An Updated Preconditioner for Sequences of General Nonsymmetric Linear Systems

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1. Introduction

- The solution of *sequences* of linear systems arises in numerous applications
- Rather few work has been done in our community on efficient solution of *general* sequences of linear systems
- The central question of such work will be:

  How can we share part of the computational effort throughout the sequence ?

- Below we list some known strategies.

1. Introduction

- Very simple trick: Hot starts, i.e. use the solution of the previous system as initial guess.

- Sometimes exact updating of the factorizations for large problems is feasible: Rank-one updates of LU factorizations have been used since decades in the simplex method where the change of one system matrix to another is restricted to one column [Bartels, Golub, Saunders - 1970; Suhl, Suhl - 1993].

- General rank-one updates of an LU decomposition are discussed in [Stange, Griewank, Bollhoefer - 2005].

- If the linear solver is a Krylov subspace method, strategies to recycle information gained from previously generated Krylov subspaces have shown to be beneficial in many applications [Parks, de Sturler, Mackey, Johnson, Maiti - 2006], [Giraud, Gratton, Martin - 2007], [Frank, Vuik - 2001].

1. Introduction

- When shifted linear systems with identical right hand sides have to be solved, Krylov subspace methods allow advantageous implementations based on the fact that all systems generate the same subspace [Frommer, Glässner - 1998]

- In nonlinear systems solved with a Newton-type method one can skip evaluations of the (approximate) Jacobian during some iterations, leading to Shamanskii's combination of the chord and Newton method [Brent - 1973] $\Rightarrow$ linear solving techniques with multiple right hand sides can be exploited.

- Another option: Allow changing the system matrices but freeze the preconditioner [Knoll, Keyes - 2004].

1. Introduction

To enhance the power of a frozen preconditioner one may also use approximate updates:

- In [Meurant - 2001] we find approximate updates of incomplete Cholesky factorizations and
- in [Benzi, Bertaccini - 2003, 2004] banded updates were proposed for both symmetric positive definite approximate inverse and incomplete Cholesky preconditioners.
- In Quasi-Newton methods the difference between system matrices is of small rank and preconditioners may be efficiently adapted with approximate small-rank updates; this has been done in the symmetric positive definite case, see e.g. [Bergamaschi, Bru, Martínez, Putti - 2006, Nocedal, Morales - 2000].

2. The proposed preconditioner updates

- We focus on a black-box approximate preconditioner update for *general nonsymmetric* systems solved by arbitrary iterative methods.
- Updating frozen preconditioners for preconditioned iterative methods instead of their recomputation.
- Simple algebraic updates which can be considered in matrix-free computations.

Notation: Consider two systems

$$Ax = b, \quad A^+ x^+ = b^+; \text{ preconditioned by } M,\ M^+,$$

$$\text{let} \qquad B \equiv A - A^+.$$

We would like the update M^+ to become as powerful as M.

2. The proposed preconditioner updates

If $||A - M||$ is the accuracy of the preconditioner M for A, we will try to find an updated M^+ for A^+ with comparable accuracy,

$$||A - M|| \approx ||A^+ - M^+||.$$

Let M be factorized as $M = LDU$, then the choice

$$M^+ = LDU - B$$

would give $||A - M|| = ||A^+ - M^+||$. We will approximate this ideal update $LDU - B$ in two steps, similarly to the techniques in [Benzi, Bertaccini - 2003, Bertaccini - 2004]. First we use

$$LDU - B = L(DU - L^{-1}B) \approx L(DU - B) \quad \text{or}$$

$$LDU - B = (LD - BU^{-1})U \approx (LD - B)U$$

depending on whether L is closer to identity or U.

2. The proposed preconditioner updates

Define the standard splitting

$$B = L_B + D_B + U_B.$$

Then the second approximation step is

$$LDU - B \approx L(DU - B) \approx L(DU - D_B - U_B) \equiv M^+$$

(upper triangular update) or

$$LDU - B \approx (LD - B)U \approx (LD - L_B - D_B)U \equiv M^+$$

(lower triangular update). Then M^+ is for free and its application asks for one forward and one backward solve.

