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Numerische Mathematik

The Numerically Stable Reconstruction of Jacobi Matrices from Spectral Data

Dedicated to Professor F.L. Bauer on the occasion of his 60th birthday

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Summary. We present an exposé of the elementary theory of Jacobi matrices and, in particular, their reconstruction from the Gaussian weights and abscissas. Many recent works propose use of the diagonal Hermitian Lanczos process for this purpose. We show that this process is numerically unstable. We recall Rutishauser's elegant and stable algorithm of 1963, based on plane rotations, implement it efficiently, and discuss our numerical experience. We also apply Rutishauser's algorithm to reconstruct a persymmetric Jacobi matrix from its spectrum in an efficient and stable manner.

Subject Classifications: AMS(MOS): 15A18, 30A22, 41A55, 65F15; CR: G.1.3, G.1.4.

1. Jacobi Matrices

An infinite Jacobi matrix is a real symmetric tridiagonal matrix,

$$T=\begin{bmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \alpha_2 & \beta_2 & & \\ & \beta_2 & \alpha_3 & \beta_3 & \\ & & \beta_3 & \alpha_4 & \ddots \\ & & & \ddots & \ddots \end{bmatrix},$$

with *positive* subdiagonal elements $\{\beta_n\}$.

Associated with T, and another positive number β_0, is the *Jacobi continued fraction*

$$J(\lambda)=\frac{\beta_0^2}{|\lambda-\alpha_1}-\frac{\beta_1^2}{|\lambda-\alpha_2}-\frac{\beta_2^2}{|\lambda-\alpha_3}-\cdots$$

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whose approximants

$$\phi_n(\lambda) := \frac{\beta_0^2}{|\lambda-\alpha_1|} - \frac{\beta_1^2}{|\lambda-\alpha_2|} - \ldots - \frac{\beta_{n-1}^2}{|\lambda-\alpha_n|}$$
$$= \pi_n(\lambda)/\psi_n(\lambda)$$

can be formed from the twin three term recurrence relations

$$\begin{bmatrix} \pi_{n+1} \\ \psi_{n+1} \end{bmatrix} := \begin{bmatrix} \pi_n & \pi_{n-1} \\ \psi_n & \psi_{n-1} \end{bmatrix} \begin{bmatrix} \lambda-\alpha_{n+1} \\ -\beta_n^2 \end{bmatrix}, \quad \begin{bmatrix} \pi_0 & \pi_{-1} \\ \psi_0 & \psi_{-1} \end{bmatrix} := \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}.$$

Equivalently,

$$\psi_n(\lambda) = \det(\lambda I - T_n)$$

and

$$\pi_n(\lambda) = \beta_0^2 \det(\lambda I - T_n')$$

with T_n the nth leading principal submatrix of T, and T_n' obtained from T_n by deleting its first row and column. Hence

$$\phi_n(\lambda) = \beta_0^2 e_1^*(\lambda I - T_n)^{-1} e_1$$

is proportional with the (1, 1) element of the resolvent of T_n.

We also have

$$\begin{bmatrix} \pi_n & \pi_{n-1} \\ \psi_n & \psi_{n-1} \end{bmatrix} = \begin{bmatrix} \pi_{n-1} & \pi_{n-2} \\ \psi_{n-1} & \psi_{n-2} \end{bmatrix} \begin{bmatrix} \lambda-\alpha_n & 1 \\ -\beta_{n-1}^2 & 0 \end{bmatrix}$$

and its corollary,

$$\pi_n \psi_{n-1} - \psi_n \pi_{n-1} \equiv \beta_0^2 \beta_1^2 \ldots \beta_{n-1}^2 > 0,$$

the *determinant formula.*

It follows by induction, from the recurrence relation for $\{\psi_n\}$, the positivity of the numbers $\{\beta_n^2\}$, and the intermediate value theorem, that ψ_n has n real distinct zeros,

$$\lambda_{n,1} > \lambda_{n,2} > \ldots > \lambda_{n,n},$$

which are strictly interlaced by the zeros of ψ_{n-1}. More precisely, $\psi_n'(\lambda_{n,k})$ and $\psi_{n-1}(\lambda_{n,k})$ each have strict sign $(-1)^{k-1}$.

The determinant formula shows that $\pi_n(\lambda_{n,k})$ also has strict sign $(-1)^{k-1}$. Hence the spectrum, $\lambda(T_n)$, of T_n is also strictly interlaced by $\lambda(T_n')$.

We conclude that the *partial fraction decomposition* of ϕ_n is

$$\phi_n(\lambda) = \sum_{k=1}^{n} \frac{\omega_{n,k}}{\lambda - \lambda_{n,k}}$$

with positive *weights*

$$\omega_{n,k} = \frac{\pi_n(\lambda_{n,k})}{\psi_n'(\lambda_{n,k})}.$$

Apart from the common constant factor β_0^2 this expresses the weights in terms of the spectra $\lambda(T_n)$ and $\lambda(T_n')$.

Define

$$\chi_n := \psi_n - \pi_n \qquad (n \geqq -1).$$

Then $\{\chi_n\}$ satisfies the same linear homogeneous difference equation as $\{\psi_n\}$ and $\{\pi_n\}$ with initial conditions $\chi_{-1} = \chi_0 = 1$. In particular, $\chi_1 = \lambda - \alpha_1 - \beta_0^2$. It follows that χ_n is the monic characteristic polynomial of the Jacobi matrix

$$T_n + \beta_0^2 e_1 e_1^*.$$

Now $\chi_n(\lambda_{n,k}) = -\pi_n(\lambda_{n,k})$ has strict sign $(-1)^k$. Hence the spectra $\lambda(T_n)$ and $\lambda(T_n + \beta_0^2 e_1 e_1^*)$ strictly interlace each other, with respect to the extended real line, with the right-most point of the latter being algebraically greater than that of the former. The weights are expressed in terms of these two spectra as

