Stable Computation of High Order Gauss Quadrature Rules Using Discretization for Measures in Radiation Transfer

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Abstract

The solution of the radiation transfer equation for the Earth's atmosphere needs to account for the reflectivity of the ground. When using the spherical harmonics method, the solution for this term involves an integral with a particular measure that presents numerical challenges. We are interested in computing a high order Gauss quadrature rule for this measure. We show that the two classical algorithms to compute the desired Gauss quadrature rule, namely the Stieltjes algorithm and the method using moments are unstable in this case. In their place, we present a numerically stable method to compute Gauss quadrature rules of arbitrary high order. The key idea is to discretize the measure in the integral before computing the recurrence coefficients of the orthogonal polynomials which lead to the quadrature rule. For discrete measures, one can use a numerically stable orthogonal reduction method to compute the recurrence coefficients. Refining the discretization we arrive at the nodes and weights of the Gauss quadrature rule for the continuous case in a stable fashion. This technique is completely general and can be applied to other measures whenever high order Gauss quadrature rules are needed.

1 Introduction

The standard problem in radiation transport is illustrated in Figure 1. We have a homogeneous, plane parallel layer with internal sources,

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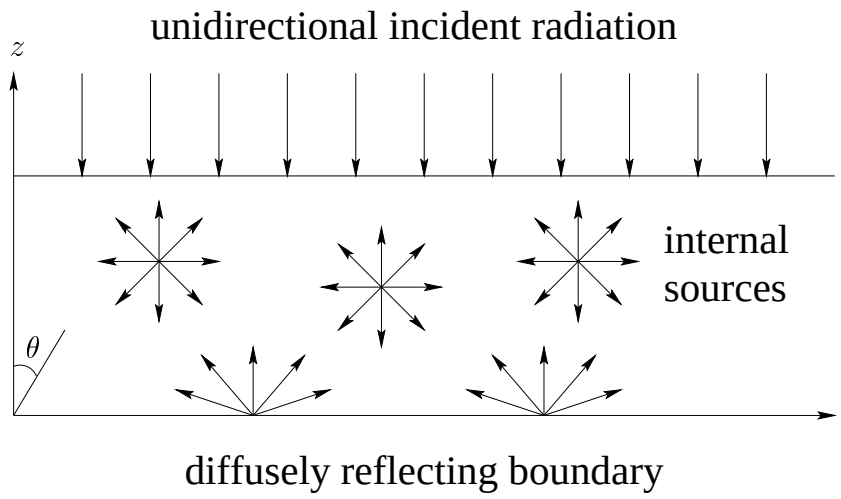

Figure 1: Basic problem of radiation transport.

unidirectional radiation normally incident on the top, and a diffusely reflecting lower boundary. As an example you can think of the earth atmosphere. The sunlight would be the incident radiation on top, thermal radiation would correspond to internal sources and the earth's surface the diffuse boundary underneath. We model the radiation transport in the z dimension only. For convenience we define two new variables: first $\tau := \kappa z$ where the constant κ equals the sum of the scattering and absorption coefficients per unit distance; in our example the scattering and absorption would be caused by tiny particles in the atmosphere. Secondly $\mu := \cos(\theta)$, the cosine of the zenith angle. The specific intensity $I(\tau, \mu)$ is defined as the amount of radiation moving in a particular direction μ at a point τ in space. The governing equation for $I(\tau, \mu)$ is

$$\mu \frac{dI}{d\tau} = I - \frac{\omega}{2} \int_{-1}^{1} P(\mu, \mu') I(\tau, \mu') d\mu' + S, \tag{1.1}$$

where ω is the fraction of the radiation that is scattered on each interaction, $P(\mu, \mu')$ describes how the radiation changes direction when it is scattered, and S represents all internal sources. To get an understanding for equation (1.1) we look at a special case: Suppose there are no sources, $S \equiv 0$, and the radiation is not scattered in the interior, $\omega \equiv 0$. Then the equation for the specific intensity simplifies to

$$\frac{dI}{d\tau} = \frac{1}{\mu} I,$$

with the exponential solution $I(\tau, \mu) = Ce^{\tau/\mu}$. For each direction μ we have to determine the constant C using the given boundary conditions.

