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SOME MODIFIED MATRIX EIGENVALUE PROBLEMS*

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Dedicated to the memory of Professor H. Rutishauser

Abstract. We consider the numerical calculation of several matrix eigenvalue problems which require some manipulation before the standard algorithms may be used. This includes finding the stationary values of a quadratic form subject to linear constraints and determining the eigenvalues of a matrix which is modified by a matrix of rank one. We also consider several inverse eigenvalue problems. This includes the problem of determining the coefficients for the Gauss–Radau and Gauss–Lobatto quadrature rules. In addition, we study several eigenvalue problems which arise in least squares.

Introduction and notation. In the last several years, there has been a great development in devising and analyzing algorithms for computing eigensystems of matrix equations. In particular, the works of H. Rutishauser and J. H. Wilkinson have had great influence on the development of this subject. It often happens in applied situations that one wishes to compute the eigensystem of a slightly modified system or one wishes to specify some of the eigenvalues and then compute an associated matrix. In this paper we shall consider some of these problems and also some statistical problems which lead to interesting eigenvalue problems. In general, we show how to reduce the modified problems to standard eigenvalue problems so that the standard algorithms may be used. We assume that the reader has some familiarity with some of the standard techniques for computing eigensystems.

We ordinarily indicate matrices by capital letters such as A, B, Σ; vectors by boldface lower-case letters such as $\mathbf{x}$, $\mathbf{y}$, $\boldsymbol{\alpha}$, and scalars by lower-case letters. We indicate the eigenvalues of a matrix as $\lambda(X)$ where X may be an expression, e.g., $\lambda(A^2 + I)$ indicates the eigenvalues of $A^2 + I$, and in a similar fashion we indicate the singular values of a matrix by $\sigma(X)$. We assume that the reader has some familiarity with singular values (cf. [9]). Usually we order the singular values $\sigma(A) = [\lambda(A^TA)]^{1/2}$ of a matrix A so that $\sigma_1(A) \leqq \sigma_2(A) \leqq \cdots \leqq \sigma_n(A)$ and if A is symmetric, the eigenvalues so that $\lambda_1(A) \leqq \lambda_2(A) \leqq \cdots \leqq \lambda_n(A)$.

1. Stationary values of a quadratic form subject to linear constraints. Let A be a real symmetric matrix of order n, and $\mathbf{c}$ a given vector with $\mathbf{c}^T\mathbf{c} = 1$.

In many applications (cf. [10]) it is desirable to find the stationary values of

$$\mathbf{x}^T A\mathbf{x} \tag{1.1}$$

subject to the constraints

$$\mathbf{x}^T\mathbf{x} = 1, \tag{1.2}$$

$$\mathbf{c}^T\mathbf{x} = 0. \tag{1.3}$$

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Let

$$\varphi(\mathbf{x}, \lambda, \mu) = \mathbf{x}^T A\mathbf{x} - \lambda(\mathbf{x}^T\mathbf{x} - 1) + 2\mu\mathbf{x}^T\mathbf{c}, \tag{1.4}$$

where λ, μ are Lagrange multipliers. Differentiating (1.4), we are led to the equation

$$A\mathbf{x} - \lambda\mathbf{x} + \mu\mathbf{c} = \mathbf{0}. \tag{1.5}$$

Multiplying (1.5) on the left by $\mathbf{c}^T$ and using the condition that $\|\mathbf{c}\|_2 = 1$, we have

$$\mu = -\mathbf{c}^T A\mathbf{x}. \tag{1.6}$$

Then substituting (1.6) into (1.5), we obtain

$$PA\mathbf{x} = \lambda\mathbf{x}, \tag{1.7}$$

where $P = I - \mathbf{c}\mathbf{c}^T$. Although P and A are symmetric, PA is not necessarily so. Note that $P^2 = P$, so that P is a projection matrix.

It is well known (cf. [14, p. 54]) that for two arbitrary square matrices G and H, the eigenvalues of GH equal the eigenvalues of HG. Thus,

$$\lambda(PA) = \lambda(P^2A) = \lambda(PAP).$$

The matrix PAP is symmetric and hence one can use one of the standard algorithms for finding its eigenvalues. Then if

$$K = PAP$$

and if

$$K\mathbf{z}_i = \lambda_i\mathbf{z}_i,$$

it follows that

$$\mathbf{x}_i = P\mathbf{z}_i, \qquad i = 1, 2, \cdots, n,$$

where $\mathbf{x}_i$ is the eigenvector which satisfies (1.7). At least one eigenvalue of K will be equal to zero, and $\mathbf{c}$ will be an eigenvector associated with a zero eigenvalue.

Now suppose we replace the constraint (1.3) by the set of constraints

$$C^T\mathbf{x} = \mathbf{0}, \tag{1.8}$$

where C is an $n \times p$ matrix of rank r. It can be verified that if

$$P = I - CC^-, \tag{1.9}$$

where C^- is a generalized inverse which satisfies

$$CC^-C = C, \qquad CC^- = (CC^-)^T, \tag{1.10}$$

then the stationary values of $\mathbf{x}^T A\mathbf{x}$ subject to (1.2) and (1.8) are eigenvalues of $K = PAP$. At least r of the eigenvalues of K will be equal to zero, and hence it would be desirable to deflate the matrix K so that these eigenvalues are eliminated.

