

# Computation of error bounds via generalized Gauss–Radau and Gauss–Lobatto rules

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## Abstract

Many functionals of a large symmetric matrix of interest in science and engineering can be expressed as a Stieltjes integral with a measure supported on the real axis. These functionals can be approximated by quadrature rules. Golub and Meurant proposed a technique for computing upper and lower error bounds for Stieltjes integrals with integrands whose derivatives do not change sign on the convex hull of the support of the measure. This technique is based on evaluating pairs of a Gauss quadrature rule and a suitably chosen Gauss–Radau or Gauss–Lobatto quadrature rule. However, when derivatives of the integrand change sign on the convex hull of the support of the measure, this technique is not guaranteed to give upper and lower error bounds for the functional. We describe an extension of the technique by Golub and Meurant that yields upper and lower error bounds for the functional in situations when only some derivatives of the integrand do not change sign on the convex hull of the support of the measure. This extension is based on the use of pairs of Gauss, and suitable generalized Gauss–Radau or Gauss–Lobatto rules. New methods to evaluate generalized Gauss–Radau and Gauss–Lobatto rules also are described.

*Keywords:* Quadrature formula, generalized Gauss–Radau formula, generalized Gauss–Lobatto formula.

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## 1. Introduction

The need to evaluate matrix functionals of the form

$$F(A) := \mathbf{v}^T f(A) \mathbf{v}, \quad (1.1)$$

where  $A \in \mathbb{R}^{n \times n}$  is a large symmetric matrix,  $\mathbf{v} \in \mathbb{R}^n$ ,  $f$  is a function that is defined on the convex hull of the spectrum of  $A$ , and the superscript  $T$  denotes transposition arises in many applications, including in Tikhonov regularization and network analysis; see, e.g., [1, 3, 4, 5, 19] for illustrations. For notational simplicity, we will assume that  $\|\mathbf{v}\| = 1$ . Here and throughout this paper  $\|\cdot\|$  denotes the Euclidean vector norm.

Golub and Meurant [13, 14] describe a technique for computing upper and lower error bounds for matrix functionals of the form (1.1) based on the connection between the Lanczos process, orthogonal polynomials, and Gauss-type quadrature rules. Their technique considers the expression (1.1) as a Stieltjes integral with integrand  $f$ . This indicates that Gauss-type quadrature rules can be applied to compute approximations of (1.1). Assuming that derivatives of the integrand  $f$  do not change sign in the convex hull of the spectrum of  $A$ , Golub and Meurant [13, 14] observed that pairs of Gauss, and suitable Gauss–Radau or Gauss–Lobatto rules, provide upper and lower bounds for (1.1). This follows straightforwardly from the sign of the remainder terms for these quadrature rules.

When derivatives of the integrand  $f$  change sign in the convex hull of the spectrum of  $A$ , the technique developed by Golub and Meurant [13, 14] is not guaranteed to provide upper and lower error bounds for (1.1).

**Example 1.1.** Let  $A \in \mathbb{R}^{200 \times 200}$  be the symmetric Toeplitz matrix with first row  $[2/3, 2/5, \dots, 2/401]$ . Its largest and smallest eigenvalues are given by  $\lambda_{min} = 0.19175$  and  $\lambda_{max} = 8.0626$ , respectively. Consider the approximation of the functional

$$F(A) := \mathbf{v}^T \exp\left(-\frac{A}{4}\right) \sin\left(\frac{A}{4}\right) \mathbf{v}. \quad (1.2)$$

and define the integrand

$$f(x) := \exp\left(-\frac{x}{4}\right) \sin\left(\frac{x}{4}\right). \quad (1.3)$$

Some derivatives of this integrand change sign on the interval  $[\lambda_{min}, \lambda_{max}]$ . We illustrate in Example 4.1 of Section 4 that pairs of Gauss and Gauss–Radau rules, or pairs of Gauss and Gauss–Lobatto rules, do not furnish upper and lower error bounds for (1.2).

We are interested in exploring whether the technique of Golub and Meurant can be extended to give upper and lower error bounds for (1.1) also in situations when some derivatives of the integrand  $f$  change sign in the convex hull of the spectrum of  $A$ . Specifically, we will show that pairs of Gauss rules and suitably chosen generalized Gauss–Radau or generalized Gauss–Lobatto rules give upper and lower error bounds for (1.1) in some situations when pairs of Gauss and (standard) Gauss–Radau or Gauss–Lobatto rules are not guaranteed to furnish upper and lower bounds.

Generalized Gauss–Radau rules are Gauss–Radau-type rules, in which the fixed node has multiplicity larger than one; similarly, generalized Gauss–Lobatto rules are Gauss–Lobatto-type rules, in which at least one of the fixed nodes has multiplicity larger than one. Generalized Gauss–Radau and Gauss–Lobatto rules have received considerable attention; see, e.g., [6, 8, 9, 11, 12, 20, 23]. Applications of these quadrature rules include the computation of spline approximations that reproduce as many consecutive moments of the integrand  $f$  as possible; see Gautschi [7, Section 3.3] for details.

This paper is organized as follows: Section 2 reviews generalized Gauss–Radau quadrature rules, and describes a novel way to evaluate these quadrature rules. Generalized Gauss–Lobatto rules are considered in Section 3, and a few computed examples are presented in Section 4. Concluding remarks can be found in Section 5.

We conclude this section by discussing how the matrix functional (1.1) is related to a Stieltjes integral. The development follows Golub and Meurant [13, 14]. Introduce the spectral factorization

$$A = S\Lambda S^T, \quad \Lambda = \text{diag}[\lambda_1, \lambda_2, \dots, \lambda_n],$$

with the eigenvalues  $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$  and  $S \in \mathbb{R}^{n \times n}$  an orthogonal matrix, whose columns are eigenvectors. Then we define

$$f(A) = Sf(\Lambda)S^T;$$

see, e.g., [15, 16] for discussions on the definition of matrix functions. Introduce the row vector  $[\nu_1, \nu_2, \dots, \nu_n] := \mathbf{v}^T S$ . Then the functional (1.1) can be written as

$$F(A) = \mathbf{v}^T S f(\Lambda) S^T \mathbf{v} = \sum_{j=1}^n f(\lambda_j) \nu_j^2. \quad (1.4)$$

The right-hand side can be expressed as a Stieltjes integral

$$\mathcal{I}f := \int_a^b f(x) d\lambda(x), \quad (1.5)$$

where the distribution function  $\lambda$  associated with the measure  $d\lambda$  can be chosen to be piece-wise constant and defined by

$$\lambda(x) := \begin{cases} 0, & \text{if } x < a = \lambda_1, \\ \sum_{j=1}^i \nu_j^2, & \text{if } \lambda_i \leq x < \lambda_{i+1}, \quad i = 1, 2, \dots, n-1, \\ \sum_{j=1}^n \nu_j^2, & \text{if } b = \lambda_n \leq x. \end{cases}$$

The  $m$ -point (standard) Gauss quadrature rule associated with the measure  $d\lambda(x)$  is of the form

$$\mathcal{G}_m f := \sum_{i=1}^m w_i f(x_i),$$

and is characterized by the property that

$$\mathcal{I}f = \mathcal{G}_m f, \quad \forall f \in \mathbb{P}^{2m-1},$$

where  $\mathbb{P}^{2m-1}$  denotes the set of polynomials of degree at most  $2m - 1$ . The nodes  $x_i$  of the quadrature rule are distinct and known to be the zeros of an  $m$ th degree orthogonal polynomial with respect to the inner product

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

When the integrand  $f$  is  $2m$  times continuously differentiable in the interval  $[a, b]$ , the error in the quadrature rule can be expressed as

$$\mathcal{E}_m f := (\mathcal{I} - \mathcal{G}_m)f = \frac{f^{(2m)}(x_G)}{(2m)!} \cdot \int_a^b \prod_{i=1}^m (x - x_i)^2 d\lambda(x), \tag{1.7}$$

for some  $x_G \in [a, b]$ , where  $f^{(2m)}(x)$  denotes the  $2m$ th derivative; see, e.g., [7, 14] for proof.

