Inverse Eigenvalue Problems for Jacobi Matrices

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Submitted by Gene H. Golub

ABSTRACT

It is proved that a real symmetric tridiagonal matrix with positive codiagonal elements is uniquely determined by its eigenvalues and the eigenvalues of the largest leading principal submatrix, and can be constructed from these data. The matrix depends continuously on the data, but because of rounding errors the investigated algorithm might in practice break down for large matrices.

1. INTRODUCTION

In this paper we will prove that a real symmetric tridiagonal matrix of order n with positive off-diagonal elements is uniquely determined by its eigenvalues and the eigenvalues of the leading principal submatrix of order $n-1$ (see Sec. 2). An alternative proof for this result has recently been published by H. Hochstadt, who uses a constructive method; see [6]. In Sec. 3 we present a computational method and show that the algorithm will work provided the two sets of eigenvalues interlace.

In Sec. 4 we establish the well-posedness of the inverse eigenvalue problem. In Sec. 5 we discuss several physical interpretations of the uniqueness result. In particular, we show that a swinging necklace is uniquely determined by its eigenfrequencies and the eigenfrequencies of the same necklace, but with the first bead fixed. Finally, in Sec. 6 we consider the algorithm from a computational point of view and present a numerical example.

2. UNIQUENESS THEOREM FOR JACOBI MATRICES

Let J be a Jacobi matrix of order n with diagonal elements $a_1,\dots,a_n$ and codiagonal elements $b_1,\dots,b_{n-1}$, where we assume that all b_i are strictly positive. The truncated matrix K is obtained by deleting the last row and column of J.

THEOREM 1 (Hochstadt). *The Jacobi matrix J is uniquely determined by the eigenvalues $\{\lambda_j\}$ and $\{\mu_j\}$ of J and K respectively.*

REMARK. Hochstadt has proved that if the codiagonal elements of J are fixed, then the diagonal elements are uniquely determined by the given data; see [5]. The full result is presented in [6]. In this paper, Hochstadt abandons the previous technique in favor of a constructive approach which, however, presupposes the existence of a solution. The validity of this assumption is investigated in Sec. 3. The proof below is based on our extension of Hochstadt's earlier technique.

Proof. Let $u_i = u_i(\lambda)$ be the solution of the difference equation

$$b_{i-1}u_{i-1} + (a_i - \lambda)u_i + b_i u_{i+1} = 0 \tag{2.1}$$

for $i = 1, 2,\dots,n-1$, where $b_0 = b_n = 0$ and u_i satisfies the initial condition $u_1 = 1$. Now λ_j is an eigenvalue of J iff the solution u_i of the difference equation (2.1) with $\lambda = \lambda_j$ satisfies the boundary condition

$$b_{n-1}u_{n-1} + (a_n - \lambda_j)u_n = 0.$$

Similarly we find that μ_j is an eigenvalue of the truncated matrix K iff the solution u_i of the difference equation (2.1) with $\lambda = \mu_j$ satisfies

$$b_{n-2}u_{n-2} + (a_{n-1} - \mu_j)u_{n-1} = 0.$$

Since b_{n-1} is different from zero, we see that $u_n(\mu_j)$ vanishes.

Suppose that there exist a Jacobi matrix $\tilde{J}$ with diagonal elements $\tilde{a}_i$ and positive codiagonal elements $\tilde{b}_i$ such that the eigenvalues of $\tilde{J}$ and $\tilde{K}$ coincide with those of J and K. We will show that $J = \tilde{J}$. Let $u(\lambda_j)$ and $v(\lambda_j)$ be the eigenvectors corresponding to the eigenvalue λ_j of J and $\tilde{J}$ respectively. Thus $Ju(\lambda_j) = \lambda_j u(\lambda_j)$ and $\tilde{J}v(\lambda_j) = \lambda_j v(\lambda_j)$. If we multiply both sides of the first

equation by $v(\lambda_j)^T$ and the second equation by $u(\lambda_j)^T$, we see that

$$v(\lambda_j)^T(J-\tilde{J})u(\lambda_j)=0 \tag{2.2}$$

for $j=1, 2,\ldots,n$. Similarly we let $u(\mu_j)$ and $v(\mu_j)$ be the eigenvectors of K and $\tilde{K}$, respectively, and find by using the preceding arguments that

$$v(\mu_j)^T(K-\tilde{K})u(\mu_j)=0 \tag{2.3}$$

for $j=1, 2,\ldots,n-1$.

For any vectors $u=(u_1,\ldots,u_n)^T$ and $v=(v_1,\ldots,v_n)^T$ we have the following identity:

$$v^TJu=\sum_{i=1}^{n} a_iu_iv_i+\sum_{i=1}^{n-1} b_i(u_iv_{i+1}+u_{i+1}v_i). \tag{2.4}$$

We introduce now the function

$$F(\lambda)=\sum_{i=1}^{n}(a_i-\tilde{a}_i)u_i(\lambda)v_i(\lambda)$$

$$+\sum_{i=1}^{n-1}(b_i-\tilde{b}_i)\left[u_i(\lambda)v_{i+1}(\lambda)+u_{i+1}(\lambda)v_i(\lambda)\right],$$

where $u_i(\lambda)$ is the solution of the difference equation (2.1) and $v_i(\lambda)$ is defined correspondingly for the Jacobi matrix $\tilde{J}$. From (2.2) and (2.4) it follows that $F(\lambda_j)$ is zero for all eigenvalues λ_j of J and $\tilde{J}$. Since $u_n(\mu_j)=v_n(\mu_j)=0$ for all eigenvalues μ_j of the truncated matrices, we see that for $\lambda=\mu_j$ the last term in each of the sums of $F(\lambda)$ vanishes. What remains is the left-hand side of (2.3). Thus $F(\mu_j)$ is zero for all eigenvalues μ_j of K and $\tilde{K}$. Since the eigenvalues of J and K interlace, the function F is zero at at least $2n-1$ distinct points.

We proceed to show that $F(\lambda)$ vanishes identically. From (2.1) it follows that $u_i(\lambda)$ is a polynomial in λ of degree $i-1$ with leading term

$$u_i(\lambda)=(b_{i-1}\cdot\cdots\cdot b_1)^{-1}\lambda^{i-1}+\cdots,$$

and we obtain similarly that

$$v_i(\lambda)=(\tilde{b}_{i-1}\cdot\cdots\cdot\tilde{b}_1)^{-1}\lambda^{i-1}+\cdots.$$

The first sum in the definition of F is therefore a linear combination of n polynomials of degree exactly $0, 2, \ldots, 2n-2$. Since all b_i and $\tilde{b}_i$ are strictly positive, there can be no cancellation in the leading coefficient of $u_i(\lambda)$ $v_{i+1}(\lambda) + u_{i+1}(\lambda)v_i(\lambda)$, which is therefore a polynomial of degree exactly $2i-1$. Thus the second sum is a linear combination of $n-1$ polynomials of degree exactly $1, 3, \ldots, 2n-3$.

