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

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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 transformations 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 a spectrum of a matrix. Instead of computing eigenvectors of the matrix T directly from the corresponding sequences of Givens 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 next proceed to 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 $\{\tilde{y_k}\}$, $k = 1, 2, \ldots, n$ such that $T\tilde{y_k} \approx \tilde{\lambda}_k\tilde{y_k}\, k = 1, 2, \ldots, n$ in two steps of inverse iteration without reorthogonalization. We call this method *Iteratively Refined Spectral Deflation.* Iteratively Refined Spectral Deflation has $O(n^2)$ complexity and requires fewer steps than most existing implementations of inverse iteration. By omitting reorthogonalization from the inverse iteration step, we obtain eigenvector approximations $\{\tilde{y_k}\}$, $k = 1, 2, \ldots, n$ which in our experiments often appear to be slightly less orthogonal than eigensystems computed using explicit reorthog-

onalization. If a few extra digits of orthogonality are desired, the eigenvector approximations $\{\tilde{y_k}\}$, $k = 1, 2, \ldots, n$ may be reorthogonalized once before renormalization, which increases worst case complexity. We call this variation of the method *Reorthogonalized Iteratively Refined Spectral Deflation*.

Iteratively Refined Spectral Deflation uses an interval implementation of the bisection method [GAKK93, Mat03] to find the smallest machine representable intervals (α_k, β_k), $k = 1, 2, \ldots, n$, each guaranteed to contain λ_k—the kth largest eigenvalue of the matrix T. Next, we set $T_n = T$ to compute the two-sided Sturm sequence $S(T_n(\alpha_n, \beta_n))$ [GAKK93, Mat03]. Knowing $S(T_n(\alpha_n, \beta_n))$ we can compute rotation parameters which enable us to transform T_n to the equivalent block-diagonal form with tridiagonal block T_{n-1} and $\tilde{\lambda}_n$ on the main diagonal and to compute the eigenvector approximation $\tilde{x}_n$ of the matrix T_n corresponding to the eigenvalue λ_n. Because of the nature of Givens transformations, the spectrum $\Lambda(T_{n-1})$ is a subset of the spectrum $\Lambda(T)$. We can repeat the deflation process for T_{n-1}, computing $S(T_{n-1}(\alpha_{n-1}, \beta_{n-1}))$ to find the eigenvector approximation $\tilde{x}_{n-1}$ and to further diagonalize the matrix T, which now has tridiagonal block T_{n-2} and diagonal matrix $\mathrm{diag}(\lambda_{n-1}, \lambda_{n-2})$ on the main diagonal. Again, we have $\Lambda(T_{n-2}) \subset \Lambda(T_{n-1}) \subset \Lambda(T)$. We can repeat this process until the matrix T is fully diagonalized and we have constructed the matrix sequence $T_{n-1}, T_{n-2}, \ldots, T_1$ and the sequence of eigenvector approximations $\tilde{x}_n(T_n), \tilde{x}_{n-1}(T_{n-1}), \ldots \tilde{x}_1(T_1)$.

We implemented Iteratively Refined Spectral Deflation, Reorthogonalized Iteratively Refined Spectral Deflation, 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 $(0, 0, 0, \ldots)$ and codiagonals $(10, 0.1, 10, 0.1, 10, 0.1, \ldots\ldots)$. 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 Iteratively Refined Spectral Deflation (**irsd**), Reorthogonalized Iteratively Refined Spectral Deflation (**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** to find eigenvalue approximations; **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 $(\tilde{\lambda_i}, \tilde{y_i})$, $i = 1, \ldots, n$: 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 system $\{\tilde{y}_i\}, i = 1, 2, \ldots, n$ from the unit basis, where $\mathcal{O}(\tilde{Y}) = (\max_i \|(\tilde{Y}^T\tilde{Y} - I)e_i\|_\infty$, $\tilde{Y} = \{\tilde{y}_i\}$, $i = 1, 2, \ldots, n$, $I = e_i$, $i = 1, 2, \ldots, n$, and $\{e_i\}$, $i = 1, 2, \ldots, n$ are the unit vectors; $\mathcal{T}(\tilde{\lambda})$, 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 Iteratively Refined Spectral Deflation can produce accurate orthogonal eigensystem significantly faster than LAPACK implementations of the Inverse Iteration, Divide and Conquer, and the QR methods. Iteratively Refined Spectral Deflation results are very close to the results of the Godunov-Inverse Iteration method. Both Iteratively Refined Spectral Deflation and Godunov-Inverse Iteration produced eigensystems which were less orthogonal than the eigenvectors computed with the LAPACK routines. With Reorthogonalized Iteratively Refined Spectral Deflation we can achieve the same orthogonality as the LAPACK methods, still, overall outperforming LAPACK.

Bibliography

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