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Abstract

We show how to construct, from certain spectral data, a discrete inner product for which the associated sequence of monic orthogonal polynomials coincides with the sequence of appropriately normalized characteristic polynomials of the left principal submatrices of the Jacobi matrix. The generation of these orthogonal polynomials via their three term recurrence relation, as popularized by Forsythe, then provides a stable means of computing the entries of the Jacobi matrix. The resulting algorithm might be of help in the approximate solution of inverse eigenvalue problems for Sturm-Liouville equations.

Our construction provides, incidentally, very simple proofs of known results concerning existence and uniqueness of a Jacobi matrix satisfying given spectral data and its continuous dependence on that data.

THE NUMERICALLY STABLE RECONSTRUCTION OF A JACOBI MATRIX FROM SPECTRAL DATA

C. de Boor[1] and G. H. Golub[1, 2]

1. Introduction. Gantmacher and Krein [3] take the term "Jacobi matrix" to mean nothing more than "tridiagonal matrix". But it seems to have become accepted in papers on the problem of concern here to mean by "Jacobi matrix" a real, symmetric, tridiagonal matrix whose next-to-diagonal elements are positive. We follow such usage here, and write such a Jacobi matrix J of order n as

$$J=\begin{bmatrix} a_1 & b_1 & & & & \\ b_1 & a_2 & b_2 & & & \\ & b_2 & a_3 & b_3 & & \\ & & \ddots & \ddots & \ddots & \\ & & & b_{n-2} & a_{n-1} & b_{n-1} \\ & & & & b_{n-1} & a_n \end{bmatrix}, \quad b_i > 0, \text{ all } i \,. \tag{1}$$

Further, we denote its left principal submatrix of order r by J_r.

We consider the following inverse problem.

Problem A. Given the sequences $\lambda := (\lambda_i)_1^n$ and $\mu := (\mu_i)_1^{n-1}$ with

$$\lambda_i < \mu_i < \lambda_{i+1}, \qquad i = 1, \ldots, n-1 \,. \tag{S}$$

construct an n-th order Jacobi matrix J which has $\lambda_1, \ldots, \lambda_n$ as its eigenvalues and $\mu_1, \ldots, \mu_{n-1}$ as the eigenvalues of its left principal submatrix J_{n-1} or order $n - 1$.

It is well known that the eigenvalues of J_{n-1} strictly separate those of $J_n = J$ so that condition (S) is necessary for the existence of a solution. Hochstadt [7] proved that the problem has at most one solution. L. J. Gray and D. G. Wilson [5] showed it to have

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at least one solution, as did O. H. Hald [6]. The latter also demonstrated the continuous dependence of J on λ and μ and described an algorithm for the construction of J which, however, fails to be stable. He also announced an iterative, linearly convergent procedure for the determination of J. A different iterative procedure was developed by Barcilon [1].

By contrast, the algorithm described below in Section 4 is direct, i. e., not iterative, and is stable. Its derivation provides simple proofs of the results concerning Problem A just mentioned.

We also consider the following related problems.

Problem B. *Given two strictly increasing sequences* $\lambda := (\lambda_i)_1^n$ *and* $\lambda^* := (\lambda_i^*)_1^n$ *with* $\lambda_i < \lambda_i^*$, *all determine an* n-*th order Jacobi matrix* J *which has* $\lambda_1, \ldots, \lambda_n$ *as its eigenvalues and for which the matrix* J^*, *obtained from* J *by changing* a_n *to* a_n^*, *has* $\lambda_1^*, \ldots, \lambda_n^*$ *as its eigenvalues*.

Problem C. *Given the strictly increasing sequence* $\lambda := (\lambda_i)_1^n$, *construct an* n-*th order persymmetric Jacobi matrix* J *having* $\lambda_1, \ldots, \lambda_n$ *as its eigenvalues*.

Here, a matrix $A = (a_{ij})$ is called *persymmetric if* it is symmetric with respect to its second diagonal, i. e., if $a_{ij} = a_{n+1-j,n+1-i}$, all i and j. The Jacobi matrix (1) is persymmetric iff $a_i = a_{n+1-i}$ and $b_i = b_{n-i}$, all i.

