Enhanced Averaged Quadrature Rules with Application to Error Estimation

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Dedicated to Gradimir V. Milovanović on the occasion of his 75th birthday

Abstract Gauss quadrature is a popular approach to approximate the value of an integral determined by a measure with support on the real axis. Laurie proposed an $(n+1)$-point quadrature rule, referred to as an anti-Gauss rule, that gives an error of the same magnitude and of opposite sign as the associated n-point Gauss quadrature rule for all polynomials of degree up to $2n+1$. Laurie also described averaged rules that are the average of an n-point Gauss rule and the associated $(n+1)$-point anti-Gauss rule. The difference between an averaged rule and the associated Gauss rule have recently been used to estimate the quadrature error in the Gauss rule. For many integrands and measures the error estimate so obtained is quite accurate, but not for all integrands and measures. This paper proposes to use the difference between enhanced averaged rules introduced in [1, eq. (1.14)] and the associated Gauss rule

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to estimate the quadrature error in the latter. The enhanced averaged rules generalize averaged rules introduced by Laurie. Also enhanced averaged rules associated with Gauss rules determined by measures with support in the complex plane are described. Computed examples illustrate the performance enhanced averaged rules applied to error estimation of Gauss rules.

1 Introduction

Orthogonal polynomials and quadrature play an important role in computational mathematics; see, e.g., Gautschi [2] for discussions of many applications. Milovanović has made numerous significant contributions to both the analysis and applications of orthogonal polynomials and quadrature; see, e.g., [3, 4, 5, 6, 7, 8, 9] for some recent publications.

The present paper is concerned with error estimation for Gauss quadrature rules. Let $d\mu$ be a nonnegative measure with support on the real axis such that the integral

$$\mathcal{I}(f) := \int_a^b f(x)d\mu(x), \qquad -\infty \le a < b \le \infty, \tag{1}$$

is a *positive definite* linear functional on the space of algebraic polynomials $\mathbb{P}$, i.e., such that the bilinear form

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

is an inner product on $\mathbb{P}$. Without loss of generality we may assume that $\mathcal{I}(1) = \int d\mu = 1$. Let $p_0, p_1, p_2, \ldots$ denote the sequence of monic orthogonal polynomials with respect to the functional $\mathcal{I}$, i.e.,

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

Thus, p_j is of degree j with leading coefficient one. The polynomials p_j satisfy a three-term recursion relation of the form

$$\begin{aligned} p_1(x) &= (x - a_0)p_0(x), \qquad p_0(x) = 1, \\ p_{i+1}(x) &= (x - a_i)p_i(x) - b_i p_{i-1}(x), \qquad i = 1, 2, \ldots, \end{aligned} \tag{2}$$

with $b_i > 0$ and $a_i \in \mathbb{R}$. The recursion relations for $p_0, p_1, \ldots, p_n$ can be expressed as

$$x \begin{bmatrix} p_0(x) \\ p_1(x) \\ \vdots \\ p_{n-1}(x) \end{bmatrix} = J_n \begin{bmatrix} p_0(x) \\ p_1(x) \\ \vdots \\ p_{n-1}(x) \end{bmatrix} + \begin{bmatrix} 0 \\ \vdots \\ 0 \\ p_n(x) \end{bmatrix},$$

where

$$J_n = \begin{bmatrix} a_0 & 1 & & & 0 \\ b_1 & a_1 & 1 & & \\ & & \ddots & & \\ & & \ddots & \ddots & 1 \\ 0 & & & b_{n-1} & a_{n-1} \end{bmatrix} \in \mathbb{R}^{n\times n}. \tag{3}$$

The matrix J_n can be symmetrized by a real diagonal similarity transformation. Denote the symmetrized tridiagonal matrix so obtained by T_n.

Let the function f be continuous on the convex hull of the support of the measure $d\mu$. The n-point Gauss quadrature rule for the approximation of the functional $\mathcal{I}$ is of the form

$$\mathcal{G}_n(f) := \sum_{i=1}^{n} f(x_i) w_i \tag{4}$$

and is characterized by the property that

$$\mathcal{I}(f) = \mathcal{G}_n(f), \qquad \forall f \in \mathbb{P}_{2n-1}, \tag{5}$$

where $\mathbb{P}_{2n-1}$ denotes the set of all polynomials of degree at most $2n-1$; see Gautschi [2] or Szegő [10] for discussions on Gauss quadrature.

It is well known that the eigenvalues and the square of the first component of the normalized eigenvectors of T_n are the nodes and weights of the Gauss rule (4), respectively. They can be computed quite efficiently with the Golub-Welsch algorithm (see, e.g., [2, 11, 12]) or by a method described by Laurie [13].

The Gauss rule (4) can be expressed as

$$\mathcal{G}_n(f) = e_1^T f(T_n) e_1, \tag{6}$$

where $e_1 = [1, 0, \ldots, 0]^T \in \mathbb{R}^n$ denotes the first axis vector and the superscript ^{T} stands for transposition. This representation allows the evaluation of the Gauss rule without computing the spectral factorization of T_n. This may be attractive for some functions f. More generally,

$$\mathcal{I}(f) = e_1^T f(\hat{T}_n) e_1, \qquad \forall f \in \mathbb{P}_{2n-1}, \tag{7}$$

for any tridiagonal matrix

$$\hat{T}_n = \begin{bmatrix} \hat{a}_0 & \hat{c}_1 & & & 0 \\ \hat{b}_1 & \hat{a}_1 & \hat{c}_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \hat{b}_{n-2} & \hat{a}_{n-2} & \hat{c}_{n-1} \\ 0 & & & \hat{b}_{n-1} & \hat{a}_{n-1} \end{bmatrix} \in \mathbb{R}^{n\times n}, \tag{8}$$

such that the polynomials

$$\begin{aligned}\hat{c}_1\hat{p}_1(x) &= (x-\hat{a}_0)\hat{p}_0(x), \qquad \hat{p}_0(x) = 1,\\ \hat{c}_{i+1}\hat{p}_{i+1}(x) &= (x-\hat{a}_i)\hat{p}_i(x) - \hat{b}_i\hat{p}_{i-1}(x), \qquad i = 1,2,\ldots,n-1,\end{aligned}$$

