SIAM J. NUMER. ANAL.
Vol. 52, No. 2, pp. 832–851




# RATIONAL GAUSS QUADRATURE*

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**Abstract.** The existence of (standard) Gauss quadrature rules with respect to a nonnegative measure $d\mu$ with support on the real axis easily can be shown with the aid of orthogonal polynomials with respect to this measure. Efficient algorithms for computing the nodes and weights of an $n$-point Gauss rule use the $n \times n$ symmetric tridiagonal matrix determined by the recursion coefficients for the first $n$ orthonormal polynomials. Many rational functions that are orthogonal with respect to the measure $d\mu$ and have real or complex conjugate poles also satisfy a short recursion relations. This paper describes how banded matrices determined by the recursion coefficients for these orthonormal rational functions can be used to efficiently compute the nodes and weights of rational Gauss quadrature rules.

**Key words.** orthogonal rational functions, Gauss quadrature

**AMS subject classifications.** Primary, 65D30, 65D32, 65F15; Secondary, 41A55

**DOI.** 10.1137/120902161

## 1. Introduction.

Many problems in science and engineering require the accurate computation of integrals of the form

$$\mathcal{I}f = \int_a^b f(x)d\mu(x), \tag{1.1}$$

where $-\infty \leq a < b \leq \infty$, $f$ is a real-valued function, and the nonnegative measure $d\mu$ has infinitely many points of support in the interval $[a, b]$ and well-defined moments

$$\mu_j = \int_a^b x^j d\mu(x), \qquad j = 0, 1, 2, \ldots.$$

We will assume that the measure satisfies these conditions throughout this section and section 2. Moreover, we assume for notational simplicity that $\mu_0 = 1$.

Gauss rules are among the most popular quadrature methods, because the $n$-point Gauss rule for approximating (1.1),

$$\mathcal{G}_n f = \sum_{i=1}^{n} f(x_i)w_i, \tag{1.2}$$

is exact for polynomials of as high degree as possible, i.e.,

$$\mathcal{G}_n f = \mathcal{I}f \qquad \forall f \in \mathbb{P}_{2n}, \tag{1.3}$$

and has positive weights $w_i$. Here $\mathbb{P}_{2n}$ denotes the $2n$-dimensional space of all polynomials of degree at most $2n - 1$. We refer to Gautschi [9] and Szegő [21] for many

*Received by the editors December 11, 2012; accepted for publication (in revised form) December 6, 2013; published electronically April 3, 2014.
http://www.siam.org/journals/sinum/52-2/90216.html

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properties and applications of Gauss rules. When the space $\mathbb{P}_{2n}$ in (1.3) is replaced by a $2n$-dimensional linear space of rational functions with fixed poles, the quadrature rule analogous to (1.2) is referred to as a rational Gauss rule.

Introduce the inner product and associated norm

$$\langle f,g\rangle := \mathcal{I}(fg), \qquad \|f\| := \langle f,f\rangle^{1/2}, \tag{1.4}$$

for suitable functions $f$ and $g$. Let $p_0, p_1, p_2, \ldots$ be a family of orthonormal polynomials with respect to this inner product and norm, i.e., $p_j$ is of degree $j$ with positive leading coefficient and

$$\langle p_i, p_j\rangle = \begin{cases} 1, & i = j, \\ 0, & i \neq j. \end{cases}$$

It is well known that the polynomials $p_j$ satisfy a three-term recurrence relation. Define the vector

$$\mathbf{p}_n(x) = [p_0(x), p_1(x), \ldots, p_{n-1}(x)]^T. \tag{1.5}$$

Then the recursion relation for the $p_j$'s can be expressed as

$$x\,\mathbf{p}_n(x) = T_n\mathbf{p}_n(x) + t_{n,n+1}p_n(x)\mathbf{e}_n, \tag{1.6}$$

where $T_n \in \mathbb{R}^{n\times n}$ is a symmetric tridiagonal matrix whose nontrivial entries are the recursion coefficients for the orthonormal polynomials and $t_{n,n+1}$ is a suitable scalar. Throughout this paper $\mathbf{e}_j = [0, \ldots, 0, 1, 0, \ldots, 0]^T$ denotes the $j$th axis vector of suitable dimension. The zeros of $p_n$ are the nodes $x_i$ of the Gauss rule (1.2), and it is easy to see that they are eigenvalues of the matrix $T_n$; the vector $\mathbf{p}_n(x_i)$ is an associated eigenvector. This observation, and the fact that the weights of the Gauss rule are the squares of the first components of normalized eigenvectors, form the basis for the Golub–Welsch algorithm [13] for computing the nodes and weights of the Gauss rule (1.2) from the matrix $T_n$; see, e.g., [8, 9, 12] for fairly recent discussions of this algorithm and its numerical performance.

When the integrand $f$ has one or several singularities close to the interval $[a,b]$, a large number of nodes $x_i$ may be required for the Gauss rule (1.2) to furnish an accurate approximation of the integral (1.1). It is then necessary to evaluate $f$ at many nodes and this may be expensive. Rational Gauss rules sometimes can remedy this difficulty. These are Gauss-type quadrature rules that are exact for as many rational functions with prescribed poles as possible. They were first discussed by Gonchar and López Lagomasino [14, 17] and have subsequently received considerable attention; see, e.g., [2, 7, 9, 10, 15, 18, 22]. Recently, Deckers and Bultheel [3] showed that orthogonal rational functions satisfy three-term recursion relations with linear fractional transformations as "coefficients" and discussed their application to the computation of rational Gauss rules in [4]. The recursion relation for these orthogonal functions differs from the recursion relation described in [19], which has scalar recursion coefficients. We will comment further on the difference between the approaches in [3, 4] and the one in [19] and the present paper in Remark 3.15 of section 3.

It is shown in [19] that certain orthonormal rational functions with respect to the inner product (1.4) satisfy short recursion relations that can be expressed in the form (1.6) with the symmetric tridiagonal matrix $T_n$ replaced by a symmetric matrix $H_n$ with larger (but still small) bandwidth. Thus, $H_n \in \mathbb{R}^{n\times n}$ is the matrix determined by the recursion coefficients for the first $n$ orthonormal rational functions. We show in section 2 that the eigenvalues of $H_n$ are the nodes of the rational Gauss rule and the squares of the first components of normalized eigenvectors are the weights. This observation can be used to develop efficient numerical methods, analogous to the Golub–Welsch algorithm, for computing the nodes and weights of rational Gauss rules.

The short recursion relations represented by the matrix $H_n$ are convenient to use in many situations. For instance, orthonormal rational functions can be applied in large-scale computational problems, such as the approximation of expressions of the forms $f(A)\mathbf{v}$ or

$$\mathcal{I}f = \mathbf{v}^T f(A)\mathbf{v}, \tag{1.7}$$

where $f$ is a nonlinear function, $A \in \mathbb{R}^{N\times N}$ is a large symmetric matrix, and $\mathbf{v} \in \mathbb{R}^N$ is a vector. Section 3 is concerned with the approximation of expressions of the form (1.7). Substituting the spectral factorization of $A$ into (1.7) shows that the computational task can be written in the form (1.1) with a measure $d\mu$ with discrete support (at the eigenvalues of $A$). Therefore, Gauss quadrature rules can be applied to compute approximations of (1.7). Golub and Meurant [11, 12] have described how an $n$-point (standard) Gauss rule for (1.7) can be evaluated efficiently by carrying out $n$ steps of the (standard) Lanczos method applied to $A$ with initial vector $\mathbf{v}$. Section 3 describes how the expression (1.7) can be approximated by an $n$-point rational Gauss rule by application of $n$ steps of the rational Lanczos method. A computed example is presented in section 4 and concluding remarks can be found in section 5.

Rational Gauss rules based on orthogonal Laurent polynomials, i.e., on orthogonal rational functions with poles at zero and infinity only, have received considerable attention; see, e.g., [5, 15, 16]. This paper generalizes some of the results available for this kind of quadrature rules to rational Gauss rules with several distinct finite poles.

## 2. Orthonormal rational functions and Gauss quadrature.

Let the real distinct poles $\alpha_1, \alpha_2, \ldots, \alpha_\ell$ lie in the complement of the convex hull of $\mathrm{supp}(d\mu)$ and be of multiplicities $k_1, k_2, \ldots, k_\ell$, respectively, and let $\alpha_{\ell+1}, \alpha_{\ell+2}, \ldots, \alpha_{\ell+2\widehat{\ell}}$ be distinct complex conjugate poles. We assume the latter to be ordered so that $\alpha_{\ell+2i} = \bar{\alpha}_{\ell+2i-1}$, $i = 1, 2, \ldots, \widehat{\ell}$, where the bar denotes complex conjugation. The multiplicity of the poles $\alpha_{\ell+2i-1}$ and $\alpha_{\ell+2i}$ is denoted by $s_i$.

