Gaussian Quadrature without Orthogonal Polynomials

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Abstract

A novel development is given of the theory of Gaussian quadrature, not relying on the theory of orthogonal polynomials. A method is given for computing the nodes and weights that is manifestly independent of choice of basis in the space of polynomials. This method can be extended to compute nodes and weights for Gaussian quadrature on the unit circle and Gauss type quadrature rules with some fixed nodes.

The aim of this letter is to show how the theory of Gaussian quadrature can be developed using elementary linear algebra, without relying on the theory of orthogonal polynomials. This is certainly useful from a pedagogical point of view, showing how basic results in linear algebra can have powerful applications and allowing Gaussian quadrature to be taught in introductory courses before the rather heavier topic of orthogonal polynomials. But it is also important from a more fundamental point of view. Orthogonal polynomials are an invaluable technical tool, but they are, after all, just a choice of basis in the vector space of polynomials. In this paper we give a method for computing nodes and weights that is independent of the choice of basis.

A number of the formulae in this letter can also be found in the papers of Sack and Donovan [7] and Gautschi [5] on the "modified moment method" for computing nodes and weights. The emphasis, however, is somewhat different: these papers focus on efficient, stable computation, while the focus here is more on the conceptual issue of basis indepedence.

It also turns out that occasional benefit can be obtained by a choice of basis not covered in [7] and [5]. Our basis independent method for computing nodes and weights is described in theorem 3. It allows immediate generalization to the cases of Gaussian quadrature on the unit circle and Gauss type quadrature with some fixed nodes, as we shall show. Our view of quadrature formulae as being related to blinear forms allows a generalization to multiple dimensions, though this is discussed in a separate paper [3].

There is, of course, already a completely elementary approach to Gaussian quadrature that avoids mention of orthogonal polynomials. We seek $x_i, w_i, i = 1, ..., n + 1$, such that the quadrature formula

$$\int_{a}^{b} w(x)f(x)dx \approx \sum_{i=1}^{n+1} w_{i}f(x_{i}) , \qquad w_{i} \neq 0 ,$$
 (1)

is exact when f(x) is any polynomial of degree not more than 2n + 1. Here w(x) is a known non-negative weight function on the interval [a, b]. Substituting in turn $f(x) = 1, x, x^2, \ldots, x^{2n+1}$ we see that the nodes and weights must satisfy the equations

$$\sum_{i=1}^{n+1} w_i x_i^{\alpha} = m_{\alpha} , \qquad \alpha = 0, 1, \dots, 2n+1 , \qquad (2)$$

where m_{α} is the α th moment

$$m_{\alpha} = \int_{a}^{b} w(x)x^{\alpha}dx \ . \tag{3}$$

In principle we should be able to obtain the nodes and weights by solving the system (2) of nonlinear equations. The drawback of this approach is that there is no evident way to solve (2) except in very simple cases; it is far from clear that there even exists a solution. Also, dependence on choice of basis is hardly resolved in this approach.

A linear algebra approach to Gaussian quadrature. Let \mathcal{P}_n denote the vector space of polynomials of degree up to n (so $\dim \mathcal{P}_n = n+1$). Let w(x) be a given non-negative weight function on the interval [a, b], and write

$$\langle f|g \rangle = \int_{a}^{b} w(x)f(x)g(x) dx$$
 (4)

for any polynomials f, g. For any $n, <\cdot|\cdot>$ determines an inner product on the space \mathcal{P}_n . Define the symmetric bilinear form $X(\cdot,\cdot)$ on \mathcal{P}_n by

$$X(f,g) = \int_{a}^{b} w(x)xf(x)g(x) dx.$$
 (5)