Hochstadt [7] showed Problem C to have at most one solution. Hald [6] showed it to have at least one solution and showed the solution to depend continuously on λ.

In the analysis of these problems, the intimate connection between Jacobi matrices and orthogonal polynomials plays an essential role. We recall the salient facts of this connection in the next section.

2. Jacobi matrices and orthogonal polynomials. We continue to use the notation J_i for the left principal submatrix of order i of the Jacobi matrix (1). Let

$$p_i(t) := \det(t - J_i), \quad i = 1, \ldots, n .$$

Then p_i is a monic polynomial of degree i, all i, and one verifies easily that the sequence (p_i) satisfies the three term recurrence

$$\text{(2)} \quad \begin{aligned} & p_i(t) = (t - a_i)p_{i-1}(t) - b_{i-1}^2 p_{i-2}(t), \quad i = 1, \ldots, n, \text{ with} \\ & p_{-1}(t) := 0, \; p_0(t) := 1 . \end{aligned}$$

Conversely, if we start with a sequence (p_i) of monic polynomials with deg $p_i = i$, all i, which also satisfies the recurrence (2), then the Jacobi matrix (1) belongs to it in the sense that then $p_i(t) = \det(t - J_i)$ for $i = 1, \ldots, n$. Since the zeros of p_i are the eigenvalues of J_i, all i, we can therefore phrase Problem A equivalently as follows.

Problem A'. Given the sequences $\lambda := (\lambda_i)_1^n$ and $\mu := (\mu_i)_1^{n-1}$ with $\lambda_i < \mu_i < \lambda_{i+1}$, all i, construct sequences $a := (a_i)_1^n$ and $b := (b_i)_1^{n-1}$ so that the sequence (p_i) of polynomials given by (2) satisfies

$$p_{n-1}(t) = \prod_{j=1}^{n-1} (t - \mu_j) \text{ and } p_n(t) = \prod_{j=1}^{n} (t - \lambda_j) .$$

It is clear that this problem has at most one solution since we can always run the recurrence (2) backwards: If we already know the monic polynomials p_i and p_{i-1} (of degree i and i - 1, respectively), then a_i is uniquely determined by the requirement that

$$q(t) := p_i(t) - (t - a_i)p_{i-1}(t)$$

be a polynomial of degree i - 2. Further, the number $-b_{i-2}^2$ is then found as the leading coefficient of q, and p_{i-2} is then constructed by dividing q by its leading coefficient.

This construction of (p_i) satisfying (2) from p_{n-1} and p_n goes back to Wendroff [9] and has been used by Hald to solve Problem A or A' numerically. We, too, did try it in some examples and found it to be badly unstable. But, in trying to understand Hochstadt's procedure for the reconstruction of J from λ and μ [8], it occurred to us that it should be possible to construct a discrete inner product whose corresponding orthogonal polynomials satisfy (2), thus allowing us to generate a and b in the manner advocated by Forsythe [2].

We recall the details. Denote by $\mathbb{P}_k$ the linear space of polynomials of order k, i.e., of degree < k, with real coefficients, and let $\langle , \rangle$ be a symmetric bilinear form which is an inner product on $\mathbb{P}_n$. Then there exists exactly one sequence $(q_i)_0^n$ of monic polynomials, with q_i of degree i, all i, which is orthogonal with respect to the inner product $\langle , \rangle$, i. e., for which

$$\langle q_i, q_j \rangle = 0, \text{ for } i \neq j .$$

One may determine q_i as the error in the best approximation from $\mathbb{P}_i$ to the function $f(t) := t^i$, with respect to the norm

$$\|f\| := \langle f, f\rangle^{\frac{1}{2}}$$

in $\mathbb{P}_n$. Alternatively, one may construct $(q_i)_0^n$ by its three term recurrence, an idea popularized specifically for the case of a discrete inner product by Forsythe [2]: One computes

(3) $$q_{-1}(t) = 0,\ q_0(t) = 1,\ q_i(t) = (t - \alpha_i)q_{i-1}(t) - \beta_{i-1}^2 q_{i-2}(t), \quad i = 1, \ldots, n,$$

with the numbers α_i and β_i computed concurrently by

(4a) $$\alpha_i := \langle tq_{i-1}, q_{i-1}\rangle / \langle q_{i-1}, q_{i-1}\rangle, \quad i = \ldots, n$$

(4b) $$\beta_i := \|q\ \| / \|q_{i-1}\|, \quad i = 1, \ldots, n-1.$$

Here, it is assumed that $\langle tf(t), g(t)\rangle = \langle f(t), tg(t)\rangle$.

