Numerical computation of classical Gaussian quadrature rules

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Gauss-quadratures: basic ideas

Given $I(f) = \int_a^b f(x)w(x)dx$, with $w(x)$ a weight function, the n-point quadrature rule

$$Q_n(f) = \sum_{i=1}^{n} w_i f(x_i)$$

is a Gaussian quadrature if $I(f) = Q_n(f)$ for f any polynomial with $\deg(f) \leq 2n-1$.

Gaussian quadrature rules are optimal in a very specific sense and they are one of the more widely used methods of integration.

The difficulty is, of course, computing the nodes x_i and weights w_i.

As it is well known, the nodes x_i, $i = 1, \ldots, n$ of the Gaussian quadrature rule are the roots of the (for instance monic) orthogonal polynomial satisfying

$$\int_a^b x^i p_n(x)w(x)dx = 0,\ i = 0, \ldots, n-1.$$

Gaussian quadrature is the result of approximating the function f by the polynomial f_{n-1} ($\deg(f_{n-1}) \leq n-1$) of lowest degree such that $(f(x_i) = f_{n-1}(x_i),\ i = 1, \ldots n)$.

$$I(f) = \int_a^b f(x)w(x)dx \approx Q(f) = \int_a^b f_{n-1}(x)w(x)dx = \sum_{i=1}^{n} w_i f(x_i),$$

$$f_{n-1}(x) = \sum_{i=1}^{n} f(x_i)L_i(x),\ L_i(x_j) = \delta_{i,j},\ \deg(L_i) = n-1,$$

and then

$$w_j = \int_a^b L_i(x)w(x)dx = \int_a^b \frac{p_n(x)}{(x-x_j)p_n'(x_j)}w(x)dx$$

And with the aid of the Christoffel-Darboux formula a more practical formula is obtained in terms of monic polynomials

$$w_j = -\frac{||p_n||^2}{p_n'(x_j)p_{n+1}(x_j)},\ ||p_n||^2 = \int_a^b p_n(x)^2 w(x)dx$$

Computation the nodes and weights.
We need:

1. A method to compute the polynomials $p_n(x)$ and the first derivatives.
2. A method to compute the roots of $p_n(x)$ (nodes x_i)
3. Compute $w_j = -||p_n||^2/(p_n'(x_i)p_{n+1}(x_i))$.

Recurrence relation for monic polynomials

$$p_{k+1}(x) = (x - B_k)p_k(x) - A_k p_{k-1}(x), \quad k = 1, 2, \ldots,$$

where $A_0 p_{-1} \equiv 0$ and

$$A_k = \frac{||p_k||^2}{||p_{k-1}||^2}, \quad k \geq 1, \quad B_k = \frac{\langle xp_k, p_k \rangle}{||p_k||^2}, \quad k \geq 0.$$

$< f, g >= \int_a^b f(x)g(x)w(x)dx$, $||f|| =< f, f >$

The Golub-Welsch algorithm

Let

$$J = \begin{pmatrix} \beta_0 & \alpha_1 & 0 & \dots & 0 \\ \alpha_1 & \beta_1 & \alpha_2 & & \\ 0 & \alpha_2 & \beta_2 & & \vdots \\ & & & & \\ \vdots & & & \ddots & \alpha_{n-1} \\ & & & & \\ 0 & \dots & & \alpha_{n-1} & \beta_{n-1} \end{pmatrix}$$

$\alpha_i = \sqrt{A_i}$, $\beta_i = B_i$. Then the n different eigenvalues of J are the nodes. Furthermore, if $\vec{\Phi}^{(j)}$ is an eigenvector with eigenvalue the node x_j:

$$w_j = \mu_0 \frac{(\Phi_1^{(j)})^2}{||\vec{\Phi}^{(j)}||_E^2}$$

where $\Phi_1^{(j)}$ is the first component of $\vec{\Phi}^{(j)}$ and $\mu_0 = \int_a^b w(x)dx$.

Classical Gaussian quadrature

Alternative methods are available for the classical cases, with OPs which are solutions of second order ODEs

$$C(x)y_n''(x) + B(x)y_n'(x) + \lambda_n y(x) = 0$$

(C and B polynomials).
The classical cases are:

1. Hermite: $w(x) = e^{-x^2}$ in $(-\infty, +\infty)$
2. Laguerre: $w(x) = x^{-\alpha}e^{-x}$, $\alpha > -1$, in $(0, +\infty)$
3. Jacobi: $w(x) = (1-x)^{\alpha}(1+x)^{\beta}$, $\alpha, \beta > -1$, in $(-1, 1)$

Apart from being solution of a second order ODE, the coefficients of the three-term recurrence relation are simple, as well as the coefficients in

$$y_n'(x) = a_n(x)y_n(x) + b_n y_{n-1}(x)$$

Several approaches to compute classical Gaussian quadratures:

1. Golub-Welsch: straightforward. We just need to diagonalize a tridiagonal matrix with explicitly know entries. Not so good for large degree n.
2. Iterative methods: either we use a globally convergent method or we need previous estimations of the nodes (usually from asymptotic methods for large degree). Better for large degree than GW.
3. Asymptotic methods?: can the initial estimations from asymptotics be accurate enough? What about the weights? Best methods for large n?
4. Other methods: numerical integration of the ODE by with a non-oscillatory phase functions (Bremer). Maybe competitive for very large n, but asymptotics will be better in that case.

Recent references on the computation of classical Gauss quadrature

E. Yakimiw, Accurate computation of weights in classical Gauss-Christoffel quadrature rules.
J. Comput. Phys. (1996) I+A+R Legendre (Hermite and Laguerre $\alpha = 0$ to a lesser extent)

P. N. Swarztrauber, On computing the points and weights for Gauss-Legendre quadrature.
SIAM J. Sci. Comput. (2002) I+A+FS Legendre

A. Glaser, X. Liu, V. Rokhlin, A fast algorithm for the calculation of the roots of special functions.
SIAM J. Sci. Comput. (2007) I+A/O+TS Hermite, Laguerre ($\alpha = 0$), Legendre

J. Segura, Reliable computation of the zeros of solutions of second order linear ODEs using a fourth order method.
SIAM J. Numer. Anal. (2010) **I+ +?** Hermite, Laguerre, Jacobi (*)

N. Hale, A. Townsend, Fast and accurate computation of Gauss-Legendre and Gauss-Jacobi quadrature nodes and weights.
SIAM J. Sci. Comput. (2013) I+A+A Jacobi

I. Bogaert, Iteration-free computation of Gauss-Legendre quadrature nodes and weights.
SIAM J. Sci. Comput. (2014) **A+A+A** Legendre

A. Townsend, The race to compute high-order Gauss-Legendre quadrature.
SIAM News (2015)

A. Townsend, T. Trogdon, S. Olver, Fast computation of Gauss quadrature nodes and weights on the whole real line.
IMA J. Numer. Anal (2016) I+A+A Hermite

J. Bremer, On the numerical calculation of the roots of special functions satisfying second order ordinary differential equations.
SIAM J. Sci. Comput (2017) O Laguerre, Jacobi. Very high degree.

In the previous list, there is an iterative-only method and an asymptotic-only one, namely:

JS, Reliable computation of the zeros of solutions of second order linear ODEs using a fourth order method.

SIAM J. Numer. Anal. (2010) I+ +? Hermite, Laguerre, Jacobi (*)

I. Bogaert, Iteration-free computation of Gauss-Legendre quadrature nodes and weights.

SIAM J. Sci. Comput. (2014) A+A+A Legendre

We argue that these are the best (and complementary) approaches:

1. Iterative-only methods with no asymptotic approximations lead to arbitrary precision algorithms provided that the computations are based on finite or convergent expansions.
2. Asymptotic-only methods can not be used for arbitary precision, but these are the fastests methods, and they can be accurate (15-16 digits) for moderately large degrees (as proved for Gauss-Legendre in Bogaert's paper).

Methods which combine both iterative and asymptotic methods, like

N. Hale, A. Townsend, Fast and accurate computation of Gauss-Legendre and Gauss-Jacobi quadrature nodes and weights.

SIAM J. Sci. Comput. (2013) I+A+A Jacobi

are accurate and efficient, but no so accurate as a purely iterative method and not as fast as a purely asymptotic method.

Iterative computation of classical Gauss quadratures

Several remarks regarding iterative methods in the literature:

◯ All papers use Newton's method for computing the roots (order 2), with the exception of Yakimiw paper (higher derivatives are needed) and JS.

Newton's method:

The NM, $x_{n+1} = x_n - \dfrac{f(x_n)}{f'(x_n)}$, has order of convergence 2 because

$$\frac{\epsilon_{n+1}}{\epsilon_n^2} = \frac{f''(\alpha)}{2f'(\alpha)} + \mathcal{O}(\epsilon_n) \text{ as } n \to \infty,\ \epsilon_n = x_n - \alpha.$$

◯ The only proof of convergence for Newton method is for the Legendre case (Petras, 1999).

◯ The defining ODE can be used to speed up the method and also to improve the convergence without increasing the complexity.

