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NUMERICAL CONSTRUCTION OF THE GENERALIZED HERMITE POLYNOMIALS

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In this paper we are concerned with polynomials orthogonal with respect to the generalized Hermite weight function $w(x) = |x - z|^\gamma \exp(-x^2)$ on $\mathbb{R}$, where $z \in \mathbb{R}$ and $\gamma > -1$. We give a numerically stable method for finding recursion coefficients in the three term recurrence relation for such orthogonal polynomials, using some nonlinear recurrence relations, asymptotic expansions, as well as the discretized Stieltjes-Gautschi procedure.

1. INTRODUCTION

The main purpose of this paper is the construction and investigation of a stable numerical method for finding recursion coefficients in the fundamental three term recurrence relation for polynomials orthogonal with respect to the following weight function

$$w(x) = w(x; z) = |x - z|^\gamma e^{-x^2} \quad \text{on} \ \ \mathbb{R}, \tag{1}$$

where $\gamma > -1$ and $z \in \mathbb{R}$. This weight function is a direct generalization of the generalized Hermite weight function $w(x; 0) = |x|^\gamma \exp(-x^2)$, $\gamma > -1$.

Knowing the first n of these recursion coefficients, one can easily obtain the corresponding N-point Gaussian quadrature formula for any N, with $1 \le N \le n$, using QR algorithm (cf. [**2**], [**4**]).

Applications of the previous weight functions, as well as the corresponding orthogonal polynomials, are various. Such weights appear frequently as density functions for some random variables in statistical mechanics, quantum mechanics, etc.

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2. NONLINEAR RECURRENCE RELATIONS

By $\pi_n = \pi_n(\cdot; z)$ we denote monic orthogonal polynomial of degree n with respect to weight function $w = w(\cdot; z)$. Then, since the weight function w is positive, we know that the monic orthogonal polynomials can be constructed (see [**1**]) and they satisfy the following orthogonality condition

$$\int_{\mathbb{R}} \pi_n(x)\pi_m(x)w(x)\,\mathrm{d}x = ||\pi_n||^2\delta_{n,m}, \quad ||\pi_n|| > 0, \quad n, m \in \mathbb{N}_0. \tag{2}$$

Using Favard theorem (see e.g., [**1**]), we know that the monic orthogonal polynomial sequence satisfy the following three term recurrence relation

$$\pi_{n+1}(x) = (x - \alpha_n)\pi_n(x) - \beta_n\pi_{n-1}(x),\ n \in \mathbb{N}_0,\ \pi_0(x) = 1,\ \pi_{-1}(x) = 0. \tag{3}$$

It is known that the recursion coefficients are such that $\alpha_n \in \mathbb{R}$ and $\beta_n > 0,\ n \in \mathbb{N}_0$, where β_0 can be chosen arbitrarily. Sometimes, it is convenient to define it by $\beta_0 = \int_{\mathbb{R}} w(x)\,\mathrm{d}x$.

By simple change of the variable $x := -x$ in (2), it can be seen that $\pi_n(x; z) = (-1)^n\pi_n(-x; -z)$, as well as $\alpha_n(z) = -\alpha_n(-z),\ \beta_n(z) = \beta_n(-z),\ n \in \mathbb{N}_0$. Thus, we will consider only the case when $z > 0$.

Defining $s_n,\ n \in \mathbb{N}_0$, in the following way

$$s_n = \int_{\mathbb{R}} (x - z)\pi_n^2 w\,\mathrm{d}x,$$

and using (3), we have ([**1**], [**4**])

$$\alpha_n - z = \frac{1}{||\pi_n||^2}\int_{\mathbb{R}} (x - z)\pi_n^2 w\,\mathrm{d}x = \frac{s_n}{||\pi_n||^2}, \quad \beta_n = \frac{||\pi_n||^2}{||\pi_{n-1}||^2}, \quad n \in \mathbb{N}_0,$$

where we put, by convention, $||\pi_{-1}|| = 1$. Also, it can be proved easily, using the three term recurrence relation (3), that the following holds

$$||\pi_n||^2 = \int_{\mathbb{R}} (x - z)\pi_n\pi_{n-1}w\,\mathrm{d}x, \quad n \in \mathbb{N}.$$

Replacing in this equation π_n, expressed from the three term recurrence relation, we get the following relation

$$\beta_n + \beta_{n-1} + (\alpha_{n-1} - z)^2 = \frac{1}{||\pi_{n-1}||^2}\int_{\mathbb{R}} (x - z)^2\pi_{n-1}^2 w\,\mathrm{d}x, \quad n \in \mathbb{N}.$$

Also, applying the same transformation to the definition of s_n, we get the second recurrence relation for the three term recurrence coefficients, i.e.,

$$\alpha_n + \alpha_{n-1} - 2z = \frac{1}{||\pi_n||^2}\int_{\mathbb{R}} (x - z)^2\pi_n\pi_{n-1}w\,\mathrm{d}x, \quad n \in \mathbb{N}.$$

These relations are know for a long time, although, in a different settings $z = 0$. They are presented, for example, in [**2**] and [**3**].

It is a basic fact that integrals appearing on the right hand sides of the equations can be integrated by parts which enables an interpretation of these integrals over three term recurrence coefficients.

