Robust Structured Multifrontal Preconditioning For Discretized PDEs

J. Xia
Department of Mathematics, Purdue University, West Lafayette, IN 47907, USA
M. Gu
Department of Mathematics, University of California, Berkeley, CA 94720, USA

We present a preconditioning technique based on an approximate structured factorization method which is efficient, robust, and also relatively insensitive to ill conditioning, high frequencies, or wave numbers for some discretized PDEs. The factorization fully integrates graphical sparse matrix techniques, rank structures of fill-in, and automatic robustness enhancement techniques. The factorization has controllable accuracy and can work as an effective black-box preconditioner.

In iterative methods for solving large discretized PDEs arising from practical problems, classical preconditioners such as incomplete factorization or orthogonalization methods can break down due to numerical instability. In this work, we present a reliable and effective preconditioner based on structured data compression with any specified accuracy.

Consider a symmetric positive definite matrix A arising from the discretization of certain PDEs. A is usually large and sparse. In the Cholesky factorization $A = \mathcal{L}\mathcal{L}^T$, new nonzeros or fill-in are introduced into $\mathcal{L}$. One way to reduce fill-in is to reorder the rows and columns of A. For example, for an $N \times N$ regular mesh, the factorization with the nested dissection ordering [8] and its generalizations take $\mathcal{O}(n^{3/2})$ flops and $\mathcal{O}(n \log n)$ storage, where $n = N^2$ is the order of A. For two-dimensional problems, these are shown to be lower bounds for exact factorizations with any ordering [10] (ignoring special techniques such as Strassen's algorithm). Nest dissection uses separators to recursively divide the mesh into subregions.

A direct factorization with nested dissection is still expensive when used as a preconditioner. In this work, we compute structured approximate factorizations of A based on a rank property of the problems. It has been indicated in [1, 2, 3, 9, 14, etc.] that for some PDEs such as elliptic equations, during the direct factorization of A, the fill-in has a low-rank property, or, the off-diagonal blocks have small numerical ranks. This property can be used to improve the efficiency of the factorization. Rank structured matrices such as quasiseparable or semiseparable matrices [7, 13] can be used to approximate the dense intermediate matrices. The factorization can then provide a structured preconditioner.

Here, we organize the factorization with a supernodal multifrontal method together with the nest dissection ordering of mesh points. The multifrontal method is a very important direct methods for sparse matrix solutions [6, 12]. It keeps the propagation of information local between nodes and their parents. The supernodal version multifrontal method we use has nice data locality and takes good advantage of dense matrix operations. The factorization follows an elimination tree of the separators. The intermediate matrices are called frontal matrices and update matrices [6]. A frontal matrix is formed before the elimination of each separator and carries the information of the separator and its upper level neighbors. An update matrix is the Schur complement after the partial factorization of a frontal matrix. If the problem has the low-rank property, the frontal matrices can be approximated with rank structured matrices such as semiseparable matrices.

In [14], semiseparable matrices are used to approximate all intermediate matrices. This makes the assembly of structured matrices extremely complicated. The algorithm in [14] needs a careful implementation to ensure high efficiency. In this work, we simply form the dense intermediate matrices first and then approximately factorize them into rank structured matrices. The algorithm in [15] is used. After the factorization, the Schur complement matrix (update matrix) is still a regular dense matrix. Thus, standard matrix assembly is used in the multifrontal process. That is, all frontal and update matrices are in dense forms, but the factors are structured. This makes the algorithm much simpler than the one in [14].

Furthermore, the algorithm in [14] may suffer from the problem of breakdown, or the lose of positive definiteness, especially when a large tolerance is used in the structured approximation. Here, when directly factorizing dense frontal matrices, we use a robustness technique where Schur complements are automatically compensated. This compensation is done implicitly during the approximation of off-diagonal blocks. Thus, the low-rank approximation improves not only the efficiency but also the reliability. The total cost of this approximate factorization is only $\mathcal{O}(rn\log n)$, where r is the maximum off-diagonal numerical rank. This has an extra $\log n$ factor compared to the complexity of the algorithm in [14]. However, the computation time is still very competitive due to the dense block operations. In addition, even for problems where the low-rank property is not very significant, our approximate factorization with a relatively large tolerance can still provide attractive preconditioning results with satisfactory condition bounds. That is, the preconditioner does not need highly strict low-rank structural requirement to be effective like many other structured algorithms.

The semiseparable structure we use for the factors is a tree structured hierarchically semiseparable (HSS) matrix [4, 5]. Thus, the overall Cholesky factor is given by two layers of tree structures, an outer elimination tree of separators, and an inner HSS tree corresponding to each separator. The preconditioner has a good potential to be parallelized. We tested the structured preconditioner on various problems including elliptic problems, linear elasticity equations, Helmholtz equations, Maxwell equations, etc. Preliminary numerical results indicate that the preconditioner is relatively insensitive to frequency, wave numbers, etc. Comparisons with other methods and tools such as Hypre [11] demonstrate the effectiveness of this preconditioner. The factorization algorithm works as a black-box preconditioner and is also easy to use. It can work on A directly without the mesh information.

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