We have now shown that F is a polynomial of degree at most $2n-2$. However, $F(\lambda)$ has at least $2n-1$ roots and must therefore vanish identically. Because the polynomials $u_i v_i$ and $u_i v_{i+1} + u_{i+1} v_i$ are linearly independent, we conclude finally that all coefficients $a_i - \tilde{a}_i$ and $b_i - \tilde{b}_i$ are zero. This completes the proof. ■

From the recursion formula for the principal minors of a symmetric tridiagonal matrix it follows that the eigenvalues depend on a_i and b_i^2; see [11, p. 300]. This shows that Theorem 1 is false if the signs of the off-diagonal elements are undetermined. Indeed, if there is one Jacobi matrix which satisfies the requirements, then the inverse problem has 2^{n-1} different solutions. In practice this is not a serious difficulty, because the sign of the off-diagonal elements is normally given by the physical model (see, e.g., Sec. 5 below).

3. A COMPUTATIONAL METHOD

In this section, we will show that given two sets of real numbers $\{\lambda_j\}$ and $\{\mu_j\}$ which satisfy

$$\lambda_1 < \mu_1 < \lambda_2 < \mu_2 < \cdots < \lambda_{n-1} < \mu_{n-1} < \lambda_n, \tag{3.1}$$

we can construct a Jacobi matrix J such that λ_j and μ_j are the eigenvalues of J and K, respectively, where K is the leading principal submatrix of order $n-1$ of J.

Assume that the inverse problem has a solution J with non-zero off-diagonal elements. By denoting the leading principal minor of order i of $J-\lambda$ by $p_i(\lambda)$, we have the recursion formula

$$p_0(\lambda) = 1,$$

$$p_1(\lambda) = a_1 - \lambda,$$

$$p_i(\lambda) = (a_i - \lambda)\, p_{i-1}(\lambda) - b_{i-1}^2\, p_{i-2}(\lambda)$$

for $i=2, 3,\ldots,n$; see [11, p. 300]. Since the zeros λ_j and μ_j of $p_n(\lambda)$ and $p_{n-1}(\lambda)$ are the eigenvalues of J and K, respectively, we see that $\{\lambda_j\}$ and $\{\mu_j\}$ satisfy (3.1) and

$$p_n(\lambda)=\prod_j(\lambda_j-\lambda), \qquad p_{n-1}(\lambda)=\prod_j(\mu_j-\lambda).$$

These two polynomials are completely determined by the given data. The existence of a solution to the inverse problem is a consequence of the following result.

LEMMA 1. *Assume that the zeros of $p_n(\lambda)$ and $p_{n-1}(\lambda)$ satisfy* (3.1). *There exist two real constants a and c such that*

$$p_n(\lambda)=(a-\lambda)\,p_{n-1}(\lambda)-cp_{n-2}(\lambda), \tag{3.2}$$

where p_{n-2} is a polynomial of degree $n-2$ with leading coefficient $(-1)^{n-2}$. Moreover, c is strictly positive, and the zeros of p_{n-1} and p_{n-2} interlace.

Proof. By introducing $-x$ in place of λ we can write

$$p_n=x^n+\alpha_{n-1}x^{n-1}+\cdots+\alpha_0,$$

$$p_{n-1}=x^{n-1}+\beta_{n-2}x^{n-2}+\cdots+\beta_0,$$

$$p_{n-2}=x^{n-2}+\gamma_{n-3}x^{n-3}+\cdots+\gamma_0.$$

We determine a and c by identifying the coefficients of equal powers in x in Eq. (3.2) and obtain formally

$$a=\alpha_{n-1}-\beta_{n-2}, \tag{3.3}$$

$$c=a\beta_{n-2}+\beta_{n-3}-\alpha_{n-2}, \tag{3.4}$$

$$\gamma_j=\frac{a\beta_j+\beta_{j-1}-\alpha_j}{c} \qquad \text{for} \quad j=n-3,\ldots,1, \tag{3.5}$$

$$\gamma_0=\frac{a\beta_0-\alpha_0}{c}. \tag{3.6}$$

The calculation of the coefficients of the polynomial p_{n-2} is meaningful

provided c is different from zero. From the definition of p_n and p_{n-1} it follows that

$$\alpha_{n-1} = \sum_{j=1}^{n} \lambda_j, \qquad \alpha_{n-2} = \sum_{j=1}^{n-1} \lambda_{j+1} \sum_{k=1}^{j} \lambda_k,$$

$$\beta_{n-2} = \sum_{j=1}^{n-1} \mu_j, \qquad \beta_{n-3} = \sum_{j=1}^{n-1} \mu_j \sum_{k=j+1}^{n-1} \mu_k.$$

By using (3.3) and (3.4), straightforward calculation shows that

$$a = \sum_{j=1}^{n} \lambda_j - \sum_{j=1}^{n-1} \mu_j,$$

$$c = \sum_{j=1}^{n-1} (\lambda_{j+1} - \mu_j) \sum_{k=1}^{j} (\mu_k - \lambda_k).$$

Since the data satisfy the interlacing condition (3.1), it is obvious from the last expression that c is strictly positive. The decomposition (3.2) is therefore uniquely determined, and p_{n-2} is a real polynomial of degree $n-2$.

We will now prove that the zeros of p_{n-1} and p_{n-2} interlace. Since p_{n-1} vanishes at all points μ_k, we obtain from (3.2) that

$$\prod_{j=1}^{n} (\lambda_j - \mu_k) = 0 - c p_{n-2}(\mu_k),$$

for $k = 1, 2, \ldots, n-1$. From this equation and the interlacing condition (3.1) it follows that the sign of $p_{n-2}(\mu_k)$ is $(-1)^{k+1}$. Consequently, the polynomial $p_{n-2}(\lambda)$ will have a zero ν_k in each of the intervals (μ_k, μ_{k+1}). This characterizes all the roots of $p_{n-2}(\lambda) = 0$, and we conclude finally that

$$\mu_1 < \nu_1 < \mu_2 < \cdots < \mu_{n-2} < \nu_{n-2} < \mu_{n-1}.$$

■

THEOREM 2. *Let $\{\lambda_j\}$ and $\{\mu_j\}$ be given and satisfy* (3.1). *There exists a Jacobi matrix J of order n such that λ_j are the eigenvalues of J and μ_j are the eigenvalues of the leading principal submatrix of order $n-1$.*

Proof. The solution of the inverse eigenvalue problem is obtained in the

following way. We construct the polynomials p_n and p_{n-1} from the data $\{\lambda_j\}$ and $\{\mu_j\}$ and determine the constants a and c and the polynomial p_{n-2} by the formulas (3.3)–(3.6). Set $a_n = a$ and $b_{n-1} = +\sqrt{c}$ or $-\sqrt{c}$. We can now repeat the process by using p_{n-1} and p_{n-2} to determine a_{n-1} and b_{n-2} and so on. The last coefficient a_1 is determined from $p_1 = a_1 - \lambda$. This algorithm cannot break down, at least in theory, because at the end of each step the roots of the two polynomials interlace, and we can therefore take one step more, according to Lemma 1. ■

We mention that Hochstadt assumes the existence of a solution to the inverse eigenvalue problem, and then suggests a computational method; see [6]. A consequence of our theorem is that if the data satisfy the interlacing condition (3.1), then Hochstadt's algorithm will succeed.