are orthogonal with respect to the functional $\mathcal{I}$. The matrices $\hat{T}_n$ and J_n are related in the following way:

$$a_i = \hat{a}_i, \qquad b_i = \hat{b}_i\hat{c}_i. \tag{9}$$

An analogous discussion holds in the case when the functional $\mathcal{I}$ is not positive definite but *quasi-definite* on $\mathbb{P}_{n-1}$. The functional $\mathcal{I}$ is said to be quasi-definite if all $k \times k$ leading principal submatrices (for $k = 1, 2, \ldots, n$) of the Hankel matrix

$$H_n = \begin{bmatrix} \mu_0 & \mu_1 & \mu_2 & \mu_3 & \cdots & \mu_{n-1} \\ \mu_1 & \mu_2 & \mu_3 & \cdots & & \mu_n \\ \mu_2 & \mu_3 & & & & \vdots \\ \mu_3 & & & & & \\ \vdots & & & & \ddots & \\ \mu_{n-1} & \cdots & & & & \mu_{2n-2} \end{bmatrix}$$

determined by the moments

$$\mu_j := \mathcal{I}(x^j), \qquad j = 0, 1, 2, \ldots,$$

are nonsingular; see, e.g., [14]. The crucial difference with respect to the case of a positive definite functional $\mathcal{I}$ is that the coefficients b_i in the three-term recurrence relation (2) are not necessarily positive; they only are known to be nonvanishing. If $\mathcal{I}$ is real-valued functional, then the coefficients b_i and a_i are real for all i. It follows that the symmetrization of the matrix (8) may have complex entries, and the eigenvalues of the symmetrized matrix may be complex-valued and have multiplicity larger than one. However, formula (7) remains valid and we may consider it an n-point Gauss quadrature rule for $\mathcal{I}$. We remark that if the matrix $\hat{T}_n$ has multiple eigenvalues, then expression (7) is not of the form (4); see, for example, [15, p. 10]. Since the matrix $\hat{T}_n$ is unreduced, i.e., all subdiagonal entries are nonvanishing, this matrix has n distinct eigenvalues if and only if it is diagonalizable, in which case the Gauss rule is of the form (4). Non-real nodes and weights in (4) (if they exist) come in complex conjugate pairs. Therefore the value of $\mathcal{G}_n(f)$ is a real number if the integrand f is real-valued.

This paper is concerned with enhanced averaged rules that are associated with a quasi-definite functional $\mathcal{I}$. Consider the enhanced averaged rule that is the average of the $(n+k)$-point generalized anti-Gauss quadrature rule

$$\widetilde{\mathcal{G}}_{n+k}^{(k)}(f) := \sum_{i=1}^{n+k} f(\widetilde{x}_i^{(k)})\widetilde{w}_i^{(k)} \tag{10}$$

and the Gauss rule (4). The rule (10) satisfies

$$(\mathcal{I} - \widetilde{\mathcal{G}}_{n+k}^{(k)})(f) = -(\mathcal{I} - \mathcal{G}_n)(f), \qquad \forall f \in \mathbb{P}_{2n+2k-1}, \tag{11}$$

for some $k \geq 2$; see Section 2. This rule was introduced in [1] for a positive definite functional $\mathcal{I}$ and generalizes the $(n+1)$-point anti-Gauss rule described by Laurie [16]. The latter is obtained when $k = 1$. The present paper is concerned with the more general case when the functional $\mathcal{I}$ is allowed to be quasi-definite. It follows from (5) that

$$\widetilde{\mathcal{G}}_{n+k}^{(k)}(f) = \mathcal{I}(f), \qquad \forall f \in \mathbb{P}_{2n-1}. \tag{12}$$

We can express (11) as

$$\widetilde{\mathcal{G}}_{n+k}^{(k)}(f) = (2\mathcal{I} - \mathcal{G}_n)(f), \qquad \forall f \in \mathbb{P}_{2n+2k-1}.$$

This shows that when the quadrature rule $\widetilde{\mathcal{G}}_{n+k}^{(k)}$ exists, we may consider it an $(n+k)$-point Gauss quadrature rule associated with the functional $2\mathcal{I} - \mathcal{G}_n$. Existence of the quadrature rule $\widetilde{\mathcal{G}}_{n+k}^{(k)}$ is guaranteed if the functional $2\mathcal{I} - \mathcal{G}_n$ is quasi-definite on $\mathbb{P}_{n+k-1}$.

Let $\pi_0, \pi_1, \pi_2, \ldots, \pi_{n+k}$ be the unique family of monic orthogonal polynomials associated with the bilinear form

$$\langle f, g \rangle := (2\mathcal{I} - \mathcal{G}_n)(fg).$$

These polynomials satisfy the recursion formulas

$$x \begin{bmatrix} \pi_0(x) \\ \pi_1(x) \\ \vdots \\ \pi_{n+k-1}(x) \end{bmatrix} = \widetilde{J}_{n+k}^{(k)} \begin{bmatrix} \pi_0(x) \\ \pi_1(x) \\ \vdots \\ \pi_{n+k-1}(x) \end{bmatrix} + \begin{bmatrix} 0 \\ \vdots \\ 0 \\ \pi_{n+k}(x) \end{bmatrix},$$

where

$$\widetilde{J}_{n+k}^{(k)} = \begin{bmatrix} \alpha_0 & 1 & & & 0 \\ \beta_1 & \alpha_1 & 1 & & \\ & & \ddots & & \\ & & \ddots & \ddots & 1 \\ 0 & & & \beta_{n+k-1} & \alpha_{n+k-1} \end{bmatrix} \in \mathbb{R}^{(n+k)\times(n+k)} \tag{13}$$

for $n \geq 2$ and $k \geq 1$. Then we have

$$\widetilde{\mathcal{G}}_{n+k}^{(k)}(f) = e_1^T f(\widetilde{J}_{n+k}^{(k)}) e_1.$$

There is an interesting relation between the matrices J_n and $\widetilde{J}_{n+k}^{(k)}$. Note that the functionals $\mathcal{I}$ and $2\mathcal{I} - \mathcal{G}_n$ coincide on $\mathbb{P}_{2n-1}$. This means that $a_i = \alpha_i$ and $b_i = \beta_i$ for $i = 0, 1, \ldots, n-1$. Only the last k rows of $\widetilde{J}_{n+k}^{(k)}$ have to be computed to determine the quadrature rule $\widetilde{\mathcal{G}}_{n+k}^{(k)}$ if we already know the matrix J_n.