The computational process (3)-(4) for the vectors α and β is very stable. We will, therefore, have solved Problem A in a satisfactory manner provided we can construct a suitable inner product for which $q_i = p_i$ for $i = n - 1$ and $i = n$. This we now do.

From a computational point of view, the simplest bilinear form $\langle\, ,\, \rangle$ which is an inner product on $\mathbb{P}_n$ is of the form

$$\langle f, g \rangle := \sum_{i=1}^{n} f(\xi_i)g(\xi_i)w_i, \quad \text{all } f, g , \tag{5}$$

with $\xi_1 < \ldots < \xi_n$, and $w_i > 0$, $i = 1, \ldots, n$.

<u>Lemma 1. Let</u> $(q_i)_0^n$ <u>be the sequence of monic orthogonal polynomials for the inner product</u> (5). <u>Then</u>

$$\prod_{j=1}^{n} (t - \xi_j) = q_n(t) \tag{6}$$

<u>and</u>

$$w_i = \gamma/(q_{n-1}(\xi_i)q_n'(\xi_i)), \; i = 1, \ldots, n, \quad \underline{\text{with}} \; \gamma := \|q_{n-1}\|^2 / \sum_{j=1} q_{n-1}(\xi_j)/q_n'(\xi_j) \tag{7}$$

<u>Consequently, we can recover</u> (5) <u>from</u> q_{n-1} <u>and</u> q_n.

<u>Proof</u>. The polynomial $q(t) := \prod_{j=1}^{n} (t - \xi_j)$ is a monic polynomial of degree n which is orthogonal with respect to the inner product (5) to all functions, hence must agree with q_n. This proves (6). As to (7), we know that q_{n-1} is orthogonal to $\mathbb{P}_{n-1}$. This means that the linear functional L given by the rule

$$Lf := \langle f, q_{n-1} \rangle = \sum_{i=1}^{n} f(\xi_i)q_{n-1}(\xi_i)w_i, \text{ all } f ,$$

vanishes on $\mathbb{P}_{n-1}$. Since any $n - 1$ distinct point evaluations are linearly independent on $\mathbb{P}_{n-1}$, this implies that

$$q_{n-1}(\xi_i) \neq 0, \text{ all } i .$$

For the same reason, there is, up to multiplication by a scalar, exactly one linear functional M, of the form $Mf = \Sigma_1^n f(\xi_i)m_i$, all f, which vanishes on $\mathbb{P}_{n-1}$. Since both L and the $(n-1)$st divided difference $[\xi_1, \ldots, \xi_n]$ on the points $\xi_1, \ldots, \xi_n$ are such linear functionals, it follows that, for an appropriate scalar γ,

$$Lf = \gamma[\xi_1, \ldots, \xi_n]f = \gamma \sum_{i=1}^{n} f(\xi_i) / \prod_{\substack{j=1 \\ j \neq i}}^{n} (\xi_i - \xi_j), \quad \text{all } f .$$

But this states, with (6), that

$$q_{n-1}(\xi_i) w_i = \gamma / q_n'(\xi_i), \qquad i = 1, \ldots, n ,$$

and, in particular,

$$\|q_{n-1}\|^2 = \gamma \sum_{i=1}^{n} q_{n-1}(\xi_i) / q_n'(\xi_i) ,$$

thus proving (7). |||

One may view Lemma 1 as giving a way to construct the computationally simplest inner product with respect to which a given sequence $(p_i)_0^n$ of monic polynomials satisfying a three term recurrence (2) is orthogonal.

