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Memory-Efficient Incomplete Factorizations for Sparse Symmetric Systems

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Introduction

Focus in this talk is on 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

Introduction

- Lots of papers on this in recent years ... too many names to mention.
- There are a number of direct solvers that are primarily designed for symmetric indefinite problems (including `MA57`, `HSL_MA86` and `HSL_MA97`) that perform well on these systems.
- For very large problems, need an iterative method and a good preconditioner. Many possibilities ... here we consider a class of incomplete factorization preconditioners.
- Recent related work includes Orban (2013) and Greif et al (see later).

Introduction

Consider the factorization

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

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

$$L_{11} L_{21} = B$$

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

This factorization always exists without pivoting although numerical stability **not** guaranteed.

Introduction

If we 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.

Introduction

In practice, to obtain a preconditioner

$$A \approx \tilde{L}_{11}\tilde{L}_{11}^T \text{ (incomplete Cholesky)}$$

$$\tilde{L}_{11}^T\tilde{L}_{21} = B^T \text{ (triangular solve)}$$

$$\tilde{S} = C + \tilde{L}_{21}\tilde{L}_{21}^T \approx \tilde{L}_{22}\tilde{L}_{22}^T \text{ (incomplete Cholesky)}$$

Key question: how to sparsify $\tilde{L}_{21}^T$? (need $\tilde{S}$ sparse)

We will 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 of K.

Constrained ordering: find permutation Q such that QKQ^T can be factorized stably **without** numerical pivoting and **without** modifying entries in K, while maintaining 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 can prove 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 a 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 (thus more work and more memory)

Our experiments found generally better to use a state-of-the-art indefinite direct solver (such as `HSL_MA97`) that allows sparsity-preserving ordering and incorporates threshold pivoting.

What about the incomplete case?

- For the incomplete case, having the best sparsity-preserving ordering may not be so important.
  A good ordering may be sufficient.
- Would like to be able to exploit incomplete Cholesky factorizations that have proved memory efficient and robust for SPD problems.

Incomplete Cholesky

Let's consider the case of a symmetric positive definite A.

Variants of incomplete Cholesky (IC) factorizations include:

- $IC(\tau)$: 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: eg. Axelsson, Munksgaard '83; Jones, Plassman '95; Saad '94.

Tismenetsky '91 approach

Tismenetsky's approach is based on decomposing A into the 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

- Consider first step of Gaussian elimination. Let $a_{2:n}$ denote the off-diagonal part of column 1 of A.
- Let $a_{2:n} = l_{2:n} + r_{2:n}$ where if $a_i \neq 0$ either $l_i = 0$ and $r_i = a_i$ or $l_i = a_i$ and $r_i = 0$.
- The Schur complement S is

$$S = A_{2:n,2:n} - a_{2:n} a_{2:n}^T$$

- That is,

$$S = A_{2:n,2:n} - (l_{2:n} + r_{2:n})(l_{2:n} + r_{2:n})^T$$

- Tismenetsky computes an incomplete factorization by not subtracting the term $r_{2:n} r_{2:n}^T$, using $l_{2:n}$ as first column of the incomplete factor L and not including $r_{2:n}$ in computed factorization.

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, symmetric positive semi definite matrix is implicitly added to A and factorization is guaranteed breakdown free.

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

Tismenetsky approach is robust and can achieve high quality preconditioner **but**

- memory demands prohibitively high;
- can be very expensive to compute.

Thus 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.
- We tried various approaches to overcome this (modifying small pivot Kershaw '78, Jennings-Malik approach ...)
- Found we obtained best results using a global diagonal shift (Manteuffel '80)

$$A \Leftarrow A - \alpha I$$

  Note: multiple restarts may be required.
- Ideas implemented in the software package `HSL_MI28`.

HSL_MI28

- User specifies the amount of fill allowed in each column of L and maximum number of entries in each column of R.
- The user may specify drop tolerances τ_1 and τ_2 for L and R.
- The matrix is optionally preordered and prescaled (both can significantly enhance performance).

Note: the widely-used ICFS code of Lin and Moré '99 implements a special case in which ordering is not incorporated, there is no dropping and $R = 0$.

HSL_MI28 results

- Very encouraging results for wide range of positive definite problems (see Scott and Tuma ACM TOMS 2014 and SISC 2014).
- In particular, found it is beneficial to use intermediate memory ($R \neq 0$) in the construction of L.
- To assess performance we define the efficiency of a preconditioner to be