For any symmetric bilinear form on an inner product space there exists an orthonormal basis in which the form is diagonal. In other words, we can find eigenvalues $x_1, \ldots, x_{n+1} \in \mathbf{R}$ and

eigenvectors $u_1(x), \ldots, u_{n+1}(x) \in \mathcal{P}_n$ such that

$$\langle u_i|u_i\rangle = \delta_{ij}$$
, (6)

$$X(u_i, u_j) = x_i \delta_{ij} . (7)$$

Theorem 1. Let x_1, \ldots, x_{n+1} be the eigenvalues of the bilinear form $X(\cdot, \cdot)$ with corresponding orthonormal eigenvectors $u_1(x), \ldots, u_{n+1}(x)$. Then for any polynomial $p(x) \in \mathcal{P}_{2n+1}$

$$\int_{a}^{b} w(x)p(x)dx = \sum_{i=1}^{n+1} \langle 1|u_{i} \rangle^{2} p(x_{i}) , \qquad (8)$$

i.e. the quadrature rule

$$\int_{a}^{b} w(x)f(x)dx \approx \sum_{i=1}^{n+1} w_{i}f(x_{i}) , \qquad (9)$$

where $w_i = <1|u_i>^2$, is exact whenever $f(x) \in \mathcal{P}_{2n+1}$.

The proof proceeds via a lemma.

The δ Lemma. For any polynomial $p \in \mathcal{P}_{n+1}$, we have

$$< p|u_i> = <1|u_i> p(x_i)$$
 (10)

In other words, up to a normalization factor, the projection of p(x) on $u_i(x)$ is found by simply evaluating p(x) at $x = x_i$.

Proof of The δ **Lemma**. We prove the result for $p(x) = 1, x, \dots, x^{n+1}$, the general result follows by linearity. For p(x) = 1 the result is trivial. For $j = 1, \dots, n+1$ we have

$$\langle x^{j}|u_{i}\rangle = \int_{a}^{b} w(x)x^{j}u_{i}(x) dx = X(x^{j-1}, u_{i}) = x_{i} \langle x^{j-1}|u_{i}\rangle$$
 (11)

Iterating this procedure j times we obtain $\langle x^j | u_i \rangle = x_i^j \langle 1 | u_i \rangle$, as required. •

Proof of Theorem 1. We prove the result for $p(x) = 1, x, \dots, x^{2n+1}$, the general result follows by linearity. For p(x) = 1 we have

$$\int_{a}^{b} w(x) dx = \langle 1|1 \rangle = \sum_{i=1}^{n+1} \langle 1|u_{i} \rangle \langle u_{i}|1 \rangle = \sum_{i=1}^{n+1} \langle 1|u_{i} \rangle^{2}$$
(12)

as required. For $p(x) = x^j$, j = 1, ..., 2n + 1, we can write $p(x) = x^{j_1 + j_2 + 1}$, where $j_1, j_2 \in \{1, 2, ..., n\}$, and thus

$$\int_{a}^{b} w(x)x^{j} dx = X(x^{j_{1}}, x^{j_{2}})$$

$$= \sum_{i_{1}=1}^{n+1} \sum_{i_{2}=1}^{n+1} \langle x^{j_{1}} | u_{i_{1}} \rangle \langle x^{j_{2}} | u_{i_{2}} \rangle X(u_{i_{1}}, u_{i_{2}})$$

$$= \sum_{i=1}^{n+1} \langle 1 | u_{i} \rangle^{2} x_{i}^{j}, \qquad (13)$$

where in the last step we have used the δ Lemma. \bullet

Theorem 1 proves the existence of a Gaussian quadrature formula for any interval [a, b] and non-negative weight function w(x). The proof is based just on diagonalization of the bilinear form $X(\cdot, \cdot)$ with no prior knowledge needed of orthogonal polynomials. The next theorem shows that some of the main results on Gaussian quadrature are easily obtained within our approach.

Theorem 2.

- 1) The Gaussian quadrature formula of theorem 1 is unique.
- 2) The nodes of the Gaussian quadrature formula lie in the interval [a, b].
- 3) The nodes of the Gaussian quadrature formula are roots of any nontrivial degree n + 1 polynomial that is orthogonal to all polynomials of degree at most n.

