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On a class of Gauss-like quadrature rules

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Abstract. We consider a problem that arises in the evaluation of computer graphics illumination models. In particular, there is a need to find a finite set of wavelengths at which the illumination model should be evaluated. The result of evaluating the illumination model at these points is a sampled representation of the spectral power density of light emanating from a point in the scene. These values are then used to determine the RGB coordinates of the light by evaluating three definite integrals, each with a common integrand (the SPD) and interval of integration but with distinct weight functions. We develop a method for selecting the sample wavelengths in an optimal manner.

More abstractly, we examine the problem of numerically evaluating a set of m definite integrals taken with respect to distinct weight functions but related by a common integrand and interval of integration. It is shown that when $m \geq 3$ it is not efficient to use a set of m Gauss rules because valuable information is wasted. We go on to extend the notions used in Gaussian quadrature to find an optimal set of *shared abcissas* that maximize precision in a well-defined sense. The classical Gauss rules come out as the special case $m = 1$ and some analysis is given concerning the existence of these rules when $m > 1$. In particular, we give conditions on the weight functions that are sufficient to guarantee that the shared abcissas are real, distinct, and lie in the interval of integration. Finally, we examine some computational strategies for constructing these rules.

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1. Introduction

A fundamental problem in computer graphics is the determination of the color of light emanating from a point P on a surface toward the viewer. To accomplish this task with a high degree of realism, researchers have developed a number of illumination models which incorporate the basic elements of light propagation into a highly simplified algebraic model (by algebraic model we mean one that requires only algebraic

operations). A simple example of such a model is the Phong model [14] which looks like

$$E_P(\lambda) = E_{\mathrm{A}}(\lambda) + \rho(\lambda) \sum_{j=1}^{ls} \left(\mathbf{n}^{\mathrm{T}}\mathbf{l}_j\right) E_j(\lambda) + k_S \sum_{j=1}^{ls} \left(\mathbf{n}^{\mathrm{T}}\mathbf{l}_j^*\right)^n E_j(\lambda) \tag{1}$$

Where:

$E_P(\lambda)$ is the spectral power distribution of light emanating from the point P towards the viewer.
$E_{\mathrm{A}}(\lambda)$ is the spectral power distribution of ambient light.
$E_j(\lambda)$ is the spectral power distribution of light emanating from the j'th light source.
$\rho(\lambda)$ is the spectral reflectance of the surface.
$\mathbf{n}$ is the unit normal to the surface at the point P.
$\mathbf{l}_j$ is the unit vector direction from the point P to the j'th light source.
k_S is the specular reflection coefficient of the surface.
$\mathbf{l}_j^*$ is the unit vector direction from the point P to a point halfway between the viewer and the j'th light source.
n an exponent that determines the apparent glossiness (or *albedo*) of the surface.
ls is the number of light sources in the scene.

Physically, the spectral power distributions and reflectance functions are assumed to be continuous functions over the interval of visible wavelengths (roughly 380 to 780nm). In a typical graphics algorithm this model must be evaluated one million or more times since there are roughly this many pixels on a color monitor and we have to determine the color of each one. Of course, it would be prohibitive to use continuous function representations in such an application and so we must rely on some kind of simplification. Historically, two simplification schemes have found common use. Both of these schemes find their origin in the fact that after evaluating the model one really needs the RGB values of the light emanating from the point, not the spectral power distribution. These values can be obtained, using the Young-Helmholtz theory of trichromatic vision, by evaluating the following definite integrals

$$\begin{aligned} R &= \int_{\mathscr{V}} E_P(\lambda)\bar{\mathbf{r}}(\lambda)d\lambda \\ G &= \int_{\mathscr{V}} E_P(\lambda)\bar{\mathbf{g}}(\lambda)d\lambda \\ B &= \int_{\mathscr{V}} E_P(\lambda)\bar{\mathbf{b}}(\lambda)d\lambda \end{aligned} \tag{2}$$

where $\mathscr{V}$ is the visible interval and $\bar{\mathbf{r}}(\lambda), \bar{\mathbf{g}}(\lambda)$, and $\bar{\mathbf{b}}(\lambda)$ are the *color matching functions*, a set of empirically determined weights whose existence follows from the linearity of color vision and the invariant color appearance of monochromatic light, see [16].

The first, and most common, simplification scheme is to discard the spectral data and replace it with RGB values. Since the transformation from the spectral domain to RGB is linear this scheme gives exact answers for any linear model. However, with the algebraic model shown above it introduces an approximation in the second term (usually called the *diffuse component*). Practical experience shows that this method works relatively well and a mathematical analysis is presented in [1, 2].

The second option is to evaluate the model at a finite set of sample points or abcissas. The values of the spectral power density at the abcissas are then used to

numerically evaluate the definite integrals in (2). This method is also widely used and some analysis of the use of Gauss quadrature methods for selecting the abcissas exists [15]. Motivated by this, we will examine the more abstract problem of numerically evaluating a finite collection of definite integrals with the following form

$$\begin{array}{c} \int_a^b f(x)\omega_1(x)dx \\ \int_a^b f(x)\omega_2(x)dx \\ \vdots \\ \int_a^b f(x)\omega_m(x)dx \end{array} \tag{3}$$

where $f(x)$ is a single *common* integrand, and the $\omega_i(x)$ are distinct weight functions. We will assume that each weight function is bounded, continuous, and non-negative on the interval $[a, b]$.

As a point of departure consider the classical numerical quadrature problem; we wish to evaluate a definite integral of the form

$$\int_a^b f(x)\omega(x)dx. \tag{4}$$

The weight function, $\omega(x)$, is fixed and subject to certain admissibility conditions, and the integrand, $f(x)$, may be any element of a given family $\mathscr{F}$ of functions. This is a well investigated problem and almost any text on numerical analysis contains a wide variety of techniques for approximating the solution (see [4] for a particularly enlightened explanation of many of these methods). Generally, an approximate quadrature rule is a linear functional $\tilde{\mathbf{Q}} : \mathscr{F} \to \Re$ such that

$$\tilde{\mathbf{Q}}f \approx \int_a^b f(x)\omega(x)dx.$$

The set of definite integrals in (3) can be regarded as a collection of simple quadrature problems like that in (4); there are many numerical methods for evaluating (4), and we can use them piecemeal to solve the more general problem.