We are in a position to introduce the enhanced averaged quadrature rule

$$\mathcal{A}_{n+k}^{(k)} := \frac{1}{2}(\mathcal{G}_n + \widetilde{\mathcal{G}}_{n+k}^{(k)}),$$

associated with quasi-definite functionals $\mathcal{I}$. These rules have previously been defined for positive definite functionals in [1]. They generalizes the averaged rule $\mathcal{A}_{n+1}^{(1)}$ defined by Laurie [16]. We will show in Section 2 that the averaged rule $\mathcal{A}_{n+k}^{(k)}$ integrates a larger set of polynomials exactly than $\mathcal{G}_n$ and $\widetilde{\mathcal{G}}_{n+k}^{(k)}$. Therefore, the difference

$$\mathcal{A}_{n+k}^{(k)}(f) - \mathcal{G}_n(f) \tag{14}$$

may be a useful estimate of the quadrature error

$$\mathcal{I}(f) - \mathcal{G}_n(f). \tag{15}$$

We illustrate in Section 4 that this is indeed the case.

Having a fairly accurate estimate of the quadrature error (15) is important in many applications in which Gauss quadrature rules are used, because this allows us to determine a suitable number of nodes, n, in the Gauss rule (4). We note that a too small value of n yields an approximation of $\mathcal{I}(f)$ of insufficient accuracy, while a too large value of n requires that unnecessarily many evaluations of the integrand f are carried out. The latter may increase the computational cost significantly when it is expensive to evaluate f.

The estimation of the quadrature error in an n-point Gauss quadrature rule has received considerable attention in the literature. The classical approach to estimate this error is to evaluate a $(2n+1)$-node Gauss-Kronrod rule associated with the Gauss rule; see Notaris [17] for an insightful discussion on this approach. However, Gauss-Kronrod rules are not guaranteed to exist for all measures $d\mu$ and numbers of nodes n, and they are somewhat complicated to compute when they exist. Therefore, the application of the optimal averaged rule S_{2n+1} associated with the Gauss rule (4) has recently attracted some attention. These rules were proposed by Spalević [18] for positive definite functionals $\mathcal{I}$. The rule S_{2n+1} has $2n+1$ real nodes and exists for all positive definite functionals. Moreover, it is easy to evaluate; see [19]. The application of these rules for more general measures is discussed in [20]. The difference

$$\mathcal{S}_{2n+1}(f) - \mathcal{G}_n(f) \tag{16}$$

furnishes in many situations a quite accurate estimate of the quadrature error (15); see [21] for computed examples. However, when the integrand f is not smooth, the quality of the quadrature error estimate (16) may be poor. We therefore are interested in investigating the performance of the error estimate (14).

We also derive error estimates that are analogous to (14) for approximations of matrix functionals of the form

$$\mathcal{L}(f) = \mathcal{L}^{(A,u,v)}(f) = u^T f(A) v, \tag{17}$$

where $A \in \mathbb{R}^{N\times N}$ is a large possibly nonsymmetric matrix, f is a function such that $f(A) \in \mathbb{R}^{N\times N}$ is well defined, and $u, v \in \mathbb{R}^N$ such that $u^T v = 1$. Obviously, $\mathcal{L}$ is a real-valued linear functional.

This paper is organized as follows. Section 2 discusses properties of generalized anti-Gauss rules and describes the entries of the matrix (13). Section 3 reviews how the non-symmetric Lanczos process determines a nonsymmetric tridiagonal matrix that is analogous to the matrix (3). We derive enhanced averaged quadrature rules for the approximation of (17). Section 4 presents a few computed examples and Section 5 contains concluding remarks.

2 Enhanced anti-Gauss rules $\widetilde{\mathcal{G}}_{n+k}^{(k)}$ for $k < 4$.

This section reviews results from [1, 16], where it is shown how to compute the coefficients α_n, α_{n+1}, α_{n+2}, β_n, β_{n+1}, and β_{n+2} in (13) when the matrix J_{n+3} is known. These formulas are in [1] derived under the assumption that the functional $\mathcal{I}$ is positive definite. Here we show that they are valid in the more general case when $\mathcal{I}$ is quasi-definite.

Laurie showed in [16] that

$$\alpha_n = a_n, \quad \beta_n = 2b_n,$$

which indicates that the quadrature rule $\widetilde{\mathcal{G}}_{n+1}^{(1)}$ exists whenever $\mathcal{I}$ is quasi-definite. If $\mathcal{I}$ is positive definite, then the nodes of $\widetilde{\mathcal{G}}_{n+1}^{(1)}$ are real and simple.

We turn to the rule $\widetilde{\mathcal{G}}_{n+2}^{(2)}$. This rule is defined by the matrix $\widetilde{J}_{n+2}^{(2)}$. The expressions for the entries

$$\begin{aligned}\alpha_{n+1} &= \frac{a_{n+1}b_{n+1} - a_{n-1}b_n}{\beta_{n+1}},\\ \beta_{n+1} &= b_{n+1} - b_n,\end{aligned}$$

of this matrix are shown in [1] for the situation when $\mathcal{I}$ is positive definite. These expressions also hold when $\mathcal{I}$ is quasi-definite. Note that when β_{n+1} vanishes, the coefficient α_{n+1} is not defined. It is not straightforward to define the generalized anti-Gauss rule in this situation. When $\beta_{n+1} > 0$ and $\mathcal{I}$ is positive definite, the rule $\widetilde{\mathcal{G}}_{n+1}^{(1)}$ exists and has real and simple nodes.

