BIT
2002, Vol. 43, No. 2, pp. 001–004

0006-3835/00/4004-0001 $15.00


# SYMMETRIC GAUSS-LOBATTO AND MODIFIED ANTI-GAUSS RULES*

DANIELA CALVETTI[1] and LOTHAR REICHEL[2] †

[1] *Department of Mathematics, Case Western Reserve University Cleveland, OH 44106, USA. email: dxc57@po.cwru.edu*

[2] *Department of Mathematical Sciences, Kent State University Kent, OH 44242, USA. email: reichel@math.kent.edu*

**Abstract.**

The present paper is concerned with symmetric Gauss-Lobatto quadrature rules, i.e., with Gauss-Lobatto rules associated with a nonnegative symmetric measure on the real axis. We propose a modification of the anti-Gauss quadrature rules recently introduced by Laurie, and show that the symmetric Gauss-Lobatto rules are modified anti-Gauss rules. It follows that for many integrands, symmetric Gauss quadrature rules and symmetric Gauss-Lobatto rules give quadrature errors of opposite sign.

*AMS subject classification:* 65D30, 65D32.

*Key words:* Gauss quadrature, error estimation.

## 1 Introduction

Let $\mu(t)$ be a nondecreasing function with infinitely many points of increase in the finite interval $[-a, a]$ of the real axis, and assume that the induced nonnegative measure $\mathrm{d}\mu(t)$ is symmetric with respect to the origin and has finite moments of all orders. Introduce, for polynomials $f$ and $g$, the inner product

$$(f, g) := \int_{-a}^{a} f(t)g(t)\mathrm{d}\mu(t). \tag{1.1}$$

Let $p_j$, $j = 0, 1, 2, \ldots$ , denote a family of orthonormal polynomials with respect to this inner product, i.e., $p_j$ is a polynomial of degree $j$ with positive leading coefficient and satisfies

$$(p_j, p_k) = \begin{cases} 1, & j = k, \\ 0, & j \neq k. \end{cases}$$

The polynomials $p_j$ satisfy a three-term recurrence relation of the form

$$\beta_j p_j(t) = t p_{j-1}(t) - \beta_{j-1} p_{j-2}(t), \qquad 2 \leq j \leq m, \tag{1.2}$$

where $p_1(t) := \beta_1^{-1} t p_0(t)$, $p_0(t) := 1/\mu_0^{1/2}$ and

$$\mu_0 := \int_{-a}^{a} \mathrm{d}\mu(t). \tag{1.3}$$

*Received September 2002. Revised May 2003. Communicated by Åke Björck.
†Research supported in part by NSF grants DMS-0107841 and DMS-0107858.

It follows that

$$p_j(t) = (\beta_j \beta_{j-1} \cdots \beta_1 \beta_0)^{-1} t^j + \mathcal{O}(t^{j-1}), \qquad t \to \infty, \tag{1.4}$$

where $\beta_0 := \mu_0^{1/2}$. We note for future reference that

$$\beta_j^2 = (tp_{j-1} - \beta_{j-1} p_{j-2}, tp_{j-1} - \beta_{j-1} p_{j-2}). \tag{1.5}$$

The present paper is concerned with the approximation of integrals of the form

$$\mathcal{I}f := \int_{-a}^{a} f(t) \mathrm{d}\mu(t) \tag{1.6}$$

by quadrature rules of Gauss-type, in particular by Gauss, Gauss-Lobatto and modified anti-Gauss quadrature rules.

The $m$-point Gauss quadrature rule associated with the measure $\mathrm{d}\mu$ is given by

$$\mathcal{G}_m f := \sum_{j=1}^{m} f(t_j) w_j^2. \tag{1.7}$$

The nodes $t_j$ and weights $w_j^2$ are uniquely determined by the requirement that

$$\mathcal{I}f = \mathcal{G}_m f, \qquad \forall f \in \mathbb{P}_{2m-1}, \tag{1.8}$$

where $\mathbb{P}_{2m-1}$ denotes the set of polynomials of degree at most $2m-1$.

Introduce the symmetric tridiagonal $m \times m$ matrix

$$T_m := \begin{bmatrix} 0 & \beta_1 & & & & & \text{\Large 0} \\ \beta_1 & 0 & \beta_2 & & & & \\ & \beta_2 & 0 & & & & \\ & & & & \ddots & & \\ & & & \ddots & \ddots & \beta_{m-2} & \\ & & & & \beta_{m-2} & 0 & \beta_{m-1} \\ \text{\Large 0} & & & & & \beta_{m-1} & 0 \end{bmatrix}. \tag{1.9}$$

It is well known that the nodes $t_j$, $1 \le j \le m$, are the eigenvalues of $T_m$, and the weight $w_j^2$ is the square of the first component of the eigenvector of $T_m$ of length $\mu_0^{1/2}$ associated with the eigenvalue $t_j$; see, e.g., Golub and Welsch [6] or Stoer and Bulirsch [8, Chapter 3].

The $(m+1)$-point Gauss-Lobatto rule associated with the measure $\mathrm{d}\mu$ is given by

$$\hat{\mathcal{G}}_{m+1} f := f(-a)\hat{w}_1^2 + \sum_{j=2}^{m} f(\hat{t}_j)\hat{w}_j^2 + f(a)\hat{w}_{m+1}^2, \tag{1.10}$$

and the nodes $\hat{t}_j$, $2 \le j \le m$, and weights $\hat{w}_j^2$, $1 \le j \le m+1$, are uniquely determined by the requirement that

$$\mathcal{I}f = \hat{\mathcal{G}}_{m+1} f, \qquad \forall f \in \mathbb{P}_{2m-1}. \tag{1.11}$$

Golub [4] described how to determine a symmetric tridiagonal matrix of order $m+1$, whose eigenvalues are the nodes $\hat{t}_j$ of the Gauss-Lobatto rule (1.10). The square of the first component of orthogonal eigenvectors of this matrix, normalized to have length $\mu_0^{1/2}$, yield the weights $\hat{w}_j^2$. Details are discussed in Section 2.