$$\omega_{n,k} = -\frac{\chi_n(\lambda_{n,k})}{\psi_n'(\lambda_{n,k})}.$$

We now briefly relate the above results with the *Gaussian quadrature formulas*,

$$\mathscr{G}_n(\phi) := \sum_{k=1}^{n} \omega_{n,k} \phi(\lambda_{n,k}),$$

associated with β_0 and T. Let

$$\phi_n(\lambda) =: \sum_{k=0}^{\infty} \frac{\mu_{n,k}}{\lambda^{k+1}}$$

be the Taylor expansion of ϕ_n about $\lambda = \infty$. From the partial fraction decomposition and the geometric series,

$$\mu_{n,k} \equiv \mathscr{G}_n(\lambda^k).$$

From the determinant formula,

$$\phi_{n+1}(\lambda) - \phi_n(\lambda) = \frac{\beta_0^2 \beta_1^2 \dots \beta_n^2}{\lambda^{2n+1}} \left[1 + O\left(\frac{1}{\lambda}\right)\right]$$

as $\lambda \to \infty$. Consequently,

$$\mu_{n+1,k} \equiv \mu_{n,k}, \qquad 0 \leqq k < 2n,$$

and

$$\mu_{n+1,2n} = \mu_{n,2n} + \beta_0^2 \beta_1^2 \dots \beta_n^2.$$

Hence the *moments*

$$\mu_k := \lim_{n \to \infty} \mu_{n,k}$$

all exist,

$$\mathscr{G}_n(\lambda^k) = \mu_k, \qquad 0 \leqq k < 2n,$$

and

$$\mu_{2n} - \mathscr{G}_n(\lambda^{2n}) = \beta_0^2 \beta_1^2 \dots \beta_n^2 > 0.$$

For a complete classical treatment of this whole circle of ideas, including solution of the *Hamburger moment problem* associated with β_0 and T, and interpretation of the $\{\psi_n\}$ as *orthogonal polynomials*, consult Akhiezer [1].

Let

$$T_n = U_n \Lambda_n U_n^*$$

be a spectral resolution of T_n, with U_n orthogonal and

$$\Lambda_n := \operatorname{diag}[\lambda_{n,k}]_{k=1}^n.$$

Then

$$\begin{aligned}\phi_n(\lambda) &= \beta_0^2 e_1^*(\lambda I - T_n)^{-1} e_1 \\ &= \beta_0^2 u_n^*(\lambda I - \Lambda_n)^{-1} u_n \\ &= \beta_0^2 \sum_{k=1}^n \frac{v_{n,k}^2}{\lambda - \lambda_{n,k}}\end{aligned}$$

with

$$u_n^* := [v_{n,1}, v_{n,2}, \ldots, v_{n,n}] := e_1^* U_n.$$

Hence the weights,

$$\omega_{n,k} = \beta_0^2 v_{n,k}^2,$$

are proportional with the squares of the first elements of the normalized eigenvectors of T_n. This also gives

$$\beta_0^2 = \sum_{k=1}^n \omega_{n,k}.$$

We prefer to work with columns rather than rows. Thus put

$$d_n := [\delta_{n,i}]_{i=1}^n := \beta_0 u_n \quad \text{and} \quad Q_n := U_n^*.$$

The above relations are then equivalent with

$$\Lambda_n Q_n = Q_n T_n, \qquad d_n = Q_n e_1 \beta_0,$$

with Q_n orthogonal, and

$$\omega_{n,k} \equiv \delta_{n,k}^2, \qquad \beta_0 = \|d_n\|_2.$$

2. Inverse Eigenvalue Problems for Finite Jacobi Matrices

In this *theoretical* section we obtain converses of the previous results for finite Jacobi matrices $T := T_n$. Since n is now fixed, we omit the corresponding subscripts. We also treat direct and inverse eigenvalue problems for $n \times n$ *persymmetric* Jacobi matrices.

Thus let

$$\Lambda := \operatorname{diag}[\lambda_k]_1^n \in \mathbb{R}^{n \times n}$$

have distinct eigenvalues, let

$$d := [\delta_i]_1^n \in \mathbb{R}^n$$

be such that the weights

$$\omega_k := \delta_k^2$$

are all positive, and put

$$\beta_0 := \|d\|_2 = (\sum \omega_k)^{1/2}.$$

We first show that there are a unique orthogonal matrix Q and a unique Jacobi matrix T, such that

$$\Lambda Q = QT \quad \text{and} \quad d = Q e_1 \beta_0.$$

The *Krylov matrix*,

$$K := [d, \Lambda d, \ldots, \Lambda^{n-1} d],$$

is nonsingular. In fact the *Gram matrix* of K is the *moment matrix*

$$M := K^* K = V W V^T$$

with the *weight matrix*

$$W := \operatorname{diag}[\omega_k]_1^n$$

and the *Vandermonde matrix*

$$V := [\lambda_j^{i-1}]_{i,j=1}^n.$$

Hence

$$\det M = \prod_{k=1}^{n} \omega_k \prod_{i>j} (\lambda_i - \lambda_j)^2 > 0.$$

Put

$$k := \Lambda^n d.$$

Then

$$\Lambda K = KE + k e_n^*$$

with the *downshift matrix*

$$E := [e_2, e_3, \ldots, e_n, 0].$$

Let f solve

$$Kf + k = 0.$$

Then

$$\Lambda K = KF$$

with the *Frobenius matrix*

$$F := E - f e_n^*.$$

Let

$$K = QR$$

be *the* QR factorization of K, with Q orthogonal and R right triangular with *positive* diagonal elements $\{\rho_k\}_0^{n-1}$. Then

$$\Lambda Q = QH$$

with the *right Hessenberg matrix*

$$H := RFR^{-1}$$

having subdiagonal elements

$$\beta_k = \rho_k / \rho_{k-1} > 0, \qquad 1 \leqq k < n.$$

In fact, since Q is orthogonal and Λ is Hermitian, we see that

$$H = Q^* \Lambda Q = H^* =: T$$

is a Jacobi matrix. Hence we have

$$\Lambda Q = QT$$

with

$$d = K e_1 = QR e_1 = Q e_1 \beta_0$$

and

$$\beta_0 := \rho_0 = \|d\|_2 > 0.$$

This completes the existence portion of the proof.

