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A Parallel Divide and Conquer Algorithm for the Generalized Real Symmetric Definite Tridiagonal Eigenproblem

Carlos F. Borges* *and William B. Gragg*†

Abstract.

We develop a parallel divide and conquer algorithm, by *extension*, for the generalized real symmetric definite tridiagonal eigenproblem. The algorithm employs techniques first proposed by Gu and Eisenstat to prevent loss of orthogonality in the computed eigenvectors for the *modification* algorithm. We examine numerical stability and adapt the insightful error analysis of Gu and Eisenstat to the arrow case. The algorithm incorporates an elegant zero finder with global monotone cubic convergence that has performed well in numerical experiments. A complete set of tested matlab routines implementing the algorithm is available on request from the authors.

1 Introduction

We consider the problem of finding a matrix $U \in \Re^{n \times n}$ such that

$$U^T (T - S\lambda) U \equiv \Lambda - I\lambda,$$

is diagonal, or equivalently

$$U^T S U = I \quad \text{and} \quad U^T T U = \Lambda, \tag{1}$$

where

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$$T = \begin{bmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \alpha_2 & \beta_2 & & \\ & \beta_2 & & \ddots & \\ & & \ddots & & \beta_{n-1} \\ & & & \beta_{n-1} & \alpha_n \end{bmatrix}, \quad S = \begin{bmatrix} \delta_1 & \gamma_1 & & & \\ \gamma_1 & \delta_2 & \gamma_2 & & \\ & \gamma_2 & & \ddots & \\ & & \ddots & & \gamma_{n-1} \\ & & & \gamma_{n-1} & \delta_n \end{bmatrix},$$

and S is assumed to be positive definite. This generalized eigenvalue problem has two special cases that are of interest in themselves. They are:

1. $S = I$, the ordinary tridiagonal eigenproblem.

2. $S = I$ and $\alpha_k \equiv 0$, the bidiagonal singular value problem (BSVP), by *perfect shuffle* of the Jordan matrix

$$\begin{bmatrix} 0 & B^T \\ B & 0 \end{bmatrix}$$

with B upper bidiagonal [16].

There are two phases to the divide and conquer algorithm, the divide (or split) phase, and the conquer (or consolidate) phase. We shall address these in order.

2   The algorithm

2.1   The divide phase

Denote by e_i the ith axis vector where the dimension will be clear from the context. Let $s, 1 \leq s \leq n$, be an integer, the *split index*, and consider the following block forms:

$$T = \begin{bmatrix} T_1 & e_{s-1}\beta_{s-1} & \\ \beta_{s-1}e_{s-1}^T & \alpha_s & \beta_s e_1^T \\ & e_1\beta_s & T_2 \end{bmatrix},$$

$$S = \begin{bmatrix} S_1 & e_{s-1}\gamma_{s-1} & \\ \gamma_{s-1}e_{s-1}^T & \delta_s & \gamma_s e_1^T \\ & e_1\gamma_s & S_2 \end{bmatrix}.$$

Note that $s = n$ is possible; then T_2, S_2, and e_1 are empty [9, 10]. Suppose we solve the subproblems

$$U_k^T (T_k - S_k \lambda) U_k \equiv \Lambda_k - I\lambda \qquad (k = 1, 2). \tag{2}$$

The form of the subproblems is preserved. In particular, the matrices S_k are positive definite and, if T has a zero diagonal, so do the matrices T_k. Let

$$\hat{U} = \begin{bmatrix} U_1 & & \\ & 1 & \\ & & U_2 \end{bmatrix}.$$

Then

$$\hat{U}^T (T - S\lambda) \hat{U} =$$
$$\begin{bmatrix} U_1^T(T_1 - S_1\lambda)U_1 & U_1^T e_{s-1}(\beta_{s-1} - \gamma_{s-1}\lambda) & \\ (\beta_{s-1} - \gamma_{s-1}\lambda)e_{s-1}^T U_1 & \alpha_s - \delta_s\lambda & (\beta_s - \gamma_s\lambda)e_1^T U_2 \\ & U_2^T e_1(\beta_s - \gamma_s\lambda) & U_2^T(T_2 - S_2\lambda)U_2 \end{bmatrix}.$$

2.2 The conquer phase

The conquer phase consists of solving the subproblems (2) from the divide phase, consolidating the solutions, and finally, solving the consolidated problem. Let

$$u_1 = U_1^T e_{s-1}, \qquad u_2 = U_2^T e_1,$$

where the U_k are solutions to (2). Then

$$\hat{U}^T (T - S\lambda) \hat{U} = \begin{bmatrix} \Lambda_1 - I\lambda & u_1(\beta_{s-1} - \gamma_{s-1}\lambda) & \\ (\beta_{s-1} - \gamma_{s-1}\lambda)u_1^T & \alpha_s - \delta_s\lambda & (\beta_s - \gamma_s\lambda)u_2^T \\ & u_2(\beta_s - \gamma_s\lambda) & \Lambda_2 - I\lambda \end{bmatrix}.$$

The right side is the sum of a diagonal and a *Swiss cross*:

$$\hat{U}^T (T - S\lambda) \hat{U} = \begin{bmatrix} x & & & & \\ & x & & & \\ & & x & & \\ & & & x & \\ & & & & x \end{bmatrix} + \begin{bmatrix} & & x & & \\ & & x & & \\ x & x & x & x & x \\ & & x & & \\ & & x & & \end{bmatrix}.$$