First, note that for each $x \in \mathbb{R}\backslash\{z\}$ we have that the following is satisfied

$$[(x-z)|x-z|^\gamma]' = (\gamma+1)|x-z|^\gamma,$$

so that, for the first integral, we have

$$\begin{aligned}\beta_n \;+\; \beta_{n-1} + (\alpha_{n-1}-z)^2 &= \frac{1}{||\pi_{n-1}||^2}\int_{\mathbb{R}} (x-z)^2\pi_{n-1}^2 w\,\mathrm{d}x \\ &= -z(\alpha_{n-1}-z) - \frac{1}{2||\pi_{n-1}||^2}\int_{\mathbb{R}} (x-z)|x-z|^\gamma \pi_{n-1}^2 (e^{-x^2})'\,\mathrm{d}x \\ &= -z(\alpha_{n-1}-z) + \frac{1}{2||\pi_{n-1}||^2}\int_{\mathbb{R}} \left[(\gamma+1)\pi_{n-1}^2 + 2(x-z)\pi_{n-1}\pi_{n-1}'\right] w\,\mathrm{d}x \\ &= -z(\alpha_{n-1}-z) + \frac{1}{2}(2n-1+\gamma).\end{aligned}$$

This gives the following relation

$$\beta_n + \beta_{n-1} + \alpha_{n-1}(\alpha_{n-1}-z) = \frac{2n-1+\gamma}{2}. \tag{4}$$

For the second integral, applying the same integration by parts, substituting

$$(x-z)\pi_{n-1} = \pi_n + (\alpha_{n-1}-z)\pi_{n-1} + \beta_{n-1}\pi_{n-2}$$

and

$$\pi_n' = \pi_{n-1} + (x-\alpha_{n-1})\pi_{n-1}' - \beta_{n-1}\pi_{n-2}',$$

we get

$$\begin{aligned}||\pi_n||^2(\alpha_n \;+\; \alpha_{n-1}-z) &= \frac{1}{2}\int_{\mathbb{R}} (x-z)\pi_n'\pi_{n-1} w\,\mathrm{d}x \\ &= \frac{1}{2}\left[(\alpha_{n-1}-z)||\pi_{n-1}||^2 + (n-1)(\alpha_{n-1}-z)||\pi_{n-1}||^2\right. \\ &\quad \left.+\beta_{n-1}(z-\alpha_{n-1})(n-1)||\pi_{n-2}||^2\right] + \frac{\beta_{n-1}}{2}\int_{\mathbb{R}} (x-z)\pi_{n-1}'\pi_{n-2} w\,\mathrm{d}x \\ &= \left[\frac{1}{2}(\alpha_{n-1}-z) + \beta_{n-1}(\alpha_{n-1}+\alpha_{n-2}-z)\right]||\pi_{n-1}||^2,\end{aligned}$$

i.e.,

$$\beta_n(\alpha_n + \alpha_{n-1} - z) = \frac{1}{2}(\alpha_{n-1}-z) + \beta_{n-1}(\alpha_{n-1}+\alpha_{n-2}-z). \tag{5}$$

As in [**3**], multiplying (5) by α_{n-1} and substituting $\alpha_{n-1}(\alpha_{n-1}-z)$ from (4), we obtain

$$\alpha_n\alpha_{n-1}\beta_n-\left(\frac{n+\gamma/2}{2}-\beta_n\right)^2=\alpha_{n-1}\alpha_{n-2}\beta_{n-1}-\left(\frac{n-1+\gamma/2}{2}-\beta_{n-1}\right)^2.$$

It is clear, this quantity is independent on n. For $n=1$, from (4) and (5), we find

$$\beta_1+\alpha_0(\alpha_0-z)=\frac{\gamma+1}{2},\quad \beta_1(\alpha_1+\alpha_0-z)=\frac{1}{2}(\alpha_0-z),$$

which after some manipulation gives

$$\alpha_1\alpha_0\beta_1-\left(\frac{1+\gamma/2}{2}-\beta_1\right)^2=\alpha_n\alpha_{n-1}\beta_n-\left(\frac{n+\gamma/2}{2}-\beta_n\right)^2=-\frac{\gamma^2}{16}. \quad (6)$$

Note that choosing a combination (4) and (6), as starting values we need only α_0, i.e., we need only s_0 and $||\pi_0||^2$.

In order (4) and (5) to be applicable for calculations we need the coefficient α_0, which can be expressed in an explicit form

$$\alpha_0=-z\left((\gamma+1)\frac{{}_1F_1(-\gamma/2,3/2,-z^2)}{{}_1F_1(-\gamma/2,1/2,-z^2)}+1\right).$$

Also, we have

$$\beta_0=\int_{\mathbb{R}}w(x)\,\mathrm{d}x=e^{-z^2}\Gamma\left(\frac{1+\gamma}{2}\right){}_1F_1\left(\frac{1+\gamma}{2},\frac{1}{2},z^2\right).$$

3. NUMERICAL CONSTRUCTION OF THREE TERM RECURRENCE COEFFICIENTS

In this section we give a numerical methods for construction recursion coefficients α_n and β_n for the weight function w. Our method depends strongly on z. According to the range z, different methods should be applied in construction of the three term recurrence coefficients.

All computations, presented in this section, are performed in double precision arithmetic with machine precision (m.p. $\approx 2.22\times10^{-16}$).

Case $\mathbf{z}\in(\mathbf{0},\mathbf{5})$. Given α_0 the construction proceeds straightforward. Namely, for a given α_{n-1} we calculate β_n using (4), and then for such β_n we calculate α_n using (5).

