MATRICES, MOMENTS, AND RATIONAL QUADRATURE

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Dedicated to Richard S. Varga on the occasion of his 80th birthday.

Abstract. Many problems in science and engineering require the evaluation of functionals of the form $F(A) = u^T f(A)u$, where A is a large symmetric matrix, u a vector, and f a nonlinear function. A popular and fairly inexpensive approach to determining upper and lower bounds for such functionals is based on first carrying out a few steps of the Lanczos procedure applied to A with initial vector u, and then evaluating pairs of Gauss and Gauss-Radau quadrature rules associated with the tridiagonal matrix determined by the Lanczos procedure. The present paper extends this approach to allow the use of rational Gauss quadrature rules.

1. Introduction.

Richard Varga has made many significant contributions to numerical analysis, approximation theory, linear algebra, and analysis. His work is concerned with iterative methods, matrices, moments, polynomial and rational approximation, as well as quadrature; see, e.g., [5, 6, 9, 19, 20, 21, 23]. This paper combines results from these areas to develop a new method for determining fairly easily computable upper and lower bounds for functionals of the form

$$F(A) = u^T f(A)u, \tag{1.1}$$

where $A \in \mathbf{R}^{n\times n}$ is a large, sparse or structured, symmetric matrix, $u \in \mathbf{R}^n$, and f is a nonlinear function. The need to evaluate this kind of functionals arises in many applications, such as inverse problems, lattice quantum cromodynamics, and fractals; see, e.g., [2, 4, 11, 17] and references therein. However, the computation of $f(A)$ may be prohibitively expensive for large matrices A. It is therefore important to be able to evaluate upper and lower bounds with fairly little computational effort.

Introduce the spectral decomposition

$$A = S\Lambda S^T, \quad \Lambda = \mathrm{diag}[\lambda_1, \lambda_2, \ldots, \lambda_n] \in \mathbf{R}^{n\times n}, \quad S \in \mathbf{R}^{n\times n}, \quad S^T S = I,$$

where I denotes the identity matrix, and define

$$f(A) = S f(\Lambda) S^T. \tag{1.2}$$

The function f is required to be differentiable sufficiently many times in an interval containing the spectrum of A. The exact requirements on f are specified in Sections 2 and 3. For notational simplicity, we order the eigenvalues according to

$$\lambda_1 \le \lambda_2 \le \cdots \le \lambda_n$$

and scale the vector u in (1.1) so that $\|u\| = 1$, where $\|\cdot\|$ denotes the Euclidean vector norm.

Golub and Meurant [11] describe an elegant technique for computing upper and lower bounds for $F(A)$ based on the connection between the Lanczos procedure, orthogonal polynomials, and Gauss-type quadrature rules. The quality of the bounds

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obtained by application of m steps of the Lanczos procedure to A depends on how well the function f can be approximated by a polynomial of degree $2m-1$ on the spectrum of A. We extend the approach in [11] to allow rational approximation of f. This extension allows cancellation of poles of the integrand, which makes it possible to determine upper and lower bounds for functionals that cannot be bounded using the technique in [11]. Our approach also can be attractive when the technique in [11] requires more Lanczos steps to give bounds of comparable accuracy. Our method requires the solution of linear systems of equations of the form $(A+sI)y=u$ for one or a few values of the scalar s.

This paper is organized as follows. The remainder of this section reviews properties of Gauss quadrature rules. Section 2 discusses the connection between the Lanczos procedure, orthogonal polynomials, and Gauss-type quadrature rules, and describes how these quadrature rules can be applied to compute upper and lower bounds for the functional (1.1). Further details on these connections can be found in the survey by Golub and Meurant [11]. Section 3 presents an extension that allows rational approximation of f. In particular, properties of rational Gauss quadrature rules are discussed. Section 4 describes a few computed examples and Section 5 contains concluding remarks.

Define the vector $[\mu_1, \mu_2, \ldots, \mu_n] = u^T S$ and, using (1.2), express the functional (1.1) in the form

$$F(A) = u^T S f(\Lambda) S^T u = \sum_{j=1}^{n} f(\lambda_j)\mu_j^2. \tag{1.3}$$

The right-hand side of (1.3) is a Stieltjes integral

$$\mathcal{I}f = \int_{-\infty}^{\infty} f(s)d\mu(s)$$

with a nonnegative measure $d\mu$, such that μ is a nondecreasing step function defined on $\mathbf{R}$ with jumps at the eigenvalues λ_j. It follows from $\|u\|=1$ that the measure $d\mu$ has total mass one. The m-point Gauss quadrature rule associated with $d\mu$,

$$\mathcal{G}_m f = \sum_{j=1}^{m} f(\theta_j)\gamma_j^2, \tag{1.4}$$

is characterized by

$$\mathcal{I}f = \mathcal{G}_m f \qquad \forall f \in \mathbf{P}_{2m-1}, \tag{1.5}$$

where $\mathbf{P}_{2m-1}$ denotes the set of polynomials of degree at most $2m-1$. The nodes θ_j of the quadrature rule are the zeros of the mth degree orthonormal polynomial with respect to the inner product

$$(f,g) = \mathcal{I}(fg). \tag{1.6}$$

It is well known that for a $2m$ times continuously differentiable function f in the interval $\Omega = [\lambda_1, \lambda_n]$, the error of the quadrature rule (1.4) can be expressed as

$$\mathcal{E}_m f = (\mathcal{I} - \mathcal{G}_m) f = \frac{f^{(2m)}(\theta_{\mathcal{G}})}{(2m)!} \cdot \int_{-\infty}^{\infty} \prod_{j=1}^{m} (s-\theta_j)^2 d\mu(s) \tag{1.7}$$

for some $\theta_{\mathcal{G}}$ in the interior of Ω; see, e.g., Gautschi [7, p. 24]. It follows that if the derivative $f^{(2m)}$ is of known constant sign in the interior of Ω, then the sign of the error $\mathcal{E}_m f$ can be determined without evaluating the right-hand side of (1.7). For instance if $f^{(2m)}$ is nonnegative on Ω, then so is $\mathcal{E}_m f$.