The formulas for the entries α_{n+2} and β_{n+2} of $\widetilde{J}_{n+3}^{(3)}$ are more complicated. They are in [1, Theorem 2.1] shown to be

$$\beta_{n+2} = \frac{\beta_{n+1}(b_{n+2}b_{n+1} - b_n b_{n-1}) - b_{n+1}b_n(a_{n+1} - a_{n-1})^2}{\beta_{n+1}^2}$$

and

$$\alpha_{n+2} = \frac{b_{n+2}b_{n+1}(a_{n+2} + 2a_{n+1} - 2\alpha_{n+1}) + b_n b_{n-1}(2\alpha_{n+1} - 2a_{n-1} - a_{n-2})}{\beta_{n+2}\beta_{n+1}}$$
$$+ \frac{a_{n+1}b_{n+1}(a_{n+1} - \alpha_{n+1})^2 - a_{n-1}b_n(a_{n-1} - \alpha_{n+1})^2}{\beta_{n+2}\beta_{n+1}}$$

when $\mathcal{I}$ is positive definite. These expressions for β_{n+2} and α_{n+2} also are valid when $\mathcal{I}$ is quasi-definite. It is possible, but tedious, to compute the entries of the matrices $\widetilde{J}_{n+k}^{(k)}$ for $k \geq 4$.

It is shown in [1, Section 3] that the enhanced averaged rule $\mathcal{A}_{n+k}^{(k)}$ satisfies

$$\mathcal{A}_{n+k}^{(k)}(f) = \mathcal{I}(f), \qquad \forall f \in \mathbb{P}_{2n+2k-1},$$

when $\mathcal{I}$ is positive definite, and this formula remains valid when $\mathcal{I}$ is quasi-definite. It follows that the enhanced averaged rule $\mathcal{A}_{n+k}^{(k)}$ is exact for polynomials of higher degree than the Gauss and generalized anti-Gauss rules that determine it; cf. (5) and (12).

3 Enhanced averaged rules for measures with support in the complex plane

We consider the approximation of the functional (17) with $A \in \mathbb{R}^{N\times N}$ and the vectors $u, v \in \mathbb{R}^N$ such that $u^T v = 1$. We assume that N is large so that the evaluation of (17) by computing $f(A)$ is too expensive to be attractive.

The functional (17) can be associated with a measure with support in the complex plane. Assume for the moment that the matrix A has the spectral factorization

$$A = S\Lambda S^{-1},$$

where the columns of $S \in \mathbb{C}^{N\times N}$ are linearly independent eigenvectors of A, and the diagonal entries of

$$\Lambda = \mathrm{diag}[\lambda_1, \lambda_2, \ldots, \lambda_N]$$

are eigenvalues. Since the matrix A is real, the eigenvalues are real or appear in complex conjugate pairs. Substituting the spectral factorization into (17) gives

$$\mathcal{L}(f) = \mathcal{L}^{(A,u,v)}(f) = u^T S f(\Lambda) S^{-1} v = \sum_{j=1}^{N} f(\lambda_j)\mu_j\mu'_j,$$

where $[\mu_1, \mu_2, \ldots, \mu_N] = u^T S$ and $[\mu'_1, \mu'_2, \ldots, \mu'_N]^T = S^{-1}v$. The right-hand side can be expressed as an integral

$$\mathcal{L}(f) = \mathcal{L}^{(A,u,v)}(f) = \int f(t) d\mu_{A,u,v}(t)$$

with the measure

$$d\mu_{A,u,v}(t) = \sum_{j=1}^{N} \delta(t-\lambda_j)\mu_j\mu_j',$$

where $\delta(\cdot)$ denotes the Dirac delta-function. We can determine an approximation of (17) by carrying out ℓ steps of the nonsymmetric Lanczos method applied to A with initial vectors u and v. This method is described by Algorithm 1 below.

Algorithm 1 The nonsymmetric Lanczos process

Require: $A \in \mathbb{R}^{N\times N}$; $u, v \in \mathbb{R}^N$ such that $u^T v = 1$; number of steps ℓ.

$u_0 := v_0 := 0 \in \mathbb{R}^N$; $u_1 := u$; $v_1 := v$; $\beta_0 := 0$; $\gamma_0 := 0$;
for $j = 1, 2, \ldots, \ell$ **do**
  $\alpha_{j-1} := u_j^T A v_j$;
  $r := Av_j - \alpha_{j-1}v_j - \gamma_{j-1}v_{j-1}$;
  $s := A^T u_j - \alpha_{j-1}u_j - \beta_{j-1}u_{j-1}$;
  $\beta_j := |r^T s|^{1/2}$; $\gamma_j := r^T s/\beta_j$;
  $v_{j+1} := r/\beta_j$; $u_{j+1} := s/\gamma_j$;
end for

Ensure: Tridiagonal matrix $T_\ell \in \mathbb{R}^{\ell\times\ell}$ with diagonal entries $\{\alpha_j\}_{j=0}^{\ell-1}$, subdiagonal entries $\{\beta_j\}_{j=1}^{\ell-1}$, and superdiagonal entries $\{\gamma_j\}_{j=1}^{\ell-1}$ (see (18) below) and vectors $u_1, u_2, \ldots, u_{\ell+2}$ and $v_1, v_2, \ldots, v_{\ell+2}$ in $\mathbb{R}^N$.

We assume that the linear functional $\mathcal{L}$ is quasi-definite on the set of polynomials P_{n+k} with k small enough so that all quantities of interest can be computed. This is equivalent to the fact that it is possible to carry out $n+k$ steps of Algorithm 1 without breakdown, i.e., without $\beta_j = 0$ for some $1 \le j \le n+k$; see [15, Section 2]. Properties and implementation details of Algorithm 1 are discussed, e.g., by Saad [22] and Ye [23].