From the algorithm (3.3)–(3.6) follows that the Jacobi matrix J depends continuously on the data $\{\lambda_j\}$ and $\{\mu_j\}$ as long as condition (3.1) is satisfied (see also Hochstadt [6]). The well-posedness of the inverse problem is studied in more detail in Sec. 4.

We have shown that from two interlacing spectra we can construct the Jacobi matrix. This result can be used to prove that one spectrum is sufficient to determine a Jacobi matrix uniquely if, in addition, we require that the tridiagonal matrix is symmetric around the secondary diagonal. Such a matrix is called a persymmetric Jacobi matrix.

THEOREM 3. *Let* $\{\lambda_j\}$ *be given and satisfy*

$$\lambda_1 < \lambda_2 < \cdots < \lambda_N. \tag{3.7}$$

There exists a Jacobi matrix J *of order* N *which satisfies the symmetry conditions*

$$a_i = a_{N+1-i} \quad \text{and} \quad b_i = b_{N-i} \tag{3.8}$$

such that λ_j *are the eigenvalues of* J. *If all off-diagonal elements are positive, then* J *is uniquely determined by the given data.*

REMARK. We shall not prove this theorem, but mention that the uniqueness result can be shown in several ways; see, e.g., Hochstadt [6] and Hald [4, p. 76]. The solution can be computed either by minor modifications of the algorithms due to Anderson [1], Gantmacher and Krein [2, p. 322] or Hald [4, p. 126], or by using Hochstadt's method (see [6]). Finally, we remark that the existence statement in Theorem 3 implies that Hochstadt's algorithm will succeed.

4. WELL-POSEDNESS OF THE INVERSE EIGENVALUE PROBLEM

In this section we will study how the solution of the inverse eigenvalue problem depends on a perturbation of the data. The main result is Theorem 4. To prove this theorem we will first show that all elements in the Jacobi matrix can be bounded in terms of the data.

LEMMA 2. *Let J be a real symmetric tridiagonal matrix of order n with diagonal elements a_i and positive codiagonal elements b_i. Then*

$$\lambda_1 < a_i < \lambda_n, \qquad i = 1,2,\ldots,n, \tag{4.1}$$

$$\delta\sqrt{\frac{\varepsilon}{2\delta+\varepsilon}} \leqslant b_i < \lambda_n - \lambda_1, \qquad i = 1,2,\ldots,n-1. \tag{4.2}$$

Here λ_j and μ_j are the eigenvalues of J and the leading principal submatrix of order $n-1$ of J, and

$$\varepsilon = \min_{j,k} |\lambda_j - \mu_k|,$$

$$\delta = \tfrac{1}{2} \min_{j \neq k} (|\lambda_j - \lambda_k|, |\mu_j - \mu_k|).$$

REMARK. By using the Bauer-Fikes theorem (see [11, p. 87]), it is easy to show that all codiagonal elements are larger than $\varepsilon/2$. However, because $\varepsilon \leqslant \delta$, the lower bound in (4.2) is always larger than $\varepsilon/\sqrt{3}$. The improvement is best when $\varepsilon \ll \delta$.

Proof. Let e_i be the ith column of the identity matrix. Since $a_i = e_i^T J e_i$, we obtain the inequality (4.1) from the extremal property of the Rayleigh quotient; see Wilkinson [11, p. 99]. We cannot have equality in (4.1), because in that case e_i would be an eigenvector of J. This is impossible, since an eigenvector of a symmetric tridiagonal matrix with non-zero off-diagonal elements cannot vanish in its first or last component; see Wilkinson [11, p. 316].

To obtain the upper bound for b_i we set $v = e_i + e_{i+1}$ and consider the Rayleigh quotient

$$\frac{a_i + a_{i+1} + 2b_i}{2} = \frac{v^T J v}{v^T v}.$$

The right side is less than λ_n. By using (4.1) we see that the left side is strictly greater than $\lambda_1 + b_i$, and this establishes the bound.

It is more complicated to prove the lower bound. Assume that one of the codiagonal elements, say b_p, violates the lower bound, i.e.,

$$b_p^2 < \frac{\varepsilon\delta^2}{2\delta+\varepsilon}.$$

Let $\tilde{J}$ be equal to the matrix J except for the pth codiagonal elements, which we set equal to zero. In addition we let K and $\tilde{K}$ be the leading principal submatrices of order $n-1$ of J and $\tilde{J}$ respectively. Since one of the off-diagonal elements in $\tilde{J}$ vanishes, we conclude that $\tilde{J}$ and $\tilde{K}$ have at least one common eigenvalue, say $\hat{\lambda}$. It can now be shown (see Wilkinson [11, p. 312]) that there exist an eigenvalue λ_r of J and an eigenvalue μ_s of K such that

$$|\hat{\lambda}-\lambda_r| \leqslant \frac{b_p^2/d_1}{1-b_p^2/d_1^2},$$

$$|\hat{\lambda}-\mu_s| \leqslant \frac{b_p^2/d_2}{1-b_p^2/d_2^2}.$$

Here all eigenvalues of J except λ_r lie at a distance greater than d_1 from $\hat{\lambda}$. Similarly d_2 is the smallest distance between $\hat{\lambda}$ and the eigenvalues of K different from μ_s. Since no eigenvalue of J is closer to $\hat{\lambda}$ than λ_r, we find that $d_1 \geqslant \min_{j\neq k}|\lambda_j-\lambda_k|/2$. In the same manner we obtain $d_2 \geqslant \min_{j\neq k}|\mu_j-\mu_k|/2$. Consequently, both d_1 and d_2 are greater than or equal to δ. We can therefore estimate the distance between λ_r and μ_s by

$$|\lambda_r-\mu_s| \leqslant 2\frac{b_p^2/\delta}{1-b_p^2/\delta^2}.$$

By inserting the bound for b_p^2 in the right-hand side of this inequality, we obtain by straightforward calculation that $|\lambda_r-\mu_s|<\epsilon$. This is a contradiction. Our assumption must therefore be false, and all off-diagonal elements will satisfy the bound (4.2). This completes the proof. ■

We will now discuss some consequences of Lemma 2. Let the vector $x=(a_1,\ldots,a_n,b_1,\ldots,b_{n-1})^T$ consist of the diagonal and codiagonal elements in the Jacobi matrix J, and let $y=(\lambda_1,\ldots,\lambda_n,\mu_1,\ldots,\mu_{n-1})^T$ consist of the

eigenvalues of J and the leading principal submatrix K of order $n-1$. Thus x and y have $2n-1$ components. Since λ_j and μ_k depend on a_r and b_s, we see that y is a function of x, say $y=F(x)$, where F is a non-linear vector-valued function. The eigenvalues are differentiable functions of a_r and b_s provided all b_s are different from zero. We will now investigate the Fréchet derivative F' of this mapping:

$$F'=\left[\begin{array}{c|c} \dfrac{\partial\lambda_j}{\partial a_r} & \dfrac{\partial\lambda_j}{\partial b_s} \\ \hline \dfrac{\partial\mu_k}{\partial a_r} & \dfrac{\partial\mu_k}{\partial b_s} \end{array}\right]. \tag{4.3}$$