For computing zeros of solutions of

$$w''(x) + B(x)w'(x) + C(x)w(x) = 0$$

Newton method gives **order** 2 generally. **But the ODE can be used to speed-up the method.**
Assuming that $B(x)$ is differentiable we can transform (11) by setting

$$y(x) = \exp\left(\int \frac{1}{2}B(x)dx\right) w(x)$$

Then, $y''(x) + A(x)y(x) = 0$, with $A(x) = C(x) - \frac{1}{2}B'(x) - \frac{1}{4}B(x)^2$ and

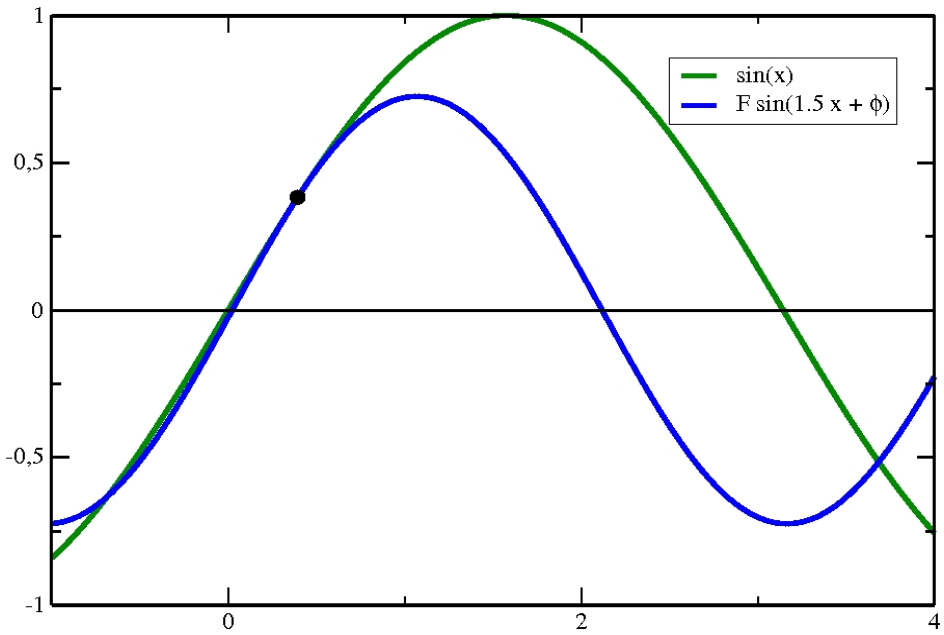
$$\frac{y(x)}{y'(x)} = \frac{w(x)}{\frac{1}{2}B'(x)w(x) + w'(x)}$$

The Newton method $x_{n+1} = x_n - \dfrac{y(x_n)}{y'(x_n)}$ is now of third order.

The reason: if α is such that $y(\alpha) = 0$, then $y''(\alpha) = 0$.
And we haven't used $A(x)$ so far...

Theorem (Sturm comparison)

Let $y(x)$ and $w(x)$ be solutions of $y''(x) + A_y(x)y(x) = 0$ and $w''(x) + A_w(x)w(x) = 0$ respectively, with $A_y(x) > A_w(x) > 0$. If $y(x_0)w'(x_0) - y'(x_0)w(x_0) = 0$ and x_y and x_w are the zeros of $y(x)$ and $w(x)$ closest to x_0 and larger (or smaller) than x_0, then $x_y < x_w$ (or $x_y > x_w$).



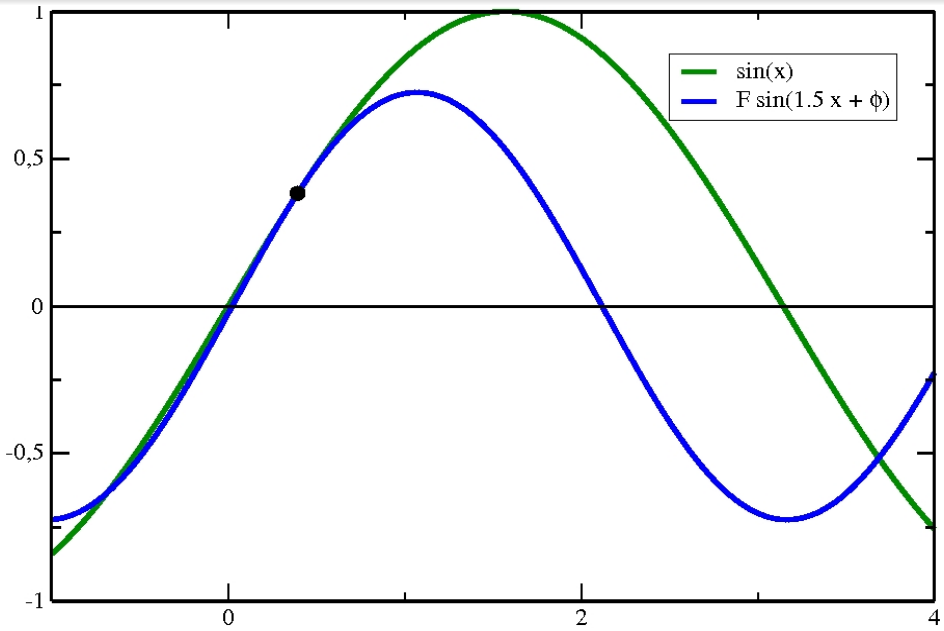
Equations: $y''(x) + y(x) = 0$, $y''(x) + 2.25y(x) = 0$

Algorithm (Zeros of $y''(x) + A(x)y(x) = 0$, $A(x)$ monotonic)

Given x_n, the next iterate x_{n+1} is computed as follows: find a solution of the equation

$$w''(x) + A(x_n)w(x) = 0$$

such that $y(x_n)w'(x_n) - y'(x_n)w(x_n) = 0$. If $A'(x) < 0$ $(A'(x) > 0)$ take as x_{n+1} the zero of $w(x)$ closer to x_n and larger (smaller) than x_n.



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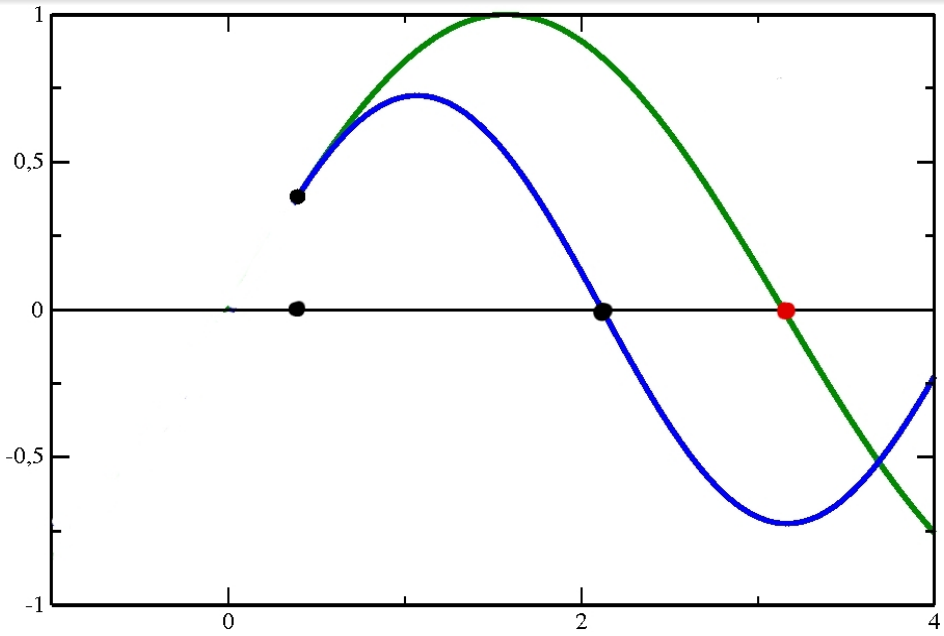


Equations: $y''(x) + A(x)y(x) = 0$, $w''(x) + A(x_n)w(x) = 0$, $(A'(x) < 0)$

The method is equivalent to iterating $x_{n+1} = T(x_n)$ with the following fixed point iteration.

Let $j = \text{sign}(A'(x))$, we define

$$T(x) = x - \frac{1}{\sqrt{A(x)}} \arctan_j(\sqrt{A(x)}h(x))$$

with

$$\arctan_j(\zeta) = \begin{cases} \arctan(\zeta) \text{ if } jz > 0, \\ \arctan(\zeta) + j\pi \text{ if } jz \leq 0, \\ j\pi/2 \text{ if } z = \pm\infty \end{cases}$$

