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Preconditioned Iterative Methods in a Subspace for Linear Algebraic Equations with Large Jumps in the Coefficients

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ABSTRACT. We consider a family of symmetric matrices $A_\omega = A_0 + \omega B$, with a nonnegative definite matrix A_0, a positive definite matrix B, and a nonnegative parameter $\omega \leq 1$. Small ω leads to a poor conditioned matrix A_ω with jumps in the coefficients. For solving linear algebraic equations with the matrix A_ω, we use standard preconditioned iterative methods with the matrix B as a preconditioner. We show that a proper choice of the initial guess makes possible keeping all residuals in the subspace $Im(A_0)$. Using this property we estimate, uniformly in ω, the convergence rate of the methods.

Algebraic equations of this type arise naturally as finite element discretizations of boundary value problems for PDE with large jumps of coefficients. For such problems the rate of convergence does not decrease when the mesh gets finer and/or ω tends to zero; each iteration has only a modest cost. The case $\omega = 0$ corresponds to the fictitious component/capacitance matrix method.

1. Introduction

In recent years, the study of preconditioners for iterative methods for solving large linear systems of equations, arising from discretizations of stationary boundary value problems of mathematical physics, has become a major focus of numerical analysts and engineers. In each iteration step of such a method, only a linear system with a special matrix, the preconditioner, has to be solved; the given system matrix has to be available only in terms of a matrix-vector multiplication. The basic theory of convergence of these methods is very well developed for the symmetric, positive definite case. It is well known that the preconditioner

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must approximate the inverse of the matrix of the original system well in order to obtain rapid convergence properties. For finite element/difference problems rapid convergence typically means that the rate of convergence is independent of the mesh size. It is common to use a conjugate gradient type method as an accelerator in such iterations.

There are several methods of constructing preconditioners, which allow the use of efficient methods, such as fast direct solvers, for solving the related linear systems. Many such methods with asymptotically optimal *a priori* estimates of the computational cost [**11**] are known, and some of these preconditioned iterative methods are among the best for solving mesh problems when the mesh parameter is small enough.

A particularly challenging class of problems arises with models described by partial differential equations (PDE) with discontinuous coefficients. Many important physical problems are of this nature. Such difficult problems arise in the design and study of numerical methods for composite materials built from essentially different components. Composites (or composite materials) are media with a large number of non-homogeneous inclusions of small sizes in at least one direction. Stationary states of such media are described by elliptic PDE with highly oscillating coefficients. Homogenization is the process of finding a set of constant coefficients such that the solution of the original PDE can be approximated well by that of the much simpler problem. The computation of homogenized coefficients for a composite with periodic structure reduces to solving a series of periodic boundary value problem for the original PDE in a domain of periodicity, see [**8**]. For composites with essentially different components, the coefficients of the PDE in the domain of periodicity are discontinuous and have large jumps.

Fictitious domain/embedding method is another source of PDE with jumps of coefficients, cf. e.g. [**19, 2, 10, 14**]. In this method, the original boundary value problem for the PDE is changed into a new boundary value problem with a domain in which the original one is embedded. In the new fictitious part of the domain the coefficients of PDE are chosen close to zero, if the original boundary condition is of Neumann type, or very large in the Dirichlet case. The solutions of these new problems approximate, or might even coincide with, the desired solutions. Therefore, the use of the fictitious domain method improves the shape of the boundary, but leads to a PDE with very large jumps of coefficients.

Similar problems occur in the semi-conductor device modelling.

There are several difficulties associated with the numerical solution of these problems using preconditioned iterative methods. For a number of methods, the larger the jumps of the coefficients, the slower the convergence. However, it has recently been shown [**4, 5, 6, 7**] that for continuous models, and with a special initial guess, the rate of convergence does not depend on the size of the jumps.

In the present paper, we explain the main idea of [**4, 5, 6, 7**] in the simplest form for algebraic systems of linear equations with a symmetric coefficient matrix.

We consider a parametric family of symmetric matrices $A_\omega = A_0 + \omega B$, with a nonnegative definite matrix A_0, a positive definite matrix B, and a parameter $\omega, 0 \le \omega \le 1$. Small ω leads to a large drop of coefficients of A_ω. For solving linear algebraic equations with matrix A_ω, we use standard preconditioned iterative methods with matrix B as a preconditioner. We show that a proper choice of the initial guess makes it possible to keep all residuals in the subspace $Im(A_0)$ and the difference between all iteration vectors and the solution in the subspace $Im(B^{-1}A_0)$. Using this property we estimate, uniformly in ω, the convergence rate of the methods.

A similar method, based on the same idea, was proposed in [**1**]. This method can only be applied for solving PDE with piece wise constant coefficients. We have to note that the proof of the mesh extension theorem in [**1**] is not correct.

In the case $\omega = 0$, these methods are closely related to the *capacitance matrix methods* [**18, 16, 17, 9, 15**].

The importance of the idea of *iterative methods in a subspace* is widely recognized in the theory of the *domain decomposition methods*, e.g. [**13**].

2. Preconditioned Iterative Methods for the symmetric positive definite case

We first consider a linear algebraic system $Au = f$ with a symmetric positive definite matrix A. In practice, a direct solution of that system often requires very considerable computational work, so iterative methods of the form

$$u^{n+1} = u^n - \gamma^n B^{-1}(Au^n - f) \tag{1}$$

with a symmetric positive definite matrix B, the preconditioner, are of great importance.