This can be permuted to an arrow matrix by a permutation similarity transformation with $P_s = [e_1, e_2, ..., e_{s-1}, e_{s+1}, ..., e_n, e_s]$. Thus

$$\begin{aligned} \hat{A}(\lambda) \ &:= \ P_s^T \hat{U}^T (T - S\lambda) \hat{U} P_s \\ &= \begin{bmatrix} \Lambda_1 & & u_1\beta_{s-1} \\ & \Lambda_2 & u_2\beta_s \\ \beta_{s-1}u_1^T & \beta_s u_2^T & \alpha_s \end{bmatrix} - \begin{bmatrix} I & & u_1\gamma_{s-1} \\ & I & u_2\gamma_s \\ \gamma_{s-1}u_1^T & \gamma_s u_2^T & \delta_s \end{bmatrix} \lambda \\ &= \begin{bmatrix} D & Bu \\ u^T B & \alpha \end{bmatrix} - \begin{bmatrix} I & Cu \\ u^T C & \gamma \end{bmatrix} \lambda, \end{aligned}$$

with

$$\mathbf{u} = \begin{bmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \end{bmatrix},$$

$$B = \begin{bmatrix} \beta_{s-1}I & \\ & \beta_s I \end{bmatrix}, \quad C = \begin{bmatrix} \gamma_{s-1}I & \\ & \gamma_s I \end{bmatrix}.$$

Since S and $\begin{bmatrix} I & C\mathbf{u} \\ \mathbf{u}^T C & \gamma \end{bmatrix}$ are congruent the latter inherits positive definiteness from the former. Its Cholesky decomposition is

$$\begin{bmatrix} I & C\mathbf{u} \\ \mathbf{u}^T C & \gamma \end{bmatrix} = \begin{bmatrix} I & \\ \mathbf{u}^T C & \rho \end{bmatrix} \begin{bmatrix} I & C\mathbf{u} \\ & \rho \end{bmatrix} = R^T R,$$

with $\rho^2 = \gamma - \mathbf{u}^T C^2 \mathbf{u} > 0$ the Schur complement in S of

$$\begin{bmatrix} S_1 & \\ & S_2 \end{bmatrix}.$$

Now

$$R^{-1} = \begin{bmatrix} I & -C\mathbf{u}/\rho \\ & 1/\rho \end{bmatrix}$$

and a second congruence transformation with R^{-1} gives

$$\begin{aligned}
A(\lambda) \quad &:= \quad R^{-T} \hat{A}(\lambda) R^{-1} \\
&= \quad R^{-T} \begin{bmatrix} D & B\mathbf{u} \\ \mathbf{u}^T B & \alpha \end{bmatrix} R^{-1} - I\lambda \\
&= \quad \begin{bmatrix} D & \mathbf{w} \\ \mathbf{w}^T & \omega \end{bmatrix} - I\lambda \quad =: \quad A - \lambda I
\end{aligned}$$

with

$$\mathbf{w} = \frac{(B - DC)\mathbf{u}}{\rho},$$

$$\omega = \frac{\alpha_s - \mathbf{u}^T (2B - DC) C\mathbf{u}}{\rho^2}.$$

We have reduced the conquer step to the problem of solving an ordinary eigenproblem for a symmetric arrow matrix. If V is an orthogonal matrix with

$$AV = V\Lambda$$

and Λ diagonal, then (1) holds with

$$\begin{aligned}
U &= \hat{U} P_s R^{-1} V \\
&= \begin{bmatrix} U_1 & -U_1 \mathbf{u}_1 \gamma_{s-1}/\rho \\ & 1/\rho \\ U_2 & -U_2 \mathbf{u}_2 \gamma_s/\rho \end{bmatrix} V.
\end{aligned}$$

It is useful that $\mathbf{v}_k = U_k\mathbf{u}_k$ can be computed in $O(n)$ time by solving $S_1\mathbf{v}_1 = \mathbf{e}_{s-1}$ and $S_2\mathbf{v}_2 = \mathbf{e}_1$ using the Cholesky factorization $S_1 = L_1L_1^T$ and the reverse Cholesky factorization $S_2 = L_2^T L_2$. In the case that only the eigenvalues are wanted it is only necessary to compute the first and last rows of the U-matrices which constitutes a further savings.

In summary, the conquer phase proceeds by consolidating the subproblems and building a full eigenproblem for an arrow matrix.

3   Solving the eigenproblem for the arrow

In this section we consider the solution of the eigenproblem for a real symmetric arrow matrix

$$A = \begin{bmatrix} D & \mathbf{b} \\ \mathbf{b}^T & \gamma \end{bmatrix}$$

where $A \in \Re^{n \times n}$ is symmetric, $D = \mathrm{diag}(\mathbf{a})$, $\mathbf{a} = [\alpha_1, ..., \alpha_{n-1}]^T$, $\alpha_1 \geq \alpha_2 \geq ... \geq \alpha_{n-1}$, and $\mathbf{b} = [\beta_1, ..., \beta_{n-1}]^T \geq 0$. When A arises from the BSVD then $\mathbf{a}$ is odd and $\mathbf{b}$ is even, that is $\mathbf{a} + J\mathbf{a} = 0$ and $\mathbf{b} = J\mathbf{b}$, with J the *counter-identity*, the identity matrix with its columns reversed, and $\gamma = 0$.

If any $\beta_j = 0$ then it is possible to set $\lambda_j = \alpha_j$ and deflate the matrix since $\mathbf{e}_j$ is clearly an eigenvector [28]. We shall call this β-deflation and note that if $\beta_j < tol_\beta \|\mathbf{b}\|$ where tol_β is a small tolerance then a *numerical* deflation occurs. We derive a precise value for tol_β in section 4.4.

A second type of deflation occurs if applying a 2×2 rotation similarity transformation in the $(j, j+1)$-plane that takes β_j to zero introduces a sufficiently small element in the $(j, j+1)$ position of the matrix. This will be called a *combo*-deflation (see [15]). At each consolidation step we perform a sweep to check for β-deflations followed by a sweep to check for *combo*-deflations. The *combo*-deflation can be arranged so that the ordering of the α_j is preserved whenever one occurs. After deflation the new $\beta_{j+1}^* := \sqrt{\beta_j^2 + \beta_{j+1}^2} \geq \beta_{j+1}$ and hence no further β-deflation can occur. The *combo*-deflations can be disposed of with a single pass by backing up a single element whenever one occurs. Note that deflation is backward stable since it results in *small* backward errors in A. Deflation for the BSVD is more delicate involving a simultaneous sweep from both ends of the matrix. Care must be exercised at the center of the matrix.