We will approximate the integral (1.5), and therefore the functional (1.1), by Gauss-type quadrature rules. Under suitable conditions, the sign of the quadrature error can be inferred from the remainder terms of the quadrature rules used. While our discussion focuses on functionals of the form (1.1), a generalization to functionals  $\mathbf{u}^T f(A)\mathbf{v}$  with  $\mathbf{u} \in \mathbb{R}^n$  different from  $\mathbf{v}$  is straightforward by using the identity

$$\mathbf{u}^T f(A)\mathbf{v} = \frac{1}{4} \left( (\mathbf{u} + \mathbf{v})^T f(A)(\mathbf{u} + \mathbf{v}) - (\mathbf{u} - \mathbf{v})^T f(A)(\mathbf{u} - \mathbf{v}) \right).$$

## 2. Generalized Gauss–Radau formulas

This section considers generalized Gauss–Radau rules of the form

$$\mathcal{G}_{m,r} f = \sum_{i=1}^m w_i f(x_i) + \sum_{j=0}^{r-1} w_j^{(0)} f^{(j)}(x_0) \tag{2.1}$$

for approximating the integral (1.5), where the  $x_i$ ,  $1 \leq i \leq m$ , are “free” distinct nodes in the open interval  $(a, b)$ , and  $x_0$  is a prescribed node of multiplicity  $r \geq 2$  outside this interval. Let  $\text{int}(a, b, x_0)$  denote the convex hull of the set  $\{a, b, x_0\}$ , where  $-\infty < x_0 \leq a$  or  $b \leq x_0 < \infty$ . We assume that  $f$  and its required derivatives (see below) are defined in  $\text{int}(a, b, x_0)$ . Many properties of generalized Gauss–Radau rules are discussed in [6, 7, 8, 9, 11, 12, 20, 23]. Here we recall that the nodes  $x_1, x_2, \dots, x_m$  are the zeros of the  $m$ th degree orthogonal polynomial with respect to the measure  $(x - a)^r d\lambda(x)$ . The generalized Gauss–Radau quadrature rule satisfies

$$\mathcal{I}f = \mathcal{G}_{m,r} f, \quad \forall f \in \mathbb{P}^{2m+r-1}; \tag{2.2}$$

see, e.g., [7] for details.

When the integrand  $f$  is  $2m + r$  times continuously differentiable in  $\text{int}(a, b, x_0)$ , the error in the generalized Gauss–Radau quadrature rule (2.1) can be expressed as

$$\mathcal{E}_{m,r}f := (\mathcal{I} - \mathcal{G}_{m,r})f = \frac{f^{(2m+r)}(x_{\text{GR}})}{(2m+r)!} \cdot \int_a^b (x-x_0)^r \prod_{i=1}^m (x-x_i)^2 d\lambda(x), \quad (2.3)$$

for some  $x_{\text{GR}} \in \text{int}(a, b, x_0)$ ; see, e.g., [18] for a proof of (2.3). If the derivative  $f^{(2m+r)}$  is of known constant sign in  $\text{int}(a, b, x_0)$ , then we can tell the sign of  $\mathcal{E}_{m,r}f$ . For instance, when  $f^{(2m+r)}(x) \leq 0$  for  $x \in \text{int}(a, b, x_0)$ , and  $x_0 = a$ , the quadrature rule  $\mathcal{G}_{m,r}f$  furnishes an upper bound for  $\mathcal{I}f$ .

Gautschi [6, 8, 9] describes several ways of computing the nodes and weights of generalized Gauss–Radau rules (2.1). We will describe a new approach to evaluate these quadrature rules that is convenient to use when the measure is implicitly defined by a sum (1.4). Our approach does not require the explicit evaluation of the nodes and weights.

Application of  $m + r$  steps of the Lanczos process to the matrix  $A$  with initial unit vector  $\mathbf{v}$  gives the Lanczos decomposition

$$AU_{m+r} = U_{m+r}J_{m+r} + \sqrt{\beta_{m+r}}\mathbf{u}_{m+r+1}\mathbf{e}_{m+r}^T, \quad (2.4)$$

where the matrix  $U_{m+r} = [\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_{m+r}] \in \mathbb{R}^{n \times (m+r)}$  and vector  $\mathbf{u}_{m+r+1} \in \mathbb{R}^n$  satisfy  $\mathbf{u}_1 = \mathbf{v}$ ,  $U_{m+r}^T U_{m+r} = I_{m+r}$ ,  $\|\mathbf{u}_{m+r+1}\| = 1$ , and  $U_{m+r}^T \mathbf{u}_{m+r+1} = \mathbf{0}$ . Throughout this paper  $\mathbf{e}_j = [0, \dots, 0, 1, 0, \dots, 0]^T$  is the  $j$ th axis vector of suitable dimension, and  $I_j$  stands for the identity matrix of order  $j$ . Moreover,  $\beta_{m+r} \in \mathbb{R}_+$  and the matrix

$$J_{m+r} := \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & & \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & & \\ & \sqrt{\beta_2} & \alpha_2 & \ddots & & \\ & & & \ddots & \ddots & \\ & & & & \ddots & \sqrt{\beta_{m+r-1}} \\ & & & & \sqrt{\beta_{m+r-1}} & \alpha_{m+r-1} \end{bmatrix} \in \mathbb{R}^{(m+r) \times (m+r)},$$

is symmetric and tridiagonal. The Lanczos procedure is a discrete analogue of the Stieltjes procedure in the sense that the former is applied to a matrix and a vector; it requires the support of the measure to be a finite discrete point set. Of course, continuous analogues of the Lanczos procedure can be defined, in which case the matrix  $A$  is replaced by a symmetric operator. The Stieltjes procedure is described, e.g., by Gautschi [7] and the (discrete) Lanczos procedure is discussed by Golub and Meurant [13, 14]. Typically,  $1 < m + r \ll n$  in computations. We tacitly assume that  $m + r$  is small enough so that the decomposition (2.4) with the stated properties exists. This is the generic situation. In the rare event that the Lanczos process breaks down before  $m + r$  steps have been carried out, the computations simplify. We will not dwell on the ramification of breakdown.

The dominant computational effort required for the calculation of the decomposition (2.4) by the Lanczos process is the evaluation of  $m+r$  matrix-vector products with the matrix  $A$ ; see, e.g., [13, 14]. Each matrix-vector product evaluation with  $A$  requires  $\mathcal{O}(cn)$  arithmetic floating-point operations (flops), where  $c$  is the average number of nonvanishing entries of  $A$  per row.

The relation (2.4) shows that the columns  $\mathbf{u}_j$  of  $U_{m+r}$  can be expressed as

$$\mathbf{u}_j = p_{j-1}(A)\mathbf{v}, \quad j = 1, 2, 3, \dots, \quad (2.5)$$

for certain polynomials  $p_{j-1} \in \mathbb{P}^{j-1}$ .

It follows from the orthonormality of the vectors  $\mathbf{u}_j$  and (2.5) that

$$\begin{aligned} (p_{j-1}, p_{k-1}) &= \int_a^b p_{j-1}(x)p_{k-1}(x)d\lambda(x) = \mathbf{v}^T S p_{j-1}(\Lambda) p_{k-1}(\Lambda) S^T \mathbf{v} \\ &= \mathbf{v}^T p_{j-1}(A) p_{k-1}(A) \mathbf{v} = \mathbf{u}_j^T \mathbf{u}_k = \begin{cases} 0, & j \neq k, \\ 1, & j = k. \end{cases} \end{aligned}$$

Thus, the polynomials  $p_j$  are orthonormal with respect to the inner product (1.6).