3. <u>A solution of Problems A, B, C</u>. Lemma 1 shows how to reconstruct the discrete inner product (5) from its last two orthogonal polynomials. It also shows the well known facts that q_n has n real zeros, all simple, and that the n - 1 zeros of q_{n-1} strictly separate those of q_n. Indeed, the positivity of the w_i's demands by (7) that $q_{n-1}(\xi_i)q_n'(\xi_i)\,\mathrm{signum}\,\gamma > 0$, all i, while, clearly, $(-)^{n-i}q_n'(\xi_i) > 0$, all i, therefore

$$q_{n-1}(\xi_i)q_{n-1}(\xi_{i+1}) < 0, \qquad i = 1, \ldots, n-1,$$

showing q_{n-1} to have a simple zero between any two zeros of q_n.

Conversely, if we compute w by

(8a) $$w_i := 1/(p_{n-1}(\xi_i)p_n'(\xi_i)), \qquad i = 1, \ldots, n$$

where

(8b) $$\xi_i := \lambda_i, \qquad i = 1, \ldots, n$$

(8c) $$p_{n-1}(t) := \prod_{j=1}^{n-1} (t - \mu_j)$$

(8d) $$p_n(t) := \prod_{j=1}^{n} (t - \lambda_j)$$

with $\lambda_i < \mu_i < \lambda_{i+1}$, all i, then $w_i > 0$, all i, hence (5) is then an inner product on $\mathbb{P}_n$, and necessarily $p_n = q_n$, by (6), and $p_{n-1} = q_{n-1}$ since $p_{n-1}(\lambda_i) = q_{n-1}(\lambda_i)$, $i = 1, \ldots, n$, by (7), and both polynomials are of degree < n.

This proves that <u>Problem A has exactly one solution for given λ and μ satisfying</u> (2). Further, since $a = \alpha$ and $b = \beta$ as determined by (3)-(4) depend continuously on ξ and w, while the latter, as determined by (8), depend continuously on λ and μ, it follows that J <u>depends continuously on λ and μ</u>.

Problem B is closely related to Problem A. In terms of the monic polynomials

$$p_i(t) = \det(t - J_i), \qquad i = 1, \ldots, n,$$

we are given the information that

$$\prod_{j=1}^{n}(t-\lambda_j) = p_n(t) = (t-a_n)p_{n-1}(t) - b_{n-1}^2 p_{n-2}(t)$$

and that

$$\prod_{j=1}^{n}(t-\lambda_j^*) = p_n^*(t) = (t-a_n^*)p_{n-1}(t) - b_{n-1}^2 p_{n-2}(t) .$$

We conclude that

$$\prod_{j=1}^{n}(t-\lambda_j^*) - \prod_{j=1}^{n}(t-\lambda_j) = (a_n - a_n^*)p_{n-1}(t) ,$$

and therefore, comparing coefficients (or else, comparing the trace of J with that of J^*),

$$\sum_{j=1}^{n}(\lambda_j - \lambda_j^*) = a_n - a_n^* .$$

This allows calculation of a_n^* once we know a_n. Further, since we only need to know the weights w for the inner product (5) up to a scalar multiple in order to reconstruct a and b via (3)-(4), it follows that we get J (and uniquely so) by choosing

$$\xi_i := \lambda_i, \quad i = 1, \ldots, n$$

(9)

$$w_i := 1/(p_n'(\lambda_i) \prod_{j=1}^{n}(\lambda_j^* - \lambda_j)) .$$

Note how the assumption $\lambda_i < \lambda_i^* < \lambda_{i+1}$, all i, insures that $w_i > 0$, all i.

The solution of Problem C leads to an intriguing fact which is also of help in the final algorithm for the solution of these problems. We came upon this fact accidentally. We had somehow gained the impression in reading Hochstadt's paper [8] that the correct weights in Lemma 1 would probably be

(10) $$w_i = q_{n-1}(\xi_i)/q_n'(\xi_i), \qquad i = 1, \ldots, n ,$$

and a quick numerical experiment confirmed this guess. Yet, when it came to proving it, we could only prove that $w_i = 1/(q_{n-1}(\xi_i)q_n'(\xi_i))$, all i. This seeming contradiction is resolved by consideration of the characteristic polynomials of the right principal submatrices of J.