After deflation the resulting matrix can be taken to have all $\beta_j > 0$ and the elements of the arrow *shaft* distinct and ordered, that is $\alpha_1 > \alpha_2 > ... > \alpha_{n-1}$. An arrow matrix of this form will be called *ordered* and *reduced*. Henceforth, we shall assume A is of this form.

The block Gauss factorization of $A - \lambda I$ is

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

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

$$f(\lambda) = \lambda - \gamma + \sum_{j=1}^{n-1} \frac{\beta_j^2}{\alpha_j - \lambda}.$$

This is a rational Pick function with a pole at infinity [1]. The *most general* form of a rational Pick function is

$$f(\lambda) = \delta\lambda - \gamma + \sum_{j=1}^{n-1} \frac{\beta_j^2}{\alpha_j - \lambda}, \qquad \delta \geq 0. \tag{3}$$

In relation to the various divide and conquer schemes, the case $\delta > 0$ corresponds with *extension*, $\delta = 0$ with *modification*, and $\delta = \gamma = 0$ with *restriction* [7].

Inspection of the graph of the spectral function reveals that the elements of the shaft interlace the eigenvalues

$$\lambda_1 > \alpha_1 > \lambda_2 > ... > \alpha_{n-1} > \lambda_n. \tag{4}$$

Moreover, in the present case, the derivative of the spectral function is bounded below by one so that its zeros are, in a certain sense, well determined.

3.1 The zero finder

The fundamental problem in finding the eigenvalues of an arrow 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 zero finding algorithm we present is globally convergent in the sense that the iteration will converge to the unique zero of f in (α_k, α_{k-1}) from any starting value in the closed interval $[\alpha_k, \alpha_{k-1}]$, where we put $\alpha_0 = +\infty$ and $\alpha_n = -\infty$. The zero finder converges monotonically at a *cubic* rate and applies to a general Pick function as given in formula (3).

3.2 Interior intervals

The iterative procedure for finding the unique zero of f in one of the interior intervals (α_k, α_{k-1}) proceeds as follows. Let x_0, $\alpha_k < x_0 < \alpha_{k-1}$, be an initial approximation to λ_k. If x_j is known choose

$$\phi_j(x) = \sigma + \frac{\omega_0}{\alpha_{k-1} - x} + \frac{\omega_1}{\alpha_k - x}$$

so that

$$\phi_j^{(i)}(x_j) = f^{(i)}(x_j), \quad i = 0, 1, 2. \tag{5}$$

Thus σ, ω_0, and ω_1 must satisfy

$$\begin{bmatrix} 1 & (\alpha_{k-1} - x_j)^{-1} & (\alpha_k - x_j)^{-1} \\ 0 & (\alpha_{k-1} - x_j)^{-2} & (\alpha_k - x_j)^{-2} \\ 0 & (\alpha_{k-1} - x_j)^{-3} & (\alpha_k - x_j)^{-3} \end{bmatrix} \begin{bmatrix} \sigma \\ \omega_0 \\ \omega_1 \end{bmatrix} = \begin{bmatrix} f(x_j) \\ f'(x_j) \\ f''(x_j) \end{bmatrix}$$

and we find

$$\sigma = 3x_j - (\gamma + \alpha_{k-1} + \alpha_k) + \sum_{i \neq k-1,k} \frac{\beta_i^2}{\alpha_i - x_j} \frac{\alpha_i - \alpha_{k-1}}{\alpha_i - x_j} \frac{\alpha_i - \alpha_k}{\alpha_i - x_j},$$

$$\omega_0 = \beta_{k-1}^2 + \frac{(\alpha_{k-1} - x_j)^3}{\alpha_{k-1} - \alpha_k} \left(1 + \sum_{i \neq k-1,k} \frac{\beta_i^2}{(\alpha_i - x_j)^2} \frac{\alpha_i - \alpha_k}{\alpha_i - x_j} \right),$$

$$\omega_1 = \beta_k^2 + \frac{(x_j - \alpha_k)^3}{\alpha_{k-1} - \alpha_k} \left(1 + \sum_{i \neq k-1,k} \frac{\beta_i^2}{(\alpha_i - x_j)^2} \frac{\alpha_i - \alpha_{k-1}}{\alpha_i - x_j} \right).$$

Since $\omega_0 > 0$ and $\omega_1 > 0$ it follows that ϕ_j is a Pick function. Thus ϕ_j has a unique zero $x_{j+1} \in (\alpha_k, \alpha_{k-1})$. Also

$$\omega_0 > \beta_{k-1}^2 > 0 \quad , \quad \omega_1 > \beta_k^2 > 0.$$

The error function

$$f(x) - \phi(x) = x - (\gamma + \sigma) + \sum_{i \neq k-1,k} \frac{\beta_i^2}{\alpha_i - x} + \frac{\beta_{k-1}^2 - \omega_0}{\alpha_{k-1} - x} + \frac{\beta_k^2 - \omega_1}{\alpha_k - x}$$

has n zeros, counting multiplicities. There are $n-3$ zeros exterior to (α_k, α_{k-1}) and three more at x_j. Thus the error function crosses zero exactly once in the interval (α_k, α_{k-1}). Hence x_{j+1} lies between x_j and λ_k, and the iteration is monotonically convergent from any starting guess $x_0 \in [\alpha_k, \alpha_{k-1}]$ as claimed. The cubic rate of convergence follows from (5).