By permuting the columns of C, we may compute the orthogonal decomposition

$$C = Q^T\begin{bmatrix} R & S \\ 0 & 0 \end{bmatrix}\Pi, \tag{1.11}$$

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where R is an upper triangular matrix of order r, S is $r \times (p - r)$, $Q^TQ = I_n$, and Π is a permutation matrix. The matrix Q may be constructed as the product of r Householder transformations (cf. [8]). A simple calculation shows

$$P = Q^T \begin{bmatrix} 0 & 0 \\ 0 & I_{n-r} \end{bmatrix} Q \equiv Q^T J Q, \tag{1.12}$$

and thus

$$\lambda(PAP) = \lambda(Q^TJQAQ^TJQ) = \lambda(JQAQ^TJ).$$

Then if

$$G = QAQ^T = \begin{bmatrix} G_{11} & G_{12} \\ G_{12}^T & G_{22} \end{bmatrix}, \tag{1.13}$$

where G_{11} is an $r \times r$ matrix and G_{22} is an $(n - r) \times (n - r)$ matrix,

$$JQAQ^TJ = \begin{bmatrix} 0 & 0 \\ 0 & G_{22} \end{bmatrix}.$$

Hence the stationary values of $\mathbf{x}^TA\mathbf{x}$ subject to (1.2) and (1.8) are simply the eigenvalues of the $(n - r) \times (n - r)$ matrix G_{22}. Finally, if

$$G_{22}\mathbf{z}_i = \lambda_i \mathbf{z}_i, \qquad i = 1, 2, \cdots, n - r,$$

then

$$\mathbf{x}_i = Q^T \begin{bmatrix} 0 \\ I_{n-r} \end{bmatrix} \mathbf{z}_i.$$

The details of the algorithm are given in [10].

From (1.13) we see that $\lambda(G) = \lambda(A)$. Then by the Courant–Fischer theorem (cf. [14, p. 101]),

$$\lambda_j(A) \leqq \lambda_j(G_{22}) \leqq \lambda_{r+j}(A), \qquad j = 1, 2, \cdots, n - r, \tag{1.14}$$

when

$$\lambda_j(A) \leqq \lambda_{j+1}(A) \quad \text{and} \quad \lambda_j(G_{22}) \leqq \lambda_{j+1}(G_{22}).$$

Furthermore, if the columns of the matrix C span the same space as the r eigenvectors associated with the r smallest eigenvalues of A,

$$\lambda_j(G_{22}) = \lambda_{r+j}(A). \tag{1.15}$$

Thus, we see that there is a strong relationship between the eigenvalues of A and the stationary values of the function

$$\varphi(\mathbf{x}, \lambda, \boldsymbol{\mu}) = \mathbf{x}^TA\mathbf{x} - \lambda(\mathbf{x}^T\mathbf{x} - 1) + 2\boldsymbol{\mu}^TC^T\mathbf{x}, \tag{1.16}$$

where $\boldsymbol{\mu}$ is a vector of Lagrange multipliers.

2. Stationary values of a bilinear form subject to linear constraints. Now let us consider the problem of determining the nonnegative stationary values of

$$(\mathbf{x}^TA\mathbf{y})/(\|\mathbf{x}\|_2\|\mathbf{y}\|_2), \tag{2.1}$$

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where A is an $m \times n$ matrix, subject to the constraints

$$C^T\mathbf{x} = \mathbf{0}, \qquad D^T\mathbf{y} = \mathbf{0}. \tag{2.2}$$

The nonnegative stationary values of (2.1) are the singular values of A (i.e., $\sigma(A) = [\lambda(A^TA)]^{1/2}$). It is easy to verify that the nonnegative stationary values of (2.1) subject to (2.2) are the singular values of

$$P_CAP_D\,, \tag{2.3}$$

where

$$P_C = I - CC^-, \qquad P_D = I - DD^-.$$

The singular values of P_CAP_D can be computed using the algorithm given in [9].

Again it is not necessary to compute the matrices P_C and P_D explicitly. If, as in (1.11),

$$C = Q_C^T\begin{bmatrix} R_C & S_C \\ 0 & 0 \end{bmatrix}\Pi_C, \qquad D = Q_D^T\begin{bmatrix} R_D & S_D \\ 0 & 0 \end{bmatrix}\Pi_D,$$

then

$$P_C = Q_C^T\begin{bmatrix} 0 & 0 \\ 0 & I_{n-r} \end{bmatrix}Q_C \equiv Q_C^TJ_CQ_C,$$

$$P_D = Q_D^T\begin{bmatrix} 0 & 0 \\ 0 & I_{n-s} \end{bmatrix}Q_D \equiv Q_D^TJ_DQ_D,$$

where r is the rank of C and s is the rank of D. Then

$$\begin{aligned}\sigma(P_CAP_D) &= \sigma(Q_C^TJ_CQ_CAQ_D^TJ_DQ_D) \\ &= \sigma(J_CQ_CAQ_D^TJ_D).\end{aligned}$$

Hence if

$$G = Q_CAQ_D^T = \begin{bmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{bmatrix},$$

where G_{11} is $r \times s$ and G_{22} is $(m-r) \times (n-s)$, then

$$J_CQ_CAQ_D^TJ_D = \begin{bmatrix} 0 & 0 \\ 0 & G_{22} \end{bmatrix}.$$

Thus the desired stationary values are the singular values of G_{22}.

3. Some inverse eigenvalue problems. Suppose we are given a symmetric matrix A with eigenvalues $\{\lambda_i\}_{i=1}^n$ $(\lambda_i < \lambda_{i+1})$ and we are given a set of values $\{\bar{\lambda}_i\}_{i=1}^{n-1}$ $(\bar{\lambda}_i < \bar{\lambda}_{i+1})$ with

$$\lambda_i < \bar{\lambda}_i < \lambda_{i+1}. \tag{3.1}$$

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We wish to determine the linear constraint $\mathbf{c}^T\mathbf{x} = 0$ so that the stationary values of $\mathbf{x}^T A\mathbf{x}$ subject to $\mathbf{x}^T\mathbf{x} = 1$ and $\mathbf{c}^T\mathbf{x} = 0$ ($\mathbf{c}^T\mathbf{c} = 1$) are the set of $\{\bar{\lambda}_i\}_{i=1}^{n-1}$. From (1.5) we have

$$\mathbf{x} = -\mu(A - \lambda I)^{-1}\mathbf{c},$$

and hence,

$$\mathbf{c}^T\mathbf{x} = -\mu\mathbf{c}^T(A - \lambda I)^{-1}\mathbf{c} = 0. \tag{3.2}$$

Assuming $\mu \neq 0$, and given $A = Q\Lambda Q^T$ where Λ is the diagonal matrix of eigenvalues of A and Q is the matrix of orthonormalized eigenvectors, substitution into (3.2) gives

$$\sum_{i=1}^{n} \frac{d_i^2}{(\lambda_i - \lambda)} = 0 \tag{3.3a}$$

with

$$\sum_{i=1}^{n} d_i^2 = 1 \tag{3.3b}$$

where $Q\mathbf{d} = \mathbf{c}$. Setting $\lambda = \bar{\lambda}_j$, $j = 1, 2, \cdots, n-1$, then leads to a system of linear equations defining the d_i^2. We shall, however, give an explicit solution to this system.