LEMMA 3. *Consider all Jacobi matrices J of order n which satisfy*

$$0 \leqslant a_i \leqslant 1 \qquad \text{for} \quad i=1,2,\ldots,n, \tag{4.4}$$

$$\eta \leqslant b_i \leqslant 1 \qquad \text{for} \quad i=1,2,\ldots,n-1, \tag{4.5}$$

where η is a fixed positive constant. There exists a positive constant σ such that $\sigma \leqslant \sigma_{2n-1}(F')$ for all F'. Here F' is the Fréchet derivative (4.3) *corresponding to the Jacobi matrix J, and σ_{2n-1} is the smallest singular value of F'.*

Proof. Let the elements a_r and b_s of the Jacobi matrix J satisfy the inequalities (4.4) and (4.5). Since all eigenvalues of J and K are distinct, we conclude that λ_j and μ_k are holomorphic functions of a_r and b_s (see Kato [7, p. 124]). Let u_j and v_k be the eigenvectors of J and K, respectively, corresponding to λ_j and μ_k, and normalized so that their first component is equal to one. Then $(J-\lambda_j)u_j=0$, and by differentiating with respect to a_r and b_s we get (see Gantmacher and Krein [2, p. 126])

$$\frac{\partial\lambda_j}{\partial a_r}=\frac{(u_{rj})^2}{u_j^T u_j} \quad \text{and} \quad \frac{\partial\lambda_j}{\partial b_s}=\frac{2u_{sj}u_{s+1,j}}{u_j^T u_j},$$

where u_{rj} is the rth component of the eigenvector u_j. Similarly, by using $(K-\mu_k)v_k=0$, we find that

$$\frac{\partial\mu_k}{\partial a_r}=\frac{(v_{rk})^2}{v_k^T v_k} \quad \text{and} \quad \frac{\partial\mu_k}{\partial b_s}=\frac{2v_{sk}v_{s+1,k}}{v_k^T v_k},$$

where v_{rk} is the rth component of the eigenvector v_k. Since all eigenvalues of K are independent of a_n and b_{n-1}, we see that $\partial\mu_k/\partial a_n$ and $\partial\mu_k/\partial b_{n-1}$ vanish for all k. Consequently we have

$$F' = \begin{bmatrix} \Sigma_r u_{rj}^2 & & \\ & \ddots & \\ & & \Sigma_s v_{sk}^2 \end{bmatrix}^{-1} \left[\begin{array}{c|c} u_{rj}^2 & 2u_{sj}u_{s+1,j} \\ \hline v_{rk}^2 & 2v_{sk}v_{s+1,k} \end{array}\right],$$

where the last columns of the two lower submatrices vanish. The diagonal matrix is invertible because $u_{1j} = v_{1k} = 1$.

We will now prove that the second matrix is non-singular. Assume that $F'z = 0$, where $z = (\alpha_1, \ldots, \alpha_n, \beta_1, \ldots, \beta_{n-1})^T$ is an arbitrary vector. From the first n components of $F'z$ it follows that

$$\sum_{r=1}^{n} \alpha_r u_{rj}^2 + \sum_{s=1}^{n-1} \beta_s 2u_{sj}u_{s+1,j} = 0$$

for $j = 1, 2, \ldots, n$, and from the last $n-1$ components we see that

$$\sum_{r=1}^{n-1} \alpha_r v_{rk}^2 + \sum_{s=1}^{n-2} \beta_s 2v_{sk}v_{s+1,k} = 0$$

for $k = 1, 2, \ldots, n-1$. Since the eigenvectors u_{rj} and v_{sk} can be computed by using the difference equation (2.1), we conclude that

$$g(\lambda) = \sum_{r=1}^{n} \alpha_r u_r^2(\lambda) + \sum_{s=1}^{n-1} \beta_s 2u_s(\lambda)u_{s+1}(\lambda)$$

vanishes for λ equal to $\lambda_1, \ldots, \lambda_n$ and $\mu_1, \ldots, \mu_{n-1}$. As in the proof for Theorem 1, we use the fact that $v_n(\mu_k)$ vanishes for all eigenvalues μ_k of K. We can now apply the same arguments as in Sec. 2 to show that $u_r^2(\lambda)$ and $u_s(\lambda)u_{s+1}(\lambda)$ are polynomials in λ of degree exactly $2r-2$ and $2s$-1 respectively. Since the degree of the polynomial $g(\lambda)$ is at most $2n$-2 and $g(\lambda)$ has at least $2n$-1 roots, we conclude that $g(\lambda)$ vanishes identically. Consequently all α_r and β_s are zero, because the polynomials $u_r^2(\lambda)$ and $u_s(\lambda)u_{s+1}(\lambda)$ are linearly independent. This shows that the matrix F' is nonsingular, and hence its lowest singular value $\sigma_{2n-1}(F')$ is strictly positive.

It can be shown that the normalized eigenvectors u_{rj} and v_{sk} are holomorphic functions of J (see Kato [7, p. 121]). The matrix F' is therefore a

continuous function of a_r and b_s. Moreover, the singular value $\sigma_{2n-1}(F')$ depends continuously on F'. Since the elements a_r and b_s of J are restricted to a compact set, we finally conclude that there exists a positive constant σ which is less than $\sigma_{2n-1}(F')$ for all Jacobi matrices J which satisfy (4.4) and (4.5). We mention that σ depends only on the lower bound η for the off-diagonal elements. This completes the proof. ■

The following result shows that for fixed n the inverse eigenvalue problem is well posed.

THEOREM 4. *Let J and $\tilde{J}$ be solutions of the inverse eigenvalue problem with data*

$$\lambda_1 < \mu_1 < \lambda_2 < \cdots < \mu_{n-1} < \lambda_n, \tag{4.6}$$

$$\tilde{\lambda}_1 < \tilde{\mu}_1 < \tilde{\lambda}_2 < \cdots < \tilde{\mu}_{n-1} < \tilde{\lambda}_n. \tag{4.7}$$

There exists a constant K such that

$$\|J - \tilde{J}\|_E \leqslant K\left[\sum_{j=1}^{n} (\lambda_j - \tilde{\lambda}_j)^2 + \sum_{j=1}^{n-1} (\mu_j - \tilde{\mu}_j)^2\right]^{1/2}, \tag{4.8}$$

where $\|\cdot\|_E$ denotes the Frobenius norm. The constant K can be bounded in terms of n and η_0, where

$$\eta_0 = \delta_0 \sqrt{\frac{\varepsilon_0}{2\delta_0 + \varepsilon_0}},$$

$$\varepsilon_0 = d^{-1} \min_{j,k} \left(|\lambda_j - \mu_k|, |\tilde{\lambda}_j - \tilde{\mu}_k|\right),$$

$$\delta_0 = \frac{1}{2} d^{-1} \min_{j \neq k} \left(|\lambda_j - \lambda_k|, |\mu_j - \mu_k|, |\tilde{\lambda}_j - \tilde{\lambda}_k|, |\tilde{\mu}_j - \tilde{\mu}_k|\right),$$

$$d = \max(\lambda_n, \tilde{\lambda}_n) - \min(\lambda_1, \tilde{\lambda}_1).$$

REMARK. The basic idea in the proof of this result is that the smallest distance between the eigenvalues gives, via Lemma 2, a lower bound for the off-diagonal elements. This guarantees, via Lemma 3, that the Fréchet derivative F' is a non-singular matrix, and consequently we can apply the implicit-function theorem.

