Gaussian quadratures with respect to Discrete measures

Stefan Engblom[1] *

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[1] *Div of Scientific Computing, Dept of Information Technology*
Uppsala University, SE-75105 Uppsala, Sweden
email: stefane@it.uu.se

Abstract

In analogy to the subject of Gaussian integration formulas we present an overview of some Gaussian *summation* formulas. The derivation involve polynomials that are orthogonal under discrete inner products and the resulting formulas are useful as a numerical device for summing fairly general series. Several illuminating examples are provided in order to present various aspects of this not very well-known technique.

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1 Introduction

Gaussian quadratures and the classical orthogonal polynomials have been around for a long time and have been subject to intense studies. The inner

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products associated with most orthogonal polynomials can be written as an integral with respect to some measure over a certain domain. That is,

$$(f, g) \equiv \int_\Omega f(x)g(x)dw(x), \tag{1.1}$$

where $w(x)$ is the (positive) weight-function. The corresponding mechanical quadrature is then of the form

$$\int_\Omega f(x)dw(x) = \sum_{i=1}^{n} f(x_i)w_i + R_n, \tag{1.2}$$

for some weights w_i and abscissas x_i. In general, the form of the remainder R_n makes the formula exact when f is a polynomial up to a certain degree.

Some less classical polynomials [3, 1] are generated by a *discrete* measure instead, implying that the resulting inner product is to be understood as a weighted sum,

$$(f, g) \equiv \sum_{x\in\Omega} f(x)g(x)w(x), \tag{1.3}$$

over some discrete set of points Ω. Interestingly, in complete analogy with the theory for mechanical integration formulas, we will show that this gives rise to *Gaussian summation formulas*;

$$\sum_{x\in\Omega} f(x)w(x) = \sum_{i=1}^{n} f(x_i)w_i + R_n. \tag{1.4}$$

It came as a great surprise to the author when several searches in the literature indicated that this technique seems not to have been discussed thoroughly.

We now review some of the relevant references that we did find. In [8] the authors undertake a theoretical study of the convergence of quadratures for series of the form

$$L_a^{p,q} = \frac{p-1}{p} \sum_{\nu\geq 0} \frac{1}{p^\nu} f\left(\frac{a}{q^\nu}\right) \qquad |p|, |q| > 1. \tag{1.5}$$

Serveral questions of theoretical nature are considered but the concluding numerical section does not relate directly to the traditional orthogonal polynomials with respect to discrete measures.

In [11] several authors describe an algorithm for computing the heat capacity of molecular systems. The resulting formula is a quadrature for series on the special form

$$C_v = \sum_{i=1}^{n} H(\omega_i)/n, \tag{1.6}$$

where

$$H(\omega) = k_B \frac{\left(h\omega c/k_B T\right)^2 e^{-h\omega c/k_B T}}{\left(1 - e^{-h\omega c/k_B T}\right)^2}. \tag{1.7}$$

Again, the classical orthogonal polynomials of discrete measures are not explicitly mentioned.

The present author came across the subject in a computational problem where the unknown is a discrete probability distributions in many dimensions. The *master equation* of chemical reactions [10] can be written as a time-dependent difference equation in the unknown discrete probability density. A natural solution strategy in the continuous case would be a spectral method since the geometry of the problem is simple. The corresponding method in the discrete case then leads to the construction of quadratures with respect to discrete measures.

The rest of the paper deals with these quadrature formulas. We start by reviewing the classical theory of mechanical quadratures aiming specifically at discrete inner products. We comment on some practical aspects on using the resulting formulas and give several illuminating and interesting examples. It will be shown that the formulas work well as a purely numerical tool for summing quite general series and open up interesting possibilities. We finally conclude the paper by a short discussion of the found properties.

2 Excerpts of the classical theory

In this section we will briefly review the link between orthogonal polynomials and Gaussian quadrature formulas. In order to be complete and since the elementary proofs are rather short we generally prefer to give them here. Most of the material presented here is found in the classical literature — see the reference [9] in particular. We have commented those few places were the discrete measure poses a difference to the more common parts of the theory.

To this end, we will use the inner product defined by (1.3) where Ω is a real but possibly unbounded set of points. We assume that there is a (possibly finite) corresponding system $\{p_n\}_{n \geq 0}$ of orthogonal polynomials associated with the product. In practise, this rules out some exotic inner products since they must at least be well-defined for polynomial inputs f and g. It is furthermore reasonable to assume $w(x)$ to be strictly positive since points for which $w(x) = 0$ could just be exclude from Ω.

