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Parallel Divide and Conquer Algorithms for the Symmetric Tridiagonal Eigenproblem and Bidiagonal Singular Value Problem

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Abstract

Recent advances [2, 7, 9, 13] can improve run times for certain matrix eigenvalue problems by orders of magnitude. In this paper we consider applying permutations to a real symmetric tridiagonal matrix T to produce a bordered symmetric matrix with two tridiagonal blocks on its diagonal. The spectral decompositions of the tridiagonal blocks are found recursively and then combined with the border to produce a symmetric arrow matrix A. The eigenvalues of A are the zeros of a rational function, f, and are interlaced by the poles, which are the eigenvalues of the unbordered matrix. The eigenvalues of A can be found using a novel zero finder with global monotone cubic convergence. The zero finder can be started at either of the two poles which the zero interlaces. The eigenvectors of A are found by formulas and the spectral decomposition of T can then be computed directly.

The bidiagonal singular value problem is equivalent with the case in which T has a zero diagonal. In this important special case the subproblems retain this structure.

1 Introduction

We will develop a recursive divide and conquer algorithm for finding the spectral decomposition of a real symmetric tridiagonal matrix

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$$T = \begin{bmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \alpha_2 & \beta_2 & & \\ & \beta_2 & & \ddots & \\ & & \ddots & & \beta_{n-1} \\ & & & \beta_{n-1} & \alpha_n \end{bmatrix}. \tag{1}$$

Because T is real symmetric it has the spectral decomposition $T = U\Lambda U^T$ where U is orthogonal and Λ is diagonal with n real eigenvalues. There are three parts to the algorithm – divide phase, conquer phase, and the zero finder. We will present them in this order.

2 The divide phase

We denote by $\mathbf{e}_i$ the ith axis vector where the dimension will be clear from the context. We define the bordering permutation P_k to be the $n \times n$ permutation matrix given by $P_k = [\mathbf{e}_1, \mathbf{e}_2, ..., \mathbf{e}_{k-1}, \mathbf{e}_{k+1}, ..., \mathbf{e}_n, \mathbf{e}_k]$. Then

$$P^T T P = \begin{bmatrix} T_1 & & \mathbf{e}_{k-1}\beta_{k-1} \\ & T_2 & \mathbf{e}_1\beta_1 \\ \mathbf{e}_{k-1}^T\beta_{k-1} & \mathbf{e}_1^T\beta_1 & \alpha_k \end{bmatrix} \tag{2}$$

where the T_1 and T_2 blocks are real symmetric tridiagonal matrices and $\mathbf{e}_1$ and $\mathbf{e}_{k-1}$ are axis vectors of appropriate size.

3 The conquer phase

Suppose we know the spectral decompositions $T_1 = U_1\Lambda_1 U_1^T$ and $T_2 = U_2\Lambda_2 U_2^T$ of the tridiagonal subblocks from equation 2 above. Then it follows that

$$P^T T P = \begin{bmatrix} U_1 & & \\ & U_2 & \\ & & 1 \end{bmatrix} \begin{bmatrix} \Lambda_1 & & \mathbf{u}_1 \\ & \Lambda_2 & \mathbf{u}_2 \\ \mathbf{u}_1^T & \mathbf{u}_2^T & \alpha_k \end{bmatrix} \begin{bmatrix} U_1 & & \\ & U_2 & \\ & & 1 \end{bmatrix}^T \tag{3}$$

with $\mathbf{u}_1 = U_1^T\mathbf{e}_{k-1}\beta_{k-1}$ and $\mathbf{u}_2 = U_2^T\mathbf{e}_1\beta_n$. The original problem is now replaced by that of computing the spectral decomposition of the arrow matrix

$$A = \begin{bmatrix} \Lambda_1 & & \mathbf{u}_1 \\ & \Lambda_2 & \mathbf{u}_2 \\ \mathbf{u}_1^T & \mathbf{u}_2^T & \alpha_k \end{bmatrix} = \begin{bmatrix} \delta_1 & & & \upsilon_1 \\ & \delta_2 & & \upsilon_2 \\ & & \ddots & \vdots \\ & & \delta_{n-1} & \upsilon_{n-1} \\ \upsilon_1 & \upsilon_2 & \upsilon_{n-1} & \alpha \end{bmatrix} = \begin{bmatrix} D & \mathbf{u} \\ \mathbf{u}^T & \alpha \end{bmatrix}. \tag{4}$$