Let $\hat{\theta} \in \mathbf{R}$ satisfy $\hat{\theta} \leq \lambda_1$ or $\hat{\theta} \geq \lambda_n$, and let $\hat{\Omega}$ denote the convex hull of the set $\{\lambda_1, \lambda_n, \hat{\theta}\}$. The $(m+1)$-point Gauss-Radau quadrature rule associated with the measure $d\mu$ and with a prescribed node at $\hat{\theta}$ is an expression of the form

$$\hat{\mathcal{G}}_{m+1} f = \sum_{j=1}^{m} f(\hat{\theta}_j)\hat{\gamma}_j^2 + f(\hat{\theta})\hat{\gamma}^2. \tag{1.8}$$

Properties of the nodes $\hat{\theta}_j$ and weights $\hat{\gamma}_j^2$ are reviewed in Section 2. The Gauss-Radau rule (1.8) satisfies

$$\mathcal{I} f = \hat{\mathcal{G}}_{m+1} f \qquad \forall f \in \mathbf{P}_{2m}. \tag{1.9}$$

Let the function f be $2m+1$ times continuously differentiable in $\hat{\Omega}$.. Then the error in the quadrature rule (1.8) is given by

$$\hat{\mathcal{E}}_{m+1} f = (\mathcal{I} - \hat{\mathcal{G}}_{m+1}) f = \frac{f^{(2m+1)}(\theta_{\hat{\mathcal{G}}})}{(2m+1)!} \cdot \int_{-\infty}^{\infty} (s-\hat{\theta}) \prod_{j=1}^{m} (s-\hat{\theta}_j)^2 d\mu(s) \tag{1.10}$$

for some $\theta_{\hat{\mathcal{G}}}$ in the interior of $\hat{\Omega}$; see, e.g., Gautschi [7, p.. 26]. We note for future reference that if the derivative $f^{(2m+1)}$ is of known constant sign in $\hat{\Omega}$, then the sign of the error $\hat{\mathcal{E}}_{m+1} f$ can be determined from (1.10) without explicit evaluation of the right-hand side expression.

2. Bounds via the Lanczos procedure. The discussion of the present section reviews results by Golub and Meurant [11] and Hanke [15]. More details can be found in [11]. Gauss quadrature rules with respect to the measure $d\mu$ can be determined conveniently by the Lanczos procedure. Application of m steps of the Lanczos procedure to the matrix A with initial vector $v_1 = u$ yields the decomposition

$$AV_m = V_m T_m + \beta_m v_{m+1} e_m^T, \tag{2.1}$$

where $V_m = [v_1, v_2, \ldots, v_m] \in \mathbf{R}^{n \times m}$ and $v_{m+1} \in \mathbf{R}^n$ satisfy $V_m^T V_m = I$, $\|v_{m+1}\| = 1$, $V_m^T v_{m+1} = 0$, and $\beta_m \geq 0$. Moreover, e_m denotes the mth axis vector and

$$T_m = \begin{bmatrix} \alpha_1 & \beta_1 & & & & 0 \\ \beta_1 & \alpha_2 & \beta_2 & & & \\ & \beta_2 & \alpha_3 & & & \\ & & & \ddots & & \\ & & & \ddots & \ddots & \beta_{m-1} \\ 0 & & & & \beta_{m-1} & \alpha_m \end{bmatrix} \in \mathbf{R}^{m \times m} \tag{2.2}$$

is a symmetric tridiagonal matrix with positive subdiagonal entries; see, e.g., [12, Chapter 9] for a detailed discussion on the Lanczos procedure. We tacitly assume that m is sufficiently small so that the decomposition (2.1) with the stated properties exists.

If $\beta_m = 0$, then we set $v_{m+1} = 0$, and obtain from (2.1) that

$$F(A) = e_1^T f(T_m) e_1.$$

Thus, $F(A)$ can be evaluated exactly. Henceforth, we assume that $\beta_m > 0$.

The relation (2.1) between the columns v_j of V_m shows that

$$v_j = p_{j-1}(A)u, \qquad 1 \le j \le m+1, \tag{2.3}$$

for certain polynomials p_{j-1} of degree $j-1$. It follows from the orthonormality of the vectors v_j that

$$\begin{aligned}(p_{j-1}, p_{k-1}) &= \int_{-\infty}^{\infty} p_{j-1}(s) p_{k-1}(s) d\mu(s) = u^T S p_{j-1}(\Lambda) p_{k-1}(\Lambda) S^T u \\ &= u^T p_{j-1}(A) p_{k-1}(A) u = v_1^T p_{j-1}(A) p_{k-1}(A) v_1 \\ &= v_j^T v_k = \begin{cases} 0, & j \ne k, \\ 1, & j = k. \end{cases}\end{aligned}$$

This shows that the polynomials p_j are orthonormal with respect to the inner product (1.6). Combining (2.1) and (2.3) yields a recurrence relation for the polynomials,

$$\begin{aligned}\beta_1 p_1(s) &= (s - \alpha_1) p_0(s), \qquad p_0(s) = 1, \\ \beta_j p_j(s) &= (s - \alpha_j) p_{j-1}(s) - \beta_{j-1} p_{j-2}(s), \qquad 2 \le j \le m.\end{aligned} \tag{2.4}$$

Thus, the Lanczos procedure is equivalent to the Stieltjes procedure for generating orthonormal polynomials. It follows from the recurrence relation (2.4) that only the columns v_j and v_{j-1} have to be available in order to determine the next column, v_{j+1}.