Let the characteristic polynomial be

$$\varphi(\lambda) = \prod_{j=1}^{n-1} (\bar{\lambda}_j - \lambda). \tag{3.4}$$

We convert the rational form (3.3a) to a polynomial,

$$\begin{aligned} \psi(\lambda) &\equiv \prod_{j=1}^{n} (\lambda_j - \lambda)\left[\sum_{i=1}^{n} \frac{d_i^2}{(\lambda_i - \lambda)}\right] \\ &= \sum_{i=1}^{n} d_i^2 \prod_{\substack{j=1 \\ j\neq i}}^{n} (\lambda_j - \lambda). \end{aligned} \tag{3.5}$$

We wish to compute $\mathbf{d}$ ($\mathbf{d}^T\mathbf{d} = 1$) so that $\psi(\lambda) \equiv \varphi(\lambda)$. Then let us equate the two polynomials at n points. Now

$$\varphi(\lambda_k) = \prod_{j=1}^{n-1} (\bar{\lambda}_j - \lambda_k),$$

$$\psi(\lambda_k) = d_k^2 \prod_{\substack{j=1 \\ j\neq k}}^{n} (\lambda_j - \lambda_k).$$

Hence $\varphi(\lambda_k) = \psi(\lambda_k)$ for $k = 1, 2, \cdots, n$, if

$$d_k^2 = \frac{\prod_{j=1}^{n-1} (\bar{\lambda}_j - \lambda_k)}{\prod_{j=1, j\neq k}^{n} (\lambda_j - \lambda_k)}. \tag{3.6}$$

The condition (3.1) guarantees that the right-hand side of (3.6) will be positive. Note that we may assign d_k a positive or negative value so that there are 2^n different solutions. Once the vector $\mathbf{d}$ has been computed, it is an easy matter to compute $\mathbf{c}$.

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We have seen in § 1 that the stationary values of (1.16) interlace the eigenvalues of A. In certain statistical applications [4] the following problem arises. Given a matrix A and an $n \times p$ matrix C, we wish to find an orthogonal matrix H so that the stationary values of

$$\varphi(\mathbf{x}, \lambda, \boldsymbol{\mu}) = \mathbf{x}^T A\mathbf{x} - \lambda(\mathbf{x}^T\mathbf{x} - 1) + \boldsymbol{\mu}^T(HC)^T\mathbf{x} \tag{3.7}$$

are equal to the $n - r$ largest eigenvalues of A.

As was pointed out in the last paragraph of § 1, the stationary values of (3.7) will be equal to the $n - r$ largest eigenvalues of A providing the columns of HC span the space associated with the r smallest eigenvalues of A. For simplicity, we assume that rank $(C) = p$. From (1.11), we see that we may write

$$C = Q^T\begin{bmatrix} R \\ 0 \end{bmatrix}.$$

Let us assume that the columns of some $n \times p$ matrix V span the same space as eigenvectors associated with the p smallest eigenvalues. We can construct the decomposition

$$V = W^T\begin{bmatrix} S \\ 0 \end{bmatrix},$$

where $W^TW = I_n$ and S is upper triangular. Then the constraints

$$(HC)^T\mathbf{x} = \mathbf{0}$$

are equivalent to

$$[R^T \vdots 0]QH^T\mathbf{x} = \mathbf{0},$$

and thus if H is chosen to be

$$H = W^TQ,$$

the stationary values of (3.7) will be equal to the $n - p$ largest eigenvalues of A.

4. Intersection of spaces. Suppose we are given two symmetric $n \times n$ matrices A and B with B positive definite and we wish to compute the eigensystem for

$$A\mathbf{x} = \lambda B\mathbf{x}. \tag{4.1}$$

One ordinarily avoids computing $C = B^{-1}A$ since the matrix C is usually not symmetric. Since B is positive definite, it is possible to compute a matrix F such that

$$F^TBF = I$$

and we can verify from the determinantal equation that

$$\lambda(F^TAF) = \lambda(B^{-1}A).$$

The matrix F^TAF is symmetric and hence one of the standard algorithms may be used for computing its eigenvalues.

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Now let us consider the following example. Suppose

$$A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \qquad B = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \varepsilon & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

where ε is a small positive value. Note B is no longer positive definite. When $\mathbf{x}^T = [1, 0, 0]$, then $A\mathbf{x} = B\mathbf{x}$ and hence $\lambda = 1$. When $\mathbf{x}^T = [0, 1, 0]$, then $A\mathbf{x} = \varepsilon^{-1}B\mathbf{x}$. Here $\lambda = \varepsilon^{-1}$ and hence as ε gets arbitrarily small, $\lambda(\varepsilon)$ becomes arbitrarily large. This eigenvalue is unstable; such problems have been carefully studied by Fix and Heiberger [5]. Finally for $\mathbf{x}^T = [0, 0, 1]$, $A\mathbf{x} = \lambda B\mathbf{x}$ for all values of λ. Thus we have the situation of continuous eigenvalues. We shall now examine ways of eliminating the problem of continuous eigenvalues.