Proof. Let $c=\min(\lambda_1,\tilde{\lambda}_1)$ and $d=\max(\lambda_n,\tilde{\lambda}_n)-c$. From Theorem 1 it follows that if J is the solution of the inverse eigenvalue problem with data $\{\lambda_j\}$ and $\{\mu_j\}$, then $d^{-1}(J-cI)$ is the solution corresponding to the data $\{(\lambda_j-c)/d\}$ and $\{(\mu_j-c)/d\}$. The inequality (4.8) and the constants ε_0 and δ_0 are independent of the linear transformation $\lambda\to(\lambda-c)/d$ of the eigenvalues. We may therefore assume that λ_j, μ_j, $\tilde{\lambda}_j$ and $\tilde{\mu}_j$ lie in the interval $[0,1]$, and after the transformation c is zero and d is one.

We will now consider intermediate inverse problems with data $\lambda_j(t)=t\tilde{\lambda}_j+(1-t)\lambda_j$ for $j=1,2,\ldots,n$ and $\mu_j(t)=t\tilde{\mu}_j+(1-t)\mu_j$ for $j=1,2,\ldots,n-1$, where $0\leqslant t\leqslant 1$. For each t in this interval we have

$$\lambda_1(t)<\mu_1(t)<\lambda_2(t)<\cdots<\mu_{n-1}(t)<\lambda_n(t). \tag{4.9}$$

From Theorem 2 we conclude that there exist a Jacobi matrix $J(t)$ which is the solution of the inverse eigenvalue problem with data (4.9). Since $\lambda_1(t)$ and $\lambda_n(t)$ are convex combinations of numbers in the interval $[0,1]$, we see that $0\leqslant\lambda_1(t)$ and $\lambda_n(t)\leqslant 1$ for all t in $[0,1]$. Let

$$\varepsilon(t)=\min_{j,k}|\lambda_j(t)-\mu_k(t)|$$

$$\delta(t)=\tfrac{1}{2}\min_{j\neq k}(|\lambda_j(t)-\lambda_k(t)|,|\mu_j(t)-\mu_k(t)|).$$

Since d is one for the modified eigenvalues, we see that $\varepsilon(t)\geqslant\varepsilon_0$ and $\delta(t)\geqslant\delta_0$ for all t in $[0,1]$. Because the lower bound in (4.2) is a monotone increasing function of ε and δ, we conclude from Lemma 2 that

$$0\leqslant a_i(t)\leqslant 1, \qquad i=1,2,\ldots,n, \tag{4.10}$$

$$\eta_0\leqslant b_i(t)\leqslant 1, \qquad i=1,2,\ldots,n-1, \tag{4.11}$$

where $\eta_0=\delta_0\sqrt{\varepsilon_0/(2\delta_0+\varepsilon_0)}$, and $a_i(t)$ and $b_i(t)$ are the diagonal and codiagonal elements of the Jacobi matrix $J(t)$.

We associate with the data (4.9) the vector

$$y(t)=(\lambda_1(t),\ldots,\lambda_n(t),\mu_1(t),\ldots,\mu_{n-1}(t))^T$$

and let $y=y(0)$ and $\tilde{y}=y(1)$. Thus y and $\tilde{y}$ correspond to (4.6) and (4.7), respectively, and $y(t)=t\tilde{y}+(1-t)y$. Let

$$x(t)=(a_1(t),\ldots,a_n(t),b_1(t),\ldots,b_{n-1}(t))^T.$$

Since the components of $y(t)$ are eigenvalues of Jacobi matrices with elements $a_i(t)$ and $b_i(t)$, we see that $F(x(t))=y(t)$. By differentiating with respect to t we obtain the linear system of equations $F'(x(t))dx/dt=\tilde{y}-y$, where F' is the square matrix (4.3). The elements in $x(t)$ satisfy (4.10) and (4.11) for all t in $[0,1]$. The matrix F' is therefore non-singular according to Lemma 3, and the ordinary differential equation has the solution

$$x(t)=x(0)+\int_0^t [F'(x(\tau))]^{-1}[\tilde{y}-y]\,d\tau.$$

Let $\eta=\eta_0$. From (4.10), (4.11) and Lemma 3 it follows that for all τ in $[0,1]$ the 2-norm of the inverse of $F'(x(\tau))$ is less than σ^{-1}, and we conclude finally that

$$\|x(1)-x(0)\|_2 \leqslant \sigma^{-1}\|\tilde{y}-y\|_2.$$

The vectors $x(0)$ and $x(1)$ consist of the diagonal and codiagonal elements of $J(0)=J$ and $J(1)=\tilde{J}$, corresponding to the data (4.6) and (4.7). We can therefore estimate the difference between J and $\tilde{J}$ by

$$\|\tilde{J}-J\|_E \leqslant 2\alpha^{-1}\left[\sum_{j=1}^{n}(\tilde{\lambda}_j-\lambda_j)^2+\sum_{j=1}^{n-1}(\tilde{\mu}_j-\mu_j)^2\right]^{1/2},$$

where we use the fact that $\|J\|_E^2 \leqslant 2(\Sigma_1^n a_i^2+\Sigma_1^{n-1}b_i^2)$. This completes the proof. ∎

Since the distance between the spectra (4.6) and (4.7) may be arbitrarily large, the statement in Theorem 4 is global. However, the constant K depends on both spectra. The effect of small perturbations of the data is given in the following

COROLLARY 1. *Let J be the Jacobi matrix corresponding to the data* (4.6). *Let ε and δ be defined as in Lemma* 2. *There exists a constant K, which depends only on the data, such that for all real numbers $\{\tilde{\lambda}_j\}$ and $\{\tilde{\mu}_j\}$ which satisfy* $\max(|\lambda_j-\tilde{\lambda}_j|, |\mu_j-\tilde{\mu}_j|)<\varepsilon/4$, *the corresponding Jacobi matrix $\tilde{J}$ satisfies*

$$\|J-\tilde{J}\|_E \leqslant K\left[\sum_{j=1}^{n}(\lambda_j-\tilde{\lambda}_j)^2+\sum_{j=1}^{n-1}(\mu_j-\tilde{\mu}_j)^2\right]^{1/2}.$$