Since

$$M = R^* R$$

we have

$$\det M = \prod_0^{n-1} \rho_k^2.$$

Hence from

$$\rho_k = \beta_0 \beta_1 \dots \beta_k, \qquad 0 \leqq k < n,$$

we find the amusing formula

$$(\beta_0^n \beta_1^{n-1} \dots \beta_{n-1})^2 = \prod_{k=1}^{n} \omega_k \prod_{i>j} (\lambda_i - \lambda_j)^2.$$

The uniqueness of Q and T, for a *Jacobi* matrix T, is a well-known theme of numerical linear algebra [25]. In fact, setting

$$Q =: [q_0, q_1, \dots, q_{n-1}],$$

equating columns in $\Lambda Q = QT$, and using the orthogonality of Q, we see that T and the columns of Q are uniquely determined by the *Lanczos process*,

$q_{-1} := 0, \quad q'_0 = d,$
for $k = 0, 1, 2, \dots, n-1$

$\beta_k = \|q'_k\|_2, \quad q_k = q'_k / \beta_k,$
$q'_{k+1} \leftarrow \Lambda q_k - q_{k-1} \beta_k,$
$\alpha_{k+1} = q_k^* q'_{k+1},$
$q'_{k+1} \leftarrow q'_{k+1} - q_k \alpha_{k+1},$

given here in the *modified Gram-Schmidt* formulation. This algorithm requires approximately $10 n^2$ arithmetic operations to orthogonally tridiagonalize Λ, subject to $Q e_1 = d/\beta_0$.

There are many variants of the Lanczos process, especially in this case when the Hermitian matrix $A := \Lambda$ is diagonal. The following *rational* variant seems to be a most efficient process which is closest in spirit to those advo-

cated in [12, 9, 20, 10, 15]:

$$p_{-1} := 0, \quad p_0 = d, \quad \rho_{-1}^2 := 1,$$
$$\textbf{for } k = 0, 1, 2, \ldots, n-1$$
$$\begin{aligned} &w_k = p_k \circ p_k, \quad \rho_k^2 = e^* w_k, \\ &\beta_k^2 = \rho_k^2 / \rho_{k-1}^2, \quad \alpha_{k+1} = l^* w_k / \rho_k^2, \\ &p_{k+1} = (l - \alpha_{k+1} e) \circ p_k - p_{k-1} \beta_k^2. \end{aligned}$$

Here $\circ$ denotes the Schur, or elementwise, product, $e := [1, 1, \ldots, 1]^*$ and $l := \Lambda e$. This algorithm uses only about $8n^2$ arithmetic operations for the tridiagonalization of Λ.

These results show that, in theory, β_0^2 and the Jacobi matrix T can be "reconstructed" from the Gaussian data $\{\omega_k\}_1^n$ and $\{\lambda_k\}_1^n$, where $\omega_k = \delta_k^2$. Combining them with the results of section one we can state the following facts.

Given real numbers

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

there is a unique Jacobi matrix T for which

$$\lambda(T) = \{\lambda_k\}_1^n \quad \text{and} \quad \lambda(T') = \{\mu_k\}_1^{n-1},$$

where T' is the trailing principal submatrix of T of order $n-1$. The weights associated with $\beta_0^2 = 1$ and T are

$$\omega_k = \frac{\prod_{j=1}^{n-1} (\mu_j - \lambda_k)}{\prod_{j \neq k} (\lambda_j - \lambda_k)}.$$

Given real numbers

$$\lambda_1 < \mu_1 < \lambda_2 < \ldots < \lambda_n < \mu_n,$$

there are unique Jacobi matrices T and $T + \beta_0^2 e_1 e_1^*$ for which

$$\lambda(T) = \{\lambda_k\}_1^n \quad \text{and} \quad \lambda(T + \beta_0^2 e_1 e_1^*) = \{\mu_k\}_1^n.$$

The weights associated with β_0^2 and T are

$$\omega_k = \frac{\prod_{j=1}^{n} (\mu_j - \lambda_k)}{\prod_{j \neq k} (\lambda_j - \lambda_k)}.$$

A finite square matrix A is *persymmetric* if it is invariant with respect to reflection in its secondary diagonal. This means that

$$A = A^P := J A^T J,$$

with J the *reversal matrix*, that is the identity matrix with its columns reversed.

The $n \times n$ real symmetric tridiagonal matrix T is persymmetric if and only if

$$T=\begin{bmatrix} S^P & \beta e_{k-1} & \\ \beta e_{k-1}^* & \alpha & \beta e_1^* \\ & \beta e_1 & S \end{bmatrix} \quad \text{if } n=2k-1$$

or

$$T=\begin{bmatrix} S^P & \beta e_k e_1^* \\ \beta e_1 e_k^* & S \end{bmatrix} \quad \text{if } n=2k.$$

Hence

$$T=\tfrac{1}{2}\begin{bmatrix} 0 & J & -J \\ \sqrt{2} & 0^* & 0^* \\ 0 & I & I \end{bmatrix}\begin{bmatrix} \alpha & \sqrt{2}\beta e_1^* & \\ \sqrt{2}\beta e_1 & S & \\ & & S \end{bmatrix}\begin{bmatrix} 0^* & \sqrt{2} & 0^* \\ J & 0 & I \\ -J & 0 & I \end{bmatrix} \quad \text{if } n=2k-1$$

and

$$T=\tfrac{1}{2}\begin{bmatrix} J & -J \\ I & I \end{bmatrix}\begin{bmatrix} S+\beta e_1 e_1^* & \\ & S-\beta e_1 e_1^* \end{bmatrix}\begin{bmatrix} J & I \\ -J & I \end{bmatrix} \quad \text{if } n=2k.$$

These orthogonal similarity transformations reduce the eigenvalue problem for T to two real symmetric tridiagonal eigenvalue problems of half the size. If the QR algorithm with Wilkinson's shift [20] is used to find $\lambda(T)$, this reduces the work by about a factor of two.