The decomposition (2.4) defines a recurrence relation for the columns  $\mathbf{u}_j$  of  $U_{m+r}$ , which, in view of (2.5), gives the following recurrence relation for the polynomials  $p_j$ ,

$$\begin{aligned} \sqrt{\beta_1} p_1(x) &= (x - \alpha_0) p_0(x), \quad p_0(x) = 1, \\ \sqrt{\beta_j} p_j(x) &= (x - \alpha_{j-1}) p_{j-1}(x) - \sqrt{\beta_{j-1}} p_{j-2}(x), \quad 2 \leq j \leq m+r, \end{aligned} \quad (2.6)$$

where

$$\alpha_{j-1} = (p_{j-1}, x p_{j-1}). \quad j = 1, 2, \dots, m+r,$$

and the  $\beta_j > 0$  are determined by the requirements  $(p_j, p_j) = 1$  for all  $j$ .

Introduce the vector

$$\mathbf{p}(x) = \begin{bmatrix} p_0(x) \\ p_1(x) \\ \vdots \\ p_{m+r-1}(x) \end{bmatrix}.$$

Then the recurrence relation (2.6) can be written in the form

$$x \mathbf{p}(x) = J_{m+r} \mathbf{p}(x) + \sqrt{\beta_{m+r}} p_{m+r}(x) \mathbf{e}_{m+r}, \quad (2.7)$$

which shows that the eigenvalues of  $J_{m+r}$  are the zeros of the polynomial  $p_{m+r}$ . It can be shown that the  $(m+r)$ -node (standard) Gauss quadrature rule associated with the measure  $d\lambda$  in (1.5) can be expressed as

$$\mathcal{G}_{m+r} f = \mathbf{e}_1^T f(J_{m+r}) \mathbf{e}_1. \quad (2.8)$$

Here we have used the fact that the vector  $\mathbf{v}$  in (1.4) is of unit norm; see [14] for details. Note that the Gauss rule (2.8) can be computed by evaluating the function  $f$  of the generally fairly small matrix  $J_{m+r}$ , without explicitly calculating the nodes

and weights of the Gauss rule. Many algorithms for evaluating functions of a small to moderately-sized matrix are described and analyzed by Higham [16].

We now show how the generalized Gauss–Radau rule (2.1) can be evaluated without explicitly computing its nodes and weights. Let  $\pi_0, \pi_1, \pi_2, \dots$  be orthonormal polynomials with respect to the inner product

$$(f, g)_r = \int_a^b f(x)g(x)(x - x_0)^r d\lambda(x), \quad (2.9)$$

where the measure  $d\lambda$  is the same as in (1.5). Thus,

$$(\pi_i, \pi_j)_r = \begin{cases} 1, & i = j, \\ 0, & i \neq j, \end{cases}$$

and  $\pi_i \in \mathbb{P}^i$ . Define the polynomial  $q_{m+r}(x) = \pi_m(x)(x - x_0)^r$ . Then

$$xp_{m+r-1}(x) = \sum_{i=0}^{m+r-1} d_i p_i(x) + s_{m+r} q_{m+r}(x), \quad (2.10)$$

for suitable coefficients  $d_i$  and  $s_{m+r}$ . The orthonormality of the polynomials  $p_i$  with respect to the inner product (1.6) gives, for  $i = 0, 1, \dots, m + r - 1$ ,

$$d_i = \int_a^b xp_{m+r-1}(x)p_i(x)d\lambda(x) - s_{m+r} \int_a^b \pi_m(x)p_i(x)(x - x_0)^r d\lambda(x).$$

Now using the orthogonality of the polynomials  $p_i$  with respect to the inner product (1.6) and the orthogonality of the polynomials  $\pi_j$  with respect to the inner product (2.9) shows that  $d_i = 0$  for  $0 \leq i < m$ . It follows that (2.10) simplifies to

$$xp_{m+r-1}(x) = \sum_{i=m}^{m+r-1} d_i p_i(x) + s_{m+r} q_{m+r}(x). \quad (2.11)$$

We obtain analogously to (2.7) the relation

$$x \mathbf{p}(x) = J_{m+r}^R \mathbf{p}(x) + s_{m+r} q_{m+r}(x) \mathbf{e}_{m+r}, \quad (2.12)$$

where the matrix  $J_{m+r}^R \in \mathbb{R}^{(m+r) \times (m+r)}$  is obtained from  $J_{m+r}$  by replacing the last row by the vector

$$[0, \dots, 0, d_m, d_{m+1}, \dots, d_{m+r-1}].$$

It follows from (2.7) that the nodes  $x_0, x_1, \dots, x_m$  of the quadrature rule (2.1) are eigenvalues of  $J_{m+r}^R$ , and the vectors  $\mathbf{p}(x_i)$ ,  $i = 0, 1, \dots, m$ , are corresponding eigenvectors. We will show below that the eigenvalue  $x_0$  has algebraic multiplicity  $r$  and geometric multiplicity 1.

Let  $p_i^{(j)}$  denote the  $j$ th derivative of the polynomial  $p_i$ . The nontrivial entries of the last row of  $J_{m+r}^R$  can be determined by solving the linear system of equations

$$x_0 p_{m+r-1}^{(j)}(x_0) + j p_{m+r-1}^{(j-1)}(x_0) = \sum_{i=m}^{m+r-1} d_i p_i^{(j)}(x_0), \quad j = 1, \dots, r-1, \quad (2.13)$$

which is obtained by differentiating (2.11) and using the fact that  $q_{m+r}^{(j)}(x_0) = 0$  for  $j = 0, 1, \dots, r-1$ .

We next verify that the Gauss–Radau rule (2.1) can be expressed as

$$\mathcal{G}_{m,r} f = \mathbf{e}_1^T f (J_{m+r}^R) \mathbf{e}_1. \quad (2.14)$$

This formula is analogous to (2.8). We show (2.14) by deriving the Jordan decomposition of the matrix  $J_{m+r}^R$ ; see [21, Section 4] for details for more general situations. Differentiating equation (2.12)  $j$  times yields

$$x \mathbf{p}^{(j)}(x) + j \mathbf{p}^{(j-1)}(x) = J_{m+r}^R \mathbf{p}^{(j)}(x) + s_{m+r} q_{m+r}^{(j)}(x) \mathbf{e}_{m+r}, \quad j = 1, 2, \dots, r-1,$$

where  $\mathbf{p}^{(j)}(x)$  denotes  $j$  times component-wise differentiation of  $\mathbf{p}(x)$  with respect to  $x$ . Dividing the right-hand side and left-hand side by  $j!$  and setting  $x = x_0$  gives

$$(J_{m+r}^R - x_0 I) \frac{1}{j!} \mathbf{p}^{(j)}(x_0) = \frac{1}{(j-1)!} \mathbf{p}^{(j-1)}(x_0),$$

i.e.,  $\mathbf{p}^{(j)}(x_0)/(j!)$ ,  $j = 1, \dots, r-1$ , are principal (generalized eigen-) vectors of  $J_{m+r}^R$ . Introduce the  $(m+r) \times (m+r)$  matrix

$$W = [\mathbf{p}(x_1), \dots, \mathbf{p}(x_m), \mathbf{p}(x_0), \mathbf{p}^{(1)}(x_0), \dots, \frac{1}{(r-1)!} \mathbf{p}^{(r-1)}(x_0)]. \quad (2.15)$$

We have derived the Jordan factorization

$$J_{m+r}^R W = W \Lambda, \quad \Lambda = \left[ \begin{array}{cccccccc} x_1 & & & & & & & \\ & \ddots & & & & & & \\ & & x_m & & & & & \\ & & & x_0 & 1 & & & \\ & & & & x_0 & 1 & & \\ & & & & & \ddots & \ddots & \\ & & & & & & x_0 & 1 \\ & & & & & & & x_0 \end{array} \right]. \quad (2.16)$$

Thus, the matrix  $\Lambda \in \mathbb{R}^{(m+r) \times (m+r)}$  has a leading  $m \times m$  diagonal block matrix and a trailing  $r \times r$  Jordan block associated with the eigenvalue  $x_0$ .