There is an equivalent form of the method for residuals $r^n = Au^n - f$:

$$\begin{aligned} r^{n+1} &= r^n - \gamma^n AB^{-1}r^n, r^0 = Au^0 - f, \\ \sigma^{n+1} &= \sigma^n + r^{n+1}, \sigma^0 = r^0, \\ u^{n+1} &= u^0 - \gamma^n B^{-1}\sigma^n. \end{aligned} \tag{2}$$

Preconditioned iterative methods of this kind can be very effective for the solution of systems of equations arising from discretizations of elliptic operators and their effectiveness can, of course, be further enhanced by the use of conjugate gradient type methods. For an appropriate choice of the preconditioner B, the convergence does not slow down when the mesh is refined and each iteration has a small cost; see e.g. [**11**].

Let

$$0 < \delta_0(Bv, v) \le (Av, v) \le \delta_1(Bv, v), v \ne 0. \tag{3}$$

The importance of choosing the preconditioner B such that δ_1/δ_0, the condition number of $B^{-1}L$, either is independent of N, the size of the system, or depends weakly, e.g. polylogarithmically in N, is widely recognized. At the same time, the numerical solution of the system with the matrix B should ideally require on the order of N, or $N \ln N$ arithmetic operations for single processor computers.

It is well known that, typically, the smaller the ratio δ_0/δ_1, the slower the convergence.

We cite here the simplest convergence estimate. Let $\gamma_k = \delta_1$; then

$$(B(u^n - u), u^n - u) \leq q^n (B(u^0 - u), u^0 - u), \quad q \equiv 1 - \delta_0/\delta_1, \tag{4}$$

for an arbitrary initial guess u^0.

3. The symmetric nonnegative definite case

We now consider the case $A = A_0$ where A_0 is a symmetric nonnegative definite matrix. The matrix B may also be symmetric nonnegative definite with the kernel $Ker B \subseteq Ker A_0$. Such matrices B and A_0 arise, for example, when considering periodic boundary value problems. In the present paper, however, we, for simplicity, consider only positive definite B.

Inequality (3) can not be true any longer, because the matrix A_0 has a kernel. Let, instead of (3), the following analogous inequalities hold:

$$0 < \delta_0 (Bv, v) \leq (A_0 v, v) \leq \delta_1 (Bv, v), v \neq 0, v \in Im(B^{-1}A_0), \tag{5}$$

and, thereby, δ's *have been redefined.* The subspace $Im(B^{-1}A_0)$ will play the key role and we denote it by $Im = Im(B^{-1}A_0)$.

LEMMA 1. *The subspace Im consists of all B-normal, i.e. normal in the scalar product $(B\star, \star)$, solutions of the system $A_0 u = f$ for all possible right-hand sides f.*

The following theorem is well known, cf. [**2**].

THEOREM 1. *Let u be a B-normal solution of $A_0 u = f$ for a given $f \in Im A_0$ and let the initial guess u^0 be chosen such that $u^0 \in Im$. Then the iterative method (1) with $A = A_0$ and $\gamma_k = \delta_1$ converges to this B-normal solution and convergence estimate (4) holds with δ's from (5).*

The proof is based on the fact that the subspace Im is invariant with respect to the operator $B^{-1}A_0$.

4. The symmetric positive definite case

We finally consider a parametric family of symmetric positive definite matrices $A = A_\omega = A_0 + \omega B$, with a parameter $\omega, 0 < \omega \leq 1$. The condition number of the matrix A_ω as well as that of the preconditioned matrix $B^{-1}A_\omega$ tends to infinity as ω tends to zero, and the common convergence theory of the method (1) for the positive definite case becomes useless.

We can improve the convergence by using a special initial guess, however.

THEOREM 2. *Let the initial guess u^0 be chosen such that $u^0 - B^{-1}f/\omega \in Im$. Then the iterative method (1) with $A = A_\omega$ and $\gamma_k = \delta_1 + 1$ converges and the convergence estimate (4) holds with $q = 1 - \delta_0/(\delta_1 + 1)$ and δ's from (5).*

The proof is very similar to the proof of the previous theorem. The subspace Im is invariant with respect to the operator $B^{-1}A_\omega = B^{-1}A_0 + \omega I$ and the initial error $u^0 - u$ is in this subspace.

We also note that the initial residual and, therefore, all residuals of the method (2) lie in the subspace ImA_0.

Analogous convergence results may be, evidently, obtained for preconditioned conjugate gradient methods with this choice of the initial guess.

A dual approach to the numerical solution of problems with large jumps of coefficients, using a mixed variational formulation, is described in [**12**]. For a general saddle point problem

$$(6) \qquad \begin{pmatrix} F_\omega & G \\ G^* & 0 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} 0 \\ f \end{pmatrix},$$

where $F_\omega = F_0 + \omega I$, F_0 symmetric nonnegative definite, and ω is a parameter, $0 \le \omega \le 1$, we obtain

$$\begin{cases} P^\perp F_\omega v &= 0, \quad P = G(G^*G)^{-1}G^*, P^\perp = I - P, \\ Pv &= p, \quad p = G(G^*G)^{-1}f. \end{cases}$$

P is an orthoprojector and the system is further reformulated as a single matrix equation with a symmetric, nonnegative definite matrix $P^\perp F_\omega P^\perp$. This matrix, as well as our preconditioned matrix $B^{-1}A_\omega$, is an ωI perturbation in the subspace $Im(P^\perp)$ of a symmetric nonnegative definite matrix. Therefore, our trick with the special initial guess for a standard iterative method is useful for this matrix, too; see [**12**].

This approach was applied in [**3**] to the diffusion equation taking A^{-1} as the diffusion coefficient and $-G$ as the gradient operator. The method is most efficient when multiplication by P can be calculated using a fast direct method, e.g. for a problem with a periodic boundary condition, which arises naturally in homogenization and fictitious domain methods.

In the near future we are planning to consider a case of a nonsymmetric family $A_\omega = A_0 + \omega B$, by using symmetrization in the form $(B^{-1}A_\omega)^*B^{-1}A_\omega$.

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