The recurrence relation (2.4) can be expressed as

$$\begin{aligned}[p_0(s), p_1(s), \dots, p_{m-1}(s)] T_m &= s[p_0(s), p_1(s), \dots, p_{m-1}(s)] \\ &- \beta_m [0, \dots, 0, p_m(s)],\end{aligned} \tag{2.5}$$

which shows that the zeros of p_m are the eigenvalues of T_m.

Introduce the spectral decomposition

$$T_m = Q_m D_m Q_m^T, \qquad D_m = \mathrm{diag}[\theta_1, \theta_2, \dots, \theta_m], \qquad Q_m^T Q_m = I_m.$$

The weights of the Gauss rule (1.4) are given by $\gamma_j^2 = (e_1^T Q_m e_j)^2$, $1 \le j \le m$, see, e.g., Gautschi [7, Theorem 3.1] or Golub and Meurant [11], and it follows that the Gauss rule (1.4) can be expressed as

$$\mathcal{G}_m f = e_1^T Q_m f(D_m) Q_m^T e_1 = e_1^T f(T_m) e_1. \tag{2.6}$$

Hence, $\mathcal{G}_m f$ can be determined by first computing the Lanczos decomposition (2.1) and then evaluating one of the expressions (2.6). The following result is an immediate consequence of the above discussion. The matrix T_{m-1} in Theorem 2.1 is the leading principal submatrix of order $m-1$ of T_m.

THEOREM 2.1. *Let the function f be $2m$ times continuously differentiable in the interval $\Omega = [\lambda_1, \lambda_n]$. Assume that $\beta_m > 0$ in (2.1). Then*

$$e_1^T f(T_{m-1}) e_1 < e_1^T f(T_m) e_1 < u^T f(A) u, \qquad \text{if } f^{(2m)} > 0 \text{ in } \Omega, \tag{2.7}$$

$$e_1^T f(T_{m-1}) e_1 > e_1^T f(T_m) e_1 > u^T f(A) u, \qquad \text{if } f^{(2m)} < 0 \text{ in } \Omega. \tag{2.8}$$

Proof. It follows from $\beta_m > 0$ that the integral on the right-hand side of (1.7) does not vanish. Therefore, the right-hand side inequality of (2.7) follows from (1.7). The nodes and weights of the m-point Gauss quadrature rule $\mathcal{G}_m$ associated with the measure $d\mu$, given by (2.6), defines a discrete measure on the real axis. The $(m-1)$-point Gauss rule

$$\mathcal{G}_{m-1}f = e_1^T f(T_{m-1})e_1$$

associated with the measure $d\mu$ also is a Gauss rule associated with the discrete measure determined by the nodes and weights of $\mathcal{G}_m$. This shows the left-hand side inequality of (2.7). The inequalities (2.8) can be shown similarly. □

We turn to the computation of Gauss-Radau quadrature rules associated with the measure $d\mu$ with a preassigned node $\hat{\theta}$, and follow the approach in [10]; see also [7, Theorem 3.2]. Introduce the symmetric tridiagonal matrix

$$\hat{T}_{m+1} = \begin{bmatrix} \alpha_1 & \beta_1 & & & & \mathbf{0} \\ \beta_1 & \alpha_2 & \beta_2 & & & \\ & \beta_2 & \alpha_3 & \ddots & & \\ & & \ddots & \ddots & \beta_{m-1} & \\ & & & \beta_{m-1} & \alpha_m & \beta_m \\ \mathbf{0} & & & & \beta_m & \hat{\alpha}_{m+1} \end{bmatrix} \in \mathbf{R}^{(m+1)\times(m+1)} \tag{2.9}$$

with the leading $m \times m$ principal submatrix (2.2). The last subdiagonal entry, β_m, is defined by (2.1) and the last diagonal entry, $\hat{\alpha}_{m+1}$, is chosen so that $\hat{T}_{m+1}$ is semidefinite and has the eigenvalue $\hat{\theta}$ as follows. Introduce the polynomial

$$\hat{p}_{m+1}(s) = (s - \hat{\alpha}_{m+1})p_m(s) - \beta_m p_{m-1}(s). \tag{2.10}$$

Then analogously to (2.5),

$$\begin{aligned} [p_0(s), p_1(s), \ldots, p_m(s)]\hat{T}_{m+1} &= s[p_0(s), p_1(s), \ldots, p_m(s)] \\ &- [0, \ldots, 0, \hat{p}_{m+1}(s)], \end{aligned}$$

which shows that $\hat{\alpha}_{m+1}$ should be chosen so that $\hat{\theta}$ is a zero of $\hat{p}_{m+1}$. Substituting $s = \hat{\theta}$ into (2.10) yields

$$\hat{\alpha}_{m+1} = \hat{\theta} - \beta_m \frac{p_{m-1}(\hat{\theta})}{p_m(\hat{\theta})}.. \tag{2.11}$$

This determines the Gauss-Radau matrix (2.9) and we obtain similarly to (2.6) that

$$\hat{\mathcal{G}}_{m+1}f = e_1^T f(\hat{T}_{m+1})e_1. \tag{2.12}$$

Hence, $\hat{\mathcal{G}}_{m+1}f$ can be computed by applying m steps of the Lanczos procedure and then evaluating the expressions (2.11) and (2.12).

The following result is analogous to Theorem 2.1. The symmetric tridiagonal matrix $\hat{T}_m \in \mathbf{R}^{m\times m}$ in Theorem 2.2 is associated with the m-point Gauss-Radau rule for the measure $d\mu$ with a prescribed node at $\hat{\theta}$.