Introduce the matrices for $\ell = n+k$ for a suitable k,

$$U_\ell = [u_1, \ldots, u_\ell] \in \mathbb{R}^{N\times\ell}, \qquad V_\ell = [v_1, \ldots, v_\ell] \in \mathbb{R}^{N\times\ell},$$

where the vectors u_j and v_k are determined by Algorithm 1. The vectors u_j and v_k are biorthonormal, i.e., $U_\ell^T V_\ell = I$. Define the tridiagonal matrix

$$T_\ell = \begin{bmatrix} \alpha_0 & \gamma_1 & & & 0 \\ \beta_1 & \alpha_1 & \gamma_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \beta_{\ell-2} & \alpha_{\ell-2} & \gamma_{\ell-1} \\ 0 & & & \beta_{\ell-1} & \alpha_{\ell-1} \end{bmatrix} \in \mathbb{R}^{\ell\times\ell}. \tag{18}$$

Its sub-diagonal and super-diagonal entries are nonvanishing.

The recursions of Algorithm 1 can be written as

$$AV_\ell = V_\ell T_\ell + \beta_\ell v_{\ell+1} e_\ell^T,$$
$$A^T U_\ell = U_\ell T_\ell^T + \gamma_\ell u_{\ell+1} e_\ell^T.$$

Moreover, the recursion formulas show that

$$u_{j+1} = q_j(A^T)u, \qquad v_{j+1} = p_j(A)v, \qquad 0 \le j \le \ell, \tag{19}$$

for some polynomials p_j and q_j of degree j. It follows that

$$\mathcal{L}(q_j p_k) = u^T q_j(A) p_k(A) v = u_{j+1}^T v_{k+1} = \begin{cases} 1, & j = k, \\ 0, & j \neq k. \end{cases}$$

This shows that the Lanczos polynomial p_k is orthogonal to any polynomial from $\text{span}\{q_0, q_1, \ldots, q_{k-1}\} = \mathbb{P}_{k-1}$ with respect to the functional $\mathcal{L}$. In other words, $p_0, p_1, \ldots, p_\ell$ is a family of orthogonal polynomials with respect to $\mathcal{L}$. It follows from (19) that the polynomials p_j satisfy the same recursion relations as the vectors v_j, i.e.,

$$\beta_j p_j(x) = (x - \alpha_{j-1}) p_{j-1}(x) - \gamma_{j-1} p_{j-2}(x), \qquad j = 1, 2, \ldots, \ell + 1,$$

with $p_{-1}(x) := 0$, $\gamma_0 := 0$, and $\beta_0 := 0$. We conclude that

$$\mathcal{L}(f) = e_1^T f(T_\ell) e_1, \qquad \forall f \in \mathbb{P}_{2\ell-1}, \tag{20}$$

i.e., the right-hand side of (20) is an ℓ-point Gauss quadrature rule for approximating $\mathcal{L}$. This quadrature rule is of the form (4) if and only if T_ℓ is diagonalizable; see [15] for details.

We can construct the generalized anti-Gauss quadrature rules $\widetilde{\mathcal{G}}_{n+k}^{(k)}$ for $1 \le k \le 3$ in the following way. Carry out $\ell = n + k$ steps of Algorithm 1 to generate the matrix T_{n+k}. Using (9), we compute the matrix J_{n+k}, and then by formulas from Section 2, we update the last k rows of J_{n+k} to construct the matrix $\widetilde{J}_{n+k}^{(k)}$. Thus, we get

$$\widetilde{\mathcal{G}}_{n+k}^{(k)}(f) = e_1^T f(\widetilde{J}_{n+k}^{(k)}) e_1.$$

4 Numerical examples

This section presents a few computed examples that illustrate the quality of the approximations and error estimates discussed in this paper. All computations were carried out in double precision arithmetic (i.e., with about 15 significant decimal digits) using MATLAB R2021a on a 64-bit personal computer.

We compute the exact value (up to the influence of round-off errors) of the functional $\mathcal{L}(f) = u^T f(A) v$ for several different matrices A, vectors u and v, and functions f. We will assume that the functions f can be evaluated not only at A, but also at the reduced matrices T_n and $\widetilde{J}_{n+k}^{(k)}$. We compare $u^T f(T_n) v$ to approximations

determined by the standard and generalized anti-Gauss rules and the standard and enhanced averaged rules. Estimates of the approximation errors by the techniques discussed in Sections 2 and 3 are tabulated.

Example 4.1. This example shows an application of the techniques of this paper to network analysis. Let $A = [\alpha_{i,j}] \in \mathbb{R}^{500\times 500}$ be the adjacency matrix for the network Air500, which describes flight connections between the top 500 airports within one year from July 1, 2007, to June 30, 2008; see [24, 25]. The airports are modeled by vertices ν_i and the flights are modeled by edges in the directed graph determined by the network. The matrix A has the entry $\alpha_{i,j} = 1$ if there is a flight from airport i to airport j; otherwise $\alpha_{i,j} = 0$. Generally, but not always, $\alpha_{i,j} = 1$ implies that $\alpha_{j,i} = 1$. This makes A nonsymmetric. The number of edges is much smaller than 500^2. Therefore the adjacency matrix A is sparse. A walk of length k in a graph is a sequence of vertices $\nu_{i_1}, \nu_{i_2}, \ldots, \nu_{i_{k+1}}$ such that there is an edge from vertex ν_{i_j} to vertex $\nu_{i_{j+1}}$ for $j = 1, 2, \ldots, k$. Vertices in a walk may be repeated. The entry $\alpha_{i,j}^{(\ell)}$ of the matrix $A^\ell = [\alpha_{i,j}^{(\ell)}]$ is equal to the number of walks of length ℓ starting at vertex i and ending at vertex j. Short walks are generally considered more important than long walks. This motivates the use of the exponential function in network analysis. The subgraph centrality of node v_j is defined as $e_j^T \exp(A) e_j$; see [26]. We are interested in computing the *total communicability* of the graph, which is defined as $v^T \exp(A) v$, where $v = [1, 1, \ldots, 1]^T/\sqrt{500}$; see, e.g., [27].