In particular, we can construct a set of approximate quadrature rules, $\tilde{\mathbf{Q}}_k$, such that

$$\tilde{\mathbf{Q}}_k f \approx \int_a^b f(x)\omega_k(x)dx$$

for $k = 1, 2, ..., m$.

We shall restrict ourselves to the case where each of the $\tilde{\mathbf{Q}}_k$ is an n-point primitive rule, that is, the individual rules have the form:

$$\tilde{\mathbf{Q}}_k f = \sum_{i=1}^{n} f(x_{k,i})w_{k,i}.$$

where the $x_{k,i}$ are a fixed set of *abcissas* and the $w_{k,i}$ are fixed weights. The primitive rules are categorized by different methods of choosing the weights and abcissas.

Note that the problem in (3) does not in any way demand uniformity in the rules. If the problem is viewed as a collection of independent, unrelated definite integrals then any haphazard collection of rules is a solution. However, there are obvious advantages

to uniformity – it will reduce book-keeping, it will enhance performance, and it will simplify error analysis.

We need only decide on the method of choosing the weights and abcissas to complete the specification of a set of quadrature rules. It seems reasonable to derive each of the $\tilde{\mathbf{Q}}_k$ in the same way. We propose

Method I. Let $\tilde{\mathbf{Q}}_k$ be the n-point Gauss rule for the admissible[1] weight function $\omega_k(x)$.

This approach is straightforward. There are many techniques (see [4, 5, 7, 10, 13]) for finding the abcissas and weights, $x_{k,i}$ and $w_{k,i}$. Each Gauss rule has degree of precision $2n-1$. For our particular problem, such a set of rules will be said to have an *overall* degree of precision $2n-1$. Since Gauss rules give the maximum achievable degree of precision for n-point primitive rules, it follows that no other collection of n-point primitive rules has a higher overall degree of precision (i.e. $2n-1$ is maximal).

Unfortunately, this method uses data poorly. In particular, when $m > 2$ method I requires that $f(x)$ be evaluated more often than necessary to achieve the observed degree of precision. We illustrate this with a simple example.

Consider the case $m = 3$. Each rule, $\tilde{\mathbf{Q}}_k$, has a set of n associated abcissas, $\{x_{k,i}\}_{i=1}^{n}$. There is no reason to suspect redundancies, so we probably need to evaluate the integrand at $3n$ distinct points. Were we to use all of this data in each rule we could easily construct three rules with an overall degree of precision $3n-1$. Important information is being wasted; this can be seen if we introduce the notion of a performance ratio, defined as:

$$R = \frac{\text{Overall degree of precision + 1}}{\text{Number of integrand evaluations}}$$

This ratio indicates how many degrees of overall precision we get in return for each integrand evaluation. It is easy to see that for this approach $R = 2/m$ and hence $R < 1$ for all $m > 2$. This indicates rather poor performance.

Another method for choosing the weights and abcissas, one that accepts a lower degree of precision in return for a more efficient use of information, is:

Method II. Select a set of n distinct abcissas, $\{x_1, x_2, ..., x_n\}$, in the interval $[a, b]$ and let each $\tilde{\mathbf{Q}}_k$ be of the form

$$\tilde{\mathbf{Q}}_k f = \sum_{i=1}^{n} f(x_i) w_{k,i}.$$

Choose the weights $w_{k,i}$ so that they satisfy the following Vandermonde system[2]

$$V(x_1, x_2, ..., x_n) \begin{bmatrix} w_{k,1} \\ w_{k,2} \\ \vdots \\ w_{k,n} \end{bmatrix} = \begin{bmatrix} \mu_0^{(k)} \\ \mu_1^{(k)} \\ \vdots \\ \mu_{n-1}^{(k)} \end{bmatrix}$$

for $k = 1, 2, ..., m$. Where

[1] For the Gauss rules a weight function is admissible if it is bounded, continuous, and non-negative over the interval of integration

[2] This is always possible if the x_i are distinct

$$\mu_i^{(k)} = \int_a^b x^i \omega_k(x)dx$$

This method binds the rules together with a single set of abcissas (we will call these *shared-abcissa rules*). The integrand must be evaluated n times, and the overall degree of precision is $n-1$. This method uses information efficiently; each rule uses all of the available data about the integrand.

This method has a performance ratio of $R = 1$. This is better but there is still room for improvement. Because the selection of abcissas is arbitrary, the rule may not be the best possible. A clever method for choosing the shared abcissas could increase the precision of this approach.

Our goal in this paper is to find an "optimal" set of shared abcissas by mimicking the development of the Gauss rules. Recall that the derivation of a Gauss rule involves simultaneously finding a set of abcissas and weights that satisfy the following equations

$$\begin{aligned}
\textstyle\sum_{i=1}^n w_i &= \textstyle\int_a^b \omega(x)dx \\
\textstyle\sum_{i=1}^n x_i w_i &= \textstyle\int_a^b x\omega(x)dx \\
\textstyle\sum_{i=1}^n x_i^2 w_i &= \textstyle\int_a^b x^2\omega(x)dx \\
&\vdots \\
\textstyle\sum_{i=1}^n x_i^j w_i &= \textstyle\int_a^b x^j\omega(x)dx
\end{aligned}$$

for the largest possible value of j.

It is well known that if the weight function satisfies the admissibility conditions then this can always be done for $j = 2n-1$ since there are a total of $2n$ unknowns (n weights and n abcissas). Moreover, it is not generally possible to do it for a larger value of j. We propose an analogous approach. Note that for a set of m shared abcissa rules we have a total of $n(m+1)$ unknowns (n weights for each of the m weight functions, plus n abcissas) so it seems reasonable to try and satisfy a total of $n(m+1)$ equations. To simplify the derivation assume that m is a factor of n. In particular

$$n = ml$$

for some integer l, and consider the following method:

Method III. Let each $\tilde{\mathbf{Q}}_k$ be of the form

$$\tilde{\mathbf{Q}}_k f = \sum_{i=1}^n f(x_i) w_{k,i}$$

where the weights, $w_{k,i}$, and the abcissas, $\{x_1, x_2, ..., x_n\}$, satisfy the following equations

$$\begin{aligned}
\textstyle\sum_{i=1}^n w_{k,i} &= \textstyle\int_a^b \omega_k(x)dx \\
\textstyle\sum_{i=1}^n x_i w_{k,i} &= \textstyle\int_a^b x\omega_k(x)dx \\
\textstyle\sum_{i=1}^n x_i^2 w_{k,i} &= \textstyle\int_a^b x^2\omega_k(x)dx \\
&\vdots \\
\textstyle\sum_{i=1}^n x_i^{n+l-1} w_{k,i} &= \textstyle\int_a^b x^{n+l-1}\omega_k(x)dx
\end{aligned} \tag{5}$$

for $k = 1, 2, ..., m$.