Our proof of the representation (2.14) requires explicit formulas for the entries in the first column of  $W^{-1}$ . Introduce the matrix  $V \in \mathbb{R}^{(m+r) \times (m+r)}$ , whose  $i$ th row is  $\mathbf{v}_i^T$ , where

$$\begin{aligned} \mathbf{v}_i &= w_i \mathbf{p}(x_i), \quad i = 1, 2, \dots, m, \\ \mathbf{v}_{m+s} &= \sum_{u=s-1}^{r-1} u! w_u^{(0)} \mathbf{p}^{(u+1-s)}(x_0), \quad s = 1, 2, \dots, r. \end{aligned}$$

Denote the  $i$ th row of  $W$  by  $\mathbf{a}_i^T = [a_1, a_2, \dots, a_{m+r}]$ , and the  $j$ th column of  $V$  by  $\mathbf{b}_j = [b_1, b_2, \dots, b_{m+r}]^T$ . We will show that

$$\mathbf{a}_i^T \mathbf{b}_j = \mathcal{G}_{m+r}(p_{i-1} p_{j-1}).$$

Note that

$$a_k = p_{i-1}(x_k), \quad b_k = w_k p_{j-1}(x_k), \quad k = 1, 2, \dots, m$$

and

$$a_{m+s} = \frac{1}{(s-1)!} p_{i-1}^{(s-1)}(x_0), \quad b_{m+s} = \sum_{u=s-1}^{r-1} u! w_u^{(0)} \frac{p_{j-1}^{(u+1-s)}(x_0)}{(u+1-s)!}, \quad s = 1, 2, \dots, r.$$

It follows that

$$\begin{aligned} \sum_{k=1}^{m+r} a_k b_k &= \sum_{k=1}^m w_k p_{i-1}(x_k) p_{j-1}(x_k) + \sum_{s=1}^r \sum_{u=s-1}^{r-1} p_{i-1}^{(s-1)}(x_0) \binom{u}{s-1} w_u^{(0)} p_{j-1}^{(u+1-s)}(x_0) \\ &= \sum_{k=1}^m w_k p_{i-1}(x_k) p_{j-1}(x_k) + \sum_{\ell=0}^{r-1} w_\ell^{(0)} \sum_{q=0}^{\ell} \binom{\ell}{q} p_{i-1}^{(q)}(x_0) p_{j-1}^{(\ell-q)}(x_0) \\ &= \sum_{k=1}^m w_k (p_{i-1} p_{j-1})(x_k) + \sum_{\ell=0}^{r-1} w_\ell^{(0)} (p_{i-1} p_{j-1})^{(\ell)}(x_0) \\ &= \mathcal{G}_{m,r}(p_{j-1} p_{i-1}). \end{aligned} \tag{2.17}$$

In view of (2.2), we have for  $i + j - 2 \leq 2m + r - 1$  that

$$\mathcal{G}_{m,r}(p_{j-1} p_{i-1}) = \begin{cases} 1, & i = j, \\ 0, & i \neq j. \end{cases}$$

It now follows from (2.17) that the first  $m + 1$  columns of the matrix  $V$  are the first  $m + 1$  columns of  $W^{-1}$ . In particular,

$$W^{-1} \mathbf{e}_1 = [w_1, w_2, \dots, w_m, w_0^{(0)}, \dots, (r-1)! w_{r-1}^{(0)}]^T. \tag{2.18}$$

We obtain from (2.15) that

$$W^T \mathbf{e}_1 = [1, 1, \dots, 1, 0, \dots, 0]^T. \tag{2.19}$$

Finally, equations (2.16), (2.18), and (2.19) give

$$\mathbf{e}_1^T f(J_{m+r}^R) \mathbf{e}_1 = \mathbf{e}_1^T W f(\Lambda) W^{-1} \mathbf{e}_1 = \mathcal{G}_{m,r} f,$$

which shows (2.14).

We conclude that the generalized Gauss–Radau rule  $\mathcal{G}_{m,r} f$  can be evaluated by using either (2.1) or (2.14). Which one of these expressions is most convenient to compute depends on whether software for computing the integrand  $f$  at the small matrix  $J_{m+r}^R$  is available or easily can be written. This is the case, for instance, for the exponential function, logarithm, square root, and rational expressions. When the form (2.1) is used, the nodes and weights have to be evaluated. This can be done with software written by Gautschi [10].

We note that if the moments  $\mu_i := \int_a^b x^i d\lambda(x)$ ,  $i = 0, 1, 2, \dots$ , are explicitly known, which is the case for many classical positive measures on the real line, the modified moments

$$\nu_i = \int_a^b x^i (x - x_0)^r d\lambda(x), \quad i = 0, 1, 2, \dots,$$

can be easily computed. Then the coefficients  $d_i$  in (2.13) can be evaluated without solving linear systems of equations.

Taking  $f(x) = (x - x_0)^r P(x)$ , where  $P(x) \in \mathbb{P}^{2m-1}$ , in (2.1) we verify that the first sum on the right-hand side in (2.1) is actually the (standard)  $m$ -point Gauss quadrature for the integral

$$\tilde{\mathcal{I}} f = \int_a^b f(x) d\tilde{\lambda}(x), \quad d\tilde{\lambda}(x) = (x - x_0)^r d\lambda(x).$$

Thus the quadrature  $\mathcal{G}_{m,r} f$  can be written in the form

$$\mathcal{G}_{m,r} f = \tilde{m}_0 \mathbf{e}_1^T f(\tilde{J}_m) \mathbf{e}_1 + \sum_{j=0}^{r-1} w_j^{(0)} f^{(j)}(x_0),$$

where  $\tilde{J}_m$  is the Jacobi matrix of dimension  $m \times m$  associated with the modified positive measure  $d\tilde{\lambda}(x)$ , and  $\tilde{m}_0 = \int_a^b d\tilde{\lambda}(x)$ . This formula can be used for the computation of the generalized Gauss–Radau quadrature when the measure  $d\lambda(x)$  is explicitly known, but not in the case when  $d\lambda(x)$  is implicitly defined by the matrix  $A$  and the vector  $\mathbf{v}$ .

### 3. Generalized Gauss–Lobatto formulas

This section discusses the application and computation of generalized Gauss–Lobatto rules

$$\mathcal{G}_{m,r,s} f = \sum_{j=0}^{r-1} w_j^{(0,1)} f^{(j)}(x_{0,1}) + \sum_{i=1}^m w_i f(x_i) + \sum_{j=0}^{s-1} w_j^{(0,2)} f^{(j)}(x_{0,2}) \quad (3.1)$$

for the approximation of the functional (1.1) or, equivalently, of the Stieltjes integral (1.5). Here the  $x_i$ ,  $1 \leq i \leq m$ , are “free” distinct nodes in the open interval  $(a, b)$ ,

$-\infty < x_{0,1} \leq a$  is a prescribed node of multiplicity  $r \geq 1$ , and  $b \leq x_{0,2} < \infty$  is a prescribed node of multiplicity  $s \geq 1$ . We assume that  $\max\{r, s\} \geq 2$  to avoid discussing “standard” Gauss–Lobatto rules. The nodes  $x_1, x_2, \dots, x_m$  are the zeros of the  $m$ th degree orthogonal polynomial  $\pi_m$  with respect to the modified measure

$$(x - x_{0,1})^r (x_{0,2} - x)^s d\lambda(x).$$

Many properties of generalized Gauss–Lobatto rules are discussed in [6, 7, 8, 9, 11, 12, 18, 20]. For instance, it is shown that

$$\mathcal{I}f = \mathcal{G}_{m,r,s}f, \quad \forall f \in \mathbb{P}^{2m+r+s-1}. \quad (3.2)$$