- Ideal for upwind/downwind modifications
- Our experiments cover broader spectrum of problems

2. The proposed preconditioner updates

As an example consider a two-dimensional nonlinear convection-diffusion model problem: It has the form

$$-\Delta u + Ru\left(\frac{\partial u}{\partial x} + \frac{\partial u}{\partial y}\right) = 2000x(1-x)y(1-y), \tag{1}$$

on the unit square, discretized by 5-point finite differences on a uniform grid.

- The initial approximation is the discretization of $u_0(x, y) = 0$.
- We use here $R = 100$ and different grid sizes.
- We solve the resulting linear systems with BiCGSTAB with right preconditioning.
- Iterations were stopped when the Euclidean norm of the residual was decreased by seven orders.
- Matlab implementation.

2. The proposed preconditioner updates

BiCGSTAB iteration counts; reference factorization ILU(0)			
Matrix	Recomp	Freeze	Triangular update
$A^{(0)}$	40	40	40
$A^{(1)}$	25	37	37
$A^{(2)}$	24	41	27
$A^{(3)}$	20	48	26
$A^{(4)}$	17	56	30
$A^{(5)}$	16	85	32
$A^{(6)}$	15	97	35
$A^{(7)}$	14	106	43
$A^{(8)}$	13	97	44
$A^{(9)}$	13	108	45
$A^{(10)}$	13	94	50
$A^{(11)}$	15	104	45
$A^{(12)}$	13	156	49
overall time	13 s	13 s	7.5 s

2. The proposed preconditioner updates

The upper triangular update

$$M^+ = L(DU - D_B - U_B)$$

combines an incomplete LU factorization with the structural, Gauss-Seidel type preconditioner

$$DU - B \approx triu(DU - B).$$

However it does not take into account both triangular parts of $DU - B$. This can be simply corrected through the splitting

$$DU - B = \hat{L} + \hat{D} + \hat{U}$$

and defining the Gauss-Seidel update

$$M^+ = L\,(\hat{L} + \hat{D})\hat{D}^{-1}(\hat{D} + \hat{U})$$

and similarly for lower triangular update [Duintjer Tebbens, Tůma - 2007].