To motivate the first part of the proof we make the observation that by setting $p(x) = u_j(x)$ in the δ Lemma we obtain

$$u_j(x_i) = \frac{\delta_{ij}}{\langle 1|u_i \rangle} \,, \tag{14}$$

implying the interesting result that the functions $u_i(x)$ are actually proportional to the Lagrange cardinal functions for the points x_1, \ldots, x_{n+1} . Note that by setting $p(x) = u_i(x)$ in (10) we see that $< 1|u_i>$ cannot be zero. Note also that the last equation implies the x_i are distinct. We mention in passing that the fact that $u_i(x_j)$ is proportional to δ_{ij} is one reason we gave the δ Lemma its name.

Proof. 1) Suppose $X_i, W_i, i = 1, ..., n+1$ are nodes and weights for a Gaussian quadrature formula, i.e. for any polynomial $p(x) \in \mathcal{P}_{2n+1}$

$$\int_{a}^{b} w(x)p(x) dx = \sum_{i=1}^{n+1} W_{i} p(X_{i}) , \qquad (15)$$

with the X_i distinct and $W_i > 0$. Define the *n*th degree polynomials $U_1(x), \ldots, U_{n+1}(x)$ by requiring

$$U_j(X_i) = \frac{\delta_{ij}}{\sqrt{W_i}}, \quad i, j = 1, \dots, n+1.$$
 (16)

We then have

$$\langle U_i|U_j \rangle = \int_a^b w(x)U_i(x)U_j(x) \ dx = \sum_{k=1}^{n+1} W_k U_i(X_k)U_j(X_k) = \delta_{ij}$$
 (17)

and

$$X(U_i|U_j) = \int_a^b w(x)xU_i(x)U_j(x) \ dx = \sum_{k=1}^{n+1} W_k X_k U_i(X_k)U_j(X_k) = X_i \delta_{ij} \ . \tag{18}$$

Thus the X_i are necessarily the eigenvalues of the bilinear form X, and the U_i are the orthonormal eigenvectors. Furthermore we have

$$<1|U_i> = \int_a^b w(x)U_i(x) \ dx = \sum_{k=1}^{n+1} W_k U_i(X_k) = \sqrt{W_i} \ ,$$
 (19)

so $W_i = <1|U_i>^2$, as before.

2) We have

$$\int_{a}^{b} w(x)au_{i}^{2}(x) dx \leq \int_{a}^{b} w(x)xu_{i}^{2}(x) dx \leq \int_{a}^{b} w(x)bu_{i}^{2}(x) dx ,$$

so $a \leq X(u_i, u_i) \leq b$ and therefore $a \leq x_i \leq b$.

3) Note that the δ Lemma holds for all $p(x) \in \mathcal{P}_{n+1}$. If p(x) is a polynomial of degree n+1 that is orthogonal to all polynomials of degree at most n, then it is orthogonal to all the $u_i(x)$, and thus, by the δ Lemma, $p(x_i) = 0$ for all i.

Calculation of the nodes and weights. Having presented our nonstandard development of the theory of Gaussian quadrature, we turn our attention to the question of computing nodes and weights using an algorithm that allows for an arbitrary choice of basis in \mathcal{P}_n . To find the nodes and weights we clearly need information on the inner product $\langle \cdot | \cdot \rangle$ and the blinear form $X(\cdot, \cdot)$ on \mathcal{P}_n . So assume the functions $q_1(x), q_2(x), \ldots, q_{n+1}(x)$ are a basis of \mathcal{P}_n and that we are given the $(n+1) \times (n+1)$ matrices B, A defined by

$$B_{ij} = \langle q_i | q_j \rangle = \int_a^b w(x)q_i(x)q_j(x)dx , \qquad i, j = 1, \dots, n+1 ,$$
 (20)

$$A_{ij} = X(q_i, q_j) = \int_a^b w(x)xq_i(x)q_j(x)dx$$
, $i, j = 1, ..., n+1$. (21)

We are about to see that knowledge of the matrices B, A and just one of the functions $q_i(x)$ is sufficient to determine the nodes x_i and weights w_i . As a prelude, note that there exists a diagonal matrix D and a matrix V satisfying

$$V^T B V = I , \qquad AV = B V D . \tag{22}$$

This is nothing but the statement that $X(\cdot,\cdot)$ has orthonormal eigenvectors, written in the basis $\{q_i\}$. In Matlab Release 14 the matrices D,V are computed from A,B by the command [V D]=eig(A,B,'chol').