THEOREM 2.2. *Let the function f be $2m+1$ times continuously differentiable in $\hat{\Omega}$, the convex hull of the set $\{\lambda_1, \lambda_n, \hat{\theta}\}$, and assume that the step function μ has at least $m+2$ points of increase. If $\hat{\theta} \leq \lambda_1$, then*

$$e_1^T f(\hat{T}_m) e_1 < e_1^T f(\hat{T}_{m+1}) e_1 < u^T f(A) u, \qquad \text{if } f^{(2m+1)} > 0 \text{ in } \hat{\Omega}, \tag{2.13}$$

$$e_1^T f(\hat{T}_m) e_1 > e_1^T f(\hat{T}_{m+1}) e_1 > u^T f(A) u, \qquad \text{if } f^{(2m+1)} < 0 \text{ in } \hat{\Omega}. \tag{2.14}$$

If instead $\hat{\theta} \geq \lambda_n$, then

$$e_1^T f(\hat{T}_m) e_1 < e_1^T f(\hat{T}_{m+1}) e_1 < u^T f(A) u, \qquad \text{if } f^{(2m+1)} < 0 \text{ in } \hat{\Omega}, \tag{2.15}$$

$$e_1^T f(\hat{T}_m) e_1 > e_1^T f(\hat{T}_{m+1}) e_1 > u^T f(A) u, \qquad \text{if } f^{(2m+1)} > 0 \text{ in } \hat{\Omega}. \tag{2.16}$$

Proof. The requirement that μ have at least $m+2$ points of increase secures that the integral on the right-hand side of (1.10) is nonvanishing. Assume that $\hat{\theta} \leq \lambda_1$ and $f^{(2m+1)} > 0$ in $\hat{\Omega}$. Then the right-hand side inequality of (2.13) follows from (1.10).

The nodes and weights of the $(m+1)$-point Gauss-Radau rule $\hat{\mathcal{G}}_{m+1}$ associated with the measure $d\mu$ define a discrete measure on the real axis. The m-point Gauss-Radau rule

$$\hat{\mathcal{G}}_m f = e_1^T f(\hat{T}_m) e_1$$

associated with the same measure $d\mu$ also is a Gauss-Radau rule associated with the discrete measure determined by the nodes and weights of $\hat{\mathcal{G}}_{m+1}$. This shows the left-hand side inequality of (2.13). The inequalities (2.14)-(2.16) follow similarly. □

3. Rational Gauss rules. This section is concerned with an extension of Gauss quadrature rules that is exact for certain rational functions with preselected poles. These rules are known as rational Gauss rules. They were first discussed in [13, 16] and have subsequently received considerable attention; see, e.g., [3, 7, 8, 14, 22] for discussions on the rate of convergence, error bounds, and the selection of poles. Pairs of rational Gauss and Gauss-Radau rules can be used to bound certain functionals (1.1) for which pairs of standard Gauss and Gauss-Radau rules are not guaranteed to provide upper and lower bounds. This is illustrated in Section 4. Moreover, when the integrand f is analytic in a set that contains the interval $[\lambda_1, \lambda_n]$ and has a singularity close to this interval, quadrature rules that are exact for rational functions with poles at or near the singularity of f may yield significantly higher accuracy than standard Gauss quadrature rules with the same number of nodes. Therefore, for some integrands rational Gauss rules provide tighter bounds than standard Gauss rules using the same number of nodes.

We review properties of rational Gauss rules and discuss their application to the computation of upper and lower bounds for functionals of the form (1.1). Let $\{z_j\}_{j=1}^k$ be a set of not necessarily distinct real or complex numbers outside the interval $[\lambda_1, \lambda_n]$, and assume that the set is symmetric with respect to the real axis. The z_j will be poles of rational functions that are integrated exactly by the rational Gauss quadrature rules. Introduce the polynomial

$$w(s) = \sigma \prod_{j=1}^{k} (s - z_j), \tag{3.1}$$

where we choose the scaling factor $\sigma \in \mathbf{R}\backslash\{0\}$ so that the measure

$$d\mu^{(w)}(s) = \frac{d\mu(s)}{w(s)} \tag{3.2}$$

has total mass one. The m-point Gauss quadrature rule associated with this measure,

$$\mathcal{G}_m^{(w)} f = \sum_{j=1}^{m} f(\theta_j^{(w)})(\gamma_j^{(w)})^2, \tag{3.3}$$

is the basis of the rational Gauss quadrature rules.

THEOREM 3.1. *Let $\{\theta_j^{(w)}, (\gamma_j^{(w)})^2\}_{j=1}^m$ be the node-weight pairs of the Gauss rule (3.3). Assume that $m \geq \frac{1}{2}(k+1)$, where k is the degree of the polynomial w; cf. (3.1). Then the m-point rational Gauss quadrature rule*

$$\mathcal{R}_m^{(w)} f = \sum_{j=1}^{m} f(\theta_j^{(w)}) w(\theta_j^{(w)})(\gamma_j^{(w)})^2 \tag{3.4}$$

satisfies

$$\mathcal{I} f = \mathcal{R}_m^{(w)} f \qquad \forall f \in \mathbf{Q}_k \oplus \mathbf{P}_{2m-1-k}, \tag{3.5}$$

where

$$\mathbf{Q}_k = \mathrm{span}\{\prod_{j=1}^{\ell} (\cdot - z_j)^{-1},\ 1 \leq \ell \leq k\} \tag{3.6}$$

with $\mathbf{Q}_0 = \emptyset$. Moreover,

$$\begin{aligned} \mathcal{E}_m^{(w)} f &= (\mathcal{I} - \mathcal{R}_m^{(w)}) f \\ &= \frac{d^{2m}}{ds^{2m}} (fw)_{s=\theta_{\mathcal{R}}} \frac{1}{(2m)!} \cdot \int_{-\infty}^{\infty} \prod_{j=1}^{m} (s - \theta_j^{(w)})^2 d\mu^{(w)}(s), \end{aligned} \tag{3.7}$$

where $\theta_{\mathcal{R}}$ is in the interior of $\Omega = [\lambda_1, \lambda_n]$.

