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AN ACCELERATED DEFLATION TECHNIQUE FOR LARGE SYMMETRIC GENERALIZED EIGENPROBLEMS

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Abstract

An accelerated optimization technique combined with a stepwise deflation procedure is presented for the efficient evaluation of a few of the smallest eigenvalues and their corresponding eigenvectors of the generalized eigenproblems. The optimization is performed on the Rayleigh quotient of the deflated matrices by the aid of a preconditioned conjugate gradient scheme with the incomplete Cholesky factorization.

1. Introduction. In this paper, we shall be concerned with computing a few of the smallest eigenvalues and their corresponding eigenvectors of the generalized eigenvalue problem

$$Ax = \lambda Bx, \tag{1}$$

where A and B are large sparse symmetric positive definite matrices. Such a partial eigenproblem often arises in many engineering and science applications, e.g., structural mechanics, hydrodynamics and plasma physics. Due to the large number of applications of this problem, considerable effort has been devoted to the development of efficient and reliable methods for solving such a problem. A detailed list of references and a review of these methods can be found in [3,10].

Recently iterative algorithms based on the optimization of the Rayleigh quotient have been developed[1,7], and a conjugate gradient(CG) scheme for the optimization of the Rayleigh quotient has proven a very attractive and promising technique for large sparse eigenproblems[4,13]. As in the case of a system of linear equations, successful application of CG method to eigenproblems depends also upon the preconditioning techniques. In particular incomplete Cholesky(IC) factorization preconditioner turned out to be a reliable and efficient tool for the solution to both linear systems and eigenproblems in a finite element context[9].

The aim of this papar is to apply IC preconditioning for the CG optimization of the Rayleigh quotient together with a shifting deflation technique to evaluate several of the smallest eigenpairs. The result proved very encouraging and the method rather cost-effective.

Key Words : Generalized eigenvalue problem, preconditioned conjugate gradient scheme, deflation
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2. Generalized eigenproblem via preconditioned CG Scheme.

2.1. Conjugate gradient scheme. Let A and B be symmetric positive definite matrices of order n. We look for the m smallest eigenvalues

$$0 < \lambda_1 < \lambda_2 \leq \lambda_3 \leq \cdots \leq \lambda_m \tag{2}$$

and for the corresponding eigenvectors $z_1, z_2, \cdots, z_m$ of (1) such that

$$Az_j = \lambda_j B z_j, \quad {z_j}^T B z_j = 1, \quad j = 1, 2, \cdots, m. \tag{3}$$

The number m of the desired eigenpairs (λ_j, z_j) is much smaller than the order n of the matrices.

We recall that the eigenvectors of (1) are the stationary points of the Rayleigh quotient

$$R(x) = \frac{x^T A x}{x^T B x}, \tag{4}$$

and the minimum of the Rayleigh quotient $R(x)$ corresponding to (1) is equal to λ_1 and is attained at z_1:

$$\min_{x \neq 0} R(x) \;=\; \lambda_1 \;=\; \frac{{z_1}^T A z_1}{{z_1}^T B z_1}.$$

The minimum of $R(x)$ is determined iteratively by CG method. For an iterate $x^{(k)}$ the corresponding gradient of $R(x)$,

$$\nabla R(x^{(k)}) = g^{(k)} = g(x^{(k)}) = 2 \left[\frac{Ax^{(k)} - R(x^{(k)}) B x^{(k)}}{{x^{(k)}}^T B x^{(k)}} \right], \tag{5}$$

is used to fix the direction of descent $p^{(k+1)}$ in which $R(x)$ is minimized. These directions of descent are defined by

$$p^{(1)} = -g^{(0)}, \quad p^{(k+1)} = -g^{(k)} + \beta^{(k)} p^{(k)}, \quad k = 1, 2, \cdots.$$

Different explicit values for the parameter $\beta^{(k)}$ exist. Comparison of CG methods for computing the smallest eigenpair with various forms of $\beta^{(k)}$ and their asymptotic behaviors are discussed in [3]. The expression for $\beta^{(k)}$, which is given by the A-conjugacy[8],

$$\beta^{(k)} = \frac{{g^{(k)}}^T g^{(k)}}{{g^{(k-1)}}^T g^{(k-1)}},$$

is commonly used.

The subsequent iterate $x^{(k+1)}$ along $p^{(k+1)}$ through $x^{(k)}$ is written as

$$x^{(k+1)} = x^{(k)} + \alpha^{(k+1)} p^{(k+1)}, \quad k = 0, 1, \cdots, \tag{6}$$

where $\alpha^{(k+1)}$ is obtained by minimizing $R(x^{(k+1)})$,

$$R(x^{(k+1)}) = \frac{{x^{(k)}}^T A x^{(k)} + 2\alpha^{(k+1)} {p^{(k+1)}}^T A x^{(k)} + {\alpha^{(k+1)}}^2 {p^{(k+1)}}^T A p^{(k+1)}}{{x^{(k)}}^T B x^{(k)} + 2\alpha^{(k+1)} {p^{(k+1)}}^T B x^{(k)} + {\alpha^{(k+1)}}^2 {p^{(k+1)}}^T B p^{(k+1)}}.$$

A detailed explanation to get the values for $\alpha^{(k+1)}$ can be found in [7].