Table 1 Example 4.1: Magnitude of the relative errors of computed approximations of $\mathcal{L}(f) = v^T \exp(A)v$, where $A \in \mathbb{R}^{500\times 500}$ and $v = [1, 1, \cdots, 1]^T/\sqrt{500}$.

	$n = 6$	$n = 8$
$\mathcal{A}_{n,1}^{(1)}(f)$	$4.61 \cdot 10^{-6}$	$1.16 \cdot 10^{-9}$
$\mathcal{A}_{n,2}^{(2)}(f)$	$1.11 \cdot 10^{-6}$	$2.38 \cdot 10^{-9}$
$\mathcal{A}_{n,3}^{(3)}(f)$	$1.59 \cdot 10^{-7}$	$8.28 \cdot 10^{-12}$
$\widetilde{\mathcal{G}}_{n,1}^{(1)}(f)$	$4.66 \cdot 10^{-4}$	$2.46 \cdot 10^{-7}$
$\widetilde{\mathcal{G}}_{n,2}^{(2)}(f)$	$4.59 \cdot 10^{-4}$	$2.39 \cdot 10^{-7}$
$\widetilde{\mathcal{G}}_{n,3}^{(3)}(f)$	$4.57 \cdot 10^{-4}$	$2.43 \cdot 10^{-7}$
$\mathcal{G}_n(f)$	$4.57 \cdot 10^{-4}$	$2.44 \cdot 10^{-7}$

Table 1 displays the relative error of computed approximations of the total communicability for the network. The approximations of the total communicability determined by the enhanced averaged rules $\mathcal{A}_{n,k}^{(k)}(f)$, $k \in \{1, 2, 3\}$, can be seen to be more accurate than the approximations determined by the standard Gauss rule and related Gauss-type formulas. This suggests that one may use the enhanced averaged quadrature rules to estimate the error in the Gauss rule. Table 2 reports the relative difference (14) for several enhanced averaged rules. All of the differences provide a quite accurate estimate of the quadrature error (15) in the Gauss rules. The error estimates obtained with the rules $\mathcal{A}_{n+3}^3(f)$ are very accurate. □

Table 2 Example 4.1: Magnitude of the relative differences of enhanced averaged and Gauss rules, where $\mathcal{L}$, A, v, and f are the same as in Table 1.

N		Error $n=6$	$n=8$
500	$\frac{\mathcal{A}_{n+1}^{(1)}(f)-\mathcal{G}_n(f)}{\mathcal{L}(f)}$	$4.61\cdot 10^{-4}$	$2.45\cdot 10^{-7}$
	$\frac{\mathcal{A}_{n+2}^{(2)}(f)-\mathcal{G}_n(f)}{\mathcal{L}(f)}$	$4.58\cdot 10^{-4}$	$2.41\cdot 10^{-7}$
	$\frac{\mathcal{A}_{n+3}^{(3)}(f)-\mathcal{G}_n(f)}{\mathcal{L}(f)}$	$4.57\cdot 10^{-4}$	$2.44\cdot 10^{-7}$
	$\frac{\mathcal{I}(f)-\mathcal{G}_n(f)}{\mathcal{L}(f)}$	$4.57\cdot 10^{-4}$	$2.44\cdot 10^{-7}$

Example 4.2. Let $N = 200$ and let $A \in \mathbb{R}^{N\times N}$ be the nonsymmetric Toeplitz matrix with first row $[1, 1/2, \ldots, 1/N]$ and first column $[1, 1/2^2, \ldots, 1/N^2]$. We seek to approximate $\mathcal{L}(f) = v^T f(A)v$ by Gauss rules, where $v = [1, \ldots, 1]^T/\sqrt{N} \in \mathbb{R}^N$ and $f(x) = \exp(x)$. Table 3 shows the magnitude of the relative errors in the computed approximations. We note that the smallest errors are achieved by the approximations furnished by the enhanced averaged rules. Table 4 reports the magnitude of the relative differences determined by (14) and (15). The table shows all the enhanced averaged rules to provide accurate estimates of the error in the Gauss quadrature rules. □

Table 3 Example 4.2: Magnitude of the relative errors of computed approximations of $\mathcal{L} = v^T f(A)v$ for $A \in \mathbb{R}^{N\times N}$ a nonsymmetric Toeplitz matrix, $f(t) = \exp(t)$, and $v = [1, 1, \ldots, 1]^T/\sqrt{N}$.

N		$n=4$	$n=6$
200	$\mathcal{A}_{n,1}^{(1)}(f)$	$1.16\cdot 10^{-7}$	$2.72\cdot 10^{-11}$
	$\mathcal{A}_{n,2}^{(2)}(f)$	$1.12\cdot 10^{-9}$	$4.78\cdot 10^{-14}$
	$\mathcal{A}_{n,3}^{(3)}(f)$	$1.70\cdot 10^{-10}$	0
	$\widetilde{\mathcal{G}}_{n,1}^{(1)}(f)$	$1.81\cdot 10^{-5}$	$2.65\cdot 10^{-9}$
	$\widetilde{\mathcal{G}}_{n,2}^{(2)}(f)$	$1.79\cdot 10^{-5}$	$2.60\cdot 10^{-9}$
	$\widetilde{\mathcal{G}}_{n,3}^{(3)}(f)$	$1.79\cdot 10^{-5}$	$2.60\cdot 10^{-9}$
	$\mathcal{G}_n(f)$	$1.79\cdot 10^{-5}$	$2.60\cdot 10^{-9}$

Table 4 Example 4.2: Magnitude of the relative differences of enhanced averaged and Gauss rules, where $\mathcal{L}$, A, v, and f are the same as in Table 3.