The key to finding the eigenvalues of A is to note that when λ is not an eigenvalue of D, the block Gauss factorization of A is

$$A - \lambda I = \begin{bmatrix} I & 0 \\ \mathbf{u}^T(D-\lambda I)^{-1} & 1 \end{bmatrix} \begin{bmatrix} D-\lambda I & \mathbf{u} \\ 0^T & -f(\lambda) \end{bmatrix} \tag{5}$$

where f is the *spectral function* of A and is given by

$$f(\lambda) = \lambda - \alpha + \sum_{i=1}^{n-1} \frac{v_i^2}{\delta_i - \lambda}. \tag{6}$$

The spectral function is a rational Pick function [3] with a pole at infinity; it maps the open upper half plane into itself. Note that the block Gauss factorization exists if and only if $\lambda \neq \delta_i$ for $i = 1, 2, ..., n-1$. In this case, λ is an eigenvalue of A if and only if $f(\lambda) = 0$. There is a second possibility. If $\lambda = \delta_i$ for some i then the block factorization does not exist. In this case we will be able to *deflate* the matrix A and replace it with a smaller arrow matrix.

4 Deflation

In order for this problem to be well-posed it is important that the block Gauss factorization 5 of $A - \lambda I$ exists. Inspection of 5 shows that this is true whenever λ is not an eigenvalue of D, that is, whenever $\lambda \neq \delta_i$ for $i = 1, 2, ..., n-1$. If this condition fails then it is possible to *deflate* the arrow matrix A and replace it with a smaller arrow matrix for which the condition does hold.

Suppose that the kth eigenvalue δ_k of D is an eigenvalue of A with associated eigenvector $[\nu_1, \nu_2, ..., \nu_n]^T$. The kth scalar equation in the expansion of the linear system $A\mathbf{v} = \delta_k \mathbf{v}$ is

$$\delta_k \nu_k + v_k \nu_n = \delta_k \nu_k$$

whence $v_k \nu_n = 0$ so that either $v_k = 0$ or $\nu_n = 0$ or both. We consider two mutually exclusive subcases:

Case I: $v_k = 0$

In this case the axis vector $\mathbf{e}_k$ is an eigenvector of A corresponding to δ_k. Moreover, by the orthogonality of the eigenvectors of A, all other eigenvectors lie in the orthogonal complement of $\mathbf{e}_k$ having zero in the kth place. We can restrict our search for eigenvectors of A to this $n-1$ dimensional subspace. Equivalently, we can replace A by a deflated A_D which results from deleting the kth row and column from A, and recover the remaining eigenvectors of A by inserting zeros into the eigenvectors of A_D in the obvious way.

Case II: $v_k \neq 0$ and $\nu_n = 0$

In this case it must happen that δ_k is a repeated element of D. To see that there must be a $j \neq k$ such that $\delta_j = \delta_k$ assume, to the contrary, that there is

no such j. Consider the linear system $A\mathbf{v} = \delta_k \mathbf{v}$. Since $\nu_n = 0$ the first $n-1$ scalar equations of the system take the form

$$\delta_j \nu_j = \delta_k \nu_j \tag{7}$$

for $j = 1, 2, ..., n-1$. Our assumption leads directly to the conclusion that $\nu_j = 0$ for all $j \neq k$. It would then follow that $\mathbf{v}$ is a scalar multiple of the axis vector $\mathbf{e}_k$. But $\mathbf{e}_k$ cannot be an eigenvector since $\upsilon_k \neq 0$, establishing by contradiction that δ_k is repeated in D.

If D contains at least one repeated diagonal element then we can construct an orthogonal matrix Q so that $Q^T A Q$ is an arrow with a zero entry in its last column. In particular, if $\delta_j = \delta_k$ with $j \neq k$ then the matrix Q is a Givens rotation in the $j-k$ plane chosen so that when applied to the last column of A either the jth or the kth element of that column becomes zero; see [9].

If $Q^T A Q$ is to be an arrow then the off-diagonal fill in the (j,k) and (k,j) elements of $Q^T A Q$ must be zero. If s and c are the sine and cosine of the Givens rotation then a simple calculation shows that these elements take the common value $cs(\delta_j - \delta_k)$. Hence if, as we are assuming here, $\delta_j = \delta_k$ the arrow form is preserved. In practice, even if the true values of δ_j and δ_k were equal, they would almost surely be corrupted by roundoff error. For this reason we adopt the numerical convention that we perform a deflation step and neglect the off-diagonal fill whenever $|cs(\delta_j - \delta_k)| < tol$ where tol is some tolerance chosen to be a few machine units in size (possibly scaled by the norm of $\mathbf{u}$).