Recently, Laurie [7] introduced quadrature rules that he referred to as anti-Gauss rules associated with the measure $\mathrm{d}\mu$. The nodes and weights of the $(m+1)$-point anti-Gauss rule, denoted by $\tilde{\mathcal{G}}_{m+1}$, are uniquely determined by the requirement that

$$(\mathcal{I}-\tilde{\mathcal{G}}_{m+1})f = -\mathcal{E}_m f, \qquad \forall f \in \mathbb{P}_{2m+1}, \tag{1.12}$$

where

$$\mathcal{E}_m f := (\mathcal{I}-\mathcal{G}_m)f \tag{1.13}$$

is the quadrature error of the Gauss rule (1.7).

Because of the relation (1.12), the $(m+1)$-point anti-Gauss rule gives for many integrands $f$ a quadrature error of opposite sign as the $m$-point Gauss rule (1.7). This property has been exploited in schemes described in [1, 2] for the estimation of the error in the approximate solutions determined by iterative methods for the solution of large linear systems of equations with a symmetric matrix.

In Section 3 we present a modification of anti-Gauss rules $\tilde{\mathcal{G}}_{m+1}$, which transforms symmetric anti-Gauss rules into symmetric Gauss-Lobatto rules. It follows that for many integrands $f$, the Gauss rule (1.7) and Gauss-Lobatto rule (1.10) yield quadrature errors of opposite sign. Hence, for many integrands we can bracket the integration error by evaluating pairs of symmetric Gauss and Gauss-Lobatto quadrature rules. This is illustrated by numerical examples in Section 4.

We conclude this section with an outline of a few other approaches to bound the error in quadrature rules of Gauss-type. When the derivative of $f$ of order $2m$, denoted by $f^{(2m)}$, is continuous in the interval of integration, the integration error $\mathcal{E}_m f$ can be expressed as

$$\mathcal{E}_m f = \frac{f^{(2m)}(\theta)}{(2m)!}\int_{-a}^{a}\prod_{j=1}^{m}(t-t_j)^2\mathrm{d}\mu(t), \tag{1.14}$$

where the $t_j$ are the nodes of the Gauss rule $\mathcal{G}_m$, and $\theta$ depends on $m$ and $f$, and lives in the open interval $]-a,a[$; see, e.g., [8, p. 158]. When $|f^{(2m)}(t)|$ does not vary much in the interval of integration and a fairly accurate bound of $\max_{t\in[-a,a]}|f^{(2m)}(t)|$ is available, this bound may yield a useful bound for the integration error $\mathcal{E}_m f$.

Similarly, the integration error

$$\hat{\mathcal{E}}_{m+1} f := (\mathcal{I}-\hat{\mathcal{G}}_{m+1})f, \tag{1.15}$$

can be expressed as

$$\hat{\mathcal{E}}_{m+1} f = \frac{f^{(2m)}(\hat{\theta})}{(2m)!}\int_{-a}^{a}(t^2-a^2)\prod_{j=2}^{m-1}(t-\hat{t}_j)^2\mathrm{d}\mu(t), \tag{1.16}$$

where the $\hat{t}_j$ are nodes of the Gauss-Lobatto rule $\hat{\mathcal{G}}_{m+1}$, and $\hat{\theta} \in ]-a, a[$ depends on $m$ and $f$. The expression (1.16) can be derived analogously as (1.14). If $f^{(2m)}$ is of constant sign in $]-a, a[$, then the right-hand sides of (1.14) and (1.16) are of opposite sign and, hence, the values $\mathcal{G}_m f$ and $\hat{\mathcal{G}}_{m+1} f$ bracket $\mathcal{I}f$. Note that the evaluation of $\mathcal{G}_m f$ and $\hat{\mathcal{G}}_{m+1} f$ gives error bounds without evaluation of $f^{(2m)}$. Results of this kind are discussed, e.g., by Golub and Meurant [5]. A nice recent review of these and related results is provided by Gautschi [3]. The present paper is concerned with the computation of upper and lower bounds of $\mathcal{I}f$ when the formula (1.14) does not give useful computable bounds of $\mathcal{E}_m f$, and when $f^{(2m)}$ changes sign in the interval of integration, so that $\mathcal{G}_m f$ and $\hat{\mathcal{G}}_{m+1} f$ cannot be guaranteed to be of opposite sign.

## 2 Symmetric Gauss-Lobatto rules

Golub [4] observed that the nodes of the $(m+1)$-point Gauss-Lobatto quadrature rule are the eigenvalues of a symmetric tridiagonal matrix of order $m+1$ that is closely related to the matrix (1.9) associated with the $m$-point Gauss rule (1.7). In the case of a symmetric measure, the formulas derived by Golub [4] show that the nodes $\hat{t}_j$ of (1.10) are the eigenvalues of the symmetric tridiagonal $(m+1) \times (m+1)$ matrix

$$\hat{T}_{m+1} := \begin{bmatrix} 0 & \hat{\beta}_1 & & & & & 0 \\ \hat{\beta}_1 & 0 & \hat{\beta}_2 & & & & \\ & \hat{\beta}_2 & 0 & & & & \\ & & & \ddots & & & \\ & & & \ddots & \ddots & \hat{\beta}_{m-1} & \\ & & & & \hat{\beta}_{m-1} & 0 & \hat{\beta}_m \\ 0 & & & & & \hat{\beta}_m & 0 \end{bmatrix}$$

and the weights $\hat{w}_j^2$ are the squares of the first components of orthogonal eigenvectors normalized to be of length $\mu_0^{1/2}$, where

$$\hat{\beta}_j := \beta_j, \qquad 1 \le j < m,$$

and

$$\hat{\beta}_m := \left( \beta_m \frac{a p_m(a)}{p_{m-1}(a)} \right)^{1/2}. \tag{2.1}$$

Since $p_j(a) > 0$ for all $j$, it follows that $\hat{\beta}_m > 0$.