N		Error $n=4$	Error $n=6$
200	$\frac{\mathcal{A}_{n+1}^{(1)}(f)-\mathcal{G}_n(f)}{\mathcal{L}(f)}$	$1.80\cdot 10^{-5}$	$2.62\cdot 10^{-9}$
	$\frac{\mathcal{A}_{n+2}^{(2)}(f)-\mathcal{G}_n(f)}{\mathcal{L}(f)}$	$1.79\cdot 10^{-5}$	$2.60\cdot 10^{-9}$
	$\frac{\mathcal{A}_{n+3}^{(3)}(f)-\mathcal{G}_n(f)}{\mathcal{L}(f)}$	$1.79\cdot 10^{-5}$	$2.60\cdot 10^{-9}$
	$\frac{\mathcal{I}(f)-\mathcal{G}_n(f)}{\mathcal{L}(f)}$	$1.79\cdot 10^{-5}$	$2.60\cdot 10^{-9}$

The following examples are concerned with functionals $\mathcal{L} = u^T f(A)v$ with a symmetric matrix A. Generalized anti-Gauss rules and enhanced averaged rules for these kinds of functionals with $u = v$ have previously been introduced in [1]. However, the application of enhanced averaged rules for the estimation of the quadrature error in Gauss rules has not been illustrated before.

Example 4.3. Let $A \in \mathbb{R}^{300\times 300}$ be the symmetric tridiagonal Toeplitz matrix with first row $[0, 1, 0, \ldots, 0]$. The vector $v \in \mathbb{R}^{300}$ has normally distributed random entries with zeros mean and is scaled to have unit Euclidean norm. We let $f(t) = \frac{\exp(t)}{t^2+1}$. This example allows the application of the quadrature rules of Section 2; the other examples of this section require the quadratures of Section 3 based on the nonsymmetric Lanczos process. Table 5 depicts the magnitude of the relative errors in the computed approximations. We can observe that the smallest errors are achieved with the enhanced averaged rules. Table 6 shows the error estimates furnished by the averaged rules $\mathcal{A}_{n+k}^{(k)}(f)$ for $k \in \{2, 3\}$ to give very accurate estimates of the errors in $\mathcal{G}_n f$. We remark that the errors in Table 6 are close to the relative errors, because $\mathcal{L}(f) = v^T f(A)v = 0.8063$.

Table 5 Example 4.3: Magnitude of the relative errors of computed approximations of $v^T f(A)v$ for $A \in \mathbb{R}^{N\times N}$ a symmetric banded Toeplitz matrix, $f(t) = \frac{\exp(t)}{(t^2+1)}$, and v with normally distributed random entries.

N		$n=4$	$n=8$
300	$\mathcal{A}_{n,1}^{(1)}(f)$	$1.10\cdot 10^{-3}$	$3.83\cdot 10^{-5}$
	$\mathcal{A}_{n,2}^{(2)}(f)$	$7.26\cdot 10^{-4}$	$6.88\cdot 10^{-6}$
	$\mathcal{A}_{n,3}^{(3)}(f)$	$2.15\cdot 10^{-4}$	$4.00\cdot 10^{-6}$
	$\widetilde{\mathcal{G}}_{n,1}^{(1)}(f)$	$1.26\cdot 10^{-2}$	$2.71\cdot 10^{-4}$
	$\widetilde{\mathcal{G}}_{n,2}^{(2)}(f)$	$1.33\cdot 10^{-2}$	$2.08\cdot 10^{-4}$
	$\widetilde{\mathcal{G}}_{n,3}^{(3)}(f)$	$1.52\cdot 10^{-2}$	$2.02\cdot 10^{-4}$
	$\mathcal{G}_n(f)$	$1.47\cdot 10^{-2}$	$1.94\cdot 10^{-4}$

Table 6 Example 4.3: Magnitude of the relative differences of enhanced averaged and Gauss rules, where $\mathcal{L}$, A, v, and f are the same as in Table 5.

N		Error $n=4$	$n=8$
300	$\frac{\mathcal{A}_{n+1}^{(1)}(f)-\mathcal{G}_n(f)}{\mathcal{L}(f)}$	$1.37\cdot 10^{-2}$	$2.33\cdot 10^{-4}$
	$\frac{\mathcal{A}_{n+2}^{(2)}(f)-\mathcal{G}_n(f)}{\mathcal{L}(f)}$	$1.40\cdot 10^{-2}$	$2.01\cdot 10^{-4}$
	$\frac{\mathcal{A}_{n+3}^{(3)}(f)-\mathcal{G}_n(f)}{\mathcal{L}(f)}$	$1.49\cdot 10^{-2}$	$1.98\cdot 10^{-4}$
	$\frac{\mathcal{I}(f)-\mathcal{G}_n(f)}{\mathcal{L}(f)}$	$1.47\cdot 10^{-2}$	$1.94\cdot 10^{-4}$

Example 4.4. We approximate $\mathcal{L}(f) := u^T f(A)v$, where $f(t)=\exp(t)$, $u=e_2$, $v=e_2+\frac{e_3}{\sqrt{2}}$, and the matrix $A\in\mathbb{R}^{300\times 300}$ is the same as in Example 4.3. Table 7 shows the magnitude of the relative errors in the computed approximations. The table shows the smallest errors to be achieved by the enhanced averaged rules $\mathcal{A}_{n,k}^{(k)}(f)$; the errors are particularly small for $k\in\{2,3\}$. Table 8 shows the differences $\mathcal{A}_{n+k}^{(k)}(f)-\mathcal{G}_n(f)$, $k\in\{1,2,3\}$, to be accurate estimates of the quadrature error in $\mathcal{G}_n(f)$.

Table 7 Example 4.4: Magnitude of the relative errors of computed approximations of $u^T f(A)v$ for $A\in\mathbb{R}^{N\times N}$ a symmetric banded Toeplitz matrix, $f(t)=\exp(t)$, and u different from v.