As usual, we define the norm by $\|f\|^2 = (f, f)$ and we also define λ_n and λ'_n as the coefficients of x^n and x^{n-1} in $p_n(x)$, respectively. We start by giving the three-term recurrence for the polynomials p_n.

Proposition 2.1 *Define the numbers*

$$A_n = \frac{\lambda_{n+1}}{\lambda_n}, \qquad B_n = A_n \left(\frac{\lambda'_{n+1}}{\lambda_{n+1}} - \frac{\lambda'_n}{\lambda_n} \right),$$
$$C_n = \frac{A_n}{A_{n-1}} \cdot \frac{\|p_n\|^2}{\|p_{n-1}\|^2}. \tag{2.1}$$

Then for $n \geq 0$,

$$p_{n+1} = (A_n x + B_n) p_n - C_n p_{n-1}, \tag{2.2}$$

provided that $p_{-1} = 0$ is understood.

Proof. A proof is easily constructed by taking inner products, using orthogonality and checking the leading terms of both sides of (2.2). Refer to [9] for this and some further details. □

The well-known *Christoffel-Darboux*[9] formula follows directly from the recurrence relation.

Proposition 2.2

$$\sum_{i=0}^{n} \frac{p_i(x)p_i(y)}{\|p_i\|^2} = \frac{1}{A_n \|p_n\|^2} \frac{p_{n+1}(x)p_n(y) - p_n(x)p_{n+1}(y)}{x - y}, \tag{2.3}$$

or, for $y \longrightarrow x$,

$$\sum_{i=0}^{n} \frac{p_i(x)^2}{\|p_i\|^2} = \frac{p'_{n+1}(x)p_n(x) - p'_n(x)p_{n+1}(x)}{A_n \|p_n\|^2}. \tag{2.4}$$

Proof. Inserting the recurrence relation (2.2) we find after some simplifications that

$$\frac{1}{A_n \|p_n\|^2} \frac{p_{n+1}(x)p_n(y) - p_n(x)p_{n+1}(y)}{x - y} = \frac{p_n(x)p_n(y)}{\|p_n\|^2} +$$
$$+ \frac{1}{A_{n-1} \|p_{n-1}\|^2} \frac{p_n(x)p_{n-1}(y) - p_{n-1}(x)p_n(y)}{x - y}.$$

Now, (2.3) follows from repeating this formula and (2.4) results by taking limits and using l'Hôpital's rule. □

We now proceed towards finding the abscissas x_i of the summation formula (1.4). The following result is a simple adaption of the well-known result that zeros of orthogonal polynomials are simple and lie in the domain over which the inner product is defined. For this purpose, define $R(\Omega)$ as the smallest real and connected set containing all of Ω.

Proposition 2.3 *If Ω is a real domain with $|\Omega| \geq n$ and if $w(x) > 0$ for $x \in \Omega$, then all the n zeros of p_n are simple and lies in $R(\Omega)$.*

Proof. Suppose that p_n changes sign $m < n$ times in $R(\Omega)$. Then we can find a polynomial q_m of degree $\leq m$ such that $p_n(x)q_m(x) > 0$ in $R(\Omega)$ except for possibly at the zeros of p_n. This implies that $(p_n, q_m) > 0$ and contradicts the orthogonality property. □

Remark. There are two cases when we cannot allow the number of abscissas n to be too large, namely *(i)* when the domain Ω is finite and *(ii)* when the inner product does not exists for polynomials beyond a certain order. As an example of the former case, consider $\Omega = \{0, 1, \ldots, N-1\}$ with $w(x) = 1$ (this is Chebyshev's polynomials, a special case of Hahn's polynomials, cf. Section 3.3). When $n = N$ we must have that the zeros are $x_i = i-1$ and, in fact, the weights in the quadrature are just $w_i = 1$. Trivially, this makes the summation formula exact for any function f and formulas with $n > N$ will not be considered. As an example of the other case, see Section 3.3. □

We now let $\{x_i\}_{1 \leq i \leq n}$ be n distinct points in $R(\Omega)$. Define the usual interpolating polynomials as follows;

$$\pi_n(x) = \prod_{i=1}^{n}(x - x_i), \tag{2.5}$$

$$l_i(x) = \frac{1}{x - x_i}\frac{\pi_n(x)}{\pi_n'(x_i)}, \tag{2.6}$$

so that

$$L(x) = \sum_{i=1}^{n} f(x_i) l_i(x) \tag{2.7}$$

is the Lagrangian interpolant. We now consider approximating the sum

$$I = \sum_{x \in \Omega} f(x) w(x) \tag{2.8}$$

by summing its interpolant,

$$J = \sum_{x\in\Omega} L(x)w(x) = \sum_{i=1}^{n} f(x_i) \sum_{x\in\Omega} l_i(x)w(x) = \sum_{i=1}^{n} f(x_i)w_i \tag{2.9}$$