## 3 Modified anti-Gauss rules

This section discusses a modification of the anti-Gauss rules $\tilde{\mathcal{G}}_{m+1}$ introduced by Laurie [7]. We denote the modified anti-Gauss rule by

$$\tilde{\mathcal{G}}_{m+1,\gamma} f := \sum_{j=1}^{m+1} f(\tilde{t}_j) \tilde{w}_j^2 \tag{3.1}$$

and we require the integration error

$$\mathcal{E}_{m+1,\gamma} f := (\mathcal{I} - \mathcal{G}_{m+1,\gamma}) f$$

to satisfy

$$(\mathcal{I} - \tilde{\mathcal{G}}_{m+1,\gamma}) f = -\gamma \mathcal{E}_m f, \qquad \forall f \in \mathbb{P}_{2m+1}, \tag{3.2}$$

where $\mathcal{E}_m f$ is the quadrature error (1.13) obtained with the Gauss rule (1.7) and $\gamma$ is a positive constant. When $\gamma = 1$, the modified anti-Gauss rule (3.1) agrees with the anti-Gauss rule $\tilde{\mathcal{G}}_{m+1}$ introduced by Laurie [7].

It follows from (3.2) that

$$\tilde{\mathcal{G}}_{m+1,\gamma} f = ((1+\gamma)\mathcal{I} - \gamma \mathcal{G}_m) f, \qquad \forall f \in \mathbb{P}_{2m+1}, \tag{3.3}$$

i.e., $\tilde{\mathcal{G}}_{m+1,\gamma}$ is the $(m+1)$-point Gauss rule for the functional

$$\mathcal{J}_\gamma f := ((1+\gamma)\mathcal{I} - \gamma \mathcal{G}_m) f.$$

Introduce the bilinear form

$$< f, g >:= \mathcal{J}_\gamma (fg),$$

and let $\{\tilde{p}_j\}_{j=0}^{m+1}$ be the first $m+2$ orthogonal polynomials with respect to $< \cdot, \cdot >$, normalized so that $< \tilde{p}_j, \tilde{p}_j >= 1$ for all $j$. These polynomials satisfy the recurrence relation

$$\tilde{\beta}_j \tilde{p}_j(t) = t\tilde{p}_{j-1}(t) - \tilde{\beta}_{j-1}\tilde{p}_{j-2}(t), \qquad 2 \le j \le m+1,$$

where $\tilde{p}_1(t) := \tilde{\beta}_1^{-1} t \tilde{p}_0(t)$ and $\tilde{p}_0(t) := 1/\mu_0^{1/2}$. We note that

$$\tilde{\beta}_j^2 =< t\tilde{p}_{j-1} - \tilde{\beta}_{j-1}\tilde{p}_{j-2}, t\tilde{p}_{j-1} - \tilde{\beta}_{j-1}\tilde{p}_{j-2} > . \tag{3.4}$$

It follows from (3.3) and (1.8) that

$$< f, g >= (f, g) = \mathcal{I}(fg), \qquad f \in \mathbb{P}_{m-1}, \quad g \in \mathbb{P}_m,$$

and this equality applied to (1.5) and (3.4) yields

$$\tilde{\beta}_j^2 = \beta_j^2, \qquad 1 \le j < m. \tag{3.5}$$

We may choose $\tilde{\beta}_j = \beta_j$ for $1 \le j < m$, and then $\tilde{p}_j = p_j$, $0 \le j < m$. Consider the polynomial

$$\hat{p}_m(t) := t\tilde{p}_{m-1}(t) - \tilde{\beta}_{m-1}\tilde{p}_{m-2}(t), \tag{3.6}$$

which also can be written as

$$\hat{p}_m(t) = tp_{m-1}(t) - \beta_{m-1}p_{m-2}(t). \tag{3.7}$$

Since this polynomial is a multiple of $p_m$, cf. (1.2), we have $\mathcal{G}_m \hat{p}_m^2 = 0$. We obtain from (1.5), (3.4), (3.6) and (3.7) that

$$\begin{aligned} \tilde{\beta}_m^2 &= < \hat{p}_m, \hat{p}_m >= (1+\gamma)\mathcal{I}(\hat{p}_m^2) - \gamma \mathcal{G}_m(\hat{p}_m^2) \\ &= (1+\gamma)\mathcal{I}(\hat{p}_m^2) = (1+\gamma)(\hat{p}_m, \hat{p}_m) = (1+\gamma)\beta_m^2. \end{aligned}$$

We may choose $\tilde{\beta}_m = \sqrt{1+\gamma}\beta_m$. It follows that the symmetric tridiagonal $(m+1)\times(m+1)$ matrix associated with the quadrature rule $\tilde{\mathcal{G}}_{m+1,\gamma}$ is given by

$$\tilde{T}_{m+1} = \begin{bmatrix} 0 & \beta_1 & & & & & 0 \\ \beta_1 & 0 & \beta_2 & & & & \\ & \beta_2 & 0 & & & & \\ & & & \ddots & & & \\ & & \ddots & \ddots & \beta_{m-1} & & \\ & & & \beta_{m-1} & 0 & \sqrt{1+\gamma}\beta_m \\ 0 & & & & \sqrt{1+\gamma}\beta_m & 0 \end{bmatrix}.$$

We are now in a position to discuss how to determine an approximation of $\mathcal{I}f$, as well as how upper and lower bounds of $\mathcal{I}f$ can be computed by evaluating pairs of Gauss and anti-Gauss quadrature rules. For special choices of $\gamma$, the anti-Gauss rules are Gauss-Lobatto rules.