We distinguish two cases:

1. If $0 < \mu \leq 1$ the equation describes radiation coming from above, because in that case $-\frac{\pi}{2} < \theta < \frac{\pi}{2}$. So the top boundary condition is used to determine C. Since the incident radiation on top is normal, the only non-zero solution is obtained for $\theta = 0 \Leftrightarrow \mu = 1$, and the specific intensity decays exponentially from the top to the bottom boundary in the direction $\mu = 1$ and is zero in all the other directions.

2. If $-1 \leq \mu \leq 0$ the equation describes radiation coming from the diffusely reflecting boundary at the bottom. So we need the bottom boundary condition to determine C. This boundary condition has to be computed using the incident radiation from the top. For each value of μ we get how much of the normally incident radiation is scattered into that direction at the bottom boundary. Using this value we get for each direction μ an exponentially decaying solution.

If there is some scattering, $\omega \neq 0$, equation (1.1) is more complicated, since now each direction is coupled to all the other directions by the integral. The whole system has to be solved simultaneously for all directions μ.

Chandrasekhar [3] proposed replacing the integral in equation (1.1) with a quadrature sum and solving the resulting system of equations for the specific intensity at a number of discrete ordinates, the Discrete Ordinates Method.

A different method to solve equation (1.1) is the spherical harmonics method which was proposed by Jeans [9] long before Chandrasekhar's Discrete Ordinates Method. It has a number of computational advantages and is the spectral analogue of the Discrete Ordinates Method. The key idea is to expand the intensity $I(\tau, \mu)$ and the kernel $P(\mu, \mu')$ in orthogonal polynomials such that the integral in equation (1.1) is replaced by an orthogonality condition. Write

$$I(\tau, \mu) = \sum_{k=0}^{n} f_k(\tau) P_k(\mu), \tag{1.2}$$

and as shown in Chandrasekhar [3]

$$P(\mu, \mu') = \sum_{k=0}^{n} \beta_k P_k(\mu) P_k(\mu'), \tag{1.3}$$

where the β_k are known quantities that depend on the type of scattering particle and $P_k(\mu)$ is the k-th Legendre polynomial that satisfies the standard recurrence relations and orthogonality condition [1].

Substituting equations (1.2) and (1.3) into equation (1.1) and using the recurrence relation of $P_k(\mu)$ involving the derivative [9] gives us the system of ordinary differential equations

$$\frac{k+1}{2k+1}\frac{df_{k+1}}{d\tau} + \frac{k}{2k+1}\frac{df_{k-1}}{d\tau} + \left(\frac{\omega\beta_k}{2k+1} - 1\right) f_k = s_k, \tag{1.4}$$

where s_k is the expansion coefficient of the internal sources.

There are two kinds of boundary conditions that are normally treated separately: the uni-directional solar illumination and the ground reflectivity. We are interested in the latter. In each case, we compute a pseudo-source that represents the effect of one scattering of the radiation from the boundary condition.

We assume that the ground reflects the incoming radiation with some angular distribution $h(\mu)$. The corresponding source term is shown in [4] to be

$$s_{k,\mathrm{g}}(\tau) = \frac{-R_g\beta_k}{2k+1}\int_0^1 e^{-(\tau_0-\tau)/\mu} h(\mu)P_k(\mu)d\mu, \tag{1.5}$$

where R_g is the reflectivity of the ground. Specular reflection, $h(\mu) = \delta(\mu - \mu_0)$, is usually treated separately. We will assume that $h(\mu)$ is piecewise continuous. The numerical evaluation of the integral in equation (1.5),

$$S_k(c) := \int_0^1 e^{-c/\mu} h(\mu)P_k(\mu)d\mu, \tag{1.6}$$

where $c := \tau_0 - \tau$, is the subject of this paper.