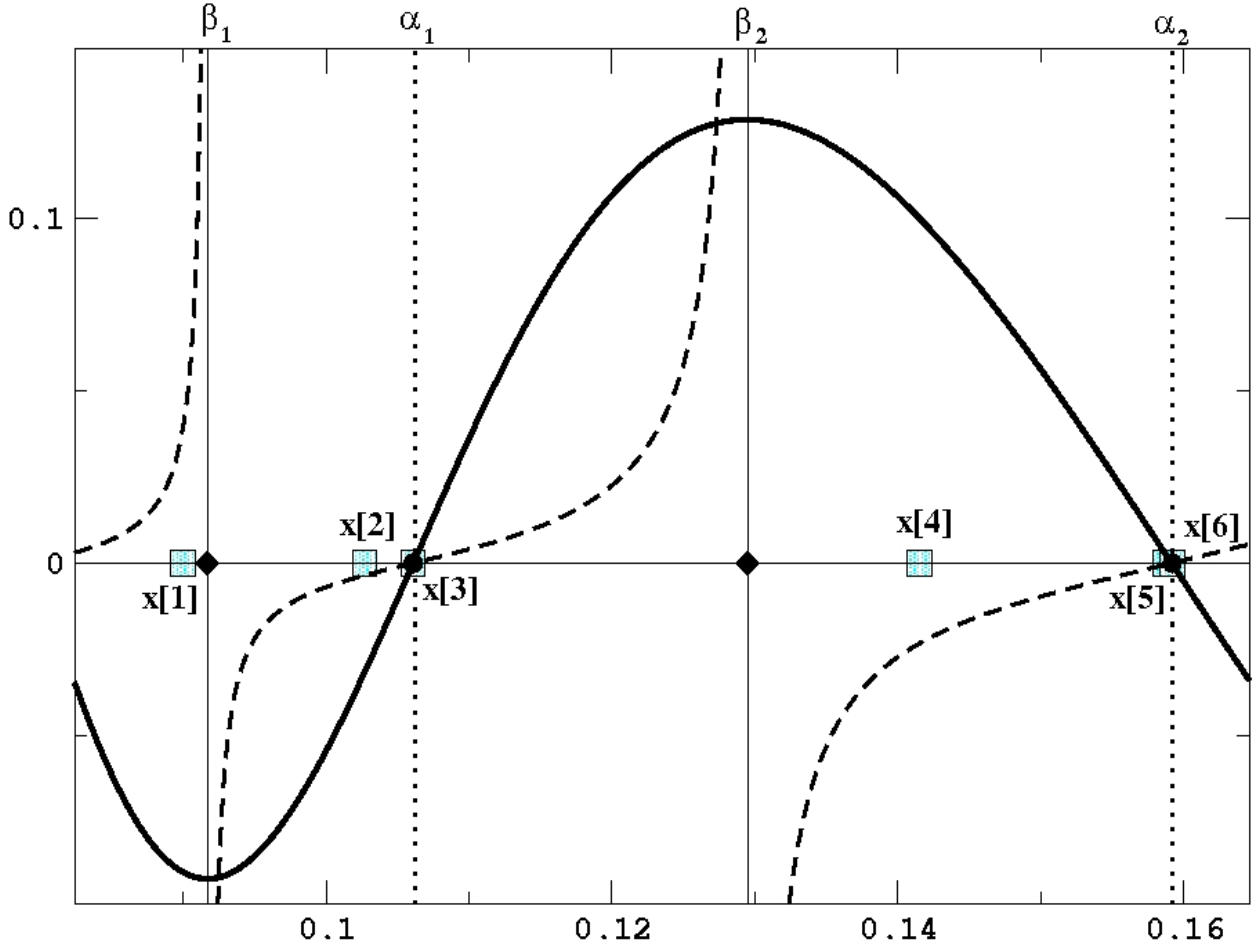
This method converges to α for any x_0 in $[\alpha', \alpha)$ if $A'(x) < 0$, with α' the largest zero smaller than α (analogously for $A'(x) > 0$).

The method has fourth order convergence:

$$\epsilon_{n+1} = \frac{A'(\alpha)}{12}\epsilon_n^4 + \mathcal{O}(\epsilon_n^5),\ \epsilon_k = x_k - \alpha$$

Computing the zeros in an interval where $A(x)$ is monotonic.

Example: zeros of $y(x) = x\sin(1/x)$, satisfying $y''(x) + x^{-4}y(x) = 0$ (4 digits of acc.).



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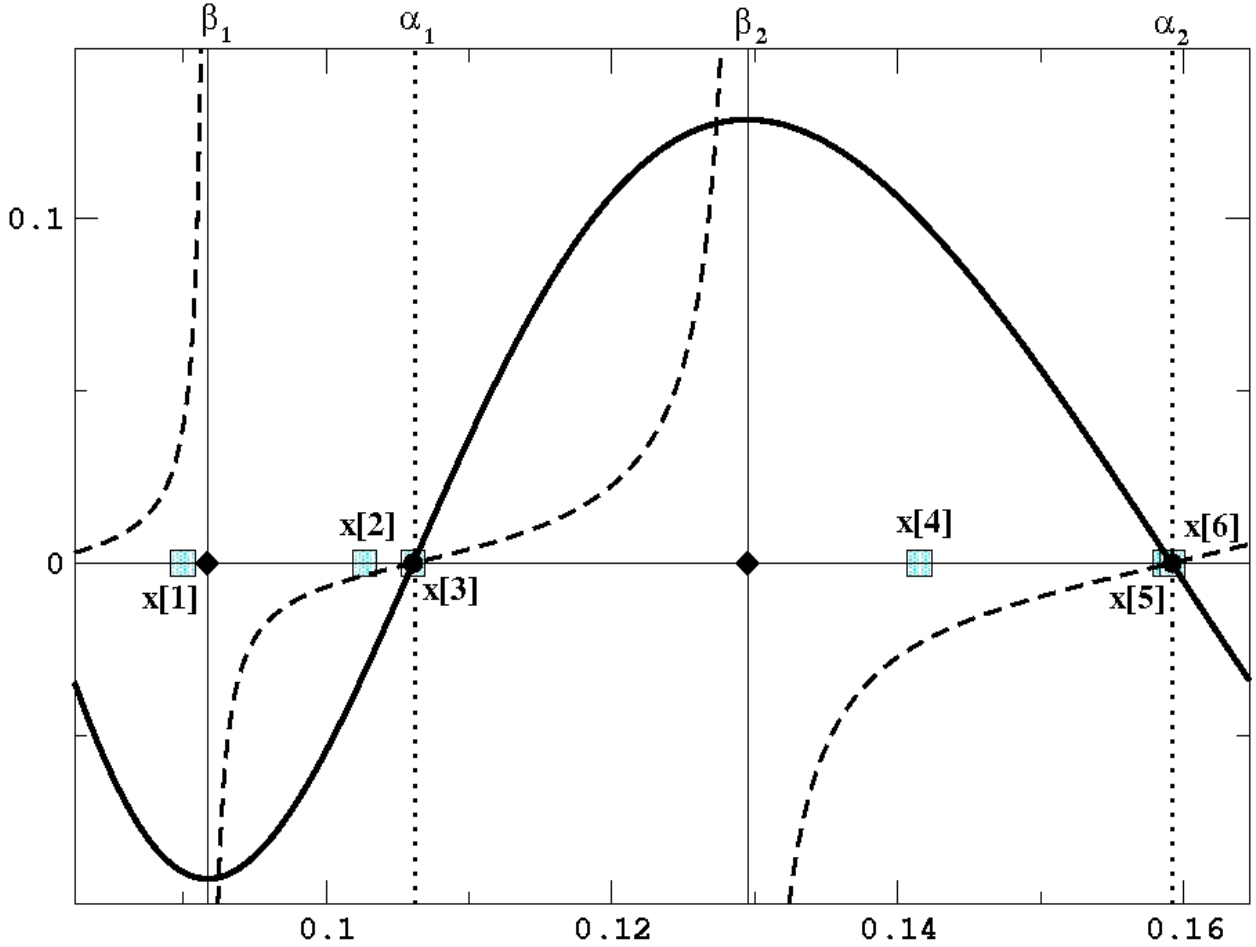

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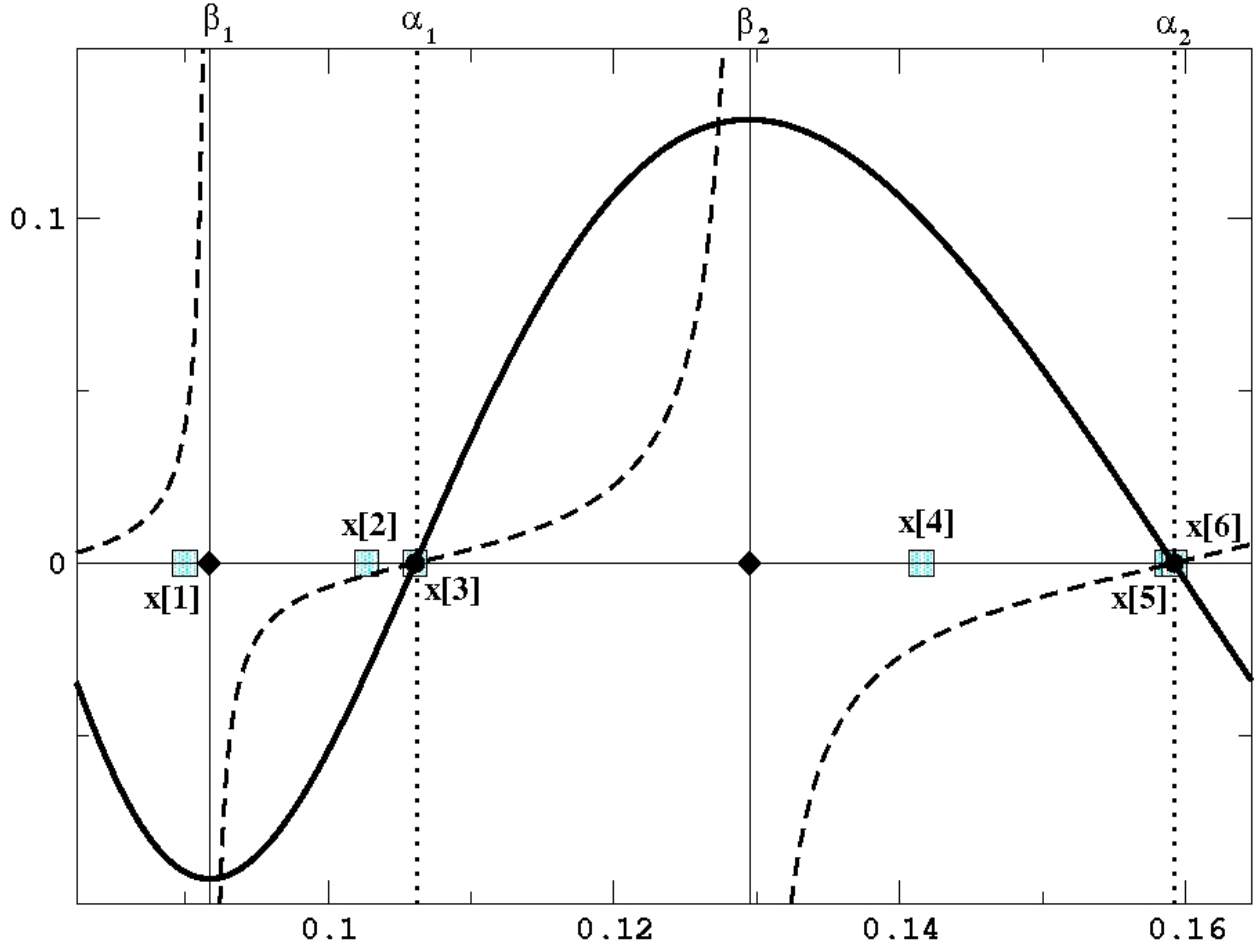

