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The Orthogonal Rayleigh Quotient Iteration (ORQI) method

by

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Abstract. This paper presents a new method for computing all the eigenvectors of a real $n \times n$ symmetric tridiagonal matrix T. The algorithm computes an orthogonal matrix $Q = [\mathbf{q}_1, \ldots, \mathbf{q}_n]$ and a diagonal matrix $\Lambda = \text{diag}\{\lambda_1, \ldots, \lambda_n\}$ such that $TQ = Q\Lambda$. The basic ideas are rather simple. Assume that $\mathbf{q}_1, \ldots, \mathbf{q}_{k-1}$ and $\lambda_1, \ldots, \lambda_{k-1}$ have already been computed. Then $\mathbf{q}_k$ is obtained via the Rayleigh Quotient Iteration (RQI) method. Starting from an arbitrary vector $\mathbf{u}_0$ the RQI method generates a sequence of vectors $\mathbf{u}_\ell$, $\ell = 1, 2, \ldots,$ and a sequence of scalars ρ_ℓ, $\ell = 0, 1, 2, \ldots$. The theory tells us that these two sequences converge (almost always) to an eigenpair $(\rho^*, \mathbf{u}^*)$. The appeal of the RQI method comes from the observation that the final rate of convergence is cubic. Furthermore, if the starting point is forced to satisfy $\mathbf{q}_i^T \mathbf{u}_0 = 0$ for $i = 1, \ldots, k-1$, as our method does, then all the coming vectors, $\mathbf{u}_\ell, \ell = 1, 2, \ldots,$ and their limit point, $\mathbf{u}^*$, should stay orthogonal to $\mathbf{q}_1, \ldots, \mathbf{q}_{k-1}$. In practice orthogonality is lost because of rounding errors. This difficulty is resolved by reorthogonalization of $\mathbf{u}_\ell$ against $\mathbf{q}_1, \ldots, \mathbf{q}_{k-1}$. The key for effective implementation of the algorithm is to use a selective orthogonalization scheme in which $\mathbf{u}_\ell$ is orthogonalized only against "close" eigenvectors. That is, $\mathbf{u}_\ell$ is orthogonalized against $\mathbf{q}_i$ only if $|\rho_\ell - \lambda_i| \leq \gamma$ where γ is a small preassigned threshold value, e.g. $\gamma = \|T\|_\infty / 100$. A further essential feature of the proposed orthogonalization scheme is the use of reorthogonalization.

The ORQI method is supported by forward and backward error analysis. Preliminary experiments on medium-size problems ($n \leq 1000$) are quite encouraging. The average number of Orthogonal Rayleigh Quotient iterations per eigenvector was less than 12, while the overall number of flops required for orthogonalizations is often below $\frac{1}{2} n^3$.

__**Key words**__: Eigenvectors, eigenvalues, real symmetric tridiagonal matrices, complete eigensystem, Rayleigh Quotient Iteration, selective orthogonalization, reorthogonalization.