Regardless of the nature of the abscissas x_i we always have that $I = J$ whenever f is a polynomial of degree $\leq n-1$ since then the Lagrangian interpolant must be exact. If in addition the abscissas are chosen as the roots of p_n we get the usual Gaussian property that the quadrature is exact for all polynomials of degree $\leq 2n-1$. For in this case, $L(x) - f(x)$ is a polynomial of degree $\leq 2n-1$ vanishing at all the zeros of p_n so that it can be written in the form $p_n(x)q_{n-1}(x)$ for some q_{n-1} of degree $\leq n-1$. And hence

$$J - I = \sum_{x\in\Omega} \left(L(x) - f(x)\right) w(x) = (p_n, q_{n-1}) = 0. \tag{2.10}$$

With the aid of the Christoffel-Darboux formula it is possible to find a closed formula for the weights w_i. By the definition (2.9),

$$w_i = \sum_{x\in\Omega} l_i(x)w(x) = \left(\frac{1}{x - x_i} \frac{\pi_n(x)}{\pi_n'(x_i)}, 1 \right). \tag{2.11}$$

Now, π_n is just $p_n(x)/\lambda_n$ and from Proposition 2.2 we have, since $p_n(x_i) = 0$ and after some manipulations,

$$-\frac{A_n\|p_n\|^2}{p_{n+1}(x_i)p_n'(x_i)} \sum_{i=0}^{n-1} \frac{p_i(x)p_i(x_i)}{\|p_i\|^2} = \frac{1}{x - x_i} \frac{p_n(x)}{p_n'(x_i)}. \tag{2.12}$$

Combining (2.11) and (2.12) we arrive at

$$w_i = -\frac{A_n\|p_n\|^2}{p_{n+1}(x_i)p_n'(x_i)}. \tag{2.13}$$

We finally turn our attention to the error term in the summation formula when f is not a polynomial but rather a sufficiently differentiable function. By the basic properties of interpolating polynomials we expect the error term to have the general appearance of

$$R_n = \frac{f^{(2n)}(\xi)}{(2n)!} \cdot K, \tag{2.14}$$

where $\xi \in R(\Omega)$ and where K is a some constant. From the special choice $f(x) = \pi_n(x)^2 = p_n(x)^2/\lambda_n^2$ we see that, in fact,

$$K = \sum_{x\in\Omega} \pi_n(x)^2 w(x) = \frac{\|p_n\|^2}{\lambda_n^2}, \tag{2.15}$$

which is identical to the standard estimate for Gaussian quadratures.

Summarizing our results so far we have just finished the proof of the following theorem.

Theorem 2.4 *Define the abscissas $\{x_i\}_{1\le i\le n} \in R(\Omega)$ as the roots of $p_n(x)$ and let the weights be defined by (2.13). Assume that f is $2n$ times continuously differentiable. Then we have the Gaussian summation formula*

$$\sum_{x\in\Omega} f(x)w(x) = \sum_{i=1}^{n} f(x_i)w_i + R_n, \tag{2.16}$$

with error

$$R_n = \frac{f^{(2n)}(\xi)}{(2n)!} \cdot \frac{\|p_n\|^2}{\lambda_n^2}, \tag{2.17}$$

where $\xi \in R(\Omega)$. In particular, $R_n \equiv 0$ whenever f is a polynomial of degree $\le 2n-1$.

Of course, Theorem 2.4 is nothing else but the usual quadrature theorem for the case when the measure is built up by Dirac delta functions,

$$dw(x) = \sum_{x\in\Omega} w(x)\delta_x. \tag{2.18}$$

It is interesting then that the resulting quadrature formulas seem not to have been investigated before.