2. The proposed preconditioner updates

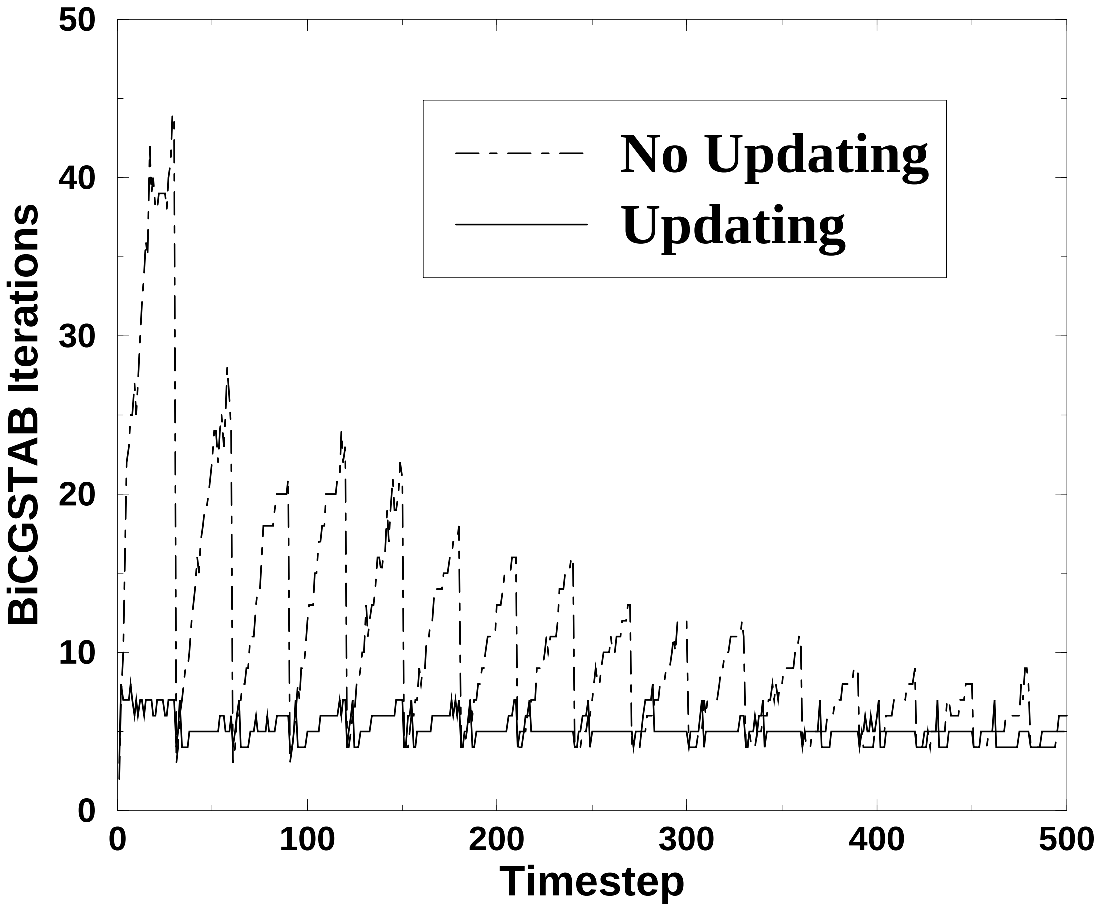
BiCGSTAB iteration counts; reference factorization ILU(0)				
Matrix	Recomp	Freeze	Triangular update	Gauss-Seidel update
$A^{(0)}$	40	40	40	40
$A^{(1)}$	25	37	37	27
$A^{(2)}$	24	41	27	27
$A^{(3)}$	20	48	26	19
$A^{(4)}$	17	56	30	21
$A^{(5)}$	16	85	32	25
$A^{(6)}$	15	97	35	29
$A^{(7)}$	14	106	43	31
$A^{(8)}$	13	97	44	40
$A^{(9)}$	13	108	45	38
$A^{(10)}$	13	94	50	44
$A^{(11)}$	15	104	45	35
$A^{(12)}$	13	156	49	42
overall time	13 s	13 s	7.5 s	6.5 s

2. The proposed preconditioner updates

The following CFD problem (compressible supersonic flow) is a less academic example:

- Frontal flow with Mach-number 10 around a cylinder, which leads to a steady state.
- 3000 steps of the implicit Euler method are performed.
- The grid consists of 20994 points, we use Finite Volume discretization and system matrices are of dimension 83976. The number of nonzeroes is about 1.33$\cdot 10^6$ for all matrices of the sequence.
- In the beginning, a strong shock detaches from the cylinder, which then slowly moves backward through the domain until reaching the steady state position.
- The iterative solver is BiCGSTAB with stopping criterion 10^{-7}, the implementation is in C++.

2. The proposed preconditioner updates



BiCGSTAB iterations for the first 500 systems in the cylinder problem

2. The proposed preconditioner updates

Can we define a good indicator of the quality of the update compared to the frozen preconditioner ? For ILU(0) and lower triangular updates we can prove

Lemma 1 *Let*

$$\rho = \frac{\|(D_B + L_B)(I - U)\|_F \, (2\,\|E - U_B\|_F + \|(D_B + L_B)(I - U)\|_F)}{\|D_B + L_B\|_F^2} < 1,$$

where $E = A - LDU$. Then the accuracy $\|A^+ - (LD - D_B - L_B)U\|_F$ of the updated preconditioner is higher than the accuracy of the frozen preconditioner $\|A^+ - LDU\|_F^2$ with

$$\|A^+ - (LD - D_B - L_B)U\|_F \leq \sqrt{\|A^+ - LDU\|_F^2 - (1-\rho)\|D_B + L_B\|_F^2}. \qquad (2)$$

2. The proposed preconditioner updates

For the first systems of the CFD problem the previous bound has the values

i	$\Vert A^{(i)} - LDU \Vert_F$	$\Vert A^{(i)} - M^{(i)} \Vert_F$	Bound from (2)	ρ from (2)
2	37.454	34.277	36.172	0.571
3	37.815	34.475	36.411	0.551
4	42.096	34.959	36.938	0.245
5	50.965	35.517	37.557	0.104
6	55.902	36.118	38.308	0.083

Accuracy of the preconditioners and theoretical bounds

However, the indicator-value ρ

- describes only accuracy, not stability $\Vert I - A^{(i)}(M^{(i)})^{-1} \Vert$ of the update
- is not fully for free because of the matrix product $(D_B + L_B)(I - U)$.