Introduce the linear spaces associated with the elementary rational functions with a finite real pole,

$$\mathbb{Q}_{i,k_i} = \mathrm{span}\left\{ \frac{1}{(x-\alpha_i)^j} \;:\; j = 1, 2, \ldots, k_i \right\}, \qquad i = 1, 2, \ldots, \ell. \tag{2.1}$$

Since we are interested in integrating real-valued functions, it suffices to consider linear combinations of pairs of elementary complex-valued rational functions

$$\frac{1}{(x-\alpha_{\ell+2i-1})^j}, \qquad \frac{1}{(x-\bar{\alpha}_{\ell+2i-1})^j}$$

that are real. Therefore, we replace each such pair of functions by a pair

$$\frac{1}{(x^2+\beta_i x+\gamma_i)^j}, \qquad \frac{x}{(x^2+\beta_i x+\gamma_i)^j}, \tag{2.2}$$

where the coefficients $\beta_i, \gamma_i \in \mathbb{R}$ are determined by $x^2 + \beta_i x + \gamma_i = (x - \alpha_{\ell+2i-1})(x - \bar{\alpha}_{\ell+2i-1})$. We define the spaces, analogous to (2.1),

$$\mathbb{W}_{i,2s_i} = \mathrm{span}\left\{ \frac{1}{(x^2+\beta_i x+\gamma_i)^j}, \frac{x}{(x^2+\beta_i x+\gamma_i)^j} \;:\; j = 1, 2, \ldots, s_i \right\},$$

for $i = 1, 2, \ldots, \widehat{\ell}$. Thus, $\dim(\mathbb{W}_{i,2s_i}) = 2s_i$.

Let

$$k = \sum_{i=1}^{\ell} k_i, \qquad s = \sum_{i=1}^{\widehat{\ell}} s_i, \tag{2.3}$$

and introduce the $n$-dimensional linear space

$$\mathbb{S}_n := \mathbb{P}_{n-k-2s} \oplus \mathbb{Q}_{1,k_1} \oplus \cdots \oplus \mathbb{Q}_{\ell,k_\ell} \oplus \mathbb{W}_{1,2s_1} \oplus \cdots \oplus \mathbb{W}_{\widehat{\ell},2s_{\widehat{\ell}}}, \tag{2.4}$$

where we assume that the $k_i$ and $s_i$ are chosen so that $0 \leq k + 2s < n$. A proof of the following result for a slightly more general situation is provided by Gautschi [9, Theorem 3.25]. We present a proof for the case of interest to us, because of its importance for the development below.

THEOREM 2.1. *Let the real poles $\alpha_1, \alpha_2, \ldots, \alpha_\ell$ lie in outside the convex hull of the support of $d\mu$ and be of multiplicities $k_1, k_2, \ldots, k_\ell$, respectively, and let $\alpha_{\ell+1}, \alpha_{\ell+2}, \ldots, \alpha_{\ell+2\widehat{\ell}}$ be distinct complex conjugate poles ordered so that $\alpha_{\ell+2i} = \bar{\alpha}_{\ell+2i-1}$. Let the multiplicity of the poles $\alpha_{\ell+2i-1}$ and $\alpha_{\ell+2i}$ be $s_i$. Assume that $0 \leq k + 2s < n$ with $k$ and $s$ given by (2.3) and define the coefficients $\beta_i$ and $\gamma_i$ as described following (2.2). Then the $n$-point rational Gauss quadrature rule,*

$$\widetilde{\mathcal{G}}_n f = \sum_{j=1}^{n} f(\widetilde{x}_j)\widetilde{w}_j, \tag{2.5}$$

*associated with the measure $d\mu$, satisfying*

$$\widetilde{\mathcal{G}}_n f = \mathcal{I} f \qquad \forall f \in \mathbb{S}_{2n}, \tag{2.6}$$

*where*

$$\mathbb{S}_{2n} := \mathbb{P}_{2n-2k-4s} \oplus \mathbb{Q}_{1,2k_1} \oplus \cdots \oplus \mathbb{Q}_{\ell,2k_\ell} \oplus \mathbb{W}_{1,4s_1} \oplus \cdots \oplus \mathbb{W}_{\widehat{\ell},4s_{\widehat{\ell}}}, \tag{2.7}$$

*exists, is unique, and has positive weights $\widetilde{w}_j$.*

*Proof.* Introduce the polynomial

$$\omega(x) = \prod_{i=1}^{\ell} (x - \alpha_i)^{k_i} \prod_{j=1}^{\widehat{\ell}} (x^2 + \beta_j x + \gamma_j)^{s_j}. \tag{2.8}$$

Thus, $\mathbb{S}_{2n} = \mathbb{P}_{2n}/\omega^2(x)$. The (standard) $n$-point Gauss quadrature rule

$$\widehat{\mathcal{G}}_n f = \sum_{i=1}^{n} f(\widehat{x}_i)\widehat{w}_i \tag{2.9}$$

connected to the nonnegative measure $d\mu(x)/\omega^2(x)$ evidently exists:

$$\widehat{\mathcal{G}}_n f = \int_a^b f(x) \frac{d\mu(x)}{\omega^2(x)} \qquad \forall f \in \mathbb{P}_{2n}.$$

Associating $\omega^2$ with $f$ instead of with $d\mu$ yields

$$\widehat{\mathcal{G}}_n f = \sum_{i=1}^{n} \left( \frac{f(\widehat{x}_i)}{\omega^2(\widehat{x}_i)} \right) \omega^2(\widehat{x}_i)\widehat{w}_i = \int_a^b \left( \frac{f(x)}{\omega^2(x)} \right) d\mu(x) \qquad \forall f \in \mathbb{P}_{2n}. \tag{2.10}$$

The above sum suggests that we identify $\widetilde{\mathcal{G}}_n(f/\omega^2)$ with $\widehat{\mathcal{G}}_n(f)$ to obtain

$$\widetilde{\mathcal{G}}_n\left(\frac{f}{\omega^2}\right) = \widehat{\mathcal{G}}_n(f) = \sum_{i=1}^{n}\left(\frac{f(\widehat{x}_i)}{\omega^2(\widehat{x}_i)}\right)\omega^2(\widehat{x}_i)\widehat{w}_i. \tag{2.11}$$

Combining (2.10) and (2.11) shows that the quadrature rule (2.5) with $\widetilde{x}_i = \widehat{x}_i$ and $\widetilde{w}_i = \omega^2(\widehat{x}_i)\widehat{w}_i$ satisfies (2.6). ∎

In this section, we will assume that $0 \leq k + 2s \leq n - 2$. Then the space (2.4) contains linear functions. Let $\Psi_{n+1} = \{\psi_0, \psi_1, \ldots, \psi_n\}$ denote an elementary basis for the space $\mathbb{S}_n \cup \{x^{n-k-2s}\}$, i.e., $\psi_0(x) = 1$ and each basis function $\psi_i(x)$, for $i = 1, 2, \ldots, n$, is one of the functions

$$x^j, \ \frac{1}{(x-\alpha_i)^j}, \ \frac{1}{(x^2+\beta_i x+\gamma_i)^j}, \ \frac{x}{(x^2+\beta_i x+\gamma_i)^j}$$

for some positive integers $i$ and $j$. We write $\psi_s \prec \psi_t$ if the basis function $\psi_s$ comes before $\psi_t$. The ordering of the basis functions $\Psi_{n+1}$ is said to be *natural* if $\psi_0(x) = 1$, and the remaining functions $\psi_j$, $j = 1, 2, \ldots, n$, satisfy:

1. $x^j \prec x^{j+1}$ for all integers $j > 0$,
2. $\frac{1}{(x-\alpha_i)^j} \prec \frac{1}{(x-\alpha_i)^{j+1}}$ for all integers $j > 0$ and every real pole $\alpha_i$,
3. $\frac{1}{(x^2+\beta_i x+\gamma_i)^j} \prec \frac{x}{(x^2+\beta_i x+\gamma_i)^j} \prec \frac{1}{(x^2+\beta_i x+\gamma_i)^{j+1}}$ for all positive integers $j$ and every pair $\{\beta_i, \gamma_i\}$,
4. if $\psi_j(x) = \frac{1}{(x^2+\beta_j x+\gamma_j)^p}$, then $\psi_{j+1}(x) = \frac{x}{(x^2+\beta_j x+\gamma_j)^p}$.

The above definition of natural ordering differs from the definition in [19] in that we impose the additional requirement 4. We refer to the ordering as "natural" because lower powers come before higher ones. In addition, we assume that $\psi_{n-1}(x) = x^{n-k-2s-1}$ and $\psi_n(x) = x^{n-k-2s}$. This condition leads to simplifications of the remainder term in (2.13) below. We comment on the situation when this condition is violated in Remarks 3.12 and 3.13 of section 3.

Application of the Gram–Schmidt process with respect to the inner product and norm (1.4) to the basis $\Psi_{n+1}$ yields an orthonormal basis $\Phi_{n+1} = \{\phi_0, \phi_1, \ldots, \phi_n\}$. Define the vector

$$\boldsymbol{\phi}_n(x) = [\phi_0(x), \phi_1(x), \ldots, \phi_{n-1}(x)]^T \tag{2.12}$$

and express the functions $x\phi_j(x)$, $j = 0, 1, \ldots, n-1$, as linear combinations of the basis functions $\Phi_{n+1}$. Then, similarly to (1.6), we obtain

$$x\,\boldsymbol{\phi}_n(x) = H_n\boldsymbol{\phi}_n(x) + h_{n-1,n}\phi_n(x)\mathbf{e}_n, \tag{2.13}$$

where $H_n = [h_{ij}]_{i,j=0}^{n-1}$ and $h_{n-1,n}$ is a suitable scalar.

The structure of the matrix $H_n$ depends on the orthonormal basis $\Phi_{n+1}$ and, thus, on the choice of elementary basis $\Psi_{n+1}$. We point out that the remainder term in (2.13) is of the form $h_{n-1,n}\phi_n(x)\mathbf{e}_n$ only when both elementary basis functions $\psi_{n-1}$ and $\psi_n$ are monomials. This is a consequence of Theorem 2.2 below and the discussion following the theorem.