This method yields a total of $n(m+1)$ equations in the unknown weights and abcissas. These equations have been carefully divided among the m weight functions

so that, whenever the system has a solution, the set of quadrature rules will have an overall degree of precision of $n + l - 1$. Since there are only $nm + n = (n + l)m$ unknowns, one can expect to satisfy no more than $n + l$ equations for each weight function. Hence, $n + l - 1$ is the maximum achievable overall degree of precision. Note also that the performance ratio is

$$R = \frac{n+l}{n} = \frac{m+1}{m}$$

so that $R > 1$ for all values of m.

2. Finding the weights and abcissas

Solving the equations in (5) is not trivial since they are not linear in the unknowns. We could apply Prony's method to change them into a form which can be solved more easily. The idea is to assume that the abcissas are known and then set up a system of linear equations for the coefficients of an n'th degree polynomial whose roots are those same abcissas. In the classical one-weight case the matrix of interest is an $n \times n$ Hankel matrix constructed from the moment sequence associated with the weight function. When applied to the problem now under consideration the structure of the matrix is somewhat different. In particular, we get a matrix where the first $l \times n$ block is Hankel in the moments of the first weight function, the next $l \times n$ block is Hankel in the moments of the second weight function, and so on for each of the m blocks.

It is known that this approach suffers from problems of numerical stability in the classical one-weight case; the resulting matrix equation can be very poorly conditioned and much effort has been directed toward avoiding its use (see [5, 13]). Part of the problem comes from the fact that moment sequences usually decrease in magnitude rather quickly. As a result, matrices that are constructed from moments, like the generalized Gram matrix, tend to exhibit large discrepancies in the relative sizes of the various entries – a known cause of ill-conditioning.

Experience indicates that the multi-weight case suffers from similar conditioning problems (although they are not as severe) and we would like to avoid this. We can appeal to our understanding of the classical Gauss rules and alleviate this by using the properties of orthogonal polynomials to find the abcissas. The fundamental theorem of Gaussian quadrature, [4], states that, for an admissible weight function $\omega(x)$, the Gauss abcissas for the n-point rule and the roots of the n'th orthogonal polynomial are the same. Since there are stable methods for finding these roots, we can avoid the ill-conditioning inherent in Prony's method.

We can use orthogonal polynomials to solve the multi-weight problem as well, but this will require an extended definition of the concept of orthogonality.

Definition 1. Given a set of admissible weight functions $\mathscr{W} = \{\omega_k(x)\}_{k=1}^m$ and an interval $[a, b]$, two functions $f(x)$ and $g(x)$ are said to be orthogonal with respect to $\mathscr{W}$ if

$$\langle f(x), g(x) \rangle_k = 0$$

for each $k = 1, 2, \ldots, m$. Where

$$\langle f(x), g(x) \rangle_k = \int_a^b f(x) g(x) \omega_k(x) dx \ .$$

We now give a counterpart to the fundamental theorem of Gaussian quadrature for the multi-weight case using the more general concept of orthogonality defined above.

Theorem 1. *Let $n = lm$ and consider the quadrature rules:*

$$\int_a^b \omega_k(x) f(x) dx \approx \sum_{j=1}^{n} w_{k,j} f(x_j)$$

where $k = 1, 2, ..., m$.

These rules are each exact for all polynomials of degree $\leq n + (l-1)$ if and only if:

1. *They are exact for all polynomials of degree $\leq n - 1$.*
2. *$\int_a^b \omega_k(x) q(x) p(x) dx = 0$ for every polynomial $p(x)$ of degree $\leq l - 1$ and for $k = 1, 2, ..., m$. Where $q(x) = \prod_{j=1}^{n}(x - x_j)$.*

Proof. ($\Rightarrow$) For part 1 note that if the quadrature rules are exact for all polynomials of degree $\leq n + (l-1)$ then they are certainly exact for those of degree $\leq n - 1$.

For part 2 assume that $p(x)$ has degree $\leq l - 1$. Then $q(x)p(x)$ has degree $\leq n + (l-1)$. Since the quadrature rules are exact for all such polynomials it follows that

$$\int_a^b \omega_k(x) q(x) p(x) dx = \sum_{j=1}^{n} w_{k,j} q(x_j) p(x_j) \ .$$

But $q(x_j) = 0$ for $j = 1, 2, ..., n$. Hence the above sum is identically zero since all of its terms are zero. Thus

$$\int_a^b \omega_k(x) q(x) p(x) dx = 0$$

and 2 follows.

($\Leftarrow$) Let $p(x)$ be a polynomial of degree $\leq n + (l-1)$. We can certainly write $p(x) = q(x)s(x) + r(x)$ where $s(x)$ is a polynomial of degree $\leq l - 1$ and $r(x)$ is of degree $\leq n - 1$. Then

$$\begin{aligned} \int_a^b \omega_k(x) p(x) dx &= \int_a^b \omega_k(x)[q(x)s(x) + r(x)]dx \\ &= \int_a^b \omega_k(x) q(x) s(x) dx + \int_a^b \omega_k(x) r(x) dx \ . \end{aligned}$$

But $\int_a^b \omega_k(x) q(x) s(x) dx = 0$ from (2) so that

$$\int_a^b \omega_k(x) p(x) dx = \int_a^b \omega_k(x) r(x) dx$$

since $r(x)$ is of degree $\leq n - 1$ it follows from 1 that

$$\int_a^b \omega_k(x) r(x) dx = \sum_{j=1}^{n} w_{k,j} r(x_j)$$

hence

$$\int_a^b \omega_k(x)p(x)dx = \sum_{j=1}^{n} w_{k,j} r(x_j)$$

and finally, since $q(x_j) = 0$ for $j = 1, 2, ..., n$, it follows that

$$\begin{aligned}\int_a^b \omega_k(x)p(x)dx &= \sum_{j=1}^{n} w_{k,j}[q(x_j)s(x_j) + r(x_j)] \\ &= \sum_{j=1}^{n} w_{k,j} p(x_j)\end{aligned}$$

and the quadrature rule is exact for all polynomials of degree $\leq n + (l - 1)$. □

This is important because it leads to an algorithm for finding the shared abcissas without resorting to Prony's method, thereby avoiding the associated numerical difficulties. In particular, it is sufficient to find, through any means possible, an n'th degree polynomial $q(x)$ that is orthogonal to $\mathscr{P}_{l-1}$ with respect to $\mathscr{W}$. The roots of this polynomial will be the shared abcissas.

