach, optionally combined with Jennings and Malik modifications or diagonal shifts.

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- Propose memory-efficient variant of Tismenetsky approach, optionally combined with Jennings and Malik modifications or diagonal shifts.
- Present comprehensive numerical results.

Positive semi-definite modifications I

- Diagonal modification scheme first introduced by Jennings and Malik '77, '78 (also Jennings and Ajiz '84).
- Every time off-diagonal entry discarded, corresponding diagonal entries modified by adding SPSD matrix

$$
\begin{array}{c} \\ i \\ \\ j \\ \\ \end{array}
\begin{array}{c}
\begin{array}{ccccc} & & i & & j \end{array} \\
\begin{pmatrix}
\ddots & & & & \\
& |a_{ij}| & & -|a_{ij}| & \\
& & \ddots & & \\
& -|a_{ij}| & & |a_{ij}| & \\
& & & & \ddots
\end{pmatrix}
\end{array}
$$

Jennings-Malik approach

- Breakdown-free factorization that can be expressed as

$$A = LL^T - E$$

  where error matrix E is sum of SPSD matrices.

- But modifications to A can be significant.
- Popular in some engineering applications.

Positive semi-definite modifications II

- More sophisticated modification scheme due to Tismenetsky '91 (and Kaporin '98).
- Introduces use of intermediate memory that is employed during construction of L but then discarded.
- Shown to be very robust but it "has unfortunately attracted surprisingly little attention" (Benzi '02).
- One possible reason for this is it suffers from a serious drawback: memory requirements can be prohibitively high.

We aim to address memory problem, while retaining robustness.

Tismenetsky approach

Based on matrix decomposition of form

$$A = (L + R)(L + R)^T - E$$

- L is lower triangular with positive diagonal entries used for preconditioning,
- R is strictly lower triangular with small entries that is used to stabilise the factorization process, and
- E has the structure

$$E = RR^T.$$

Tismenetsky approach

- On j-th step, decompose col. 1 of Schur complement S into

$$l_j + r_j \quad \text{with} \quad |l_j|^T |r_j| = 0,$$

  where entries of l_j are retained in incomplete factorization and those in r_j are discarded.

- On next step, S updated by subtracting

$$(l_j + r_j)(l_j + r_j)^T.$$

- Tismenetsky omits the term

$$E_j = r_j r_j^T. \tag{1}$$

- Thus, SPSD matrix implicitly added to A.

Kaporin's use of drop tolerances

- Obvious choice for r_j are smallest off-diagonal entries in col j.
- Controls size of L but not memory required to compute it.
- Kaporin '98: entries of magnitude at least τ_1 kept in L and those smaller than τ_2 are dropped from R.
- Now E has structure

$$E = RR^T + F + F^T,$$

F strictly lower triangular matrix that is not computed;
R used in computation of L but discarded.

Problem of unrestricted L and R

- With no restriction on size of L and R, can achieve high quality preconditioner but memory demands high.
- Also can be very expensive to compute making approach impractical for the very large problems iterative methods designed for.

Remedy: impose memory limit on L and R.

What about breakdown?

- If we impose memory limit and/or drop small entries, Tismenetsky approach not guaranteed breakdown free.
- Use global diagonal shift? (Manteuffel)
  Note: multiple restarts may be required so potentially expensive.
- Or combine with Jennings-Malik compensation?

How to combine approaches?

There are a number of possibilities:

- Compensate for all entries not retained in L or R.
- Allow entries in RR^T that do not lead to any further fill-in and compensate for all remaining entries of RR^T.

Test environment

- Problems from University of Florida Collection.
- Selected all non-diagonal SPD matrices with $n > 1000$.
- Removed those with duplicate sparsity patterns.
- All problems prescaled (this is important).
- Following initial experiments, 8 problems discarded as unable to achieve convergence without large amount of fill.
- Test set of 145 problems.

Test environment (continued)

- CG used with $x_0 = 0$, b computed so that $x = 1$, and stopping criteria

$$\|Ax_k - b\| \leq 10^{-10}\|b\|$$

  with limit of 2000 iterations.

- All software written in Fortran.