It is an amazing fact, this construction works for the weight function w, provided z is sufficiently small. As an example, we present results for $z=1/3$ and $\gamma=-1/2$ in Table 1. Numbers in parentheses indicate decimal exponents, i.e., $x(m)=x\times10^m$.

n	α_n	$r_n^{(1)}$	$r_n^{(2)}$	β_n
0	1.604974533946931(−1)	m.p.	m.p.	3.433209278590652
1	−1.383113351931182(−1)	m.p.	m.p.	2.777397185853827(−1)
2	1.163735907797128(−1)	m.p.	m.p.	9.070264775740081(−1)
3	−9.784310002138714(−2)	m.p.	m.p.	1.368221906721599
4	7.984368934809036(−2)	1(−15)	4(−16)	1.839590454382810
5	−6.455428349329288(−2)	7(−16)	4(−16)	2.430649094004505
6	4.995871370080372(−2)	7(−16)	5(−16)	2.793665555980398
7	−3.752641420292943(−2)	8(−16)	7(−16)	3.470491475511898
8	2.586370101338528(−2)	7(−16)	1(−15)	3.765591487990863
9	−1.593470946824870(−2)	5(−15)	4(−16)	4.492360814650156
10	6.789555242436285(−3)	1(−14)	9(−15)	4.752073700561257
11	9.604656281837112(−4)	2(−13)	1(−14)	5.500143386459166
12	−7.954348185129339(−3)	4(−14)	6(−15)	5.750175846256006
13	1.382125980653763(−2)	3(−14)	5(−16)	6.497109432693900
14	−1.898687887021462(−2)	2(−14)	7(−16)	6.757306626685639
15	2.323925670588782(−2)	2(−14)	1(−15)	7.486003912121723
16	−2.686128871467686(−2)	1(−14)	7(−16)	7.771202443727997
17	2.974176256843383(−2)	1(−14)	2(−15)	8.469122264535697
18	−3.207084600755667(−2)	1(−14)	2(−15)	8.789907083879770
19	3.379754383265745(−2)	2(−14)	2(−15)	9.448374094954070
20	−3.505402513131707(−2)	1(−14)	2(−15)	9.811749479021028
21	3.582208040587151(−2)	1(−14)	2(−15)	1.042533706125729(1)
22	−3.619929812410516(−2)	1(−14)	1(−15)	1.083532041076673(1)
23	3.618238733331904(−2)	1(−14)	7(−16)	1.140130276734056(1)
24	−3.584956518330079(−2)	9(−15)	3(−16)	1.185944886328407(1)
25	3.520144786001178(−2)	9(−15)	m.p.	1.237731609033100(1)
26	−3.430625453994549(−2)	8(−15)	m.p.	1.288317858369090(1)
27	3.316229361164631(−2)	9(−15)	m.p.	1.335420907902856(1)
28	−3.183311728564849(−2)	8(−15)	m.p.	1.390574528112441(1)
29	3.031176214840014(−2)	1(−14)	m.p.	1.433263033242426(1)
30	−2.865973918507802(−2)	1(−14)	9(−16)	1.492655478536734(1)
99	−5.853017337313245(−4)	4(−12)	1(−12)	4.949983398795690(1)
100	−2.527116010163625(−4)	1(−11)	3(−12)	4.974997056888707(1)
101	1.074640398629048(−3)	2(−12)	7(−13)	5.049994513004944(1)
199	−8.458109437422345(−3)	2(−13)	3(−15)	9.928135827367433(1)
200	8.739329900268865(−3)	2(−13)	1(−15)	9.996575081689794(1)

Table 1: Recursion coefficients for $z = 1/3$, $\gamma = -1/2$ and the relative errors in α-coefficients: $r_n^{(1)}$ (using (4) and (5)) and $r_n^{(2)}$ (using (7) and (5))

As it can be seen in this case, the maximal relative error in α-coefficients is of order $1(-12)$. However, β-coefficients are constructed with machine precision. It is important to say that the error is not propagated. The maximal relative error for α-coefficients appears for $n = 100$, but for $n = 200$ the relative error in α_{200} is of order $1(-15)$.

A construction can be even improved if the equation (4) is rewritten in the form

$$\begin{aligned} \beta_n - \beta_{n-2} + \alpha_{n-1}(\alpha_{n-1} - z) \;&-\; \alpha_{n-2}(\alpha_{n-2} - z) \\ &= \frac{2n-1+\gamma}{2} - \frac{2n-3+\gamma}{2} = 1. \end{aligned} \tag{7}$$

Using this equation instead of (4) for the calculation of β_n, we save at least one significant digit in the calculation.

Increasing γ produces even better results. For example, taking $\gamma = 10$ and $z = 1/3$ gives the maximal relative error in α-coefficients of order of magnitude $1(-14)$, while β-coefficients are given with machine precision (in our case, m.p. $\approx 2.22 \times 10^{-16}$).

It is important to say that since the limit of α-coefficients is zero, the errors in α-coefficients should be measured as absolute errors instead of relative errors. Using this criterion, the error in α-coefficients have a magnitude of $1(-15)$, i.e., only one significant digit is lost and the error is not propagated.

A reason for such good results can be understood straightforward. It is known that for the weight function w, the asymptotical behavior of the three term recurrence coefficients is given by

$$\alpha_n \to 0, \quad \beta_n \to \frac{n}{2}, \qquad n \to +\infty.$$

If we look at equation (7) it can be seen clearly that asymptotically it really reduces to $\beta_n \approx \beta_{n-2} + 1$, which means no cancellation effect is present. Also, investigating (5) it can be seen clearly that we have the following asymptotic form $\alpha_n \approx \alpha_{n-2} + O(1/n)$, which again makes it asymptotically perfect for calculations.