Consider the expansion

$$f(t) = \sum_{j=0}^{\infty} \eta_j p_j(t), \qquad -a < t < a, \tag{3.8}$$

and assume that the series in the right-hand side converges sufficiently rapidly to allow term-wise integration. Because of $\mathcal{I}p_0 = \mu_0^{1/2}$ and $\mathcal{I}p_j = 0$ for $j > 0$, application of the integral operator $\mathcal{I}$ to (3.8) yields $\mathcal{I}f = \eta_0\mu_0^{1/2}$. Moreover, it follows from the symmetry of the measure $\mathrm{d}\mu$ with respect to the origin that

$$\mathcal{G}_m p_{2j+1} = \tilde{\mathcal{G}}_{m+1,\gamma} p_{2j+1} = 0, \qquad j = 0,1,2,\ldots\ . \tag{3.9}$$

Therefore, applying the Gauss rule $\mathcal{G}_m$ and modified anti-Gauss rule $\tilde{\mathcal{G}}_{m+1,\gamma}$ to (3.8), using the properties (1.8) and (3.9), yields

$$\begin{aligned} \mathcal{G}_m f &= \sum_{j=0}^{\infty} \eta_{2j}\mathcal{G}_m p_{2j} = \mathcal{I}f + \sum_{j=m}^{\infty} \eta_{2j}\mathcal{G}_m p_{2j}, \qquad (3.10) \\ \tilde{\mathcal{G}}_{m+1,\gamma} f &= \sum_{j=0}^{\infty} \eta_{2j}\tilde{\mathcal{G}}_{m+1,\gamma} p_{2j} \\ &= \sum_{j=0}^{m} \eta_{2j}((1+\gamma)\mathcal{I} - \gamma\mathcal{G}_m)p_{2j} + \sum_{j=m+1}^{\infty} \eta_{2j}\tilde{\mathcal{G}}_{m+1,\gamma} p_{2j} \\ &= \sum_{j=0}^{m} \eta_{2j}(1+\gamma)\mathcal{I}p_{2j} - \sum_{j=0}^{m} \eta_{2j}\gamma\mathcal{G}_m p_{2j} + \sum_{j=m+1}^{\infty} \eta_{2j}\tilde{\mathcal{G}}_{m+1,\gamma} p_{2j} \\ &= \mathcal{I}f - \eta_{2m}\gamma\mathcal{G}_m p_{2m} + \sum_{j=m+1}^{\infty} \eta_{2j}\tilde{\mathcal{G}}_{m+1,\gamma} p_{2j}. \qquad (3.11) \end{aligned}$$

Related expansions for the case when $\gamma = 1$ and the measure $\mathrm{d}\mu$ is not required to be symmetric can be found in [2].

Assume that the coefficients $\eta_j$ converge rapidly to zero with increasing index. Then the leading terms in the expansions (3.10) and (3.11) dominate and the integration errors $\mathcal{E}_m f$ and $\tilde{\mathcal{E}}_{m+1,\gamma} f$ are of opposite sign, or equivalently,

$$\mathcal{G}_m f \leq \mathcal{I} f \leq \tilde{\mathcal{G}}_{m+1,\gamma} f \quad \text{or} \quad \mathcal{G}_m f \geq \mathcal{I} f \geq \tilde{\mathcal{G}}_{m+1,\gamma} f. \tag{3.12}$$

We formulate this observation as a theorem.

THEOREM 3.1. *Let the function $f(t)$, $-a < t < a$, have an expansion (3.8) that converges sufficiently rapidly to allow term-wise integration. In addition, assume that*

$$|\eta_{2m} \mathcal{G}_m p_{2m}| \geq |\sum_{j=m+1}^{\infty} \eta_{2j} \mathcal{G}_m p_{2j}|, \tag{3.13}$$

$$|\eta_{2m} \gamma \mathcal{G}_m p_{2m}| \geq |\sum_{j=m+1}^{\infty} \eta_{2j} \tilde{\mathcal{G}}_{m+1,\gamma} p_{2j}|. \tag{3.14}$$

*Then (3.12) holds.*

PROOF. It follows from (3.10) that

$$\mathcal{E}_m f = (\mathcal{I} - \mathcal{G}_m) f = -\eta_{2m} \mathcal{G}_m p_{2m} - \sum_{j=m+1}^{\infty} \eta_{2j} \mathcal{G}_m p_{2j},$$

and the inequality (3.13) yields

$$\operatorname{sign}(\mathcal{E}_m f) = -\operatorname{sign}(\eta_{2m} \mathcal{G}_m p_{2m}) \tag{3.15}$$

or $\mathcal{E}_m f = 0$. Similarly, we obtain from (3.11) that

$$\tilde{\mathcal{E}}_{m+1,\gamma} f = (\mathcal{I} - \tilde{\mathcal{G}}_{m+1,\gamma}) f = \eta_{2m} \gamma \mathcal{G}_m p_{2m} - \sum_{j=m+1}^{\infty} \eta_{2j} \tilde{\mathcal{G}}_{m+1,\gamma} p_{2j},$$

and it follows from (3.14) that

$$\operatorname{sign}(\tilde{\mathcal{E}}_{m+1,\gamma} f) = \operatorname{sign}(\eta_{2m} \mathcal{G}_m p_{2m}) \tag{3.16}$$

or $\tilde{\mathcal{E}}_{m+1,\gamma} f = 0$. This shows (3.12). □

The following auxiliary result will help us to draw further conclusions from the expansions (3.10) and (3.11).