1. $T(x[1]) = x[2]$, $T(x[2]) = x[3]$ (with four digits acc.)
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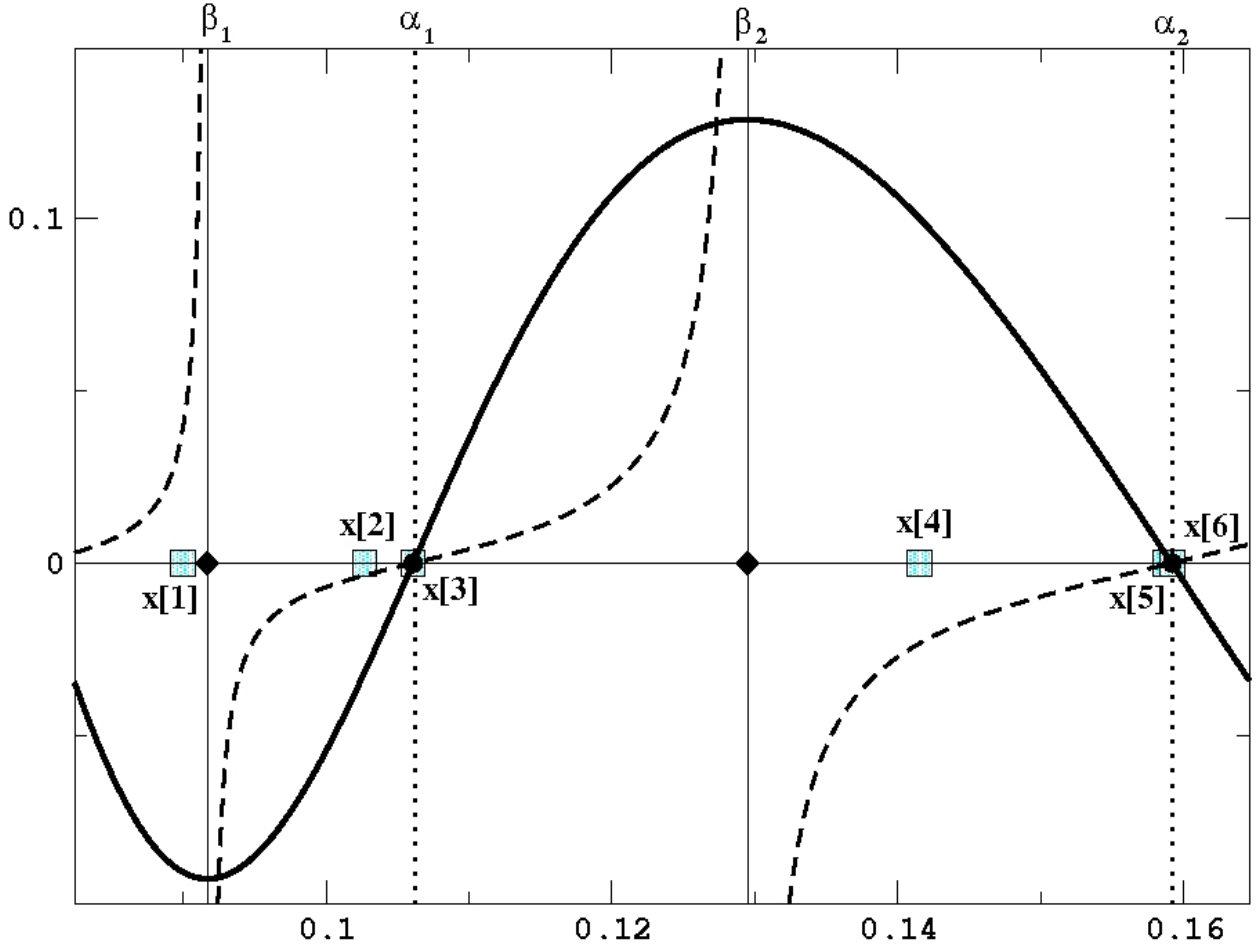

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3. $T(x[4]) = x[5]$, $T(x[5]) = x[6]$ (with four digits acc.)

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Gauss-Hermite quadrature

We have that $y_n(x) = C_n e^{-x^2/2} H_n(x)$ satisfies

$$y_n''(x) + A(x) y_n(x) = 0,\ A(x) = 2n + 1 - x^2.$$

$A(x)$ has its maximum at $x = 0$. The nodes are symmetric around the origin.

We compute the positive roots in the direction of decreasing $A(x)$, starting at $x = 0$ until we have computed $\lfloor n/2 \rfloor$ zeros.
The first step is

$$x = T_{-1}(0) = \begin{cases} \dfrac{\pi}{\sqrt{2n+1}}, & n \text{ odd} \\ \dfrac{\pi}{2\sqrt{2n+1}}, & n \text{ even} \end{cases}$$

As $n \to +\infty$ the coefficient $A(x)$ is essentially constant for not too large x.
In this sense, the method will be asymptotically exact.

Methods are available for computing efficiently and reliably $y_n(x)$ (see A. Gil , JS, N.M. Temme. ACM Trans. Math. Softw. (2006)), but here we prefer to avoid asymptotics so that arbitary accuracy for any degree is available:

The three-term recurrence relation IS NOT a good idea, particularly for large degree: the complexity is bad as for Golub-Welsch. A good alternative: use local Taylor series (as done in Glaser, Liu, Rokhlin (2007)).

Given $y(x) = C_n e^{-x^2/2} H_n(x)$, and assuming that the derivatives at x_0 are known:

$$y(x) = \sum_{k=0}^{\infty} \frac{y^{(k)}(x_0)}{k!}(x - x_0)^k.$$

and similarly for $y'(x)$, truncating the series for a given precision.

From $y(x_0)$ and $y'(x_0)$, we compute the sucessive derivatives by differentiating $y''(x) + (2n + 1 - x^2)y(x) = 0$:

$$y^{(k+2)} + (2n + 1 - x^2)y^{(k)} - 2kxy^{(k-1)} - k(k-1)y^{(k-2)} = 0.$$

Perron-Kreuser theorem: all the solutions of the difference equation are such that $\limsup_{k \to +\infty} \left(|y^{(k)}|/(k!)^{2/3} \right)^{1/k} = 1$ (the series converges everywhere, as expected).

$h = x - x_0$ will be always less than the maximal distance between zeros of $H_n(x)$.

Algorithm for Gauss-Hermite based on local Taylor series.
Take $y(x) = (2^n n!)^{-1/2} e^{-x^2/2} H_n(x)$.

1. With $x = \pi/\sqrt{2n+1}$ for n odd and $x = \pi/(2\sqrt{2n+1})$ for n even, compute $y(x)$ and $y'(x)$ by Taylor series starting from the known values $y(0)$ and $y'(0)$ **(alternatively, we can take $y(0) = 1$ and $y'(0) = 0$ for n even and $y(0) = 0$ and $y'(0) = 1$ for n odd, and rescale later)**. Let $i = 1$.
2. Iterate the fixed point method