There is one more effect which makes calculation stable. It seems that α-coefficients satisfy the condition $\alpha_n \alpha_{n-1} < 0$, which disables the cancellation of significant digits since in (7) we do not have a subtraction of the terms $\alpha_n(\alpha_n - z)$, but rather their addition, since two terms are of different signs.

Equation (6) is not useful for calculations, which can be easily understood, since it has serious cancellation problems. Namely, as $n \to +\infty$ it is clear that the term $((n + \gamma/2)/2 - \beta_n)^2 - \gamma^2/16$ introduces a cancellation of significant digits which grows linearly with n.

The system of equations (7) and (5) gives good results for a sufficiently small z and it can be used for a construction provided $z < 5$. For example, taking $z = 5$, $\gamma = -1/2$, we get the maximal relative error in α-coefficients of order $1(-7)$, and for β-coefficients of order $1(-12)$, for first 200 coefficients.

Case z > 50. To understand what is happening with calculations when z is increased, we introduce

$$g_n = \frac{n+\gamma/2}{2} - \beta_n, \quad n \in \mathbb{N}.$$

According to (4) it is clear that α-coefficients can be given by

$$\alpha_n(\alpha_n - z) = g_{n+1} + g_n.$$

Using $\alpha_n \to 0,\ n \to +\infty$, we know that

$$\alpha_n = \frac{z}{2}\big(1 - \sqrt{1+4G_n'}\,\big), \quad G_n' = \frac{g_{n+1}+g_n}{z^2}, \quad n \in \mathbb{N}.$$

To have shorter expressions we introduce $Y = n + \gamma/2$.

Using all previously defined quantities, and using squaring to the equation (5) to eliminate square roots, we have

$$\begin{aligned}
&A_n = \beta_n - \beta_{n-1} - 1/2, \quad G_n = z^2 G_n',\\
&z^2 B_n = \beta_n^2(z^2+4G_n) + \beta_{n-1}^2(z^2+4G_{n-2}) - (z^2+4G_{n-1})A_n^2,\\
&z^4 C_n = (z^2B_n)^2 + 4\beta_n^2\beta_{n-1}^2(z^2+4G_n)(z^2+4G_{n-2}) - z^2(z^2+4G_{n-1})A_n^2,\\
&(z^4C_n)^2 - 16\beta_n^2\beta_{n-1}^2(z^2B_n)^2(z^2+4G_n)(z^2+4G_{n-2}) = 0. \qquad (8)
\end{aligned}$$

The last equation is really an equation to which (5) is transformed. It can be checked (using some computer algebra, for example Mathematica, Maple), that highest term in Y survives. For z small enough, the equation can always be written in terms of two most dominant terms in Y, which are Y^8 and Y^7. It becomes

$$Y^8(G_n - G_{n-2}) + 2Y^7\big\{4[G_{n-2}(1+2g_{n-1}) - 2g_nG_n] + z^2(1+2g_{n-1}-2g_n)\big\} = 0$$

or it can be rewritten in the form

$$g_{n+1} = -g_n + \frac{YG_{n-2}}{Y-16g_n} - \frac{8G_{n-2}(1+2g_{n-1}) - 2z^2(1+2g_{n-1}+2g_n)}{Y-16g_n}. \qquad (9)$$

This clearly shows that this equation is stable, since the error in g_n is not amplified when g_{n+1} is evaluated. Note, also that for $z=0$, three term recurrence coefficients are $\alpha_k = 0,\ k \in \mathbb{N}_0,\ \beta_{2k} = k,\ \beta_{2k-1} = (2k-1+\gamma)/2,\ k \in \mathbb{N}$, we have $g_{2k} = \gamma/4$ and $g_{2k-1} = -\gamma/4,\ k \in \mathbb{N}$. Letting z to be very close to zero, the values for g_n are not changed to much, we can expect lost of significant digits in α-coefficients, since $\alpha_n \approx G_n/z$. Actually, this effect does not take place or rather is very hard to catch it. For example, taking $z = 1(-10),\ \gamma = -1/2$, the maximal relative error in α-coefficients does not exceed $1(-15)$, while with $z = 1(-5),\ \gamma = -1/2$, it produces the maximal relative error of the order $1(-12)$. A full effect of the loss of significant digits in α-coefficients, as $z \to 0$, can be seen if we choose γ close to zero. However, this loss of significant digits appears only in α-coefficients and can be fully understood, since in that case, also, we have that α-coefficients are nearly zero. For example, with $z = 1(-5)$ and $\gamma = 1(-10)$ there are only $5-6$ significant digits in α-coefficients and almost all 16 in β-coefficients. This can be understood in site of (9), since in this case G_{n-2} is calculated with a very small precision.

An analysis for large z and n relatively small can also be performed using the same definition for g_n and (8). It turns out that the coefficient with z^8 is cancelled out identically which really produces loss of significant digits in calculations. Also, the corresponding term with z^6 is

$$32\Big(g_{n-1} - \frac{Y-1}{2}\Big)\Big(g_{n-1} - \frac{Y}{2}\Big)\Big(g_n - \frac{Y-1}{2}\Big)\Big(g_n - \frac{Y}{2}\Big)\Big[1 + 2(g_{n-1} - g_n)\Big] \times$$
$$\times (g_n - g_{n-1})\big[2g_ng_{n+1} - 2g_{n-1}g_{n-2} - G_{n-2} + Y(G_{n-2} - G_n)\big],$$

and the term with z^4 is to complicated to be written. It can be seen that degree of Y which appears in the coefficient with z^6 is Y^5, and in the coefficient with z^4 is Y^6. From this information it can be understood that while $n < z^2$ the dominant terms in (8) are those with z^6 and z^4. When n becomes larger then z^2 again the equation is dominated by the terms in Y. However, equation (8) is unstable for numerical calculations while $n < z^2$, this because of the fact that term with z^8 is cancelled out. Taking $z = 10, \gamma = -1/2$, it produces complete loss of significant digits in α- and β-coefficients for $n = 10$. In each iteration two significant digits are lost. Note that we are using n rather than $Y = n + \gamma/2$ for the reasons we discuss in the sequel.