2.1 Practical aspects

Turn now to some practical aspects of using Gaussian summation formulas. Firstly, the task of finding the abscissas and weights should in general *not* be performed by a root-finding algorithm. Instead, the usual observation [5] is that the recurrence relation (2.2) can be written in matrix form as

$$x \begin{bmatrix} p_0 \\ p_1 \\ \vdots \\ p_{n-1} \end{bmatrix} = \begin{bmatrix} \alpha_0 & \gamma_0 & & & \\ \beta_1 & \alpha_1 & \gamma_1 & & \\ & \vdots & \vdots & & \\ & & \beta_{n-2} & \alpha_{n-2} & \gamma_{n-2} \\ & & & \beta_{n-1} & \alpha_{n-1} \end{bmatrix} \begin{bmatrix} p_0 \\ p_1 \\ \vdots \\ p_{n-1} \end{bmatrix} + \gamma_{n-1} \begin{bmatrix} 0 \\ 0 \\ \vdots \\ p_n \end{bmatrix}, \tag{2.19}$$

in terms of which

$$\alpha_n = -\frac{B_n}{A_n}, \qquad \beta_n = \frac{C_n}{A_n}, \qquad \gamma_n = \frac{1}{A_n}. \tag{2.20}$$

If $p_n(x) = 0$ this is just an eigenvalue problem for a tridiagonal matrix T which can be symmetrized through a diagonal similar transform,

$$J = DTD^{-1} = \begin{bmatrix} \alpha_0 & \delta_1 & & & & \\ \delta_1 & \alpha_1 & \delta_2 & & & \\ & \vdots & \vdots & & & \\ & & \delta_{n-2} & \alpha_{n-2} & \delta_{n-1} & \\ & & & \delta_{n-1} & \alpha_{n-1} & \end{bmatrix}, \tag{2.21}$$

where

$$\delta_n = \frac{\lambda_{n-1}}{\lambda_n} \cdot \frac{\|p_n\|}{\|p_{n-1}\|}, \tag{2.22}$$

i.e. the associated *Jacobian* matrix. Moreover, if $y^{(i)}$ is the eigenvector corresponding to the abscissa x_i, normalized so that $y^T y = 1$, then the weights can be found according to $y_1^{(i)} = w_i/\mu_0$ where $\mu_0 = \|1\|^2$ is the 0th moment of the measure. This follows as a fairly straightforward application of the second Christoffel-Darboux formula in Proposition 2.2. Finding the eigenvalues and -vectors of a symmetric tridiagonal matrix is a relatively well-conditioned problem for which fast algorithms exist[4].

Building programs with orthogonal polynomials with respect to discrete measures is quite similar to using the classical orthogonal polynomials. —It is straightforward to use the recurrence formula (2.2) to evaluate the polynomials at arbitrary points x and also to use *Clenshaw summation*[2] to evaluate sums of the polynomials times some coefficients.

However, there is one minor difference in the stability of such recursion formulas. For orthogonal polynomials in general, the roots of $p_{n+1}(x)$ are located in between those of $p_n(x)$[9]. For discrete measures, however, as n grows large we must have that the roots converge towards the points in Ω. This means that eventually, the roots of p_n will be quite close to those of p_{n+1}. At points $x \in \Omega$, $p_n(x)$ may well end up as an almost cancelling linear combination of numbers of decreasing magnitude. For high order n, a direct evaluation of the recurrence at points close to points in Ω should therefore be avoided. In such cases, a preferable technique could be to use the backward recursion instead (*Miller's algorithm* [1]).

3 Examples and experiments

In this section we will explicitly give three Gaussian summation formulas. We have not been able to find any of them in the literature despite several searches. The associated polynomials are given in Table 3.1 together with the various coefficients needed to derive each new formula. In subsequent sections we investigate the performance of each case by performing numerical experiments on different sums and comment on various aspects of the usage of the technique.

Name	Parameter(s)	$-A_n$, $-C_n/A_n$	$(-1)^n\lambda_n$, $\|p_n\|^2$
Charlier $C_n(x;a)$	$a>0$	$1/a$ n	a^{-n} $a^{-n}n!$
Meixner $M_n(x;\beta,c)$	$0<c<1$ $\beta>0$	$\frac{1-c}{c(n+\beta)}$ $n/(1-c)$	$\frac{(1-c)^n}{c^n(\beta)_n}$ $\frac{n!}{c^n(\beta)_n}$
Hahn $q_n(x;a,b,c)$	a, b, c $w:=c-a-b$ $w\geq 2n$	$\frac{(w-2n)(w-2n-1)}{(w-n)(a+n)(b+n)}$ $\frac{n(w+a-n)(w+b-n)}{(w-2n)(w-2n+1)}$	$\frac{(w+1-2n)_n}{(a)_n(b)_n}$ See (3.15).

Table 3.1: Orthogonal polynomials with respect to discrete measures. For brevity, we suppress $B_n = 1 + C_n$. With the exception of the Hahn polynomials, we use the notation and normalization in [6] but we have changed the measure so that $\mu_0 = \|1\| = 1$ in all cases. In the numerical computations we also always normalize the polynomials to unity. The inner products are given explicitly in the following sections.