Proof. It is sufficient to show that the constant η_0 in Theorem 4 can be bounded from below, independent of the perturbation. We will estimate η_0, ε_0, δ_0 and d from the data (4.6). Clearly $d \leqslant \lambda_n - \lambda_1 + \varepsilon/2 = d_1$. To estimate ε_0 we note that $|\tilde{\lambda}_j - \tilde{\mu}_k| \geqslant |\lambda_j - \mu_k| - \varepsilon/2$ for all j and k. Thus $\varepsilon_0 \geqslant d_1^{-1}\varepsilon/2 = \varepsilon_1$. Similarly we find for j different from k that $|\tilde{\lambda}_j - \tilde{\lambda}_k| \geqslant |\lambda_j - \lambda_k| - \varepsilon/2$ and $|\tilde{\mu}_j - \tilde{\mu}_k| \geqslant |\mu_j - \mu_k| - \varepsilon/2$. Consequently $\delta_0 \geqslant d_1^{-1}(\delta - \varepsilon/4) = \delta_1$, where δ is defined in Lemma 2. By substituting ε_1 and δ_1 instead of ε_0 and δ_0 in the definition of η_0, we conclude by simple calculations that for all small perturbations of the data (4.6) the corresponding η_0 satisfies

$$\eta_0 \geqslant \delta_1 \sqrt{\frac{\varepsilon_1}{2\delta_1 + \varepsilon_1}}$$

$$\geqslant \frac{4\delta - \varepsilon}{8(\lambda_n - \lambda_1) + 4\varepsilon} \sqrt{\frac{\varepsilon}{\delta}} \, .$$

By using the fact that $\varepsilon \leqslant \delta$ and $\varepsilon < (\lambda_n - \lambda_1)/2$, we get the slightly simpler bound $\eta_0 \geqslant 0.3\sqrt{\varepsilon\delta}\,/(\lambda_n - \lambda_1) = \eta_1$. These lower bounds for η_0 depend only on the data. For each perturbation $\{\tilde{\lambda}_j\}$ and $\{\tilde{\mu}_j\}$ of the data, the associated constant K, which can be bounded in terms of n and η_0, will be less than $K_1 = \sigma_1^{-1}$. The existence of σ_1 is proven in Lemma 3, and σ_1 can be bounded in terms of n and η_1. This completes the proof. ∎

These results can be extended to the case where only one spectrum is given and the Jacobi matrix is required to be persymmetric. In particular, we mention without proof

THEOREM 5. *Let J be a Jacobi matrix corresponding to the data* (3.7) *and satisfy the symmetry conditions* (3.8). *Set $\varepsilon = \min_j(\lambda_{j+1} - \lambda_j)$. There exists a constant K such that for all real data $\{\tilde{\lambda}_j\}$ which satisfy $\max_j|\lambda_j - \tilde{\lambda}_j| < \varepsilon/4$, the corresponding Jacobi matrix $\tilde{J}$ satisfies*

$$\|J - \tilde{J}\|_E \leqslant K\left[\sum_{j=1}^{n} (\lambda_j - \tilde{\lambda}_j)^2\right]^{1/2} .$$

In this section we have considered the stability of the inverse eigenvalue problem from a mathematical point of view, not a computational one. It is not clear whether the algorithm given in Sec. 3 is stable, and indeed,

numerical experiments indicate the opposite (see Sec. 6). The advantage of the method is that it gives the solution in a finite number of steps. In a later paper we will present a linearly convergent method which is slow in practice, but extremely stable. The convergence proof for this iterative method will be based on the stability results presented here.

5. PHYSICAL EXAMPLES

In this section we will study several physical interpretations of Hochstadt's uniqueness result, i.e., Theorem 1. We begin by considering a composite pendulum—that is, a pendulum which is suspended from a fixed point and consists of n beads of masses $m_i > 0$ connected by weightless infinite flexible strings of length l_i. Here m_1 is the mass of the lowest bead. We will only study small vibrations of the pendulum and assume that the strings do not stretch under tension. The derivation of the linearized equation of motion for this system can be found in Gantmacher and Krein [2, pp. 130, 146] and Hadeler [3].

Our starting point is the following eigenvalue problem, which is obtained after a separation of variables:

$$-\frac{\sigma_{i-1}}{l_{i-1}}u_{i-1}+\left(\frac{\sigma_{i-1}}{l_{i-1}}+\frac{\sigma_i}{l_i}\right)u_i-\frac{\sigma_i}{l_i}u_{i+1}=\lambda m_i u_i \tag{5.1}$$

for $i=1, 2,\ldots,n$, where $\sigma_0=0$ and we have the end conditions $u_0=u_{n+1}=0$. The deviation of the ith bead from its position at rest is called amplitude and denoted by u_i. The tension of the ith string is $\sigma_i=g\sum_{j=1}^{i} m_j$ where g is the gravity. Our goal is to find the masses of the beads and the length of the connecting strings from eigenvalue data. An inspection of (5.1) shows that the eigenvalues are unchanged if all masses are multiplied by a constant. Thus we can at most determine the ratios between the masses m_i and the lengths l_i, and we choose the normalization $m_1=1$.

Let now the uppermost bead, with mass m_n, be fixed. What remains is a smaller composite pendulum which consists of $n-1$ beads and $n-1$ strings. It will be called the truncated pendulum. We can now give the physical interpretation of Hochstadt's uniqueness result.

THEOREM 6. *The lengths of the strings $(l_1,\ldots,l_n)$ and the ratio of the masses $(m_1:m_2:\cdots:m_n)$ are uniquely determined by the eigenfrequencies of the composite pendulum and the eigenfrequencies of the truncated pendulum.*

Proof. If p is an eigenfrequency of the pendulum, then $\lambda = p^2$ is an eigenvalue of (5.1). Let $\alpha_i = \sigma_i / l_i$ for $i = 1, 2, \ldots, n$. The eigenvalue problem (5.1) can be written in the form $Au = \lambda Mu$, where

$$A = \begin{bmatrix} \alpha_1 & -\alpha_1 & & & & \\ -\alpha_1 & \alpha_1 + \alpha_2 & -\alpha_2 & & & \\ & \ddots & \ddots & \ddots & & \\ & & -\alpha_{n-2} & \alpha_{n-2} + \alpha_{n-1} & -\alpha_{n-1} & \\ & & & -\alpha_{n-1} & \alpha_{n-1} + \alpha_n \end{bmatrix},$$

$M = \operatorname{diag}(m_1, \ldots, m_n)$ and $u = (u_1, \ldots, u_n)^T$. Let $\lambda_1, \ldots, \lambda_n$ be the eigenvalues. Similarly $Bv = \mu Nv$, where $v = (v_1, \ldots, v_{n-1})^T$ is the eigenvalue problem for the truncated pendulum. The matrices B and N of order $n-1$ are obtained by removing the last column and row from A and M, respectively.