To understand fully behavior of g_n for large z, we use equation (6), which we transform into the form

$$A_n = 4\frac{g_n^2 - \gamma^2/16}{\beta_n},$$
$$4A_n^2(z^2 + 4G_n)(z^2 + 4G_{n-1}) = \big[(A_n - z^2)^2 - z^4 + 16G_nG_{n-1}\big]^2.$$

Performing all calculations we get the following reduced form

$$a_n = g_n^2 - \gamma^2/16,$$
$$z^2 a_n\beta_n(a_n + \beta_nG_n)(a_n + \beta_nG_{n-1}) - \big(a_n^2 - \beta_n^2G_nG_{n-1}\big)^2 = 0. \tag{10}$$

It is clear that the original equation (6) is not stable for calculation for large z, since terms with z^8, z^6, z^4 are identically cancelled out. What can be seen from this equation is the behavior of g_n. In order for two terms to be comparable, g_n is very close to $\gamma/4$ for small n. This conclusion can be drown, also, from the definition of $g_n = (n + \gamma/2)/2 - \beta_n$. For large z it is clear that the influence of the factor $|x - z|^\gamma$ in w is almost neglectful, for small powers of x, since, the influence of $|x - z|^\gamma$ to the moments of w is neglectful. For small values of n and large z, it is quite understandable that β-coefficients are almost the same as for the Hermite weight $w(x; 0) = \exp(-x^2)$, i.e., $n/2$.

According to the fact $g_n \approx \gamma/4$, it can be easily understood, why we need that z^2 has to be dominated by n instead of $n + \gamma/2$. If latter is the case, then we know that $g_n \approx \gamma/4$. Applying this to equation (9) we can easily find that the second term is amplified for $Y \approx 16 g_n$, which produces an amplification of error in g_{n+1} of the term G_{n-2}, but also of the term with z^2, i.e., term $1 + 2g_{n-1} - 2g_n$. This causes a loss of significant digits when Y instead of n dominates z.

Performing all numerical calculations in an extended precision (using Mathematica, for example, we can work with 1000 digits length in mantissa), a typical behavior of the sequence g_n is given in Figure 1 for $z = 1,\ \gamma = -1/2$ (top) and for $z = 10,\ \gamma = -1/2$ (bottom).

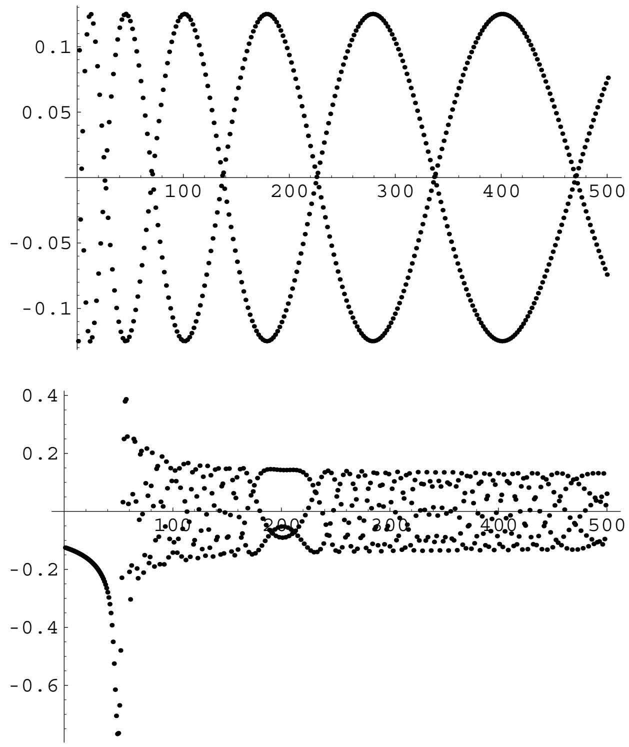

Figure 1: The sequence g_n for $z = 1,\ \gamma = -1/2$ (top) and $z = 10,\ \gamma = -1/2$ (bottom)

The pick in Figure 1 (bottom) can be explained using equation (10). As it can be seen from the figure for $z = 10,\ \gamma = -1/2$, when $n < z^2/2$, the sequence g_n has quite different behavior than for $n > z^2/2$. For $n > z^2/2$ the behavior is pretty much the same as for $z = 1,\ \gamma = -1/2$. Substituting $d_n = g_n - \gamma/4$, performing all calculations and neglecting all terms, except linear in terms of the sequence $\{d_n\}$

(note that for small n we have $d_n \approx 0$), we can develop the following relation

$$d_n \approx n \frac{\gamma/4 + (d_{n+1} + d_{n-1})/2}{z^2/2 - n + \gamma}.$$

It is clear that the mentioned pick in the sequence g_n appears for $z^2/2 - n + \gamma \approx 0$. This point also shows that "the transient regime" ends for $n > z^2/2 + \gamma$. After this point, the calculation can be continued using equations (7) and (5), and this calculation is numerically stable.

For a large z, we can search for an asymptotic formula for g_n.