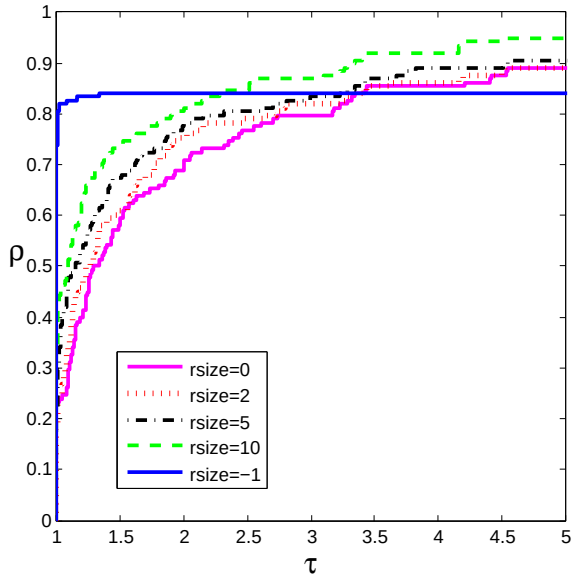
$$iter \times nz(L)$$

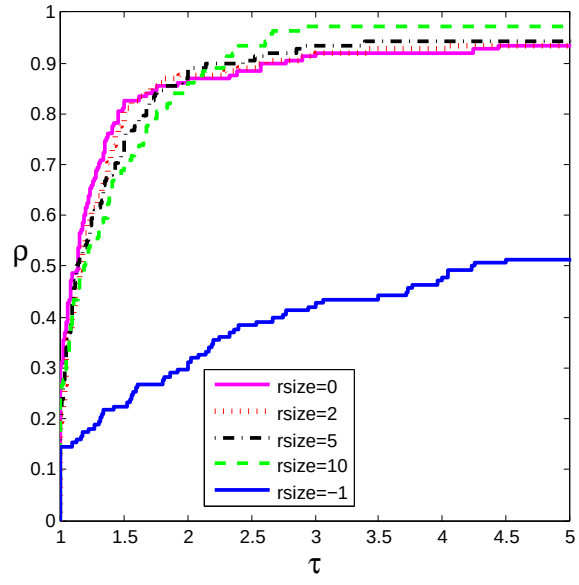
and use performance profiles (Moré, Dolan '02).

- Test set of 145 SPD problems from University of Florida Collection of order $n > 1000$.

Results for `rsize` varying

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





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

What about saddle-point systems?

Recall: we want an incomplete factorization preconditioner for saddle-point matrices

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

What about signed *IC*?

Challenge: can we adapt our *IC* code to compute a signed *IC* factorization preconditioner for K?

Two basic changes:

- Identify C-nodes and post process the pivot order so C-node is ordered only after all its A-node neighbours (constrained ordering).
- Allow use of two shifts and thus we factorize

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

where S is diagonal scaling, Q permutation.

Results $C = 0$

GMRES(100) convergence results. $\alpha(1) = 0.0$.
$fill_{IC} = nz(L)/nz(K)$

Identifier	*lsize*	*rsize*	$\alpha(2)$	$fill_{IC}$	iters
boyd1	20	20	0.0	0.82	7
d_pretok	5	5	2.56×10^{-1}	1.96	28
ncvxqp9	10	10	4.19×10^{3}	3.98	2
sit100	20	20	0.0	3.61	14
stokes64	10	10	0.0	2.73	157
tuma1	20	20	0.0	5.79	20
turon_m	20	20	1.60×10^{-2}	4.36	56

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

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

Identifier	$\alpha(1)$	$\alpha(2)$	$fill_{IC}$	iters
c-55	0.01	0.64	2.08	117
c-68	0.01	2.56	2.31	44
c-69	0.01	0.64	2.35	70
c-70	0.01	0.64	2.32	72
c-71	0.01	0.04	2.17	83
c-big	0.01	0.64	2.63	109

Some comparisons with SYM_ILDL

SYM_ILDL is code by Greif, He and Liu (2013).

- Based on the earlier work by Li and Saad (2005).
- Performs an incomplete factorization of sparse symmetric indefinite matrices with Bunch-Kaufman pivoting for numerical stability and to prevent breakdown.
- Incomplete factorization LDL^T, where D is block diagonal, with blocks of order 1 and 2, corresponding to 1×1 and 2×2 pivots.
- User parameters *fill* and *tol* control $nz(L)$.

Some comparisons with SYM_ILDL

GMRES(100) results with $lsize = rsize = 30$ and $\alpha_{in}(1:2) = 0.01$.
SYM-ILDL is run with $fill = 12.0$ and $tol = 0.003$.

Identifier	Signed *IC*				SYM-ILDL	
	$\alpha_{out}(1)$	$\alpha_{out}(2)$	$fill_{IC}$	iters	$fill_{IC}$	iters
GHS_indef/c-55	0.01	0.08	3.37	41	4.35	78
GHS_indef/c-68	0.01	0.01	4.06	14	4.31	61
GHS_indef/c-69	0.0025	0.01	4.00	30	3.81	42
GHS_indef/c-70	0.01	0.01	3.88	45	3.61	22
GHS_indef/c-71	0.01	0.01	3.51	53	4.03	37

Future directions

- Results suggest signed *IC* approach can provide good preconditioners for saddle-point systems.
  But can we do better?
- Currently developing limited memory incomplete LDL^T factorization code for general indefinite systems, again using intermediate memory that is discarded.
- Also exploring effects of matching-based orderings (used by Hagemann and Schenk '06 for incomplete factorizations).

Thank you!

HSL_MI28 (incomplete Cholesky) and HSL_MI30 (signed incomplete Cholesky for saddle-point systems) are available as part of HSL 2013. Free for academic use so please try and feedback!

MATLAB interfaces are available `http://www.hsl.rl.ac.uk`

More details and results: see Technical Report RAL-P-2014-003

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