Successive iterates can be found by solving quadratic equations. Rather than solve $\phi_j(x) = 0$ for x_{j+1} it is better to solve

$$\phi_j(x_j - \Delta) = 0$$

for the *increment* $\Delta = x_j - x_{j+1}$. Some rearrangement using (5) reduces this to

$$a\Delta^2 + \beta\Delta - f = 0, \tag{6}$$

with

$$\alpha = \frac{\sigma}{(\alpha_{k-1} - x_j)(x_j - \alpha_k)}, \tag{7}$$

$$\beta = f'(x_j) - \left(\frac{1}{\alpha_{k-1} - x_j} + \frac{1}{\alpha_k - x_j}\right) f(x_j). \tag{8}$$

When shifts of the origin to the nearest pole [15] are used then one of α_{k-1} or α_k is zero. The computation of $\beta = \beta(x_j)$ should account for the fact that it has only *simple* poles at α_{k-1} and α_k.

If we start at the midpoint of the interval, $x_0 = (\alpha_{k-1} + \alpha_k)/2$, then we always have $\beta = \beta(x_j) \geq f'(x_j) \geq 1$. This can be seen by noting that $\beta(x_0) = f'(x_0)$ and that when $x_0 > \lambda_k$ then for all of the succeeding iterates $f(x_j) > 0$, by monotonicity, and $\frac{1}{\alpha_{k-1} - x_j} + \frac{1}{\alpha_k - x_j}$ is negative. If $x_0 < \lambda_k$ a similar argument applies. It follows that the increment can *always* be computed stably as

$$\Delta = \frac{2f/\beta}{1 + \sqrt{1 + \frac{2\alpha}{\beta}\frac{2f}{\beta}}}. \tag{9}$$

3.3 Exterior intervals

The treatment of the two exterior intervals is *geometrically* the same as above. Again, the approximating function has poles at the endpoints and the residues at these poles, and the constant term, are chosen to satisfy (5). We present the case for the interval (α_1, ∞), the case for the other exterior interval being similar. Now

$$\phi_j(x) = \omega_0 x - \sigma + \frac{\omega_1}{\alpha_1 - x}$$

with

$$\omega_0 = 1 + \sum_{i=2}^{n-1} \frac{\beta_i^2}{(x_j - \alpha_i)^2} \frac{\alpha_1 - \alpha_i}{x_j - \alpha_i} \geq 1,$$

$$\omega_1 = \beta_1^2 + \sum_{i=2}^{n-1} \beta_i^2 \left(\frac{x_j - \alpha_1}{x - \alpha_i}\right)^3 \geq \beta_1^2.$$

The inequalities are strict unless $n = 2$. Again we find (6) where now

$$\alpha = -\frac{1 + \sum_{i=2}^{n-1} \frac{\beta_i^2}{(x_j - \alpha_i)^2} \frac{\alpha_1 - \alpha_i}{x_j - \alpha_i}}{x_j - \alpha_1},$$

$$\beta = f'(x_j) + \frac{f(x_j)}{x_j - \alpha_1}.$$

These are limiting cases of (7) and (8) (introduce another pole $\alpha_0 > \alpha_1$ and let $\alpha_0 \to +\infty$). If $x_0 > \lambda_1$ then $f(\lambda) > 0$ so $\beta > f' > 1$ and Δ is again computed stably using (9). We obtain global monotone cubic convergence as before.

Contrary to the algorithms of [11, 12, 15] our algorithm is well-defined when starting at the endpoints of the intervals. The algorithm of [23] can start at the endpoints but has only quadratic convergence.

To guarantee that $x_0 \geq \lambda_1$ we take x_0 to be the iterate in $(\alpha_1, +\infty)$ from $+\infty$. As $x_0 \to +\infty$ the approximate Pick function tends to

$$\phi(x) = x - \gamma + \frac{\|\mathbf{b}\|^2}{\alpha_1 - x}. \tag{10}$$

Our *actual* starting guess is the zero of (10) in $(\alpha_1, +\infty)$:

$$x_0 = \begin{cases} \alpha_1 + \frac{\gamma - \alpha_1}{2} + \sqrt{\left(\frac{\gamma - \alpha_1}{2}\right)^2 + \|\mathbf{b}\|^2} & , \quad \gamma > \alpha_1, \\[3mm] \alpha_1 + \dfrac{\|\mathbf{b}\|^2}{\frac{\alpha_1 - \gamma}{2} + \sqrt{\left(\frac{\gamma - \alpha_1}{2}\right)^2 + \|\mathbf{b}\|^2}} & , \quad \gamma \leq \alpha_1. \end{cases}$$

When shifts are used we have $\alpha_1 = 0$.

3.4 Orthogonality of the eigenvectors

It is essential that the computed eigenvectors of the arrow matrix be numerically orthogonal. As a point of entry into the further analysis of the algorithm we now examine the orthogonality of the eigenvectors following [15].

Consider the divided difference

$$\begin{aligned} f(\lambda, \mu) &= \frac{f(\lambda) - f(\mu)}{\lambda - \mu} = 1 + \sum_{j=1}^{n-1} \frac{\beta_j^2}{(\alpha_j - \lambda)(\alpha_j - \mu)} \\ &= 1 + \mathbf{b}^T (D - \lambda I)^{-1} (D - \mu I)^{-1} \mathbf{b}. \end{aligned} \tag{11}$$

Note that $\mu = \lambda$ gives $f'(\lambda) = 1 + \|(D - \lambda I)^{-1}\mathbf{b}\|_2^2$. If $f(\lambda) = 0$ then

$$v(\lambda) = \begin{bmatrix} \frac{\beta_j}{\lambda - \alpha_j} \\ 1 \end{bmatrix} = \begin{bmatrix} (\lambda I - D)^{-1}\mathbf{b} \\ 1 \end{bmatrix}$$

is an eigenvector of the arrow matrix $A = \begin{bmatrix} D & \mathbf{b} \\ \mathbf{b}^T & \gamma \end{bmatrix}$ associated with the eigenvalue λ, and

$$u(\lambda) = \frac{v(\lambda)}{\sqrt{f'(\lambda)}}$$

is the normalized eigenvector whose last element is positive. The ordering of A implies that its matrix of eigenvectors can be taken positive below and on the diagonal, and negative above.