Theorem 3. If D, V are matrices satisfying (22), with D diagonal, then the nodes and weights of the Gaussian quadrature formula (that is exact for polynomials in \mathcal{P}_{2n+1}) are determined by

$$x_i = D_{ii} , \qquad w_i = \left(\frac{(V^{-1})_{ij}}{q_j(x_i)}\right)^2 .$$
 (23)

(The second relation holds for arbitrary j).

Proof. Since all the integrals needed to compute B and A are integrals of polynomials of degree up to 2n + 1, we have

$$B_{ij} = \sum_{k=1}^{n+1} w_k q_i(x_k) q_j(x_k) = \sum_{k=1}^{n+1} Q_{ik} W_{kk} Q_{jk} , \qquad (24)$$

$$A_{ij} = \sum_{k=1}^{n+1} w_k x_k q_i(x_k) q_j(x_k) = \sum_{k=1}^{n+1} Q_{ik} W_{kk} X_{kk} Q_{jk} , \qquad (25)$$

where we have introduced diagonal matrices X, W with the nodes x_i and the weights w_i along their diagonals, and the matrix Q with entries $Q_{ik} = q_i(x_k)$. More concisely, we have

$$B = QWQ^T , \qquad A = QWXQ^T . (26)$$

Inserting these into the second relation in (22) we obtain

$$QWXQ^TV = QWQ^TVD , (27)$$

and therefore

$$X = (Q^T V)D(Q^T V)^{-1} . (28)$$

Since diagonal matrices are conjugate if and only if they are equal, up to reordering of the diagonal entries, we deduce the first statement in the theorem. Furthermore, after reordering the nodes if necessary, we see that the matrix Q^TV commutes with X. But X is a diagonal matrix with distinct entries on the diagonal, so Q^TV must also be diagonal. Write $\sqrt{W}Q^TV = Y$. Then $Y^TY = V^TQWQ^TV = I$ (by (26) and the first relation in (22)). So the diagonal entries of Y are all plus or minus 1. Writing $\sqrt{W}Q^T = YV^{-1}$ we obtain $w_iQ_{ji}^2 = ((V^{-1})_{ij})^2$ for all i, j, giving the second statement in the theorem. \bullet

Notes: 1. Under a change of the basis $\{q_i\}$ we will have $Q \to MQ$, $A \to MAM^T$, $B \to MBM^T$, $V \to M^{-T}V$, where M is a suitable nonsingular matrix. The nodes and the weights, however, remain unchanged.

- 2. Once the nodes x_i are known, then the weights can be obtained from the first equation in (26). This, however, requires full knowledge of the basis q_i , whereas the formula for the weights in the theorem requires knowledge of just a single basis element.
- 3. The simplest cases of theorem 3 are well-known. If we choose $q_i(x)$ to be the orthormal basis of \mathcal{P}_n formed by Gram-Schmidt orthonormalization of the basis $1, x, \ldots, x^n$, then B = I and A is tridiagonal. The method for finding nodes and weights reduces to the classic and widely used method of [6] (see [1] for an exposition). If we choose $q_i(x) = x^{i-1}$ then the matrices A and B are Hankel matrices (A_{ij} and B_{ij} both depend only on i+j), and

the computation of D and V is numerically unstable (at least for all but the smallest values of n). For more general bases the method is essentially equivalent to that of [7] and [5], but the formulation here makes the issue of basis independence much clearer. The papers [7] and [5] focus on bases in which the $q_i(x)$ satisfy a recursion of the form

$$xq_i(x) = a_i q_{i+1}(x) + b_i q_i(x) + c_i q_{i-1}(x) . (29)$$

This makes most of the entries of A expressible in terms of the entries of B and the coefficients a_i, b_i, c_i .

