A robust limited-memory incomplete Cholesky factorization

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Introduction

Consider the large sparse symmetric linear system

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

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 factorization

$$A \simeq LL^T$$

Some entries that occur in complete factorization are ignored.

Long history ($>$ 50 years) and many possible variants:

- Structure-based $IC(\ell)$: potential fill entries allowed only if their level of fill is less than ℓ.
- Threshold-based $IC(\tau)$: entries greater than τ dropped.
- Memory-based $IC(p)$: dropping of entries based on memory available.

$IC(\ell)$

- Location of permissible fill entries using sparsity pattern of A prescribed in advance.
- Aim to mimic how pattern of A is developed during complete factorization.
- But although entries of $E = A - LL^T$ are zero inside prescribed sparsity pattern, outside can be large.
- Increasing ℓ can be prohibitive (storage requirements and time to compute and apply the preconditioner).

$IC(\tau)$

- Entries of computed factors or intermediate quantities that exceed drop tolerance τ discarded.
- Success depends on suitable τ: highly problem dependent.
- Trade-off between sparsity and quality.
- Memory not predictable.

$IC(p)$

- Prescribe maximum number of entries allowed in each column of L and retain only largest entries.
- Memory predictable.
- Example is widely-used dual threshold $ILUT(p, \tau)$ (Saad '94).
  - Designed for non symmetric problems.
  - Combines use of drop tolerance τ with prescribed maximum column and row counts.
  - Ignores symmetry in A (if A symmetric, patterns of L and U^T normally different).

ICFS

ICFS code of Lin and Moré '99:

- Given p, retains $n_j + p$ largest entries in the lower triangular part of L_j, where n_j is number of entries in lower triangular part of A_j.
- Incorporates l_2-norm based scaling.
- In the event of breakdown, uses global diagonal shift ($A + \alpha I$ factorized for some $\alpha > 0$ (Manteuffel '80)).
- Widely used for large-scale trust region subproblems.

But, as we will see, efficiency of resulting preconditioner not very sensitive to choice of p.
So how to improve preconditioner quality?

Positive semi-definite modifications I

Alternative way to prevent breakdown:

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

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

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).
- Suffers from a serious drawback: memory requirements can be prohibitively high.

Our aims

- Develop generalisation of ICFS such that efficiency of preconditioner improves with prescribed memory.
- Develop memory-efficient variant of Tismenetsky-Kaporin approach using global shifts to avoid breakdown.
- Combine in "black-box" *IC* factorization code that is demonstratively robust, efficient and flexible.

New package is `HSL_MI28`.

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.

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.

Problems of Tismenetsky-Kaporin approach

- How to choose tolerances τ_1 and τ_2? Problem dependent.
- Method not guaranteed breakdown free ... combine with diagonal compensation or global shift.
- With no restriction on size of L and R, can achieve high quality preconditioner but memory demands high.
- Also too expensive. Impractical for the very large problems iterative methods designed for.

Remedy: impose memory limit on L and R.

Limited memory Tismenetsky-Kaporin approach

- `lsize`: max. number of fill entries in each col. of L

$$nz(L) \le nz(A) + \texttt{lsize} * (n-1)$$

- `rsize`: max. number of entries in each col. of R.
  Amount of intermediate memory and work involved in computing preconditioner depends on `rsize`.
  Note: if $\texttt{rsize} = 0$, R not used.

- Retain largest entries in l_j, provided at least τ_1 in magnitude; then retain next largest entries in r_j, provided at least τ_2 in magnitude.

Left-looking algorithm outline

Input: A, `lsize`, `rsize`, τ_1, τ_2

Set $w(1:n) = 0$
for $j = 1 : n$ **do**
  Scatter col. A_j into w
  Apply $LL^T + RL^T + LR^T$ updates from columns $1 : j-1$ to w
  (Partially) sort entries in w by magnitude
  Keep $n_j +$ `lsize` entries of largest magnitude in l_j provided
    they are at least τ_1
  Keep `rsize` additional entries that are next largest in magnitude
    in r_j provided they are at least τ_2
  Reset entries of w to zero
  end do
end do

Output: L

Coping with breakdown

- When using limited memory (and/or dropping), factorization may breakdown.
- We hold a copy of diagonal entries and, at each step j, keep them updated. If any becomes zero or negative, restart factorization with

$$A \leftarrow A + \alpha I$$

  for some positive α.
- More than one restart may be required.

Test environment

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

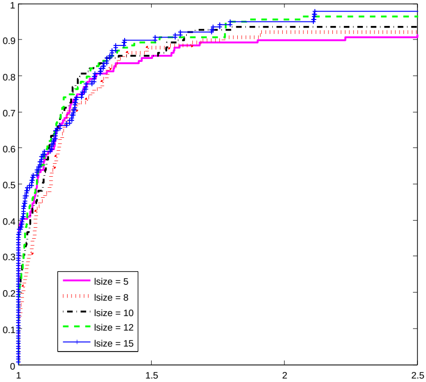
Test environment (continued)

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

$$iter \times nz(L)$$

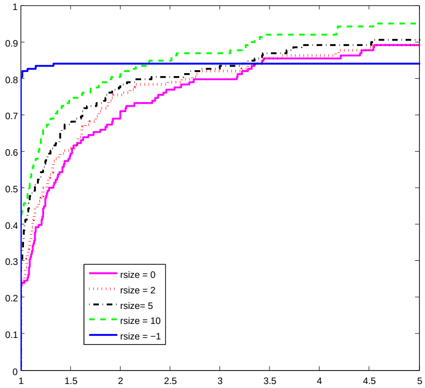
- Performance profiles (Moré, Dolan '02) used to assess performance.
- All software written in Fortran.