$$T(x) = x - \frac{1}{\sqrt{A(x)}} \arctan_{-1}(\sqrt{A(x)} h(x))$$

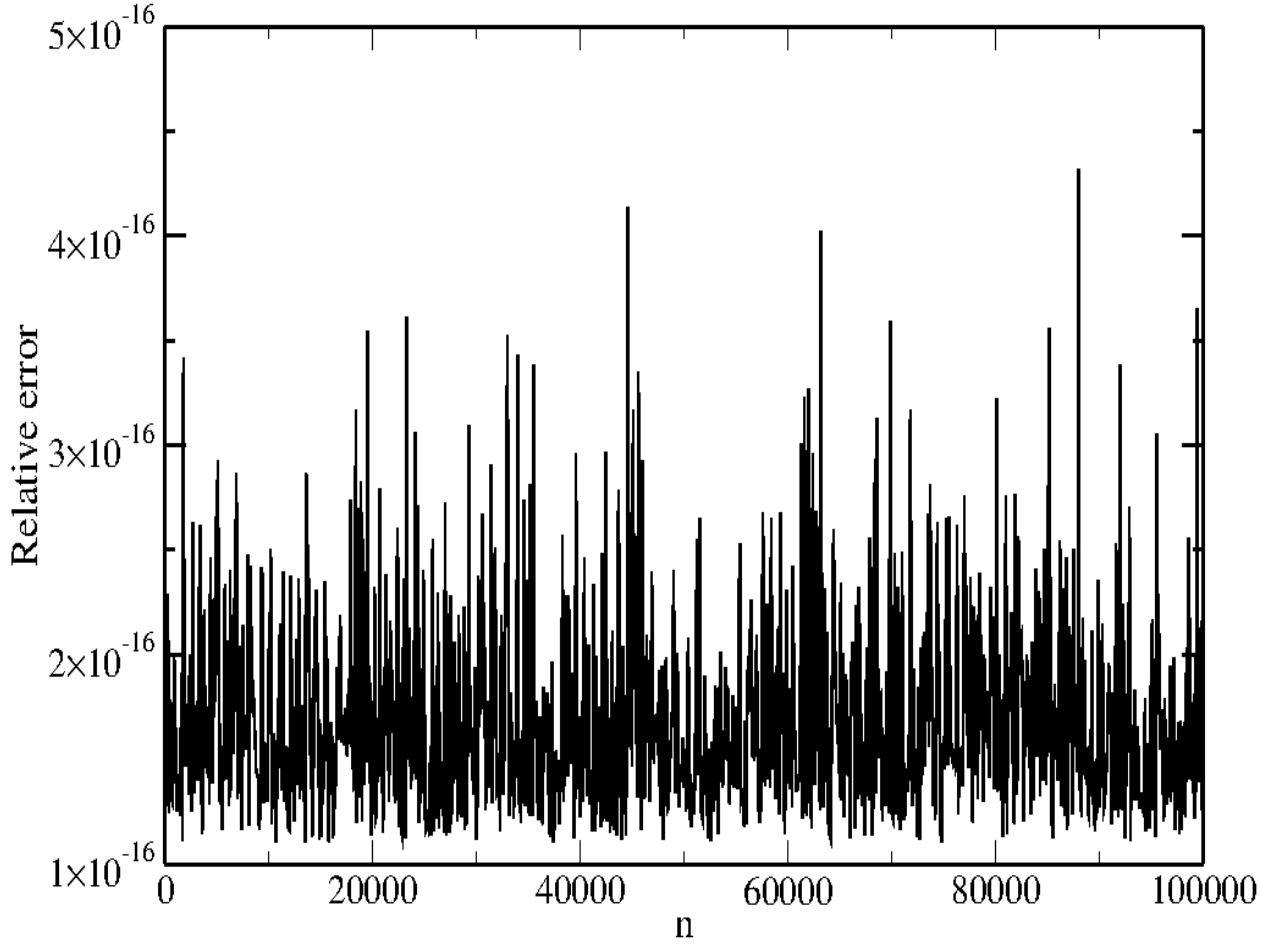
   until convergence is reached within a given accuracy. The values of $y(x)$ and $y'(x)$ are computed from Taylor series, starting with the values at the previous point. Let x_i be the resulting zero (node)
3. The corresponding weight is given by $w_i = 2e^{-x_i^2}/(y_n'(x_i))^2$.
4. Set $x = x_i + \pi/\sqrt{A(x_i)}$, $i = i + 1$, and if additional nodes have to be computed then go to 2.

If rescaling is used, we just have to take into account that the sum of all the weights is $\sqrt{\pi}$.

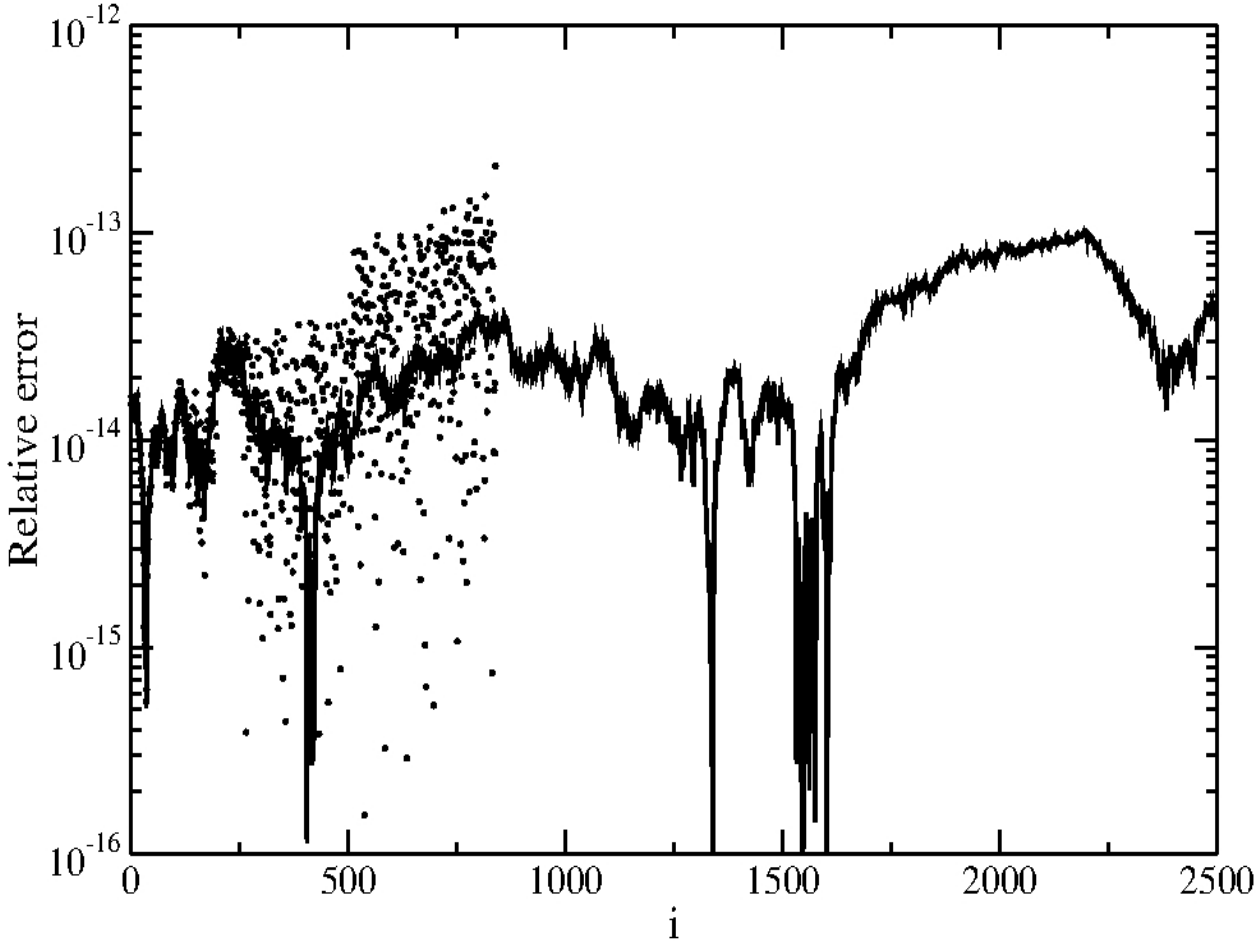
Some (nice) features of the algorithm

1. The cost of local Taylor series is essentially the same irrespectively of the order.
2. The cost of computing each zero decreases as $n \to \infty$ (asymptotic exactness)
3. Because of the fourth order convergence, when two succesive iterates are such that $|x^{(n+1)}/x^{(n)} - 1| < 10^{-p}$ then we can estimate that $|x_{n+1}/\alpha - 1| < 10^{-4p}$.
4. The so-called scaled weights $\omega_i = 1/y'(x_i)^2$ are well-conditioned as a function of x_i because $\omega_i = W(x_i)$ with $W'(x_i) = 0$.
5. The code is short (30-40 lines), reliable and efficient.