2.2. Preconditioned CG scheme. The convergence of the sequence of iterates $x^{(k)}$ in (6) towards the direction of z_1 depends on the condition number of the Hessian matrix $H(x)$ of $R(x)$,

$$H(x) = \frac{2}{x^T Bx}\left[A - R(x)B - g(x)(Bx)^T - (Bx)g(x)^T\right]$$

evaluated at z_1[9]. Due to the B-orthonormality of z_1 and $g(z_1) = 0$, $H(z_1) = 2(A - \lambda_1 B)$ holds and the norm of $H(z_1)$, subordinate to the norms $\|x\|_B = \sqrt{x^T Bx}$ and $\|x\|_{B^{-1}} = \sqrt{x^T B^{-1} x}$, is given by

$$\|H(z_1)\|_{B,B^{-1}} = \sup_{x\neq 0} \frac{\|H(z_1)x\|_{B^{-1}}}{\|x\|_B} = 2(\lambda_n - \lambda_1).$$

Since $H(z_1)$ is positive semidefinite, the corresponding condition number is defined by

$$\kappa_{B,B^{-1}}(H(z_1)) = \frac{\lambda_n - \lambda_1}{\lambda_2 - \lambda_1},$$

and the condition number of the Hessian matrix can be essentially decreased by the use of suitable preconditioning techniques[11].

The idea behind the PCG is to apply CG method to the transformed system

$$\tilde{A}\tilde{x} = \lambda \tilde{B}\tilde{x},$$

where $\tilde{A} = C^{-1}AC^{-1}$, $\tilde{B} = C^{-1}BC^{-1}$, $\tilde{x} = Cx$, and C is nonsingular symmetric matrix. By substituting $x = C^{-1}\tilde{x}$ into (4), we obtain

$$R(\tilde{x}) = \frac{\tilde{x}^T C^{-1}AC^{-1}\tilde{x}}{\tilde{x}^T C^{-1}BC^{-1}\tilde{x}} = \frac{\tilde{x}^T \tilde{A}\tilde{x}}{\tilde{x}^T \tilde{B}\tilde{x}}, \tag{7}$$

where the matrices $\tilde{A}$ and $\tilde{B}$ are symmetric positive definite. The transformation (7) leaves the stationary values of (4) unchanged, which are eigenvalues of (1), while the corresponding stationary points are obtained from $\tilde{x}_j = Cz_j, \quad j = 1, 2, \cdots, n$. In fact the Hessian matrix of $R(\tilde{x})$, evaluated at the eigenvector $\tilde{x}_1$, is similar to

$$C^{-1}H(\tilde{x}_1)C = 2(C^2)^{-1}(A - \lambda_1 B) = (C^2)^{-1}H(z_1).$$

The matrix $M = C^2$ is called the preconditioner.

There are a number of choices of M, ranging from simple to complicated forms, among which the incomplete Cholesky decomposition that preserves exactly the nonzero pattern of A exhibits both efficiency and robustness[3-6,11]. In our work, the preconditioning matrix $M = HH^T$ is used, H being the pointwise incomplete Cholesky factor of A. The PCG algorithm for solving the smallest eigenpair with implicit preconditioning is summarized as follows.

The PCG algorithm for computing the smallest eigenpair

Step 1. Compute the preconditioner $M = HH^T$.
Step 2. Choose an initial guess $x^{(0)} \neq 0$.
Step 3. Construct the initial gradient direction $g^{(0)}$.

$$\text{Set } \; p^{(1)} = -g^{(0)} \; \text{ and } \; Mh^{(0)} = g^{(0)}.$$

Step 4. Iterate for $k = 0$ to NMAX(maximum number of iterations).
Step 5. If $k = 0$ then set $\beta^{(k)} = 0$, otherwise compute

$$Mh^{(k)} = g^{(k)} \; \text{ and } \; \beta^{(k)} = \frac{{g^{(k)}}^T h^{(k)}}{{g^{(k-1)}}^T h^{(k-1)}}.$$

Step 6. Compute $p^{(k+1)} = -h^{(k)} + \beta^{(k)} p^{(k)}$.
Step 7. Compute $\alpha^{(k+1)}$ by minimizing $R(x^{(k+1)})$(see [7] for details).
Step 8. Compute $x^{(k+1)} = x^{(k)} + \alpha^{(k+1)} p^{(k+1)}$.
Step 9. Test on convergence.