We exploit this result by examining the orthogonal polynomial systems of the various weight functions in $\mathscr{W}$. Let p_j^* be the orthogonal polynomial of degree j associated with $\omega_1(x)$, the first weight function (we do not lose any generality in choosing the first weight function). Clearly then, p_n^* is orthogonal to $\mathscr{P}_{l-1}$ with respect to the weight function $w_1(x)$. Indeed, any element of the linear manifold

$$\mathscr{M} = \text{span}\,\{p_l^*, p_{l+1}^*, ..., p_n^*\}$$

will be orthogonal to $\mathscr{P}_{l-1}$ with respect to the weight function $\omega_1(x)$. Moreover, any polynomial of degree n that is orthogonal to $\mathscr{P}_{l-1}$ with respect to $\omega_1(x)$ is necessarily an element of $\mathscr{M}$. So it follows that $q(x) \in \mathscr{M}$ since $q(x)$ is certainly orthogonal to $\mathscr{P}_{l-1}$ with respect to $\omega_1(x)$ if it is orthogonal to $\mathscr{P}_{l-1}$ with respect to $\mathscr{W}$. Hence

$$q(x) = \sum_{i=l}^{n} \gamma_i p_i^* \tag{6}$$

for some real coefficients γ_i.

Of course, $q(x)$ must also be orthogonal to $\mathscr{P}_{l-1}$ with respect to the remaining weight functions, that is

$$\langle q(x), p(x) \rangle_k = 0 \tag{7}$$

for any $p(x) \in \mathscr{P}_{l-1}$ and $k = 2, 3, ..., m$. It will be convenient to take $\{p_0^*, p_1^*, p_2^*, ..., p_{l-1}^*\}$ as our basis for $\mathscr{P}_{l-1}$, so that the orthogonality conditions from equation (7) become

$$\langle q(x), p_i^* \rangle_k = 0 \tag{8}$$

for $i = 0, 1, ..., l - 1$ and $k = 2, 3, ..., m$. Substituting for $q(x)$ with equation (6) and using the linearity of the inner product transforms equation (8) into

$$\gamma_l \langle p_l^*, p_i^* \rangle_k + \gamma_{l+1} \langle p_{l+1}^*, p_i^* \rangle_k + \cdots + \gamma_n \langle p_n^*, p_i^* \rangle_k = 0\ . \tag{9}$$

Assume, without loss of generality, that $\gamma_n = 1$ so that equation (9) becomes

$$\gamma_l \langle p_l^*, p_i^* \rangle_k + \gamma_{l+1} \langle p_{l+1}^*, p_i^* \rangle_k + \cdots + \gamma_{n-1} \left\langle p_{n-1}^*, p_i^* \right\rangle_k = - \langle p_n^*, p_i^* \rangle_k \ .$$

For convenience let

$$\mu_{i,j}^{(k)} = \int_a^b p_i^*(x) p_j^*(x) \omega_k(x) dx \ .$$

This yields the following linear system for the coefficients γ_i

$$\begin{bmatrix} \mu_{l,0}^{(2)} & \mu_{l+1,0}^{(2)} & \cdots & \mu_{n-1,0}^{(2)} \\ \mu_{l,1}^{(2)} & \mu_{l+1,1}^{(2)} & \cdots & \mu_{n-1,1}^{(2)} \\ \mu_{l,2}^{(2)} & \mu_{l+1,2}^{(2)} & \cdots & \mu_{n-1,2}^{(2)} \\ \vdots & \vdots & & \vdots \\ \mu_{l,l-1}^{(2)} & \mu_{l+1,l-1}^{(2)} & \cdots & \mu_{n-1,l-1}^{(2)} \\ \mu_{l,0}^{(3)} & \mu_{l+1,0}^{(3)} & \cdots & \mu_{n-1,0}^{(3)} \\ \vdots & \vdots & & \vdots \\ \vdots & \vdots & & \vdots \\ \mu_{l,l-1}^{(m)} & \mu_{l+1,l-1}^{(m)} & \cdots & \mu_{n-1,l-1}^{(m)} \end{bmatrix} \begin{bmatrix} \gamma_l \\ \gamma_{l+1} \\ \vdots \\ \gamma_{n-1} \end{bmatrix} = - \begin{bmatrix} \mu_{n,0}^{(2)} \\ \mu_{n,1}^{(2)} \\ \mu_{n,2}^{(2)} \\ \vdots \\ \mu_{n,l-1}^{(2)} \\ \mu_{n,0}^{(3)} \\ \vdots \\ \vdots \\ \mu_{n,l-1}^{(m)} \end{bmatrix} .$$

We shall call the matrix that appears on the left of equation (2) the *mixed modified Gram matrix*. This equation can be written more compactly by introducing the matrix $M_{i,j,n}^{(k)}$ defined to be

$$M_{i,j,n}^{(k)} = \begin{bmatrix} \mu_{j,0}^{(k)} & \mu_{j+1,0}^{(k)} & \cdots & \mu_{n,0}^{(k)} \\ \mu_{j,1}^{(k)} & \mu_{j+1,1}^{(k)} & \cdots & \mu_{n,1}^{(k)} \\ \mu_{j,2}^{(k)} & \mu_{j+1,2}^{(k)} & \cdots & \mu_{n,2}^{(k)} \\ \vdots & \vdots & & \vdots \\ \mu_{j,i-1}^{(k)} & \mu_{j+1,i-1}^{(k)} & \cdots & \mu_{n,i-1}^{(k)} \end{bmatrix} .$$

A matrix with the form of $M_{i,j,n}^{(k)}$ shall be known as a *modified Gram block* (or matrix) because of its similarity with the matrices of modified moments used in [13, 5]. The linear system for the coefficients γ_i can be rewritten as

$$\begin{bmatrix} M_{l,l,n-1}^{(2)} \\ M_{l,l,n-1}^{(3)} \\ \vdots \\ M_{l,l,n-1}^{(m)} \end{bmatrix} \begin{bmatrix} \gamma_l \\ \gamma_{l+1} \\ \vdots \\ \gamma_{n-1} \end{bmatrix} = - \begin{bmatrix} M_{l,n,n}^{(2)} \\ M_{l,n,n}^{(3)} \\ \vdots \\ M_{l,n,n}^{(m)} \end{bmatrix} . \tag{10}$$

3. A generalized formulation

In the original derivation we assumed that the number of abcissas, n, was a multiple of the number of weight functions, m. Although this assumption simplifies the derivation, it is not mathematically necessary; it only eases the task of allocating of the n additional degrees of precision to the various weight functions. By assuming that $n = ml$ and giving l extra equations to each weight function we maximize the overall degree of precision.