Proof. Rational Gauss rules of the form (3.4) are discussed, e.g., by Gautschi [7, Section 3.1.4], where also (3.5) is shown. The proof follows by choosing suitable polynomials f in (1.5) with $d\mu$ replaced by (3.2). The remainder formula (3.7) is obtained by replacing $d\mu$ by (3.2) and f by fw in the remainder formula (1.7) for standard Gauss quadrature. The lower bound for m secures that the quadrature rule integrates constants exactly. □

Rational Gauss-Radau rules can be defined analogously. Thus, let the prescribed node $\hat{\theta}$ satisfy $\hat{\theta} \leq \lambda_1$ or $\hat{\theta} \geq \lambda_n$, and introduce the $(m+1)$-point Gauss-Radau quadrature rule associated with the measure (3.2),

$$\hat{\mathcal{G}}_{m+1}^{(w)} f = \sum_{j=1}^{m} f(\hat{\theta}_j^{(w)})(\hat{\gamma}_j^{(w)})^2 + f(\hat{\theta})(\hat{\gamma}^{(w)})^2. \tag{3.8}$$

The following result, which is based on properties of this Gauss-Radau rule, is analogous to Theorem 3.1.

THEOREM 3.2. *Let* $\{\hat{\theta}_j^{(w)}, (\hat{\gamma}_j^{(w)})^2\}_{j=1}^m \cup \{\hat{\theta}, (\hat{\gamma}^{(w)})^2\}$ *be the node-weight pairs of the Gauss-Radau rule (3.8). Assume that* $m \geq k/2$*, where* k *is the degree of the polynomial* w*; cf. (3.1). Then the* $(m+1)$*-point rational Gauss-Radau quadrature rule*

$$\hat{\mathcal{R}}_{m+1}^{(w)} f = \sum_{j=1}^{m} f(\hat{\theta}_j^{(w)}) w(\hat{\theta}_j^{(w)}) (\hat{\gamma}_j^{(w)})^2 + f(\hat{\theta}) w(\hat{\theta}) (\hat{\gamma}^{(w)})^2 \tag{3.9}$$

satisfies

$$\mathcal{I} f = \hat{\mathcal{R}}_{m+1}^{(w)} f \qquad \forall f \in \mathbf{Q}_k \oplus \mathbf{P}_{2m-k}, \tag{3.10}$$

where $\mathbf{Q}_k$ *is defined by (3.6). Moreover,*

$$\begin{aligned} \hat{\mathcal{E}}_{m+1}^{(w)} f &= (\mathcal{I} - \hat{\mathcal{R}}_{m+1}^{(w)}) f \\ &= \frac{d^{2m+1}}{ds^{2m+1}} (fw)_{s=\theta_{\hat{\mathcal{R}}}} \frac{1}{(2m+1)!} \cdot \int_{-\infty}^{\infty} (s - \hat{\theta}) \prod_{j=1}^{m} (s - \hat{\theta}_j^{(w)})^2 d\mu^{(w)}(s), \end{aligned} \tag{3.11}$$

where $\theta_{\hat{\mathcal{R}}}$ *is in the interior of* $\hat{\Omega}$*, the convex hull of the set* $\{\lambda_1, \lambda_n, \hat{\theta}\}$.

Proof. Rational Gauss-Radau rules (3.9) are discussed by Gautschi [7, Section 3.1.4.4]. The theorem can be shown similarly as Theorem 3.1. Thus, the property (3.10) is obtained by choosing suitable polynomials f in (1.9) with $d\mu$ replaced by (3.2). The remainder formula (3.11) follows by replacing $d\mu$ by (3.2) and f by fw in (1.10). □

Let $T_m^{(w)} \in \mathbf{R}^{m \times m}$ be the symmetric tridiagonal matrix associated with the Gauss quadrature rule (3.3), i.e., the nodes $\{\theta_j^{(w)}\}_{j=1}^m$ are the eigenvalues of $T_m^{(w)}$ and the weights $\{(\gamma_j^{(w)})^2\}_{j=1}^m$ are the square of the first component of the normalized eigenvectors. Thus, the matrix $T_m^{(w)}$ relates to the Gauss rule (3.3) similarly as the matrix (2.2) relates to the Gauss rule (1.4). Analogously to the right-hand side of (2.6), the rational Gauss rule (3.4) can be expressed as

$$\mathcal{R}_m^{(w)} f = e_1^T f(T_m^{(w)}) w(T_m^{(w)}) e_1. \tag{3.12}$$

Substituting the function $f \equiv 1$ into (3.4) and (3.5) yields

$$1 = \mathcal{R}_m^{(w)} f = \sum_{j=1}^{m} w(\theta_j^{(w)}) (\gamma_j^{(w)})^2 = e_1^T w(T_m^{(w)}) e_1,$$

which determines the scaling factor

$$\sigma = (e_1^T \prod_{j=1}^{k} (T_m^{(w)} - z_j I) e_1)^{-1}$$

in (3.1). Whether it is preferable to determine the spectral decomposition of $T_m^{(w)}$ and evaluate (3.4) or to compute (3.12) depends on the function f, the degree k of the polynomial (3.1), the order m of the quadrature rule, as well as on the number of times the quadrature rule is to be evaluated.