2 Earlier Work

If $h(\mu)$ is a constant, $h(\mu) \equiv H$, we can use the exponential integral [1]

$$E_j(c) := \int_1^\infty e^{-cx}\frac{1}{x^j}d\mu \tag{2.1}$$

to integrate (1.6). Let a_k be the coefficients of the polynomial $P_k(\mu)$,

$$P_k(\mu) = \sum_{j=0}^{k} a_j\mu^j.$$

Inserting this expression into $S_k(c)$ and using the exponential integral (2.1) we obtain

$$S_k(c) = H \cdot \sum_{j=0}^{k} a_j E_{j+2}(c), \tag{2.2}$$

Unfortunately, the coefficients a_j of $P_k(\mu)$ vary widely in magnitude and differ in sign making the summation numerically unstable. Table 1 shows how the positive and negative components in the sum balance each other and lead to cancellation.

k	positive part	negative part
5	0.31593286828701e+00	-0.32273434246716e+00
10	1.06529837121543e+01	-1.06537713711572e+01
25	1.60087271890534e+06	-1.60087271891255e+06
50	2.14468963201455e+15	-2.14468963201455e+15

Table 1: Positive and negative values in the sum (2.2) summed separately reveal cancellation

Dave [5] used Simpson's rule between the zeros of $P_k(\mu)$ and Karp, Greenstadt and Fillmore [10] used a 50-point Gauss quadrature to evaluate this integral. While for both approaches the absolute accuracy is good and the methods are efficient, neither of these approaches is mathematically elegant.

More than a decade passed with no further publications in this area until Settle [11] derived a 5-term recurrence relation that is valid when $h(\mu) = \mu^r$, where $r > -1$ is a real number. Hence, any reflectivity of this form can be computed. The backward recurrence of

$$\begin{aligned} 0 \;=\; & (2k+3)(k-1)(k-r-2)S_{k-2} \\ & -c(2k-1)(2k+3)S_{k-1} \\ & +(2k+1)(2k^2+2k-3-r)S_k \\ & +c(2k-1)(2k+3)S_{k+1} \\ & +(k+2)(k+r+3)(2k-1)S_{k+2} \end{aligned} \tag{2.3}$$

is only mildly unstable, allowing the evaluation of the integral for this class of reflectivity coefficients.

3 Gauss Quadrature Rule

Our approach is to note that the integral can be viewed as integrating a polynomial over a finite interval with the non-negative measure

$$w(\mu) := e^{-c/\mu} h(\mu) \geq 0, \tag{3.1}$$

since the angular distribution $h(\mu)$ is in general non-negative [1]. It is always possible to derive Gauss quadrature rules for non-negative

[1] If a certain model requires $h(\mu)$ to attain negative values as well, one would exclude $h(\mu)$ from the measure and integrate it together with $P_k(\mu)$ when the quadrature rule is applied.

measures [6]. The nodes and weights can be obtained from the polynomials which are orthogonal on the finite interval under the given measure $w(\mu)$.

It is well known that the orthogonal polynomials $\pi_k(\mu)$ satisfy a three term recurrence relation

$$\begin{aligned} \pi_{k+1}(x) = (x - \alpha_k)\pi_k(x) - \beta_k \pi_{k-1}(x), \quad k = 0, 1, \ldots \\ \pi_0(x) = 1, \quad \pi_{-1}(x) = 0 \end{aligned} \tag{3.2}$$

and from the recurrence coefficients α_k and β_k the Golub-Welsch algorithm [8] computes in a stable fashion the nodes and weights of the desired Gauss quadrature rule. It is thus essential to be able to compute the recurrence coefficients α_k and β_k in the recurrence relation (3.2) to compute a Gauss quadrature rule for a given measure $w(\mu)$ [7].

3.1 Continuous Measures

There are two classical methods to compute the recurrence coefficients α_k and β_k for continuous measures $w(\mu)$: the Stieltjes algorithm and the method of moments.

The Stieltjes algorithm uses the fact that the recurrence coefficients α_k and β_k can be expressed in terms of the orthogonal polynomials (3.2) and the related inner product

$$(f, g) = \int_a^b f(\mu) g(\mu) w(\mu) d\mu. \tag{3.3}$$

The relations are

$$\begin{aligned} \alpha_k = \tfrac{(x\pi_k, \pi_k)}{(\pi_k, \pi_k)}, \quad k \geq 0; \\ \beta_0 = (\pi_0, \pi_0), \quad \beta_k = \tfrac{(\pi_k, \pi_k)}{(\pi_{k-1}, \pi_{k-1})}, \quad k > 0. \end{aligned} \tag{3.4}$$

To compute the orthogonal polynomials the following iterative procedure can be used: compute α_0 and β_0 using the known initial polynomial $\pi_0 = 1$. Then use the recurrence relation for the polynomials (3.2) to compute π_1. With π_1 we can compute α_1, β_1 using (3.4) and so on. This procedure can however exhibit instabilities for measures $w(\mu)$ arising in applications. We will show in Section 4 that we can only obtain low order quadrature rules with the Stieltjes algorithm in our application.