The eigenvalue problem $A\mathbf{x} = \lambda B\mathbf{x}$ can have continuous eigenvalues if the null space associated with A and the null space associated with B intersect. Therefore we wish to determine a basis for the intersection of these two null spaces. Let us assume we have determined X and Y so that

$$AX = 0, \qquad BY = 0$$

with

$$X^T X = I_p \quad \text{and} \quad Y^T Y = I_q. \tag{4.2}$$

Let

$$Z = [X \vdots Y]. \tag{4.3}$$

Suppose H is an $n \times v$ basis for the null space of Z with

$$H = \begin{bmatrix} E \\ \cdots \\ F \end{bmatrix},$$

where E is $p \times v$ and F is $q \times v$. Then

$$ZH = XE + YF = 0.$$

Hence the nullity of Z determines the rank of the basis for the intersection of the two spaces.

Consider the matrix

$$L = Z^T Z.$$

Note nullity(L) = nullity(Z). From (4.3), we see that

$$L = \begin{bmatrix} I_p & X^T Y \\ Y^T X & I_q \end{bmatrix} \equiv I_{p+q} + \begin{bmatrix} 0_p & T \\ T^T & 0_q \end{bmatrix} \equiv I_{p+q} + W. \tag{4.4}$$

Since $\lambda(L) = \lambda(I + W) = 1 + \lambda(W)$,

$$\lambda(L) = 1 \pm \sigma(T). \tag{4.5}$$

Therefore, if $\sigma_j(T) = 1$ for $j = 1, 2, \cdots, t$, from (4.5) we see that the nullity $(L) = t$.

Consider the singular value decomposition of the matrix

$$T = X^T Y = U \Sigma V^T,$$

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where

$$U = [\mathbf{u}_1, \cdots, \mathbf{u}_p], \qquad V = [\mathbf{v}_1, \cdots, \mathbf{v}_q].$$

The matrices $\tilde{X} = XU$ and $\tilde{Y} = YV$ yield orthonormal bases for the null space of the matrices A and B, respectively. Since $\sigma(T) = 1$ for $j = 1, \cdots, t$,

$$\tilde{\mathbf{x}}_j = X\mathbf{u}_j = Y\mathbf{v}_j = \tilde{\mathbf{y}}_j \quad \text{for } j = 1, \cdots, t,$$

and thus the vectors $\{\tilde{\mathbf{x}}_j\}_{j=1}^t$ yield a basis for the intersection of the two spaces.

The singular values of X^TY can be thought of as the cosines between the spaces generated by X and Y. An analysis of the numerical methods for computing angles between linear subspaces is given in [2]. There are other techniques for computing a basis for the intersection of the subspaces, but the advantage of this method is that it also gives a way of finding vectors which are *almost* in the intersection of the subspaces.

5. Eigenvalues of a matrix modified by a rank one matrix. It is sometimes desirable to determine some eigenvalues of a diagonal matrix which is modified by a matrix of rank one. In this section, we give an algorithm for determining in $O(n^2)$ numerical operations some or all of the eigenvalues and eigenvectors of $D + \sigma\mathbf{u}\mathbf{u}^T$, where $D = \operatorname{diag}(d_i)$ is a diagonal matrix of order n.

Let $C = D + \sigma\mathbf{u}\mathbf{u}^T$; we denote the eigenvalues of C by $\lambda_1, \lambda_2, \cdots, \lambda_n$ and we assume $\lambda_i \leqq \lambda_{i+1}$ and $d_i \leqq d_{i+1}$. It can be shown (cf. [14]) that

(i) if $\sigma \geqq 0$,

$$d_i \leqq \lambda_i \leqq d_{i+1}, \qquad i = 1, 2, \cdots, n-1,$$
$$d_n \leqq \lambda_n \leqq d_n + \sigma\mathbf{u}^T\mathbf{u};$$

(ii) if $\sigma \leqq 0$,

$$d_{i-1} \leqq \lambda_i \leqq d_i, \qquad i = 2, \cdots, n,$$
$$d_1 + \sigma\mathbf{u}^T\mathbf{u} \leqq \lambda_1 \leqq d_1.$$

Thus, we have precise bounds on each of the eigenvalues of C.

The eigenvalues of the matrix C satisfy the equation

$$\det(D + \sigma\mathbf{u}\mathbf{u}^T - \lambda I) = 0,$$

which after some manipulation can be shown to be equivalent to the characteristic equation

$$\varphi_n(\lambda) = \prod_{i=1}^{n} (d_i - \lambda) + \sigma \sum_{i=1}^{n} u_i^2 \prod_{\substack{j=1 \\ j \neq i}}^{n} (d_j - \lambda) = 0. \tag{5.1}$$

Now if we write

$$\varphi_k(\lambda) = \prod_{i=1}^{k} (d_i - \lambda) + \sigma \sum_{i=1}^{k} u_i^2 \prod_{\substack{j=1 \\ j \neq i}}^{k} (d_j - \lambda),$$

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then it is easy to verify that

$$\begin{aligned} \varphi_{k+1}(\lambda) &= (d_{k+1} - \lambda)\varphi_k(\lambda) + \sigma u_{k+1}^2 \psi_k(\lambda), && k = 0, 1, \cdots, n-1, \\ \psi_k(\lambda) &= (d_k - \lambda)\psi_{k-1}(\lambda), && k = 1, 2, \cdots, n-1, \end{aligned} \tag{5.2}$$

with

$$\psi_0(\lambda) = \varphi_0(\lambda) = 1.$$

Thus it is a simple matter to evaluate the characteristic equation for any value of λ. Several well-known methods may be used for computing the eigenvalues of C. For instance, it is a simple matter to differentiate the expressions (5.2) with respect to λ and hence determine $\varphi_n'(\lambda)$ for any value of λ. Thus Newton's method can be used in an effective manner for computing the eigenvalues.

An alternative method has been given in [1] and we shall describe that technique. Let K be a bidiagonal matrix of the form

$$K = \begin{bmatrix} 1 & r_1 & & & & \\ & 1 & r_2 & & 0 & \\ & & \cdot & \cdot & & \\ & & & \cdot & \cdot & \\ & & & & \cdot & \cdot \\ & 0 & & & \cdot & r_{n-1} \\ & & & & & 1 \end{bmatrix},$$

and let $M = \operatorname{diag}(\mu_i)$. Then KMK^T is a symmetric tridiagonal matrix with elements $\{\mu_k r_{k-1}, (\mu_k + \mu_{k+1} r_k^2), \mu_{k+1} r_k\}_{k=1}^n$, $r_0 = r_n = \mu_{n+1} = 0$.

