1995

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ABSTRACT

We consider the problem of reconstructing Jacobi matrices and real symmetric arrow matrices from two eigenpairs. Algorithms for solving these inverse problems are presented. We show that there are reasonable conditions under which this reconstruction is always possible. Moreover, it is seen that in certain cases reconstruction can proceed with little or no cancellation. The algorithm is particularly elegant for the tridiagonal matrix associated with a bidiagonal singular value decomposition.

Keywords: Jacobi matrix, Arrow matrix, inverse problem.

1 Introduction

We consider the problem of reconstructing Jacobi matrices and real symmetric arrow matrices from two eigenpairs. The algorithms we present for solving these inverse problems are simple, and useful for constructing test matrices for eigenproblems. The algorithm for reconstructing Jacobi matrices was applied to the problem of model identification of reciprocal stochastic processes in [3].

2 Jacobi matrices

Let T be an unreduced real symmetric tridiagonal matrix (i.e. a Jacobi matrix)

$$T = \begin{bmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \alpha_2 & \beta_2 & & \\ & \beta_2 & & \ddots & \\ & & \ddots & & \beta_{n-1} \\ & & & \beta_{n-1} & \alpha_n \end{bmatrix} \tag{2.1}$$

with $\beta_i > 0$ for $i = 1, 2, ..., n-1$. We use the notation introduced in [13] and let $\mathbf{UST}(n)$ denote the set of $n \times n$ real unreduced symmetric tridiagonal matrices, and let $\mathbf{UST}_+(n)$ denote that subset of $\mathbf{UST}(n)$ with positive β_i.

We wish to develop an algorithm to reconstruct T from the knowledge of two of its eigenpairs $(\lambda, \mathbf{u})$ and $(\mu, \mathbf{v})$. The eigenvector recurrence for symmetric tridiagonal matrices is

$$\beta_{i-1}u_{i-1} + \alpha_i u_i + \beta_i u_{i+1} = \lambda u_i \tag{2.2}$$

where $(\lambda, \mathbf{u})$ is any eigenpair of T, u_i is the ith element of $\mathbf{u}$, and $\beta_0 = \beta_n = 0$. Applying this relation to both eigenpairs gives

$$\begin{aligned} \beta_{i-1}u_{i-1} + \alpha_i u_i + \beta_i u_{i+1} &= \lambda u_i \\ \beta_{i-1}v_{i-1} + \alpha_i v_i + \beta_i v_{i+1} &= \mu v_i. \end{aligned}$$

Combining these two equations and eliminating α_i gives

$$\beta_{i-1}(v_i u_{i-1} - u_i v_{i-1}) + \beta_i(u_{i+1}v_i - v_{i+1}u_i) = (\lambda - \mu)u_i v_i. \tag{2.3}$$

Since $\beta_0 = \beta_n = 0$ we get the following initial and terminal conditions

$$\beta_1(u_2 v_1 - v_2 u_1) = (\lambda - \mu)u_1 v_1 \tag{2.4}$$

$$\beta_{n-1}(v_n u_{n-1} - u_n v_{n-1}) = (\lambda - \mu)u_n v_n. \tag{2.5}$$

Combining (2.3) with (2.4) gives a special case of the Christoffel-Darboux identity,

$$\beta_i(u_{i+1}v_i - v_{i+1}u_i) = (\lambda - \mu)\sum_{k=1}^{i} u_k v_k \tag{2.6}$$

for $i = 1, 2, ..., n-1$. There is also a backward formula,

$$\beta_i(u_{i+1}v_i - v_{i+1}u_i) = -(\lambda - \mu)\sum_{k=i+1}^{n} u_k v_k, \tag{2.7}$$

which follows from (2.3) and (2.5), or from (2.6) and the orthogonality of the eigenvectors. In a similar manner, we can show that

$$2\alpha_i u_i v_i = (\lambda + \mu)u_i v_i - \beta_{i-1}(u_i v_{i-1} + v_i u_{i-1}) - \beta_i(u_{i+1}v_i + v_{i+1}u_i). \tag{2.8}$$