Let $f(\lambda_0) = f(\mu_0) = 0$ with $\lambda_0 \neq \mu_0$. Thus λ_0 and μ_0 are distinct eigenvalues of A. The eigenvectors $u(\lambda_0)$ and $u(\mu_0)$ are orthonormal:

$$u(\lambda_0)^T u(\mu_0) = f(\lambda_0, \mu_0) = 0.$$

Let λ and μ be approximate eigenvalues in the sense that

$$-\delta_j = \frac{\lambda - \lambda_0}{\alpha_j - \lambda_0}, \qquad |\delta_j| \leq \frac{\delta}{1 + \delta},$$

$$-\delta_j' = \frac{\mu - \mu_0}{\alpha_j - \mu_0}, \qquad |\delta_j'| \leq \frac{\delta}{1 + \delta}. \tag{12}$$

Here $\delta > 0$ is hopefully, but not necessarily, close to the machine unit ϵ. Note that (12) is equivalent with

$$\frac{\alpha_j - \lambda}{\alpha_j - \lambda_0} = 1 + \delta_j, \quad \frac{\alpha_j - \mu}{\alpha_j - \mu_0} = 1 + \delta_j'.$$

These conditions imply that the approximate eigenvectors $u(\lambda)$ and $u(\mu)$ are nearly orthogonal. For we have

$$
\begin{aligned}
\sqrt{f'(\lambda)f'(\mu)}u(\lambda)^T u(\mu) &= f(\lambda, \mu) - f(\lambda_0, \mu_0) \\
&= \sum_{j=1}^{n-1} \frac{\beta_j^2}{(\alpha_j - \lambda)(\alpha_j - \mu)} \left(1 - \frac{(\alpha_j - \lambda)(\alpha_j - \mu)}{(\alpha_j - \lambda_0)(\alpha_j - \mu_0)} \right) \\
&= \sum_{j=1}^{n-1} \frac{\beta_j^2}{(\alpha_j - \lambda)(\alpha_j - \mu)} \left(\delta_j + \delta_j' + \delta_j \delta_j' \right).
\end{aligned}
$$

Since

$$|\delta_j + \delta_j' + \delta_j \delta_j'| \leq \frac{2\delta}{1 + \delta} + \frac{\delta^2}{(1 + \delta)^2} \leq 2\delta$$

then

$$\sqrt{f'(\lambda)f'(\mu)}u(\lambda)^T u(\mu) = 2\delta b^T (D - \lambda I)^{-1} \Theta (D - \mu I)^{-1} b$$

with $|\Theta| \leq I$. Thus

$$\sqrt{f'(\lambda)f'(\mu)}|u(\lambda)^T u(\mu)| = 2\delta \|(D - \lambda I)^{-1} b\|_2 \|(D - \mu I)^{-1} b\|_2,$$

and so

$$|u(\lambda)^T u(\mu)| < 2\delta.$$

Condition (12) is stringent. If we let $\beta_k \to 0$ then it is easy to show that A can have an eigenvalue $\lambda_0 = \lambda_0(\beta_k) = \alpha_k + O(\beta_k^2)$; (12) then requires that the approximate eigenvalue λ satisfies a bound

$$|\lambda - \lambda_0| \leq O(\delta \beta_k^2),$$

which is difficult if $\beta_k / \|\mathbf{b}\|$ is only somewhat larger than machine precision, say $\epsilon^{3/4}$. Two techniques are used to attempt to satisfy (12) – shifts of the origin [15], and simulated extended precision (SEP) arithmetic [26, 14]. Condition (12) means that

$$|\lambda - \lambda_0| < \delta \min\{\lambda_0 - \alpha_k, \alpha_{k-1} - \lambda_0\}.$$

When shifts are used it means that λ is nearly $fl(\lambda_0)$.

4   Numerical stability of the algorithm

We now give a partial analysis of the stability of this approach to the eigenproblem for the symmetric arrow matrix. Observe that

$$f(\lambda) = \frac{p(\lambda)}{q(\lambda)} := \frac{\prod_{j=1}^{n}(\lambda - \lambda_j)}{\prod_{j=1}^{n-1}(\lambda - \alpha_j)}.$$

The following *inverse eigenvalue problem* [6] is important: given $\{\alpha_j\}$ and $\{\lambda_j\}$ satisfying (4), find $\{\beta_j\}$ and γ so that $\lambda(A) = \{\lambda_j\}$. This problem is simply solved by computing the residues of the partial fraction decomposition of f. In particular

$$\beta_k^2 = \lim_{\lambda \to \alpha_k} (\alpha_k - \lambda)\frac{p(\lambda)}{q(\lambda)}$$

$$= -\frac{\prod_{j=1}^{n}(\alpha_k - \lambda_j)}{\prod_{j \neq k}(\alpha_k - \alpha_j)}.$$

$$\gamma = \sum_{j=1}^{n} \lambda_j - \sum_{j=1}^{n-1} \alpha_j.$$

For fixed $\{\alpha_j\}$, the elements of the arrow *head*, $\{\beta_k\}$ and γ, are *explicitly known* functions of the eigenvalues.

Now let $\{\hat{\lambda}_j\}$ be a set of *approximate* eigenvalues of A satisfying (4). Then

$$\hat{\beta}_k^2 = -\frac{\prod_{j=1}^{n}(\alpha_k - \hat{\lambda}_j)}{\prod_{j \neq k}(\alpha_k - \alpha_j)} \qquad (\hat{\beta}_k > 0), \tag{13}$$

$$\hat{\gamma} = \sum_{j=1}^{n} \hat{\lambda}_j - \sum_{j=1}^{n-1} \alpha_j, \tag{14}$$

define a *modified* matrix $\hat{A}$ with $\lambda(A) = \{\hat{\lambda}_j\}$. To obtain a backward error analysis for the complete eigenvalue problem we bound the differences $\hat{\beta}_k - \beta_k$ and $\hat{\gamma} - \gamma$.