Moreover, let  $\text{int}(a, b, x_{0,1}, x_{0,2})$  denote the convex hull of the set  $\{a, b, x_{0,1}, x_{0,2}\}$  and let the integrand  $f$  be  $2m + r + s$  times continuously differentiable in  $\text{int}(a, b, x_{0,1}, x_{0,2})$ . Then analogously to (2.3), the error in the quadrature rule (3.1) can be expressed as

$$\begin{aligned} \mathcal{E}_{m,r,s}f &:= (\mathcal{I} - \mathcal{G}_{m,r,s})f \\ &= \frac{f^{(2m+r+s)}(x_{\text{GL}})}{(2m+r+s)!} \cdot \int_a^b (x - x_{0,1})^r (x - x_{0,2})^s \prod_{i=1}^m (x - x_i)^2 d\lambda(x), \end{aligned}$$

where  $x_{\text{GL}} \in \text{int}(a, b, x_{0,1}, x_{0,2})$ . If  $f^{(2m+r+s)}$  is of constant sign in  $\text{int}(a, b, x_{0,1}, x_{0,2})$ , then the sign of  $\mathcal{E}_{m,r,s}f$  can be determined by choosing suitable multiplicities  $r$  and  $s$ .

We derive a formula analogous to (2.14) for the evaluation of  $\mathcal{G}_{m,r,s}f$ . Our derivation is similar to the one for (2.14). We therefore only provide an outline. Application of  $m + r + s$  steps of the Lanczos process to the matrix  $A$  with initial unit vector  $\mathbf{v}$  gives the Lanczos decomposition

$$AU_{m+r+s} = U_{m+r+s}J_{m+r+s} + \sqrt{\beta_{m+r+s}}\mathbf{u}_{m+r+s+1}\mathbf{e}_{m+r+s}^T. \quad (3.3)$$

This decomposition is analogous to (2.4). Here we only note for future reference that the  $(m + r + s) \times (m + r + s)$  matrix

$$J_{m+r+s} := \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & & \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & & \\ & \sqrt{\beta_2} & \alpha_2 & \ddots & & \\ & & & \ddots & \ddots & \\ & & & & \ddots & \sqrt{\beta_{m+r+s-1}} \\ & & & & \sqrt{\beta_{m+r+s-1}} & \alpha_{m+r+s-1} \end{bmatrix}$$

is symmetric and tridiagonal; we assume that  $m + r + s$  is small enough so that the decomposition (3.3) exists. Using (2.5) and defining

$$\mathbf{p}(x) = \begin{bmatrix} p_0(x) \\ p_1(x) \\ \vdots \\ p_{m+r+s-1}(x) \end{bmatrix},$$

we can express (3.3) in the form

$$x \mathbf{p}(x) = J_{m+r+s} \mathbf{p}(x) + \sqrt{\beta_{m+r+s}} p_{m+r+s}(x) \mathbf{e}_{m+r+s}.$$

Introduce the inner product

$$(f, g)_{r,s} = \int_a^b f(x)g(x)(x - x_{0,1})^r (x_{0,2} - x)^s d\lambda(x),$$

and let the polynomials  $\pi_0, \pi_1, \pi_2, \dots$  be orthonormal polynomials with respect to this inner product, i.e.,

$$(\pi_i, \pi_j)_{r,s} = \begin{cases} 1, & i = j, \\ 0, & i \neq j, \end{cases}$$

and  $\pi_i \in \mathbb{P}^i$ . Define the polynomial

$$q_{m+r+s}(x) = \pi_m(x)(x - x_{0,1})^r (x_{0,2} - x)^s.$$

Then

$$xp_{m+r+s-1}(x) = \sum_{i=0}^{m+r+s-1} d_i p_i(x) + \tau_{m+r+s} q_{m+r+s}(x), \quad (3.4)$$

for suitable coefficients  $d_i$  and  $\tau_{m+r+s}$ . Using the orthogonality property of the  $p_i$ , we obtain

$$d_i = \int_a^b xp_{m+r+s-1}(x)p_i(x)d\lambda(x) - \tau_{m+r+s} \int_a^b \pi_m(x)p_i(x)(x - x_{0,1})^r (x_{0,2} - x)^s d\lambda(x),$$

for  $i = 0, 1, \dots, m+r+s-1$ . Using the orthonormality properties of the polynomials  $p_i$  and  $\pi_m$  gives that  $d_i = 0$  for  $0 \leq i < m$ . Thus, the relation (3.4) simplifies to

$$xp_{m+r+s-1}(x) = \sum_{i=m}^{m+r+s-1} d_i p_i(x) + \tau_{m+r+s} q_{m+r+s}(x). \quad (3.5)$$

The coefficients  $d_m, d_{m+1}, \dots, d_{m+r-1}$  can be determined by solving the linear system of equations

$$x_{0,1} p_{m+r+s-1}^{(j)}(x_{0,1}) + j p_{m+r+s-1}^{(j-1)}(x_{0,1}) = \sum_{i=m}^{m+r-1} d_i p_i^{(j)}(x_{0,1}), \quad j = 1, \dots, r-1, \quad (3.6)$$

and the coefficients  $d_{m+r}, d_{m+r+1}, \dots, d_{m+r+s-1}$  are similarly obtained by solving the linear system of equations

$$x_{0,2} p_{m+r+s-1}^{(j)}(x_{0,2}) + j p_{m+r+s-1}^{(j-1)}(x_{0,2}) = \sum_{i=m+r}^{m+r+s-1} d_i p_i^{(j)}(x_{0,2}), \quad j = 1, \dots, s-1. \quad (3.7)$$

We remark that the systems (3.6) and (3.7) are obtained from (3.5) by using the fact that  $q_{m+r+s}^{(j)}(x_{0,1}) = 0$  for  $j = 0, 1, \dots, r-1$ , and  $q_{m+r+s}^{(j)}(x_{0,2}) = 0$  for  $j = 0, 1, \dots, s-1$ .



Thus, the matrix  $\Lambda \in \mathbb{R}^{(m+r+s) \times (m+r+s)}$  is bidiagonal with a leading  $m \times m$  principal diagonal matrix, which is followed by a Jordan block associated with the eigenvalue  $x_{0,1}$  of order  $r$ , and another Jordan block associated with the eigenvalue  $x_{0,2}$  of order  $s$ . We have the Jordan factorization

$$J_{m+r+s}^L W = W \Lambda.$$

Similarly as at the end of Section 2, we need the first row of the matrix  $W$  and the first column of  $W^{-1}$  to define an expression for the quadrature rule (3.1) that does not require explicit knowledge of the nodes and weights. It follows from (3.9) that the first row of  $W$  is of the form

$$[1, \dots, 1, 0, \dots, 0, 1, 0, \dots, 0];$$

the ones are in the positions where there is no derivative. To determine the first column of  $W^{-1}$ , we define the matrix  $V$ , whose rows are  $\mathbf{v}_i^T$ ,  $i = 1, 2, \dots, m+r+s$ , are defined as follows:

$$\begin{aligned} \mathbf{v}_k &= w_k \mathbf{p}(x_k), \quad k = 1, 2, \dots, m, \\ \mathbf{v}_{m+k} &= \sum_{u=k-1}^{r-1} u! w_u^{(0,1)} \frac{\mathbf{p}^{(u+1-k)}(x_{0,1})}{(u+1-k)!}, \quad k = 1, 2, \dots, r, \\ \mathbf{v}_{m+r+k} &= \sum_{u=k-1}^{r-1} u! w_u^{(0,2)} \frac{\mathbf{p}^{(u+1-k)}(x_{0,2})}{(u+1-k)!}, \quad k = 1, 2, \dots, s. \end{aligned}$$