These generalized eigenvalue problems are equivalent to the normal eigenvalue problem for the matrices $J = M^{-1/2} A M^{-1/2}$ and $K = N^{-1/2} B N^{-1/2}$. Here K is the leading principal submatrix of order $n-1$ of J. Since all off-diagonal elements of J are different from zero,

$$\lambda_1 < \mu_1 < \lambda_2 < \cdots < \mu_{n-1} < \lambda_n.$$

Assume now that there exists a different composite pendulum with masses $\tilde{m}_i$, where $\tilde{m}_1 = 1$, and strings of length $\tilde{l}_i$, such that λ_i and μ_i are also the eigenvalues of $\tilde{A}u = \lambda \tilde{M}u$ and $\tilde{B}v = \mu \tilde{N}v$. Here $\tilde{A}$, $\tilde{M}$, $\tilde{B}$ and $\tilde{N}$ are defined in the same manner as above. Thus the eigenvalues of $\tilde{J} = \tilde{M}^{-1/2} \tilde{A} \tilde{M}^{-1/2}$ and $\tilde{K} = \tilde{N}^{-1/2} \tilde{B} \tilde{N}^{-1/2}$ coincide with those of J and K. From Theorem 1 follows that the elements in the Jacobi matrix J are uniquely determined by the eigenvalues λ_i and μ_i. Consequently

$$\frac{\alpha_1}{m_1} = \frac{\tilde{\alpha}_1}{\tilde{m}_1},$$

$$\frac{\alpha_{i-1} + \alpha_i}{m_i} = \frac{\tilde{\alpha}_{i-1} + \tilde{\alpha}_i}{\tilde{m}_i}, \qquad i = 2, 3, \ldots, n,$$

$$\frac{\alpha_i}{\sqrt{m_i m_{i+1}}} = \frac{\tilde{\alpha}_i}{\sqrt{\tilde{m}_i \tilde{m}_{i+1}}}, \qquad i = 1, 2, \ldots, n-1.$$

Since the mass of the lowest bead is one in both cases, the first equation shows that $\alpha_1 = \tilde{\alpha}_1$. For $i = 1$ the last equation gives $m_2 = \tilde{m}_2$ and the middle

equation implies for $i=2$ that $\alpha_2=\tilde{\alpha}_2$, and so on. The masses m_i of the beads and the coefficients α_i are therefore uniquely determined by the spectra $\{\lambda_j\}$ and $\{\mu_j\}$. Moreover, since $\alpha_i=\sigma_i/l_i$ and the σ_i only depend on the masses of the beads, we conclude that the lengths of the strings l_i are also uniquely determined by the eigenfrequencies. This completes the proof. ■

We mention that Eq. (5.1) has a different interpretation. If $\sigma_0=0$ but all other σ_i are equal to a positive constant τ, then Eq. (5.1) determines the normal frequencies for a vibrating horizontal string with beads. The string has tension τ, and the masses of the beads are (from left to right) $m_1,\ldots,m_n$. The string is free at its left end and fixed at its right end. The distance from the last bead to the right end is l_n, and l_i is the distance between the beads with masses m_i and m_{i+1}. Our goal is to determine the string from eigenvalue data. However, we cannot hope to find the distance l_0 between the left end of the string and the first bead, because Eq. (5.1) is independent of this quantity. If we fix the last bead at the right, the remaining string is called the truncated string. We can now formulate

THEOREM 7. *Let the tension τ and the distance from the last bead to the end of the string be given. The masses m_i of the beads and the distances l_i between the beads are uniquely determined by the fundamental tones and the overtones of the string and the truncated string.*

Proof. The eigenvalue problem (5.1) for the string can be written in the form $Au=\lambda Mu$, where $M=\operatorname{diag}(m_1,\ldots,m_n)$ and $u=(u_1,\ldots,u_n)^T$. The nonzero elements of $A=(a_{ij})$ are $a_{11}=\tau/l_1$, $a_{ii}=\tau(1/l_{i-1}+1/l_i)$ for $i=2,3,\ldots,n$ and $a_{i,i+1}=a_{i+1,i}=-\tau/l_i$ for $i=1,2,\ldots,n-1$. Let $J=M^{-1/2}A\,M^{-1/2}$. The eigenvalues of J are the square of the fundamental tone and the overtones of the string (see Gantmacher and Krein [2, p. 136]). As in Theorem 6, we see that the eigenvalues corresponding to the truncated string are the eigenvalues of the leading principal submatrix K of order $n-1$ of J. The diagonal and codiagonal elements of J—i.e.,

$$a_1=\frac{\tau}{l_1m_1},$$

$$a_i=\left(\frac{1}{l_{i-1}}+\frac{1}{l_i}\right)\frac{\tau}{m_i}, \qquad i=2,\ldots,n,$$

$$b_i=-\frac{\tau}{l_i\sqrt{m_im_{i+1}}}, \qquad i=1,\ldots,n-1$$

—are therefore uniquely determined by the eigenfrequencies of the string and the truncated string. By setting $m_1 = 1$, the remaining coefficients l_i and m_i can be found successively from a_i and b_i. Determine c such that cl_n equals the given distance between the last bead and the right end of the string. The string with beads of masses m_i/c and distance cl_i between the beads is the unique solution of the inverse problem. ∎

The examples in this section have been discussed from different points of view by Hadeler and Hochstadt. Given the masses of the beads and the frequencies of the composite pendulum, Hadeler was able, under certain conditions, to determine the distances between the beads (see [3]). If the pendulum has n beads, the inverse problem has in general $n!$ solutions.

The case of a vibrating string with beads was considered by Hochstadt (see [5]). Assume that the string is fixed at both ends. Hochstadt proves that provided the positions of the beads are known, the masses of the beads are uniquely determined by the frequencies of the string and the frequencies of the same string with the last bead fixed at its position of rest. Note that in this case we determine n unknowns from $3n$ data, and consequently we cannot hope, in general, to obtain a solution to this inverse problem. Additional interpretations, with special emphasis on strings with the beads distributed symmetrically, can be found in Gantmacher and Krein [2, pp. 322–338] and Hald [4, pp. 119–138].

6. A NUMERICAL EXAMPLE

In this section we will present some numerical experiments. The computations were carried out on the IBM 370/155 at Uppsala University. The programs were written in ALGOL and run in double precision.

As data for the inverse problem we choose the zeros of the Laguerre polynomials L_n and L_{n-1}. The Laguerre polynomials can be represented explicitly by

$$L_i(\xi) = \sum_{\nu=0}^{i} \binom{i}{\nu} \frac{(-\xi)^\nu}{\nu!} \tag{6.1}$$

(see Szegö [8, p. 97]) and satisfy the three-step recurrence relation

$$(i-1)L_{i-2} + (\xi - 2i + 1)L_{i-1} + iL_i = 0 \tag{6.2}$$

for $i = 1, 2, \ldots$ with $L_0 = 1$.

Let ξ be a root of $L_n(\xi)=0$. From (6.2) follows that ξ is actually a solution to the eigenvalue problem $Ju=\xi u$, where J is the Jacobi matrix of order n with diagonal elements $a_i=2i-1$ for $i=1, 2,\ldots,n$ and codiagonal elements $b_i=-i$ for $i=1, 2,\ldots,n-1$. Moreover, the ith component of the eigenvector u is simply $u_i=\text{const}\times L_{i-1}(\xi)$ for $i=1, 2,\ldots,n$. Similarly we find that ξ is a root of $L_{n-1}(\xi)=0$ if and only if $Kv=\xi v$, where K is the leading principal submatrix of order $n-1$ of J.

From a physical point of view, the eigenvalues of J and K can be interpreted as the squares of the eigenfrequencies for the composite and the truncated pendulum if we assume that all beads have the same mass and are placed equidistantly.

