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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 without reorthogonalization for real symmetric tridiagonal matrices. We achieve this by choosing initial vectors from well-defined subspaces generated using Godunov's two-sided Sturm sequence-based spectral deflation. 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 $T_{n-1} \in R^{n-1\times n-1}, T_{n-2} \in R^{n-2\times n-2}, \dots , T_1 \in R^{1\times 1}$, such that $\Lambda(T_1) \subset \Lambda(T_2) \dots \Lambda(T_{n-1}) \subset \Lambda(T)$, 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 $\tilde{x}_n(T_n) \in R^n, \tilde{x}_{n-1}(T_{n-1}) \in R^{n-1}, \dots \tilde{x}_1(T_1) \in R^1$ corresponding to the eigenvalues $\lambda_n(T) = \lambda_n(T_n) \geq \lambda_{n-1}(T) = \lambda_{n-1}(T_{n-1}) \geq \lambda_1(T) = \lambda_1(T_1)$. We construct initial vectors y_k^0, $k = 1, 2, \dots , n$ 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)*. If a few extra digits of orthogonality are desired, IRSD eigenvector may be reorthogonalized once. We call this variation of the method *Reorthogonalized Iteratively Refined Spectral Deflation (RIRSD)*.

We implemented IRSD and RIRSD along with an interval version of the eigenvalue bisection (which we use in both 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 test eigenproblem with tridiagonal matrix T of size $n = 2500$ with main diagonal $(0, 0, 0, \dots)$ and co-

diagonals $(10, 0.1, 10, 0.1, 10, 0.1, \ldots \ldots)$. This matrix has two very tight eigenvalue clusters. We solve this test problem using IRSD (**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**, a double-precision implementation of inverse iteration which uses bisection procedure **dstebz**; **dsteqr**, a double-precision implementation of the QR algorithm; and, **dstedc**, a double-precision 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 approximate eigensystem $\tilde{Y} = \{\tilde{y}_i\}$, $i = 1, 2, \ldots, n$ from the unit basis $I = \{e_i\}$, $i = 1, 2, \ldots, n$, 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, $\Sigma_{\mathcal{T}} \equiv \mathcal{T}(\tilde{\lambda}) + \mathcal{T}(\tilde{Y})$.

	$\mathcal{R}(\tilde{\lambda},\, \tilde{Y})$	$\mathcal{O}(\tilde{Y})$	$\mathcal{T}(\tilde{\lambda}), \mathrm{s}$	$\mathcal{T}(\tilde{Y}), \mathrm{s}$	$\Sigma_{\mathcal{T}}, \mathrm{s}$
irsd	$\mathbf{2.03e-15}$	$4.16e-11$	16.21	**4.40**	**20.61**
rirsd	$7.66e-15$	$\mathbf{5.05e-15}$	16.21	46.09	62.30
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