Denote the  $i$ th row of  $W$  by  $\mathbf{a}_i^T = [a_1, \dots, a_{m+r+s}]$ , and the  $j$ th column of  $V$  by  $\mathbf{b}_j = [b_1, \dots, b_{m+r+s}]^T$ . We will show that

$$\mathbf{a}_i^T \mathbf{b}_j = \mathcal{G}_{m,r,s}(p_{i-1} p_{j-1}).$$

Note that, in view of (3.2),

$$\mathcal{G}_{m,r,s}(p_{i-1} p_{j-1}) = \int_a^b p_{i-1}(x) p_{j-1}(x) d\lambda(x) = \begin{cases} 1, & i = j, \\ 0, & i \neq j, \end{cases}$$

for  $i + j - 2 \leq 2m + r + s - 1$ . We have

$$\begin{aligned} a_k &= p_{i-1}(x_k), \quad b_k = w_k p_{j-1}(x_k), \quad k = 1, 2, \dots, m, \\ a_{m+k} &= \frac{1}{(k-1)!} p_{i-1}^{(k-1)}(x_{0,1}), \quad k = 1, 2, \dots, r, \\ b_{m+k} &= \sum_{u=k-1}^{r-1} u! w_u^{(0,1)} \frac{p_{j-1}^{(u+1-k)}(x_{0,1})}{(u+1-k)!}, \quad k = 1, 2, \dots, r, \\ a_{m+r+k} &= \frac{1}{(k-1)!} p_{i-1}^{(k-1)}(x_{0,2}), \quad k = 1, 2, \dots, s, \\ b_{m+r+k} &= \sum_{u=k-1}^{s-1} u! w_u^{(0,2)} \frac{p_{j-1}^{(u+1-k)}(x_{0,2})}{(u+1-k)!}, \quad k = 1, 2, \dots, s. \end{aligned}$$

After some computations similar to those at the end of Section 2, we obtain

$$\begin{aligned} \sum_{k=1}^{m+r+s} a_k b_k &= \sum_{k=1}^m w_k(p_{i-1}p_{j-1})(x_k) + \sum_{\ell=0}^{r-1} w_\ell^{(0,1)}(p_{i-1}p_{j-1})^{(\ell)}(x_{0,1}) \\ &\quad + \sum_{h=0}^{s-1} w_h^{(0,2)}(p_{i-1}p_{j-1})^{(h)}(x_{0,2}) = \mathcal{G}_{m+r+s}(p_{j-1}p_{i-1}). \end{aligned}$$

It follows similarly as in Section 2 that

$$W^{-1}\mathbf{e}_1 = \left[ w_1, w_2, \dots, w_m, w_0^{(0,1)}, \dots, (r-1)!w_{r-1}^{(0,1)}, w_0^{(0,2)}, \dots, (s-1)!w_{s-1}^{(0,2)} \right]^T.$$

We finally obtain the desired representation of the quadrature rule,

$$\mathbf{e}_1^T f(J_{m+r+s}^L) \mathbf{e}_1 = \mathbf{e}_1^T W f(\Lambda) W^{-1} \mathbf{e}_1 = \mathcal{G}_{m,r,s}(f). \quad (3.10)$$

Similarly as at the end of Section 2, we conclude that the generalized Gauss–Lobatto rule  $\mathcal{G}_{m,r,s}f$  can be evaluated by using either (3.1) or (3.10). Which one of these expressions is most convenient to use depends on the integrand.

#### 4. Computed examples

In this section, we present three examples to illustrate the performance of the generalized Gauss–Radau and generalized Gauss–Lobatto quadrature rules. The examples show pairs of a Gauss rule and a generalized Gauss–Radau or generalized Gauss–Lobatto rule to provide upper and lower error bounds for the expression (1.1) in situations when pairs of Gauss rules and standard Gauss–Radau or standard Gauss–Lobatto rules do not. All computations were carried out using MATLAB R2017b on a 64-bit MacBook Pro personal computer with about 15 significant decimal digits.

**Example 4.1.** This example continues the discussion of Example 1.1. Thus, we would like to determine an approximation of the functional (1.2) with the matrix  $A$  defined as in Example 1.1. The vector  $\mathbf{v}$  has normally distributed entries with zero mean and is normalized to be of unit norm. The exact value is  $F(A) \approx 0.1183$ .

We first consider the approximation of (1.2) by pairs of a Gauss rule and a standard or generalized Gauss–Radau rule with a fixed node  $x_0 = \lambda_{min}$ , and by pairs of a Gauss rule and standard or generalized Gauss–Lobatto rule with fixed nodes  $x_{0,1} = \lambda_{min}$  and  $x_{0,2} = \lambda_{max}$ . Let  $\mathcal{G}_{m,1}f$  and  $\mathcal{G}_{m,1,1}f$  denote (standard) Gauss–Radau and Gauss–Lobatto quadrature rules, respectively. We observe that the derivatives  $f^{(2m+r)}$  and  $f^{(2m+r+s)}$  of the integrand (1.3) change sign on the interval  $[\lambda_{min}, \lambda_{max}]$  when  $m = 2k$  and  $r = s = 1$ . This implies that pairs of the Gauss rule  $\mathcal{G}_m f$  and the standard Gauss–Radau rule  $\mathcal{G}_{m,1}f$ , or pairs of the Gauss rule  $\mathcal{G}_m f$  and the standard Gauss–Lobatto rule  $\mathcal{G}_{m,1,1}f$ , are not guaranteed to bracket the value  $F(A)$ . Indeed, for  $m = 2$  we have  $F(A) - \mathcal{G}_{m,1}f = -2.991 \cdot 10^{-5}$  and  $F(A) - \mathcal{G}_{m,1,1}f = -1.021 \cdot 10^{-6}$ . Table 4.1 shows

that  $F(A) - \mathcal{G}_m f$  also is negative. Thus, the value  $F(A)$  is not bracketed by  $\mathcal{G}_{m,1}f$  and  $\mathcal{G}_{m,1,1}f$ . We conclude that the technique described in [13, 14] for bounding  $F(A)$  based on evaluating pairs of Gauss and (standard) Gauss–Radau or Gauss–Lobatto quadrature rules fails to yield upper and lower bounds for the expression (1.2). These quadrature rules therefore are not useful for assessing the errors in  $\mathcal{G}_{m,1}f$  or  $\mathcal{G}_{m,1,1}f$ .

The derivatives  $f^{(4\ell)}$  in (1.7), when  $\ell$  is odd, are of negative sign in the interval  $[\lambda_{min}, \lambda_{max}]$ . This yields errors of negative sign and therefore the quadrature rule provides an upper bound for  $\mathcal{I}f$ . In addition, the derivatives  $f^{(4\ell)}$ , when  $\ell$  is even, are of positive sign in the interval  $[\lambda_{min}, \lambda_{max}]$ . In this case, we have a positive error and the quadrature rule furnishes a lower bound for  $\mathcal{I}f$ . However, note that the derivatives  $f^{(4\ell+1)}$  and  $f^{(4\ell+2)}$  change sign in the interval  $[\lambda_{min}, \lambda_{max}]$ . Therefore, pairs of a Gauss rule and a (standard) Gauss–Radau or Gauss–Lobatto rule are not guaranteed to give upper and lower error bounds for (1.2).