We would like $H_n$ to have small bandwidth. The following result, shown in [19, Theorem 1], indicates how this can be achieved.

THEOREM 2.2. *Let the basis $\Psi_{n+1} = \{\psi_0, \psi_1, \ldots, \psi_n\}$ satisfy conditions* 1, 2, *and* 3 *of natural ordering. Assume that every sequence of $m_1$ consecutive basis functions*

*$\psi_j, \psi_{j+1}, \ldots, \psi_{j+m_1-1}$ contains at least one nonnegative power $x^\ell$ and that between every pair of basis functions*

$$\left\{ \frac{1}{(x^2+\beta_i x+\gamma_i)^j}, \frac{x}{(x^2+\beta_i x+\gamma_i)^j} \right\}, \qquad j = 1, 2, 3, \ldots, \quad i = 1, 2, 3, \ldots,$$

*there are at most $m_2$ basis functions. Then the orthonormal rational functions $\phi_0, \phi_1, \ldots, \phi_{n-1}$ satisfy a $(2m+1)$-term recurrence relation of the form*

$$x\phi_t(x) = \sum_{j=-m}^{m} c_{t,t+j}\phi_{t+j}(x), \qquad t = 0, 1, 2, \ldots, \tag{2.14}$$

*with $m = \max\{m_1, m_2+1\}$. By convention, coefficients $c_{t,t+j}$ and functions $\phi_{t+j}$ with negative index $t + j$ are defined to be zero. The parameter $t$ has to be small enough for all required terms in the sum* (2.14) *to exist.*

It follows from Theorem 2.2 that if there are no finite poles, then $m = 1$ and we obtain the standard three-term recurrence relation for orthonormal polynomials. If there are finite poles and at least every other elementary basis function $\psi_j$ is a nonnegative power of $x$ ($m_1 = 2$), then we can achieve that $m_2 \le 1$, i.e., $m = 2$. This yields recurrence relations with at most five terms.

The proof of Theorem 2.2 or direct computations show that the recurrence formula (2.14) may be further simplified by including condition 4 of natural ordering (which means that $m_2 = 0$) and by letting the number of terms in the sum (2.14) depend on the index $t$. We obtain

$$x\phi_t(x) = \sum_{j=-m_3}^{m_4} c_{t,t+j}\phi_{t+j}(x), \qquad t = 0, 1, 2, \ldots, \tag{2.15}$$

where $m_3 = m_3(t)$, $t - m_3$ is the largest integer smaller than $t$ such that $\psi_{t-m_3}$ is a monomial, $m_4 = m_4(t)$, and $t + m_4$ is the smallest integer larger than $t$ such that $\psi_{t+m_4}$ is a monomial. It implies the following block-diagonal structure of the matrix $H_n$ from (2.13). The matrix has $n-k-2s-1$ square blocks along the diagonal. Two consecutive blocks overlap in one diagonal element. The $j$th block is of dimension $t \times t$, where $t-2$ is the number of rational functions between consecutive monomials $x^{j-1}$ and $x^j$. Precisely, the $j$th block of $H_n$ is $H_n(t_1 : t_2, t_1 : t_2)$, where $\psi_{t_1}(x) = x^{j-1}$ and $\psi_{t_2}(x) = x^j$. Here $H_n(t_1 : t_2, t_1 : t_2)$ denotes the submatrix of $H_n = [h_{ij}]_{i,j=0}^{n-1}$ with the entries $h_{ij}$, $t_1 \le i, j \le t_2$. Also, $t = t_2 - t_1 + 1$. The following examples provide illustrations.

*Example* 2.3. Let all the poles $\alpha_i$ be real and consider the elementary basis

$$\begin{aligned} &1, \frac{1}{x-\alpha_1}, x, \frac{1}{(x-\alpha_1)^2}, x^2, \ldots, \frac{1}{(x-\alpha_1)^{k_1}}, x^{k_1}, \frac{1}{(x-\alpha_2)}, x^{k_1+1}, \ldots, \\ &\frac{1}{(x-\alpha_2)^{k_2}}, x^{k_1+k_2}, \ldots, \frac{1}{x-\alpha_\ell}, \ldots, \frac{1}{(x-\alpha_\ell)^{k_\ell}}, x^k, \end{aligned} \tag{2.16}$$

where $k$ is defined by (2.3) and $n = 2k + 1$. This basis together with the function $\psi_n(x) = x^{k+1}$ satisfy the requirements of natural ordering. The use of $n \ne 2k + 1$ is commented on below.

In the setting of this example, formula (2.15) reduces to

$$x\phi_t(x) = \sum_{j=t-2}^{t+2} h_{t,j}\, \phi_j(x), \quad t = 0, 1, 2, \ldots,$$

where

$$h_{t,j} = \langle x\, \phi_t(x), \phi_j(x)\rangle = \langle x\, \phi_j(x), \phi_t(x)\rangle = h_{j,t}, \tag{2.17}$$

and $h_{t,t+2} = h_{t,t-2} = 0$ for $t$ odd. Moreover, $h_{n-1,n+1} = 0$. This shows that the matrix $H_n = [h_{ij}]_{i,j=0}^{n-1}$ in (2.13) is symmetric and pentadiagonal with $k$ $3 \times 3$ blocks along the diagonal:

$$H_n = \begin{bmatrix} * & * & * & & & & & & & & \\ * & * & * & & & & & & & & \\ * & * & * & * & * & & & & & & \\ & & * & * & * & & & & & & \\ & & * & * & * & * & * & & & & \\ & & & & * & * & * & & & & \\ & & & & & & \ddots & & & & \\ & & & & & & * & * & * & & \\ & & & & & & * & * & * & * & * \\ & & & & & & & & * & * & * \\ & & & & & & & & * & * & * \end{bmatrix}. \tag{2.18}$$

We remark that when $n$ is odd, the value $k = (n-1)/2$, where $k$ is defined by (2.3), is the largest possible to achieve a pentadiagonal structure of $H_n$. A larger value of $k$ with $n$ fixed yields at least one diagonal block of $H_n$ of size $4 \times 4$ or larger. If we assign a smaller value to $k$, while keeping $n$ fixed, then $H_n$ will have at least one $2 \times 2$ diagonal block.

So far we have assumed that $n$ is odd. When $n$ is even, we have to omit one basis function in (2.16), either a monomial or a rational function. If we would like $\psi_n$ to be a monomial and that no two consecutive elementary basis functions, say, $\psi_j$ and $\psi_{j+1}$, are both rational nonpolynomial functions, then we must omit a rational function in (2.16). Therefore, when $n$ is even, we move the elementary rational function between the functions 1 and $x$ in (2.16) to be between the powers $x$ and $x^2$ and adjust the remaining elementary rational functions accordingly, i.e., we order the elementary basis functions according to

$$1, x, \frac{1}{x-\alpha_1}, x^2, \frac{1}{(x-\alpha_1)^2}, x^3, \dots.$$

The structure of the matrix (2.18) changes in that the first $3 \times 3$ diagonal block shrinks to a $2 \times 2$ diagonal block. The case when we omit the last function in (2.16) is discussed in Remark 3.15 below. $\square$

The following example is concerned with the structure of the matrix $H_n$ in (2.13) when in addition to the functions (2.16), we use elementary basis functions of the form (2.2).

*Example* 2.4. Let the finite poles $\alpha_1, \alpha_2, \dots, \alpha_{\ell+2\widehat{\ell}}$ be enumerated as described in the beginning of this section, and let the coefficients $\beta_i$ and $\gamma_i$ be defined as stated following (2.2). This can give the following sequence of $n$ elementary basis functions:

$$\begin{gathered} 1, \frac{1}{x-\alpha_1}, x, \frac{1}{(x-\alpha_1)^2}, x^2, \dots, \frac{1}{x-\alpha_\ell}, x^{k-k_\ell+1}, \dots, \frac{1}{(x-\alpha_\ell)^{k_\ell}}, x^k, \\ \frac{1}{x^2+\beta_1 x+\gamma_1}, \frac{x}{x^2+\beta_1 x+\gamma_1}, x^{k+1}, \dots, \frac{1}{(x^2+\beta_1 x+\gamma_1)^{s_1}}, \end{gathered}$$

$$\frac{x}{(x^2+\beta_1 x+\gamma_1)^{s_1}}, x^{k+s_1}, \frac{1}{x^2+\beta_2 x+\gamma_2}, \frac{x}{x^2+\beta_2 x+\gamma_2}, x^{k+s_1+1}, \ldots,$$
$$\frac{1}{(x^2+\beta_{\widehat{\ell}} x+\gamma_{\widehat{\ell}})^{s_{\widehat{\ell}}}}, \frac{x}{(x^2+\beta_{\widehat{\ell}} x+\gamma_{\widehat{\ell}})^{s_{\widehat{\ell}}}}, x^{k+s}, \tag{2.19}$$

where $k$ and $s$ are given by (2.3) and $n = 1 + 2k + 3s$. This basis together with $\psi_n(x) = x^{k+s+1}$ fulfill the demands of natural ordering.

The structure of the matrix $H_n \in \mathbb{R}^{n\times n}$ of recursion coefficients of the orthonormal rational functions associated with the elementary functions (2.19) differs from the structure of the matrix (2.18) in that the present matrix has $s$ trailing $4 \times 4$ diagonal blocks. This makes $H_n$ septadiagonal.