Using the above results we can (theoretically) reconstruct a persymmetric Jacobi matrix T from its spectrum,

$$\lambda(T)\colon\ \lambda_1<\lambda_2<\ldots<\lambda_n,$$

as follows.

If $n=2k-1$ then the Jacobi matrix

$$\begin{bmatrix} \alpha & \sqrt{2}\beta e_1^* \\ \sqrt{2}\beta e_1 & S \end{bmatrix}$$

is uniquely determined by its spectrum $\{\lambda_{2j-1}\}_1^k$ and weights

$$\omega_j=\omega_j' := \frac{\prod_{i=1}^{k-1}(\lambda_{2i}-\lambda_{2j-1})}{\prod_{i\neq j}(\lambda_{2i-1}-\lambda_{2j-1})}.$$

This is turn determines T uniquely.

If $n=2k$ we construct the Jacobi matrix $S-\beta e_1 e_1^*$ from its spectrum $\{\lambda_{2j-1}\}_1^k$ with the weights

$$\begin{aligned}\omega_j=\omega_j^0 &:= \frac{\prod_{i=1}^{k}(\lambda_{2i}-\lambda_{2j-1})}{\prod_{i\neq j}(\lambda_{2i-1}-\lambda_{2j-1})} \\ &=(\lambda_n-\lambda_{2j-1})\,\omega_j'.\end{aligned}$$

This choice of weights ensures that $S+\beta e_1 e_1^*$ has spectrum $\{\lambda_{2j}\}_1^k$, where

$$2\beta=\beta_0^2=\sum_1^k \omega_j.$$

These relations determine T uniquely.

3. The Rutishauser-Kahan-Pal-Walker Algorithm

It is well-known, and will be easily shown in section four, that the Lanczos process is *manifestly numerically unstable*. This has been observed to some extent in [13], p. 293. The use of reorthogonalization [18, 7, 20, 5] enhances the numerical stability of the Lanczos process at the expense of additional work. In fact if each vector q'_{k+1} is reorthogonalized *at least once* against *all* the previous vectors $q_0, q_1, \ldots, q_k$ then we obtain an $O(n^3)$-process.

However, this added expense is unnecessary, for we shall presently show that Q can be computed, as a product of $n(n-1)/2$ plane rotations, and that T can be *reconstructed* with at most $6n^2$ arithmetic operations. This stabilization of the diagonal Hermitian Lanczos process is due in essence to Rutishauser [22]. When properly implemented it turns out to be even cheaper than the cheapest of the Lanczos processes. Rutishauser's algorithm seems to have been rather completely overlooked, perhaps because it was couched in the language of continued fractions. It has recently been rediscovered, and extended in a certain way to band matrices, by Biegler-König [3].

Let

$$d:=[\delta_i]_1^n\in\mathbb{R}^n$$

and

$$\Lambda:=\operatorname{diag}[\lambda_k]_1^n\in\mathbb{R}^{n\times n}.$$

It is a manifestation of the numerical stability of Rutishauser's process, to be studied experimentally in section four, that the *weights* $\omega_k=\delta_k^2$ are now not required to be positive, nor are the *abscissas* $\{\lambda_k\}_1^n$ required to be distinct. In this generality the problem of reconstructing T from d and Λ can be *ill-posed*; T need not be unique, even if its subdiagonal elements are restricted to be nonnegative. However, we can establish the existence of a suitable T by induction on n.

Suppose that

$$\begin{bmatrix}1 & \\ & Q^*\end{bmatrix}\begin{bmatrix}\alpha_0 & d^* \\ d & \Lambda\end{bmatrix}\begin{bmatrix}1 & \\ & Q\end{bmatrix}=\begin{bmatrix}\alpha_0 & \beta_0 e_1^* \\ \beta_0 e_1 & T\end{bmatrix} \tag{1}$$

with Q orthogonal and T (symmetric) tridiagonal with diagonal elements $\{\alpha_k\}_1^n$ and subdiagonal elements $\{\beta_k\}_1^{n-1}$. We shall show how to *update* β_0 and T when the pair (δ, λ) is adjoined to the data (d, Λ). Thus we show how to orthogonally tridiagonalize the matrix

$$\begin{bmatrix}\alpha_0 & \beta_0 e_1^* & \delta \\ \beta_0 e_1 & T & 0 \\ \delta & 0^* & \lambda\end{bmatrix}=\begin{bmatrix}1 & & \\ & Q^* & \\ & & 1\end{bmatrix}\begin{bmatrix}\alpha_0 & d^* & \delta \\ d & \Lambda & 0 \\ \delta & 0^* & \lambda\end{bmatrix}\begin{bmatrix}1 & & \\ & Q & \\ & & 1\end{bmatrix} \tag{2}$$

without changing α_0. We "chase" the common $(n+1,0)$ and $(0,n+1)$ element δ into positions $(n+1,n)$ and $(n,n+1)$ by means of a sequence of n orthogonal similarity transformations based on rotations in planes $(1,n+1)$, $(2,n+1),\ldots,(n,n+1)$, and implement the process in analogy with the Kahan-Pal-Walker formulation [20] of the shifted QR algorithm. We denote the corresponding updated matrix elements by $\{\bar{\alpha}_k\}_1^{n+1}$ and $\{\bar{\beta}_k\}_0^n$.