Of course, if m is not a factor of n then the equations can not be allocated in such an equitable a manner. Some of the weights must have more than others, hence some of the $\tilde{\mathbf{Q}}_k$ will have a higher degree of precision than others.

We introduce the notion of a *degree sequence*.

Definition 2. An indexed set, $S = \{\nu_1, \nu_2, ...\nu_m\}$, containing m non-negative integers such that:

$$\sum_{i=1}^{m} \nu_i = n$$

will be called an (m, n) *degree sequence*.

We can generalize these quadrature rules as follows:

Definition 3. Let $\mathscr{W} = \{\omega_k(x)\}_{k=1}^{m}$ be a set of admissible weight functions on the interval $[a, b]$, and $S = \{\nu_1, \nu_2, ...\nu_m\}$ be an (m, n) degree sequence, a set of rules $\tilde{\mathbf{Q}}_k$ of the form:

$$\tilde{\mathbf{Q}}_k f = \sum_{i=1}^{n} f(x_i) w_{k,i}$$

will be called an *optimal* set with respect to $\mathscr{W}$ and S if and only if the weights, $\{w_{k,i}\}$, and the abcissas, $\{x_i\}$, satisfy the following equations:

$$\begin{array}{rcl} \sum_{i=1}^{n} w_{k,i} & = & \int_a^b \omega_k(x)dx \\ \sum_{i=1}^{n} x_i w_{k,i} & = & \int_a^b x\omega_k(x)dx \\ \sum_{i=1}^{n} x_i^2 w_{k,i} & = & \int_a^b x^2\omega_k(x)dx \\ & \vdots & \\ \sum_{i=1}^{n} x_i^{n+\nu_k-1} w_{k,i} & = & \int_a^b x^{n+\nu_k-1}\omega_k(x)dx \end{array} \tag{11}$$

for $k = 1, 2, ..., m$.

The previous derivation is now a special case where $n = ml$ and the degree sequence $\{l, l, ..., l\}$ is used. We shall call such a set of rules *uniform*.

Once again we can avoid using Prony's method to find the coefficients of the polynomial $q(x)$ by exploiting the concept of orthogonal polynomials. However, before proceeding it will be worthwhile to mention a concept introduced by M. Riesz in his study, [11, 12], of the moment problem. In particular:

Definition 4 (Chihara). A polynomial $q(x)$, not identically zero, is called a *quasi-orthogonal polynomial of order* $n + 1$ if and only if it is of degree at most $n + 1$ and:

$$\int_a^b q(x)x^i\omega(x)dx = 0$$

for $i = 0, 1, ..., n - 1$.

This concept can be used to derive a trivial extension of the Gauss quadrature rules, [3]. In particular, given $q(x)$, a quasi-orthogonal polynomial of order $n + 1$, there is a set of weights $\{w_i\}_{i=1}^{n+1}$ such that:

$$\int_a^b p(x)\omega(x)dx = \sum_{i=1}^{n+1} w_i p(x_i) \tag{12}$$

for all polynomials of degree at most $2n$. The abcissas x_i are the roots of $q(x)$, and can be shown to be real and distinct.

Note that, in general, this rule is not Gaussian since the Gauss rule of this order would have degree of precision $2n+1$. It is, however, very close to the Gauss rule. In effect, this extension gives up a single degree of precision in exchange for the lifting of a single orthogonality condition on $q(x)$.

The *optimal rules* presented here are quite similar in that they also trade precision in return for relaxed orthogonality conditions. The difference is that the excess orthogonality conditions are used to increase the precision of other rules based on the same abcissas. Although an optimal set of rules cannot be improved upon without degrading at least one of its members, the rule in equation (12) can be unilaterally improved.

Once more we broaden our definition of orthogonality.

Definition 5. Let $q(x)$ be a polynomial of degree $d > n$, and let $\mathscr{W}$ and S be as in Definition 3. If, for $k = 1, 2, ..., m$, the following holds:

$$\langle q(x), p(x) \rangle_{\omega_k} = 0$$

for every polynomial $p(x)$ of degree less than ν_k. Then $q(x)$ will be said to be *quasi-orthogonal with respect to* $\mathscr{W}$ *and* S.

This definition leads to a generalization of Theorem 1, the key theorem to developing an alternate method for finding the abcissas.

Theorem 2. *Consider the quadrature rules:*

$$\tilde{\mathbf{Q}}_k f = \sum_{j=1}^{n} w_{k,j} f(x_j)$$

where $k = 1, 2, ..., m$. *These rules form an optimal set with respect to* $\mathscr{W}$ *and* S *if and only if:*

1. *They are exact for all polynomials of degree* $\leq n - 1$.
2. *The polynomial* $q(x) = \prod_{j=1}^{n}(x - x_j)$ *is quasi-orthogonal with respect to* $\mathscr{W}$ *and* S.

The proof of this theorem proceeds along the same lines as that for Theorem 1 with l replaced by ν_k so it is omitted.

The next fact establishes the connection between, $q(x)$, a polynomial which is quasi-orthogonal with respect to $\mathscr{W}$ and S, and the orthogonal polynomial systems associated with the various elements of $\mathscr{W}$.

Fact 3. Let $q(x)$ be a polynomial of degree n that is quasi-orthogonal with respect to $\mathscr{W}$ and S. And let $p_i^*(x)$ be the i'th element of the orthogonal polynomial system associated with the weight function $\omega_1(x) \in \mathscr{W}$. Then, there exist coefficients $\gamma_{\nu_1}, \gamma_{\nu_1+1}, ..., \gamma_n$ such that:

$$q(x) = \sum_{i=\nu_1}^{n} \gamma_i p_i^*(x)$$

Moreover, $\gamma_n \neq 0$.