LEMMA 3.2.

$$\mathcal{G}_m p_{2m} = -\mu_0^{1/2} \frac{\beta_1 \beta_2 \cdots \beta_m}{\beta_{m+1} \beta_{m+2} \cdots \beta_{2m}}, \qquad m = 1, 2, 3, \dots , \tag{3.17}$$

*where $\mu_0$ is defined by (1.3) and the $\beta_j$ are the recursion coefficients of the orthonormal polynomials $p_j$; see (1.2).*

PROOF. Substituting $f = p_{2m}$ into (1.13) and (1.14), and using the fact that $\mathcal{I} p_{2m} = 0$, yields

$$-\mathcal{G}_m p_{2m} = \frac{p_{2m}^{(2m)}(\theta)}{(2m)!} \int_{-a}^{a} \prod_{j=1}^{m} (t - t_j)^2 \mathrm{d}\mu(t). \tag{3.18}$$

It follows from (1.4) that

$$\frac{p_{2m}^{(2m)}(\theta)}{(2m)!} = \beta_0^{-1}\beta_1^{-1}\cdots\beta_{2m}^{-1} \tag{3.19}$$

and

$$\prod_{j=1}^{m}(t-t_j) = \beta_0\beta_1\cdots\beta_m p_m(t),$$

where $\beta_0 = \mu_0^{1/2}$. Therefore

$$\int_{-a}^{a}\prod_{j=1}^{m}(t-t_j)^2 \mathrm{d}\mu(t) = \beta_0^2\beta_1^2\cdots\beta_m^2 \tag{3.20}$$

Substituting (3.19) and (3.20) into (3.18) yields (3.17). □

COROLLARY 3.3. *Under the conditions of Theorem 3.1, we have*

$$\mathrm{sign}(\mathcal{E}_m f) = \mathrm{sign}(\eta_{2m}), \qquad \mathrm{sign}(\mathcal{E}_{m+1,\gamma} f) = -\mathrm{sign}(\eta_{2m}).$$

PROOF. The corollary follows by substituting (3.17) into (3.15) and (3.16). □

The following theorem gives sufficient conditions, that do not explicitly depend on the quadrature rules, for the Gauss and anti-Gauss rules to give quadrature errors of opposite sign.

THEOREM 3.4. *Let the function $f(t)$, $-a < t < a$, have an expansion (3.8) that converges sufficiently rapidly to allow term-wise integration. If*

$$|\eta_{2m}| \geq \mu_0^{1/2}\max\{1, \frac{1}{\gamma}\}\frac{\beta_{m+1}\beta_{m+2}\cdots\beta_{2m}}{\beta_1\beta_2\cdots\beta_m}\max_{-a\leq t\leq a}|\sum_{j=m+1}^{\infty}\eta_{2j}p_{2j}(t)|, \tag{3.21}$$

*where $\mu_0$ is defined by (1.3), then (3.12) holds.*

PROOF. In view of Lemma 3.2, the inequality (3.21) is equivalent to

$$|\eta_{2m}\mathcal{G}_m p_{2m}| \geq \max\{1, \frac{1}{\gamma}\}\mu_0 \max_{-a\leq t\leq a}|\sum_{j=m+1}^{\infty}\eta_{2j}p_{2j}(t)|. \tag{3.22}$$

Using the fact that the weights $w_k^2$ and $\tilde{w}_k^2$ of the Gauss and anti-Gauss rules $\mathcal{G}_m$ and $\tilde{\mathcal{G}}_{m+1,\gamma}$, respectively, are positive and sum to $\mu_0$ yields the following two lower bounds for the sum in the right-hand side of (3.22),

$$\begin{aligned}
\mu_0 \max_{-a\leq t\leq a}|\sum_{j=m+1}^{\infty}\eta_{2j}p_{2j}(t)| &\geq |\sum_{k=1}^{m}(\sum_{j=m+1}^{\infty}\eta_{2j}p_{2j}(t_k))w_k^2| \\
= |\mathcal{G}_m(\sum_{j=m+1}^{\infty}\eta_{2j}p_{2j})| &= |\sum_{j=m+1}^{\infty}\eta_{2j}\mathcal{G}_m p_{2j}| \\
\mu_0 \max_{-a\leq t\leq a}|\sum_{j=m+1}^{\infty}\eta_{2j}p_{2j}(t)| &\geq |\sum_{k=1}^{m+1}(\sum_{j=m+1}^{\infty}\eta_{2j}p_{2j}(\tilde{t}_k))\tilde{w}_k^2| \\
= |\tilde{\mathcal{G}}_{m+1,\gamma}(\sum_{j=m+1}^{\infty}\eta_{2j}p_{2j})| &= |\sum_{j=m+1}^{\infty}\eta_{2j}\tilde{\mathcal{G}}_{m+1,\gamma}p_{2j}|.
\end{aligned}$$

Substituting these bounds into (3.22) shows that

$$|\eta_{2m}\mathcal{G}_m p_{2m}| \geq \mu_0 \max_{-a\leq t\leq a} |\sum_{j=m+1}^{\infty} \eta_{2j} p_{2j}(t)| \geq |\sum_{j=m+1}^{\infty} \eta_{2j}\mathcal{G}_m p_{2j}|$$

and

$$|\eta_{2m}\mathcal{G}_m p_{2m}| \geq \frac{\mu_0}{\gamma} \max_{-a\leq t\leq a} |\sum_{j=m+1}^{\infty} \eta_{2j} p_{2j}(t)| \geq \frac{1}{\gamma}|\sum_{j=m+1}^{\infty} \eta_{2j}\tilde{\mathcal{G}}_{m+1,\gamma} p_{2j}|.$$

Thus, the inequality (3.21) implies (3.13) and (3.14), and the theorem follows from Theorem 3.1. □

Theorem 3.4 suggests how a set of functions for which pairs of Gauss and anti-Gauss rules $\mathcal{G}_m$ and $\mathcal{G}_{m+1,\gamma}$ give quadrature errors of opposite sign can be defined. Thus, let $\mathbb{Q}_\gamma(\mathrm{d}\mu)$ be the set of functions $f$ with a term-wise integrable expansion (3.8), such that the inequality (3.21) holds for $m = 1, 2, 3, \ldots$ .