This formula uses all of the available information but it is possible to obtain an equation for the α_i using the β_i and a single eigenpair with the formula

$$\alpha_i v_i = \mu v_i - \beta_{i-1}v_{i-1} - \beta_i v_{i+1}. \tag{2.9}$$

We can use these equations to reconstruct the original matrix from the two eigenpairs provided that no element of the two eigenvectors is zero and that $v_i u_{i+1} - u_i v_{i+1} \neq 0$ for any $i = 1, 2, ..., n-1$. If this is true, then the equations for the α_i simplify to

$$2\alpha_i = (\lambda+\mu) - \beta_{i-1}\left(\frac{v_{i-1}}{v_i} + \frac{u_{i-1}}{u_i}\right) - \beta_i\left(\frac{v_{i+1}}{v_i} + \frac{u_{i+1}}{u_i}\right) \tag{2.10}$$

or

$$\alpha_i = \lambda - \beta_{i-1}\frac{u_{i-1}}{u_i} - \beta_i\frac{u_{i+1}}{u_i}. \tag{2.11}$$

Notice that (2.10) is just the simple average of (2.11) over both eigenpairs. Using (2.11), (2.6), and (2.7) we can reconstruct the original matrix in $13n-12$ flops.

In order to determine when these formulas can be applied, we need some additional results. We introduce the following fact from [12].

Fact 1 *Let $T \in \mathbf{UST}_+(n)$ and assume that the eigenvalues are ordered so that $\lambda_1 > \lambda_2 > \ldots > \lambda_n$. Then the number of sign changes between consecutive elements of the kth eigenvector of T, denoted s_k, is $k-1$.*

We refer the reader to [12] for a proof but note that it can be derived from the Sturm sequence property for the characteristic polynomials of the principal submatrices. With this fact in hand we can prove the following theorem.

Theorem 1 *If $T \in \mathbf{UST}_+(n)$ and if $(\lambda, \mathbf{u})$ and $(\mu, \mathbf{v})$ are the extremal eigenpairs of T, that is $\lambda = \lambda_1$ and $\mu = \lambda_n$, then $v_i u_{i+1} - u_i v_{i+1} \neq 0$ for any $i = 1, 2, ..., n-1$.*

Proof. The proof follows trivially by noting that the strict interlacing property for unreduced symmetric tridiagonals (see [14] p. 300) guarantees that none of the numbers $u_i, u_{i+1}, v_i, v_{i+1}$ can be zero. And, since u_i and u_{i+1} must have the same sign and v_i and v_{i+1} must have opposite signs (from fact 1), it follows that both terms in $u_i v_{i+1} - v_i u_{i+1}$ have opposite signs and are nonzero so this difference is really a sum of two strictly positive (negative) numbers and hence is not zero. □

Hence, if we choose the two extremal eigenpairs of a given element of $\mathbf{UST}_+$ we can always reconstruct the original matrix using the formulas above. Notice that the denominator is computed without cancellation in this case because of the sign pattern. Moreover, if we use the smallest (largest) eigenpair in (2.9) to get the α_i, then these can be reconstructed from the derived β_i and the data without further cancellation if the matrix is positive (negative) definite. If the matrix is indefinite then there is only one additional cancellation for each of the α_i. If the matrix is singular then choosing the eigenvector associated with the zero eigenvalue prevents further cancellation.

Note that any element of $\mathbf{UST}(n)$ has exactly $2n-1$ real degrees of freedom and that two eigenpairs contain $2n+2$ numbers but, in fact, also have $2n-1$ real degrees of freedom since there are two arbitrary scaling parameters for the eigenvectors and a single orthogonality condition. The eigenpairs contain precisely the right amount of information.

This algorithm is especially robust when applied to the tridiagonal matrix associated with the bidiagonal SVD. It is well known [8] that the Jordan-Lanczos matrix

$$A = \begin{bmatrix} 0 & B^T \\ B & 0 \end{bmatrix}, \tag{2.12}$$

where $B \in \Re^{n \times n}$ is an unreduced bidiagonal with positive elements, can be reduced via the *perfect shuffle* to an unreduced tridiagonal T of the form

$$T = \begin{bmatrix} 0 & \beta_1 & & & & \\ \beta_1 & 0 & \beta_2 & & & \\ & \beta_2 & & \ddots & & \\ & & \ddots & & & \beta_{2n-1} \\ & & & & \beta_{2n-1} & 0 \end{bmatrix}. \tag{2.13}$$

The matrix T is $2n \times 2n$ and its eigenvalues occur in plus-minus pairs. It is not difficult to show that if $(\lambda, \mathbf{u})$ is an eigenpair of T then $(-\lambda, S\mathbf{u})$ is also an eigenpair where S is diagonal with 1 and -1 alternating as the diagonal elements. The reconstruction formula for this matrix simplifies considerably since we need only a single eigenpair. In particular, the β_i are given by

$$\beta_i = \frac{(-1)^i \lambda}{u_{i+1} u_i} \sum_{k=1}^{i} (-1)^k u_k u_k. \tag{2.14}$$