Proof. Since $q(x)$ has degree n, and since the set of orthogonal polynomials $\{p_i^*(x)\}_{i=0}^n$ is a basis for $\mathscr{P}_n$, it follows that there is a Fourier expansion of $q(x)$ in terms of the $p_i^*(x)$. In particular

$$q(x) = \sum_{i=0}^{n} \frac{\langle q, p_i^* \rangle}{\langle p_i^*, p_i^* \rangle} p_i^*(x) \tag{13}$$

$$= \sum_{i=\nu_1}^{n} \frac{\langle q, p_i^* \rangle}{\langle p_i^*, p_i^* \rangle} p_i^*(x) \tag{14}$$

$$= \sum_{i=\nu_1}^{n} \gamma_i p_i^*(x) \ . \tag{15}$$

(16)

Finally, note that $\gamma_n \neq 0$ because if this were not true $q(x)$ could have degree no greater than $n-1$ which is a contradiction. □

This, of course, gives a method for finding $q(x)$ just as it did in the uniform case. We get the following linear system of equations for the coefficients

$$\begin{bmatrix} M^{(2)}_{\nu_2,\nu_1,n-1} \\ M^{(3)}_{\nu_3,\nu_1,n-1} \\ \vdots \\ M^{(m)}_{\nu_m,\nu_1,n-1} \end{bmatrix} \begin{bmatrix} \gamma_l \\ \gamma_{l+1} \\ \vdots \\ \gamma_{n-1} \end{bmatrix} = - \begin{bmatrix} M^{(2)}_{\nu_2,n,n} \\ M^{(3)}_{\nu_3,n,n} \\ \vdots \\ M^{(m)}_{\nu_m,n,n} \end{bmatrix} . \tag{17}$$

If the *mixed modified Gram matrix* matrix has a non-zero determinant then $q(x)$ exists and has real coefficients, however, this is not sufficient to guarantee that it has real, or distinct roots.

4. Existence and location of the abcissas

The classical Gauss rules have the useful property that the abcissas for the n'th order rule are real, distinct, and lie in the interval $[a, b]$ as long as $\omega(x) \geq 0$ in the same interval. Unfortunately this result does not extend to the abcissas of the rules we are considering. If the only condition placed on the elements of $\mathscr{W}$ is that they be non-negative over the interval $[a, b]$ many examples can be given where this is not true.

It is possible, however, to give a sufficient condition on the weight functions that guarantees real, distinct roots inside the interval of integration. Towards this end, we introduce the notion of an *integrable Markov system* (see [9]).

Definition 1. A sequence of real valued functions $m_i(x)$, $i = 1, 2, ..., n$ is called an *integrable Markov system* on (a, b) if:

1. $m_i(x)$ is defined at every point $x \in (a, b)$ and is integrable, for each $i = 1, 2, ..., n$.
2. The linear combination
$$\sum_{i=1}^{n} a_i m_i(x)$$
does not have more than $n-1$ zeros in (a, b) for any non-trivial set of coefficients $a_1, a_2, ..., a_n$.

We now state a theorem of Kershaw [9], that can be used to guarantee real, distinct roots in the interval of integration.

Theorem 4 (Kershaw). *If* $\{m_i(x)\}_{i=1}^n$ *is an integrable Markov system on* (a, b) *then*

1. *There exists a polynomial* $p_n(x)$*, of degree* n*, which is unique up to an arbitrary non-zero scalar multiplier, such that*

$$\int_a^b m_i(x)p_n(x)dx = 0, \qquad i = 1, 2, ..., n. \tag{18}$$

2. *The zeros of* $p_n(x)$ *are real, distinct, and lie in* (a, b)*.*
3. *If* $p_{n+1}(x)$ *is a polynomial of degree* $n + 1$ *that satisfies*

$$\int_a^b m_i(x)p_{n+1}(x)dx = 0, \qquad i = 1, 2, ..., n.$$

and has real, distinct zeros then between any pair of adjacent zeros of $p_{n+1}(x)$ *lies a zero of* $p_n(x)$*, all lying in* (a, b)*.*

We refer the reader to [9] for the proof of this elegant theorem. With this in hand, we can prove the following theorem.

Theorem 5. *Let* $\mathscr{W} = \{\omega_k(x)\}_{k=1}^m$ *be a set of weight functions defined and integrable on the interval* $[a, b]$*, and* $S = \{\nu_1, \nu_2, ...\nu_m\}$ *be an* (m, n) *degree sequence. If the induced sequence of functions*

$$\mathscr{W} \times \mathbf{S} = \{\omega_1(x), x\omega_1(x), ...x^{\nu_1-1}\omega_1(x), \omega_2(x), ..., x^{\nu_m-1}\omega_m(x)\}$$

is an integrable Markov system on (a, b)*, then there is a polynomial* $q(x)$ *of degree* n*, that is unique up to an arbitrary non-zero scalar multiplier, that is quasi-orthogonal with respect to* $\mathscr{W}$ *and* **S***. Moreover, the polynomial* $q(x)$ *has* n *real, distinct roots in the interval* (a, b)*.*

Proof. Existence of the polynomial $q(x)$ with real distinct roots follows directly from theorem 4. To see that $q(x)$ is quasi-orthogonal with respect to $\mathscr{W}$ and **S** consider any polynomial $p(x)$ of degree less than ν_k. Obviously we can write

$$p(x) = \sum_{i=0}^{\nu_k-1} \gamma_i x^i \ .$$

Now consider

$$\int_a^b p(x)q(x)\omega_k(x)dx = \sum_{i=0}^{\nu_k-1} \gamma_i \int_a^b q(x)x^i\omega_k(x)dx \ .$$

Clearly all of the terms on the right vanish as a result of (18) from Theorem 4. And it follows that $q(x)$ is quasi-orthogonal with respect to $\mathscr{W}$ and **S**. □

This is a strong result but it requires that the weight functions satisfy a rather stringent condition. One immediate advantage is that we have dismissed the restriction that the weight functions must be non-negative over the interval of integration. Clearly, non-negativity is not implicit in Theorem 5. However, if we do enforce the non-negativity condition then we can account for some of the zeros without resorting to the conditions of Theorem 5.