In the following analogue of Theorem 2.1, $T_{m-1}^{(w)}$ denotes the leading principal submatrix of $T_m^{(w)}$ of order $m-1$; the matrix $T_{m-1}^{(w)}$ is associated with the $(m-1)$-point Gauss rule $\mathcal{G}_{m-1}^{(w)}$ analogous to (3.3). The requirement in the theorem below that the $(m+1)$-node Gauss rule exists is equivalent to the requirement $\beta_m > 0$ in Theorem 2.1.

THEOREM 3.3. *Let the function f be $2m$ times continuously differentiable in the interval $\Omega = [\lambda_1, \lambda_n]$ and assume that the $(m+1)$-point Gauss rule analogous to (3.3) exists. If $d^{2m}(fw)/dt^{2m} > 0$ in Ω, then*

$$e_1^T f(T_{m-1}^{(w)}) w(T_{m-1}^{(w)}) e_1 < e_1^T f(T_m^{(w)}) w(T_m^{(w)}) e_1 < u^T f(A) u. \tag{3.13}$$

Similarly, if $d^{2m}(fw)/dt^{2m} < 0$ in Ω, then

$$e_1^T f(T_{m-1}^{(w)}) w(T_{m-1}^{(w)}) e_1 > e_1^T f(T_m^{(w)}) w(T_m^{(w)}) e_1 > u^T f(A) u. \tag{3.14}$$

Proof. The theorem follows from the observation that the rational Gauss rule (3.4) is the Gauss rule (3.3) applied to the function fw. The inequalities (3.13) and (3.14) are a consequence of Theorem 2.1. □

We turn to Gauss-Radau quadrature rules (3.8) associated with the measure (3.2) with a preassigned node $\hat{\theta}$. Let $\hat{T}_{m+1}^{(w)} \in \mathbf{R}^{(m+1)\times(m+1)}$ be the symmetric tridiagonal matrix associated with the Gauss-Radau rule (3.8). Then the rational Gauss-Radau rule (3.9) can be evaluated as

$$\hat{\mathcal{R}}_{m+1}^{(w)} f = e_1^T f(\hat{T}_{m+1}^{(w)}) w(\hat{T}_{m+1}^{(w)}) e_1.$$

In the following theorem, $\hat{T}_m^{(w)}$ denotes the symmetric tridiagonal matrix associated with the m-point Gauss-Radau rule $\hat{\mathcal{G}}_m^{(w)}$ analogous to the $(m+1)$-point rule $\hat{\mathcal{G}}_{m+1}^{(w)}$.

THEOREM 3.4. *Let the function f be $2m+1$ times continuously differentiable in $\hat{\Omega}$, the convex hull of the set $\{\lambda_1, \lambda_n, \hat{\theta}\}$. Assume that the $(m+2)$-point Gauss-Radau rule analogous to (3.9) exists. If $d^{2m+1}(fw)/dt^{2m+1} > 0$ in $\hat{\Omega}$, then*

$$e_1^T f(\hat{T}_m^{(w)}) w(\hat{T}_m^{(w)}) e_1 < e_1^T f(\hat{T}_{m+1}^{(w)}) w(\hat{T}_{m+1}^{(w)}) e_1 < u^T f(A) u. \tag{3.15}$$

Similarly, if $d^{2m+1}(fw)/dt^{2m+1} < 0$ in $\hat{\Omega}$, then

$$e_1^T f(\hat{T}_m^{(w)}) w(\hat{T}_m^{(w)}) e_1 > e_1^T f(\hat{T}_{m+1}^{(w)}) w(\hat{T}_{m+1}^{(w)}) e_1 > u^T f(A) u. \tag{3.16}$$

Proof. The theorem follows from the observation that the rational Gauss rule (3.4) is the Gauss rule (3.3) applied to the function fw. The inequalities (3.15) and (3.16) are a consequence of Theorem 2.2. □

We turn to the computation of the m-point rational Gauss rule (3.4) when the measure $d\mu$ is defined by (1.3). In view of Theorem 3.1, we need to determine the symmetric tridiagonal matrix $T_m^{(w)} \in \mathbf{R}^{m\times m}$ associated with the Gauss rule (3.3). The nontrivial entries of this matrix are recurrence coefficients for orthonormal polynomials with respect to the inner product

$$(f, g)^{(w)} = u^T f(A) g(A) (w(A))^{-1} u. \tag{3.17}$$

The matrix $T_m^{(w)}$ can be computed in several ways. First assume that the polynomial (3.1) can be factored according to

$$w(s) = (\widetilde{w}(s))^2, \tag{3.18}$$

where $\widetilde{w}$ is a polynomial of degree $k/2$, say,

$$\widetilde{w}(s) = \prod_{j=1}^{k/2} (s - z_j).$$

Then m steps of the standard Lanczos procedure with initial vector $(\widetilde{w}(A))^{-1} u$ yields the matrix $T_m^{(w)}$. We note that the first $k/2$ steps of the Lanczos procedure can be carried out without evaluating matrix-vector products with A if the intermediate vectors

$$w_j = (A - z_j I)^{-1} w_{j-1}, \qquad j = 1, 2, \ldots, \frac{k}{2} - 1,$$

are stored with $w_0 = u$.

If the polynomial w cannot be factored according to (3.18), then a Lanczos-type procedure that generates two biorthogonal vector sequences with respect to the inner product (3.17), such as

$$v_j = p_{j-1}(A)u, \qquad w_j = p_{j-1}(A)(w(A))^{-1}u, \qquad j = 1, 2, 3, \ldots\ ,$$

can be used to compute $T_m^{(w)}$. Such a procedure requires the evaluation of two matrix-vector products with the matrix A in each step. The need to determine two biorthogonal sequences arises when it is infeasible or impractical to compute the vector $(w(A))^{-1/2}u$.

