On positive semidefinite modification schemes for incomplete Cholesky factorization

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Introduction

We are interested in the efficient and robust solution of large sparse symmetric linear systems

$$Ax = b, \ A \in R^{n \times n}$$

In this talk, we focus on Incomplete Cholesky (IC) factorizations

$$A \simeq LL^T$$

used with the conjugate gradient (CG) method.

Incomplete factorization: some entries that occur in complete factorization are ignored.

Introduction

- 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:
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  - 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

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

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

$$A = LL^T + LR^T + RL^T + \hat{E}$$

- 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
- $\hat{E}$ has the structure
$$\hat{E} = RR^T.$$

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

$$\hat{E}_j = r_j r_j^T. \tag{1}$$

- Thus, SPSD matrix implicitly added to A.

Can we compare the two approaches?

- Standard tool in modified IC (Gill, Murray, Wright '81, survey by Fang, O'Leary '08): consider norm of error matrix $E = A - LL^T$.
- Jennings-Malik implies a smaller $\| E \|$:

Theorem (Scott and Tůma)
At stage j, assume S has been computed and its first column split into l_j and r_j. Then the 2-norm of the Jennings-Malik modification that compensates for all the dropped entries is not larger than the 2-norm of the Tismenetsky modification corresponding to adding $r_j r_j^T$ to the corresponding positions.

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 $\hat{E}$ has structure

$$\hat{E} = RR^T + F + F^T,$$

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.

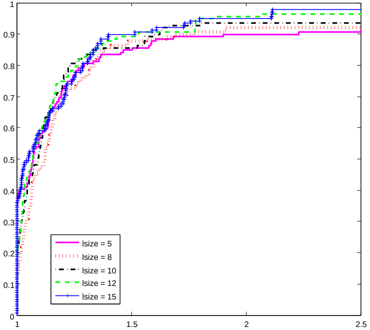
Test environment (continued)

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

$$iter \times nz(L)$$

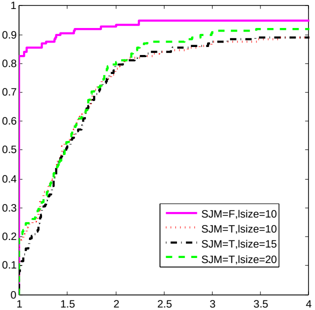
- Performance profiles (Moré, Dolan '02) used to assess performance.
- In our tests, `lsize` is max. number of fill entries in each col. of L and `rsize` is max. number of entries in each col. of R.

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 in 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.

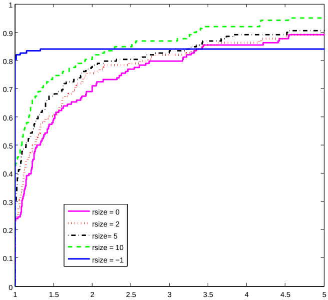
Results for `rsize` varying

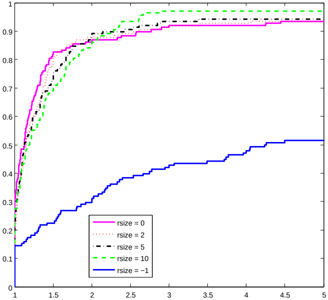
We now consider using intermediate memory (`rsize`$>$0).

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

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

where F is not computed but R is.

Results with/without diagonal compensation

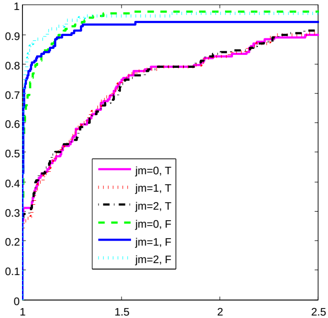
Consider three strategies for dealing with RR^T:

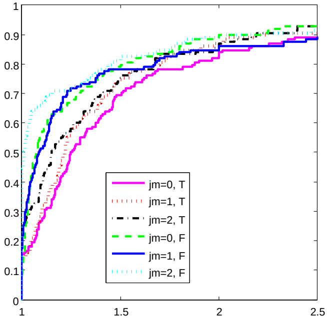
- `jm = 0`: allow entries of RR^T that cause no further fill in $LL^T + LR^T + L^T R$ and discard all other entries of RR^T.
- `jm = 1`: as above but use Jennings-Malik compensation for discarded entries of RR^T.
- `jm = 2`: discard all entries of RR^T.

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`)





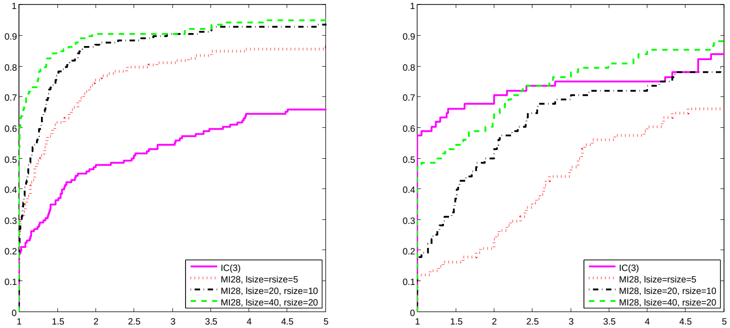
- Compensating for dropped entries of R generally not beneficial.
- Reliability slightly improved if entries of RR^T allowed (`jm=0`) but faster and better efficiency to ignore RR^T (`jm=2`).

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.

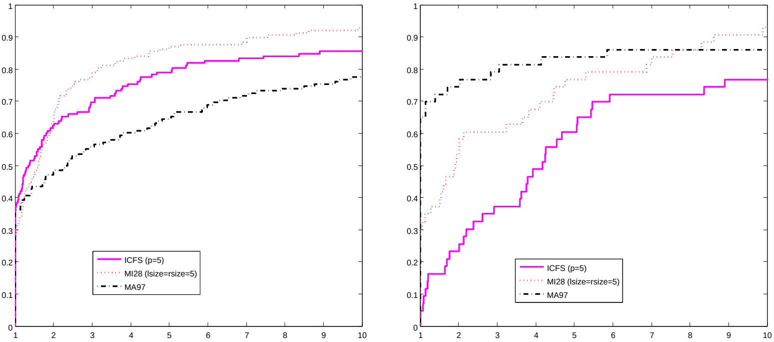
Comparison with level-based approach ($IC(3)$)

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 succeeds when HSL_MA97 runs out of memory).

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- But diagonal compensation to prevent breakdown appears less important than generally supposed.

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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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- Using restricted intermediate memory improves efficiency.
- 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`.

Thank you!

HSL_MI28 is available (without charge) as part of HSL 2013.

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