Single Precision Calculation of Iterative Refinement of Pairs of a Real Symmetric-Definite Generalized Eigenproblem by Using a Filter Composed of a Single Resolvent

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1 INTRODUCTION

For a given generalized eigenproblem $A\mathbf{v} = \lambda B\mathbf{v}$ whose matrices A and B are real symmetric and B is positive definite, we solve all those approximate pairs whose eigenvalues are in the specified real interval $[a, b]$ by using a filter. There are many references of methods which can be classified as filter diagonalization methods [1, 2, 4–7, 10].

The filter is usually composed of several resolvents $\mathcal{R}(\rho_i) \equiv (A - \rho_i B)^{-1}B$ whose shift ρ_i are complex numbers.

For a given vector $\mathbf{x}$, an application of the resolvent $\mathbf{y} \leftarrow \mathcal{R}(\rho)\mathbf{x}$ is to solve a system of linear equations $C(\rho)\mathbf{y} = B\mathbf{x}$ for $\mathbf{y}$, here $C(\rho) \equiv A - \rho B$ is the shifted matrix corresponds to both matrices of the generalized eigenproblem. In this study, for the solution of this kind of system, we assume to use some direct method which uses matrix factorization.

When the shift ρ is a real number, the matrix $C(\rho)$ is real symmetric. When the shift is a real number less than the minimum eigenvalue $\lambda_{\min}$ of the eigenproblem, the matrix is real symmetric positive definite. When the shift is an imaginary number, the matrix is complex symmetric and non-singular. For a symmetric matrix either real or complex, the modified Cholesky method can be used to solve the system of linear equations by a matrix decomposition and forward and backward substitutions (The modified Cholesky method for complex symmetric matrices is derived from the method for real symmetric matrices by replacing numbers and arithmetic expressions from real to complex).

When computing resources are limited but the problem size is large, the filtering calculation tends to be restricted by both amounts of computation to factor shifted matrices and especially storage to hold factors of matrices. Both are proportional to the number of resolvents to construct the filter. So it is desirable to reduce the number of resolvents. There are two kinds of filters composed of only a single resolvent: 1) The filter which is a real polynomial of a resolvent with a real shift, 2) The filter which is a real polynomial of the imaginary part of a resolvent with an imaginary shift. In this study, in order to make the filter design simple, a Chebyshev polynomial is used to express the "real polynomial". When the interval is located at the lower-end of the eigenvalue distribution, we use a filter $\mathcal{F} = g_s\, T_n(2\,\gamma\,\mathcal{R}(\rho) - I)$ which is an n-th degree Chebyshev polynomial of a single resolvent $\mathcal{R}(\rho)$ whose shift ρ is real and less than the minimum eigenvalue. When the interval is in the middle of the eigenvalue distribution, we use a filter $\mathcal{F} = g_s\, T_n(2\,\gamma'\,\mathrm{Im}\,\mathcal{R}(\rho') - I)$ which is an n-th degree Chebyshev polynomial of the imaginary part of a single resolvent $\mathcal{R}(\rho')$ whose shift ρ' is imaginary. Here, g_s is the tight upper-bound of the transfer function magnitude of the filter in the stop-band, γ and γ' are real constants, and I is the identity operator.

However, properties of these simple filters are not very well, because they are composed of a single resolvent rather than many, and also their real polynomials are expressed by just using Chebyshev polynomials. For example, their transfer functions cannot have steep changes of values, thus $\mu - 1$ the geometrical ratio of the width of transition-bands to the width of the pass-band cannot be made very small. Also, if the value of g_s is set very small, which is the upper-bound of the transfer-rates in stop-bands, the value of $1/g_p$ will be large, which is the max-min ratio of the transfer function of the filter in the passband $\lambda \in [a, b]$. When this max-min ratio is very large, the contained rates of required eigenvectors in the set of vectors after a filtration tend to have different orders of magnitudes. Therefore, within a vector, suppressed by large values of those eigenvectors whose transfer-rates are larger, smaller values of those eigenvectors whose transfer-rates are smaller lose accuracy by rounding errors. By this reason, those eigenvectors whose transfer-rates are smaller, which are extracted from a set of filtered vectors, tend to have lower accuracy. Therefore, some approximate pairs may not attain the level of required accuracy.

In the above explanation about the filtering method, we assumed to apply the filter only once to a set of random initial vectors. The following procedure shows how to calculate approximate pairs with a single application of the filter.