Let S be the permutation matrix carrying $(1, 2, \ldots, n)$ into $(n, n-1, \ldots, 1)$, i.e.,

$$S := (\delta_{i+j,\,n+1})_{i,j=1}^{n} = S^{-1},$$

and denote by $\bar{J}$ the reflection of J across its second diagonal,

$$\bar{J} := S^{-1}JS =: \begin{bmatrix} \bar{a}_1 & \bar{b}_1 & & \\ \bar{b}_1 & \bar{a}_2 & \bar{b}_2 & \\ & \ddots & \ddots & \ddots \\ & & \bar{b}_{n-1} & \bar{a}_n \end{bmatrix}$$

with $\bar{a}_i = a_{n+1-i}$, $\bar{b}_i = b_{n-i}$, all i. Correspondingly, let

$$\bar{p}_{-1}(t) := 0,\ \bar{p}_0(t) := 1,\ \bar{p}_i(t) := \det(t - \bar{J}_i), \qquad i = 1, \ldots, n.$$

<u>Lemma 2</u>. <u>For</u> $i = 1, \ldots, n$, $p_{n-1}(\lambda_i)\bar{p}_{n-1}(\lambda_i) = (b_1 \cdot \ldots \cdot b_{n-1})^2$.

<u>Proof</u>. For each i, $p_{n-1}(\lambda_i)\bar{p}_{n-1}(\lambda_i)$ is the product of the $(n-1)$st order left principal minor with the $(n-1)$st order right principal minor of the singular matrix

$$A := \lambda_i - J,$$

i.e., $p_{n-1}(\lambda_i) = \det A\begin{pmatrix}1, \ldots, n-1\\ 1, \ldots, n-1\end{pmatrix}$ and $\bar{p}_{n-1}(\lambda_i) = \det A\begin{pmatrix}2, \ldots, n\\ 2, \ldots, n\end{pmatrix}$, and $\det A = 0$. Apply Sylvester's identity (see, e.g., [3, p. 15]), using $A\begin{pmatrix}2, \ldots, n-1\\ 2, \ldots, n-1\end{pmatrix}$ as pivotal block, to get that

$$0 = \det A\begin{pmatrix}2, \ldots, n-1\\ 2, \ldots, n-1\end{pmatrix}\det A = \det \begin{bmatrix} \det A\begin{pmatrix}1, \ldots, n-1\\ 1, \ldots, n-1\end{pmatrix} & \det A\begin{pmatrix}1, \ldots, n-1\\ 2, \ldots, n\end{pmatrix} \\ \det A\begin{pmatrix}2, \ldots, n\\ 1, \ldots, n-1\end{pmatrix} & \det A\begin{pmatrix}2, \ldots, n\\ 2, \ldots, n\end{pmatrix} \end{bmatrix}$$

$$= p_{n-1}(\lambda_i)\bar{p}_{n-1}(\lambda_i) - ((-)^{n-1}b_1 \cdot \ldots \cdot b_{n-1})^2 \qquad |||$$

Here, we have used the abbreviation

$$A\begin{pmatrix} i_1, \dots, i_r \\ j_1, \dots, j_s \end{pmatrix} := (a_{i_\rho j_\sigma})_{\rho=1, \sigma=1}^{r \quad s} .$$

If now J is persymmetric, then $J = \bar{J}$ and so $p_i = \bar{p}_i$, all i. The lemma then implies that $(p_{n-1}(\lambda_i))^2 = (b_1 \cdot \dots \cdot b_{n-1})^2$, all i. Since we only need to know the weight vector w up to a scalar multiple, it follows that we only need to know p_n in order to reconstruct a persymmetric J, thus solving Problem C.

We conclude further that the computations (3)-(4) always generate the diagonals α and β of a persymmetric Jacobi matrix if we use the discrete inner product

$$\langle f, g \rangle := \sum_{i=1}^{n} f(\xi_i) g(\xi_i) / \prod_{\substack{j=1 \\ j \neq i}}^{n} |\xi_i - \xi_j| .$$

We were interested in Lemma 2 because of its importance for the algorithm in the next section and have therefore not followed the more customary treatment of Problem C. This treatment goes back to Gantmacher and Krein and consists in using the persymmetry of J to construct an equivalent problem of the form B and of half the size, thus reducing it to a problem with a known solution.