The second method, the method of moments, uses the fact that the first n recursion coefficients α_k and β_k, $k = 0, 1, \ldots, n-1$ are uniquely determined by the first $2n$ moments m_k, $k = 0, 1, \ldots, 2n-1$ of the given measure $w(\mu)$,

$$m_k := \int_a^b \mu^k w(\mu) d\mu.$$

Formulas are known which express α_k and β_k in terms of Hankel determinants in these moments. Unfortunately this algorithm is unstable as well for the measures in our application, as will be shown in Section 4. In fact, we were not able to compute Gauss quadrature rules of the order required in our application using the classical two methods.

3.2 Discrete Measures

For discrete measures

$$w(\mu) = \sum_{i=1}^{n} w_i \delta(\mu - \mu_i)$$

there is a third method to compute the orthogonal polynomials which is based on an observation by Boley and Golub [2], that the tridiagonal matrix containing the desired recurrence coefficients

$$J_n := \begin{bmatrix} 1 & \sqrt{\beta_0} & & & 0 \\ \sqrt{\beta_0} & \alpha_0 & \sqrt{\beta_1} & & \\ & \sqrt{\beta_1} & \alpha_1 & \ddots & \\ & & \ddots & \ddots & \sqrt{\beta_{n-1}} \\ 0 & & & \sqrt{\beta_{n-1}} & \alpha_{n-1} \end{bmatrix}$$

is orthogonally similar to the matrix

$$A_n := \begin{bmatrix} 1 & \sqrt{w_1} & \sqrt{w_2} & \dots & \sqrt{w_n} \\ \sqrt{w_1} & \mu_1 & & & \\ \sqrt{w_2} & & \mu_2 & & \\ \vdots & & & \ddots & \\ \sqrt{w_n} & & & & \mu_n \end{bmatrix},$$

where w_i are the values of the discrete measure at the nodes μ_i. Hence the desired entries of the matrix J_n can be obtained by applying Givens rotations or Householder reflections to the matrix A_n. This process is by its definition numerically stable.

Thus for cases where the two classical methods for continuous measures fail and it is impossible to compute the needed Gauss quadrature rule, we propose to benefit from the stability of the discrete algorithm to obtain the desired recurrence coefficients. We discretize the measure $w(\mu)$ and compute a sequence of approximations to the inner product (3.3) by a sum using a suitable quadrature scheme Q^i, $i = 1, 2, \ldots$,

$$(f,g) = \int_a^b f(\mu)g(\mu)w(\mu)d\mu \approx Q^i(f \cdot g) = \sum_{j=1}^{N_i} f(\mu_j^i)g(\mu_j^i)w_j^i,\ N_{i+1} > N_i. \tag{3.5}$$

Then we compute the recurrence coefficients $\tilde{\alpha}_k^i$ and $\tilde{\beta}_k^i$ of the discrete measure w^i in a stable fashion using the Boley-Golub algorithm. The obtained recurrence coefficients are an approximation of the recurrence coefficients of the continuous measure,

$$\tilde{\alpha}_k^i \approx \alpha_k, \quad \tilde{\beta}_k^i \approx \beta_k.$$

By refining the discretization of the measure using higher and higher order quadrature schemes Q^i as i increases in (3.5), we can compute an approximation to the recurrence coefficients α_k and β_k up to a required accuracy. Furthermore there is no need to implement this discretization procedure: the procedure 'mcdis' from the ORTHPOL package by Gautschi [7] which was designed to compute quadrature rules for measures with continuous and discrete parts uses discretization to achieve its goal. Applied to a measure with continuous part only it performs precisely the calculations we need. The stability of these calculations when every other method fails for continuous measures is in our opinion a new result. Indeed we were not able to find this result when we searched for a way to compute the high order Gauss quadrature rules in our application described in the following section.