Consider the matrix equation

$$(D + \sigma \mathbf{u}\mathbf{u}^T)\mathbf{x} = \lambda \mathbf{x}. \tag{5.3}$$

Multiplying (5.3) on the left by K and letting $\mathbf{x} = K^T\mathbf{y}$, we have

$$K(D + \sigma \mathbf{u}\mathbf{u}^T)K^T\mathbf{y} = \lambda K K^T \mathbf{y}$$

or

$$(KDK^T + \sigma K\mathbf{u}\mathbf{u}^T K^T)\mathbf{y} = \lambda K K^T \mathbf{y}.$$

Let us assume that we have reordered the elements of $\mathbf{u}$ (and hence of D, also) so that

$$u_1 = u_2 = \cdots = u_{p-1} = 0 \quad \text{and} \quad 0 < |u_p| \leqq |u_{p+1}| \leqq \cdots \leqq |u_n|.$$

Now it is possible to determine the elements of K so that

$$K\mathbf{u} = \begin{bmatrix} 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \\ u_n \end{bmatrix}. \tag{5.4}$$

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Specifically,

$$r_i = \begin{cases} 0 & \text{for } i < p, \\ -u_i/u_{i+1} & \text{for } i \geqq p, \end{cases}$$

and we note $|r_i| \leqq 1$. Therefore, if $K\mathbf{u}$ satisfies (5.4), we see that $KDK^T + \sigma K\mathbf{u}\mathbf{u}^T K^T$ is a symmetric tridiagonal matrix and so is KK^T. Thus we have a problem of the form $A\mathbf{y} = \lambda B\mathbf{y}$, where A and B are symmetric, tridiagonal matrices and B is positive definite.

Peters and Wilkinson [13] have shown how linear interpolation may be used effectively for computing the eigenvalues of such matrices when the eigenvalues are isolated. The algorithm makes use of $\det(A - \lambda B)$ which is quite simple to compute when A and B are tridiagonal. Once the eigenvalues have been computed it is easy to compute the eigenvectors by inverse iteration. Even if several of the eigenvalues are equal, it is often possible to compute accurate eigenvectors. This can be accomplished by choosing the initial vector in the inverse iteration process to be orthogonal to all the previously computed eigenvectors and by forcing the computed vector after the inverse iteration to be orthogonal to the previously computed eigenvectors. In some unusual situations, however, this procedure may fail.

Another technique which is useful for finding the eigenvalues of (5.3) is to note that if $u_i \neq 0$ for $i = 1, 2, \cdots, n$, then

$$\begin{aligned} \det(D + \sigma\mathbf{u}\mathbf{u}^T - \lambda I) &= \det(D - \lambda I)\det(I + \sigma(D - \lambda I)^{-1}\mathbf{u}\mathbf{u}^T) \\ &= \prod_{i=1}^{n} (d_i - \lambda)\left(1 + \sigma \sum_{i=1}^{n} \frac{u_i^2}{(d_i - \lambda)}\right). \end{aligned}$$

Thus, the eigenvalues of (5.3) can be computed by finding the zeros of the secular equation

$$\omega(\lambda) \equiv 1 + \sigma \sum_{i=1}^{n} \frac{u_i^2}{(d_i - \lambda)}.$$

6. Least squares problems. In this section we shall show how eigenvalue problems arise in linear least squares problems. The first problem we shall consider is that of performing a fit when there is error in the observations and in the data. The approach we take here is a generalization of the one in [9]. Let A be a given $m \times n$ matrix and let $\mathbf{b}$ be a given vector with m components. We wish to construct a vector $\hat{\mathbf{x}}$ which satisfies the constraints

$$(A + E)\mathbf{x} = \mathbf{b} + \boldsymbol{\delta} \tag{6.1}$$

and for which

$$\|P[E \vdots \boldsymbol{\delta}]Q\| = \text{minimum}, \tag{6.2}$$

where P is a given diagonal matrix with $p_i > 0$, Q is a given diagonal matrix with $q_j > 0$, and $\|\cdot\|$ indicates the Euclidean norm of the matrix. We rewrite (6.1) as

$$[A \vdots \mathbf{b}]\begin{bmatrix} \mathbf{x} \\ -1 \end{bmatrix} + [E \vdots \boldsymbol{\delta}]\begin{bmatrix} \mathbf{x} \\ -1 \end{bmatrix} = \mathbf{0},$$

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or equivalently as

$$B\mathbf{y} + F\mathbf{y} = \mathbf{0}, \tag{6.3}$$

where

$$B = [A \vdots \mathbf{b}]Q, \quad F = [E \vdots \boldsymbol{\delta}]Q, \quad \mathbf{y} = Q^{-1}\begin{bmatrix} \mathbf{x} \\ -1 \end{bmatrix}. \tag{6.4}$$

Our problem now is to determine $\hat{\mathbf{y}}$ so that (6.3) is satisfied, and

$$\|PF\| = \text{minimum}.$$

Again we use Lagrange multipliers as a device for minimizing $\|PF\|$ subject to (6.3).