COROLLARY 3.5. *Let $f \in \mathbb{Q}_\gamma(\mathrm{d}\mu)$. Then (3.12) holds for $m = 1, 2, 3, \ldots$ .*

PROOF. The corollary follows from Theorem 3.4. □

It follows from (3.10) and (3.11) that

$$(1+\gamma)^{-1}(\tilde{\mathcal{G}}_{m+1,\gamma} f - \mathcal{G}_m f) \approx -\eta_{2m}\mathcal{G}_m p_{2m}, \tag{3.23}$$

and therefore evaluation of the left-hand side of (3.23) yields an estimate of the error in $\mathcal{G}_m f$. Similarly, evaluation of the left-hand side of

$$\frac{-\gamma}{1+\gamma}(\tilde{\mathcal{G}}_{m+1,\gamma} f - \mathcal{G}_m f) \approx \eta_{2m}\gamma\mathcal{G}_m p_{2m} \tag{3.24}$$

gives an estimate of the error in $\tilde{\mathcal{G}}_{m+1,\gamma} f$.

The formulas (3.10) and (3.11) suggest that the quadrature rule

$$\mathcal{L}_{2m+1,\gamma} f := (1+\gamma)^{-1}(\tilde{\mathcal{G}}_{m+1,\gamma} + \gamma\mathcal{G}_m) f \tag{3.25}$$

yields a good approximation of $\mathcal{I}f$. Indeed, it follows from (3.10) and (3.11) that

$$\mathcal{L}_{2m+1,\gamma} f = \mathcal{I}f + \frac{\gamma}{1+\gamma}\sum_{j=m+1}^{\infty} \eta_{2j}\mathcal{L}_{2m+1,\gamma} p_{2j},$$

which shows that the quadrature rule (3.25) is exact for all polynomials of degree up to $2m+1$. We refer to $\mathcal{L}_{2m+1,\gamma}$ as the average integration rule. Laurie [7] introduced this quadrature rule for $\gamma = 1$.

The following connection between Gauss-Lobatto rules and modified anti-Gauss rules suggests, in view of Theorems 3.1 and 3.4, that for many integrands the $m$-point Gauss rule $\mathcal{G}_m$ and the associated $(m+1)$-point Gauss-Lobatto rule $\hat{\mathcal{G}}_{m+1}$ give integration errors of opposite sign.

THEOREM 3.6. *The Gauss-Lobatto quadrature rule (1.10) is a modified anti-Gauss rule (3.1) with*

$$\gamma = \frac{a p_m(a)}{\beta_m p_{m-1}(a)} - 1. \tag{3.26}$$

*In particular, $\gamma$ is positive.*

PROOF. The expression (3.26) follows from (2.1) and by requiring the matrices $\hat{T}_{m+1}$ and $\tilde{T}_{m+1}$ to have the same last subdiagonal entries. Then $\hat{T}_{m+1} = \tilde{T}_{m+1}$.

It remains to be shown that $\gamma$ defined by (3.26) is positive. Since $p_j(a) > 0$ and $\beta_j > 0$ for all $j$, it suffices to show that

$$ap_m(a) - \beta_m p_{m-1}(a) > 0.$$

But the left-hand side of this inequality equals $\beta_{m+1}p_{m+1}(a)$, which is positive. □

Introduce

$$\gamma(t) := \frac{tp_m(t)}{\beta_m p_{m-1}(t)} - 1, \qquad t \geq a. \tag{3.27}$$

This formula generalizes (3.26). It follows from (2.1) with $a$ replaced by $t$ that the symmetric tridiagonal matrix obtained by replacing the last subdiagonal entry $\sqrt{1+\gamma}\beta_m$ in $\tilde{T}_{m+1}$ by $\sqrt{1+\gamma(t)}\beta_m$ has eigenvalues at $\pm t$.

THEOREM 3.7. *The parameter $\gamma(t)$ defined by (3.27) is a positive and strictly increasing function of $t$ for $t \geq a$. Moreover,*

$$\lim_{t\to\infty} \frac{\gamma(t)}{t^2} = 1. \tag{3.28}$$

PROOF. Since the zeros of the polynomials $p_j$ are in the open interval $]-a, a[$ for all $j$, the quantity $\gamma(t)$ is well defined for all $t \geq a$. Theorem 3.6 established that $\gamma(a) > 0$. The inequality

$$p'_m(t)p_{m-1}(t) - p'_{m-1}(t)p_m(t) > 0, \qquad t \in \mathbb{R},$$

is well known; see, e.g., [9, eq. (3.3.6)]. It shows that $p_m(t)/p_{m-1}(t)$ has a positive derivative for $t \geq a$. Therefore $\frac{d}{dt}\gamma(t) > 0$ for $t \geq a$. The limit (3.28) is a consequence of (1.4). □

Theorem 3.7 shows that for any $\tilde{\gamma} \geq \gamma(a)$ the modified anti-Gauss rule $\tilde{\mathcal{G}}_{m+1,\tilde{\gamma}}$ can be considered a Gauss-Lobatto rule associated with the measure $d\mu$ with prescribed nodes at $\pm t(\tilde{\gamma})$, where $t(\gamma)$ is the inverse function of $\gamma(t)$.