Consider the matrix

$$\begin{bmatrix} \bar{\alpha}_{k-1} & \beta'_{k-1} & 0^* & \delta_{k-1} \\ \beta'_{k-1} & \alpha_k & \beta_k e_1^* & \bar{\delta}_{k-1} \\ 0 & \beta_k e_1 & T_{k+1} & 0 \\ \delta_{k-1} & \bar{\delta}_{k-1} & 0^* & \lambda_{k-1} \end{bmatrix} \tag{3}$$

in which

$$\lambda_{k-1}=\lambda+\tau_{k-1}, \tag{4}$$

$$\begin{bmatrix} \beta'_{k-1} & \bar{\delta}_{k-1} \\ \delta_{k-1} & \tau_{k-1} \end{bmatrix} = \begin{bmatrix} \beta_{k-1} \\ \pi_{k-1} \end{bmatrix} [\gamma_{k-1}, \sigma_{k-1}], \tag{5}$$

$$\gamma_{k-1}^2+\sigma_{k-1}^2=1, \tag{6}$$

and T_{k+1} is the trailing principal submatrix of T of order $n-k$. Initially, for $k=1$, we have

$$\tau_0=0, \quad \gamma_0=1, \quad \sigma_0=0, \ \pi_0=\delta$$

and

$$\bar{\alpha}_0=\alpha_0, \quad \beta'_0=\beta_0, \quad \delta_0=\delta, \ \bar{\delta}_0=0.$$

Annihilate the element δ_{k-1} by means of a classical plane rotation applied to the second and last rows of (3). Thus choose γ_k and σ_k with

$$\gamma_k^2+\sigma_k^2=1 \tag{6'}$$

so that

$$\begin{bmatrix} \gamma_k & -\sigma_k \\ \sigma_k & \gamma_k \end{bmatrix} \begin{bmatrix} \beta'_{k-1} \\ \delta_{k-1} \end{bmatrix} = \begin{bmatrix} \bar{\beta}_{k-1} \\ 0 \end{bmatrix},$$

that is

$$\begin{bmatrix} \gamma_k & -\sigma_k \\ \sigma_k & \gamma_k \end{bmatrix} \begin{bmatrix} \beta_{k-1} \\ \pi_{k-1} \end{bmatrix} \gamma_{k-1} = \begin{bmatrix} \bar{\beta}_{k-1} \\ 0 \end{bmatrix}.$$

Put

$$\rho_k := (\beta_{k-1}^2+\pi_{k-1}^2)^{1/2}, \tag{7}$$

$$\gamma_k := \beta_{k-1}/\rho_k, \quad \sigma_k := -\pi_{k-1}/\rho_k \quad \text{if } \rho_k>0 \tag{8a}$$

and

$$\gamma_k := 1, \quad \sigma_k := 0 \quad \text{if } \rho_k=0. \tag{8b}$$

In either case

$$\bar{\beta}_{k-1} := \gamma_{k-1}\rho_k \tag{9}$$

and

$$\sigma_k \beta_{k-1}+\gamma_k \pi_{k-1}=0. \tag{10}$$

The vector $[\beta_k, 0]^*$ is transformed into

$$\begin{bmatrix} \beta'_k \\ \bar{\delta}_k \end{bmatrix} := \begin{bmatrix} \gamma_k & -\sigma_k \\ \sigma_k & \gamma_k \end{bmatrix} \begin{bmatrix} \beta_k \\ 0 \end{bmatrix};$$

hence

$$[\beta'_k, \bar{\delta}_k] = \beta_k [\gamma_k, \sigma_k]. \tag{5a'}$$

Complete the orthogonal similarity transformation of (3) to obtain the symmetric matrix

$$\begin{bmatrix} \bar{\alpha}_{k-1} & \bar{\beta}_{k-1} & 0^* & 0^* \\ \bar{\beta}_{k-1} & \bar{\alpha}_k & \beta'_k e_1^* & \delta_k \\ 0 & \beta'_k e_1 & T_{k+1} & \bar{\delta}_k e_1 \\ 0 & \delta_k & \bar{\delta}_k e_1^* & \lambda_k \end{bmatrix} \tag{3'}$$

in which

$$\begin{bmatrix} \bar{\alpha}_k & \delta_k \\ \delta_k & \lambda_k \end{bmatrix} := \begin{bmatrix} \gamma_k & -\sigma_k \\ \sigma_k & \gamma_k \end{bmatrix} \begin{bmatrix} \alpha_k & \bar{\delta}_{k-1} \\ \bar{\delta}_{k-1} & \lambda_{k-1} \end{bmatrix} \begin{bmatrix} \gamma_k & \sigma_k \\ -\sigma_k & \gamma_k \end{bmatrix}. \tag{11}$$

Some direct computations, using (4), (5), (6') and (10), now show that

$$\lambda_k = \lambda + \tau_k \tag{4'}$$

with

$$[\delta_k, \tau_k] := \pi_k [\gamma_k, \sigma_k], \tag{5b'}$$

$$\pi_k := \sigma_k (\alpha_k - \lambda) + \gamma_k \sigma_{k-1} \beta_{k-1}, \tag{12}$$

and

$$\tau_k = \sigma_k^2 (\alpha_k - \lambda) - \gamma_k^2 \tau_{k-1}. \tag{13}$$

Hence the matrix obtained from (3') by deleting the first row and column is of the form (3) with k increased by one. Finally, equality of the traces of the two similar matrices in (11) gives, on account of (4),

$$\bar{\alpha}_k = \alpha_k - (\tau_k - \tau_{k-1}). \tag{14}$$

The Kahan-Pal-Walker version of Rutishauser's algorithm for orthogonally tridiagonalizing the initial matrix (2), without changing α_0, is obtained by squaring equations (7), (8) and (9), computing τ_k from (13) and $\bar{\alpha}_k$ from (14), and noting from (5b'), (6') and (12) that

$$\begin{aligned} \pi_k^2 &= \tau_k^2 / \sigma_k^2 && \text{if } \sigma_k^2 > 0, \\ &= \sigma_{k-1}^2 \beta_{k-1}^2 && \text{if } \sigma_k^2 = 0. \end{aligned}$$