5 The zero finder

The fundamental problem in finding the eigenvalues by this method is that of providing a stable and efficient method for finding the zeros of the spectral function. We now examine this problem in some detail. The spectral function is given by

$$f(\lambda) = \lambda - \alpha + \sum_{k=1}^{n-1} \frac{\upsilon_k^2}{\delta_k - \lambda}.$$

If the δ_k are ordered so that $\delta_1 > \delta_2 > ... > \delta_{n-1}$ then f has exactly one zero in each of the open intervals $(-\infty, \delta_{n-1}), (\delta_{n-1}, \delta_{n-2}), ..., (\delta_1, +\infty)$. Moreover, the derivative of the spectral function is bounded below by one ($f'(\lambda) \geq 1$) so that its zeros are, in a certain sense, well determined.

The zero finding algorithm we present here is globally convergent in the sense that within any of the intervals mentioned above any starting estimate will converge to the unique zero of f inside that interval. Convergence of the zero finder is monotone, which yields a simple stopping criterion for the numerical procedure – terminate when strict monotonicity fails. Moreover, the zero finding algorithm converges at a *cubic* rate, so it is fast.

The iterative procedure for finding the unique zero of f in one of the intervals I given above proceeds as follows. Choose an initial starting guess $x_0 \in I$. For each iterate x_j construct a rational function ϕ_j which behaves like f over the interval I — is monotonically increasing with poles at the endpoints — and approximates $f(x)$ at x_j to third order. Then, take x_{j+1} to be the unique solution to $\phi_j(x) = 0$.

In particular, on interior intervals, those of the form $I = (\delta_{k+1}, \delta_k)$, each $\phi_j(x)$ has the form

$$\phi_j(x) = \gamma + \frac{\omega_0}{\delta_k - x} + \frac{\omega_1}{\delta_{k+1} - x}$$

where we choose γ, ω_0, and ω_1 so that

$$\begin{aligned} \phi_j(x_j) &= f(x_j), \\ \phi_j'(x_j) &= f'(x_j), \\ \phi_j''(x_j) &= f''(x_j). \end{aligned} \tag{8}$$

It is clear that γ, ω_0, and ω_1 must satisfy

$$\begin{bmatrix} 1 & (\delta_k - x_j)^{-1} & (\delta_{k+1} - x_j)^{-1} \\ 0 & (\delta_k - x_j)^{-2} & (\delta_{k+1} - x_j)^{-2} \\ 0 & (\delta_k - x_j)^{-3} & (\delta_{k+1} - x_j)^{-3} \end{bmatrix} \begin{bmatrix} \gamma \\ \omega_0 \\ \omega_1 \end{bmatrix} = \begin{bmatrix} f(x_j) \\ f'(x_j) \\ f''(x_j) \end{bmatrix} \tag{9}$$

which has the solution

$$\gamma = 3x_j - (\alpha + \delta_k + \delta_{k+1}) + \sum_{i \neq k, k+1} \frac{v_i^2}{\delta_i - x_j} \frac{\delta_i - \delta_k}{\delta_i - x_j} \frac{\delta_i - \delta_{k+1}}{\delta_i - x_j}, \tag{10}$$

$$\omega_0 = v_k^2 + \frac{(\delta_k - x_j)^3}{\delta_k - \delta_{k+1}} \left(1 + \sum_{i \neq k, k+1} \frac{v_i^2}{(\delta_i - x_j)^2} \frac{\delta_i - \delta_{k+1}}{\delta_i - x_j} \right), \tag{11}$$

$$\omega_1 = v_{k+1}^2 + \frac{(x_j - \delta_{k+1})^3}{\delta_k - \delta_{k+1}} \left(1 + \sum_{i \neq k, k+1} \frac{v_i^2}{(\delta_i - x_j)^2} \frac{\delta_i - \delta_k}{\delta_i - x_j} \right). \tag{12}$$

Notice that all of the terms in the sums defining ω_0 and ω_1 are positive (this follows from the fact that $\lambda_{k+1} > x_j > \lambda_k$). This implies that ϕ_j has a zero in the interval (δ_{k+1}, δ_k).