4.1 Error analysis for the Dongarra-Sorensen condition

We give an error analysis using the Dongarra-Sorensen condition

$$-\frac{\hat{\lambda}_j - \lambda_j}{\alpha_k - \lambda_j} = \delta_{j,k}, \quad |\delta_{j,k}| \leq \delta, \tag{15}$$

where $\delta = O(\epsilon)$ is of the order of the machine unit, simplifying that in [6].
    Rearrangement of (15) gives

$$\hat{\lambda}_j - \alpha_k = (\lambda_j - \alpha_k)(1 + \delta_{j,k}).$$

It follows that

$$\hat{\beta}_k^2 = \beta_k^2 \prod_{j=1}^{n}(1 + \delta_{j,k}) = \beta_k^2 \left(1 + \sum_{j=1}^{n}\delta'_{j,k}\right),$$

and

$$\hat{\beta}_k = \beta_k \left(1 + \frac{1}{2}\sum_{j=1}^{n}\delta''_{j,k}\right),$$

with the $\delta'_{j,k}$ and $\delta''_{j,k}$ at most only slightly larger than the $\delta_{j,k}$. Thus

$$\left|\frac{\hat{\beta}_k - \beta_k}{\beta_k}\right| \leq \frac{n}{2}\delta'',$$

where $\delta'' = O(\epsilon)$ is only slightly larger than δ.
    Now (14) becomes

$$\hat{\gamma} = \gamma + \sum_{j=1}^{n}(\lambda_j - \alpha_{k(j)})\delta_{j,k(j)}$$

with $\alpha_{k(j)}$ one of the poles of f. Thus

$$|\hat{\gamma} - \gamma| \leq \delta \sum_{j=1}^{n}|\lambda_j - \alpha_{k(j)}|.$$

To minimize this bound we choose $\alpha_{k(j)}$ to be a pole of f closest to λ_j. Clearly, $\alpha_{k(1)} = \alpha_1$ and $\alpha_{k(n)} = \alpha_{n-1}$, so

$$|\hat{\gamma} - \gamma| \leq \delta \left((\lambda_1 - \alpha_1) + \sum_{j=2}^{n-1}|\lambda_j - \alpha_{k(j)}| + (\alpha_{n-1} - \lambda_n)\right).$$

For $1 < j < n$ a closest pole to λ_j is either α_j or α_{j-1}. The distance

$$|\lambda_j - \alpha_{k(j)}| = \min\{\lambda_j - \alpha_j, \alpha_{j-1} - \lambda_j\}$$

is maximized when λ_j is the midpoint of the interval (α_j, α_{j-1}), and the value of the maximum is $(\alpha_j + \alpha_{j-1})/2$. Thus

$$
\begin{aligned}
|\hat{\gamma} - \gamma| &\leq \delta\left((\lambda_1 - \alpha_1) + \frac{1}{2}\sum_{j=2}^{n-1}(\alpha_{j-1} - \alpha_j) + (\alpha_{n-1} - \lambda_n)\right) \\
&= \delta\left((\lambda_1 - \lambda_n) - \frac{\alpha_1 - \alpha_{n-1}}{2}\right) \\
&\leq \delta(\lambda_1 - \lambda_n) \leq 2\delta\|A\|_2.
\end{aligned}
$$

In summary, the Dongarra-Sorensen condition implies small relative errors in each β_k and a small absolute error in γ. For the BSVD this implies small element-wise relative errors since the condition $\gamma = \hat{\gamma} = 0$ is enforced by $\hat{\lambda}_j + \hat{\lambda}_{n+1-j} = 0$ (only half of the eigenvalues are actually computed, the rest follow from this condition).

4.2 Rounding error analysis of the computation of $f(\lambda)$

The choice of a termination criterion depends on a careful rounding error analysis of the particular manner in which we compute $f(\lambda)$. Let $\{\alpha_i\}$, $\{\beta_i\}$, and γ be floating point numbers. We *represent* λ as the ordered pair of floating point numbers (σ, μ) where the *shift* σ is a pole closest to λ, and $\lambda := \sigma + \mu$. For the exterior intervals we have $\sigma = \alpha_1$ or $\sigma = \alpha_{n-1}$. For the interior intervals σ can be determined by evaluating f at the midpoint and checking the sign. We compute $f(\lambda)$ as

$$
f_\sigma(\mu) = \sum_{j=1}^{n-1} \frac{\beta_j^2}{\alpha_j' - \mu} + (\mu - \gamma'),
$$

with the standard operation precedence rules, where

$$
\alpha_j' = \alpha_j - \sigma \quad \text{and} \quad \gamma' = \gamma - \sigma.
$$

We use Wilkinson's notation: $fl(x * y) = (x * y)(1 + \delta)$ with $|\delta| \leq \epsilon/(1 + \epsilon)$ and $\epsilon = 2^{-t}$ the machine unit. More generally, ϵ denotes numbers not essentially larger than 2^{-t} [27] and the rounding errors δ satisfy $|\delta| < \epsilon$.