The above discussion suggests that pairs of suitable Gauss and generalized Gauss–Radau or generalized Gauss–Lobatto rules may be used to bracket (1.2). Let  $r = 4$  and  $x_0 = \lambda_{min}$  for the generalized Gauss–Radau rules  $\mathcal{G}_{m,r}f$ , and let  $r = 2$ ,  $s = 2$ ,  $x_{0,1} = \lambda_{min}$ , and  $x_{0,2} = \lambda_{max}$ , for the generalized Gauss–Lobatto rules  $\mathcal{G}_{m,r,s}f$ . Then pairs of Gauss rules and these generalized Gauss–Radau or generalized Gauss–Lobatto rules bracket (1.2). This is illustrated by Table 4.1.

Errors	$m = 2$	$m = 4$	$m = 6$
$F(A) - \mathcal{G}_m f$	$-1.900 \cdot 10^{-3}$	$2.112 \cdot 10^{-7}$	$-1.653 \cdot 10^{-13}$
$F(A) - \mathcal{G}_{m,r} f$	$3.312 \cdot 10^{-5}$	$-1.143 \cdot 10^{-10}$	$2.636 \cdot 10^{-16}$
$F(A) - \mathcal{G}_{m,r,s} f$	$1.050 \cdot 10^{-6}$	$-4.096 \cdot 10^{-11}$	$5.134 \cdot 10^{-16}$

Table 4.1: Example 4.1: Errors for computed approximations of  $F(A) := \mathbf{v}^T \exp(-\frac{A}{4}) \sin(\frac{A}{4}) \mathbf{v}$ ,  $A$  a symmetric Toeplitz matrix,  $r = 4$  in  $\mathcal{G}_{m,r}$ , and  $r = s = 2$  in  $\mathcal{G}_{m,r,s}$ .

**Example 4.2.** We consider the approximation of the functional

$$F(A) := \mathbf{v}^T \exp(A)(\cos(A) - \sin(A))\mathbf{v}, \quad (4.1)$$

where  $A = \frac{1}{6}(B + \frac{3\pi}{7}I) \in \mathbb{R}^{200 \times 200}$  with  $B \in \mathbb{R}^{200 \times 200}$  a symmetric Toeplitz matrix with first row  $[1, 1/2, \dots, 1/200]$ . The vector  $\mathbf{v}$  has normally distributed entries with zero mean and is normalized to be of unit norm. The exact value is  $F(A) \approx 0.7343$ . In this example, the extreme eigenvalues of  $A$  are  $\lambda_{min} = 0.28878$  and  $\lambda_{max} = 1.7141$ . Consider the integrand

$$f(x) := \exp(x)(\cos(x) - \sin(x)).$$

We compute approximations of (4.1) by pairs of Gauss rules and standard or generalized Gauss–Radau rules with a fixed node  $x_0 = \lambda_{min}$ , and by pairs of Gauss rules and standard or generalized Gauss–Lobatto rules with fixed nodes  $x_{0,1} = \lambda_{min}$  and  $x_{0,2} = \lambda_{max}$ .



The derivatives  $f^{(2m+r)}$  and  $f^{(2m+r+s)}$  of the integrand change sign on the interval  $[\lambda_{min}, \lambda_{max}]$  when  $m = 2k + 1$  and  $r = s = 1$ . This indicates that pairs of Gauss rules  $\mathcal{G}_m f$  and standard Gauss–Radau rules  $\mathcal{G}_{m,1} f$ , or pairs of Gauss rules  $\mathcal{G}_m f$  and standard Gauss–Lobatto rules  $\mathcal{G}_{m,1,1} f$ , are not guaranteed to bracket (4.1). For instance, we find for  $m = 5$  that  $F(A) - \mathcal{G}_{m,1} f = -6.452 \cdot 10^{-13}$  and  $F(A) - \mathcal{G}_{m,1,1} f = -6.246 \cdot 10^{-11}$ . Comparison with results of Tables 4.2 shows that the pairs of rules  $\{\mathcal{G}_m f, \mathcal{G}_{m,1} f\}$  and  $\{\mathcal{G}_m f, \mathcal{G}_{m,1,1} f\}$  do not bracket the value (4.1).

Note that the derivatives  $f^{(4\ell+2)}$  are positive in the interval  $[\lambda_{min}, \lambda_{max}]$  when  $\ell$  is odd. This shows that the errors are positive, and then the quadrature rule yields a lower bound for  $\mathcal{I}f$ . Moreover, the derivatives  $f^{(4\ell+2)}$  are negative in the interval  $[\lambda_{min}, \lambda_{max}]$  when  $\ell$  is even. Hence, we have negative errors and the quadrature rule yields an upper bound for  $\mathcal{I}f$ . We therefore can determine upper and lower error bounds for (4.1) by suitable pairs of Gauss and generalized Gauss–Radau or generalized Gauss–Lobatto rules. Let  $r = 4$  and  $x_0 = \lambda_{min}$  for the generalized Gauss–Radau rules  $\mathcal{G}_{m,r} f$ , and let  $r = 2, s = 2, x_{0,1} = \lambda_{min}$ , and  $x_{0,2} = \lambda_{max}$  for the generalized Gauss–Lobatto rules  $\mathcal{G}_{m,r,s} f$ . Table 4.2 shows pairs of Gauss rules and these generalized Gauss–Radau or generalized Gauss–Lobatto rules to bracket (4.1).

Errors	$m = 3$	$m = 5$
$F(A) - \mathcal{G}_m f$	$3.862 \cdot 10^{-5}$	$-1.331 \cdot 10^{-10}$
$F(A) - \mathcal{G}_{m,r} f$	$-1.735 \cdot 10^{-8}$	$1.054 \cdot 10^{-14}$
$F(A) - \mathcal{G}_{m,r,s} f$	$-3.993 \cdot 10^{-9}$	$4.662 \cdot 10^{-15}$

Table 4.2: Example 4.2: Errors for computed approximations of  $F(A) := \mathbf{v}^T \exp(A)(\cos(A) - \sin(A))\mathbf{v}$ ,  $A$  a symmetric Toeplitz matrix,  $r = 4$  in  $\mathcal{G}_{m,r}$ , and  $r = s = 2$  in  $\mathcal{G}_{m,r,s}$ .

**Example 4.3.** We would like to compute an approximation of the functional

$$F(A) := \mathbf{v}^T \exp\left(-\frac{A}{7}\right) \cos\left(\frac{A}{7}\right) \mathbf{v}, \quad (4.2)$$

where  $A \in \mathbb{R}^{2114 \times 2114}$  is the symmetric adjacency matrix for the Yeast network; see [17, 22]. This matrix is available at [2]. We let the vector  $\mathbf{v}$  have normally distributed entries with zero mean and to be of unit norm. The extreme eigenvalues of  $A$  are  $\lambda_{min} = -7.5159$  and  $\lambda_{max} = 7.5412$ . Introduce the integrand

$$f(x) := \exp\left(-\frac{x}{7}\right) \cos\left(\frac{x}{7}\right). \quad (4.3)$$

We consider the approximation of (4.2) by pairs of Gauss rules and standard or generalized Gauss–Radau rules with a fixed node  $x_0 = \lambda_{min}$ , and by pairs of Gauss rules and standard or generalized Gauss–Lobatto rules with fixed nodes  $x_{0,1} = \lambda_{min}$  and  $x_{0,2} = \lambda_{max}$ . We observe that the derivatives  $f^{(2m+r)}$  and  $f^{(2m+r+s)}$  of the integrand (4.3) change sign on the interval  $[\lambda_{min}, \lambda_{max}]$  when  $m = 2k$  and  $r = s = 1$ . Therefore,

pairs of Gauss rules  $\mathcal{G}_m f$  and standard Gauss–Radau rules  $\mathcal{G}_{m,1} f$ , or pairs of Gauss rules  $\mathcal{G}_m f$  and standard Gauss–Lobatto rules  $\mathcal{G}_{m,1,1} f$ , are not guaranteed to bracket the value (4.2). For instance, we obtain for  $m = 4$  that  $F(A) - \mathcal{G}_{m,1} f = 2.672 \cdot 10^{-8}$  and  $F(A) - \mathcal{G}_{m,1,1} f = 1.499 \cdot 10^{-6}$ . Comparison with results of Table 4.3 shows that the pairs of rules  $\{\mathcal{G}_m f, \mathcal{G}_{m,1} f\}$  and  $\{\mathcal{G}_m f, \mathcal{G}_{m,1,1} f\}$  do not bracket (4.2).