Lemma. *Let*

$$\begin{aligned}
a_n^{(1)} &= \frac{\gamma n}{4}, \quad a_n^{(2)} = \frac{3}{8}\gamma n(n-\gamma), \quad a_n^{(3)} = \frac{5}{16}\gamma n(2n^2 - 5\gamma n + 2\gamma^2 + 1),\\
a_n^{(4)} &= \frac{7}{32}\gamma n(n-\gamma)(5n^2 - 17\gamma n + 5\gamma^2 + 10),\\
a_n^{(5)} &= \frac{9}{64}\gamma n \left[14n^4 - 93\gamma n^3 + (70 + 164\gamma^2)n^2 - (167 + 93\gamma^2)\gamma n\right.\\
&\qquad \left. +21 + 70\gamma^2 + 14\gamma^4\right],\\
a_n^{(6)} &= \frac{11}{128}\gamma n(n-\gamma)\left[(42n^4 - 344\gamma n^3 + (420 + 686\gamma^2)n^2 - (1300 + 344\gamma^2)\gamma n\right.\\
&\qquad \left. +483 + 420\gamma^2 + 42\gamma^4\right],\\
a_n^{(7)} &= \frac{13}{256}\gamma n \left[132n^6 - 1586\gamma n^5 + (2310 + 5868\gamma^2)n^4 - (14065 + 8885\gamma^2)\gamma n^3\right.\\
&\qquad +(6468 + 24169\gamma^2 + 5868\gamma^4)n^2 - (15018 + 14065\gamma^2 + 1586\gamma^4)\gamma n\\
&\qquad \left. +1485 + 6468\gamma^2 + 2310\gamma^4 + 132\gamma^6\right]
\end{aligned}$$

and

$$\begin{aligned}
\Delta_n \;=\; & \frac{15}{32768}\gamma^4 n^4 (n-\gamma)\big[429n^6 - 6047\gamma n^5 + (12012 + 25341\gamma^2)n^4\\
& -(88144 + 40613\gamma^2)\gamma n^3 + (66066 + 167972\gamma^2 + 25341\gamma^4)n^2\\
& -(192906 + 88144\gamma^2 + 6047\gamma^4)\gamma n + 56628 + 66066\gamma^2 + 12012\gamma^4 + 429\gamma^6\big].
\end{aligned}$$

Then, choosing

$$g_n = \frac{\gamma}{4} + \frac{a_n^{(1)}}{z^2} + \frac{a_n^{(2)}}{z^4} + \frac{a_n^{(3)}}{z^6} + \frac{a_n^{(4)}}{z^8} + \frac{a_n^{(5)}}{z^{10}} + \frac{a_n^{(6)}}{z^{12}} + \frac{a_n^{(7)}}{z^{14}},$$

the left hand side in equation (10) *reduces to*

$$z^2 a_n \beta_n (a_n + \beta_n G_n)(a_n + \beta_n G_{n-1}) - \left(a_n^2 - \beta_n^2 G_n G_{n-1}\right)^2 = \frac{\Delta_n}{z^{14}} + O\left(\frac{1}{z^{16}}\right).$$

Proof. The proof can be given by a direct calculation. However, a such calculation can be done hardly by hand, instead some computer algebra should be used. We used MATHEMATICA. □

Using this Lemma for a large z we can give some asymptotic formulae for coefficients α_n and β_n. For α-coefficients we have

$$\alpha_n \approx \frac{1}{2}\left(\frac{A_n^{(1)}}{z}+\frac{A_n^{(2)}}{z^3}+\frac{A_n^{(3)}}{z^5}+\frac{A_n^{(4)}}{z^7}+\frac{A_n^{(5)}}{z^9}+\frac{A_n^{(6)}}{z^{11}}+\frac{A_n^{(7)}}{z^{13}}\right), \tag{11}$$

where

$$\begin{aligned}
A_n^{(1)} &= -\gamma, \quad A_n^{(2)} = \frac{1}{2}(\gamma^2 - 4Sa_n^{(1)}), \quad A_n^{(3)} = \frac{1}{2}(-4Sa_n^{(2)} + 4\gamma Sa_n^{(1)} - \gamma^3),\\
A_n^{(4)} &= \frac{1}{8}\left(16(Sa_n^{(1)})^3 - 16Sa_n^{(3)} + 16Sa_n^{(2)} - 24\gamma^2 Sa_n^{(1)} + 5\gamma^4\right),\\
A_n^{(5)} &= \frac{1}{8}\Big(32Sa_n^{(1)}Sa_n^{(2)} - 16Sa_n^{(4)} - 48\gamma(Sa_n^{(1)})^2 + 16\gamma Sa_n^{(3)} - 24\gamma^2 Sa_n^{(2)}\\
&\quad +40\gamma^3 Sa_n^{(1)} - 7\gamma^5\Big),\\
A_n^{(6)} &= \frac{1}{16}\Big(-64(Sa_n^{(1)})^2 + 32(Sa_n^{(2)})^2 + 64Sa_n^{(1)}Sa_n^{(3)} - 32Sa_n^{(5)} - 192\gamma Sa_n^{(1)}Sa_n^{(2)}\\
&\quad +32\gamma Sa_n^{(4)} + 240\gamma^2(Sa_n^{(1)})^2 - 48\gamma^2 Sa_n^{(3)} + 80\gamma^3 Sa_n^{(2)} - 140\gamma^4 Sa_n^{(1)} + 21\gamma^6\Big),\\
A_n^{(7)} &= \frac{1}{16}\Big(-192(Sa_n^{(1)})^2 Sa_n^{(2)} + 64Sa_n^{(2)}Sa_n^{(3)} + 64Sa_n^{(1)}Sa_n^{(4)} - 32Sa_n^{(6)} + 32\gamma Sa_n^{(5)}\\
&\quad +320\gamma(Sa_n^{(1)})^3 - 96\gamma(Sa_n^{(2)})^2 - 192\gamma Sa_n^{(1)}Sa_n^{(3)} + 480\gamma^2 Sa_n^{(1)}Sa_n^{(2)}\\
&\quad -48\gamma^2 Sa_n^{(4)} - 560\gamma^3(Sa_n^{(1)})^2 + 80\gamma^3 Sa_n^{(3)} - 140\gamma^4 Sa_n^{(2)} + 252\gamma^5 Sa_n^{(1)} - 33\gamma^7\Big)
\end{aligned}$$

