Anna Matsekh

Using Spectral Deflation to Accelerate Convergence of Inverse Iteration for Symmetric Tridiagonal Eigenproblems.

CCS-3
Los Alamos National Laboratory
P O Box 1663
MS B256
Los Alamos
NM 87544
USA
matsekh@lanl.gov

We present a new fast implementation of inverse iteration for real symmetric tridiagonal matrices. This implementation does not require reorthogonalization of eigenvectors in tight clusters. We achieve this by choosing initial vectors from well-defined subspaces generated using two-sided Sturm sequence-based spectral deflation [GAKK93].

We apply spectral deflation to the tridiagonal matrix $T \in R^{n\times n}$, $T = T^T$ to find a sequence of Givens rotations to obtain matrices $T_{n-1} \in R^{n-1\times n-1}, T_{n-2} \in R^{n-2\times n-2}, \ldots, T_1 \in R^{1\times 1}$, such that $\Lambda(T_1) \subset \Lambda(T_2) \ldots \Lambda(T_{n-1}) \subset \Lambda(T)$, where $\Lambda(\cdot)$ denotes matrix spectrum. Instead of computing eigenvectors of the matrix T directly from the corresponding sequences of rotation parameters, as it is done in the Godunov et al. version of the method (which in our studies fails to give satisfactory residuals because of rounding errors), we compute eigenvector approximations $\tilde{x}_n(T_n) \in R^n, \tilde{x}_{n-1}(T_{n-1}) \in R^{n-1}, \ldots \tilde{x}_1(T_1) \in R^1$ corresponding to the eigenvalues $\lambda_n(T) = \lambda_n(T_n) \geq \lambda_{n-1}(T) = \lambda_{n-1}(T_{n-1}) \geq \lambda_1(T) = \lambda_1(T_1)$ in $O(n^2)$ floating point operations. We construct initial vectors y_k^0, $k = 1, 2, \ldots, n$ for inverse iteration by padding the vector $\tilde{x}_k(T_k)$ with $n - k$ zeros. Even if two consecutive eigenvalues λ_k and λ_{k-1} are very close or coincident, the corresponding vectors y_k^0 and y_{k-1}^0 differ in at least one component, while $\tilde{x}_k$ and $\tilde{x}_{k-1}$ approximately solve the respective eigenproblems $T_k\tilde{x}_k \approx \tilde{\lambda}_k\tilde{x}_k$ and $T_k\tilde{x}_{k-1} \approx \tilde{\lambda}_k\tilde{x}_{k-1}$. This approach appears sufficient to produce an accurate orthogonal eigensystem in two steps of inverse iteration without reorthogonalization. We call this method *Iteratively Refined Spectral Deflation (IRSD).* IRSD has $O(n^2)$ complexity and requires fewer steps than most existing implementations of inverse iteration. If a few extra digits of orthogonality are desired, the eigenvector may be reorthogonalized once, before renormalization. We call this variation of the method *Reorthogonalized Iteratively Refined Spectral Deflation (RIRSD).*

We implemented IRSD, RIRSD, and the Godunov-Inverse Iteration method [Mat03], along with an interval version of the eigenvalue bisection (which we use in all three algorithms) in ANSI C (GNU C compiler, version 3.2) using IEEE double-precision arithmetic. In the table below we present computational times and residuals for the eigenproblem with tridiagonal matrix T of size $n = 2500$ with main diagonal $(0, 0, 0, \dots)$ and codiagonals $(10, 0.1, 10, 0.1, 10, 0.1, \dots \dots)$. Computing a system of orthogonal eigenvectors of this matrix may be challenging because we are dealing with two very tight eigenvalue clusters. We solve this test problem using IRSD method (**irsd**), RIRSD (**rirsd**), Godunov–Inverse Iteration (**gii**) and LAPACK dste*xx* routines on the 1800 MHz Intel® Pentium 4 Mobile® CPU. We used the following LAPACK routines in our tests: **dstein**, an implementation of inverse iteration which uses a bisection procedure **dstebz**; **dsteqr**, an implementation of the QR algorithm; and, **dstedc**, an implementation of the Divide and Conquer algorithm.

In the table below we report the following characteristics for the computed eigenpairs $(\tilde{\lambda}_i, \tilde{y}_i)$, $i = 1, \dots, n$: the maximum residual $\mathcal{R}(\tilde{\lambda}, \tilde{Y}) = \max_i \|(T - \tilde{\lambda}_i I)\tilde{y}_i\|_\infty$; the maximum deviation $\mathcal{O}(\tilde{Y})$ of the approximate eigensystem $\tilde{Y} = \{\tilde{y}_i\}$, $i = 1, 2, \dots, n$ from the unit basis $I = \{e_i\}$, $i = 1, 2, \dots, n$, where $\mathcal{O}(\tilde{Y}) = (\max_i \|(\tilde{Y}^T\tilde{Y} - I)e_i\|_\infty$; $\mathcal{T}(\tilde{\lambda})$, the time in seconds spent computing all eigenvalue approximations; $\mathcal{T}(\tilde{Y})$, the time in seconds spent computing all eigenvector approximations; and, the cumulative time, $\Sigma_\mathcal{T} \equiv \mathcal{T}(\tilde{\lambda}) + \mathcal{T}(\tilde{Y})$.

	$\mathcal{R}(\tilde{\lambda}, \tilde{Y})$	$\mathcal{O}(\tilde{Y})$	$\mathcal{T}(\tilde{\lambda})$, s	$\mathcal{T}(\tilde{Y})$, s	$\Sigma_\mathcal{T}$, s
irsd	$2.03e-15$	$4.16e-11$	16.21	**4.40**	**20.61**
rirsd	$7.66e-15$	$\mathbf{5.05e-15}$	16.21	46.09	62.30
gii	$\mathbf{2.02e-15}$	$3.32e-11$	16.21	5.13	21.34
dstein	$9.77e-15$	$5.06e-15$	11.76	119.33	131.09
dstedc	$1.07e-13$	$6.32e-15$	**0.76**	52.30	53.06
dsteqr	$2.35e-13$	$9.10e-15$	1.21	249.57	250.78

The table shows that IRSD can produce accurate orthogonal eigensystem significantly faster than LAPACK implementations of the Inverse Iteration, Divide and Conquer, and the QR methods. IRSD results are very close to the results of the Godunov-Inverse Iteration method. Both IRSD and Godunov-Inverse Iteration produced eigensystems which were less orthogonal than the eigenvectors computed with the LAPACK routines. With explicit reorthogonalization in RIRSD we can achieve the same orthogonality as the LAPACK methods, still, overall outperforming LAPACK.

Bibliography

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