We define

$$
fl(\alpha_j - \lambda) := fl(\alpha_j' - \mu) = fl((\alpha_j - \sigma) - \mu).
$$

If $\sigma = \alpha_k$ then

$$
fl(\alpha_k - \lambda) = -\mu = \alpha_k - \lambda,
$$

with no rounding error. For $j \neq k$,

$$fl(\alpha_j - \lambda) = (\alpha_j - \lambda)\left(1 + \frac{\alpha_j - \alpha_k}{\alpha_j - \lambda}\delta + \delta'\right),$$

and since α_k is a pole *closest* to λ then $\left|\frac{\alpha_j - \alpha_k}{\alpha_j - \lambda}\right| \leq 2$. Thus all terms $\alpha_j - \lambda$ are computed with small relative errors:

$$fl(\alpha_j - \lambda) = (\alpha_j - \lambda)(1 + 3\delta_j), \quad |\delta_j| < \epsilon. \tag{16}$$

When computing $f(\lambda) = f_\sigma(\mu)$ we add the term $\lambda - \gamma = (\lambda - \sigma) - (\gamma - \sigma)$ last. A routine error analysis using (16) and

$$|\lambda - \gamma| \leq |f(\lambda)| + \sum_{j=1}^{n-1} \frac{\beta_j^2}{|\alpha_j - \lambda|}$$

to eliminate the term $|\lambda - \gamma|$ from the error bound gives

$$|fl(f(\lambda)) - f(\lambda)| \leq \epsilon \left(3|f(\lambda)| + |\sigma - \lambda| + (n+5)\sum_{j=1}^{n-1}\frac{\beta_j^2}{|\alpha_j - \lambda|}\right)$$

which implies

$$|fl(f(\lambda))| \leq (1 + 3\epsilon)|f(\lambda)| + \epsilon\left(|\sigma - \lambda| + (n+5)\sum_{j=1}^{n-1}\frac{\beta_j^2}{|\alpha_j - \lambda|}\right). \tag{17}$$

4.3 Termination

Our goal is to choose a termination criterion so that we stop when λ is as close to the true eigenvalue λ_k as possible. Let $\mu = \lambda_k$ in (11) with $f(\lambda_k) = 0$. Now $\alpha_k < \lambda_k < \alpha_{k-1}$. Also let $\alpha_k < \lambda < \alpha_{k-1}$. Then the terms $\alpha_j - \lambda$ and $\alpha_j - \lambda_k$ have the same sign and

$$|\lambda - \lambda_k| \leq \frac{|f(\lambda)|}{1 + \sum_{j=1}^{n-1}\frac{\beta_j^2}{|\alpha_j - \lambda||\alpha_j - \lambda_k|}}. \tag{18}$$

To obtain an upper bound for $|\lambda - \lambda_k|$ we need an upper bound for $|f(\lambda)|$ and a lower bound for the denominator. For the latter we have

$$1 + \sum_{j=1}^{n-1}\frac{\beta_j^2}{|\alpha_j - \lambda||\alpha_j - \lambda_k|} \geq 1 + \frac{\sum_{j=1}^{n-1}\frac{\beta_j^2}{|\alpha_j - \lambda|}}{\max_j |\alpha_j - \lambda_k|}. \tag{19}$$

Let us determine how small $|f(\lambda)|$ is when λ is the *rounded representation* of λ_k. This is

$$\tilde{\lambda} \quad := \quad \sigma + fl(\mu_k) = \sigma + \mu_k(1+\delta)$$
$$= \quad \lambda_k + \mu_k\delta = \lambda_k + (\lambda_k - \sigma)\delta$$

and we have

$$|\sigma - \lambda_k| = \min_j |\alpha_j - \lambda_k|.$$

Thus

$$|f(\tilde{\lambda})| = |\tilde{\lambda} - \lambda_k| \left(1 + \sum_{j=1}^{n-1} \frac{\beta_j^2}{(\alpha_j - \tilde{\lambda})(\alpha_j - \lambda_k)}\right)$$

$$= |(\sigma - \lambda_k)\delta| \left(1 + \sum_{j=1}^{n-1} \frac{\beta_j^2}{(\alpha_j - \tilde{\lambda})(\alpha_j - \lambda_k)}\right)$$

$$\leq \epsilon \left(|\sigma - \lambda_k| + \sum_{j=1}^{n-1} \frac{\beta_j^2}{|\alpha_j - \tilde{\lambda}|}\right).$$

From (17),

$$|fl(f(\tilde{\lambda}))| \leq \epsilon \left(|\sigma - \lambda_k| + |\tilde{\lambda} - \sigma| + (n+6) \sum_{j=1}^{n-1} \frac{\beta_j^2}{|\alpha_j - \tilde{\lambda}|}\right).$$

Since $\lambda_k - \sigma = (\tilde{\lambda} - \sigma)/(1+\delta)$ then

$$|fl(f(\tilde{\lambda}))| \leq \epsilon \left(2|\tilde{\lambda} - \sigma| + (n+6) \sum_{j=1}^{n-1} \frac{\beta_j^2}{|\alpha_j - \tilde{\lambda}|}\right).$$

We terminate and set $\lambda_k := \lambda$ when

$$|fl(f(\lambda))| \leq 2\epsilon \left(2|\lambda - \sigma| + (n+6) \sum_{j=1}^{n-1} \frac{\beta_j^2}{|\alpha_j - \lambda|}\right).$$

Inequality (17) also holds if $f(\lambda)$ and $fl(f(\lambda))$ are interchanged. Thus

$$|f(\hat{\lambda}_k)| \leq \epsilon \left(5|\lambda_k - \sigma| + (3n+17) \sum_{j=1}^{n-1} \frac{\beta_j^2}{|\alpha_j - \lambda_k|}\right). \tag{20}$$

From (18) and (19)

$$|\hat{\lambda}_k - \lambda_k| \leq \epsilon \max_j |\lambda_k - \alpha_j| \frac{5|\sigma - \tilde{\lambda}_k| + (3n+17) \sum_{j=1}^{n-1} \frac{\beta_j^2}{|\alpha_j - \lambda_k|}}{\max_j |\lambda_k - \alpha_j| + \sum_{j=1}^{n-1} \frac{\beta_j^2}{|\alpha_j - \lambda_k|}}.$$