Alternatively, we may first generate the symmetric tridiagonal matrix T_m associated with the standard Gauss quadrature rule $\mathcal{G}_m$ for the measure $d\mu$ by applying m steps of the Lanczos procedure to A with initial vector u, as described in Section 2, and then modifying this matrix to obtain $T_m^{(w)}$ as follows. Assume that the matrix T_m and the "next" subdiagonal element, β_m, already have been computed, cf. (2.1), and let z_1 be a real zero of the polynomial (3.1). We compute the moment $\mu_{-1} = u^T (A - z_1 I)^{-1} u$, e.g., by solving the linear system of equations

$$(A - z_1 I) y^{(1)} = u. \tag{3.19}$$

Algorithm 2.8 in Gautschi [7, p. 129], with T_m, β_m, and μ_{-1} as input, yields the symmetric tridiagonal matrix $T_m^{(1)}$, associated with the m-point Gauss quadrature rule for the measure $d\mu^{(1)}(s) = \sigma^{(1)}(s - z_1)^{-1} d\mu(s)$, and the next subdiagonal entry $\beta_m^{(1)}$. Here $\sigma^{(1)}$ is a scaling factor chosen to give the measure $d\mu^{(1)}$ total mass one.

If the polynomial (3.1) has another real zero, say z_2, then we update $T_m^{(1)}$ and $\beta_m^{(1)}$ similarly as T_m and β_m. Thus, we first compute the moment μ_{-2}, e.g., by solving the linear system of equations $(A - z_2 I) y^{(2)} = y^{(1)}$, where $y^{(1)}$ satisfies (3.19), and then use $T_m^{(1)}$, $\beta^{(1)}$, and μ_{-2} as input for Algorithm 2.8 in [7]. The algorithm determines the symmetric tridiagonal matrix $T_m^{(2)}$, associated with the m-point Gauss quadrature rule for the measure $d\mu^{(2)}(s) = \sigma^{(2)}(s - z_1)^{-1}(s - z_2)^{-1} d\mu(s)$, and the next subdiagonal entry $\beta_m^{(2)}$. The coefficient $\sigma^{(2)}$ is a scaling factor.

When the polynomial (3.1) has a pair of complex conjugate zeros, say z_3 and z_4, Algorithm 2.9 in [7, p. 131] can be used to compute the tridiagonal matrix $T_m^{(4)}$, associated with the m-point Gauss quadrature rule for the measure

$$d\mu^{(4)}(s) = \sigma^{(4)} \prod_{j=1}^{4} (s - z_j)^{-1} d\mu(s), \tag{3.20}$$

and the next subdiagonal entry $\beta_m^{(4)}$. The algorithm computes the tridiagonal matrix associated with the poles z_3 and z_4 without using complex arithmetic. It requires the matrix $T_m^{(2)}$, the next sudiagonal entry $\beta_m^{(2)}$, and the moment $\mu_{-3} = u^T(A - z_3 I)^{-1} y^{(2)}$ as input. The output from Algorithms 2.8 and 2.9 in [7] allows the computation of the matrix $\hat{T}_{m+1}^{(4)}$ associated with the $(m+1)$-point Gauss-Radau quadrature rule for the measure (3.20) and a specified node, $\hat{\theta}$, as described in Section 2.

Given T_m, β_m, and the moments μ_{-j}, $1 \le j \le 3$, the computation of the tridiagonal matrices $T_m^{(4)}$ and $\hat{T}_{m+1}^{(4)}$ by Algorithms 2.8 and 2.9 in [7] requires only $\mathcal{O}(m)$ arithmetic floating point operations. In the applications of the present paper, k typically is small and m is not large. Algorithms 2.8 and 2.9 in [7] perform well in this situation.

4. Computed examples. The numerical examples of this section illustrate the application of rational Gauss quadrature rules to compute bounds for functionals of the form (1.1). All computations are carried out in MATLAB with approximately 16 significant decimal digits.

m	$F(A) - \mathcal{R}_m^{(w)} f$	$F(A) - \hat{\mathcal{R}}_{m+1}^{(w)} f$
2	$1.1 \cdot 10^{-1}$	$-9.5 \cdot 10^{-2}$
4	$3.7 \cdot 10^{-5}$	$-2.1 \cdot 10^{-5}$
6	$1.9 \cdot 10^{-9}$	$-7.6 \cdot 10^{-10}$

TABLE 4.1

Example 4..1: $f(s) = (s+1)^{-1}\exp(s/2)$, $w(s) = s+1$, $F(A) = 3.25117509770 \cdot 10^1$, and A is a symmetric positive definite Toeplitz matrix.

Example 4.1. Let $A \in \mathbf{R}^{n\times n}$ be the symmetric Toeplitz matrix with first row $[1, 1/2, \ldots, 1/n]$ and $n = 1024$. Its smallest and largest eigenvalues are $\lambda_{\min}(A) = 3.86 \cdot 10^{-1}$ and $\lambda_{\max}(A) = 1.22 \cdot 10^1$, respectively. Let $u = n^{-1/2}[1, 1, \ldots, 1]^T \in \mathbf{R}^n$. We seek to determine upper and lower bounds for the functional (1.1) with

$$f(s) = \frac{1}{s+1} \exp\left(\frac{s}{2}\right).$$

The polynomial $w(s) = s+1$ determines the rational Gauss and Gauss-Radau quadrature rules $\mathcal{R}_m f$ and $\hat{\mathcal{R}}_{m+1} f$, respectively. The latter have the fixed node $\hat{\theta} = 13$. We compute the tridiagonal matrices for the quadrature rules by Algorithm 2.8 in [7]. The computations require the solution of a linear system of equations (3.19) with the symmetric positive definite Toeplitz matrix $A + I$. Fast algorithms are available for this purpose; they require only $\mathcal{O}(n \log_2^2 n)$ arithmetic floating point operations, see, e.g., [1]. This is not much more computational work than the $\mathcal{O}(n \log_2 n)$ arithmetic floating point operations needed for the evaluation of a matrix-vector product with the matrix A; see, e.g., [18, Section 3.4] for a discussion of the latter.