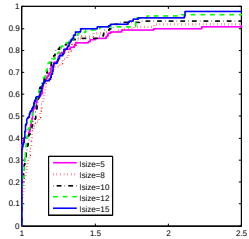
Test environment (continued)

- What to measure? iteration counts? timings? sparsity of L?
- We define the efficiency of preconditioner to be

$$iter \times nz(L)$$

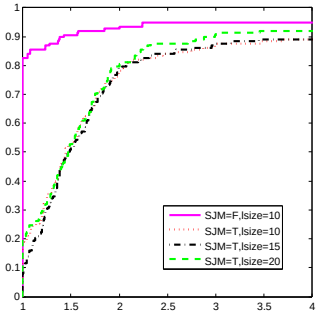
- Performance profiles (Moré, Dolan '02) used to assess performance.
- In our tests, `lsize` is max. number of fill entries in each col. of L and `rsize` is max. number of entries in each col. of R.

Efficiency for `rsize`=0, no diagonal compensation



- These results are without diagonal compensation and no dropping of small entries .... equilavent to ICFS code of Lin and Moré '99.
- Rather insensitive to choice of `lsize`.

Efficiency for rsize=0, with/without SJM



- These results are with and without standard Jennings-Malik (SJM) diagonal compensation.
- Conclude that compensation not generally useful in this case.

Iterations and time for rsize=0, with/without SJM

Comparison of using global diagonal shifts (GDS) with the Jennings-Malik strategy (SJM) (lsize = 10).
Figures in parentheses are number of shifts and final shift; times are seconds

Problem	Iterations		Total time	
	GDS	SJM	GDS	SJM
HB/bcsstk28	232 (2, $4.0 * 10^{-3}$)	468	0.120	0.221
Cylshell/s3rmq4m1	648 (2, $4.0 * 10^{-3}$)	838	0.381	0.459
GHS_psdef/ldoor	437 (3, $8.0 * 10^{-3}$)	643	66.4	91.5
GHS_psdef/audikw_1	707 (2, $2.0 * 10^{-3}$)	1442	157	303

- Our experience: generally better to use diagonal shift.

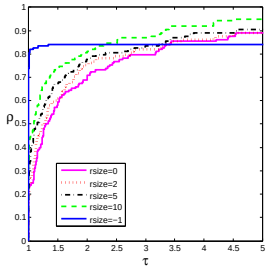
Results for `rsize` varying

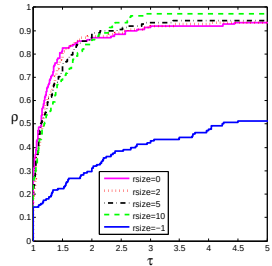
We now consider using intermediate memory (`rsize`>0).

We start by performing no diagonal compensation.

Results for `rsize` varying

Efficiency (left) and total time (right) (`lsize`=5)





- `rsize`=−1 is unlimited memory for R (not practical).

Results with/without diagonal compensation

Recall:

Limited memory Tismenetsky approach based on decomposition

$$A = LL^T + LR^T + L^T R - E, \qquad E = RR^T + F + F^T,$$

where F is not computed but R is.

Results with/without diagonal compensation

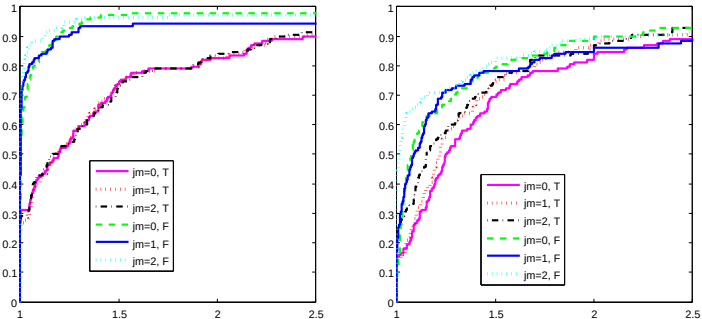
Consider three strategies for dealing with RR^T:

- `jm = 0`: allow entries of RR^T that cause no further fill in $LL^T + LR^T + L^TR$ and discard all other entries of RR^T.
- `jm = 1`: as above but use Jennings-Malik compensation for discarded entries of RR^T.
- `jm = 2`: discard all entries of RR^T.

We run these options with (T) and without (F) diagonal compensation for entries discarded from R.