Theorem 6. *Let $\mathscr{W}$ and S be as before and assume that the mixed Gram determinant with respect to $\mathscr{W}$ and S is non-zero. If there exists a $\omega_k(x) \in \mathscr{W}$ such that $\omega_k(x) \geq 0$ on $[a,b]$, then the n'th degree polynomial $q(x)$ that is quasi-orthogonal with respect to $\mathscr{W}$ and S has at least ν_k distinct, real roots in the interval $[a,b]$. Moreover, if ν_k and n differ in parity then $q(x)$ has at least $\nu_k + 1$ distinct, real roots, although one of them may lie outside the interval $[a,b]$.*

Proof. Proceed by contradiction. Let $y_1, y_2, ..., y_j$ be the real zeros of $q(x)$ that lie in $[a,b]$ and have odd multiplicity. Assume that $j < \nu_k$ and let $r(x) = \prod_{i=1}^{j}(x - y_i)$. Then, since the product $q(x)r(x)$ does not change sign in the interval $[a,b]$, it must be true that:

$$\int_a^b q(x)r(x)\omega_k(x)dx \neq 0 \ .$$

But this is a contradiction since $r(x) \in \mathscr{P}_{\nu_k - 1}$. Hence, it follows that $j \geq \nu_k$, and so $q(x)$ has at least ν_k real, distinct zeros in the interval $[a,b]$.

It is seen that $q(x)$ has at least ν_k real, distinct roots of odd multiplicity in the interval $[a,b]$. This means that the number of roots that have been accounted for, including multiplicities, has the same parity as ν_k. If ν_k and n differ in parity then, since $q(x)$ has real coefficients and complex roots can only occur with even multiplicity, it follows that $q(x)$ has at least one more distinct real root of odd multiplicity, although nothing can be said about its location. □

Corollary 7 follows directly from the theorem:

Corollary 7. *Let $\mathscr{W}$ and S be as before and assume that the mixed Gram determinant with respect to $\mathscr{W}$ and S is non-zero. Assume $\omega_k(x) \geq 0$ on $[a,b]$ for each $\omega_k(x) \in \mathscr{W}$. Then the n'th degree polynomial, $q(x)$, that is quasi-orthogonal with respect to $\mathscr{W}$ and S has at least t distinct, real roots in the interval $[a,b]$, where:*

$$t = \max_{1 \leq k \leq m} \nu_k \ .$$

Moreover, if t and n differ in parity then $q(x)$ has at least $t + 1$ distinct, real roots, although one of them may lie outside the interval $[a,b]$.

Note that Theorem 6 implies that all of the roots are real, distinct, and in $[a,b]$ if $m = 1$ (this is the special case of a Gauss rule). There is one other case, closely related to the quasi-orthogonal polynomials of Riesz, for which a stronger result may be given.

Theorem 8. *Assume $\mathscr{W}$ has only two elements, S is given by $\{n-1, 1\}$, and $\omega_1(x) \geq 0$ on $[a,b]$. If there exists a polynomial, $q(x)$, of degree n that is quasi-orthogonal with respect to $\mathscr{W}$ and S, then all of its roots are real and at least $n-1$ of them lie in the interval $[a,b]$.*

Proof. It follows directly from Theorem 6 that $q(x)$ has at least $n-1$ distinct, real zeros in $[a,b]$ and that the remaining zero is real since n and $n-1$ obviously differ in parity. Note that it is not possible to determine whether or not the remaining root lies in the interval $[a,b]$ using the conditions of the theorem. □

5. Computational strategies for constructing the rules

In order to implement the methods developed in the last few sections and maintain some degree of numerical stability we need to do a bit more work. In this section we derive an algorithm that allows these rules to be more easily constructed. In particular, we show how the abcissas and weights can be found by looking at a related eigenvalue problem involving a rank one change to the Jacobi matrix associated with the weight function ω_1.

The first step in finding a set of rules of the type outlined in this paper is to construct the mixed Gram matrix. We note briefly here that this can be done using only knowledge of the Jacobi matrices of the various weight functions. In particular, Gautschi [5] gives a method for computing the quantities $\mu_{i,j}^{(k)}$ given only the modified moments $\mu_i^{(k)}$, and the three-term recurrence relation[3] for the weight function ω_k. Moreover, Golub and Fischer [6] give a method for generating the modified moments from the Jacobi matrices alone. Hence, all of the data needed to solve equation (17) can be had by manipulating the Jacobi matrices of the various weight functions.

Once we have the coefficients $\gamma_{\nu_k}, \gamma_{\nu_k+1}, ..., \gamma_n$ we can find the roots of the quasi-orthogonal polynomial by solving an eigenvalue problem. Recall that the system of orthonormal polynomials associated with the weight function ω_1 satisfies a three-term recurrence relation of the form

$$x\mathbf{p}(x) = J^{(1)}\mathbf{p}(x) + \beta_n^{(1)} p_n^*(x)\mathbf{e}_n$$

where $J^{(1)}$ is a symmetric tridiagonal (Jacobi) matrix with elements $\alpha_1^{(1)}, \alpha_2^{(1)}, ..., \alpha_n^{(1)}$ on the diagonal, and elements $\beta_1^{(1)}, \beta_2^{(1)}, ..., \beta_{n-1}^{(1)}$ on the subdiagonal, and where $\mathbf{p}(x) = [p_0^*, p_1^*, ..., p_{n-1}^*]^{\mathrm{T}}$, and $\mathbf{e}_n = [0, 0, ..., 0, 1]^{\mathrm{T}}$.
Using equation (3) and the fact that $\gamma_n = 1$ gives

$$p_n^*(x) = q(x) - \sum_{i=\nu_1}^{n-1} \gamma_i p_i^*(x) \ .$$

If we let

$$\gamma = \left[0, ..., 0, \gamma_{\nu_k}, ..., \gamma_{n-1}\right]^{\mathrm{T}} \ .$$

Then clearly

$$x\mathbf{p}(x) = J^{(1)}\mathbf{p}(x) + \beta_n^{(1)} \left(q(x) - \gamma^{\mathrm{T}}\mathbf{p}(x)\right) \mathbf{e}_n \ .$$