At the last step ($k = n$) the matrix T_{k+1} is empty so (5a') does not apply. Then, from (5b') and (4'),

$$\bar{\beta}_n^2 := \delta_n^2 = \gamma_n^2 \pi_n^2, \qquad \bar{\alpha}_{n+1} := \lambda_n = \lambda + \tau_n.$$

The same results are obtained by putting

$$\beta_n^2 := 0, \qquad \alpha_{n+1} := \lambda,$$

and running the algorithm to $k=n+1$. We summarize these results in

Algorithm RKPW:

input: $n, \{\alpha_k\}_1^n, \{\beta_k^2\}_0^{n-1}, \omega := \delta^2, \lambda,$
$\gamma_0^2=1, \beta_n^2=\sigma_0^2=\tau_0=0, \alpha_{n+1}=\lambda, \pi_0^2=\omega,$
for $k=1,2,3,\ldots,n+1$
  $\rho_k^2=\beta_{k-1}^2+\pi_{k-1}^2, \bar{\beta}_{k-1}^2=\gamma_{k-1}^2\rho_k^2,$
  if $\rho_k^2=0$ **then** $\gamma_k^2=1, \sigma_k^2=0$
  else $\gamma_k^2=\beta_{k-1}^2/\rho_k^2, \sigma_k^2=\pi_{k-1}^2/\rho_k^2,$
  $\tau_k=\sigma_k^2(\alpha_k-\lambda)-\gamma_k^2\tau_{k-1},$
  $\bar{\alpha}_k=\alpha_k-(\tau_k-\tau_{k-1}),$
  if $\sigma_k^2=0$ **then** $\pi_k^2=\sigma_{k-1}^2\beta_{k-1}^2$
  else $\pi_k^2=\tau_k^2/\sigma_k^2.$

This rational algorithm uses three divisions, four multiplications and five additions per step. By using it repeatedly we can orthogonally tridiagonalize the matrix

$$\begin{bmatrix} a_0 & d^* \\ d & \Lambda \end{bmatrix}: \; d\in\mathbb{R}^n, \quad \Lambda\in\mathbb{R}^{n\times n} \text{ diagonal}, \tag{15}$$

in at most $6n^2$ arithmetic operations (including n square roots). Equivalently, we can compute β_0 and a tridiagonal T so that there exists an orthogonal Q with

$$\Lambda Q=QT, \quad d=Qe_1\beta_0. \tag{16}$$

The rotations defining Q can be stored, using Stewart's scheme [24], in at most $n(n-1)/2$ storage locations. Hence Q can be applied to a vector in $O(n^2)$ operations. But forming Q elementwise would be an $O(n^3)$-process.

If a machine infinity is available then a variant of Reinsch type [20] can be based on the computation of $\{\eta_k\}$, with

$$\eta_0 := \infty, \quad \eta_k := \alpha_k-\lambda-\beta_k^2/\eta_{k-1}.$$

Then

$$\tau_k=\sigma_k^2\eta_k, \quad \pi_k^2=\tau_k\eta_k.$$

All apparant ambiguities can be resolved resulting in a savings of one multiplication per step. The algorithm appears (intuitively) to be numerically stable.

One problem, posed in [14] and treated in detail in [4], is that of computing the spectrum of $\Lambda\pm dd^*$. One solution, not considered in [14, 4], is to apply Rutishauser's algorithm. From (16) we see that the required spectrum is that of $T\pm\beta_0^2 e_1 e_1^*$. Likewise, the spectrum of the matrix (15) is that of the matrix (1). These tridiagonal problems can now be solved by the QR algorithm with Wilkinson's shift. We do not expect this approach to be as efficient as the refined techniques of [4, 6], but it does seem to be a primary alternative.

Although we shall not pursue the matter here, it is clear that Rutishauser's algorithm has important applications to the numerical construction of Gaussian quadrature formulas [11–13]. In fact, it supplies an elegant solution to the

problem mentioned in [13], p. 314. For C^∞ weight functions with compact support, it seems possible to combine it in a useful way with repeated Richardson extrapolation [2, 17].

Combining the RKPW algorithm with the results of section two we see that it is possible to *reconstruct* an $n \times n$ persymmetric Jacobi matrix from its spectrum with at most $5n^2/2$ arithmetic operations.

As in [3], using Rutishauser's algorithm, we can extend the considerations of section two to the case of multiple eigenvalues. Thus let

$$\lambda_1 \leqq \mu_1 \leqq \lambda_2 \leqq \ldots \leqq \mu_{n-1} \leqq \lambda_n \leqq \mu_n,$$

and let

$$\lambda_1 = \lambda_{\nu(1)} < \lambda_{\nu(2)} < \ldots < \lambda_{\nu(l)} = \lambda_n$$

be the distinct eigenvalues of T with $\lambda_{\nu(k)}$ having multiplicity

$$m(k) = \nu(k) - \nu(k-1) \quad \text{and} \quad \nu(0) := 0.$$

Then

$$\psi_n(\lambda) = \prod_{k=1}^{l} (\lambda - \lambda_{\nu(k)})^{m(k)},$$

$$\pi_n(\lambda) = \prod_{k=1}^{l} (\lambda - \lambda_{\nu(k)})^{m(k)-1} \prod_{k=1}^{l-1} (\lambda - \lambda_{\nu(k)}),$$

and

$$\chi_n(\lambda) = \prod_{k=1}^{l} (\lambda - \lambda_{\nu(k)})^{m(k)-1} \prod_{k=1}^{l} (\lambda - \mu_{\nu(k)}).$$