Results with/without diagonal compensation

Efficiency (left) and total time (right) (`lsize`=`rsize`=10)



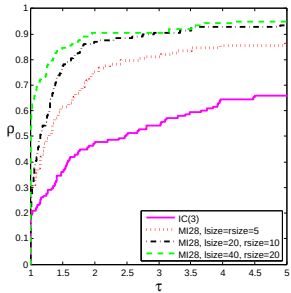
- Compensating for dropped entries of R generally not beneficial.
- Reliability slightly improved if entries of RR^T allowed (`jm`=0) but faster and better efficiency to ignore RR^T (`jm`=2).

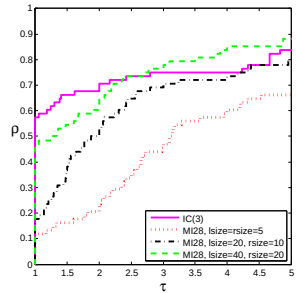
New *IC* code

- Based on our findings, we have developed a new IC code called HSL_MI28.
- Can be used as a "black-box" to compute an efficient and robust *IC* preconditioner.
- But also flexible, allowing user to choose the scaling, ordering, diagonal shift, drop tolerances etc.
- Importantly, the amount of memory used (for both L and R) is under the user's control.

Comparison with level-based approach ($IC(3)$)

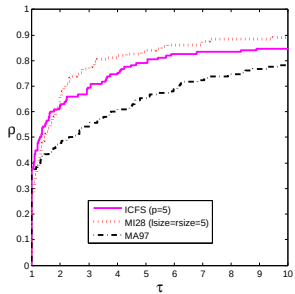
Efficiency (left) and iterations (right).

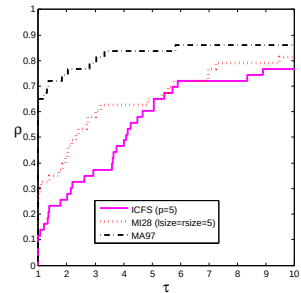




Comparison with direct solver HSL_MA97

Total time: all problems (left) and large problems (right).





HSL_MI28 can sometimes compete with direct solver (and succeed when HSL_MA97 runs out of memory).

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- Using restricted intermediate memory improves efficiency.

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- Our extensive experiments favour use of global diagonal shifts (works well provided the problem is well scaled).

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- We have explored the use of diagonal compensation with a limited memory Tismenetsky approach.
- The proposed limited memory Tismenetsky approach has been shown to be robust and efficient.
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- But diagonal compensation to prevent breakdown appears less important than generally supposed.
- Our extensive experiments favour use of global diagonal shifts (works well provided the problem is well scaled).
- New *IC* code `HSL_MI28`.

What about indefinite problems?

Saddle-point systems $Kx = b$ where

$$K = \begin{pmatrix} A & B^T \\ B & -C \end{pmatrix}$$

- A is $n \times n$ symmetric positive definite
- B is rectangular and of full rank
- C is $m \times m$ ($m \leq n$) symmetric positive semi-definite

Signed Cholesky factorization

$$K = \begin{pmatrix} L_{11} & 0 \\ L_{21} & L_{22} \end{pmatrix} \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \begin{pmatrix} L_{11}^T & L_{21}^T \\ 0 & L_{22}^T \end{pmatrix},$$

$$A = L_{11} L_{11}^T$$

$$L_{21} = B L_{11}^{-T}$$

$$S = C + L_{21} L_{21}^T = L_{22} L_{22}^T$$

This factorization always exists, without pivoting (although numerical stability is not guaranteed).

Signed Cholesky factorization

Set

$$\mathcal{L} = \begin{pmatrix} L_{11} & 0 \\ L_{21} & L_{22} \end{pmatrix},$$

then

$$P = \mathcal{L}\mathcal{L}^T$$

can be used as a (split) preconditioner.

$\mathcal{L}^{-1}K\mathcal{L}^{-T}$ has two distinct eigenvalues ± 1, so symmetric Krylov subspace method (MINRES or SYMMLQ) converges in at most two iterations.