3. Updates in matrix-free environment

In many applications the linear solver is chosen such that it is not necessary to store system matrices; a matrix-vector product subroutine suffices. Can the updates be used in matrix-free environment ?

First note that to compute an incomplete factorization like ILU in matrix-free environment at all, the system matrix has to be *estimated*. This can be done with a graph coloring algorithm that tries to minimize the number of matvecs for a good estimate [Cullum, Tůma - 2006].

Recall the upper triangular update

$$M^+ = L(DU - D_B - U_B)$$

is based on the splitting

$$L_B + D_B + U_B = B = A - A^+.$$

Thus the update needs information on A and A^+.

3. Updates in matrix-free environment

We propose two strategies:

1. Estimation of *only the upper triangular part* of A^+ (the matrix A has been estimated anyway). Depending on the sparsity structure this might cost significantly less matvecs than estimation of the whole matrix A^+.

2. The second strategy circumvents any estimation of A^+. Let the matvec be replaced with a function evaluation

$$A^+ \cdot v \quad \rightarrow \quad F^+(v), \quad F^+ : \mathbb{R}^n \rightarrow \mathbb{R}^n.$$

We assume it is possible to compute the components $F_i^+ : \mathbb{R}^n \rightarrow \mathbb{R}$ of F^+ individually,

$$e_i^T \cdot A^+ \cdot v \quad \rightarrow \quad F_i^+(v), \quad F_i^+ : \mathbb{R}^n \rightarrow \mathbb{R}.$$

- The forward solves with L in $M^+ = L(DU - D_B - U_B)$ are trivial.

3. Updates in matrix-free environment

- For the backward solves, use a mixed explicit-implicit strategy: Split $DU - D_B - U_B = DU - triu(A) + triu(A^+)$ in the explicitly given part $X \equiv DU - triu(A)$ and the implicit part $triu(A^+)$. We then have to solve the triangular systems

$\left(X + triu(A^+)\right) z = y,$ yielding the standard backward substitution cycle

$$z_i = \frac{y_i - \sum_{j>i} x_{ij} z_j - \sum_{j>i} a^+_{ij} z_j}{x_{ii} + a^+_{ii}}, \qquad i = n, n-1, \ldots, 1. \qquad (3)$$

The sum $\sum_{j>i} a^+_{ij} z_j$ can be computed by the function evaluation

$$\sum_{j>i} a^+_{ij} z_j = F^+_i\left((0, \ldots, 0, z_{i+1}, \ldots, z_n)^T\right). \qquad (4)$$

The diagonal $\{a^+_{11}, \ldots, a^+_{nn}\}$ can be found by computing

$$a^+_{ii} = F^+_i(e_i), \qquad 1 \leq i \leq n.$$

4. Conclusions, future work

- We described a black-box preconditioner update for general nonsymmetric sequences of linear systems
- It can be combined with other techniques for solving specific types of sequences
- It can be applied in matrix-free environment
- Future work includes permutations to enhance triangular dominance, incorporating a priori estimators of the quality of the update and formulation for approximate inverse factorizations

For more details see:

- Birken Ph, Duintjer Tebbens J, Meister A, Tůma M: *Preconditioner Updates Applied to CFD Model Problems*, published online in Applied Numerical Mathematics in October 2007.
- Duintjer Tebbens J, Tůma M: *Improving Triangular Preconditioner Updates for Nonsymmetric Linear Systems*, LNCS vol. 4818, pp. 737–744, 2007 (proceedings of the 6th International Conference on Large-Scale Scientific Computations).
- Duintjer Tebbens J, Tůma M: *Efficient Preconditioning of Sequences of Nonsymmetric Linear Systems*, SIAM J. Sci. Comput., vol. 29, no. 5, pp. 1918–1941, 2007.

Thank you for your attention.

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