3. Higher eigenvalues computation. Although the PCG scheme in §2 only produces the smallest eigenpair of (1), this algorithm can also be used evaluate a few of the smallest eigenpairs and their corresponding eigenvectors by using a deflation based on a partial shift of the spectrum [6,11].

When the first $r-1$ eigenpairs are approximately known, the next eigenpair (λ_r, z_r) could be obtained by minimizing the Rayleigh quotient $R(x)$ of the modified eigenproblem $A_r x = \lambda B x$, where A_r is defined by

$$A_r = A + \sum_{i=1}^{r-1} \sigma_i (Bz_i)(Bz_i)^T, \tag{8}$$

with σ_i is the shift that satisfies $\sigma_i > 0$ and $\lambda_i + \sigma_i > \lambda_r, \quad i = 1, 2, \cdots, r-1$. More details and the numerical stability of the deflation process (8) are reported in [11].

In the previous section, we chose the preconditioner M as an approximate representation of A. Thus, M also has to be modified in the same manner as A_r. The modified preconditioner M_r of A_r is defined by

$$M_r = M + \sum_{i=1}^{r-1} \sigma_i (Bz_i)(Bz_i)^T.$$

The replacement of M with M_r in *step 5* of the PCG scheme in §2 requires the solution of the linear equation

$$\left\{ M + \sum_{i=1}^{r-1} \sigma_i (Bz_i)(Bz_i)^T \right\} h = g. \tag{9}$$

To solve for h in (9), a Sherman-Morrison formula is applied. By assuming that $h_0 = M^{-1} g$ can be easily solved, the algorithm for computing (9) is given as follows.

Algorithm for computing $h = M_r^{-1} g$

Step 1. Compute $h_0 = M^{-1} g$.
Step 2. Iterate for $i = 1$ to $r - 1$.
Step 3. Compute $h_i = h_{i-1} - \dfrac{\sigma_i M^{-1}(Bz_i)(Bz_i)^T h_{i-1}}{1 + \sigma_i (Bz_i)^T M^{-1}(Bz_i)}$.

A proper choice of the shift σ_i can reduce the number of iterations significantly in the proposed method. Experience indicates that too large shifts σ_i of the computed eigenvalues have some negative influence on the convergence, so that they must be chosen in a reasonable way, taking into account the distribution of the eigenvalues. A possible strategy defines the σ_i to be a multiple of the lastly computed eigenvalue λ_{r-1}[11], where the factor decreases from a starting value to a limiting value larger than one with increasing index r. However, a potential wrong choice with $\lambda_{r-1} + \sigma_{r-1} < \lambda_r$ can easily be discovered in the deflation of using the multiple shift because the resulting minimal value of the Rayleigh quotient will be equal to $\lambda_{r-1} + \sigma_{r-1}$. A bad choice with $\lambda_r < \lambda_{r-1} + \sigma_{r-1} < \lambda_{r+1}$ results in a slow convergence. We recall that the Rayleigh quotient (4) for an arbitrary vector x provides an overestimate and an underestimate of the spectral bounds λ_n and λ_1, respectively. So the maximal value of (4) is equal to λ_n and is obtained by using opposite direction of the descent $g(x^{(k)})$ in (5). By assuming that λ_n is easily computed, a possible choice of the shift σ_i can be defined by

$$\sigma_i = \mu - \lambda_i, \quad i = 1, \cdots, r-1, \quad \text{where } \mu = \frac{\lambda_1 + \lambda_n}{2}. \tag{10}$$

In the numerical models of large hydrodynamic systems or mechanical structures $\lambda_1 \ll \lambda_n$, the eigenvalues exhibit to some extent a uniform distribution between the extreme bound and the separation is usually not to bad. Thus the way of choosing σ_i in (10) is quite effective. Actually the numerical results given in the next section show that, while the deflation with the multiple shifting fails to converge, the deflation with the shifting in (10) yields accurate results in only a few number of steps.

4. Numerical experiments. The performance of the deflation-PCG scheme presented in this paper has been analyzed for the computation of the m smallest eigenpairs of two sparse symmetric positive definite matrices. *Example 1.* The dynamic modelling of structure is considered. The matrix A, the stiffness matrix*, and the matrix B, the mass matrix†, are the result of applying "static condensation" to the oil ring model. Static condensation can be applied in cases where the mass matrix is singular to reduce the problem order while preserving the spectrum. However, the reduced stiffness matrix is usually dense, which is the case here. *Example 2.* The problem of the vibration string of length 1, fixed at both ends, is considered. The variational formulation of the Rayleigh quotient takes the form

$$R(x) = \frac{\int_0^1 (dx/dt)^2 dt}{\int_0^1 x(t)^2 dt}. \tag{11}$$

*These matrices can be obtained from the Matrix Market under the set BCSSTRUC1; `http://math.nist.gov/MatrixMarket/data/Harwell-Boeing`