However, note that the derivatives  $f^{(4\ell)}(x)$  are of a negative sign in the interval  $[\lambda_{min}, \lambda_{max}]$  when  $\ell$  is odd, and of a positive sign when  $\ell$  is even. This observation allows us to compute upper and lower error bounds for (4.2) by suitable pairs of Gauss and generalized Gauss–Radau or generalized Gauss–Lobatto rules. Let  $r = 4$  and  $x_0 = \lambda_{min}$  for the generalized Gauss–Radau rules  $\mathcal{G}_{m,r} f$ , and let  $r = 2$ ,  $s = 2$ ,  $x_{0,1} = \lambda_{min}$ , and  $x_{0,2} = \lambda_{max}$  for the generalized Gauss–Lobatto rules  $\mathcal{G}_{m,r,s} f$ . Table 4.3 and shows that pairs of Gauss rules and these generalized Gauss–Radau or generalized Gauss–Lobatto rules bracket (4.2).

Errors	$m = 2$	$m = 4$	$m = 6$
$F(A) - \mathcal{G}_m f$	$-1.600 \cdot 10^{-3}$	$2.555 \cdot 10^{-7}$	$-1.083 \cdot 10^{-11}$
$F(A) - \mathcal{G}_{m,r} f$	$2.621 \cdot 10^{-5}$	$-7.180 \cdot 10^{-10}$	$6.106 \cdot 10^{-15}$
$F(A) - \mathcal{G}_{m,r,s} f$	$2.310 \cdot 10^{-6}$	$-4.266 \cdot 10^{-11}$	$2.220 \cdot 10^{-16}$

Table 4.3: Example 4.3: Errors for computed approximations of  $F(A) := \mathbf{v}^T \exp(\frac{-A}{7}) \cos(\frac{A}{7}) \mathbf{v}$ ,  $A$  a symmetric adjacency matrix for the Yeast network,  $r = 4$  in  $\mathcal{G}_{m,r}$ , and  $r = s = 2$  in  $\mathcal{G}_{m,r,s}$ .

## 5. Conclusion

Golub and Meurant [13, 14] described a technique for computing upper and lower error bounds for a Stieltjes integral by evaluating pairs of Gauss, and suitable Gauss–Radau or Gauss–Lobatto quadrature rules. However, this technique is not guaranteed to furnish upper and lower error bounds when certain derivatives of the integrand  $f$  change sign on the convex hull of spectrum of  $A$ . This paper extends the technique by Golub and Meurant by using pairs of Gauss, and suitable generalized Gauss–Radau or generalized Gauss–Lobatto rules, to determine upper and lower error bounds for Stieltjes integrals with an integrand  $f$ , some of whose derivatives change sign on the convex hull of the support of the measure. New methods for evaluating generalized Gauss–Radau and Gauss–Lobatto rules are described. Computed examples illustrate the benefit of using these quadrature rules.

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## References

- [1] Z. Bai, M. Fahey, and G. H. Golub, *Some large scale matrix computation problems*, J. Comput. Appl. Math., 74 (1996), pp. 71–89.
- [2] V. Batagelj and A. Mrvar, *Pajek data sets*, (2006). Available at <http://vlado.fmf.uni-lj.si/pub/networks/data/>
- [3] D. Calvetti, P. C. Hansen, and L. Reichel, *L-curve curvature bounds via Lanczos bidiagonalization*, Electron. Trans. Numer. Anal., 14 (2002), pp. 20–35.
- [4] C. Fenu, D. Martin, L. Reichel, and G. Rodriguez, *Network analysis via partial spectral factorization and Gauss quadrature*, SIAM J. Sci. Comput., 35 (2013), pp. A2046–A2068.
- [5] P. Fika, M. Mitrouli, and P. Roupa, *Estimates for the bilinear form  $x^T A^{-1}y$  applications to linear algebra problems*, Electron. Trans. Numer. Anal., 43 (2014), pp. 70–89.
- [6] W. Gautschi, *High-order Gauss–Lobatto formulae*, Numer. Algorithms, 25 (2000), pp. 213–222.
- [7] W. Gautschi, *Orthogonal Polynomials: Computation and Approximation*, Oxford University Press, Oxford, 2004.
- [8] W. Gautschi, *Generalized Gauss–Radau and Gauss–Lobatto formulae*, BIT Numer. Math., 44 (2004), pp. 711–720.
- [9] W. Gautschi, *High-order generalized Gauss–Radau and Gauss–Lobatto formulae for Jacobi and Laguerre weight functions*, Numer. Algorithms, 51 (2009), pp. 143–149.
- [10] W. Gautschi, MATLAB codes for computing nodes and weights of quadrature rules described in [8] and [9] are available at <https://www.cs.purdue.edu/archives/2002/wxg/codes/>
- [11] W. Gautschi and S. Li, *The remainder term for analytic functions of Gauss–Radau and Gauss–Lobatto rules with multiple end points*, J. Comput. Appl. Math., 33 (1990), pp. 315–329.
- [12] W. Gautschi and S. Li, *Gauss–Radau and Gauss–Lobatto rules with double end points*, J. Comput. Appl. Math., 34 (1991), pp. 343–360.
- [13] G. H. Golub and G. Meurant, *Matrices, moments and quadrature*, in Numerical Analysis 1993, eds. D. F. Griffiths and G. A. Watson, Longman, Essex, England, 1994, pp. 105–156.
- [14] G. H. Golub and G. Meurant, *Matrices, Moments and Quadrature with Applications*, Princeton University Press, Princeton, 2010.

- [15] G. H. Golub and C. F. Van Loan, *Matrix Computations*, 4th ed., Johns Hopkins University Press, Baltimore, 2013.
- [16] N. J. Higham, *Functions of Matrices*, SIAM, Philadelphia, 2008.
- [17] H. Jeong, S. Mason, A.-L. Barabási, and Z. N. Oltvai, *Lethality and centrality of protein networks*, *Nature*, 411 (2001), pp. 41–42.
- [18] H. Joulak and B. Beckermann, *On Gautschi’s conjecture for generalized Gauss–Radau and Gauss–Lobatto formulae*, *J. Comput. Appl. Math.*, 233 (2009), pp. 768–774.
- [19] S. Morigi, L. Reichel, and F. Sgallari, *An iterative Lavrentiev regularization method*, *BIT Numer. Math.*, 46 (2006), pp. 589–606.
- [20] G. Petrova, *Generalized Gauss–Radau and Gauss–Lobatto formulas with Jacobi weight functions*, *BIT Numer. Math.*, 57 (2017), pp. 191–206.
- [21] S. Pozza, M. S. Pranić, and Z. Strakoš, *The Lanczos algorithm and complex Gauss quadrature*, *Electron. Trans. Numer. Anal.*, 50 (2018), pp. 1–19.
- [22] S. Sun, L. Ling, N. Zhang, G. Li, and R. Chen, *Topological structure analysis of the protein-protein interaction network in budding yeast*, *Nucleic Acids Research*, 31 (2003), pp. 2443–2450.
- [23] B. D. Welfert, *The weights of classical Gauss–Radau quadratures with double endpoint*, *Appl. Numer. Math.*, 60 (2010), pp. 574–586.