4 Numerical Experiments

We perform numerical experiments with the methods described in the previous section on the integral of radiation transfer (1.6). We illustrate in the following how the two classical algorithms fail to compute the desired Gauss quadrature rule whereas the discretization procedure succeeds. We choose as a first example

$$h(\mu) := 1 \text{ and } c := 3/2 \tag{4.1}$$

Using the Stieltjes algorithm we can directly compute the recurrence coefficients α_k and β_k with the iterative algorithm given in Section 3.1. However this process becomes very quickly unstable as k increases. Table 2 shows the results of this algorithm which required 60 digits of accuracy in Maple and several hours computing time on a workstation to obtain 14 correct digits for $k = 50$.

Table 3 shows the results of the Stieltjes algorithm with standard double precision for the example measure (4.1) and compares the results with the accurate results obtained by Maple in Table 2. Clearly the algorithm becomes unstable and there are only one resp. no significant digits left for $k = 10$. Thus the high order Gauss quadrature rules needed in our application can not be obtained with this algorithm.

k	α_k exact	β_k exact
0	.77618166448162	.073100786538480
1	.65768094525413	.026905634469467
2	.61907537016101	.034688131374812
3	.59820380841666	.039286039184924
4	.58473406996687	.042328606983553
5	.57516985728672	.044518321400496
6	.56795457810211	.046185049938023
7	.56227743900237	.047505066032515
8	.55766990937508	.048581848115053
9	.55384032530538	.049480524061563
10	.55059662985707	.050244336338481
20	.53318631545529	.054385798780231
30	.52572641062310	.056182700835241
40	.52142039580247	.057226424055389
50	.51856195909407	.057922028958190

Table 2: Coefficients α_k and β_k computed with the the Stieltjes algorithm and 60 digits accuracy in Maple.

k	α_k double precision	err α_k	β_k double precision	err β_k
0	.77618166448164	1.1e-14	.073100786538480	8.4e-16
1	.65768094525488	7.4e-13	.026905634469455	1.2e-14
2	.61907537016421	3.2e-12	.034688131374769	4.2e-14
3	.59820380936326	9.4e-10	.039286039151921	3.3e-11
4	.58473407735886	7.3e-09	.042328606683491	3.0e-10
5	.57517005348101	1.9e-07	.044518309567765	1.1e-08
6	.56795473056972	1.5e-07	.046185091997963	4.2e-08
7	.56230484613302	2.7e-05	.047502893642560	2.1e-06
8	.55788886824010	2.1e-04	.048560599223896	2.1e-05
9	.55735849056603	3.5e-03	.049247351793347	2.3e-04
10	.56153846153846	1.0e-02	.049056603773584	1.1e-03

Table 3: Coefficients α_k and β_k with standard double precision using the Stieltjes algorithm and the absolute error.

k	α_k double precision	err α_k	β_k double precision	err β_k
0	.77618166448162	1.1e-16	.073100786538480	0.0
1	.65768094525413	1.1e-16	.026905634469466	5.8e-17
2	.61907537016083	1.7e-13	.034688131374815	2.8e-15
3	.59820380840887	7.7e-12	.039286039185180	2.5e-13
4	.58473406966937	2.9e-10	.042328606993016	9.4e-12
5	.57516984500899	1.2e-08	.044518321810482	4.0e-10
6	.56795409444963	4.8e-07	.046185066228693	1.6e-08
7	.56225946568115	1.7e-05	.047505737782324	6.7e-07
8	.55751834547536	1.5e-04	.048599725384848	1.7e-05
9	.58382382821813	2.9e-02	.049051912565198	4.2e-04

Table 4: Coefficients α_k and β_k with standard double precision using the method of moments compared with the accurate values from Maple.

To use the method of moments, we note that for the constant reflectivity, the moments

$$m_k := \int_0^1 \mu^k dw(\mu) = \int_0^1 \mu^k e^{-c/\mu} d\mu$$

can be obtained explicitly using the exponential integral (2.1). Thus the method of moments would be ideal in this case to compute the recurrence coefficients α_k and β_k. However the method becomes unstable as well as k increases. We show the results obtained using the method of moments for the example measure (4.1) in Table 4. Again there are only one resp. two significant digits left for $k = 9$ and thus we can not compute the Gauss quadrature rules we need in our application.

Using however the discrete algorithm, we are able to compute the recurrence coefficients to full accuracy. Table 5 shows for the example weight (4.1) that the computation is numerically stable. To compute accurate results with the Stieltjes procedure for $k = 50$ we needed 60 digits of accuracy in Maple and several hours of computation, whereas the discretization procedure achieves the same accuracy with standard double precision in a few seconds. Figure 2 shows that even for large values of k there is no instability in the computation of the recurrence coefficients α_k and β_k. For such large k we were not able to perform the computations in Maple and thus the discretization method was the only approach which allowed us to compute the desired Gauss quadrature rule.