The two integrals are approximated using quadratic spline functions with a mesh step $h = \frac{1}{513}$ and 512 interior points. Equation (11) takes the form

$$R(x) \approx \frac{c}{h^2} \frac{x^T A x}{x^T B x}$$

with $c = 18$ and

$$A = \begin{bmatrix} 8 & -1 & -1 & & & & & \\ -1 & 6 & -2 & -1 & & & & \\ -1 & -2 & 6 & -2 & -1 & & & \\ & & \ddots & \ddots & \ddots & & & \\ & & -1 & -2 & 6 & -2 & -1 & \\ & & & -1 & -2 & 6 & -1 & \\ & & & & -1 & -1 & 8 & \end{bmatrix}, \quad B = \begin{bmatrix} 40 & 25 & 1 & & & & & \\ 25 & 66 & 26 & 1 & & & & \\ 1 & 26 & 66 & 26 & 1 & & & \\ & & \ddots & \ddots & \ddots & & & \\ & & 1 & 26 & 66 & 26 & 1 & \\ & & & 1 & 26 & 66 & 1 & \\ & & & & 1 & 25 & 40 & \end{bmatrix}.$$

The convergence criterion is set as

$$\frac{\|\lambda^{(k)} B x^{(k)} - A x^{(k)}\|}{\|A x^{(k)}\|} < \epsilon,$$

ϵ is the convergence tolerance for the required eigensolutions.

Due to the comparison of the performance of the CG scheme and the PCG-IC scheme for computing the smallest eigenvalue have been reported in [3-4,11], these two schemes are not described in this study. Also the approach with the initial guess obtained from a coarse mesh[2], which is potentially attractive, is not considered.

Figure 1 compares the performance of deflation-PCG with the multiple shift[11](DPCGM) and deflation-PCG with the shift in (10)(DPCGB) for the computation of the leftmost m eigenpairs of the matrices in Examples 1–2. Figure 1 emphasizes the improved performance of DPCGB. The DPCGB iterations needed to compute the leftmost m eigenpairs are fewer than the DPCGM iterations.

FIG. 1. *Average convergence profiles of DPCGB and DPCGM for Examles 1 and 2*

Table 1 compares the CPU times required by both schemes. The average numbers of DPCGB iterations and DPCGM iterations performed to satisfy the exit criterion with $\epsilon = 10^{-6}$ are also given.

TABLE 1. *CPU time and the average iterations of DPCGB and DPCGM*

Examples	λ_i	DPCGB		DPCGM	
		time(sec.)	iter.	time(sec.)	iter.
	4.3265013e+01	7.8000e–02	13	7.8000e–02	13
$n = 66$	4.3849748e+01	7.8000e–02	11	9.4000e–02	15
$m = 5$	4.9453708e+01	3.1000e–02	6	7.8000e–02	10
	5.6567577e+02	1.5600e–01	18	1.4840e–00	148
	5.7065179e+02	6.3000e–02	8	2.1900e–01	17
	8.9173756e+00	6.9380e+00	8	6.6410e+00	8
$n = 512$	3.5669502e+01	1.0578e+01	11	2.8906e+01	29
$m = 10$	8.0256381e+01	1.3844e+01	13	1.8828e+01	16
	1.4267801e+02	1.6297e+01	14	5.6250e+01	42
	2.2293439e+02	1.9000e+01	15	3.8109e+01	25
	3.2102553e+02	2.1906e+01	16	7.8392e+01	46
	4.3695141e+02	2.5031e+01	17	4.8796e+01	26
	5.7071205e+02	2.8359e+01	18	5.5844e+01	28
	7.2230744e+02	3.1891e+01	19	5.9110e+01	28
	8.9173758e+02	3.3859e+01	19	5.3236e+02	230

5. Conclusions. From the above numerical experiments it appears that the deflation-PCG scheme DPCGB is quite robust and the number of iterations required in the evaluation of each eigenpair does not increase significantly when the order n becomes large. In the present paper a few of the smallest eigenpairs have been computed, but the scheme can be used efficiently for the assessment of a large number of eigenpairs.

Although the DPCGB is numerically superior to the DPCGM, in case of pathological eigenvalue distributions every rule for defining the shifts may happen to fail. In a series of papers [10,5], Gambolati. et al. have developed schemes which can considerably reduce this difficulty even though they are not easy to implement practically in a computer code and their numerical behavior has been explored mainly with small and unrealistic sample problems. Comparisons of these schemes and DPCGM with various finite element examples will be reported in detail elsewhere [6].

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