Consider the function

$$\varphi(F, \mathbf{y}, \boldsymbol{\lambda}) = \sum_{i=1}^{m} \sum_{j=1}^{n+1} p_i^2 f_{ij}^2 - 2 \sum_{i=1}^{m} \lambda_i \sum_{j=1}^{n+1} (b_{ij} + f_{ij}) y_j. \tag{6.5}$$

Then

$$\frac{\partial \varphi}{\partial f_{rs}} = 2p_r^2 f_{rs} - 2\lambda_r y_s$$

so that we have a stationary point of (6.5) when

$$P^2 F = \boldsymbol{\lambda}\mathbf{y}^T. \tag{6.6}$$

Note that the matrix F must be of rank one. Substituting (6.6) into (6.3) we have

$$\boldsymbol{\lambda} = -P^2 B\mathbf{y}/(\mathbf{y}^T\mathbf{y}),$$

and hence,

$$PF = -PB\mathbf{y}\mathbf{y}^T/(\mathbf{y}^T\mathbf{y}).$$

Thus,

$$\|PF\|^2 = \mathbf{y}^T B^T P^2 B\mathbf{y}/(\mathbf{y}^T\mathbf{y}),$$

and hence $\|PF\| =$ minimum when $\hat{\mathbf{y}}$ is the eigenvector associated with the smallest eigenvalue of $B^T P^2 B$. Of course a more accurate procedure is to compute the smallest singular value of PB.

Then, in order to compute $\hat{\mathbf{x}}$, we perform the following calculations:

(a) Form the singular value decomposition of PB, viz.,

$$PB = U\Sigma V^T.$$

(It is generally not necessary to compute U.)

(b) Let $\mathbf{v}$ be the column vector of V associated with $\sigma_{\min}(PB)$ so that $\mathbf{v} = \hat{\mathbf{y}}$. Compute

$$\mathbf{z} = Q\mathbf{v}.$$

(c) From (6.4),

$$\begin{bmatrix} \hat{\mathbf{x}} \\ -1 \end{bmatrix} = -\frac{1}{z_{n+1}}\mathbf{z}.$$

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Note that $\min\|PF\| = \sigma_{\min}(PB)$, and that

$$[E \vdots \boldsymbol{\delta}] = -[A \vdots \mathbf{b}]\mathbf{v}\mathbf{v}^T Q^{-1}.$$

The solution will not be unique if the smallest singular value is multiple. Furthermore, it will not be possible to compute the solution if $z_{n+1} = 0$. This will occur, for example, if $P = I_m$, $Q = I_{n+1}$, $A^T\mathbf{b} = \mathbf{0}$ and $\sigma_{\min}(A) < \|\mathbf{b}\|_2$.

Another problem which arises frequently is that of finding a least squares solution with a quadratic constraint; we have considered this problem previously in [1]. We seek a vector $\hat{\mathbf{x}}$ such that

$$\|\mathbf{b} - A\mathbf{x}\|_2 = \text{minimum} \tag{6.7}$$

with the constraint that

$$\|\mathbf{x}\|_2 = \alpha. \tag{6.8}$$

The condition (6.8) is frequently imposed when the matrix A is ill-conditioned. Now let

$$\varphi(\mathbf{x}, \alpha) = (\mathbf{b} - A\mathbf{x})^T(\mathbf{b} - A\mathbf{x}) + \lambda(\mathbf{x}^T\mathbf{x} - \alpha^2), \tag{6.9}$$

where λ is a Lagrange multiplier. Differentiating (6.9), we are led to the equation

$$A^TA\mathbf{x} - A^T\mathbf{b} + \lambda\mathbf{x} = \mathbf{0} \tag{6.10}$$

or

$$(A^TA + \lambda I)\mathbf{x} = A^T\mathbf{b}. \tag{6.11}$$

Note that (6.10) represents the usual normal equations that arise in the linear least squares problem, with the diagonal elements of A^TA shifted by λ. The parameter λ will be positive when

$$\alpha < \|A^+\mathbf{b}\|_2,$$

and we assume that this condition is satisfied.

Since $\mathbf{x} = (A^TA + \lambda I)^{-1}A^T\mathbf{b}$, we have from (6.8) that

$$\mathbf{b}^TA(A^TA + \lambda I)^{-2}A^T\mathbf{b} - \alpha^2 = 0. \tag{6.12}$$

By repeated use of the identity

$$\det\begin{bmatrix} X & Y \\ Z & W \end{bmatrix} = \det(X)\det(W - ZX^{-1}Y) \quad \text{if } \det(X) \neq 0,$$

we can show that (6.12) is equivalent to the equation

$$\det((A^TA + \lambda I)^2 - \alpha^{-2}A^T\mathbf{b}\mathbf{b}^TA) = 0. \tag{6.13}$$

Finally if $A = U\Sigma V^T$, the singular value decomposition of A, then

$$A^TA = VDV^T, \qquad V^TV = I, \tag{6.14}$$

where $D = \Sigma^T\Sigma$ and (6.13) becomes

$$\det((D + \lambda I)^2 - \mathbf{u}\mathbf{u}^T) = 0, \tag{6.15}$$

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where $\mathbf{u} = \alpha^{-1}\Sigma^T U^T \mathbf{b}$. Equation (6.15) has $2n$ roots; it can be shown (cf. [6]) that we need the largest real root of (6.15) which we denote by λ^*. By a simple argument, it can be shown that λ^* is the unique root in the interval $[0, \mathbf{u}^T\mathbf{u}]$. Thus we have the problem of determining an eigenvalue of a diagonal matrix which is modified by a matrix of rank one.

As in § 5, we can determine a matrix K so that $K\mathbf{u}$ satisfies (5.4), and hence (6.15) is equivalent to

$$\det(K(D + \lambda I)^2 K^T - K\mathbf{u}\mathbf{u}^T K^T) = 0. \tag{6.16}$$

The matrix $G(\lambda) = K(D + \lambda I)^2 K^T - K\mathbf{u}\mathbf{u}^T K^T$ is tridiagonal so that it is easy to evaluate $G(\lambda)$ and $\det G(\lambda)$. Since we have an upper and lower bound on λ^*, it is possible to use linear interpolation to find λ^*, even though $G(\lambda)$ is quadratic in λ. Numerical experiments have indicated it is best to compute $G(\lambda) = K(D + \lambda I)^2 K^T - K\mathbf{u}\mathbf{u}^T K^T$ for each approximate value of λ^* rather than computing

$$G(\lambda) = (KD^2K^T - K\mathbf{u}\mathbf{u}^T K^T) + 2\lambda KDK^T + \lambda^2 KK^T.$$