Example: For the weight function $w(x) = (1+x)^{-1}$ on [0,1], the construction of orthogonal polynomials by Gram-Schmidt orthonormalization of the standard basis $1, x, \ldots, x^n$ is awkward. It is much more convenient to work in a basis in which most of the elements have a factor (1+x). As a first attempt, take

$$q_i(x) = \begin{cases} (1+x)x^{i-1} & i = 1, \dots, n \\ 1 & i = n+1 \end{cases}$$
 (30)

It is straightforward to compute the necessary integrals to obtain

$$B_{ij} = \begin{cases} \frac{1}{i+j-1} + \frac{1}{i+j} & i, j = 1, \dots, n \\ \frac{1}{i} & i = 1, \dots, n, j = n+1 \\ \frac{1}{j} & j = 1, \dots, n, i = n+1 \\ \ln 2 & i = j = n+1 \end{cases},$$
(31)

$$A_{ij} = \begin{cases} \frac{1}{i+j} + \frac{1}{i+j+1} & i, j = 1, \dots, n \\ \frac{1}{i+1} & i = 1, \dots, n, j = n+1 \\ \frac{1}{j+1} & j = 1, \dots, n, i = n+1 \\ 1 - \ln 2 & i = j = n+1 \end{cases}$$
(32)

For fairly small n, it is straightforward to find D, V and the nodes and weights using Matlab. As n gets larger and the conditioning of the Hankel matrices B and A becomes a concern, it is preferable to use the basis

$$q_i(x) = \begin{cases} (1+x)p_i(x) & i = 1, \dots, n \\ 1 & i = n+1 \end{cases}$$
 (33)

where the $\{p_i(x)\}$ are the standard orthonormal polynomials on [0,1] (orthonormal with respect to the weight function 1). Then B and A are tridiagonal and pentadiagonal matrices respectively.

The point in this example is that we can exploit the freedom of basis to simplify evaluation of the necessary integrals. The cost is a little more linear algebra, but this is hardly a challenge by modern standards.

Generalization 1. Gaussian Quadrature on the Unit Circle [2]. Let $w(\theta)$ be a 2π -periodic non-negative weight function. Assume there exists a quadrature formula

$$\frac{1}{2\pi} \int_0^{2\pi} f\left(e^{i\theta}\right) w(\theta) d\theta \approx \sum_{r=1}^{n+1} w_r f(z_r) , \qquad w_r \neq 0 , \qquad (34)$$

with distinct nodes z_r , which is exact for the 2n+2 functions $f(z)=z^{-n},\ldots,z^n,z^{n+1}$ and all their linear combinations. Let $q_r(z)$, $r = 1, \ldots, n+1$ be a basis for the vector space of (complex) polynomials of degree at most n in z. Define the $(n+1) \times (n+1)$ matrices B, A bv

$$B_{rs} = \frac{1}{2\pi} \int_0^{2\pi} w(\theta) \overline{q_r(e^{i\theta})} q_s(e^{i\theta}) d\theta , \qquad r, s = 1, \dots, n+1 ,$$

$$A_{rs} = \frac{1}{2\pi} \int_0^{2\pi} w(\theta) \overline{q_r(e^{i\theta})} e^{i\theta} q_s(e^{i\theta}) d\theta , \qquad r, s = 1, \dots, n+1 .$$
(35)

$$A_{rs} = \frac{1}{2\pi} \int_0^{2\pi} w(\theta) \overline{q_r(e^{i\theta})} e^{i\theta} q_s(e^{i\theta}) d\theta , \qquad r, s = 1, \dots, n+1 .$$
 (36)

Note that B is Hermitian and positive definite, but A need not be Hermitian. We assume the pair A, B is diagonalizable, i.e. that there exists a diagonal matrix D and a matrix Vsuch that

$$AV = BVD. (37)$$

The matrices D, V can be obtained in Matlab by the command [V D]=eig(A,B). We then have the following analog of theorem 3:

Theorem 3'. The nodes and weights of the quadrature formula (34) (that is exact for $f(z) = z^{-n}, \dots, z^n, z^{n+1}$) are determined by

$$z_r = D_{rr} , \qquad w_r = \frac{(V^{-1})_{rs}(BV)_{sr}}{q_s(z_r)\overline{q_s\left(\frac{1}{\overline{z_r}}\right)}} . \tag{38}$$

(The second relation holds for arbitrary s).