and $Sa_n^{(\nu)} = a_n^{(\nu)} + a_{n+1}^{(\nu)}$. For β-coefficients we have

$$\beta_n \approx \frac{n}{2} - \left(\frac{a_n^{(1)}}{z^2}+\frac{a_n^{(2)}}{z^4}+\frac{a_n^{(3)}}{z^6}+\frac{a_n^{(4)}}{z^8}+\frac{a_n^{(5)}}{z^{10}}+\frac{a_n^{(6)}}{z^{12}}+\frac{a_n^{(7)}}{z^{14}}\right). \tag{12}$$

These asymptotic formulae for α- and β-coefficients can be successfully applied for $z > 50$. For example, the error introduced in α_{100} for $z = 50$, $\gamma = -1/2$, is of order $1(-10)$, and for β_{100} it is of order $6(-11)$. For achieving all 16 significant digits, z has to be bigger than 140, with γ which is not significantly bigger than 1 in modulus. As an example, in Table 2 we present three term recurrence coefficients for $z = 200$, $\gamma = -1/2$.

Case $\mathbf{z} \in (\mathbf{4}, \mathbf{50})$. In order to calculate three term recurrence coefficients in this case, we apply the discretized STIELTJES-GAUTSCHI procedure (see [**2**]). The basic idea of this procedure is to use DARBOUX formulas for recursion coefficients

$$\alpha_k = \frac{\displaystyle\int_{\mathbb{R}} x\pi_k^2 w\,\mathrm{d}x}{\displaystyle\int_{\mathbb{R}} \pi_k^2 w\,\mathrm{d}x}, \quad \beta_k = \frac{\displaystyle\int_{\mathbb{R}} \pi_k^2 w\,\mathrm{d}x}{\displaystyle\int_{\mathbb{R}} \pi_{k-1}^2 w\,\mathrm{d}x}, \tag{13}$$

which are a direct consequence of the three term recurrence relation (3), and numerically calculate the integrals in (13). For these integrals we use a Gaussian quadrature rule with respect to some appropriate weight function W which is not very different from w. Such approach provides a sufficiently good approximation for integrals of the form $\int_{\mathbb{R}} Pw\,\mathrm{d}x$, where P is an algebraic polynomial.

n	α_n	β_n
0	1.250023438671966(−3)	1.253320012386169(−1)
1	1.250054691992686(−3)	5.000031251757959(−1)
2	1.250085947657757(−3)	1.000006250586008
3	1.250117205667472(−3)	1.500009376230666
4	1.250148466022123(−3)	2.000012502109800
5	1.250179728722005(−3)	2.500015628223438
6	1.250210993767411(−3)	3.000018754571609
7	1.250242261158633(−3)	3.500021881154344
8	1.250273530895966(−3)	4.000025007971671
9	1.250304802979701(−3)	4.500028135023618
10	1.250336077410134(−3)	5.000031262310220
11	1.250367354187558(−3)	5.500034389831500
12	1.250398633312265(−3)	6.000037517587491
13	1.250429914784550(−3)	6.500040645578220
14	1.250461198604707(−3)	7.000043773803718
15	1.250492484773028(−3)	7.500046902264014
16	1.250523773289809(−3)	8.000050030959137
17	1.250555064155342(−3)	8.500053159889117
18	1.250586357369922(−3)	9.000056289053983
19	1.250617652933842(−3)	9.500059418453764
20	1.250648950847397(−3)	1.000006254808849(1)

Table 2: Recursion coefficients for $z = 200$, $\gamma = -1/2$, calculated using asymptotic expansions (11) and (12)

Let $z \in (4, 50)$ and $w(x) = w(x; z)$, defined by (1). Then, for W we take

$$W(x) = w(x; \lambda z/2) = |x - \lambda z/2|^{\gamma} e^{-x^2}, \quad \lambda \in (0, 2),$$

supposing that we know the three term recurrence relation for this weight, i.e., we know its recursion coefficients α_n and β_n for $n \leq N - 1$, where N is a sufficiently large integer.