If we choose fewer or more positive powers of $x$ among the $n$ functions than in (2.19), then some diagonal blocks will become smaller or larger, similar to Example 2.3. We also remark that the requirement that the elementary basis functions $\psi_{n-1}$ and $\psi_n$ be monomials can be dispensed with. ☐

THEOREM 2.5. *Let the orthogonal rational functions $\phi_0, \phi_1, \ldots, \phi_n$ be determined by applying the Gram–Schmidt process to the naturally ordered elementary basis functions $\psi_0, \psi_1, \ldots, \psi_n$. If $\psi_j$ is a monomial or a rational function having a real pole outside the convex hull of the support of $d\mu$, then $\phi_j$ has $j$ zeros, which are simple and lie in the convex hull of the support of the measure $d\mu$.*

*Proof.* The result follows from properties of orthogonal polynomials. First assume that $\psi_j$ is a monomial. Then

$$\phi_j(x) = \frac{p_j(x)}{\rho(x)},$$

where $p_j \in \mathbb{P}_{j+1}$ and $\rho \in \mathbb{P}_q$, for some $q$ depending on the ordering of the elementary basis functions. The function $\phi_j$ is orthogonal to

$$\mathrm{span}\{\psi_0, \psi_1, \ldots, \psi_{j-1}\} = \mathbb{P}_j/\rho. \tag{2.20}$$

Therefore, the polynomial $p_j$ is orthogonal to $\mathbb{P}_j$ with respect to the inner product

$$[f, g] = \int_a^b f(x)g(x)\frac{d\mu(x)}{\rho^2(x)} \tag{2.21}$$

for a suitably restricted class of function. In particular, formula (2.21) defines an inner product on $\mathbb{P}_{j+1}$. The polynomial $p_j$ is the $j$th orthogonal polynomial in a family of orthogonal polynomials with respect to the inner product (2.21). It follows, e.g., from [9, Theorem 1.19] that all zeros of $p_j$ are simple and lie in the convex hull of $\mathrm{supp}(d\mu)$.

Let $\psi_j$ be a rational function having the real pole $\alpha$. Then

$$\phi_j(x) = \frac{p_j(x)}{(x-\alpha)\rho(x)}$$

for some (fixed) polynomial $\rho(x)$, and $\phi_j$ is orthogonal to the linear space (2.20). It follows that $p_j$ is orthogonal to $\mathbb{P}_j$ with respect to the inner product

$$[f, g] = \int_a^b f(x)g(x)\frac{d\mu(x)}{(x-\alpha)\rho^2(x)}.$$

Since $\alpha \notin \mathrm{supp}(d\mu)$ we conclude similarly as above that all zeros of $p_j$ are simple and live in the convex hull of $\mathrm{supp}(d\mu)$. ☐

We are in a position to discuss the relation between the matrix $H_n$ in (2.13) and the rational Gauss rule (2.5).

THEOREM 2.6. *Assuming that $\psi_{n-1}(x)$ and $\psi_n(x)$ are monomials, the eigenvalues of the matrix $H_n$ in (2.13) are the nodes $\widetilde{x}_j$ of the rational Gauss rule (2.5). The square of the first entry of the normalized eigenvector associated with the eigenvalue $\widetilde{x}_j$ is the weight $\widetilde{w}_j$.*

*Proof.* By Theorem 2.5, the function $\phi_n$ has $n$ distinct zeros $\theta_1 < \theta_2 < \cdots < \theta_n$ in the interval $[a, b]$. It follows from (2.13) that every zero $\theta_j$ of $\phi_n$ is an eigenvalue of $H_n$ and that $\boldsymbol{\phi}_n(\theta_j)$, defined by (2.12), is an associated eigenvector. Since the matrix $H_n$ is symmetric (cf. (2.17)), the eigenvectors $\{\boldsymbol{\phi}_n(\theta_1), \boldsymbol{\phi}_n(\theta_2), \ldots, \boldsymbol{\phi}_n(\theta_n)\}$ are orthogonal.

Let $c_j = 1/\|\boldsymbol{\phi}_n(\theta_j)\|$, where $\|\cdot\|$ denotes the Euclidean vector norm. Then the matrix $\Phi = [c_1\boldsymbol{\phi}_n(\theta_1), c_2\boldsymbol{\phi}_n(\theta_2), \ldots, c_n\boldsymbol{\phi}_n(\theta_n)]$ is orthogonal. Therefore $\Phi\Phi^T = I$. The entries of this matrix yield the equations

$$\sum_{i=1}^{n} c_i^2 \phi_j(\theta_i)\phi_k(\theta_i) = \begin{cases} 1, & j = k, \\ 0, & j \neq k, \end{cases} \tag{2.22}$$

for $0 \leq j, k < n$. Using the rational Gauss rule (2.5) yields

$$\langle \phi_j, \phi_k \rangle = \sum_{i=1}^{n} \phi_j(\widetilde{x}_i)\phi_k(\widetilde{x}_i)\widetilde{w}_i = \begin{cases} 1, & j = k, \\ 0, & j \neq k, \end{cases} \tag{2.23}$$

where the last equality follows from the orthonormality of the $\phi_j$. The nodes and weights of rational Gauss quadrature rules are unique. Therefore, comparing the sums (2.22) and (2.23) shows that $\theta_i = \widetilde{x}_i$ and $c_i^2 = \widetilde{w}_i$. Moreover, since $\psi_0(x) = 1$ and $\mu_0 = 1$, it follows that $\phi_0(x) = 1$. Therefore, the first component of the normalized eigenvector $c_i\boldsymbol{\phi}_n(\theta_i)$ is $c_i$. ☐

The Golub–Welsch algorithm [13] is an efficient scheme for determining the nodes and weights of standard $n$-point Gauss quadrature rules (1.2). This algorithm computes the eigenvalues and the first components of normalized eigenvectors of the tridiagonal matrix $T_n$ in (1.6), which is determined by the recursion relation of the orthonormal polynomials in the vector (1.5). It follows from Theorem 2.6 that the nodes and the weights of the rational Gauss rule (2.5) can be determined similarly, i.e., by computing the eigenvalues and first components of normalized eigenvectors of the matrix $H_n$ in (2.13).

*Remark* 2.7. The requirement in Theorem 2.6 that $\psi_{n-1}$ and $\psi_n$ be monomials is included in order for the remainder term to be of the form specified in (2.13). However, all entries of the matrix $H_n = [h_{ij}]$ can be expressed in terms of inner products involving the functions $\phi_0, \phi_1, \ldots, \phi_{n-1}$ and $x\phi_0, x\phi_1, \ldots, x\phi_{n-1}$. For instance, assume that for some $0 \leq j_1 \leq j \leq j_2 < n$ we have

$$x\phi_j(x) = h_{j,\ell_{j_1}}\phi_{\ell_{j_1}}(x) + h_{j,\ell_{j_1}+1}\phi_{\ell_{j_1+1}}(x) + \cdots + h_{j,\ell_{j_2}}\phi_{\ell_{j_2}}(x).$$

Then $h_{j,k} = \langle x\phi_j, \phi_k \rangle$ for $j_1 \leq k \leq j_2$. In particular, the entries of $H_n$ are independent of the function $\phi_n$ in the remainder term in (2.13). It follows that the elementary basis function $\psi_n$ does not have to be a monomial in order for the eigenvalues and square of the first components of normalized eigenvectors of the matrix $H_n$ to determine a rational Gauss quadrature rule (2.5). Remarks 3.12 and 3.13 in section 3 contain further comments on the role of the elementary basis function $\psi_n$ and discuss the requirement of Theorem 2.6 that the elementary function $\psi_{n-1}$ be a monomial. ☐

The following section is concerned with rational Gauss quadrature rules for the situation when the measure only has finitely many points of support. An analogue of Theorem 2.6 can then be shown using a different technique.

**3. Rational Gauss quadrature for a discrete measure.** This section discusses the approximation of expressions of the form (1.7) by a rational Gauss rule. Let the symmetric matrix $A \in \mathbb{R}^{N\times N}$ have the spectral factorization

$$A = U\Lambda U^T$$

with $U \in \mathbb{R}^{N\times N}$ orthogonal and $\Lambda = \mathrm{diag}[\lambda_1, \lambda_2, \ldots, \lambda_N] \in \mathbb{R}^{N\times N}$. Substituting this factorization into (1.7) yields

$$\mathbf{v}^T f(A)\mathbf{v} = \sum_{i=1}^{N} f(\lambda_i)\nu_i^2, \qquad [\nu_1, \nu_2, \ldots, \nu_N]^T := U^T\mathbf{v}.$$

For notational simplicity we will assume that $\|\mathbf{v}\| = 1$. Then $\mu_0 = 1$. The above sum can be written as a Stieltjes integral

$$\mathbf{v}^T f(A)\mathbf{v} = \int f(x)d\mu_N \tag{3.1}$$

determined by a piecewise constant distribution function $\mu_N(x)$ with jumps $\nu_i^2$ at the eigenvalues $\lambda_i$. We introduce the inner product and norm

$$\langle f, g\rangle := \int f(x)g(x)d\mu_N, \qquad \|f\| := \langle f, f\rangle^{1/2}, \tag{3.2}$$

for suitably restricted functions $f$ and $g$. This setting allows us to show properties of rational Gauss rules for the approximation of (3.1) by matrix methods. Our analysis extends the discussion in [15] on Laurent polynomials to rational functions with several distinct finite poles.