## 4 Computed examples

We determine the quadrature error achieved with several pairs of Gauss and Gauss-Lobatto rules. The integrands in the computed examples are chosen so that the error formulas (1.14) and (1.16) for Gauss and Gauss-Lobatto quadrature rules, respectively, do not give simply computable accurate error bounds for the quadrature errors. Moreover, the integrals can be evaluated analytically. All computations were carried using Matlab 6.1 on a personal computer with about 16 significant decimal digits.

Example 4.1. Let $f(t) := (5-10t)\exp(-5(t-t^2))$, $a := 1$ and $d\mu(t) := dt$. Then $\mu_0 = 2$ and $\mathcal{I}f = 1 - e^{-10}$. It can be shown that the anti-Gauss rule $\tilde{\mathcal{G}}_{m+1,\gamma}$ with $\gamma = 1 + 1/m$ is the Gauss-Lobatto rule $\hat{\mathcal{G}}_{m+1}f$. Tables 4.1 and 4.2 show the performance of Gauss, Gauss-Lobatto and average quadrature rules used to approximate $\mathcal{I}f$. The errors $(\mathcal{I} - \mathcal{G}_m)f$ and $(\mathcal{I} - \hat{\mathcal{G}}_{m+1})f$ are seen to be

Table 4.1: Example 4.1: Comparison of Gauss rules $\mathcal{G}_m$ and Gauss-Lobatto rules $\hat{\mathcal{G}}_{m+1}$ for $f(t) := (5-10t)\exp(-5(t-t^2))$, $-1 < t < 1$, $\mathrm{d}\mu(t) = \mathrm{d}t$. $\mathcal{I}f = 1-e^{-10}$.

| $m$ | $(\mathcal{I}-\mathcal{G}_m)f$ | $(\mathcal{I}-\hat{\mathcal{G}}_{m+1})f$ |
|---|---|---|
| 5 | $1.9\cdot 10^{-1}$ | $-2.1\cdot 10^{-1}$ |
| 10 | $5.6\cdot 10^{-6}$ | $-5.9\cdot 10^{-6}$ |
| 15 | $-2.1\cdot 10^{-10}$ | $2.2\cdot 10^{-10}$ |

Table 4.2: Example 4.1: Error of the average rule $\mathcal{L}_{2m+1,\gamma}$ and error estimate (3.23) for Gauss rules $\mathcal{G}_m$ and (3.24) for Gauss-Lobatto rules, $f(t) := (5-10t)\exp(-5(t-t^2))$, $-1 < t < 1$, $\mathrm{d}\mu(t) = \mathrm{d}t$. $\mathcal{I}f = 1-e^{-10}$.

| $m$ | $(\mathcal{I}-\mathcal{L}_{2m+1,\gamma})f$ | (3.23) | (3.24) | $\gamma$ |
|---|---|---|---|---|
| 5 | $7.1\cdot 10^{-3}$ | $1.8\cdot 10^{-1}$ | $-2.1\cdot 10^{-1}$ | 1.2000 |
| 10 | $1.3\cdot 10^{-7}$ | $5.5\cdot 10^{-6}$ | $-6.0\cdot 10^{-6}$ | 1.1000 |
| 15 | $-8.9\cdot 10^{-13}$ | $-2.1\cdot 10^{-10}$ | $2.2\cdot 10^{-10}$ | 1.0667 |

Table 4.3: Example 4.2: Comparison of Gauss rules $\mathcal{G}_m$ and Gauss-Lobatto rules $\hat{\mathcal{G}}_{m+1}$ for $f(t) = \frac{100}{3}\cos(\frac{10}{3}\arccos(t))\exp(10\sin(\frac{10}{3}\arccos(t)))$, $-1 < t < 1$, $\mathrm{d}\mu(t) = (1-t^2)^{-1/2}\mathrm{d}t$. $\mathcal{I}f = \exp(-5\sqrt{3})-1$.

| $m$ | $(\mathcal{I}-\mathcal{G}_m)f$ | $(\mathcal{I}-\hat{\mathcal{G}}_{m+1})f$ |
|---|---|---|
| 100 | $-4.4\cdot 10^{-2}$ | $9.0\cdot 10^{-2}$ |
| 200 | $-1.1\cdot 10^{-2}$ | $2.3\cdot 10^{-2}$ |
| 300 | $-5.1\cdot 10^{-3}$ | $1.0\cdot 10^{-2}$ |

Table 4.4: Example 4.2: Error of the average rule $\mathcal{L}_{2m+1,\gamma}$ and error estimates (3.23) for Gauss rules $\mathcal{G}_m$ and (3.24) for Gauss-Lobatto rules $\hat{\mathcal{G}}_{m+1}$, $f(t) = \frac{100}{3}\cos(\frac{10}{3}\arccos(t))\exp(10\sin(\frac{10}{3}\arccos(t)))$, $-1 < t < 1$, $\mathrm{d}\mu(t) = (1-t^2)^{-1/2}\mathrm{d}t$. $\mathcal{I}f = \exp(-5\sqrt{3})-1$.

| $m$ | $(\mathcal{I}-\mathcal{L}_{2m+1,\gamma})f$ | (3.23) | (3.24) | $\gamma$ |
|---|---|---|---|---|
| 100 | $2.2\cdot 10^{-2}$ | $-6.7\cdot 10^{-2}$ | $6.7\cdot 10^{-2}$ | 1 |
| 200 | $5.7\cdot 10^{-3}$ | $-1.7\cdot 10^{-2}$ | $1.7\cdot 10^{-2}$ | 1 |
| 300 | $2.5\cdot 10^{-3}$ | $-7.6\cdot 10^{-3}$ | $7.6\cdot 10^{-3}$ | 1 |

of opposite sign. Moreover, the error estimate (3.23) for the Gauss rule and the error estimate (3.24) for the Gauss-Lobatto rule are close to the actual errors obtained with the Gauss and Gauss-Lobatto rules, respectively. □