For the two basic problems of section two we can assign null values to all the weights except $\{\omega_{\nu(k)}\}_1^l$, with these weights (residues) having the respective values

$$\omega_{\nu(k)} = \omega'_{\nu(k)} := \frac{\prod_{j=1}^{l-1} (\mu_{\nu(j)} - \lambda_{\nu(k)})}{\prod_{j \neq k} (\lambda_{\nu(j)} - \lambda_{\nu(k)})}$$

or

$$\omega_{\nu(k)} = \omega^0_{\nu(k)} := (\mu_n - \lambda_{\nu(k)})\, \omega'_{\nu(k)}.$$

Numerically we consider two eigenvalues λ_i and λ_j as "equal" if

$$|\lambda_i - \lambda_j| \leqq \varepsilon \|T\|_2,$$

where ε is the basic machine unit. The integer l and the indices $\{\nu(k)\}_1^l$ are found by the following program:

$t = \max\{|\lambda_1|, |\lambda_n|\}$,
$l \leftarrow \nu(1) \leftarrow 1$,
if $n = 1$ **then go to** $l2$,
$l1$: **if** $|\lambda_{\nu(l)} - \lambda_{\nu(l)+1}| \leqq t\varepsilon$ **then** $\nu(l) \leftarrow \nu(l) + 1$
else $\nu(l+1) \leftarrow \nu(l) + 1$, $l \leftarrow l + 1$,
if $\nu(l) < n$ **then go to** $l1$,
$l2$: ....

4. Numerical Results

We implemented the three versions of the Lanczos process, denoted by LMGS, RL and RKPW, respectively, in double precision FORTRAN on an IBM 370. Our first four experiments are concerned with these implementations which execute the transformation

$$(\{v_k^2\}, \{\lambda_k\}) \to \bar{T}$$

of the normalized weights and abscissas into a computed real symmetric tridiagonal matrix $\bar{T}$ with diagonal elements $\{\bar{\alpha}_k\}$ and nonnegative subdiagonal elements $\{\bar{\beta}_k\}$.

In the first two experiments the unnormalized weights $\{\omega_k\}$ are specified; the normalized weights $\{v_k^2\}$ were computed from these in quadruple precision followed by rounding to double precision.

In the second two experiments Jacobi matrices T, with diagonal elements $\{\alpha_k\}$ and subdiagonal elements $\{\beta_k\}$, are specified. The normalized weights and abscissas were obtained by applying a quadruple precision version of the Golub-Welsch algorithm [16] to T and rounding the results to double precision. For this we used the appropriate modification of *imtql2* [26].

We also used this version of *imtql2*, applied to $\bar{T}$, to assess the errors in our computations. Thus we accepted its quadruple precision results, $\{\bar{v}_k^2\}$ and $\{\bar{\lambda}_k\}$, as the true normalized weights and abscissas associated with the computed matrix T'.

Let $\bar{u} := [\bar{v}_1, \bar{v}_2, \ldots, \bar{v}_n]^T$ and $\bar{l} := [\bar{\lambda}_1, \bar{\lambda}_2, \ldots, \bar{\lambda}_n]^T$. In Tables 1–4 the columns denoted by T, ω and λ give the number of correct decimal digits in $\bar{T}/\|T\|_2$, $\bar{u} \circ \bar{u}$ and $\bar{l}/\|T\|_2$, respectively. More precisely, these columns represent the nearest integers to the negative logarithms (base 10) of the following errors:

$$e_T := \max\{|\alpha_k - \bar{\alpha}_k|, |\beta_k - \bar{\beta}_k|\}/\|T\|_2,$$
$$e_\omega := \max|v_k^2 - \bar{v}_k^2|,$$
$$e_\lambda := \max|\lambda_k - \bar{\lambda}_k|/\|T\|_2.$$

Of course we have $\|T\|_2 = \max|\lambda_k|$.

It is easy to give examples which exhibit the numerical instability of the two classical Lanczos processes. For this one (nearly) violates the assumption that the weights are all positive and the eigenvalues are all distinct.

Experiment 1. Table 1 gives the results for the "reconstruction" of tridiagonal matrices of orders $n = 10$, 30, and 50 from the data

$$\omega_{2k-1} \equiv 1, \quad \omega_{2k} \equiv \varepsilon, \quad \lambda_k = k - 1,$$

for the cases $\varepsilon = 10^{-6}$ and $\varepsilon = 0$. For $\varepsilon = 10^{-6}$ both RL and LMGS have partially deteriorated, in the eigenvalues only, at $n = 30$. This deterioration is complete by $n = 50$.

Table 1

ε	n	RL		LMGS		RKPW	
		ω	λ	ω	λ	ω	λ
10^{-6}	10	16	15	16	16	16	16
	30	15	11	16	10	16	16
	50	*	*	2	2	16	15
0	10	1	1	1	1	16	17
	30	1	2	1	2	16	16
	50	2	2	2	2	16	16

An asterisk (*) denotes failure of our version of the algorithm. The RKPW algorithm is stable in all cases.

Experiment 2. Table 2 contains results for the data

$$\omega_k \equiv 1, \quad \lambda_{2k-1} = k-1, \quad \lambda_{2k} = k-1+\varepsilon$$

with $\varepsilon = 10^{-5}$, $\varepsilon = 10^{-10}$ and $\varepsilon = 0$. Here we have (nearly) double eigenvalues.