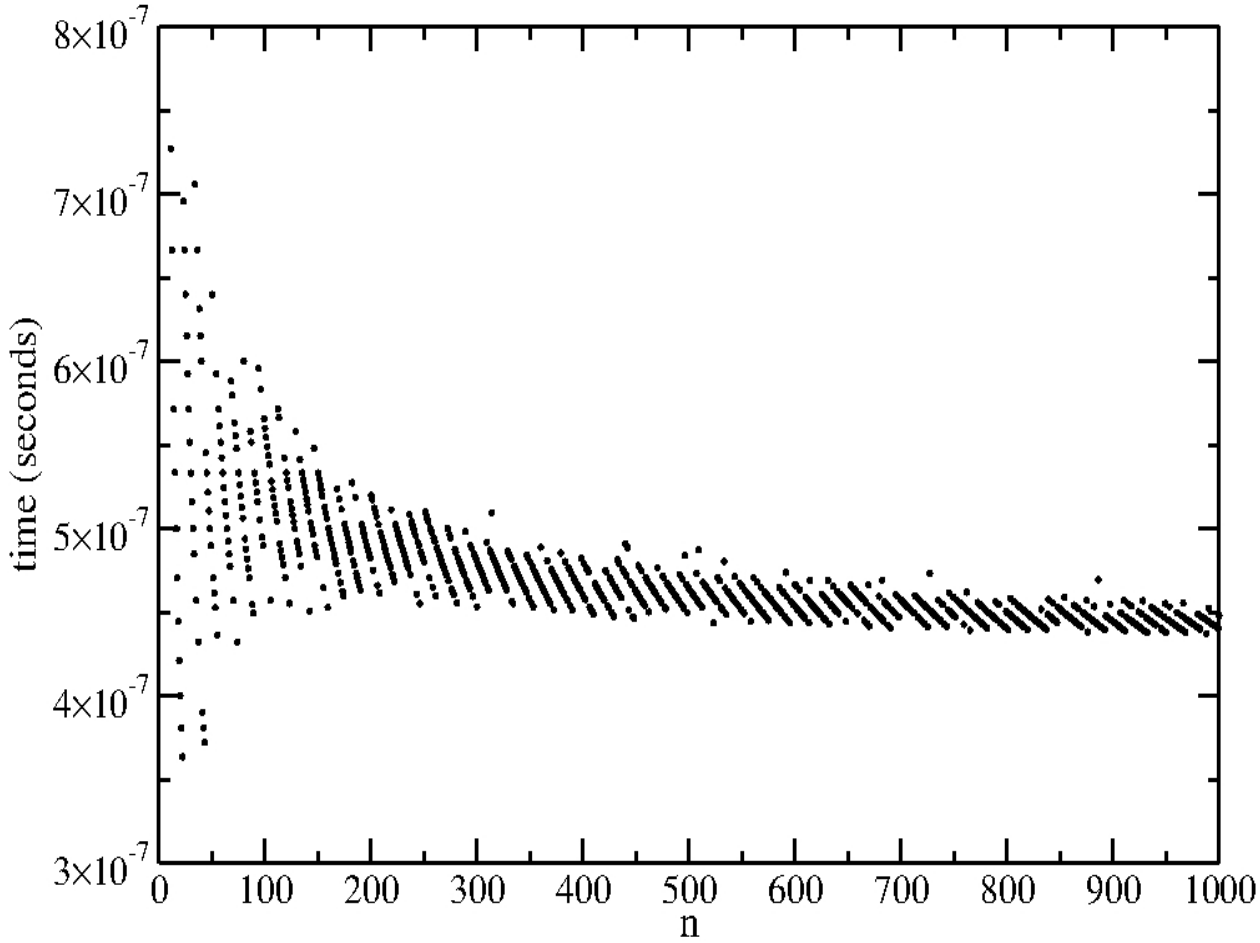
The method does not need initial estimations for the roots. It seems they don't improve significantly the performance (typically 0.5 seconds for 10^6 nodes in my laptop).



Maximum relative error in the computation of the nodes as a function of the degree n



Relative error in the computation of scaled weights (solid line) and unscaled weights (dots) for the 5000-point Gauss Hermite formula as a function of i, with i numbering the positive nodes in increasing order.



Unitary time spent (time per node and corresponding weight) in seconds as a function of the degree

Gauss-Laguerre quadrature

Take $y(z) = z^{\alpha+1/2} e^{-z^2/2} L_n^{(\alpha)}(z^2)$ which satisfies $\boldsymbol{\ddot{y}(z) + A(z)y(z) = 0}$ with

$$\boldsymbol{A(x) = A(z(x)) = -x + 2(2n + \alpha + 1) + \frac{\frac{1}{4} - \alpha^2}{x}},$$

$A(x)$ for $x > 0$: decreasing if $|\alpha| \leq 1/2$.
with a maximum at $x_e = \sqrt{\alpha^2 - 1/4}$ if $|\alpha| > 1/2$.

Depence of $A(x)$ on $n \to$ asymptotic exactness.

The Gauss-Laguerre weights are

$$w_i = \frac{4\Gamma(n + \alpha + 1)}{n!(\dot{y}(z_i))^2} x_i^{\alpha+\frac{1}{2}} e^{-x_i} \equiv \omega_i x_i^{\alpha+\frac{1}{2}} e^{-x_i},$$

where the ω_i are the so-called **scaled weights**.
Scaled weights: **well conditioned as a function of the nodes** ($\omega_i = W(z_i)$ with $\dot{W}(z_i) = 0$).
Our algorithm computes the doubly scaled weights $\hat{\omega}_i = \omega_i/\Gamma(\alpha + 1)$.

The computation of $y(z)$ for the Laguerre case is not so easy as for Hermite.

Taylor series must be supplemented with an additional starting method.
A good choice is the continued fraction which follows from iterating

$$r^{(\alpha)} = \frac{a_\alpha}{b_\alpha + r^{(\alpha+1)}},$$

where $r^{(\alpha)} = L_n^{(\alpha)}(x)/L_n^{(\alpha-1)}(x)$, $b_\alpha = -(1+\alpha/x)$, $a_\alpha = -(n+\alpha)/x$.
Using the derivative rule

$$xL_n^{(\alpha)'}(x) = -\alpha L_n^{(\alpha)}(x) + (\alpha+n)L_n^{(\alpha-1)}(x)$$

we get

$$\frac{\dot{y}(z)}{y(z)} = \frac{1/2-\alpha}{z} - z + \frac{2(n+\alpha)}{zr^{(\alpha)}(z^2)}.$$

with $y(z)$ as defined before.

We only need this for initiating Taylor series (the ratio is enough, because we can rescale with the moment of order zero).

Taylor series

The function $y(z)$ satisfies

$$P(z)y^{(2)}(z) + Q(z)y(z) = 0,$$

with

$$P(z) = z^2, \quad Q(z) = -z^4 + 2Lz^2 + \frac{1}{4} - \alpha^2$$

taking successive derivatives and using that $P^{(n)}(z) = 0$, $n > 2$ and $Q^{(n)}(z) = 0$, $n > 4$, we obtain the following recursion formula for the derivatives with respect to z:

$$\sum_{m=0}^{2} \left(\begin{array}{c} j \\ m \end{array} \right) P^{(m)}(z)y^{(j+2-m)}(z) + \sum_{m=0}^{4} \left(\begin{array}{c} j \\ m \end{array} \right) Q^{(m)}(z)y^{(j-m)}(z) = 0,$$

where $\left(\begin{array}{c} j \\ m \end{array} \right)$ are binomial coefficients.

This is a seven-term recurrence relation and therefore the space of solutions has dimension 6.

Perron-Kreuser theorem: the solutions of this difference equation lie in two subspaces: a subspace of dimension two of solutions satisfying

$$\limsup_{n\to+\infty} |y^{(n)}/n!|^{1/n} = |1/x|,$$

and a subspace of dimension four of solutions satisfying

$$\limsup_{n\to+\infty} |y^{(n)}/\sqrt{n!}|^{1/n} = 1.$$

The solutions of the first subspace are dominant over the second subspace.

The derivatives of solutions of the ODE are in this dominant subspace because the Taylor series centered at x has radius of convergence $R = |x|$ (as corresponds to a differential equation with a singularity at $x = 0$).

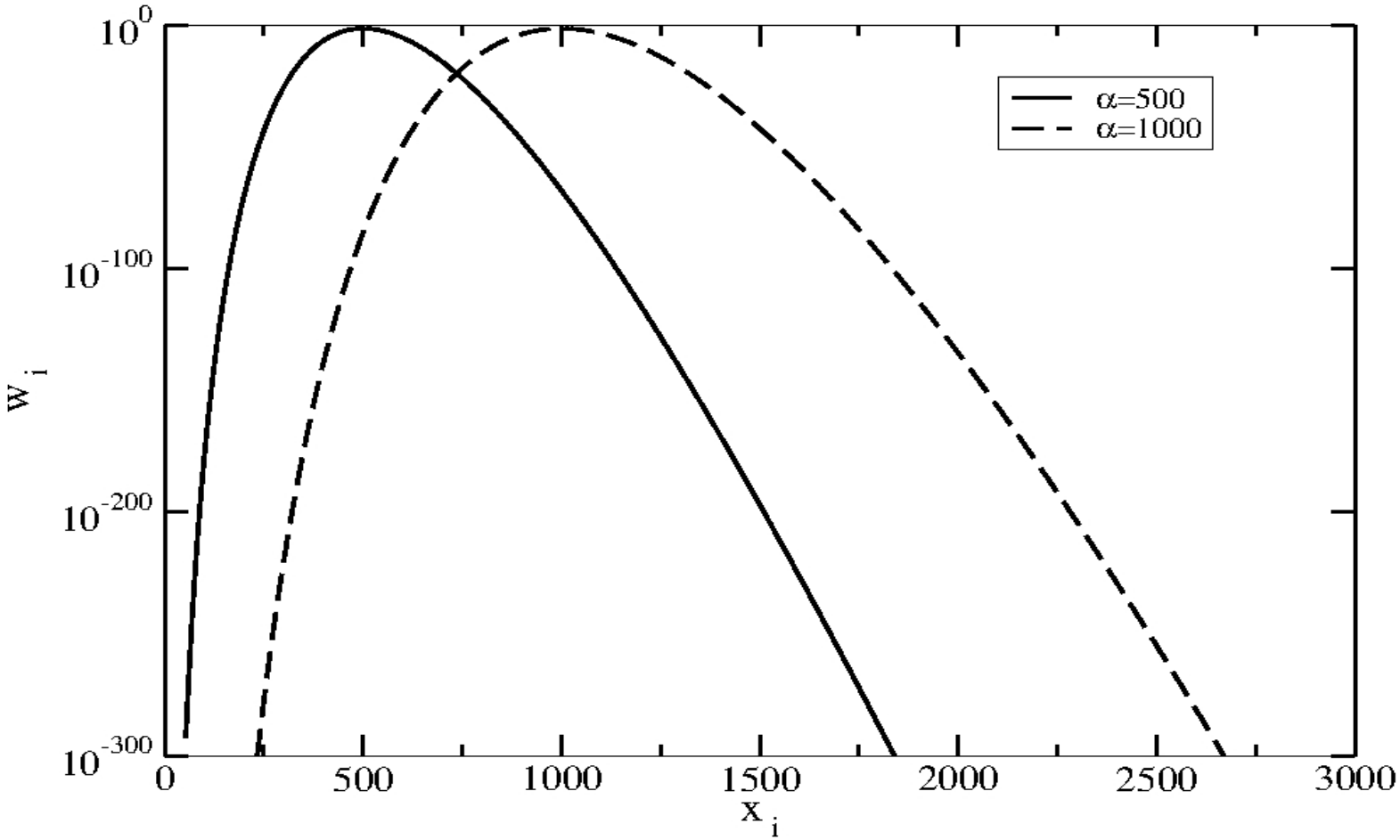
Because of the dominance of these solutions, the computation of the derivatives in the forward direction is well conditioned.