Example 4.2. Let $f(t) := \frac{100}{3}\cos(\frac{10}{3}\arccos(t))\exp(10\sin(\frac{10}{3}\arccos(t)))$, $a := 1$ and $\mathrm{d}\mu(t) := (1-t^2)^{-1/2}\mathrm{d}t$. Then $\mu_0 = \pi$ and $\mathcal{I}f = \exp(-5\sqrt{3})-1$. The anti-Gauss rules with $\gamma = 1$ are Gauss-Lobatto rules; see Laurie [7] for a discussion on anti-Gauss rules (with $\gamma = 1$) for Jacobi measures. The performance of the Gauss, Gauss-Lobatto and average quadrature rules is displayed in Tables 4.3 and 4.4. □

Example 4.3. Let $f(t) := \frac{1}{10}\exp(2\arccos(t))\sin^3(3\arccos(t))$, $a := 1$ and

Table 4.5: Example 4.3: Comparison of Gauss rules $\mathcal{G}_m$ and Gauss-Lobatto rules $\hat{\mathcal{G}}_{m+1}$ for $f(t) = \frac{1}{10}\exp(2\arccos(t))\sin^3(3\arccos(t))$, $-1 < t < 1$, $\mathrm{d}\mu(t) = (1-t^2)^{1/2}\mathrm{d}t$. $\mathcal{I}f \approx 0.9$.

| $m$ | $(\mathcal{I} - \mathcal{G}_m)f$ | $(\mathcal{I} - \hat{\mathcal{G}}_{m+1})f$ |
|---|---|---|
| 5 | $-3.6 \cdot 10^{-1}$ | $3.6 \cdot 10^{-1}$ |
| 10 | $3.9 \cdot 10^{-3}$ | $-9.3 \cdot 10^{-3}$ |
| 15 | $3.7 \cdot 10^{-4}$ | $-9.0 \cdot 10^{-4}$ |

Table 4.6: Example 4.3: Error of the average rule $\mathcal{L}_{2m+1,\gamma}$ and error estimates (3.23) for Gauss rules $\mathcal{G}_m$ and (3.24) for Gauss-Lobatto rules $\hat{\mathcal{G}}_{m+1}$, $f(t) = \frac{1}{10}\exp(2\arccos(t))\sin^3(3\arccos(t))$, $-1 < t < 1$, $\mathrm{d}\mu(t) = (1-t^2)^{1/2}\mathrm{d}t$. $\mathcal{I}f \approx 0.9$.

| $m$ | $(\mathcal{I} - \mathcal{L}_{2m+1,\gamma})f$ | (3.23) | (3.24) | $\gamma$ |
|---|---|---|---|---|
| 5 | $-6.0 \cdot 10^{-2}$ | $-3.0 \cdot 10^{-1}$ | $4.2 \cdot 10^{-1}$ | 1.4000 |
| 10 | $-2.1 \cdot 10^{-3}$ | $6.0 \cdot 10^{-3}$ | $-7.2 \cdot 10^{-3}$ | 1.2000 |
| 15 | $-2.3 \cdot 10^{-4}$ | $5.9 \cdot 10^{-4}$ | $-6.7 \cdot 10^{-4}$ | 1.1333 |

$\mathrm{d}\mu(t) := (1-t^2)^{1/2}\mathrm{d}t$. Then $\mu_0 = \pi/2$ and

$$\mathcal{I}f = \frac{365796}{212298125}(e^{2\pi} + 1).$$

Hence, $\mathcal{I}f \approx 0.9$. The anti-Gauss rule $\tilde{\mathcal{G}}_{m+1,\gamma}$ with $\gamma = 1 + 2/m$ is the Gauss-Lobatto rule $\hat{\mathcal{G}}_{m+1}$. Tables 4.5 and 4.6 illustrate the performance of the Gauss, Gauss-Lobatto and average quadrature rules. □

The above examples show Gauss and Gauss-Lobatto rules to give quadrature errors of opposite sign. They therefore provide upper and lower bounds of $\mathcal{I}f$. This behavior also has been observed for numerous other integrands.

**Acknowledgement.**

We would like to thank Sven Ehrich for comments.

## REFERENCES

1. D. Calvetti, S. Morigi, L. Reichel, and F. Sgallari, *Computable error bounds and estimates for the conjugate gradient method*, Numer. Algorithm, 25 (2000), pp. 79–88.
2. D. Calvetti, S. Morigi, L. Reichel, and F. Sgallari, *An iterative method with error estimators*, J. Comput. Appl. Math., 127 (2001), pp. 93–119.
3. W. Gautschi, *The interplay between classical analysis and (numerical) linear algebra – A tribute to Gene H. Golub*, Elec. Trans. Numer. Anal., 13 (2002), pp. 119–147.
4. G. H. Golub, *Some modified matrix eigenvalue problems*, SIAM Rev., 15 (1973), pp. 318–334.

5. 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.
6. G. H. Golub and J. H. Welsch, *Calculation of Gauss quadrature rules*, Math. Comp., 23 (1969), pp. 221–230.
7. D. P. Laurie, *Anti-Gaussian quadrature formulas*, Math. Comp., 65 (1996), pp. 739–747.
8. J. Stoer and R. Bulirsch, *Introduction to Numerical Analysis*, 2nd ed., Springer, New York, 1993.
9. G. Szegő, *Orthogonal Polynomials*, 4th ed., Amer. Math. Society, Providence, 1975.