Signed Cholesky factorization

In practice,

$$A \approx \tilde{L}_{11}\tilde{L}_{11}^T,$$

$$\tilde{L}_{11}^T\tilde{L}_{21} = B^T$$

$$\tilde{S} = C + \tilde{L}_{21}\tilde{L}_{21}^T \approx \tilde{L}_{22}\tilde{L}_{22}^T$$

- Key question: how to sparsify $\tilde{L}_{21}^T$? (need $\tilde{S}$ sparse)
- We take a different approach that does not limit working to the $(1,1)$ block and then the $(2,2)$ block.

Constrained orderings

Consider for now the complete factorization.

Constrained ordering: find permutation Q such that QKQ^T can be factorized stably **without** numerical pivoting and **without** modifying entries in K, while keeping sparsity.

Bridson (2007):

- Divide nodes of adjacency graph of K into two disjoint sets: A-nodes that correspond to diagonal entries of A and remaining nodes are C-nodes.
- A C-node can only be ordered after all its A-node neighbours K have been ordered.

Constrained orderings

- Provided A is definite and B is of full row rank, with this ordering the LDL^T factorization exists, with L unit lower triangular and D diagonal.
- Moreover, the pivots associated with A-nodes are positive and those associated with C-nodes are negative.
- Rescaling, $L \leftarrow L|D|^{1/2}$ and $D \leftarrow sign(D) = diag(\pm 1)$

This gives a signed Cholesky factorization of K.

Is this good approach?

- **Advantage:** simple modification to Cholesky code, avoiding need for pivoting (static data structures set up during analyse phase).
- **Disadvantages:**
  - no pivoting so stability not guaranteed
  - constrained ordering may lead to more fill (more work and more memory)

Our experiments showed better to use a state-of-the-art indefinite direct solver that incorporates pivoting.

But can we use it for incomplete signed *IC*?

- Want to adapt our *IC* code to compute signed *IC* factorization.
- Need to identify *C*-nodes and post process ordering so *C*-node ordered only after its *A*-node neighbours.
- Allow use of two shifts

$$\overline{K} = SQ \begin{pmatrix} A & B^T \\ B & -C \end{pmatrix} Q^T S + \begin{pmatrix} \alpha(1)I & 0 \\ & -\alpha(2)I \end{pmatrix}$$

where S is diagonal scaling, Q permutation (cf. Saunders and Tomlin '96 and also Altman and Gondzio '99 regularization of symmetric indefinite systems).

Early results $C = 0$

GMRES(100) convergence results. $\alpha(1) = 0.0$.

Identifier	*lsize*	*rsize*	$\alpha(2)$	*fill*	efficiency	iters
boyd1	20	20	0.0	0.82	3.75×10^{6}	7
d_pretok	5	5	2.56×10^{-1}	1.96	4.85×10^{7}	28
ncvxqp9	10	10	4.19×10^{3}	3.98	2.51×10^{5}	2
sit100	20	20	0.0	3.61	1.72×10^{6}	14
stokes64	10	10	0.0	2.73	3.19×10^{7}	157
tuma1	20	20	0.0	5.79	5.86×10^{6}	20
turon_m	20	20	1.60×10^{-2}	4.36	2.23×10^{8}	56

Early results $C = 10^{-8}$ (interior-point matrices)

GMRES(100) convergence results. *lsize* = *rsize* = 10.

Identifier	$\alpha(1)$	$\alpha(2)$	*fill*	efficiency	iters
c-55	0.01	0.64	2.08	5.30×10^{7}	117
c-68	0.01	2.56	2.31	3.21×10^{7}	44
c-69	0.01	0.64	2.35	5.68×10^{7}	70
c-70	0.01	0.64	2.32	6.09×10^{7}	72
c-71	0.01	0.04	2.17	8.42×10^{7}	83
c-big	0.01	0.64	2.63	3.85×10^{8}	109

Future directions

- Results suggest we can use a signed *IC* approach
  but we want to do better.
- Developing limited memory incomplete LDL^T factorization, again using intermediate memory that is discarded.
- This will involve using 2×2 pivots for stability
  (shifts will not be needed).
- **Note:** Recent work by Chen and Liu to develop SYM-ILDL code, based on the work of Li and Saad '05.
  This is giving some good results.
- Also want to explore effects of matching orderings (used by Hagemann and Schenk '06 for incomplete factorizations).

Thank you!

HSL_MI28 is available as part of HSL 2013.

Technical Reports RAL-P-2013-004 and RAL-P-2013-005
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