Let the elementary basis functions $\psi_0, \psi_1, \ldots, \psi_{n-1}$ for the space $\mathbb{S}_n$, defined by (2.4), be naturally ordered. For now, we also assume that $\psi_{n-1}$ and $\psi_n$ are monomials. This condition can be removed; see Remarks 3.12 and 3.13 below. The application of $n$ steps of the rational Lanczos process determined by these basis functions to the matrix $A$ with initial vector $\mathbf{v}$ yields an orthonormal basis $\{\phi_j(A)\mathbf{v}\}_{j=0}^{n-1}$ of rational functions $\phi_j$ in $A$ with respect to the inner product (3.2) for the rational Krylov subspace

$$\mathbb{K}_n(A, \mathbf{v}) = \mathrm{span}\{\psi_0(A)\mathbf{v}, \psi_1(A)\mathbf{v}, \ldots, \psi_{n-1}(A)\mathbf{v}\}; \tag{3.3}$$

see, e.g., [1, 6, 20] for discussions on the rational Lanczos process. This defines the matrix

$$V = [\phi_0(A)\mathbf{v}, \phi_1(A)\mathbf{v}, \ldots, \phi_{n-1}(A)\mathbf{v}] \in \mathbb{R}^{N\times n} \tag{3.4}$$

with orthonormal columns. In particular, $V\mathbf{e}_1 = \mathbf{v}$. The rational Lanczos process can be implemented with short recursion relations, analogously to the Stieltjes-type procedure (Algorithm 3.1) of [19]. We will not discuss the implementation details here, since this paper is concerned with quadrature rules. We now state the main result of this section.

THEOREM 3.1. *Let the elementary basis functions $\psi_0, \psi_1, \ldots, \psi_{n-1}$ for the space $\mathbb{S}_n$, defined by* (2.4)*, be naturally ordered, and assume that the functions $\psi_{n-1}$ and*

*$\psi_n$ are monomials. Let the matrix $V$ be given by* (3.4) *and introduce the projection of $A$ onto the rational Krylov subspace* (3.3)*:*

$$H = V^T AV. \tag{3.5}$$

*Then*

$$\mathbf{v}^T f(A)\mathbf{v} = \mathbf{e}_1^T f(H)\mathbf{e}_1 \qquad \forall f \in \mathbb{S}_{2n}, \tag{3.6}$$

*where $\mathbb{S}_{2n}$ is defined by* (2.7)*. Thus, the right-hand side is a rational Gauss quadrature rule for the approximation of the expression* (1.7)*.*

By substituting the spectral factorization of the matrix $H$ into the right-hand side of (3.6), we see that the latter can be written in the form (2.5). We will show Theorem 3.1 by using the structure of $H$ and of the projections

$$\begin{array}{rclr} G_i & = & V^T (A - \alpha_i I)^{-1} V, & i = 1, 2, \ldots, \ell, \\ M_j & = & V^T (A^2 + \beta_j A + \gamma_j I)^{-1} V, & j = 1, 2, \ldots, \widehat{\ell}. \end{array} \tag{3.7}$$

of the matrices $(A - \alpha_i I)^{-1}$ and $(A^2 + \beta_j A + \gamma_j I)^{-1}$ onto the subspace (3.3). The matrix (3.5) is analogous to the matrix $H_n$ in (2.13). To simplify notation, we do not use a subscript to indicate matrix size in this section.

We exploit the structure of the matrices $G_i$, $M_j$, and $H$ in a sequence of lemmas, which are used to establish Theorem 3.1. The following result, shown in [19], gives some insight into the structure of the matrices $G_i$.

Theorem 3.2. *Let the basis $\Psi_{n+1} = \{\psi_0, \psi_1, \ldots, \psi_n\}$ satisfy conditions* 1, 2, *and* 3 *of natural ordering and let $\alpha_i$ be a real pole of this basis. Assume that every sequence of $m_1$ consecutive basis functions $\psi_j, \psi_{j+1}, \ldots, \psi_{j+m_1-1}$ contains at least one power $(x - \alpha_i)^{-t}$, $t \geq 1$, and that between every pair of basis functions*

$$\left\{ \frac{1}{(x^2 + \beta_q x + \gamma_q)^j}, \frac{x}{(x^2 + \beta_q x + \gamma_q)^j} \right\}, \qquad j = 1, 2, 3, \ldots, \quad q = 1, 2, 3, \ldots,$$

*there are at most $m_2$ functions. Then the basis of orthonormal rational functions $\phi_0, \phi_1, \ldots, \phi_n$ with prescribed poles satisfies a $(2m+1)$-term recurrence relation of the form*

$$\frac{1}{x - \alpha_i} \phi_t(x) = \sum_{j=-m}^{m} g_{t,t+j}^{(i)} \phi_{t+j}(x), \qquad t = 0, 1, 2, \ldots, \tag{3.8}$$

*with $m = \max\{m_1, m_2 + 1\}$. Coefficients $g_{t,t+j}^{(i)}$ and functions $\phi_{t+j}$ with negative index $t + j$ are defined to be zero. The parameter $t$ has to be small enough for all required terms in the sum* (3.8) *to exist.*

The recurrences relation (3.8) can be simplified by including the fourth condition of natural ordering and by allowing the parameter $m$ to depend on $t$. We have

$$\frac{1}{x - \alpha_i} \phi_t(x) = \sum_{j=-m_3}^{m_4} g_{t,t+j}^{(i)} \phi_{t+j}(x), \qquad t = 0, 1, 2, \ldots, \tag{3.9}$$

where $m_3 = m_3(t)$, $t - m_3$ is the largest integer smaller than $t$ such that $\psi_{t-m_3}$ is a rational function with a pole at $\alpha_i$, $m_4 = m_4(t)$, and $t + m_4$ is the smallest integer larger than $t$ such that $\psi_{t+m_4}$ is a rational function with a pole at $\alpha_i$. This endows the matrix $G_i = [g_{i,j}^{(i)}]_{i,j=0}^{n-1}$ with the following block-diagonal structure: $G_i$ has $k_i + 1$ square blocks along the diagonal. Two consecutive blocks overlap in one entry. The $j$th block , for $j = 1, \ldots, k_i$,is of dimension $t \times t$, where $t-2$ is the number of elementary basis functions between $(x - \alpha_i)^{-(j-1)}$ and $(x - \alpha_i)^{-j}$. Precisely, the $j$th block of $G_i$ is $G_i(t_1 : t_2, t_1 : t_2)$, where $\psi_{t_1}(x) = (x - \alpha_i)^{-(j-1)}$ and $\psi_{t_2}(x) = (x - \alpha_i)^{-j}$. Also, $t = t_2 - t_1 + 1$.

The relation (3.9) assumes that $t$ is small enough so that $t + m_4 \leq n$. Conversely, if we would like to let $t + m_4 > n$, then we have to choose $n + m_4$ elementary basis functions $\psi_0, \psi_1, \ldots, \psi_{n+m_4}$ that satisfy requirements 1–3 of natural ordering. The following example illustrates the structure of the matrix $G_i$.

*Example* 3.3. Consider the elementary basis functions ordered as (2.19). Introduce the indices

$$z_1 = 2, \qquad z_j = 2(k_1 + \cdots + k_{j-1}) + 2, \qquad j = 2, 3, \ldots, \ell,$$

and

$$v_j = 2 + 2(k_{j+1} + k_{j+2} + \cdots + k_\ell) + 3s, \quad j = 1, 2, \ldots, \ell - 1; \quad v_\ell = 2 + 3s, \tag{3.10}$$

where $s$ is defined by (2.3). Then the matrix $G_i \in \mathbb{R}^{n \times n}$ has the following structure: $G_i$ has $k_i + 1$ square blocks along the diagonal. Adjacent blocks overlap; they share one diagonal entry. The first block is of size $z_i \times z_i$, the following $k_i - 1$ blocks are of size $3 \times 3$, and the last block is of size $v_i \times v_i$. □

We turn to the last kind of recursion relations required. The following result is shown in [19].

THEOREM 3.4. *Let the basis $\Psi_{n+1} = \{\psi_0, \psi_1, \ldots, \psi_n\}$ satisfy requirements* 1*,* 2*, and* 3 *of natural ordering, and assume that every sequence of $m$ consecutive basis functions $\psi_j, \psi_{j+1}, \ldots, \psi_{j+m-1}$ contains at least one function $(x^2 + \beta_j x + \gamma_j)^{-t}$ for some integer $t \geq 1$. Then the orthonormal rational functions $\phi_0, \phi_1, \ldots, \phi_n$ with prescribed poles satisfy a $(4m-3)$-term recurrence relation of the form*

$$\frac{1}{x^2 + \beta_j x + \gamma_j}\,\phi_t(x) = \sum_{i=-2m+2}^{2m-2} c_{t,t+i}^{(j)} \phi_{t+i}(x), \qquad t = 0, 1, 2, \ldots. \tag{3.11}$$

*Coefficients $c_{t,t+i}^{(j)}$ and functions $\phi_{t+i}$ with negative index $t+i$ are defined to be zero. The parameter $t$ has to be small enough for all required terms in the sum* (3.8) *to exist.*

The recurrences (3.11) can be simplified by including the fourth condition of natural ordering and by allowing the number of terms in the sum to depend on $t$ as follows:

$$\frac{1}{x^2 + \beta_j x + \gamma_j}\,\phi_t(x) = \sum_{i=-m_1}^{m_2} c_{t,t+i}^{(j)} \phi_{t+i}(x), \qquad t = 0, 1, 2, \ldots, \tag{3.12}$$

where $t - m_1$ is the largest integer smaller than $t$ such that

$\psi_{t-m_1}(x) = (x^2 + \beta_j x + \gamma_j)^{-s}$ if $\psi_t$ is not of the form $x(x^2 + \beta_j x + \gamma_j)^{-\tilde{s}}$ and
$\psi_{t-m_1}(x) = x(x^2 + \beta_j x + \gamma_j)^{-s}$ if $\psi_t$ is of the form $x(x^2 + p_j x + q_j)^{-\tilde{s}}$,

and $t + m_2$ is the smallest integer larger than $t$ such that

$\psi_{t+m_2}(x) = x(x^2 + \beta_j x + \gamma_j)^{-s}$ if $\psi_t$ is not of the form $(x^2 + \beta_j x + \gamma_j)^{-\tilde{s}}$ and
$\psi_{t+m_2}(x) = (x^2 + \beta_j x + \gamma_j)^{-s}$ if $\psi_t$ is of the form $(x^2 + \beta_j x + \gamma_j)^{-\tilde{s}}$.