Proof: Proceeding as in the real case we obtain

$$B = QW\tilde{Q} , \qquad A = QWX\tilde{Q} , \qquad (39)$$

where Q, \tilde{Q} are matrices with entries $Q_{rs} = q_r(z_s)$ and $\tilde{Q}_{rs} = \overline{q_s\left(\frac{1}{\overline{z_r}}\right)}$, respectively, and X, Ware diagonal matrices with diagonal entries equal to the nodes and the weights, respectively. Using these relations in (37) we rapidly obtain

$$X = (\tilde{Q}V)D(\tilde{Q}V)^{-1} , \qquad (40)$$

giving us the first result, that X = D, and also that the matrix $Y = \tilde{Q}V$ is diagonal.

From $\tilde{Q} = YV^{-1}$ we deduce that

$$\tilde{Q}_{rs} = Y_{rr}(V^{-1})_{rs} , \qquad (41)$$

for each r, s. Multiplying the first equation in (39) on the right by V, gives BV = QWY, implying

$$(BV)_{sr} = Y_{rr} w_r Q_{sr} , \qquad (42)$$

for each r, s. Finally we divide (42) by (41) to obtain the second result in the theorem. •

Notes: 1. The result in the theorem shows how to compute the weights given A, B and one of the q_r . It may be easier, if all of the q_r are known, to directly use the first formula in (39) to find the weights.

2. For each k we have $A\mathbf{v}_k = z_k B\mathbf{v}_k$, where \mathbf{v}_k denotes the vector that is the kth column of V. Thus $\mathbf{v}_k^*(A - z_k B)\mathbf{v}_k = 0$, or

$$\frac{1}{2\pi} \int_0^{2\pi} (e^{i\theta} - z_k) |a(\theta)|^2 w(\theta) d\theta = 0 , \qquad (43)$$

where $a(\theta) = \sum_r (\mathbf{v}_k)_r q_r(e^{i\theta})$. Since

$$\left| \int_0^{2\pi} e^{\sqrt{-1}\theta} |a(\theta)|^2 w(\theta) d\theta \right| \le \int_0^{2\pi} |a(\theta)|^2 w(\theta) d\theta , \qquad (44)$$

it follows that $|z_k| \leq 1$, i.e. the nodes are inside the unit circle.

Example: Taking $w(\theta) = \sin^2 \theta$ and using the standard basis $\{q_r(z)\} = \{1, z, \dots, z^n\}$ we have

$$A_{rs} = \frac{1}{2\pi} \int_0^{2\pi} e^{i(r-s)\theta} \sin^2\theta d\theta = \frac{1}{4} \left(2\delta_{r-s} - \delta_{r-s+2} - \delta_{r-s-2} \right) , \qquad (45)$$

$$B_{rs} = \frac{1}{2\pi} \int_0^{2\pi} e^{i(r-s+1)\theta} \sin^2\theta d\theta = \frac{1}{4} \left(2\delta_{r-s+1} - \delta_{r-s+3} - \delta_{r-s-1} \right) , \qquad (46)$$

where δ_r is 1 if r = 0 and 0 otherwise, and we have used $\frac{1}{2\pi} \int_0^{2\pi} e^{ir\theta} d\theta = \delta_r$. With n = 7 and these simple choices of A and B, and with a little help from Matlab, theorem 3' rapidly reproduces the nodes and weights given in the third part of table 1 in [2].

For a further reference on the use of Gaussian quadrature for complex integrals see [8].