Efficiency performance profile, `rsize`=0



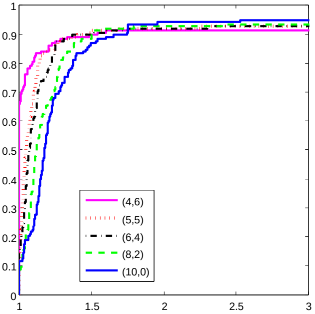
Note: rather insensitive to choice of `lsize` (ICFS).

Efficiency (= iteration) performance profile, `lsize`=5



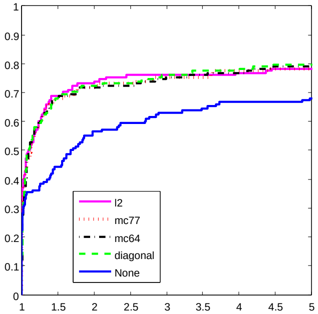
`rsize`=`-1` is unlimited memory for R (not practical).

Efficiency performance profile `lsize+rsize` constant



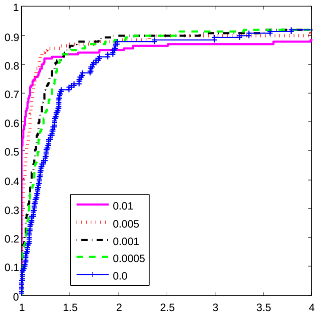
Pairs (`lsize`,`rsize`)
Intermediate memory (`rsize` > 0) can compensate for `lsize`.

Effect of scaling on efficiency (`lsize` = `rsize` = 5)



`HSL_MI28` default is l_2 scaling.

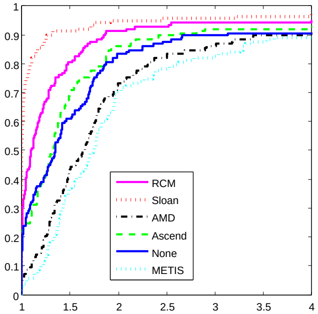
Effect of dropping on efficiency ($\texttt{lsize} = \texttt{rsize} = 5$)



Often advantageous to use small drop tolerance.

Default $\tau_1 = 0.001$.

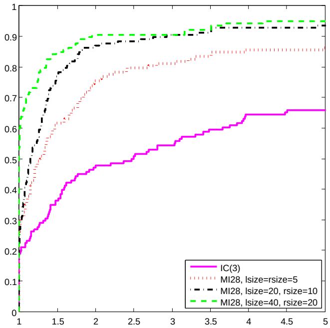
Effect of ordering on efficiency

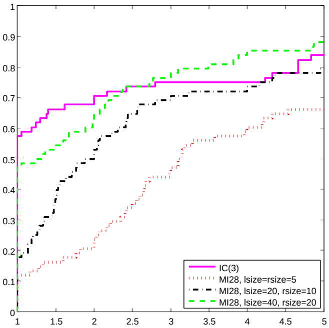


Sloan profile-reduction ordering is the winner.

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

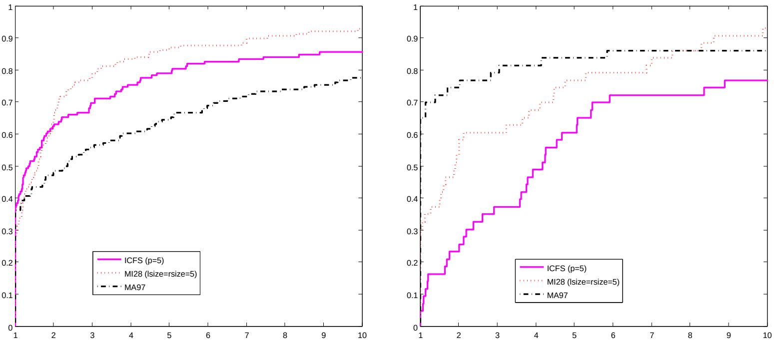
Efficiency (left) and iterations (right).





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).

Concluding remarks

- We have developed a new *IC* code HSL_MI28 that may be used as a "black box" or tuned for a particular problem.
- Memory usage is under the user's control.
- Using restricted intermediate memory improves efficiency.
- The intermediate memory can compensate for the preconditioner size.
- Based on extensive experimentation, HSL_MI28 appears robust and efficient.

Note: at the Preconditioning Conference, my talk will focus more on the use of positive semidefinite modification schemes.

Thank you!

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

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

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