4. *An algorithm*. Lemma 2 shows that we could also determine the correct weights w for the generation of a and b via (4) by

$$w_i = \bar{p}_{n-1}(\lambda_i)/p'_n(\lambda_i), \qquad i = 1, \ldots, n .$$

To say it differently, *if the inner product* (5) *is given by*

$$\begin{aligned} \xi_i &:= \lambda_i, \qquad i = 1,\ldots,n , \\ w_i &:= p_{n-1}(\lambda_i)/p'_n(\lambda_i), \qquad i = 1, \ldots, n , \end{aligned} \tag{11}$$

then the quantities generated by (3)-(4) *are* $q_i = \bar{p}_i$, $\alpha_i = \bar{a}_i$, $\beta_i = \bar{b}_i$, *all* i. This says that use of the weights (11) rather than the weights (8b) in the computations (3)-(4) also generates the nonzero entries of J, but *in reverse order*. This explains the success in our numerical experiments using the weights (10) alluded to earlier: all examples happened to have been persymmetric.

Use of the weights (11) in preference to (8b) has some computational advantages. Because of the interlacing conditions (S), we get the bounds

$$\frac{\lambda_i - \mu_{i-1}}{\lambda_i - \lambda_1} \frac{\mu_i - \lambda_i}{\lambda_n - \lambda_i} < p_{n-1}(\lambda_i)/p'_n(\lambda_i) < 1 , \tag{12}$$

where the first (last) factor in the lower bound is to be omitted in case $i = 1$ ($i = n$). This shows that overflow or underflow is highly unlikely to occur in the calculation of the weights (11). By contrast, the computation of the numbers $1/(p_{n-1}(\lambda_i)p'_n(\lambda_i))$ has to be carefully monitored, in general, for the occurrence of overflow or underflow, else, one has to compute the logarithms of these numbers, a somewhat more expensive procedure.

We offer the following algorithm for the solution of Problem A, and recall that Problems B and C can also be solved by it, if the definition of $p_{n\ 1}(\lambda_i) := \prod_1^{n-1} (\lambda_i - \mu_j)$ used here is modified appropriately.

Algorithm. Given the n eigenvalues $\lambda_1 < \ldots < \lambda_n$ of the Jacobi matrix (1) and the $n - 1$ eigenvalues $\mu_1 < \ldots < \mu_{n-1}$ of its left principal minor of order $n - 1$. Note that, necessarily, $\lambda_i < \mu_i < \lambda_{i+1}$, all i.

1. Compute the weights w from λ and μ:

   1.1 temp(i - 1) := λ_i, i = 2, . . . , n

   1.2 for i = 1, . . ., n, do:

   1.21 $w_i := \prod_{j=1}^{n-1} (\lambda_i - \mu_j)/(\lambda_i - \text{temp}(j))$

   1.22 temp(i) := λ_i

2. Generate the values at λ of the first two orthogonal polynomials:

   2.1 $s := \sum_{j=1}^{n} w_j = \langle \bar{p}_0, \bar{p}_0 \rangle$

   2.2 $\bar{a}_1 := (\sum_{j=1}^{n} w_j\lambda_j)/s = \langle \bar{p}_0, \bar{p}_1 \rangle / s$

   2.3 for i = 1, . . ., n, do:

   2.31 pkml(i) := 1 = $\bar{p}_0(\lambda_i)$

   2.32 pk(i) := $\lambda_i - \bar{a}_1 = \bar{p}_1(\lambda_i)$

3. Compute $\|\bar{p}_k\|^2$ and $\bar{a}_k$, $\bar{b}^2_{k-1}$, then use them to generate the values at λ of $\bar{p}_{k+1}$ from those of $\bar{p}_k$ and $\bar{p}_{k-1}$ by the three term recurrence:

   3.1 for k = 2 , . . ., n, do:

   3.11 S' := S = $\|\bar{p}_{k-1}\|^2$

   3.12 s := t := 0

   3.13 for i = 1, . . ., n, do:

   3.131 p := w_i*pk(i)**2

   3.132 s := s + p

   3.133 t := t + λ_i*p

3.14 $\bar{b}^2_{k-1} := s/s'$

3.15 $\bar{a}_k := t/s$

3.16 for $i = 1, \ldots, n$, do:

3.161 $p := pk(i)$

3.162 $pk(i) := (\lambda_i - \bar{a}_k)*p - \bar{b}^2_{k-1}*pkml(i)$

3.163 $pkml(i) := p$

4. Compute $\bar{b}_k$ from $\bar{b}^2_k$. Also, if a and b, rather than the vectors $\bar{a}$ and $\bar{b}$ are wanted, this is the place to reorder them.

