Advances in Engineering Software 000 (2016) 1–6

Contents lists available at ScienceDirect

Advances in Engineering Software

journal homepage: www.elsevier.com/locate/advengsoft

An adaptive multilevel factorized sparse approximate inverse preconditioning☆

Jiří Kopal[a,b,*], Miroslav Rozložník[a], Miroslav Tůma[a,c]

[a] Institute of Computer Science, Academy of Sciences of the Czech Republic, Pod Vodárenskou věží 2, CZ-182 07 Prague 8, Czech Republic
[b] Institute of Novel Technologies, Technical University of Liberec, Studentská 1402/2, CZ-461 17 Liberec 1, Czech Republic
[c] Faculty of Mathematics and Physics, Charles University in Prague,Czech Republic

ARTICLE INFO

Article history:
Received 29 February 2016
Revised 10 August 2016
Accepted 3 October 2016
Available online xxx

2010 MSC:
65F08
65F25
65F50

Keywords:
Approximate inverse
Gram–Schmidt orthogonalization
Incomplete factorization
Multilevel methods
Preconditioned conjugate gradient method

ABSTRACT

This paper deals with adaptively preconditioned iterative methods for solving large and sparse systems of linear equations. In particular, the paper discusses preconditioning where adaptive dropping reflects the quality of preserving the relation $UZ = I$ between the direct factor U and the inverse factor Z that satisfy $A = U^T U$ and $A^{-1} = ZZ^T$. The proposed strategy significantly extends and refines the approach from [1], see also [2], by using a specific multilevel framework. Numerical experiments with two levels demonstrate that the new preconditioning strategy is very promising. Namely, we show a surprising fact that in our approach the Schur complement is better to form in a more sophisticated way than by a standard sparse matrix-matrix multiplication.

1. Introduction

An important source of linear systems with positive definite matrices is represented by discretization of partial differential equations. Such equations arise in numerous applications in science and engineering and often lead to problems with sparse matrices. Let us consider the system of linear equations

$$Ax = b, \quad A \in \mathbb{R}^{n\times n}, \quad x \in \mathbb{R}^n, b \in \mathbb{R}^n, \tag{1}$$

where A is the system matrix, x is the vector of unknowns and b is the right-hand side vector. Here we will assume that the system matrix A is symmetric and positive definite.

Direct methods including the sparse Cholesky method as their standard representative are often considered as a method of choice. This approach is usually based on the factorization $A = U^T U$, where U is upper triangular. An important alternative to direct solvers are iterative Krylov space methods. In the symmetric and positive definite case, a natural choice in this class is the conjugate gradient (CG) method. In order to increase the robustness of iterative methods, the system (1) needs to be transformed, and this transformation is called preconditioning.

While in some cases preconditioning can be application-based, in other situations we have to rely on general algebraic approaches. Consequently, the need for generally reliable incomplete factorizations is strong. An important preconditioning strategy is based on incomplete Cholesky factorizations, that is on factorization $A \approx \hat{U}^T \hat{U}$, where $\hat{U}$ is upper triangular. There are a lot of possibilities to determine the way to approximate the exact Cholesky factorization.

But there are a few potential problems connected to the incomplete Cholesky factorization. First, it can break down. This means that a diagonal entry computed at some factorization step is zero or negative. Such a situation can be cured by various strategies that modify the original matrix introducing in this way an additional error. Formally the incomplete Cholesky factorization can be described as an exact factorization of a perturbed matrix

$$A + \Delta\hat{E} = \hat{U}^T \hat{U}, \tag{2}$$

where the matrix $\hat{E}$ is called the factorization error. Theoretical analysis of the incomplete Cholesky factorization that takes into

☆ Supported by the project GA13-06684S of the Grant Agency of the Czech Republic and by the ERC project MORE LL1202 financed by the MŠMT of the Czech Republic.

* Corresponding author.
E-mail addresses: jiri@cs.cas.cz, jiri.kopal@tul.cz (J. Kopal), miro@cs.cas.cz (M. Rozložník), tuma@cs.cas.cz, mirektuma@karlin.mff.cuni.cz (M. Tůma).

http://dx.doi.org/10.1016/j.advengsoft.2016.10.005
0965-9978/

account general matrix perturbations used in practice is very difficult and successful only in special cases, see, e.g., [3]. In addition, the bounds for the factorization error are often rough, they typically need additional assumptions and are difficult to apply if the factorization should be kept reasonably sparse. An important step to make factorization more robust is based on incomplete factors computed with the inverse-based dropping proposed by Bollhöfer and Saad [4–6]. Another attempt to get more reliable factorization is to evaluate simultaneously the direct approximate factor $\hat{U}$ with the approximate inverse factor $\hat{Z}$, see [7,8].

A counterpart of the Cholesky factorization is the inverse factorization introduced in [9]. It computes $A^{-1} = ZZ^T$ with Z upper triangular. Its algorithm is nothing more than the Gram–Schmidt orthogonalization of standard unit vectors with respect to a non-standard inner product induced by the matrix A. In this way we get two factors Z and U that satisfy the identities $ZU = UZ = I$. Similarly to the Cholesky factorization of A, the inverse factorization can be computed incompletely. In general, even more effort must be done to keep reasonable sparsity in the approximate inverse factorization $A^{-1} \approx \hat{Z}\hat{Z}^T$ computed by the approximate Gram–Schmidt orthogonalization, but such approximate inverse construction has also strong advantages. For example, we can get an incomplete Cholesky factor U without a breakdown and construct rather robust preconditioners for some classes of problems [10,11].