To test the method presented in Sec. 3 we computed the eigenvalues λ_j and μ_j of J and K by using the algorithm *tql* 1 (see Wilkinson and Reinsch [9, pp. 227–240]). Since J and K are diagonal dominant matrices, all eigenvalues are positive. We computed the characteristic polynomials as functions of $-x$ in place of λ, i.e.,

$$p_n=\prod_j (x+\lambda_j), \qquad p_{n-1}=\prod_j (x+\mu_j),$$

and found the solution of the inverse eigenvalue problem by using (3.3)–(3.6) recursively. We tested $n=5, 10,\ldots$. The absolute and the relative errors were smallest in the very first and the very last elements of J. The maxima of the relative errors in the elements of J are given in column 1 of Table 1. The algorithm breaks down for $n=35$, because the square of one of the off-diagonal elements becomes negative.

TABLE 1

MAXIMAL RELATIVE ERROR IN EACH OF THE ELEMENTS OF J (DOUBLE PRECISION)

n	Eigenvalues Computed	Laguerre pol. exact	Laguerre pol. appr.
5	4.4×10^{-15}	0.0	0.0
10	3.8×10^{-13}	0.0	0.0
15	9.2×10^{-11}	Overflow	0.0
20	2.4×10^{-8}		8.8×10^{-11}
25	2.4×10^{-6}		1.9×10^{-6}
30	3.1×10^{-4}		5.2×10^{-4}
35	Breakdown		1.8×10^{-1}
40			Breakdown

The effect of the errors in the computed eigenvalues and the perturbation of the characteristic polynomials can be studied by using the connection between the matrices J and K and the exact representation of the Laguerre polynomials [see (6.1)]. Since the leading coefficient of L_i is $(-1)^i/i!$, we see that $n!\,L_n$ and $(n-1)!\,L_{n-1}$ are the characteristic polynomials of J and K. To compute the coefficients

$$\alpha_\nu = \binom{n}{\nu}\frac{n!}{\nu!}$$

in L_n we use the fact that $\alpha_n = 1$ and $\alpha_\nu = \alpha_{\nu+1}(\nu+1)^2/(n-\nu)$ for $\nu = n-1,\ldots,0$. Similarly the coefficients in $(n-1)!\,L_{n-1}$ are computed by $\beta_{n-1}=1$ and $\beta_\nu = \beta_{\nu+1}(\nu+1)^2/(n-1-\nu)$ for $\nu = n-2,\ldots,0$. The coefficients α_ν and β_ν were represented as integers. By using $n!L_n$ and $(n-1)!\,L_{n-1}$ instead of p_n and p_{n-1}, we found the matrix J exactly (see column 2 of Table 1), but for $n=15$ some coefficients in the Laguerre polynomial exceeded the upper limit for integers and overflow resulted.

To extend the calculations to larger n, we represented the coefficients as real numbers. For n large, some of the coefficients will be rounded before storing. Thus for $n=20$ we have $\alpha_4 = 16^3 \times m$, where $m = 2^8\times 19\times 17\times 5\times 19!!\times 9!!\times 5!! = 1.198\times 10^{17}$. This number cannot be represented exactly in double-precision floating point. The effect of the perturbation of the coefficients in the characteristic polynomials can be studied in the last column of Table 1. Here we give the maxima of the relative errors in each of the elements in the computed solutions J of the inverse eigenvalue problems. The method breaks down at n equal to 40, because in the computation of the off-diagonal elements we try to take the square root of a negative number.

To investigate the influence of the rounding errors we tested the algorithm in single-precision arithmetic, i.e., 7–8 significant decimal digits. The results are given in Table 2. The breakdown occurred for small n, and in both cases because the square of one of the off-diagonal elements becomes negative.

TABLE 2

MAXIMAL RELATIVE ERROR IN EACH OF THE ELEMENTS OF J (SINGLE PRECISION)

n	Eigenvalues computed	Laguerre pol. exact	Laguerre pol. appr.
5	2.6×10^{-5}	0.0	0.0
10	3.3×10^{-3}	0.0	0.0
15	Breakdown	Overflow	1.1×10^{-1}
20			Breakdown

It is well known (see Wilkinson [10, pp. 41–43]) that there exist polynomials with real and simple roots for which a small perturbation of the coefficients gives a large change in some of the roots. Thus, if the Jacobi matrix is computed without rounding errors from such polynomials contaminated by small perturbations, the eigenvalues of the matrices J and K may differ drastically from the given data. As an example we consider the data $\lambda_j = j$ for $j = 1, 2, \ldots, n$ and $\mu_j = j + 0.5$ for $j = 1, 2, \ldots, n-1$, where $n = 5, 10, \ldots$. The eigenvalues are well separated, and from Lemma 1 it follows that the lower bound for the off-diagonal elements is 0.288.... The maximal deviation in the eigenvalues of the computed solutions J and K from the given data can be found in columns 1 and 2 of Table 3.

TABLE 3

MAXIMAL ERRORS IN THE EIGENVALUES FOR THE COMPUTED MATRICES J AND K

n	$\lambda_j = j$	$\mu_j = j + \frac{1}{2}$	$\lambda_j = j + \sqrt{2}$	$\mu_j = j + \frac{1}{2} + \sqrt{2}$
5	0.0	0.0	6.1×10^{-13}	1.8×10^{-13}
10	0.0	0.0	8.4×10^{-10}	1.7×10^{-9}
15	1.1×10^{-8}	5.5×10^{-9}	1.7×10^{-5}	3.6×10^{-6}
20	2.3×10^{-3}	3.1×10^{-3}	3.2×10^{-1}	7.7×10^{-2}

In this example many of the coefficients in the characteristic polynomials were computed exactly, because the data were too regular. To introduce rounding errors in all coefficients we shifted the eigenvalues by $\sqrt{2}$, i.e. $\lambda_j = j + \sqrt{2}$ for $j = 1, 2, \ldots, n$ and $\mu_j = j + 0.5 + \sqrt{2}$ for $j = 1, 2, \ldots, n-1$. The lower bound for the offdiagonal terms is still 0.288.... The errors in the eigenvalues of the computed matrices are given in columns 3 and 4 of Table 3. Generally the largest eigenvalues were most affected by the rounding errors. This is in agreement with the investigation of Wilkinson (see [10, pp. 41–43]). For n less than or equal to 20 all off-diagonal elements satisfy the bounds given above. However, the algorithm breaks down for n equal to 25 in both cases, because we try to take the square root of a negative number. Thus, even though the algorithm developed in Sec. 3 produces the solution of the inverse eigenvalue problem in a finite number of steps, the numerical results given here indicate that the method is potentially unstable. In a forthcoming paper we will present an iterative method, which is based on the theorems in Sec. 4 and is stable.

The results in Secs. 2, 3 and 5 were obtained in connection with the research leading to the author's Ph.D. thesis, written under the guidance of

Professor Olof B. Widlund, New York University. In addition, the author wants to thank Professor Harry Hochstadt and Professor Eugene Isaacson for helpful discussions. The results presented here are not included in the thesis.

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Received 31 July 1974