Table 4.1 displays the errors in the computed rational Gauss and Gauss-Radau quadrature rules. The errors are seen to decrease quickly as m increases. The table illustrates that

$$\mathcal{R}_m f < F(A) < \hat{\mathcal{R}}_{m+1} f \qquad \forall m.$$

We remark that the standard Gauss and Gauss-Radau rules of Section 2 are not guaranteed to determine approximations that bracket $F(A)$. □

m	$F(A) - \mathcal{R}_m^{(w)} f$	$F(A) - \hat{\mathcal{R}}_{m-1}^{(w)} f$
3	$-1.5 \cdot 10^{-6}$	$6.5 \cdot 10^{-7}$
4	$-5.7 \cdot 10^{-8}$	$2.3 \cdot 10^{-8}$
5	$-2.2 \cdot 10^{-9}$	$8.8 \cdot 10^{-10}$
6	$-8.5 \cdot 10^{-11}$	$3.3 \cdot 10^{-11}$

TABLE 4.2

Example 4.2: $f(s) = (s^2 + \frac{1}{4})^{-1} \log(\frac{1}{2} + s)$, $w(s) = s^2 + \frac{1}{4}$, $F(A) = 3.10166289819 \cdot 10^{-1}$, and A is a symmetric positive definite Toeplitz matrix.

Example 4.2. Let $A \in \mathbf{R}^{1024 \times 1024}$ be the symmetric Toeplitz matrix with the first row $\frac{1}{10}[1, 1/2, \dots, 1/1024]$. Its extreme eigenvalues are $\lambda_{\min}(A) = 3.86 \cdot 10^{-2}$ and $\lambda_{\max}(A) = 1.22$. The vector u is the same as in Example 4.1. We would like to compute upper and lower bounds for the functional (1.1) with

$$f(s) = \frac{1}{s^2 + \frac{1}{4}} \log(\frac{1}{2} + s).$$

The polynomial $w(s) = s^2 + \frac{1}{4}$ determines the rational Gauss and Gauss-Radau quadrature rules $\mathcal{R}_m f$ and $\hat{\mathcal{R}}_{m+1} f$, respectively. The latter have a fixed node at the origin. We compute the tridiagonal matrices for the quadrature rules by Algorithm 2.9 in [7].

Table 4.2 displays the errors in the computed rational Gauss and Gauss-Radau quadrature rules. The table illustrates that

$$\mathcal{R}_m f > F(A) > \hat{\mathcal{R}}_{m+1} f \qquad \forall m.$$

The values determined by the standard Gauss and Gauss-Radau rules of Section 2 are not guaranteed to bracket $F(A)$. □

t	$F(A) - \mathcal{G}_6 f$	$F(A) - \hat{\mathcal{G}}_7 f$	$F(A) - \mathcal{R}_6^{(w)} f$	$F(A) - \hat{\mathcal{R}}_7^{(w)} f$
0.5	$2.9 \cdot 10^{-10}$	$-1.3 \cdot 10^{-10}$	$-3.0 \cdot 10^{-12}$	$1.2 \cdot 10^{-12}$
0.6	$8.4 \cdot 10^{-11}$	$-3.1 \cdot 10^{-11}$	$-1.1 \cdot 10^{-11}$	$4.2 \cdot 10^{-12}$
0.7	$2.7 \cdot 10^{-11}$	$-9.0 \cdot 10^{-12}$	$-7.1 \cdot 10^{-12}$	$2.3 \cdot 10^{-12}$

TABLE 4.3

Example 4.3: $f(s) = (s + t)^{-9/10}$, $w(s) = s + \frac{1}{2}$, $F(A) \approx 0.6$ for the tabulated values of t, and A is a symmetric positive definite Toeplitz matrix.

Example 4.3. Let the matrix A and vector u be the same as in Example 4.2. We wish to determine upper and lower bounds for the functional (1.1) with $f(s) = (s + t)^{-9/10}$ for a few values of the parameter $t \geq 1/2$. Pairs of Gauss and Gauss-Radau rules of Section 2 yield such bounds, and so do pairs of rational Gauss and

Gauss-Radau rules of Section 3 with $w(s) = s + \frac{1}{2}$. The Gauss-Radau and rational Gauss-Radau rules have a fixed node at the origin. The so determined quadrature rules satisfy

$$\mathcal{G}_m f < F(A) < \hat{\mathcal{G}}_{m+1} f, \qquad \hat{\mathcal{R}}_{m+1} f < F(A) < \mathcal{R}_m f \qquad \forall m.$$

Table 4.3 shows the rational Gauss-Radau rule to give smaller errors of the same sign than the standard Gauss rule, and a much smaller error for $t = 1/2$. The rational Gauss rule yield smaller errors of the same sign than the standard Gauss-Radau rule. The exact values of $F(A)$ are (after rounding) $6.20904123704 \cdot 10^{-1}$ for $t = 0.5$, $5.89614813104 \cdot 10^{-1}$ for $t = 0.6$, and $5.61495157374 \cdot 10^{-1}$ for $t = 0.7$.

The accuracy of the standard Gauss rules can be improved by increasing the sizes of the corresponding tridiagonal matrices. The availability of an accurate approximation of the functional (1.1) with a small matrix can be important if the approximant is to be evaluated for many values of the parameter t. □

5. Conclusion. Rational Gauss rules can be used to bound functionals of the form (1.1) in situations when standard Gauss rules cannot. Moreover, when both standard and rational Gauss rules provide bounds, the latter may give higher accuracy with the same number of nodes.

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