4.1 $\bar{b}_k := \mathrm{sqrt}(\bar{b}^2_k)$, $k = 1, \ldots, n - 1$

Output consists of the vectors $\bar{a}$ and $\bar{b}$, with $\bar{a}_i = a_{n+1-i}$, $\bar{b}_i = b_{n-i}$, all i, and a and b the diagonals of (1).

We have carried out various numerical experiments with this algorithm and describe here only three.

For the n-th order Jacobi matrix J_n with general row 1, -2, 1, the eigenvalues are given explicitly (and in order) by the formula

$$\lambda_j = 2(\cos \frac{j\pi}{n+1} - 1), \quad j = 1, \ldots, n .$$

Starting with these values and the corresponding sequence $(\mu_j)_1^{n-1}$ for J_{n-1}, the algorithm produced approximations to the diagonal and the offdiagonal entries of J_n whose maximum and average error are recorded for n = 25, 50, 100, and 200 in the first columns of the following table. All calculations were carried out on a UNIVAC 1110 in single precision (27 binary bit floating point mantissa).

n	diagonal		offdiagonal		diagonal		offdiagonal	
	max.	ave.	max.	ave.	max.	ave.	max.	ave.
25	4.-7	2.-7	2.-7	6.-8	2.-6	5.-7	1.-6	4.-7
50	9.-7	1.-7	4.-7	2.-7	6.-4	1.-5	5.-5	2.-6
100	2.-6	7.-7	8.-7	2.-7	7.-1	3.-2	3.-1	1.-2
200	3.-6	9.-7	1.-6	3.-7	8.-1	2.-2	5.-1	1.-2

Table 1. Maximum and average error in the diagonal and offdiagonal entries of two specific Jacobi matrices as reconstructed with the algorithm of this section from (approximate) spectral data.

For variety, we also consider the n-th order Jacobi matrix J_n with general row

$$1 - i/n,\ i/n - 2,\ 1 - (i+1)/n, \qquad i = 1, \ldots, n\,.$$

We know of no simple formula for its eigenvalues, therefore used the algorithm tqℓ 1 on pp. 232-233 of Wilkinson and Reinsch' handbook [10] to compute them and those of J_{n-1}. The tolerance (relative error requirement) for tqℓ 1 we chose as 1. -7. With this spectral information, we entered the above algorithm and so reconstructed J_n approximately. Errors of this reconstruction are also given in Table 1, in the last four columns. There is a significant deterioration as n increases.

As can be expected from formula (11) for the weights (w_i), the condition of the problem of determining J_n from (λ_i) and (μ_i) deteriorates as some or more μ_i approach the corresponding λ_i since then one or more of the weights approach zero. This is shown even more strikingly when the matrix of the last example is reflected across its second diagonal, i.e., when the Jacobi matrix with the following general row

$$1 - (n+1-i)/n,\ (n+1-i)/n - 2,\ 1 - (n-i)/n, \qquad i = 1, \ldots, n\,,$$

is considered. Now the reconstruction breaks down in single precision already for n = 30 since $\mu_1 - \lambda_1$ becomes too small. Even for n = 20, we have $\mu_1 - \lambda_1 \sim$ 2. -7. In fact, in computations using tqℓ 1 to obtain the spectral information, some weights become negative for n = 30, while, for n = 10 and 20, we obtain approximations with errors of the order of 1. -4 and 2. -2, respectively.

5. <u>The connection with Gauss quadrature</u>. For the given Jacobi matrix J in (1), let $(P_i)_0^n$ be the polynomial sequence generated by the recursion

$$\text{(13)}\qquad \begin{aligned} &b_{j+1}P_{j+1}(t) = (t - a_{j+1})P_j(t) - b_j P_{j-1}(t), \qquad j = 0, \ldots, n-1 \\ &P_{-1}(t) := 0, \quad P_0(t) := 1 , \end{aligned}$$

with b_0 arbitrary, $b_n \neq 0$. The sequence (P_i) is related to the sequence (p_i) with $p_i(t) := \det(t - J_i)$, all i, of monic polynomials by

$$\text{(14)}\qquad p_i = (b_1 \cdot \ldots \cdot b_i)P_i ,$$

as one verifies easily, e.g., by comparing (13) and (2).