As a special case of the more general algorithm it is obvious that the denominator $u_{i+1}u_i$ is not zero provided we use the eigenvector associated with the largest eigenvalue. Even more intriguing is that, provided none of the principal submatrices shares an eigenvalue with the full matrix, this denominator will be non-zero for any eigenpair since in this case no element of any eigenvector can be zero. In other words, the reconstruction from any eigenpair is well-posed provided that the given eigenvector has no zero elements. The algorithm requires $5n - 6$ flops working with (2.14) and the backward equation

$$\beta_i = \frac{(-1)^{i+1} \lambda}{u_{i+1} u_i} \sum_{k=i+1}^{n} (-1)^k u_k u_k. \tag{2.15}$$

Notice that this matrix has only $n - 1$ real degrees of freedom which is exactly what is given by one eigenpair since the eigenvector contains an arbitrary scaling parameter and must satisfy the special orthogonality condition

$$\sum_{i=1}^{n} (-1)^i u_i^2 = 0. \tag{2.16}$$

We point out that this algorithm can be interpreted as the reconstruction of an unreduced bidiagonal B from its largest singular value and both associated singular vectors.

3 Arrow Matrices

We can reconstruct the arrow matrix in a similar manner to that given above. The arrow is of some importance as it occurs in certain divide and conquer schemes for finding the eigenvalues of a tridiagonal matrix. The arrow is also an element of the class of symmetric acyclic matrices (as is the Jacobi matrix) and hence it is possible, under certain conditions (e.g. if it is positive definite or scaled diagonally dominant), to find its eigenvalues with "tiny component-wise relative backward error", [6].

The general form of an arrow matrix is

$$A = \begin{bmatrix} \alpha_1 & & & & \beta_1 \\ & \alpha_2 & & & \beta_2 \\ & & \ddots & & \vdots \\ & & & \alpha_{n-1} & \beta_{n-1} \\ \beta_1 & \beta_2 & & \beta_{n-1} & \gamma \end{bmatrix}. \tag{3.1}$$

If $\beta_i \neq 0$ for $i = 1, 2, ..., n-1$ and if $\alpha_i \neq \alpha_j$ for any $i \neq j$ then we shall say that $A \in \mathbf{USA}(n)$, where $\mathbf{USA}(n)$ is the set of unreduced symmetric arrow matrices. Proceeding as before, we let $(\lambda, \mathbf{u})$ and $(\mu, \mathbf{v})$ be two eigenpairs of A. The eigenvector recurrence is

$$\alpha_i u_i + \beta_i u_n = \lambda u_i \tag{3.2}$$

$$\alpha_i v_i + \beta_i v_n = \mu v_i \tag{3.3}$$

for $i = 1, 2, ..., n-1$. Moreover, the eigenvector relation also gives

$$\gamma = \mu - \frac{1}{v_n} \sum_{i=1}^{n-1} \beta_i v_i \tag{3.4}$$

for any eigenpair $(\mu, \mathbf{v})$ of A. If we combine (3.2) and (3.3) and eliminate α_i we get

$$\beta_i (v_i u_n - u_i v_n) = (\lambda - \mu) u_i v_i. \tag{3.5}$$

Similarly, eliminating β_i gives

$$\alpha_i (v_i u_n - u_i v_n) = \mu v_i u_n - \lambda u_i v_n. \tag{3.6}$$

This gives a very simple, easily vectorizable reconstruction algorithm. The only remaining question is whether the quantities $v_n u_i - u_n v_i$ are all nonzero. In order to show that this is true under the correct conditions, we need to first establish some facts about the eigenvectors of an unreduced arrow matrix. We begin by noting that

$$A - \lambda I = \begin{bmatrix} D - \lambda I & \mathbf{b} \\ \mathbf{b}^T & \gamma - \lambda \end{bmatrix} \tag{3.7}$$

where $D = \text{diag}(\alpha_1, \alpha_2, ..., \alpha_{n-1})$, and $\mathbf{b} = [\beta_1, \beta_2, ..., \beta_{n-1}]^T$. Following [9] we compute the Gauss factorization

$$\begin{bmatrix} D - \lambda I & \mathbf{b} \\ \mathbf{b}^T & \gamma - \lambda \end{bmatrix} = \begin{bmatrix} I & 0 \\ \mathbf{b}^T (D - \lambda I)^{-1} & 1 \end{bmatrix} \begin{bmatrix} D - \lambda I & \mathbf{b} \\ 0^T & -f(\lambda) \end{bmatrix} \tag{3.8}$$