Table 2

ε	n	RL			LMGS			RKPW		
		ω	$\tilde{\omega}$	λ	ω	$\tilde{\omega}$	λ	ω	$\tilde{\omega}$	λ
10^{-5}	30	11	15	16	11	16	16	11	16	16
	40	6	15	11	7	16	12	11	16	16
	50	2	15	7	2	16	6	11	16	16
	60	*	*	*	2	2	2	11	16	16
10^{-10}	30	5	16	15	6	16	16	6	16	16
	40	2	15	11	2	16	11	6	16	16
	50	2	15	5	2	16	5	6	16	16
	60	2	2	2	2	2	2	6	16	15
0	30	2	16	15	2	16	16	2	16	16
	40	2	15	8	2	16	10	2	16	16
	50	2	15	4	2	4	2	2	16	15
	60	2	2	2	2	3	2	2	16	15

Algorithms RL and LMGS are clearly unstable. In all cases algorithm RKPW reproduces the eigenvalues accurately, with the deterioration in the weights being consistent with the perturbation theory [25, 8, 23] for the Hermitian eigenvalue problem. The $\tilde{\omega}$-columns contain the information analogous to that in the ω-columns, but now for the sums of pairs of weights

$$\tilde{v}_k^2 := v_{2k-1}^2 + v_{2k}^2.$$

These quantities are computed accurately by algorithm RKPW, but not by the other algorithms.

Experiment 3. Table 3 gives results for $n \times n$ tridiagonal matrices T_n with elements

$$\alpha_{n,k} = 1 + \frac{k-1}{n}, \qquad \beta_{n,k} = \frac{k}{n}.$$

This is essentially the same example as the third example of de Boor and Golub [9] who experienced difficulty in single precision for $n=30$ with their version of algorithm RL. The matrices T_n are positive definite with spectra in the interval (0, 4). The weights $\omega_{n,k} = v_{n,k}^2$ are initially increasing with k until $\lambda_{n,k} \doteq 1$, and then decreasing thereafter. For $n=50$ the computed weights vary in order of magnitude from 10^{-69} to 10^{-1}. After $n=50$ some underflow and are set to zero.

Table 3

n	RL			LMGS			RKPW		
	T	ω	λ	T	ω	λ	T	ω	λ
10	15	16	16	16	16	16	16	15	15
40	15	15	16	15	15	16	15	15	15
50	14	15	15	15	15	16	1	14	15
80	14	15	15	15	14	16	1	15	15
90	3	3	4	15	14	16	0	14	15
100	0	1	−1	7	14	16	0	14	15
110	*	*	*	1	14	2	0	14	15
120				1	1	1	0	14	15
300							0	13	15
500							0	13	15

With our double precision version of algorithm RL the instability is delayed until $n=90$. The results for algorithm LMGS are interesting. The computed matrix $\bar{T}_n$ is inaccurate for $n=100$, although the weights and abscissas are determined accurately in this case; the abscissas are completely inaccurate for $n=110$, and for $n=120$ the deterioration is total.

The RKPW algorithm is numerically stable in all cases, although there is a very mild deterioration in the weights which is related to the results of experiment 2. Even though the computed matrices $\bar{T}_n$ are completely inaccurate for $n \geqq 50$, their associated weights and abscissas are accurate up to $n=500$ (and further). The problem of reconstructing T_n from the weights and abscissas is *ill-conditioned.*

Experiment 4. Table 4 gives the corresponding results for the *Laguerre* tridiagonal matrices T_n with

$$\alpha_k = 2k-1, \qquad \beta_k = k.$$

The results are qualitatively the same as in experiment 3.

Table 4

n	RL			LMGS			RKPW		
	T	ω	λ	T	ω	λ	T	ω	λ
10	16	15	16	16	16	16	16	15	16
20	15	15	16	16	16	16	15	15	16
30	15	15	16	16	15	16	1	15	16
40	*	*	*	16	15	16	1	14	16
80				15	15	16	1	14	16
90				8	15	16	1	14	16
100				1	14	1	1	14	16
110				1	1	1	1	14	16
300							1	14	17
500							1	13	17

Our final two experiments concern the construction of symmetric persymmetric tridiagonal matrices, with nonnegative subdiagonal elements, with prescribed spectra. Here we use the RKPW algorithm together with the results of sections two and three. In particular, the case of multiple eigenvalues is treated. These computations were done in *single precision* FORTRAN on a VAX 11/750, with a double precision version of *imtql1* [26] used to compute the errors.

Experiment 5. For $m=1$ and $m=5$ Table 5 gives the errors $e_{m,n}:=e_{T(m,n)}$ in the construction of $n\times n$ matrices $T(m,n)$ with eigenvalues

$$\lambda_k=k-1, \qquad k=1,2,\ldots,n/m,$$

Table 5

n	$e_{1,n}$	$e_{5,n}$
1000	1.709_{10-6}	3.512_{10-7}
2000	3.371_{10-6}	7.071_{10-7}
3000	5.207_{10-6}	1.050_{10-6}
4000	6.735_{10-6}	1.397_{10-6}

each of multiplicity m. Least squares fits of the data $(\log n, \log e_{m,n})$ by linear functions $\alpha+\beta n$, on this and even more extensive data, show that the errors $e_{m,n}$ grow almost exactly linearly with n. For this data the *exponents* β are 0.998 and 0.995 for $m=1$ and $m=5$, respectively. This is interesting since the RKPW algorithm, coupled with that for generating the weights, is an $O(n^2)$-process. For $m=5$ we ran this example up to $n=10{,}000$ with error 3.396_{10-6}.

Experiment 6. The corresponding results for $n\times n$ matrices $T(m,n)$ with eigenvalues

$$\lambda_k=1/k, \qquad k=1,2,\ldots,n/m,$$

each of multiplicity m, are given in Table 6. In this case the errors $e_{m,n}$ appear to be "essentially bounded".

Table 6

n	$e_{1,n}$	$e_{5,n}$
1000	4.764_{10-7}	5.814_{10-8}
2000	2.655_{10-7}	1.391_{10-7}
3000	6.395_{10-8}	1.145_{10-7}
4000	2.804_{10-7}	1.293_{10-7}

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