3.1 Charlier's polynomials

Charlier's polynomials [6] are orthogonal with respect to the inner product

$$(f,g) = \sum_{x\geq 0} f(x)g(x)\frac{a^x}{x!}e^{-a}, \qquad a>0. \tag{3.1}$$

The Jacobian matrix is generated by

$$\left.\begin{array}{rcl}\alpha_n &=& n+a\\ \delta_n &=& -\sqrt{na}\end{array}\right\} \tag{3.2}$$

and the summation formula is then of the form

$$\sum_{x\geq 0} f(x)\frac{a^x}{x!}e^{-a} = \sum_{i=1}^{n} f(x_i)w_i + R_n, \tag{3.3}$$

where

$$R_n = a^n n! \frac{f^{(2n)}(\xi)}{(2n)!}. \tag{3.4}$$

As a fairly general numerical example of the Gauss-Charlier summation formula (3.3) we consider the hypergeometric function[1],

$$_3F_3(\bar{a}, \bar{b}, z) = \sum_{j \geq 0} \frac{z^j}{j!} \frac{(\bar{a})_j}{(\bar{b})_j}, \tag{3.5}$$

where as usual

$$([\bar{a}_1, \ldots, \bar{a}_n])_j = \prod_{i=1}^{n} \frac{\Gamma(\bar{a}_i + j)}{\Gamma(\bar{a}_i)} \tag{3.6}$$

(bars are used in order to avoid confusions with the various parameters of the polynomials themselves). In Table 3.2 and 3.3 some typical results with varying argument $a = z$ and order n of the quadrature are displayed. Over all, the numerical behavior of the technique is quite satisfactory.

$a \diagdown n$	6	8	10	14	18
0.5	$1.92 \cdot 10^{-6}$	$1.00 \cdot 10^{-8}$	$3.09 \cdot 10^{-11}$	$9.36 \cdot 10^{-16}$	$2.22 \cdot 10^{-16}$
1.0	$2.27 \cdot 10^{-5}$	$4.88 \cdot 10^{-7}$	$6.11 \cdot 10^{-9}$	$2.97 \cdot 10^{-13}$	$2.02 \cdot 10^{-16}$
4.0	$2.10 \cdot 10^{-5}$	$1.08 \cdot 10^{-5}$	$2.74 \cdot 10^{-6}$	$4.04 \cdot 10^{-8}$	$1.64 \cdot 10^{-10}$
16.0	$3.35 \cdot 10^{-8}$	$3.00 \cdot 10^{-9}$	$4.15 \cdot 10^{-10}$	$2.23 \cdot 10^{-11}$	$3.09 \cdot 10^{-11}$
64.0	$1.05 \cdot 10^{-11}$	$5.81 \cdot 10^{-14}$	$1.83 \cdot 10^{-14}$	$3.82 \cdot 10^{-14}$	$5.85 \cdot 10^{-14}$

Table 3.2: The Gauss-Charlier summation formula where, somewhat arbitrary, $\bar{a} = [1/3, 3/4, 7/5]$ and $\bar{b} = [1/2, 3/5, 1/7]$ were chosen. The table shows the relative errors for different arguments a using different orders n.

3.2 Meixner's polynomials

Meixner's polynomials [6] are associated with the inner product

$$(f, g) = \sum_{x \geq 0} f(x) g(x) c^x \frac{(\beta)_x}{x!} (1 - c)^\beta, \qquad 0 < c < 1, \quad \beta > 0. \tag{3.7}$$

The domain for the coefficients as given above actually formally excludes the special case $\beta = -N$ and $c = -p/q$ which are called *Krawtchouk's*

$a \diagdown n$	6	8	10	14	18
0.5	$1.26 \cdot 10^{-3}$	$9.71 \cdot 10^{-6}$	$4.04 \cdot 10^{-8}$	$1.90 \cdot 10^{-13}$	$8.55 \cdot 10^{-16}$
1.0	$1.27 \cdot 10^{-2}$	$4.23 \cdot 10^{-4}$	$7.33 \cdot 10^{-6}$	$5.73 \cdot 10^{-10}$	$1.24 \cdot 10^{-14}$
4.0	$1.71 \cdot 10^{-1}$	$1.85 \cdot 10^{-2}$	$4.18 \cdot 10^{-3}$	$1.10 \cdot 10^{-4}$	$7.07 \cdot 10^{-7}$
16.0	$4.42 \cdot 10^{-7}$	$1.44 \cdot 10^{-7}$	$3.90 \cdot 10^{-8}$	$5.27 \cdot 10^{-8}$	$1.80 \cdot 10^{-7}$
64.0	$4.46 \cdot 10^{-11}$	$3.01 \cdot 10^{-13}$	$1.44 \cdot 10^{-14}$	$3.46 \cdot 10^{-14}$	$7.76 \cdot 10^{-14}$