To test the robustness of the discretization method, we applied the

k	α_k double precision	α_k exact	β_k double precision	β_k exact
0	.77618166448162	6.6e-16	.073100786538480	4.1e-17
1	.65768094525413	5.5e-16	.026905634469467	1.0e-17
2	.61907537016101	6.6e-16	.034688131374812	3.4e-17
3	.59820380841666	0.0	.039286039184924	5.5e-17
4	.58473406996687	3.3e-16	.042328606983553	1.5e-16
5	.57516985728672	2.2e-16	.044518321400496	4.1e-17
6	.56795457810211	6.6e-16	.046185049938023	1.3e-16
7	.56227743900237	2.2e-16	.047505066032515	1.1e-16
8	.55766990937508	4.4e-16	.048581848115054	1.8e-16
9	.55384032530538	4.4e-16	.049480524061563	6.9e-17
10	.55059662985706	1.1e-15	.050244336338481	1.0e-16
20	.53318631545529	3.3e-16	.054385798780232	1.0e-16
30	.52572641062310	6.6e-16	.056182700835242	7.6e-17
40	.52142039580247	7.7e-16	.057226424055389	9.0e-17
50	.51856195909408	6.6e-16	.057922028958190	2.0e-17

Table 5: Coefficients α_k and β_k with standard double precision using the discretization method compared with the accurate values from Maple.

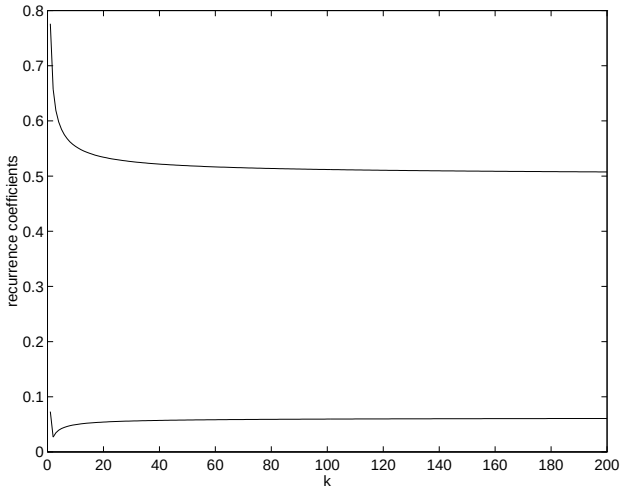

Figure 2: Coefficients α_k and β_k of the three term recurrence relation for the example measure (4.1).

algorithm to the following set of test measures from our application:

$$
\begin{aligned}
w_1(\mu) &= 2\mu e^{-5/\mu} \\
w_2(\mu) &= \begin{cases} 0 & \text{if } \mu \le a \\ \frac{1}{1-a} e^{-1/\mu} & \text{otherwise} \end{cases} \\
w_3(\mu) &= \frac{2\mathrm{erf}(b)}{\sqrt{\pi} b} e^{-b^2(1-\mu)^2} e^{-3/2\mu} \\
w_4(\mu) &= 2\sin^2(2\pi\mu) e^{-2/\mu}
\end{aligned}
$$

Note that the last three measures can not be integrated using the five term recurrence by Settle [11], since the corresponding reflectivity can not be represented in the required form. The discretization method computes again the recurrence coefficients in a stable fashion, as one can see in Figure 3 whereas with standard double precision, the Stieltjes algorithm lost all accuracy after 6 steps for w_1 and after 8 steps for the other measures. We used again 60 digits of accuracy in Maple to check our calculations, but we were only able to verify the accuracy of the discretization procedure for moderate values of k since the calculations became infeasible for k large.

Having the coefficients for the recurrence relation of the orthogonal polynomials with respect to our measure, the Golub-Welsch algorithm [8] computes in a stable fashion the nodes and weights for a Gauss Quadrature rule which is exact for polynomials up to order $2n-1$.