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

$$f(\lambda) = \lambda - \gamma + \sum_{i=1}^{n-1} \frac{\beta_i^2}{\alpha_i - \lambda}. \tag{3.9}$$

From (3.8) and (3.9) the zeros of f are the eigenvalues of A. Furthermore, if A is unreduced, then the eigenvalues of A are strictly interlaced by the α_i. It follows that the eigenvector associated with λ is

$$\mathbf{v}(\lambda) = \begin{bmatrix} (\lambda I - D)^{-1}\mathbf{b} \\ 1 \end{bmatrix}. \tag{3.10}$$

Note that distinctness of the α_i is critical since it guarantees that $(\lambda I - D)$ is nonsingular. Combining this description of the eigenvectors with the fact that the α_i interlace the eigenvalues, we have the following fact.

Fact 2 *Let A be an unreduced arrow matrix with $\beta_i > 0$ for $i = 1, 2, ..., n-1$. Then the following hold.*

1. *If $\mathbf{u}$ is any eigenvector of A then $u_i \neq 0$ for any $i = 1, 2, ..., n$.*

2. *If we order the eigenvalues of A so that $\lambda_1 > \lambda_2 > ... > \lambda_n$ and let $\mathbf{u}_k$ be the eigenvector, from (3.10), associated with λ_k, then the first $k-1$ elements of $\mathbf{u}_k$ are less than zero, and the last $n-k+1$ elements are greater than zero.*

Proof. The proof of the first fact follows directly from formula (3.10) and the interlacing property. The second fact follows from formula (3.10), the interlacing property, and the positivity of the β_i. □

This simplifies the reconstruction formula since, if we assume that the eigenvectors are normalized so that their last elements are equal to one, the reconstruction formulas can be rewritten as

$$\begin{aligned} \alpha_i &= \lambda - \frac{(\mu - \lambda)v_i}{u_i - v_i} \\ \beta_i &= \frac{(\mu - \lambda)u_i v_i}{u_i - v_i} \\ \gamma &= \mu - \frac{1}{v_n}\sum_{i=1}^{n-1} \beta_i v_i. \end{aligned} \tag{3.11}$$

Using these formulas and the fact that $(\mu - \lambda)v_i/(u_i - v_i)$ is a common subexpression, we can reconstruct the arrow matrix in $7n - 5$ flops. Under the previously mentioned conditions, it is easily shown that none of the denominators in the reconstruction formula are zero and hence we can always reconstruct the matrix from two eigenpairs.

Theorem 2 *If A is an unreduced arrow matrix, and if λ and μ are any two distinct eigenvalues of A with associated eigenvectors $\mathbf{u}$ and $\mathbf{v}$, normalized to have their last elements equal to one, then $u_i - v_i \neq 0$ for $i = 1, 2, ..., n-1$.*

Proof. Assume that $u_i = v_i$. The eigenvector relation implies that

$$\begin{bmatrix} u_i & 1 \\ v_i & 1 \end{bmatrix} \begin{bmatrix} \alpha_i \\ \beta_i \end{bmatrix} = \begin{bmatrix} \lambda u_i \\ \mu v_i \end{bmatrix} \tag{3.12}$$

which implies that $\lambda = \mu$, but this contradicts the distinctness of the eigenvalues. Hence, it follows that $u_i \neq v_i$. □

The reconstruction algorithm has another very important property: if the two extremal eigenpairs (λ_1 and λ_n and their associated eigenvectors) are used, then the β_i can be found, up to the scaling factor $\lambda_1 - \lambda_n$, without cancellation. This follows from the normalization of the eigenvectors which implies that the differences in the denominator do not involve cancellation. Moreover, if A is indefinite there are no cancellations whatsoever in computing the β_i. Conversely, if A is definite the formulas may be rearranged so that there are no cancellations in computing the α_i. If A is semi-definite (and singular) then there is no cancellation at all, including the computation of γ. The computation of γ involves one cancellation if the matrix is indefinite, and none if it is definite, or semi-definite, provided we choose the correct eigenvector for its computation. In any case, whenever there is cancellation in this algorithm, it is benign.