There is a rich history of incomplete factorizations that are based on multilevel reorderings or that explicitly use more levels in the factorization. Let us consider first the goal to achieve the multilevel effect by reorderings including also approaches for more general systems than symmetric and positive definite. In case of matrices from structured PDE discretizations we have interesting examples of recursive red-black reorderings in [12] where the author looks at conditioning of the final system matrix, studies the nested recursive factorization with two levels for nine-point difference matrices [13] and use it as a smoother in multigrid. Another combination of multigrid with incomplete factorization is described in [14]. A renumbering strategy with more levels that works also on unstructured grids was presented in [15], see also [16]. Let us also mention general matrix reorderings in [17], solving eigenvalue problems in [18] and also the use of more levels in incomplete factorizations in various applications. Such factorizations are typically used either directly, for example, for solving saddle-point problems, or as preconditioners, see, e.g., in [19–21], and also [22]. Related approximate inverse factorizations considered here is the line of research in [23–25]. We believe that the construction of the Schur complement proposed here may be combined with the framework and strategies in [26–28], but see also recent papers on other multilevel approaches from domain decomposition and nonsymmetric multilevel approximate inverse technique based on a block independent set reordering scheme and using factorized inverses as [29].

This paper presents a multilevel approach for computing the above mentioned approximate inverse factorization. The factorization uses the adaptive dropping introduced in [30], see also [1]. Here we propose the approximate inverse multilevel factorization as well as a new way to perform data transfer between levels in order to minimize the errors caused by related incomplete orthogonalization process.

If we use the computed approximate factorized inverse as a preconditioner of some Krylov space method then the transformed system is

$$\hat{Z}^T A\hat{Z}y = \hat{Z}^T b, \quad x = \hat{Z}y. \tag{3}$$

The quality of the approximation is determined by the loss of orthogonality between the column vectors of $\hat{Z}$ defined as $\Delta\hat{H} = \hat{Z}^T A\hat{Z} - I$. This quantity is an analogue of the expression $\hat{U}^{-T}A\hat{U}^{-1} - I$ introduced by Chow and Saad [31] as a measure of stability. It is clear that a small right residual $\Delta\hat{G} = I - \hat{U}\hat{Z}$ together with a small error in Cholesky factorization (2) imply a small loss of orthogonality $\Delta\hat{H}$. Indeed, we have

$$\hat{Z}^T A\hat{Z} - I = \hat{Z}^T(\hat{U}^T\hat{U} - \Delta\hat{E})\hat{Z} - I = \Delta\hat{G}^T + \Delta\hat{G} + \Delta\hat{G}^T\Delta\hat{G} - \hat{Z}^T\Delta\hat{E}\hat{Z}. \tag{4}$$

This relation is a theoretical basis of the adaptive dropping that we will use here.

The paper is organized as follows. Basics of the underlying theory are summarized in Section 2. The multilevel scheme is described in Section 3. Experimental results showing the qualitative improvements of the new approach are shown in Section 4 and the paper is finalized by conclusions and description of future work.

2. Gram–Schmidt based approximate inverse preconditioners

Let us consider the Gram–Schmidt orthogonalization of the standard unit vectors $e_1, \ldots, e_n$ with respect to the inner product $\langle \cdot, \cdot \rangle_A$ induced by the matrix A. We assume that the unit vectors are permuted so that they represent column vectors of the permutation matrix P. In this case, the Gram–Schmidt process applied to the columns of P leads to the factors Z and U satisfying

$$ZU = P, \tag{5}$$

where the columns of Z are A-orthonormal with $Z^TAZ = I$ and U is the upper triangular Cholesky factor of the matrix $P^TAP = U^TU$. It is clear that Z is the inverse factor satisfying $A^{-1} = ZZ^T$. The Gram–Schmidt process is summarized in Algorithm 1, where $Z = [z_1, \ldots, z_n]$ are the resulting A-orthonormal vectors and $U = [\alpha_{j,k}]$ contains the orthogonalization and normalization coefficients. Here we consider the modified version of the Gram–Schmidt process [32] that is equivalent to the SAINV algorithm [33] as explained in [2].

Algorithm 1 Modified version of the Gram–Schmidt process with column permutation and with respect to the inner product $\langle \cdot, \cdot \rangle_A$.

```
for k := 1 → n do
  z_k^(0) := P e_k
  for j := 1 → k − 1 do
    α_{j,k} := ⟨z_k^(j−1), z_j⟩_A
    z_k^(j) := z_k^(j−1) − α_{j,k} z_j
  end for
  α_{k,k} := ‖z_k^(k−1)‖_A
  z_k := z_k^(k−1) / α_{k,k}
end for
```

Algorithm 1 computes for each k a column z_k of the factor Z using the vector Pe_k that is A-orthogonalized against the previously computed vectors $z_1, \ldots, z_{k-1}$. This organization of the computation is known as the left-looking approach. Our goal is to obtain factor U such that its entries satisfy inequalities

$$\alpha_{1,1} \geq \alpha_{2,2} \geq \ldots \geq \alpha_{n,n} > 0 \tag{6}$$

$$\alpha_{i,i}^2 \geq \sum_{j=i}^{k} \alpha_{j,k}^2, \quad k = i+1, \ldots, n. \tag{7}$$

Note that, (6) and (7) also imply

$$\alpha_{j,j} > |\alpha_{j,k}|, \quad j = 1, \ldots, n, \quad k = j+1, \ldots, n. \tag{8}$$

The permutation P that leads to U in the above mentioned form is not a priori known and has to be computed on-the-fly. In addition, Algorithm 1 requires additional precomputation of orthogonalization coefficients using the classical variant of the Gram–Schmidt

Please cite this article as: J. Kopal et al., An adaptive multilevel factorized sparse approximate inverse preconditioning, Advances in Engineering Software (2016), http://dx.doi.org/10.1016/j.advengsoft.2016.10.005