Another approach for determining λ^* is the following: we substitute the decomposition (6.14) into (6.12) and are led to the equation

$$\varphi_n(\lambda) \equiv \sum_{i=1}^{n} \frac{u_i^2}{(d_i + \lambda)^2} - 1 = 0, \tag{6.17}$$

with $\mathbf{u} = \alpha^{-1}\Sigma^T U^T \mathbf{b}$. It is easy to verify that if

$$\begin{aligned} \psi_k(\lambda) &= \prod_{j=1}^{k} (d_i + \lambda)^2 \left[\sum_{i=1}^{k} \frac{u_i^2}{(d_i + \lambda)^2} - 1 \right], \\ \psi_{k+1}(\lambda) &= (d_{k+1} + \lambda)^2 \psi_k(\lambda) - u_{k+1}^2 \xi_k(\lambda), && k = 0, 1, \cdots, n-1, \\ \xi_k(\lambda) &= (d_k + \lambda)^2 \xi_{k-1}(\lambda), && k = 1, 2, \cdots, n-1, \end{aligned} \tag{6.18}$$

with

$$\psi_0(\lambda) = \xi_0(\lambda) = 1.$$

Then using (6.18) we can easily evaluate $\psi_n(\lambda)$ and $\psi_n'(\lambda)$, and hence use one of the standard root finding techniques for determining λ^*. It is easy to verify that $\hat{\mathbf{x}} = V(D + \lambda^* I)^{-1}\Sigma U^T \mathbf{b}$.

A similar problem arises when it is required to make

$$\|\mathbf{x}\|_2 = \text{minimum}$$

when

$$\|\mathbf{b} - A\mathbf{x}\|_2 = \beta,$$

where

$$\beta > \min_{\mathbf{x}} \|\mathbf{b} - A\mathbf{x}\|.$$

Again the Lagrange multiplier λ satisfies a quadratic equation which is similar to the equation given by (6.14).

7. Gauss-type quadrature rules with preassigned nodes. In many applications it is desirable to generate Gauss-type quadrature rules with preassigned nodes. This is particularly true for numerical methods which depend on the theory of moments

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for determining bounds (cf. [3]), and for solving boundary value problems [12]. We shall show that it is possible to generate these quadrature rules as a modified eigenvalue problem.

Let $\omega(x) \geqq 0$ be a fixed *weight function* defined on the interval $[a, b]$. For $\omega(x)$ it is possible to define a sequence of polynomials $p_0(x)$, $p_1(z)$, $\cdots$ which are orthonormal with respect to $\omega(x)$ and in which $p_n(x)$ is of exact degree n so that

$$\int_a^b p_n(x)p_m(x)\omega(x) = \begin{cases} 1 & \text{when } m = n, \\ 0 & \text{when } m \neq n. \end{cases}$$

The polynomial $p_n(x) = k_n \prod_{i=1}^n (x - t_i^{(n)})$, $k_n > 0$, has n distinct real roots $a < t_1^{(n)} < t_2^{(n)} < \cdots < t_n^{(n)} < b$. The roots of the orthogonal polynomials play an important role in Gauss-type quadrature.

THEOREM. *Let $f(x) \in C^{2N}[a, b]$; then it is possible to determine positive w_j so that*

$$\int_a^b f(x)\omega(x)\,dx = \sum_{j=1}^N w_j f(t_j^{(N)}) = R[f],$$

where

$$R[f] = \frac{f^{(2N)}(\eta)}{(2N)!} \int_a^b \left[\prod_{i=1}^N (x - t_i^{(N)}) \right]^2 \omega(x)\,dx, \qquad a < \eta < b.$$

Thus, the Gauss-type quadrature rule is exact for all polynomials of degree less than or equal to $2N - 1$.

Any set of orthonormal polynomials satisfies a three-term recurrence relationship:

$$\begin{aligned} &\beta_j p_j(x) = (x - \alpha_j)p_{j-1}(x) - \beta_{j-1}p_{j-2}(x) \quad \text{for } j = 1, 2, \cdots, N; \\ &p_{-1}(x) \equiv 0, \qquad p_0(x) \equiv 1. \end{aligned} \tag{7.1}$$

We may identify (7.1) with the matrix equation

$$x\mathbf{p}(x) = J_N\mathbf{p}(x) + \beta_N p_N(x)\mathbf{e}_N, \tag{7.2}$$

where

$$[\mathbf{p}(x)]^T = [p_0(x), p_1(x), \cdots, p_{N-1}(x)],$$
$$\mathbf{e}_N^T = [0, 0, \cdots, 1],$$

and

$$J_N = \begin{bmatrix} \alpha_1 & \beta_1 & & & & \\ \beta_1 & \alpha_2 & \beta_2 & & & 0 \\ & \cdot & \cdot & \cdot & & \\ & & \cdot & \cdot & \cdot & \\ & & & \cdot & \cdot & \beta_{N-1} \\ & 0 & & & \cdot & \cdot \\ & & & & \beta_{N-1} & \alpha_N \end{bmatrix}.$$

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Suppose that the eigenvalues of J_N are computed so that

$$J_N \mathbf{q}_j = \lambda_j \mathbf{q}_j, \qquad j = 1, 2, \cdots, N,$$

with

$$\mathbf{q}_j^T \mathbf{q}_j = 1$$

and

$$\mathbf{q}_j^T = [q_{1j}, q_{2j}, \cdots, q_{Nj}].$$

Then it is shown in [11] that

$$t_j^{(N)} = \lambda_j, \qquad w_j = (q_{1j})^2. \tag{7.3}$$

(From here on in, we drop the superscripts on the $t_j^{(N)}$'s.)

A very effective way to compute the eigenvalues of J_N and the first component of the orthonormalized eigenvectors is to use the QR method of Francis (cf. [14]).