Since $|\sigma - \tilde\lambda_k| \le |\sigma - \lambda_k| + |\tilde\lambda_k - \lambda_k|$ and $|\sigma - \lambda_k| \le \max_j |\alpha_j - \lambda_k|$ the computed eigenvalues satisfy

$$
\begin{aligned}
|\hat\lambda_k - \lambda_k| &\le (3n+17)\epsilon \max_j |\alpha_j - \lambda_k| \\
&\le 6(n+6)\epsilon \|A\|_2 .
\end{aligned}
\tag{21}
$$

4.4 Error analysis for the Gu-Eisenstat condition

From $\hat\gamma - \gamma = \sum_{j=1}^n (\hat\lambda_j - \lambda_j)$ and (21) we find

$$
|\hat\gamma - \gamma| \le 6n(n+6)\epsilon \|A\|_2 .
$$

We have noted that the Dongarra-Sorensen condition (15) is stringent. It is natural to ask for small *absolute* errors in the β_k. If we replace $\delta_{j,k}$ by $\delta_{j,k}/\beta_k$ in the analysis in section 4.1 we find that

$$
\hat\beta_k = \beta_k \left(1 + \frac{1}{2} \sum_{j=1}^{n-1} \frac{\delta_{j,k}''}{\beta_k} \right) = \beta_k + \frac{1}{2} \sum_{j=1}^{n-1} \delta_{j,k}'' ,
$$

and

$$
|\hat\beta_k - \beta_k| \le \frac{n}{2} \delta'' , \qquad |\delta''| \le \delta(1 + O(\epsilon)),
$$

are implied by the *Gu-Eisenstat condition*

$$
-\beta_k \frac{\hat\lambda_j - \lambda_j}{\alpha_j - \lambda_j} = \delta_{j,k} , \qquad |\delta_{j,k}| \le \delta .
$$

We must bound δ.
From (20)

$$
|\hat\lambda_k - \lambda_k| \left(1 + \sum_{j=1}^{n-1} \frac{\beta_j^2}{(\alpha_j - \lambda_k)(\alpha_j - \hat\lambda_k)} \right) \le m \left(|\hat\lambda_k - \sigma| + \sum_{j=1}^{n-1} \frac{\beta_j^2}{|\alpha_j - \hat\lambda_k|} \right)
$$

with $m = 3(n+6)$. Using

$$
|\hat\lambda - \sigma| \le |\hat\lambda - \hat\lambda_k| + |\hat\lambda_k - \sigma|
$$

and the Gu-Eisenstat inequality,

$$
\frac{1}{|\alpha_j - \hat\lambda|} \le \left| \frac{1}{(\alpha_j - \lambda)(\alpha_j - \hat\lambda_k)} \right|^{1/2} + \frac{|\hat\lambda_k - \hat\lambda|}{(\alpha_j - \lambda)(\alpha_j - \hat\lambda_k)} ,
$$

we get

$$|\hat{\lambda}_k - \lambda_k| \le m\epsilon \left(|\lambda_k - \sigma| + \frac{\sum_{j=1}^{n-1} \frac{\beta_j^2}{[(\alpha_j - \lambda_k)(\alpha_j - \lambda_k)]^{1/2}}}{\sum_{j=1}^{n-1} \frac{\beta_j^2}{(\alpha_j - \lambda_k)(\alpha_j - \lambda_k)}} \right),$$

where ϵ has been increased to $\epsilon/(1 - m\epsilon)$.

By Cauchy's inequality,

$$|\hat{\lambda}_k - \lambda_k| \le m\epsilon \left(|\lambda_k - \sigma| + \frac{\|\mathbf{b}\|}{\left(\sum_{j=1}^{n-1} \frac{\beta_j^2}{(\alpha_j - \lambda_k)(\alpha_j - \lambda_k)} \right)^{1/2}} \right)$$

$$\le m\epsilon \left(|\lambda_k - \sigma| + \frac{\|\mathbf{b}\|}{\beta_j} \left[(\alpha_j - \lambda_k)(\alpha_j - \lambda_k) \right]^{1/2} \right),$$

for every j. The arithmetic-geometric mean inequality and the triangle inequality yield

$$|\hat{\lambda}_k - \lambda_k| \le m\epsilon \left(|\lambda_k - \sigma| + \frac{\|\mathbf{b}\|}{\beta_j} \left(|\alpha_j - \lambda_k| + \frac{1}{2}|\hat{\lambda}_k - \lambda_k| \right) \right).$$

Thus

$$\left(1 - \frac{m\epsilon}{2} \frac{\|\mathbf{b}\|}{\beta_j} \right) |\hat{\lambda}_k - \lambda_k| \le m\epsilon \left(|\lambda_k - \sigma| + |\alpha_j - \lambda_k| \frac{\|\mathbf{b}\|}{\beta_j} \right)$$

$$= m\epsilon \|\mathbf{b}\| \frac{|\alpha_j - \lambda_k|}{\beta_j} \left(1 + \frac{|\lambda_k - \sigma|}{|\lambda_k - \alpha_j|} \frac{\beta_j}{\|\mathbf{b}\|} \right)$$

$$\le 2m\epsilon \|\mathbf{b}\| \frac{|\alpha_j - \lambda_k|}{\beta_j}.$$

If $m\epsilon \|\mathbf{b}\| \le \beta_j$ for all j, then

$$|\delta_{j,k}| \le 4 m\epsilon \|\mathbf{b}\|.$$

and consequently

$$|\hat{\beta}_k - \beta_k| \le 6n(n+6)\epsilon \|\mathbf{b}\|.$$

Thus tol_β is $m\epsilon$. If $\beta_k < 3(n+6)\epsilon \|\mathbf{b}\|$ we replace β_k by zero and accept α_k as an eigenvalue with normalized eigenvector e_k.

The computed eigenvectors of A are taken to be those of the nearby matrix $\hat{A}$. Because of (13) and (16) they are computed to high relative precision elementwise and hence are numerically orthogonal [20].

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