The ingredients for the method for Gauss-Laguerre are:

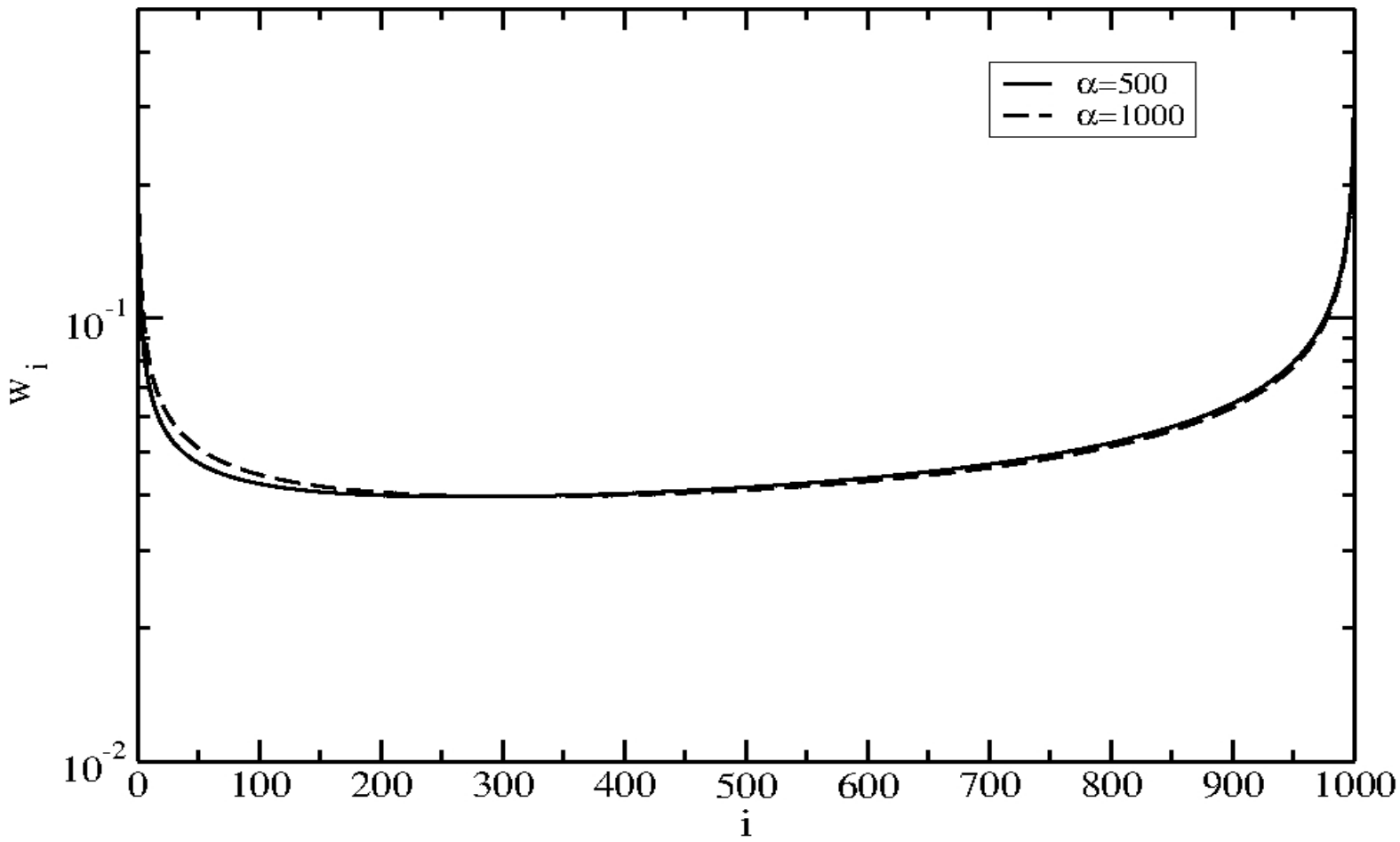
1. The fourth order fixed point method in the z variable
2. The continued fraction as a starting value (in some cases two values are required)
3. Taylor series in the z variable