The recursion relation (3.12) gives the matrix $M_j = [c_{i,t}^{(j)}]_{i,t=0}^{n-1}$ the following block-diagonal structure: $M_j$ has $s_j + 1$ square blocks along the diagonal. Two consecutive blocks overlap in a $2 \times 2$ block. The $i$th block, for $i = 1, \ldots, s_j$, is of size $t \times t$, where $t - 2$ is the number of elementary basis functions between $(x^2 + \beta_j x + \gamma_j)^{-(i-1)}$ and $x(x^2 + \beta_j x + \gamma_j)^{-i}$. Specifically, the $i$th block of $M_j$ is $M_j(t_1 : t_2, t_1 : t_2)$, where $\psi_{t_1}(x) = (x^2 + \beta_j x + \gamma_j)^{-(i-1)}$ and $\psi_{t_2}(x) = x(x^2 + \beta_j x + \gamma_j)^{-i}$. Moreover, $M_j(t_2, t_1) = M_j(t_1, t_2) = 0$. The following example shows the structure of a particular matrix $M_j$.

Formula (3.12) assumes that $t$ is small enough so that $t + m_2 \le n$. Therefore, if we would like to let $t = n - 1$, then we have to choose $n + m_2$ elementary basis functions $\psi_0, \psi_1, \ldots, \psi_{n+m_2}$ that satisfy requirements 1–3 of natural ordering.

*Example* 3.5. Analogously as in Example 3.3, we conclude that when the elementary basis functions are ordered according to (2.19), the matrices $M_j$ have a similar block-diagonal structure as the matrices $H$ and $G_i$, with one exception: Consecutive blocks overlap in a $2 \times 2$ block instead of having only one common entry. The matrices $M_j$ have $s_j + 1$ blocks. The first block is of size $\tilde{z}_i \times \tilde{z}_i$, the following $s_j - 1$ blocks are $5 \times 5$ blocks with zeros in the $(5, 1)$ and $(1, 5)$ entries, and the last block is of size $\tilde{v}_i \times \tilde{v}_i$:

$$M_j = \left[\begin{array}{ccccccccccccc}
\ddots & * & * & & & & & & & & & & \\
* & * & * & * & * & 0 & & & & & & & \\
0 & * & * & * & * & * & & & & & & & \\
 & * & * & * & * & * & & & & & & & \\
 & * & * & * & * & * & * & * & 0 & & & & \\
 & 0 & * & * & * & * & * & * & * & & & & \\
 & & & & * & * & * & * & * & & & & \\
 & & & & * & * & * & * & * & * & * & 0 & \\
 & & & & 0 & * & * & * & * & * & * & * & \\
 & & & & & & & * & * & * & * & * & \\
 & & & & & & & * & * & * & * & * & * \\
 & & & & & & & 0 & * & * & * & * & * \\
 & & & & & & & & & & * & * & \ddots
\end{array}\right].$$

The values of $\tilde{z}_i$ and $\tilde{v}_i$ are

$$\tilde{z}_1 = 2k + 3, \quad \tilde{z}_j = 2k + 3(s_1 + \cdots + s_{j-1}) + 3, \; j = 2, \ldots, \widehat{\ell},$$

$$\tilde{v}_j = 3(s_{j+1} + s_{j+2} + \cdots + s_{\widehat{\ell}}) + 3, \; j = 1, \ldots, \widehat{\ell} - 1, \quad \tilde{v}_{\widehat{\ell}} = 3. \tag{3.13}$$

□

The recurrence formulas (2.15), (3.9), and (3.12), in order, together with (3.4), give the matrix relations

$$AV = VH + \mathbf{g}\mathbf{e}_n^T, \quad V^T\mathbf{g} = \mathbf{0}, \tag{3.14}$$

$$(A - \alpha_i I)^{-1}V = VG_i + \sum_{k=1}^{v_i} \mathbf{g}_k^{(i)}\, \mathbf{e}_{n+1-k}^T, \quad V^T\mathbf{g}_k^{(i)} = \mathbf{0}, \tag{3.15}$$

$$(A^2 + \beta_j A + \gamma_j I)^{-1}V = VM_j + \sum_{k=1}^{\tilde{v}_j} \tilde{\mathbf{g}}_k^{(j)}\, \mathbf{e}_{n+1-k}^T, \quad V^T\tilde{\mathbf{g}}_k^{(j)} = \mathbf{0}, \tag{3.16}$$

for certain vectors $\mathbf{g}$, $\mathbf{g}_k^{(i)}$, and $\tilde{\mathbf{g}}_k^{(j)}$. These vectors depend on the ordering of elementary basis functions $\psi_n, \psi_{n+1}, \ldots$ that follow those that define the rational Krylov subspace (3.3). However, the explicit form of the vectors $\mathbf{g}$, $\mathbf{g}_k^{(i)}$, and $\tilde{\mathbf{g}}_k^{(j)}$ is not important in what follows; only the fact that they are orthogonal to the columns of the matrix $V$ is essential. Therefore, the choice of elementary basis functions $\psi_n, \psi_{n+1}, \ldots$ is not important for the development in this section.

We use the structure of the matrices $H$, $G_i$, and $M_j$ to show the following lemmas, which are used to establish (3.6). Recall that the matrix $H$ has $r = n - k - 2s - 1$ square partly overlapping blocks along the diagonal, the matrices $G_i$, $i = 1, 2, \ldots, \ell$, have $k_i + 1$ square partly overlapping blocks along the diagonal, and the matrices $M_j$, $j = 1, 2, \ldots, \widehat{\ell}$, have $s_j + 1$ square partly overlapping blocks along the diagonal. In other words, the number of blocks is equal to the multiplicity of the corresponding pole plus one, with one exemption: the number of blocks in $H$ equals the multiplicity of the pole at $\infty$ (the power of the last monomial in $\Psi_n$). We denote the size of the last block of $G_i$ ($M_j$) by $v_i$ ($\tilde{v}_j$).

Lemma 3.6. *The last $v_i - 1$ ($\tilde{v}_j - 1$) entries of the first column of the matrix $G_i^{k_i}$ ($M_j^{s_j}$) are zero, and at least the $v_i$ ($\tilde{v}_j$) last entries of the first column of $G_i^{k_i-1}$ ($M_j^{s_j-1}$) vanish. The last entry of the first column of $H^{r-1}$ is zero.*

*Proof.* The result can be shown by using the structure of the matrices $G_i$, $M_j$, and $H$. ∎

The following three lemmas can be proved in the same way. We therefore show only Lemma 3.8 below. In the proofs of the lemmas, we need the largest possible powers of $H$, $G_i$, and $M_j$, whose first column has $w$ vanishing entries at the bottom, where $w$ must not be less than the number of columns affected by the remainder term. For the matrices $G_i$ and $M_j$ the desired power is two less than the number of blocks, and for the matrix $H$ the desired power is one less than the number of blocks. This compensates the fact that the number of blocks in $H$ equals the multiplicity of the pole at $\infty$.

Lemma 3.7. *There holds*

$$\mathbf{v}^T A^k \mathbf{v} = \mathbf{e}_1^T H^k \mathbf{e}_1\,, \quad k = 0, 1, \ldots, 2r + 1.$$

Lemma 3.8. *There holds*

$$\mathbf{v}^T (A - \alpha_i I)^{-k} \mathbf{v} = \mathbf{e}_1^T G_i^k \mathbf{e}_1\,, \quad k = 0, 1, \ldots, 2k_i + 1. \tag{3.17}$$

*Proof.* We first show that

$$(A - \alpha_i I)^{-k} \mathbf{v} = V G_i^k \mathbf{e}_1, \quad k = 0, 1, \ldots, k_i. \tag{3.18}$$

The assertion obviously holds for $k = 0$. For $k = 1, \ldots, k_i - 1$, using Lemma 3.6 and (3.15), we obtain

$$\begin{aligned}
(A - \alpha_i I)^{-k-1} \mathbf{v} &= (A - \alpha_i I)^{-1} (A - \alpha_i I)^{-k} \mathbf{v} \\
&= (A - \alpha_i I)^{-1} (V G_i^k \mathbf{e}_1) \\
&= \left( V G_i + \sum_{j=1}^{v_i} \mathbf{g}_j^{(i)}\, \mathbf{e}_{n+1-j}^T \right) G_i^k \mathbf{e}_1 \\
&= V G_i^{k+1} \mathbf{e}_1 + \sum_{j=1}^{v_i} \mathbf{g}_j^{(i)}\, \mathbf{e}_{n+1-j}^T G_i^k \mathbf{e}_1 \\
&= V G_i^{k+1} \mathbf{e}_1.
\end{aligned}$$

Note that (3.18) might not hold for $k = k_i + 1$ since $\mathbf{e}_{n+1-s_i}^T G_i^{k_i} \mathbf{e}_1$ may be nonzero.