Table 3.3: As in Table 3.2 but now $\bar{a} = [-1/3, 3/4, 7/5]$ instead. This induces a single pole in the summand at $x = 1/3$ which means that the truncation error in the form (3.4) could formally be unbounded. This is also seen in the table where the errors in some parts are now considerably larger. For the argument $a = 16$ the relative error drops below 10^{-12} at about $n = 42$.

polynomials. They generate summation formulas for sums on the special form

$$\frac{1}{(p+q)^N} \sum_{x=0}^{N} p^x q^{N-x} \binom{N}{x}. \tag{3.8}$$

It is obvious that this special case in fact corresponds to a well-defined and positive weight-function.

The Jacobian matrix for Meixner's polynomials is given by

$$\left.\begin{array}{rcl} \alpha_n & = & \frac{c(n+\beta)+n}{1-c} \\ \delta_n & = & -\frac{\sqrt{cn(n+\beta-1)}}{1-c} \end{array}\right\} \tag{3.9}$$

and the summation formula readily follows as

$$\sum_{x \geq 0} f(x) c^x \frac{(\beta)_x}{x!} (1-c)^\beta = \sum_{i=1}^{n} f(x_i) w_i + R_n, \tag{3.10}$$

with the truncation error

$$R_n = n!(\beta)_n \frac{c^n}{(1-c)^{2n}} \frac{f^{(2n)}(\xi)}{(2n)!}. \tag{3.11}$$

Again we shall consider the hypergeometric function as a good example representing a wide class of functions. From the presence of $(\beta)_x$ in the inner product it follows that ${}_3F_2(\bar{a}, \bar{b}, z)$ is the natural target in the following experiments.

In Table 3.4 relative errors for varying c are displayed. From the formula for the error (3.11) it seems natural to let β be the smallest positive element in $\bar{a}$ since this minimizes the term $(\beta)_n$. It is seen that the summation formula performs well when c is small but that the errors become quite large when c approaches 1. This is of course reflected in the error formula and comes as no surprise as the general behavior of this type of power series near the boundary of its convergence domain can be very complicated.

$c \diagdown n$	6	8	10	14	18
0.2	$3.47 \cdot 10^{-7}$	$1.02 \cdot 10^{-8}$	$3.23 \cdot 10^{-10}$	$3.59 \cdot 10^{-13}$	$1.84 \cdot 10^{-16}$
0.4	$2.10 \cdot 10^{-5}$	$2.49 \cdot 10^{-6}$	$3.14 \cdot 10^{-7}$	$5.62 \cdot 10^{-9}$	$1.10 \cdot 10^{-10}$
0.6	$2.17 \cdot 10^{-4}$	$5.78 \cdot 10^{-5}$	$1.65 \cdot 10^{-5}$	$1.50 \cdot 10^{-6}$	$1.49 \cdot 10^{-7}$
0.8	$1.01 \cdot 10^{-3}$	$4.76 \cdot 10^{-4}$	$2.41 \cdot 10^{-4}$	$6.93 \cdot 10^{-5}$	$2.19 \cdot 10^{-5}$
0.9	$1.69 \cdot 10^{-3}$	$9.95 \cdot 10^{-4}$	$6.32 \cdot 10^{-4}$	$2.90 \cdot 10^{-4}$	$1.46 \cdot 10^{-4}$

Table 3.4: Relative errors for the Gauss-Meixner summation formula. Here $\bar{a} = [1/3, 3/4, 7/5]$ and $\bar{b} = [1/2, 3/5]$ were chosen and the summation formula uses $\beta = 1/3$ (see text). Evidently, the order n must increase when c approaches 1. For example, when $c = 0.9$, $n = 174$ is needed in order to bring the relative error below 10^{-12}.

The strength of the Gauss-Meixner summation formula lies instead in its behavior when β grows while c is kept fixed. In Table 3.5 we display some typical relative errors for this case and it is seen that the summation formula performs better as β increases.