N		$n=4$	$n=6$
300	$\mathcal{A}_{n,1}^{(1)}(f)$	$5.22\cdot 10^{-8}$	$1.49\cdot 10^{-12}$
	$\mathcal{A}_{n,2}^{(2)}(f)$	$4.78\cdot 10^{-11}$	$5.31\cdot 10^{-15}$
	$\mathcal{A}_{n,3}^{(3)}(f)$	$2.27\cdot 10^{-13}$	$5.31\cdot 10^{-16}$
	$\widetilde{\mathcal{G}}_{n,1}^{(1)}(f)$	$4.70\cdot 10^{-6}$	$2.51\cdot 10^{-10}$
	$\widetilde{\mathcal{G}}_{n,2}^{(2)}(f)$	$4.80\cdot 10^{-6}$	$2.54\cdot 10^{-10}$
	$\widetilde{\mathcal{G}}_{n,3}^{(3)}(f)$	$4.80\cdot 10^{-6}$	$2.54\cdot 10^{-10}$
	$\mathcal{G}_n(f)$	$4.80\cdot 10^{-6}$	$2.54\cdot 10^{-10}$

Table 8 Example 4.4: Magnitude of the relative differences of enhanced averaged and Gauss rules, where $\mathcal{L}$, A, v, and f are the same as in Table 7.

N		Error $n=4$	Error $n=6$
300	$\frac{\mathcal{A}_{n+1}^{(1)}(f)-\mathcal{G}_n(f)}{\mathcal{L}(f)}$	$4.75\cdot 10^{-6}$	$2.53\cdot 10^{-10}$
	$\frac{\mathcal{A}_{n+2}^{(2)}(f)-\mathcal{G}_n(f)}{\mathcal{L}(f)}$	$4.81\cdot 10^{-6}$	$2.54\cdot 10^{-10}$
	$\frac{\mathcal{A}_{n+3}^{(3)}(f)-\mathcal{G}_n(f)}{\mathcal{L}(f)}$	$4.81\cdot 10^{-6}$	$2.54\cdot 10^{-10}$
	$\frac{\mathcal{I}(f)-\mathcal{G}_n(f)}{\mathcal{L}(f)}$	$4.81\cdot 10^{-6}$	$2.54\cdot 10^{-10}$

Example 4.5. We approximate $\mathcal{L}(f) := u^T\left(A^2+I\right)^{-1}u$, where u is a random vector of unit norm with normally distributed entries with zero mean, and the symmetric matrix $A\in\mathbb{R}^{100\times 100}$ has randomly generated uniformly distributed real eigenvalues in the interval $[-1,1]$ and a random orthogonal eigenvector matrix. The exact value of $\mathcal{L}(f)$ is 0.8934. Table 9 shows the magnitude of the relative errors in the computed approximations. The table shows the smallest errors to be achieved by the the enhanced averaged rules $\mathcal{A}_{n,k}^{(k)}(f)$; the errors are particularly small for $k=3$. Table 10 shows the differences $\mathcal{A}_{n+k}^{(k)}(f)-\mathcal{G}_n(f)$, $k\in\{1,2,3\}$, to be accurate estimates of the quadrature error in $\mathcal{G}_n(f)$.

Table 9 Example 4.5: Magnitude of the relative errors of computed approximations of $u^T\left(A^2+I\right)^{-1}u$ for $A\in\mathbb{R}^{100\times 100}$ a random symmetric matrix, and u is a random vector.

N		$n=3$	$n=5$
100	$\mathcal{A}_{n,1}^{(1)}(f)$	$3.63\cdot 10^{-4}$	$4.33\cdot 10^{-6}$
	$\mathcal{A}_{n,2}^{(2)}(f)$	$5.01\cdot 10^{-5}$	$1.34\cdot 10^{-6}$
	$\mathcal{A}_{n,3}^{(3)}(f)$	$3.33\cdot 10^{-7}$	$1.28\cdot 10^{-8}$
	$\widetilde{\mathcal{G}}_{n,1}^{(1)}(f)$	$3.50\cdot 10^{-3}$	$7.88\cdot 10^{-5}$
	$\widetilde{\mathcal{G}}_{n,2}^{(2)}(f)$	$2.90\cdot 10^{-3}$	$6.74\cdot 10^{-5}$
	$\widetilde{\mathcal{G}}_{n,3}^{(3)}(f)$	$2.80\cdot 10^{-3}$	$7.02\cdot 10^{-5}$
	$\mathcal{G}_n(f)$	$2.80\cdot 10^{-3}$	$7.01\cdot 10^{-5}$

Table 10 Example 4.5: Magnitude of the relative differences of enhanced averaged and Gauss rules, where $\mathcal{L}$, A, v, and f are the same as in Table 9.

N		Error $n=3$	Error $n=5$
100	$\frac{\mathcal{A}_{n+1}^{(1)}(f)-\mathcal{G}_n(f)}{\mathcal{L}(f)}$	$3.20 \cdot 10^{-3}$	$7.45 \cdot 10^{-5}$
	$\frac{\mathcal{A}_{n+2}^{(2)}(f)-\mathcal{G}_n(f)}{\mathcal{L}(f)}$	$2.80 \cdot 10^{-3}$	$6.88 \cdot 10^{-5}$
	$\frac{\mathcal{A}_{n+3}^{(3)}(f)-\mathcal{G}_n(f)}{\mathcal{L}(f)}$	$2.80 \cdot 10^{-3}$	$7.01 \cdot 10^{-5}$
	$\frac{\mathcal{I}(f)-\mathcal{G}_n(f)}{\mathcal{L}(f)}$	$2.80 \cdot 10^{-3}$	$7.01 \cdot 10^{-5}$

5 Conclusion

This paper proposes to use enhanced averaged rule to estimate the error in Gauss quadrature rules. The enhanced averaged rules are modifications of averaged rules introduced by Laurie. They are defined with the aid of generalized anti-Gauss rules. The latter rules, as well as the enhanced averaged rules, are determined for quasi-definite functionals $\mathcal{I}$. In particular, we allow functionals that are associated with measures with support in the complex plane. Computed examples illustrate the performance of the enhanced averaged rules.

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