n	α_n	r_n	β_n	r_n
0	9.626084279022080(−3)	1(−13)	3.477033700324542(−1)	m.p.
1	9.640398301791682(−3)	2(−13)	5.001855297560273(−1)	3(−15)
2	9.654776418649182(−3)	2(−13)	1.000371888811139	2(−15)
3	9.669219109647301(−3)	1(−13)	1.500559083366045	3(−15)
4	9.683726859890307(−3)	2(−13)	2.000747119686594	8(−15)
5	9.698300159602592(−3)	2(−12)	2.500936004104657	8(−15)
6	9.712939504198404(−3)	1(−12)	3.001125743019025	5(−15)
7	9.727645394352736(−3)	2(−13)	3.501316342896322	1(−14)
8	9.742418336073406(−3)	5(−13)	4.001507810271931	m.p.
9	9.757258840774342(−3)	4(−13)	4.501700151750942	7(−15)
10	9.772167425350108(−3)	4(−13)	5.001893374009104	6(−15)
11	9.787144612251691(−3)	2(−12)	5.502087483793809	2(−15)
12	9.802190929563576(−3)	1(−13)	6.002282487925074	9(−16)
13	9.817306911082116(−3)	2(−12)	6.502478393296560	6(−16)
14	9.832493096395256(−3)	6(−13)	7.002675206876590	5(−15)
15	9.847750030963625(−3)	2(−12)	7.502872935709196	1(−15)
16	9.863078266203000(−3)	2(−13)	8.003071586915185	1(−14)
17	9.878478359568210(−3)	2(−12)	8.503271167693208	1(−14)
18	9.893950874638483(−3)	2(−13)	9.003471685320866	m.p.
19	9.909496381204272(−3)	5(−13)	9.503673147155826	m.p.
20	9.925115455355587(−3)	1(−12)	1.000387556063696(1)	1(−15)
21	9.940808679571879(−3)	2(−12)	1.050407893328549(1)	7(−15)
22	9.956576642813490(−3)	2(−12)	1.100428327270618(1)	2(−15)
23	9.972419940614706(−3)	2(−12)	1.150448858658853(1)	5(−15)
24	9.988339175178452(−3)	3(−12)	1.200469488270798(1)	m.p.
25	1.000433495547267(−2)	2(−12)	1.250490216892718(1)	5(−15)
26	1.002040789732838(−2)	1(−12)	1.300511045319721(1)	3(−15)
27	1.003655862353951(−2)	2(−12)	1.350531974355890(1)	6(−15)
28	1.005278776396452(−2)	5(−13)	1.400553004814412(1)	7(−15)
29	1.006909595562978(−2)	5(−12)	1.450574137517713(1)	1(−14)
30	1.008548384283489(−2)	3(−12)	1.500595373297588(1)	8(−15)
⋮				
98	1.143104074095088(−2)	5(−12)	4.902338279503830(1)	1(−15)
99	1.145504513978333(−2)	1(−11)	4.952369359553401(1)	3(−15)
100	1.147920159484019(−2)	3(−12)	5.002400636004121(1)	5(−15)
⋮				
198	1.499584025371824(−2)	8(−12)	9.906948217740761(1)	3(−15)
199	1.505024651932378(−2)	3(−12)	9.957018479396415(1)	2(−15)
200	1.510525109465832(−2)	2(−11)	1.000708951056180(2)	1(−15)
⋮				
297	2.823005489474894(−2)	2(−12)	1.487392040210585(2)	2(−14)
298	2.860594484503885(−2)	2(−11)	1.492439804702057(2)	4(−14)
299	2.899774410369597(−2)	6(−11)	1.497489557956849(2)	1(−13)

Table 3: Three term recurrence coefficients for $z = 26,\ \gamma = -1/2$

Then, we have

$$\begin{aligned}\int_{\mathbb{R}} P(x)w(x)\,\mathrm{d}x &= \int_{\mathbb{R}} P\Big(x+\frac{2-\lambda}{2}z\Big)\,\Big|\,x-\frac{\lambda z}{2}\,\Big|^{\gamma}\, e^{-(x+(2-\lambda)z/2)^2}\,\mathrm{d}x \\ &= e^{-(1-\lambda/2)^2z^2}\int_{\mathbb{R}} e^{-(2-\lambda)zx} P\Big(x+\frac{2-\lambda}{2}z\Big)W(x)\,\mathrm{d}x \\ &\approx e^{-(1-\lambda/2)^2z^2}\sum_{k=1}^{N} A_k e^{-(2-\lambda)zx_k} P\Big(x_k+\frac{2-\lambda}{2}z\Big),\end{aligned}$$

where A_k and x_k, $k=1,\ldots,N$, are weights and nodes of the corresponding N-point Gauss-Christoffel quadrature formula with respect to the weight function W.

Thus, applying the discretized Stieltjes-Gautschi procedure, we construct recursion coefficients for the weight $w = w(\cdot\,; z)$.

Choosing $N = 500$ and $(2-\lambda)z = 12$, it turns out that to the precision of the $A_k,\ x_k,\ k=1,\ldots,N$, we can construct safely 300 recursion coefficients. Choosing $(2-\lambda)z$ smaller, a bigger number of three term recurrence coefficients can be constructed.

An example with $\lambda z/2 = 20$, i.e., $z = 26,\ \lambda = 40/26,\ \gamma = -1/2$, is presented in Table 3. Starting with 500 recursion coefficients for the weight with $z = 20$, we can construct to the precision of $A_k,\ x_k,\ k=1,\ldots,N$, coefficients for the weight function with $z = 26$.

We keep repeating "to the precision of $A_k,\ x_k,\ k=1,\ldots,N$," since it is known that QR-algorithm, which is standardly used for the construction of Gaussian quadrature rules given in [**2**], can return weights $A_k,\ k=1,\ldots,N$, which precision can be significantly harmed (see [**5**]). There is significant error introduced in $A_k,\ k=1,\ldots,500$, which reduces precision of the constructed three term recurrence coefficients. For example, using modified version of QR-algorithm presented in [**5**], the relative error introduced in weights for $z = 20,\ \gamma = -1/2$, is of order $1(-11)$. This error causes errors in constructed recursion coefficients presented in Table 3.

The most important thing here is that the construction of coefficients using this discretized procedure does not depend on γ. Thus, it means that what is said for $\gamma = -1/2$ stays valid for all $\gamma > -1$.

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