4 Breakdown of the Jacobi reconstruction

On seeing that the reconstruction algorithm for the arrow is well posed for any two eigenpairs, it is tempting to believe that this might also hold for Jacobi matrices since the same conditions apply – unreduced, no principal submatrix shares an eigenvalue with the full matrix. To see that it is not true consider the matrix

$$\begin{bmatrix} 6 & 2 & 0 & 0 \\ 2 & 4 & 5 & 0 \\ 0 & 5 & 4 & 2 \\ 0 & 0 & 2 & 6 \end{bmatrix}. \tag{4.1}$$

This matrix is in $\mathbf{UST}_+$ and shares no eigenvalues with its principal submatrices. The eigenvalues are 10, $(5+\sqrt{65})/2$, 5, $(5-\sqrt{65})/2$ and the eigenvectors associated with 10 and 5 are $[1\ 2\ 2\ 1]^T$ and $[-2\ 1\ 1\ -2]^T$, respectively. Using these two eigenpairs the algorithm breaks down in computing β_2. Manipulation of the scalar equations shows that the two eigenpairs in question are eigenpairs of any matrix of the form

$$\begin{bmatrix} 6 & 2 & 0 & 0 \\ 2 & 9-\gamma & \gamma & 0 \\ 0 & \gamma & 9-\gamma & 2 \\ 0 & 0 & 2 & 6 \end{bmatrix}. \tag{4.2}$$

We can say a few things about breakdown. First of all, if the algorithm breaks down in the computation of β_i then it cannot break down for β_{i-1} or β_{i+1} as this implies that two distinct eigenvalues share the same eigenvector. Second, if there is a breakdown then it is possible to reconstruct a parametrized matrix with the specified eigenpairs by setting $\beta_i = \gamma$ and solving for α_i and α_{i+1} in terms of γ. Setting $\gamma = 0$ will yield a reduced tridiagonal with the specified eigenpairs.

5 Stabilizing divide and conquer algorithms

We note that there are several other important inverse problems for the symmetric arrow matrix. Of interest, is the reconstruction of the symmetric arrow from the eigenvalues and the *shaft* of the arrow (i.e. the elements α_i). In this case we can reconstruct the arrow in a straightforward manner. We need to determine the β_i and the element γ. We obtain γ from the trace formula

$$\gamma = \sum_{i=1}^{n} \lambda_i - \sum_{i=1}^{n-1} \alpha_i. \tag{5.1}$$

The β_i can be computed directly since the $-\beta_i^2$ are the residues of the *partial fraction decomposition*

$$f(\lambda) = \frac{\prod_{i=1}^{n}(\lambda - \lambda_i)}{\prod_{i=1}^{n-1}(\lambda - \alpha_i)} = \lambda - \gamma + \sum_{i=1}^{n-1} \frac{\beta_i^2}{\alpha_i - \lambda}. \tag{5.2}$$

Thus we have

$$\beta_j^2 = \lim_{\lambda \to \alpha_k} (\alpha_k - \lambda) f(\lambda) = -\frac{\prod_{i=1}^{n}(\alpha_j - \lambda_i)}{\prod_{i \neq j}(\alpha_j - \alpha_i)}. \tag{5.3}$$

This algorithm is used in [2] for the reconstruction of a periodic Jacobi matrix. It can also be applied to stabilize the extension based tridiagonal divide and conquer algorithms [9, 4].

We note that this is very similar to the inverse problem first considered in [1] and then used in [10] to stabilize the modification based Cuppen-Dongarra-Sorensen algorithm [5, 7]. In particular, the zeros of the *spectral function*

$$f(\lambda) = 1 + \sum_{i=1}^{n} \frac{\beta_i^2}{\alpha_i - \lambda} \tag{5.4}$$

are the eigenvalues of $D + \mathbf{b}\mathbf{b}^T$. The authors of [10] show that loss of orthogonality in computing the eigenvectors can be avoided by using the computed eigenvalues $\tilde{\lambda}_i$ in the reconstruction formula

$$\tilde{\beta}_j^2 = \frac{\prod_{i=1}^{n}(\tilde{\lambda}_i - \alpha_j)}{\prod_{i \neq j}(\alpha_i - \alpha_j)} \tag{5.5}$$

and then computing the eigenvectors of $D + \tilde{\mathbf{b}}\tilde{\mathbf{b}}^T$ from their explicit expressions. The enlightened use of *shifts* of the origin [10] is crucial to both algorithms.

Acknowledgements

The first and third authors were supported by direct grant from the Naval Postgraduate School. The third author also acknowledges support from the Interdisciplinary Project Center for Supercomputing at the ETH, Zürich.

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