Let now ω be a monotone function on some interval $[A, B]$ so that $(P_i)_0^n$ is <u>orthonormal</u> with respect to the inner product

$$\langle f, g\rangle_\omega := \int_A^B f(t)g(t)\omega(dt) .$$

(Lemma 1 provides a simple proof of the existence of such ω.) Then the zeros $\lambda_1 < \ldots < \lambda_n$ of P_n must lie in $[A, B]$, and there exist positive weights $w_1, \ldots, w_n$ so that, for every $f \in C^{2n}[A, B]$,

$$\text{(15)}\qquad \int_A^B f(t)\omega(dt) = \sum_{j=1}^n w_j f(\lambda_j) + b_1 \cdot \ldots \cdot b_n f^{(2n)}(\xi)/(2n)! \quad \text{for some } \xi \in\,]A, B[.$$

If we take this fact for granted, then it follows that

$$\delta_{i-j} \quad \langle P_i, P_j\rangle_\omega = \sum_{r=1}^n w_r P_i(\lambda_r)P_j(\lambda_r) \quad \text{for } i + j < 2n ,$$

showing that

$$\text{(5')}\qquad \langle f, g\rangle := \sum_{j=1}^n f(\lambda_i)g(\lambda_i)w_i$$

is an inner product on $\mathbb{P}_n$ with respect to which $(P_i)_0^{n-1}$ is orthonormal, hence for which $(p_i)_0^n$ is an orthogonal sequence.

This shows that the construction of the weights (w_i) for (5), which was crucial for our numerical solution of the various inverse eigenvalue problems, can be started from any convenient formula for the weights in a Gaussian quadrature formula.

For instance, one could start with the following consequence of the Christoffel-Darboux formula,

(16) $$w_j \underset{\sim}{P}^T(\lambda_j) \underset{\sim}{P}(\lambda_j) = 1 \text{ for } j = 1, \ldots, n \ .$$

Here, $P(\lambda)$ denotes the n-vector $(P_0(\lambda), \ldots, P_{n-1}(\lambda))$. By (13), $\underset{\sim}{P}(\lambda_j)$ is an eigenvector for J belonging to the eigenvalue λ_j. Therefore, with $\underset{\sim}{u}_j := (u_{1j}, \ldots, u_{nj})$ a unit eigenvector of J for λ_j, (16) implies that

(17) $$w_j = u_{ij}^2 / P_{i-1}^2(\lambda_j), \qquad i = 1, \ldots, n \ .$$

Since $P_0(\lambda) = 1$, we obtain in this way the formula

(18) $$w_j = u_{1j}^2, \qquad j = 1, \ldots, n \ ,$$

used by Golub and Welsch [4] to compute the weights. Problems A, B, and C can now be solved by deriving from the given data information about the eigenvectors of J.

A more direct approach might be to start with the well known formula

19) $$w_j = -\frac{k_{n+1}}{k_n} \frac{1}{P_{n+1}(\lambda_j) P'_n(\lambda_j)}, \qquad j = 1, \ldots, n \ ,$$

with k_j the leading coefficient of P_j, i.e., $k_j = 1/(b_1 \cdot \ldots \cdot b_j)$. This formula involves the "next" orthogonal polynomial P_{n+1}. But, since $P_n(\lambda_j) = 0$ for all j, we have

$$P_{n+1}(\lambda_j)/k_{n+1} = p_{n+1}(\lambda_j) = -b_n^2 p_{n-1}(\lambda_j) = -b_n^2 P_{n-1}(\lambda_j)/k_{n-1}$$

by the three-term recurrence, therefore we also have

(19') $$w_j = 1/(b_n P_{n-1}(\lambda_j) P'_n(\lambda_j)), \qquad j = 1, \ldots, n$$

which shows how equation (7) could have been derived from standard results in Gauss quadrature.

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