We have used the nodes and weights to evaluate the integral for $c = 3/2$, $h(\mu) = 1$ and k up to 199. The absolute accuracy is good, but as k increases, the value of the integral decreases causing the relative accuracy to suffer. Beyond $k = 100$ the value of the integral is less than 10^{-12}, and only few significant digits are left, as one can see in table 6. Fortunately, the computed intensity is insensitive to such

Degree of the Polynomial	Gauss Quadrature	Maple with high precision arithmetic
20	-1.238295799049847e-05	-1.238295799049653e-05
40	2.269755760984558e-07	2.269755759420927e-07
60	-6.058218490188644e-09	-6.058218535653499e-09
80	-6.269748923528706e-10	-6.269748390677194e-10
100	1.327424746795755e-10	1.327425275730553e-10
120	5.190009477008340e-12	5.190243346208851e-12
150	1.587570576573345e-12	1.587741096646863e-12
199	-2.350507619488032e-14	not feasible

Table 6: Integration using a Gauss Rule with 100 nodes

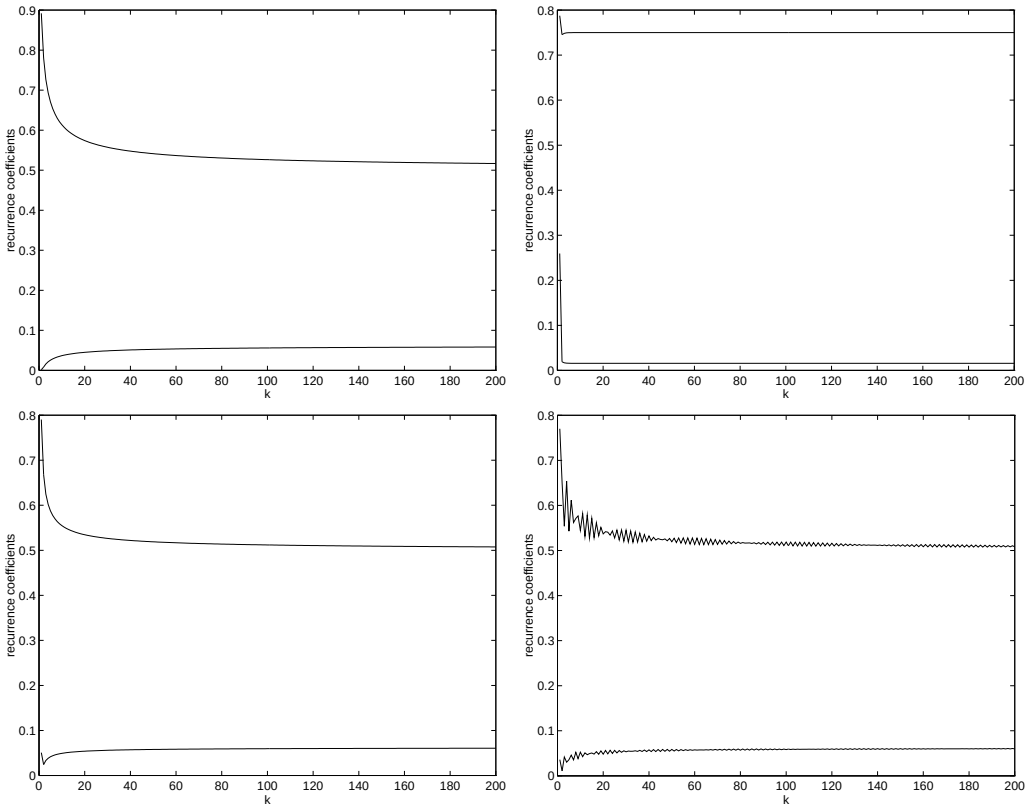

Figure 3: Coefficients α_k and β_k of the three term recurrence relation, from top left to bottom right for the measures w_1, w_2 with $a = 1/2$ and w_3 with $b = 1$ and w_4.

small contributions.

5 Conclusions

We have shown how to derive Gauss quadrature rules for an integral important in radiation transport. To overcome the numerical instabilities of the traditional Stieltjes algorithm and the method using moments we discretized the measure and applied the numerically stable orthogonal reduction method. By refining the discretization, we are able to compute high order quadrature rules for this particular integral.

Our approach makes no use of the form of the measure. Hence the method of discretization is a numerically stable tool for computing Gauss quadrature rules of high order for non-negative measures in general.

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