So that the roots x_i of the quasi-orthogonal polynomial are precisely the eigenvalues of the matrix

$$J^{(1)} - \beta_n^{(1)}\mathbf{e}_n\gamma^{\mathrm{T}} \tag{19}$$

which can be easily found using the QR algorithm. Notice also that the eigenvector associated with x_i is given by $\mathbf{v}_i = \mathbf{p}(x_i)$. We can use this fact to solve for the weights $w_{k,i}$ by requiring that each rule correctly generate the first n *modified moments*. This is mathematically equivalent to solving the Vandermonde system for the weights of an interpolatory rule but is much better numerically and is very convenient for us since we already have the eigenvectors as a byproduct of finding the roots via the QR algorithm. Note that this approach is equivalent to the method presented by Kautsky and Elhay in [8]. In particular, let

[3] This can, of course, be had from the Jacobi matrix

$$K = \left[\mathbf{p}(x_1), \mathbf{p}(x_2), ..., \mathbf{p}(x_n)\right] \ . \tag{20}$$

The vectors $\mathbf{p}(x_i)$ can be had by scaling the eigenvectors from the QR method so that their first elements are all identical and equal to the zero moment of the weight function ω_1. Then, the interpolatory weights $\mathbf{w}_k = \left[w_{k,1}, w_{k,2}, ..., w_{k,n}\right]^{\mathrm{T}}$ can be found by solving

$$K\mathbf{w}_k = \begin{bmatrix} \mu_0^{(k)} \\ \mu_1^{(k)} \\ \vdots \\ \mu_{n-1}^{(k)} \end{bmatrix} \ . \tag{21}$$

It is quite easy to verify from here that the weights for the classical Gauss rules are just the squared first elements of the normalized eigenvectors of the Jacobi matrix.

6. A brief numerical example

We present a brief numerical example in order to illustrate the process. We are looking for a four point uniform rule with two weight functions defined on $[-1, 1]$. The weight functions are

$$\begin{aligned} \omega_1(x) &= \sqrt{1-x^2} \\ \omega_2(x) &= 1 + x \ . \end{aligned}$$

The orthonormal polynomials[4] associated with $\omega_1(x)$ are the Chebyshev polynomials of the second kind. They are, in particular

$$U_0 = 1; \quad U_1 = 2x; \quad U_2 = 4x^2 - 1; \quad U_3 = 8x^3 - 4x; \quad U_4 = 16x^4 - 12x^2 + 1 \ .$$

Following equation (10) we need to solve

$$M^{(2)}_{2,2,3} \begin{bmatrix} \gamma_2 \\ \gamma_3 \end{bmatrix} = -M^{(2)}_{2,4,4} \ .$$

In particular

$$\begin{bmatrix} \frac{2}{3} & \frac{8}{15} \\ \frac{14}{15} & \frac{8}{15} \end{bmatrix} \begin{bmatrix} \gamma_2 \\ \gamma_3 \end{bmatrix} = - \begin{bmatrix} \frac{2}{5} \\ \frac{46}{105} \end{bmatrix} \ .$$

This system has a condition number of roughly $\mathscr{K} = 12.04$ which stands in strong contrast to the condition number of roughly 116 that one gets using Prony's method. Solving the equation yields $\gamma_2 = -\frac{1}{7}$ and $\gamma_3 = -\frac{4}{7}$. The Jacobi matrix of order 4 associated with ω_1 is

$$J_4^{(1)} = \begin{pmatrix} 0 & 1/2 & 0 & 0 \\ 1/2 & 0 & 1/2 & 0 \\ 0 & 1/2 & 0 & 1/2 \\ 0 & 0 & 1/2 & 0 \end{pmatrix}$$

the vector $\gamma = [0 \quad 0 \quad -1/7 \quad -4/7]$, and $\beta_4 = 1/2$ so that, following equation 19, the abcissas are the eigenvalues of the matrix

[4] Up to a scalar constant of $\sqrt{\pi/2}$

$$\begin{pmatrix} 0 & 1/2 & 0 & 0 \\ 1/2 & 0 & 1/2 & 0 \\ 0 & 1/2 & 0 & 1/2 \\ 0 & 0 & 8/14 & 2/7 \end{pmatrix}. \tag{22}$$

Using the QR method to solve for the eigenvalues yields the four abcissas, approximately

$$x_1 = -0.791263; \quad x_2 = -0.237959; \quad x_3 = 0.427455; \quad x_4 = 0.887481 .$$

Note that they are real, distinct, and lie in the interval of integration. Moreover, note that the distribution of abcissas is somewhat skewed toward the right side of the interval. This is intuitively pleasing as it appears to reflect the fact that the second weight function places far more emphasis on the right half of the interval than the left; it would seem that $\omega_2(x)$ is *pulling* the sample points to the right in order to extract more information from that part of the interval.

Finally, we form K by scaling the eigenvectors of the matrix in (22) so that their first elements are all 1 and solve

$$K\mathbf{w}_1 = \begin{bmatrix} \pi/2 \\ 0 \\ 0 \\ 0 \end{bmatrix} \qquad K\mathbf{w}_2 = \begin{bmatrix} 2 \\ 4/3 \\ 2/3 \\ 8/15 \end{bmatrix}$$

for the weights. This yields the rules

$$\begin{aligned} \tilde{\mathbf{Q}}_1 f &= \pi\,[0.079050 f(x_1) + 0.204235 f(x_2) + 0.176469 f(x_3) + 0.040245 f(x_4)] \\ \tilde{\mathbf{Q}}_2 f &= 0.082275 f(x_1) + 0.507998 f(x_2) + 0.866157 f(x_3) + 0.543569 f(x_4) . \end{aligned}$$

7. Overview and conclusions

We have examined the problem of approximating the values of a set of definite integrals with a common integrand over the same interval but taken with respect to distinct weight functions. There are many approaches to this problem but we restricted our efforts to finding a set of shared abcissa primitive quadrature rules. It was shown that these rules could be constructed to have the maximum degree of accuracy by choosing an appropriate set of shared abcissas. This is accomplished by extending the concepts used in the derivation of the classical Gauss quadrature rules. Two methods of solution were discussed. The first, Prony's method, is analogous to inverting a generalized Gram matrix. This is conceptually easy to follow but not numerically desirable. The second uses the properties of orthogonal polynomials to find the abcissas and is much better numerically than the first. We presented some results about the location and existence of the abcissas, and gave a sufficient condition on the weights that guarantee real, distinct roots in the interval of integration. Finally, we introduced a computational strategy for constructing these rules that equates this problem with an eigenvalue problem for a rank one variant of a symmetric tridiagonal Jacobi matrix.

We note that the results for the particular set of weights that motivated the problem were quite good and will appear in a future paper on numerical determination of tristimulus coordinates.

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