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1) Let $Y^{(0)}$ be an initial set of m random column vectors.
2) B-orthonormalize $Y^{(0)}$ to make $X^{(1)}$;
   $X^{(1)}$ is filtered to make $Y^{(1)}$.
3) Considering properties of the filter, approximate pairs are constructed from both sets of vectors $X^{(1)}$ and $Y^{(1)}$.

2 ITERATIVE REFINEMENT OF EIGENPAIRS BY USING A FILTER

When properties of the filter are not good, approximate pairs are also not good in accuracy which are obtained by an application of the filter to a set of initial random vectors. Even in such case, we can improve approximate pairs with a few applications of the combination of B-orthonormalization and filtering.

The following procedure shows how to calculate approximate pairs with applications of the filter `IT` times.

1) Let $Y^{(0)}$ be an initial set of m random column vectors.
2) Iterate the followings for $i = 1, \ldots, \mathrm{IT}$
   B-orthonormalize $Y^{(i-1)}$ to make $X^{(i)}$;
   $X^{(i)}$ is filtered to make $Y^{(i)}$.
3) Considering properties of the filter, approximate pairs are constructed from both sets of vectors $X^{(\mathtt{IT})}$ and $Y^{(\mathtt{IT})}$.

(During the iteration, in B-orthonormalization in the above step 2, if the effective rank of the set of vectors is found decreased, we decrease the number m of orthonormalized vectors in the set.)

The orthonormalization prevents eigenvectors of small transfer-rates from losing their accuracy by numerical rounding errors. It prevents the set of vectors from being occupied by those eigenvectors whose transfer-rates are larger. The principle to use orthogonalization of vectors in each iteration step is called "orthogonal iteration" and is well known [3, 8, 9].

3 CONCLUSION

We made some experiments to solve pairs of a real symmetric-definite generalized eigenproblem whose eigenvalues are in the specified interval by using a filter.

In this study we used filters composed of an action of a single resolvent. We used a real shift for the resolvent to solve pairs whose eigenvalues are lowest. When we used an imaginary shift, the interval for eigenvalues may be placed anywhere. The filter we used is a real polynomial of a single resolvent whose shift is real, or a real polynomial of an imaginary part of a single resolvent whose shift is imaginary. When the degree of the real polynomial is n, in an application of the filter the resolvent is applied n times. A Chebyshev polynomial is used to represent the real polynomial to make the filter design simple, and an application of the filter can be calculated by using the three-term recursion.

An application of a resolvent to a vector is to solve a system of linear equations whose coefficient is the shifted matrix made from both matrices of the generalized eigenproblem. In our study, the system of linear equations is assumed to be solved by some direct method using decomposition of the coefficient matrix. Since we use a filter consists of a single resolvent, we need to factor the coefficient matrix only once, and matrix factors are hold and used sequentially n times to solve a system of linear equations inside the filtering, here n is degree of the polynomial of the filter.

By the use of a single resolvent for the filter instead of many resolvents, we reduced both costs to factor matrix and especially to store matrix factors. However, properties of those filters which are composed of a single resolvent are not good compared from ones composed of many resolvents, especially when the precision of numbers and arithmetics used in computation is low.

The set of initial vectors generated from random numbers is B-orthonormalized and then filtered to give another set of vectors, to which we analyze and try to extract approximate pairs. If filter's properties are not good, approximate pairs obtained are inaccurate or some of them are lost, especially when the precision of computation is low.

However, in the similar way as "orthogonal iteration" [3, 8, 9] which is a well known method, we generate an initial set of vectors from random numbers, and to the set the combination of orthonormalization and filtering are applied a few times. The orthonormalization prevents the tendency to linear dependence of the set of vectors, and the filtering decrease content rates of those eigenvectors to be removed. By this refinement, the set of vectors spans better approximation of the invariant-subspace spanned by required eigenvectors. From the set of refined vectors, the basis of approximate invariant-subspace is constructed, and to the basis the Rayleigh-Ritz procedure is applied to obtain approximate pairs required.

We made some experiments for a banded real symmetric-definite generalized eigenproblem whose size of matrices is 210000 with lower-bandwidth 3051, which is a FEM discretization of the Laplacian eigenproblem in a cube with zero-Dirichlet boundary condition (Even banded matrices are sparse inside their bands, they are treated as if their bands are dense). From experiments which used only single precision for computations, even we used a filter whose properties were not good since it was composed of only a single resolvent to reduce requirements for computer resources, we found this approach of iterative refinement of eigenpairs worked well.

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