$\beta \diagdown n$	6	8	10	14	18
4	$3.77 \cdot 10^{-3}$	$2.73 \cdot 10^{-3}$	$1.92 \cdot 10^{-3}$	$7.93 \cdot 10^{-4}$	$2.55 \cdot 10^{-4}$
8	$1.93 \cdot 10^{-4}$	$1.39 \cdot 10^{-4}$	$1.08 \cdot 10^{-4}$	$6.87 \cdot 10^{-5}$	$4.12 \cdot 10^{-5}$
16	$1.93 \cdot 10^{-6}$	$6.47 \cdot 10^{-7}$	$3.12 \cdot 10^{-7}$	$1.33 \cdot 10^{-7}$	$8.24 \cdot 10^{-8}$
32	$2.48 \cdot 10^{-8}$	$2.31 \cdot 10^{-9}$	$3.31 \cdot 10^{-10}$	$1.66 \cdot 10^{-11}$	$1.94 \cdot 10^{-12}$
64	$3.60 \cdot 10^{-10}$	$9.32 \cdot 10^{-12}$	$4.09 \cdot 10^{-13}$	$2.08 \cdot 10^{-15}$	$1.62 \cdot 10^{-14}$

Table 3.5: Convergence behavior when β increases. The parameters are $\bar{a} = [1/3, 3/4, \beta]$, $\bar{b} = [1/2, 3/5]$ and $c = 0.6$.

3.3 Hahn's polynomials

The inner product now contains *three* parameters [6, 3],

$$(f,g) = \sum_{x\geq 0} f(x)g(x)\frac{(a)_x(b)_x}{(c)_x x!}\frac{\Gamma(c-a)\Gamma(c-b)}{\Gamma(c)\Gamma(c-a-b)}, \qquad c-a-b \geq 2n, \quad (3.12)$$

where the general domain of convergence has been indicated as a limitation on n, the order of the corresponding system of orthogonal polynomials. There are, however, some more restrictions on the parameters; — the measure must be *positive* which in fact allows an *even* number of the parameters to be negative. Also, in the case of a *finite* series (when either a or b is a non-positive integer), then n must not be greater than the resulting number of terms. Finally, unless the series terminates soon enough, c can not be a non-positive integer.

One special case of these polynomials is *Chebyshev's* polynomials which correspond to $a = c = 1 - N$ and $b = 1$ for some integer $N \geq 1$. This case produces summation formulas for sums of the simple form

$$\frac{1}{N}\sum_{x=0}^{N-1} f(x). \quad (3.13)$$

We mention also that the definition of the Hahn polynomials as given above differ from the polynomials $Q(x;\alpha,\beta,N)$ defined in [6]. The relation is simply

$$q(x;a,b,c) = Q(x,a-1,b-c,-b), \quad (3.14)$$

but several formulas need to be rearranged with our definition in order to avoid the various singular cases. We prefer the current angle of view since (3.12) more clearly shows the relation to the hypergeometric function ${}_2F_1([a,b],c,1)$. We note also in passing that our definition agrees with that given in the early reference [3].

The formula for $\|q_n\|^2$ that did not fit in Table 3.1 is

$$\|q_n\|^2 = \frac{\sin\pi c\cdot\sin\pi w}{\sin\pi(a+w)\cdot\sin\pi(b+w)}\cdot\frac{(a+w-n)_n(b+w-n)_n}{(a)_n(b)_n}\cdot\frac{n!(w)_{1-n}}{w-2n}, \quad (3.15)$$

where again $w = c - a - b$. The Jacobian is generated according to

$$\left.\begin{array}{rcl} \alpha_n & = & \frac{(1-a-b-c)n^2-(1-a-b-c)wn+(1+w)ab}{(w-2n-1)(w-2n+1)} \\ \delta_n & = & -\sqrt{\frac{n(w+1-n)(a+n-1)(b+n-1)(a+w-n)(b+w-n)}{(w-2n)(w-2n+1)^2(w-2n+2)}} \end{array}\right\}, \quad (3.16)$$

and the summation formula comes as no surprise,

$$\sum_{x\geq 0} f(x)\frac{(a)_x(b)_x}{(c)_x x!}\frac{\Gamma(c-a)\Gamma(c-b)}{\Gamma(c)\Gamma(c-a-b)} = \sum_{i=1}^{n} f(x_i)w_i + R_n. \tag{3.17}$$

The truncation error can be derived from (2.15) with (3.15) and the formula for the leading coefficient λ_n given in Table 3.1.

The usefulness of the Gauss-Hahn formula is very dependent on the parameters. For the *terminating* case when the sum in the inner product (3.12) is finite we are essentially summing polynomials times a combinatorial weight. When the order of the quadrature is sufficiently high the exact answer is obtained but useful approximations often emerge before this point (see Table 3.7 for a simple example). It is more challenging to use the formula for the *non-terminating* case since polynomials of a degree higher than a certain order produces a divergent sum. In Table 3.6 we list some result for the case ${}_4F_3(\bar{a}, \bar{b}, 1)$ where now the order n of the quadrature must be bounded. It is seen that the technique performs quite poorly except for possible the case when c can be chosen fairly large (i.e. when $\bar{b}$ contains a large number). Of course, the problems come from the fact that approximating a smooth function by polynomials of very limited order can be problematic.

