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

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1 FILTERS COMPOSED OF A SINGLE RESOLVENT

For a given real symmetric-definite generalized eigenproblem $A\mathbf{v} = \lambda B\mathbf{v}$, we solve those approximate eigenpairs whose eigenvalues are in the specified interval $[a, b]$ by using an appropriate filter.

Our filter is composed of some 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 $\mathbf{y} \leftarrow \mathcal{R}(\rho)\mathbf{x}$ reduces to solve $C(\rho)\mathbf{y} = B\mathbf{x}$ for $\mathbf{y}$ whose coefficient is the shifted matrix $C(\rho) \equiv A - \rho B$, which we assume to be solved by some direct method.

The shifted matrix is real-symmetric when the shift is real, and it is real-symmetric and positive-definite when the shift is real and less than the minimum eigenvalue. The matrix is complex-symmetric non-singular when the shift is imaginary. To solve a symmetric system of linear equations, we make an LDL^T decomposition and forward and backward substitutions.

Both amounts of computation to factor matrices and especially storage to hold factors of matrices tend to limit the calculation when we solve a large size problem under limited computing resources. Both are proportional to the number of resolvents to compose the filter, thus it is desirable to reduce the number.

We used two types of filters which use only a single resolvent:

1) $\mathcal{F} = g_s\, T_n(2\,\gamma\,\mathcal{R}(\rho) - I)$. **2)** $\mathcal{F} = g_s\, T_n(2\,\gamma'\,\mathrm{Im}\,\mathcal{R}(\rho') - I)$.

When the interval $[a, b]$ is located at the lower-end of the eigenvalue distribution, we can use the type-1 filter and the shift ρ is real and less than the minimum eigenvalue. For the type-2 filter, the shift ρ' is imaginary and the location of the interval may be anywhere. Here, g_s is the tight bound of the transfer function magnitude of the filter in the stop-band, γ and γ' are real constants, and I denotes the identity operator.

However, for these kinds of simple filters, shapes of transfer functions cannot be made very good, mainly because only a single resolvent is used rather than many. For example, their transfer functions cannot have steep changes of values, thus 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 to very small, the max-min ratio of the transfer function of the filter in the pass-band $\lambda \in [a, b]$ will be larger. If this max-min ratio is very large, the contained rates of required eigenvectors in the set of vectors tend to have different orders of magnitudes after the filter is applied. Thus, eigenvectors with larger transfer-rates dominate in a vector and eigenvectors with smaller transfer-rates reduce accuracy. By this reason, eigenvectors with smaller transfer-rates contained in filtered vectors tend to be inaccurate. Therefore, some approximate eigenpairs may fail to attain the level of required accuracy or lost.

In the above, we have assumed the filter is applied only once.

2 ITERATIVE REFINEMENT OF EIGENPAIRS BY USING A FILTER

Even the shape of the transfer function of the filter may not be good, we can obtain refined approximate eigenpairs if the combination of a B-orthonormalization and an application of the filter is iterated a small number (IT) of times by the following procedure.

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) Construct approximate eigenpairs from both sets $X^{(\mathrm{IT})}$ and $Y^{(\mathrm{IT})}$ considering the shape of the filter's transfer function.

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

The orthonormalization prevents the tendency of those eigenvectors whose transfer-rates are relatively smaller to lose information by numerical rounding errors. The principle to use orthogonalization of vectors in each iteration step is well known and called *orthogonal iteration* [1–3].

3 CONCLUSION

We made some experiments for a banded real symmetric-definite generalized eigenproblem whose size of matrices is 210,000 with lower-bandwidth 3,051, which is a FEM discretization of the Laplacian eigenproblem for a cube region with zero-Dirichlet boundary condition. When we solve the system of linear equations to give the action of the resolvent, the banded coefficient matrix is treated as if the band is dense even it is actually very sparse.

In experiments, filters we used did not have good shapes of their transfer functions because they were composed of only a single resolvent so to reduce computer resource requirements. However, we found present approach of iterative refinement of eigenpairs worked well even the calculation was made in single-precision.

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