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On deflation and singular symmetric positive semi-definite matrices

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Abstract

For various applications, it is well-known that the deflated ICCG is an efficient method for solving linear systems with invertible coefficient matrix. We propose two equivalent variants of this deflated ICCG which can also solve linear systems with singular coefficient matrix, arising from discretization of the discontinuous Poisson equation with Neumann boundary conditions. It is demonstrated both theoretically and numerically that the resulting methods accelerate the convergence of the iterative process.

Moreover, in practice the singular coefficient matrix has often been made invertible by modifying the last element, since this can be advantageous for the solver. However, the drawback is that the condition number becomes worse-conditioned. We show that this problem can completely be remedied by applying the deflation technique with just one deflation vector.
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1. Introduction

Recently, moving boundary problems have received much attention in literature due to their applicative relevance in many physical processes. One of the most popular moving boundary problems is modelling bubbly flows, see e.g. [15]. These bubbly flows can be simulated by solving the Navier–Stokes equations using for instance the pressure correction method [5]. The most time-consuming part of this method is solving the symmetric and positive semi-definite (SPSD) linear system on each time step, which is coming from a second-order finite-difference discretization of the Poisson equation with possibly discontinuous coefficients and Neumann boundary conditions:

$$\begin{cases} \nabla \cdot \left(\dfrac{1}{\rho(\mathbf{x})} \nabla p(\mathbf{x}) \right) = f(\mathbf{x}), & \mathbf{x} \in \Omega, \\ \dfrac{\partial}{\partial \mathbf{n}} p(\mathbf{x}) = g(\mathbf{x}), & \mathbf{x} \in \partial\Omega, \end{cases} \tag{1}$$

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where p, ρ, $\mathbf{x}$ and $\mathbf{n}$ denote the pressure, density, spatial coordinates and the unit normal vector to the boundary $\partial\Omega$, respectively. The resulting singular linear system is

$$Ax = b, \quad A = [a_{i,j}] \in \mathbb{R}^{n\times n}, \tag{2}$$

where the coefficient matrix A is SPSD. If $b \in \mathrm{Col}(A)$ then the linear system (2) is consistent and infinite number of solutions exists. Due to the Neumann boundary conditions, the solution x is determined up to a constant, i.e., if x_1 is a solution then $x_1 + c$ is also a solution where $c \in \mathbb{R}^n$ is an arbitrary constant vector. This situation presents no real difficulty, since pressure is a relative variable, not an absolute one. In this paper we concentrate on the linear system (2), which can also be derived from other problems besides the bubbly flow problems. The precise requirements can be found in the next section of this paper.

In many computational fluid dynamics packages, see also [1,4,14], one would impose an invertible A, denoted by $\widetilde{A}$. This makes the solution x unique which can be advantageous in computations, for instance,

- direct solvers like Gaussian elimination can only be used to solve the linear systems when A is invertible;
- the original singular system may be inconsistent as a result of rounding errors, whereas the invertible system is always consistent;
- the deflation technique requires an invertible matrix $E := Z^{\mathrm{T}}AZ$ which will be explained later on in this paper. The choice of Z is only straightforward if A is non-singular.

One common way to force invertibility of matrix A in literature is to replace the last element $a_{n,n}$ by $\tilde{a}_{n,n} = (1+\sigma)a_{n,n}$ with $\sigma > 0$. In fact, a Dirichlet boundary condition is imposed at one point of the domain Ω. This modification results in an invertible linear system

$$\widetilde{A}x = b, \quad \widetilde{A} = [\tilde{a}_{i,j}] \in \mathbb{R}^{n\times n}, \tag{3}$$

where $\widetilde{A}$ is symmetric and positive definite (SPD).

The most popular iterative method to solve linear systems like (3) is the preconditioned conjugate gradient (CG) method (see e.g. [3]). After k iterations of the CG method, the error is bounded by (cf. [3, Theorem 10.2.6])

$$\|x - x_k\|_{\widetilde{A}} \leqslant 2\|x - x_0\|_{\widetilde{A}} \left(\frac{\sqrt{\kappa - 1}}{\sqrt{\kappa + 1}}\right)^k, \tag{4}$$

where x_0 denotes the starting vector and $\kappa = \kappa(\widetilde{A}) = \lambda_n/\lambda_1$ denotes the spectral condition number of $\widetilde{A}$. Therefore, a smaller κ leads asymptotically to a faster convergence of the CG method. In practice, it appears that the condition number κ is relatively large, especially when σ is close to 0. Hence, solving (3) with the CG method shows slow convergence, see also [4,14]. The same holds if the ICCG method [9] is used. Since $\widetilde{A}$ is an SPD matrix with $\tilde{a}_{i,j} \leqslant 0$ for all $i \neq j$, an incomplete Cholesky (IC) decomposition always exists [4].

ICCG shows good performance for relatively small and easy problems. However, it appears that ICCG still does not give satisfactory results in more complex models, for instance when the number of grid points becomes very large or when there are large jumps in the density of (1). To remedy the bad convergence of ICCG, (eigenvalue) deflation techniques are proposed, originally from Nicolaides [13]. The idea of deflation is to project the extremely large or small eigenvalues of $\widetilde{M}^{-1}\widetilde{A}$ to zero, where $\widetilde{M}^{-1}$ is the IC preconditioner based on $\widetilde{A}$. This leads to a faster convergence of the iterative process, due to Expression (4) and due to the fact that the CG method can handle matrices with zero-eigenvalues, see also [4]. The resulting method is called DICCG.

The deflation technique has been exploited by several other authors, e.g. [2,7,8,10–12]. The resulting linear system which has to be solved is

$$\widetilde{M}^{-1}\widetilde{P}\widetilde{A}x = \widetilde{M}^{-1}\widetilde{P}b, \tag{5}$$

where $\widetilde{P}$ denotes the deflation matrix based on $\widetilde{A}$. We have already mentioned that the ICCG method shows slow convergence after forcing invertibility of A. In this paper, we will investigate this phenomenon for the DICCG method.

Another DICCG approach to solve (2) without forcing invertibility is to solve

$$M^{-1}PAx = M^{-1}Pb, \tag{6}$$

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