$n\diagdown b^*$	6	8	10	12	14
1	$1.60\cdot 10^{-2}$	$1.10\cdot 10^{-2}$	$8.39\cdot 10^{-3}$	$6.78\cdot 10^{-3}$	$5.68\cdot 10^{-3}$
2	$2.93\cdot 10^{-3}$	$1.21\cdot 10^{-3}$	$6.51\cdot 10^{-4}$	$4.07\cdot 10^{-4}$	$2.78\cdot 10^{-4}$
3	-	$4.23\cdot 10^{-4}$	$1.51\cdot 10^{-4}$	$6.99\cdot 10^{-5}$	$3.78\cdot 10^{-5}$
4	-	-	$7.01\cdot 10^{-5}$	$2.29\cdot 10^{-5}$	$9.53\cdot 10^{-6}$
5	-	-	-	$1.25\cdot 10^{-5}$	$3.85\cdot 10^{-6}$
6	-	-	-	-	$2.33\cdot 10^{-6}$

Table 3.6: Hypergeometric summation for ${}_4F_3(\bar{a}, \bar{b}, 1)$ with parameters $\bar{a} = [1/2, 1/3, 1/5, 1/7]$ and $\bar{b} = [1/4, 1/6, b^*]$, where b^* is varied. The parameters (a, b, c) of the summation formula is chosen so as to maximize the available order n of the quadrature.

As a final example we consider the terminating case in the form of the Gauss-Chebyshev formula (3.13) for the two sums

$$H_N \equiv \sum_{x=0}^{N-1} \frac{1}{x+1}, \tag{3.18}$$

$$H_N^{-1/2} \equiv \sum_{x=0}^{N-1} \frac{1}{x-1/2}, \tag{3.19}$$

where the last summand contains a singularity at $x = 1/2$. In Table 3.7 we display some relative errors for the case $N = 1000$ when the order n of the quadrature is increased. Compared to the Gauss-Charlier case, it is now seen that the impact of the singularity in the summand is slightly more problematic. Nevertheless, the convergence for both cases is reasonably monotonic anyway.

n	H_{1000}	$H_{1000}^{-1/2}$
50	$3.11 \cdot 10^{-3}$	$7.77 \cdot 10^{-1}$
60	$7.63 \cdot 10^{-4}$	$3.37 \cdot 10^{-1}$
70	$1.58 \cdot 10^{-4}$	$1.59 \cdot 10^{-1}$
80	$2.76 \cdot 10^{-5}$	$6.59 \cdot 10^{-2}$
90	$4.03 \cdot 10^{-6}$	$2.17 \cdot 10^{-2}$
100	$4.89 \cdot 10^{-7}$	$5.43 \cdot 10^{-3}$
110	$4.94 \cdot 10^{-8}$	$1.03 \cdot 10^{-3}$
120	$4.12 \cdot 10^{-9}$	$1.50 \cdot 10^{-4}$
130	$2.84 \cdot 10^{-10}$	$1.72 \cdot 10^{-5}$
140	$1.62 \cdot 10^{-11}$	$1.55 \cdot 10^{-6}$
150	$7.73 \cdot 10^{-13}$	$1.11 \cdot 10^{-7}$

Table 3.7: Results from the Gauss-Chebyshev formula (3.13) applied to harmonic sums. The table displays relative errors when the order n of the quadrature increases.

4 Conclusions

We have constructed three quite general classes of Gaussian quadratures with respect to discrete measures. The explicit construction follows more or less exactly the same path as for the classical continuous case. Each class of formulas has its own behavior and can be expected to work well in different situations.

We have also seen some difficulties arising in some of the examples; — most notably with the Gauss-Meixner formula when the parameter c approaches 1 and in the Gauss-Hahn formula when the corresponding system of polynomials must be finite due to the slowly decreasing measure. The technique works at its best when the measure, when viewed as a discrete probability distribution, has a well-defined and sharp peak. In this respect, the technique relates loosely to the steepest-descent method[7] in the theory of asymptotics of integrals.

We would finally like to mention that this technique opens up for some quite interesting applications. We immediately think of *discrete spectral methods* for difference equations of various types and also of new representations and algorithms for discrete data sets in general. In the corresponding continuous cases, the existence of mechanical quadratures resides as one of the most important practical tools.

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