Now let us consider the problem of determining the quadrature rule so that

$$\int_a^b f(x)\omega(x)\,dx \approx \sum_{j=1}^{N} w_j f(t_j) + \sum_{k=1}^{M} v_k f(z_k),$$

where the nodes $\{z_k\}_{k=1}^M$ are prescribed. It is possible to determine $\{w_j, t_j\}_{j=1}^N$, $\{v_k\}_{k=1}^M$ so that we have for the remainder

$$R[f] = \frac{f^{(2N+M)}(\eta)}{(2N+M)!} \int_a^b \prod_{k=1}^{M} (x - v_k) \left[\prod_{j=1}^{N} (x - t_j) \right]^2 \omega(x)\,dx, \qquad a < \eta < b.$$

For $M = 1$ and $z_1 = a$ or $z_1 = b$, we have the Gauss–Radau-type formula, and for $M = 2$ with $z_1 = a$ and $z_2 = b$, we have the Gauss–Lobatto-type formula.

First we shall show how the Gauss–Radau-type rule may be computed. For convenience, we assume that $z_1 = a$. Now we wish to determine the polynomial $p_{N+1}(x)$ so that

$$p_{N+1}(a) = 0.$$

From (7.1) we see that this implies that

$$0 = p_{N+1}(a) = (a - \alpha_{N+1})p_N(a) - \beta_N p_{N-1}(a)$$

or

$$\alpha_{N+1} = a - \beta_N \frac{p_{N-1}(a)}{p_N(a)}. \tag{7.4}$$

From equation (7.2) we have

$$(J_N - aI)\mathbf{p}(a) = -\beta_N p_N(a)\mathbf{e}_N,$$

or equivalently,

$$(J_N - aI)\boldsymbol{\delta}(a) = \beta_N^2 \mathbf{e}_N, \tag{7.5}$$

where

$$\delta_j(a) = -(\beta_N p_{j-1}(a))/p_N(a), \qquad j = 1, 2, \cdots, N.$$

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Thus,

$$\alpha_{N+1} = a + \delta_N(a). \tag{7.6}$$

Hence, in order to compute the Gauss–Radau-type rule, we do the following:

(a) Generate the matrix J_N and the element β_N.

(b) Solve the system of equations (7.5) for $\delta_N(a)$.

(c) Compute α_{N+1} by (7.6) and use it to replace the $(N+1, N+1)$ element of J_{N+1}.

(d) Use the QR algorithm to compute the eigenvalues and first element of the eigenvector of the tridiagonal matrix

$$\tilde{J}_{N+1} = \left[\begin{array}{c|c} J_N & \beta_N \mathbf{e}_N \\ \hline \beta_N \mathbf{e}_N^T & \alpha_{N+1} \end{array}\right].$$

Of course, one of the eigenvalues of the matrix J_{N+1} must be equal to a.

Since $a < \lambda_{\min}(J_N)$, the matrix $J_N - aI$ will be positive definite and hence Gaussian elimination without pivoting may be used to solve (7.5). It is not even necessary to solve the complete system since it is only necessary to compute the element $\delta_N(a)$. However, one may wish to use iterative refinement to compute $\delta_N(a)$ very precisely since for N large, $\lambda_{\min}(J)$ may be close to a, and hence the system of equations (7.5) may be quite ill-conditioned. When $z_1 = b$, the calculation of $\tilde{J}_{N+1}$ is identical except with b replacing a in equations (7.5) and (7.6). The matrix $J_N - bI$ will be negative definite since $b > \lambda_{\max}(J)$.

To compute the Gauss–Lobatto quadrature rule, we need to compute a matrix $\tilde{J}_{N+1}$ such that

$$\lambda_{\min}(\tilde{J}_{N+1}) = a \quad \text{and} \quad \lambda_{\max}(\tilde{J}_{N+1}) = b.$$

Thus, we wish to determine $p_{N+1}(x)$ so that

$$p_{N+1}(a) = p_{N+1}(b) = 0. \tag{7.7}$$

Now from (7.1) we have

$$\beta_{N+1} p_{N+1}(x) = (x - \alpha_{N+1}) p_N(x) - \beta_N p_{N-1}(x),$$

so that (7.7) implies that

$$\begin{aligned} \alpha_{N+1} p_N(a) + \beta_N p_{N-1}(a) &= a p_N(a), \\ \alpha_{N+1} p_N(b) + \beta_N p_{N-1}(b) &= b p_N(b). \end{aligned} \tag{7.8}$$

Using the relationship (7.2), if

$$(J_N - aI)\,\boldsymbol{\gamma} = \mathbf{e}_N \quad \text{and} \quad (J_N - bI)\boldsymbol{\mu} = \mathbf{e}_N, \tag{7.9}$$

then

$$\gamma_j = -\frac{1}{\beta_N}\frac{p_{j-1}(a)}{p_N(a)}, \qquad \mu_j = -\frac{1}{\beta_N}\frac{p_{j-1}(b)}{p_N(b)}, \qquad j = 1, 2, \cdots, N. \tag{7.10}$$

Thus, (7.8) is equivalent to the system of equations

$$\alpha_{N+1} - \gamma_N \beta_N^2 = a, \qquad \alpha_{N+1} - \mu_N \beta_N^2 = b. \tag{7.11}$$

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Hence, in order to compute the Gauss–Lobatto-type rule, we perform the following calculations:

(a) Generate the matrix J_N.
(b) Solve the systems of equations (7.9) for γ_N and μ_N.
(c) Solve (7.11) for α_{N+1} and β_N^2.
(d) Use the QR algorithm to compute the eigenvalues and first element of the eigenvectors of the tridiagonal matrix

$$\tilde{J}_{N+1} = \left[\begin{array}{c|c} J_N & \beta_N \mathbf{e}_N \\ \hline \beta_N \mathbf{e}_N^T & \alpha_{N+1} \end{array}\right].$$

Galant [7] has given an algorithm for computing the Gaussian-type quadrature rules with preassigned nodes which is based on a theorem of Christoffel. His method constructs the orthogonal polynomials with respect to a modified weight function.

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