Finally,

$$
\begin{aligned}
&\mathbf{v}^T(A-\alpha_i I)^{-k_i}(A-\alpha_i I)^{-k_i-1}\mathbf{v}\\
&=\mathbf{e}_1^T G_i^{k_i} V^T\Big(VG_i^{k_i+1}\mathbf{e}_1+\sum_{j=1}^{v_i}\mathbf{g}_j^{(i)}\,\mathbf{e}_{n+1-j}^T G_i^{k_i}\mathbf{e}_1\Big)\\
&=\mathbf{e}_1^T G_i^{2k_i+1}\mathbf{e}_1. \qquad \square
\end{aligned}
$$

Lemma 3.8 shows more than we need in what follows. For the purpose of this paper, it suffices that $k$ goes from 0 to $2k_i$ in (3.17). This will be clear after Lemma 3.10.

LEMMA 3.9. *There holds*

$$
\mathbf{v}^T(A^2+\beta_j A+q_j I)^{-k}\mathbf{v}=\mathbf{e}_1^T M_j^k\mathbf{e}_1, \quad k=0,1,\ldots,2s_j,
$$

*and*

$$
\mathbf{v}^T(A^2+\beta_j A+q_j I)^{-k}A(A^2+\beta_j A+q_j I)^{-i}\mathbf{v}=\mathbf{e}_1^T M_j^k H M_j^i\mathbf{e}_1
$$

*for* $k,i=0,1,\ldots,s_j$.

In order to show (3.6) two additional results are required.

LEMMA 3.10. *We have*

$$
\mathbf{e}_1^T(H-\alpha_i I)^{-k}\mathbf{e}_1=\mathbf{e}_1^T G_i^k\mathbf{e}_1, \quad k=0,1,\ldots,2k_i. \tag{3.19}
$$

*Proof.* We first show that

$$
(H-\alpha_i I)G_i=I+\mathbf{e}_n\mathbf{r}^T, \tag{3.20}
$$

where only the last $v_i$ elements of the vector $\mathbf{r}$ may be nonvanishing. When we transpose both the right-hand side and the left-hand side of (3.14) and add $-\alpha_i V^T$ to both sides, we get

$$
V^T(A-\alpha_i I)=(H-\alpha_i I)V^T+\mathbf{e}_n\mathbf{g}^T. \tag{3.21}
$$

From (3.15) and (3.21), we obtain

$$
I=(H-\alpha_i I)G_i+\mathbf{e}_n\mathbf{g}^T\left(\sum_{k=1}^{v_i}\mathbf{g}_k^{(i)}\,\mathbf{e}_{n+1-k}^T\right),
$$

which is equivalent to (3.20).

Further we prove that

$$
(H-\alpha_i I)^k G_i^k\mathbf{e}_1=\mathbf{e}_1, \quad k=0,1,\ldots,k_i. \tag{3.22}
$$

The equality (3.22) is trivial for $k=0$. For $k=1,2,\ldots,k_i$, using (3.20) and Lemma 3.6, we obtain

$$
\begin{aligned}
(H-\alpha_i I)^k G_i^k\mathbf{e}_1&=(H-\alpha_i I)^{k-1}[(H-\alpha_i I)G_i]G_i^{k-1}\mathbf{e}_1\\
&=(H-\alpha_i I)^{k-1}[I+\mathbf{e}_n\mathbf{r}^T]G_i^{k-1}\mathbf{e}_1\\
&=(H-\alpha_i I)^{k-1}G_i^{k-1}\mathbf{e}_1+(H-\alpha_i I)^{k-1}\mathbf{e}_n\mathbf{r}^T G_i^{k-1}\mathbf{e}_1\\
&=\mathbf{e}_1.
\end{aligned}
$$

Formula (3.22) does not hold for $k=k_i+1$, since $\mathbf{r}^T G_i^{k_i}\mathbf{e}_1$ may be nonvanishing.

We can write (3.22) in the form

$$G_i^k \mathbf{e}_1 = (H - \alpha_i I)^{-k} \mathbf{e}_1, \quad k = 0, 1, \ldots, k_i, \tag{3.23}$$

or, after transposition of both the left-hand and right-hand sides,

$$\mathbf{e}_1^T G_i^k = \mathbf{e}_1^T (H - \alpha_i I)^{-k}, \quad k = 0, 1, \ldots, k_i. \tag{3.24}$$

The equality (3.19) now follows from (3.23) and (3.24). ∎

Lemma 3.11. *There holds*

$$\mathbf{e}_1^T (H^2 + \beta_j H + \gamma_j I)^{-k} \mathbf{e}_1 = \mathbf{e}_1^T M_j^k \mathbf{e}_1\,, \quad k = 0, 1, \ldots, 2s_j,$$

*and for* $k, i = 0, 1, \ldots, s_j$,

$$\mathbf{e}_1^T (H^2 + \beta_j H + \gamma_j I)^{-k} H (H^2 + \beta_j H + \gamma_j I)^{-i} \mathbf{e}_1 = \mathbf{e}_1^T M_j^k H M_j^i \mathbf{e}_1.$$

*Proof.* The formula

$$(H^2 + \beta_j H + \gamma_j I) M_j = I + \sum_{k=1}^{\tilde{v}_j} \mathbf{e}_{n+1-k} \mathbf{r}_{(k)}^T$$

is analogous to (3.20). Only the last $\tilde{v}_j$ entries of $\mathbf{r}_{(k)}$ may be nonvanishing. The formulas

$$M_j^k \mathbf{e}_1 = (H^2 + \beta_j H + \gamma_j I)^{-k} \mathbf{e}_1, \quad k = 0, 1, \ldots, s_j, \tag{3.25}$$

and

$$\mathbf{e}_1^T M_j^k = \mathbf{e}_1^T (H^2 + \beta_j H + \gamma_j I)^{-k}, \quad k = 0, 1, \ldots, s_j, \tag{3.26}$$

are analogues of (3.23) and (3.24). The lemma follows from (3.25) and (3.26). ∎

Theorem 3.1 now can be established by combining Lemmas 3.7–3.11. Recall that $p(A)(A - cI)^{-1} = (A - cI)^{-1} p(A)$, where $p$ is a polynomial and $c$ is a scalar.

*Remark* 3.12. In addition to the set $\Psi_n$ being naturally ordered, we assumed in Theorems 2.6 and 3.1 that the functions $\psi_{n-1}$ and $\psi_n$ are monomials. We commented in Remark 2.7 that Theorem 2.6 holds independently of the choice of the elementary basis function $\psi_n$. A similar argument can be applied to Theorem 3.1. In detail, we note that the matrices $H$ in (3.5), as well as $G_i$ and $M_j$ in (3.7), are completely determined by the functions $\phi_0, \phi_1, \ldots, \phi_{n-1}$. They are formed from coefficients of recursion relations that express

$$x\phi_j(x), \quad \frac{1}{x - \alpha_i}\phi_j(x), \quad \text{or} \quad \frac{1}{x^2 + \beta_i x + \gamma_i}\phi_j(x), \quad j = 0, \ldots, n-1,$$

in terms of the functions $\phi_0, \phi_1, \ldots, \phi_{n-1}$. These recursion relations also involve certain orthonormal rational functions $\phi_k$ for $k \geq n$, which depend on some elementary functions $\psi_n, \psi_{n+1}, \psi_{n+2}, \ldots$. For instance, when both $\psi_{n-1}$ and $\psi_n$ are monomials, the remainder in (2.13) and (3.14) depends only on $\phi_n$. If $\psi_n$ is not a monomial, then the remainder depends on several functions $\phi_n, \phi_{n+1}, \ldots, \phi_{n+t}$. Precisely, the remainder depends linearly on the functions $\phi_n, \phi_{n+1}, \ldots, \phi_{n+t}$, where $\psi_{n+t}$ is the first monomial in the sequence $\psi_n, \psi_{n+1}, \ldots$. An analogous result holds for the remainder in (3.15) when we let $\psi_n$ be a power of $1/(x - \alpha_i)$ instead of a monomial. The discussion on the remainder term in (3.16) is only slightly more complicated. We illustrate this with the vectors $\mathbf{g}$, $\mathbf{g}_k^{(i)}$, $\tilde{\mathbf{g}}_k^{(j)}$ and the scalars $v_i$ and $\tilde{v}_j$ from (3.14), (3.15), and (3.16):