It also follows that

$$\omega_0 > v_k^2 > 0 \qquad \text{and} \qquad \omega_1 > v_{k+1}^2 > 0. \tag{13}$$

Now, the approximation error for any of the $\phi_j(x)$ is

$$f(x) - \phi(x) = x - (\alpha + \gamma) + \sum_{i \neq k, k+1} \frac{v_i^2}{\delta_i - x} + \frac{v_k^2 - \omega_0}{\delta_k - x} + \frac{v_{k+1}^2 - \omega_1}{\delta_{k+1} - x}. \quad (14)$$

This function has n zeros, counting multiplicities. There are $n-3$ zeros exterior to (δ_{k+1}, δ_k) and three more at x_j. Thus the error function crosses zero exactly once in the interval (δ_{k+1}, δ_k). This implies that the zero of ϕ in the interval is between the current approximation point and the true zero of f, so that the zero finder is monotonically convergent from any starting guess $x_0 \in I$ as claimed. The cubic rate of convergence follows from the manner of construction of the $\phi_j(x)$.

The treatment of the two exterior intervals is *geometrically* the same as above. In particular, the residue of a Pick function with a pole at infinity is the negative of its coefficient of x. Again, the approximating function has poles at the endpoints and the residues at these poles, and the constant term, are chosen to satisfy 9. The details, as well as the fact that the iterates make sense even when starting from the endpoints of the intervals, including the pole at infinity, are left as exercises for the reader.

6 Computing the eigenvectors

It is clear from 5 that if λ is an eigenvalue of A then the associated eigenvector $\mathbf{v}$ is the solution to

$$\begin{bmatrix} D - \lambda I & \mathbf{u} \\ 0^T & 0 \end{bmatrix} \mathbf{v} = \mathbf{0}. \quad (15)$$

It follows that we can explicitly construct the eigenvector $\mathbf{v}$ with

$$\mathbf{v} = \begin{bmatrix} \frac{v_1}{\lambda - \delta_1} \\ \frac{v_2}{\lambda - \delta_2} \\ \vdots \\ \frac{v_{n-1}}{\lambda - \delta_{n-1}} \\ 1 \end{bmatrix}. \quad (16)$$

7 Singular value decomposition

We note that the singular value decomposition (SVD) of a matrix B can be obtained from the spectral decomposition of the Hermitian matrix

$$A = \begin{bmatrix} 0 & B^H \\ B & 0 \end{bmatrix}. \quad (17)$$

The SVD is given by $B = V\Sigma U^H$, where U and V are unitary matrices and Σ is nonnegative diagonal. Then

$$\begin{aligned} A\begin{bmatrix} U \\ V \end{bmatrix} &= \begin{bmatrix} B^H V \\ BU \end{bmatrix} \\ &= \begin{bmatrix} (V^H B)^H \\ V\Sigma \end{bmatrix} \\ &= \begin{bmatrix} (\Sigma U^H)^H \\ V\Sigma \end{bmatrix} \\ &= \begin{bmatrix} U \\ V \end{bmatrix} \Sigma \end{aligned} \tag{18}$$

and similarly

$$A\begin{bmatrix} U \\ -V \end{bmatrix} = \begin{bmatrix} U \\ -V \end{bmatrix} (-\Sigma)\,. \tag{19}$$

It follows that the columns of $\begin{bmatrix} V \\ U \end{bmatrix}$ and $\begin{bmatrix} V \\ -U \end{bmatrix}$ are eigenvectors of A, and that the corresponding eigenvalues are the diagonal elements of Σ and of $-\Sigma$ respectively. Thus the eigenvalues of A occur in plus-minus pairs, the nonnegative eigenvalues of A are the singular values of B, and the singular vectors of B and B^H can be obtained by partitioning the eigenvectors of A according to 18.

If B is real bidiagonal then there is a permutation matrix S so that $T = S^H A S$ is a symmetric tridiagonal matrix with a zero main diagonal [11]. Note that the proper first step in the calculation of the SVD is Householder reduction to bidiagonal form. The problem then becomes one of finding the spectral decomposition of T, which we can calculate by the algorithm described in this paper. The zero diagonal is preserved at each stage of the divide and conquer operation, and at each stage we need calculate only half of the eigenvalues and half of the eigenvectors.

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