Generalization 2. Gauss-type rules with some fixed nodes. We seek nodes and weights $x_i, w_i, i = 1, ..., n + 1$, and weights $v_{\alpha}, \alpha = 1, ..., m$, such that the quadrature formula

$$\int_{a}^{b} f(x)w(x)dx \approx \sum_{\alpha=1}^{m} v_{\alpha}f(y_{\alpha}) + \sum_{i=1}^{n+1} w_{i}f(x_{i}) , \qquad w_{i}, v_{\alpha} \neq 0 ,$$
 (47)

is exact when f(x) is any polynomial of degree not more than 2n + m + 1. Here the y_{α} , $\alpha = 1, \ldots, m$, are given nodes in [a, b], and we assume the x_i and y_{α} are all distinct. There is no particular reason to assume w(x) is non-negative. Let $q_i(x)$, $i = 1, \ldots, n + 1$ be an arbitrary basis for the vector space of polynomials of degree at most n. Let the $(n+1) \times (n+1)$

matrices B, A be defined by

$$B_{ij} = \int_{a}^{b} w(x) \prod_{\alpha=1}^{m} (x - y_{\alpha}) \ q_{i}(x) q_{j}(x) dx , \qquad i, j = 1, \dots, n+1 ,$$

$$A_{ij} = \int_{a}^{b} w(x) \prod_{\alpha=1}^{m} (x - y_{\alpha}) \ x q_{i}(x) q_{j}(x) dx , \qquad i, j = 1, \dots, n+1 .$$

$$(48)$$

$$A_{ij} = \int_{a}^{b} w(x) \prod_{\alpha=1}^{m} (x - y_{\alpha}) x q_{i}(x) q_{j}(x) dx , \qquad i, j = 1, \dots, n+1 .$$
 (49)

Both B and A are symmetric, but in this generalization B need not be positive definite (though in the important cases m = 1, $y_1 = a$ or b, and m = 2, $y_1 = a$, $y_2 = b$, it is positive or negative definite). Assume the pair A, B is diagonalizable, i.e. that we can find a diagonal matrix D and a matrix V satisfying

$$AV = BVD. (50)$$

We then have the following:

Theorem 3". If the quadrature formula (47) is exact when f(x) is any polynomial of degree not more than 2n + m + 1, and the pair A, B is diagonalizable, then the nodes and weights are determined by

$$x_i = D_{ii} , \qquad w_i \prod_{\alpha=1}^m (x_i - y_\alpha) = \frac{(V^{-1})_{ij} (BV)_{ji}}{q_j (x_i)^2} .$$
 (51)

(The second relation holds for arbitrary j).

The proof of this is sufficiently similar to that of theorem 3' that we omit it.

Once the nodes x_i and weights w_i have been determined using this theorem, the weights v_{α} can be determined by solving the linear system arising from exactness of the quadrature formula for $f(x) = 1, x, \dots, x^{m-1}$.

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References.

- [1] P.J.Davis and P.Rabinowitz, Methods of Numerical Integration, Academic Press (1975).
- [2] L.Darius, P.González-Vera and F.Marcellan, Gaussian Quadrature Formulae on the Unit Circle, J.Comp.Appl.Math. 140 (2002) 159-183.
- [3] I.Degani, J.Schiff and D.J.Tannor, Commuting Extensions and Cubature Formulae, Numer.Math., to appear. arXiv:math.NA/0408076.

- [4] A.S.Dickinson and P.R.Certain, Calculation of Matrix Elements for One-Dimensional Quantum-Mechanical Problems, J.Chem.Phys. 49 (1968) 4209-4211.
- [5] W.Gautschi, On the Construction of Gaussian Quadrature Rules from Modified Moments, Math.Comp. 24 (1970) 245-260.
- [6] G.H.Golub and J.H.Welsch, Calculation of Gauss Quadrature Rules, Math.Comp. 23 (1969) 221-230.
- [7] R.A.Sack and A.F.Donovan, An Algorithm for Gaussian Quadrature given Modified Moments, Numer.Math. 18 (1972) 465-478.
- [8] P.E.Saylor and D.C.Smolarski, Why Gaussian Quadrature in the Complex Plane?, Numerical Algorithms 26 (2001) 251-280.