- The vector $\mathbf{g}$ is of the form $c\phi_n(A)\mathbf{v}$.
- The vectors $\mathbf{g}_k^{(i)}$, $k = 1, \ldots, v_i$, are of the form $(c_0\phi_n(A) + c_1\phi_{n+1}(A) + \cdots + c_t\phi_{n+t}(A))\mathbf{v}$, where $\psi_{n+t}$ is the first function which is a power of $1/(x - \alpha_i)$ among the functions $\psi_n, \psi_{n+1}, \ldots$. The scalar $v_i$ is such that $\psi_{n-v_i}$ is the last function among $\psi_0, \psi_1, \ldots, \psi_{n-1}$, which is a power of $1/(x - \alpha_i)$.
- The vectors $\tilde{\mathbf{g}}_k^{(j)}$, $k = 1, \ldots, \tilde{v}_j$, are of the form $(c_0\phi_n(A) + c_1\phi_{n+1}(A) + \cdots + c_t\phi_{n+t}(A))\mathbf{v}$, where $\psi_{n+t}$ is the first function of the form $x/(x^2 + \beta_j x + \gamma_j)^r$ among the functions $\psi_n, \psi_{n+1}, \ldots$. The scalar $\tilde{v}_j$ is such that $\psi_{n-\tilde{v}_j}$ is the last function among $\psi_0, \psi_1, \ldots, \psi_{n-1}$, which is of the form $1/(x^2 + \beta_j x + \gamma_j)^r$. □

*Remark* 3.13. We saw in Remark 3.12 how the ordering of $\phi_n, \phi_{n+1}, \ldots$ influences the remainder terms in (3.14), (3.15), and (3.16). Now we explain the effect of the ordering of $\phi_0, \ldots, \phi_{n-1}$. The remainder term is applied either to all last columns ending with a nonvanishing entry (in all relations except one) or only to the last column[1] (in the relation in which the pole(s) imposed by $\psi_{n-1}$ coincide(s) with the pole(s) of the function (of $A$) multiplying $V$ on the left-hand side in (3.14), (3.15), or (3.16)). The number of blocks in the matrices $G_i$, $M_j$, and $H$ is $q+1$ or $q$, where $q$ is the multiplicity of the corresponding pole. The number of blocks is $q$ in only one case: in the matrix from the relation in which the remainder term applies only to the last column (or to the last two columns for corresponding $M_j$). However, this lack of blocks is compensated for by the fact that the remainder term is not applied to all last columns ending with nonvanishing entry (see the discussion after Lemma 3.6.). It is not difficult to see that the elementary function $\psi_{n-1}$ does not have to be a monomial in order for Theorem 3.1 to hold. □

Rational Gauss rules that are exact for functions in $S_{2n}$ have $n$ distinct nodes. This follows from the analogous property that standard Gauss rules that are exact for all functions in $\mathbb{P}_{2n}$ have $n$ distinct nodes. This observation and the above discussion can be summarized as follows.

COROLLARY 3.14. *Assume that the elementary basis functions $\{\psi_0, \psi_1, \ldots, \psi_{n-1}\}$ are naturally ordered. Then the matrix $H$ in* (3.5) *has $n$ distinct eigenvalues for any choices of elementary basis functions $\psi_{n-1}$ and $\psi_n$. Here we assume that the distribution function $\mu_N$ in* (3.1) *has at least $n$ points of increase. Similarly, the matrix $H_n$ in* (2.13) *has $n$ distinct eigenvalues for any choice of elementary basis functions $\psi_{n-1}$ and $\psi_n$.*

*Remark* 3.15. Deckers and Bultheel [3, 4] describe an approach for determining orthonormal rational functions and associated rational Gauss quadrature rules different from that of the present paper. They show that the orthonormal rational functions satisfy a three-term recursion relation in which the "coefficients" are linear fractional transformations. The nodes and weights of the associated rational Gauss quadrature rules are determined by solving a generalized eigenvalue problem with tridiagonal matrices. Deckers and Bultheel [4] do not require the poles to appear in complex conjugate pairs or the integrand to be real-valued. The present paper focuses on the integration of real-valued functions on a real interval. When the poles are real or appear in complex conjugate pairs, the Gauss quadrature rule can be determined by solving a (standard) eigenvalue problem for a real symmetric matrix with small bandwidth. Our space $\mathbb{S}_{2n}$ is a special case of the space $\mathcal{R}_{n,n-1}$ when $\alpha_n = \infty$ (with the notation from [4]). In other words, we have shown that the solution of the

[1]When we are dealing with matrices $M_j$, the remainder term is applied to the last two columns.

generalized eigenvalue problem (6) in [4] can be replaced by the solution of a (standard) real symmetric eigenvalue problem when $\alpha_n = \infty$ and the poles in $\mathbb{C}\backslash\mathbb{R}$ among the set $\{\alpha_j\}_{j=1}^{n-1}$ appear in complex conjugate pairs.

We note that when the inner product is defined in terms of a discrete measure determined by a large matrix $A$ and a vector $\mathbf{v}$ (cf. (3.1)), the computation of an additional rational function with a new real pole $\alpha$ requires the solution of a linear system of equations with the matrix $A - \alpha I$ when the approach of section 3 is used. Application of the recursion formulas in [3, 4] requires the solution of two linear system of equations with the matrix $A - \alpha I$. ▯

**4. A numerical example.** Let $d\mu(x) = dx$, $a = 0.3$, and $b = 1$ in (1.1). Then we obtain the inner product

$$\langle f, g\rangle := \int_{0.3}^{1} f(x)g(x)dx;$$

cf. (1.4). Consider the elementary basis

$$1, x, \frac{1}{x-1.2}, x^2, \frac{1}{(x-1.2)^2}, x^3, \frac{1}{x}, x^4, \frac{1}{x^2}$$

and generate an associated sequence of orthonormal rational functions $\phi_0, \phi_1, \ldots, \phi_8$ and the matrix $H_9 \in \mathbb{R}^{9\times 9}$ containing recursion coefficients for the $\phi_i$'s as described in [19]. The nodes of the nine-point rational Gauss quadrature rule $\widetilde{\mathcal{G}}_9$ for the approximation of the integral (1.1) are the eigenvalues of the matrix $H_9$ (cf. Example 2.3), which is given by

$$\begin{bmatrix} 0.650 & 0.202 & & & & & & & \\ 0.202 & 0.650 & -0.164 & 0.066 & & & & & \\ & -0.168 & 0.779 & 0.165 & & & & & \\ & 0.066 & 0.165 & 0.648 & -0.164 & 0.064 & & & \\ & & & -0.164 & 0.776 & 0.164 & & & \\ & & & 0.064 & 0.164 & 0.649 & 0.168 & 0.051 & \\ & & & & & 0.168 & 0.547 & 0.168 & \\ & & & & & 0.051 & 0.168 & 0.650 & -0.168 \\ & & & & & & & -0.168 & 0.547 \end{bmatrix}.$$

The quadrature rule $\widetilde{\mathcal{G}}_9$ is exact for all functions in the space

$$\mathbb{S}_{18} := \mathbb{P}_{10} \oplus \mathbb{Q}_{1,4} \oplus \mathbb{Q}_{2,4}$$

with $\alpha_1 = 1.2$ and $\alpha_2 = 0$ in (2.1). The weights and nodes of $\widetilde{\mathcal{G}}_9$ are displayed in Table 1.

We first apply $\widetilde{\mathcal{G}}_9$ to approximate the integral (1.1) with the integrand

$$f(x) = \frac{2x - 1.2}{(1.2x - x^2)\ln^2(1.2x - x^2)}.$$

This yields a quadrature error of magnitude $1.7729 \cdot 10^{-9}$. When we instead integrate the function

$$f(x) = \frac{e^x(x - 2.2)}{(x - 1.2)^2},$$

Table 1
*Weights and nodes of the rational Gauss rule $\widetilde{\mathcal{G}}_9$.*

| $j$ | $\widetilde{w}_j$ | $\widetilde{x}_j$ |
|---|---|---|
| 1 | 0.0256 | 0.3099 |
| 2 | 0.0602 | 0.3528 |
| 3 | 0.0932 | 0.4298 |
| 4 | 0.1177 | 0.5364 |
| 5 | 0.1257 | 0.6597 |
| 6 | 0.1140 | 0.7812 |
| 7 | 0.0871 | 0.8826 |
| 8 | 0.0541 | 0.9533 |
| 9 | 0.0224 | 0.9913 |

we obtain an approximation of (1.1) with an error of magnitude $1.2434 \cdot 10^{-14}$.

We remark that leading principal submatrices $H_i \in \mathbb{R}^{i\times i}$ of $H_9$ can be used to construct $i$-point rational Gauss quadrature rules $\widetilde{\mathcal{G}}_i$. When $i \geq 3$ is odd, the nodes of $\widetilde{\mathcal{G}}_i$ are the zeros of $\phi_i(x)$. The same would hold for even values of $i$ if we replace the function $\psi_i$ by a suitable monomial.

The fact that rational Gauss quadrature rules can give much more accurate approximations of an integral than standard Gauss rules with the same number of nodes has been well demonstrated in the literature; see, e.g., [7, 9, 15, 18]. We therefore omit numerical illustrations of the benefits of rational Gauss quadrature over standard Gauss quadrature.

## 5. Conclusion.

It is well known that the nodes and weights of a (standard) Gauss quadrature rule are the eigenvalues and squares of the first components of the associated eigenvectors of the symmetric tridiagonal matrix defined by the recursion relations for the orthonormal polynomials connected with the Gauss rule. This paper shows, in section 2, an analogous result for rational Gauss quadrature rules defined by (2.5)–(2.7). When the measure has discrete support, a situation that arises when evaluating inner products involving matrix functions, we show the existence of a rational Gauss quadrature rule with linear algebra techniques by exploiting the structure of matrices determined by the recursion relations. This results extends the discussions by Golub and Meurant [11, 12] and that in [15] to rational Gauss rules determined by several distinct finite poles.

**Acknowledgment.** We would like to thank the referees for suggestions that led to improvements of the presentation.

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