In our previous notation, this is **I+ +TS/CF**

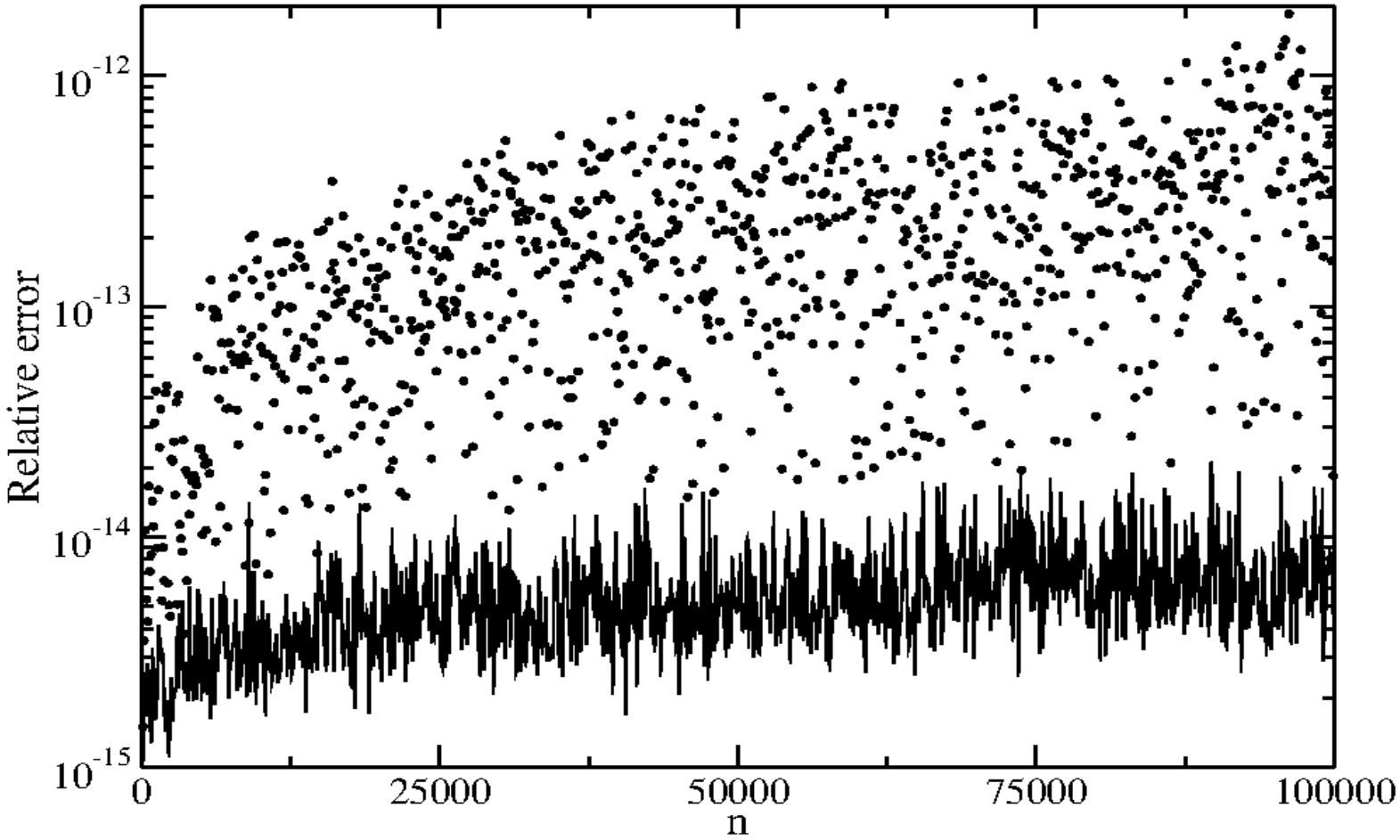
Some numerical results follow



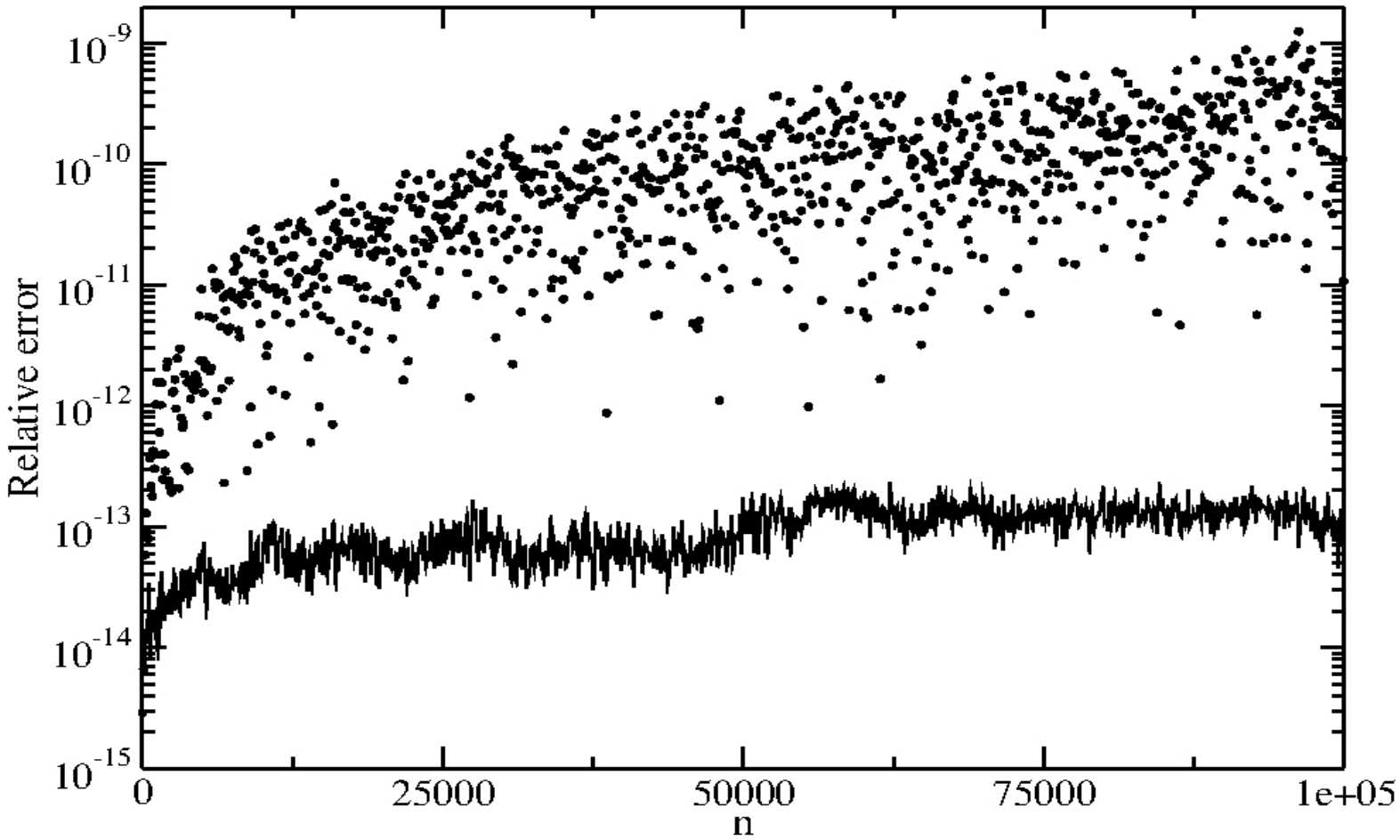
Gauss-Laguerre weights as a function of the nodes x_i, where the degree is $n = 1000$. Two values of α are considered: $\alpha = 500$ and $\alpha = 1000$



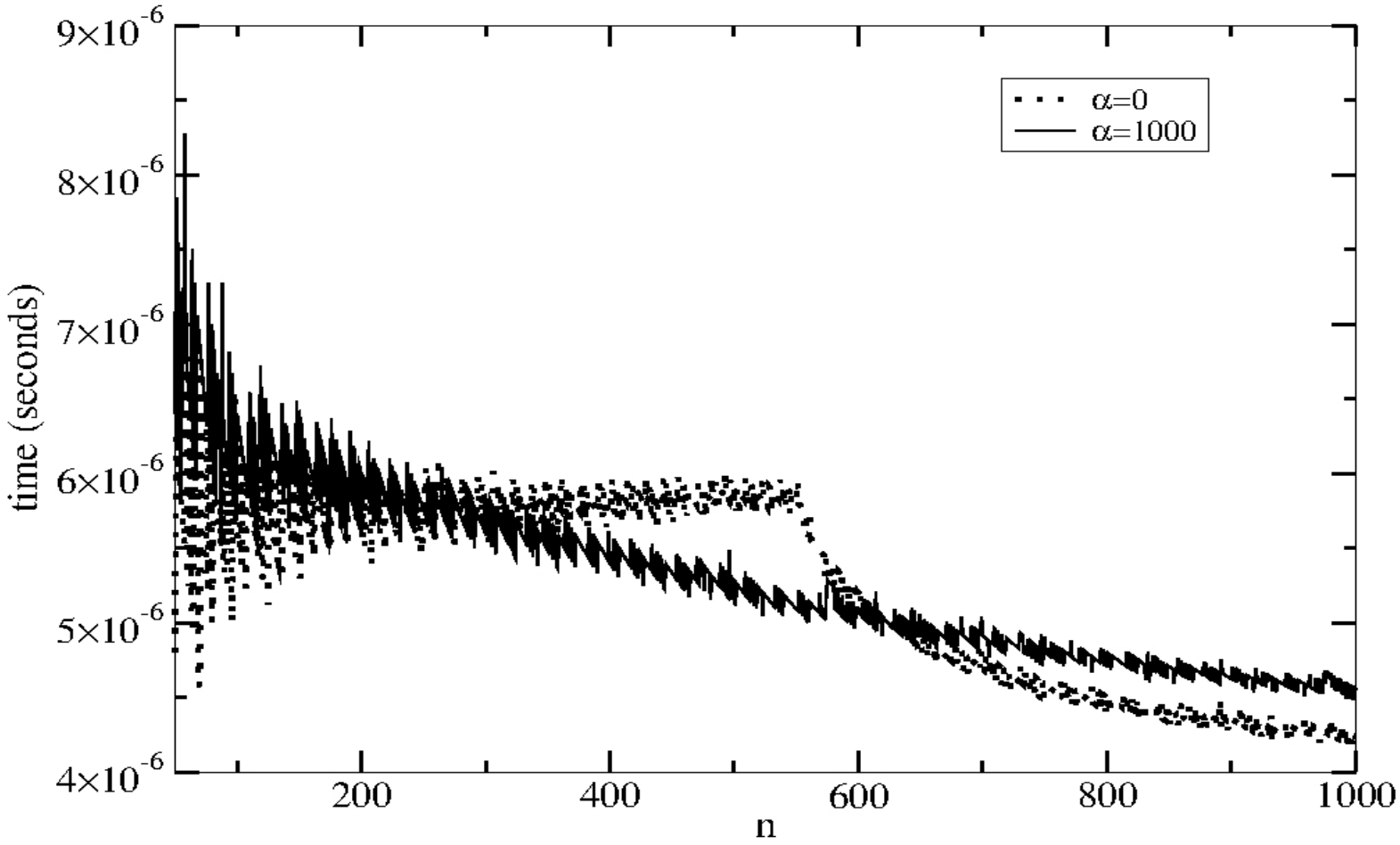
Gauss-Laguerre doubly-scaled weights as a function of the number i of the nodes x_i $(x_0 < x_1 < \cdots)$, where the degree is $n = 1000$. Two values of α are considered: $\alpha = 500$ and $\alpha = 1000$



Maximum relative errors in the computation of the nodes for n-point Gauss–Laguerre quadrature with $\alpha = 0$ (dots). We also show the maximum error when it is evaluated only for the nodes for which the weights are larger than 10^{-30} (solid line); the error in this case is smaller.



Same as the previous figure but for the scaled weights.



Unitary CPU-time spent as a function of the degree n for Gauss-Laguerre with $\alpha = 0$ and $\alpha = 1000$

Gauss-Jacobi

We only mention few details.

The most appropriate starting point is the ODE satisfied by $y(\theta) = \left(\sin\frac{\theta}{2}\right)^{\alpha+1/2}\left(\cos\frac{\theta}{2}\right)^{\beta+1/2} P_n(\cos\theta)$:

$$\frac{d^2y}{d\theta^2} + \frac{1}{4}\left[L^2 + \frac{\frac{1}{4}-\alpha^2}{\sin^2(\theta/2)} + \frac{\frac{1}{4}-\beta^2}{\cos^2(\theta/2)}\right] y = 0$$

$L = 2n + \alpha + \beta$

The change $x = \cos\theta$ is not the only possibility (see Deaño, Gil, Segura (2004)) but in this variable the method is asymptotically exact as $n \to +\infty$, and well-conditioned scaled weights are also available.

With

$$u(\theta) = M_{n,\alpha,\beta}^{-1/2} \left(\sin\frac{\theta}{2}\right)^{\alpha+1/2} \left(\cos\frac{\theta}{2}\right)^{\beta+1/2} P_n^{(\alpha,\beta)}(\cos\theta),$$

which satisfies the previous ODE, we can write the Jacobi weights as

$$w_i = |\dot{u}(\theta_i)|^{-2} \left(\sin\frac{\theta_i}{2}\right)^{2\alpha+1} \left(\cos\frac{\theta_i}{2}\right)^{2\beta+1},$$

where

$$M_{n,\alpha,\beta} = 2^{\alpha+\beta+1} \frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{n!\Gamma(n+\alpha+\beta+1)},$$

and the scaled weights can be defined as

$$\omega_i = |\dot{u}(\theta_i)|^{-2},$$

which are well conditioned as a function of θ_i.
Taylor series in the θ variable are harder, because the derivatives do not satisfy a recurrence relation with a fixed number of terms.

Asymptotic methods

Until recently, only the Gauss-Legendre quadratures were available with $15-16$ accuracy and moderately large n (Bogaert's paper).
But the same can be said now for the rest of classical Gaussian quadratures:

1. The Hermite and Laguerre cases were discussed in:

   A. Gil, J. Segura, N. M. Temme. Asymptotic approximations to the nodes and weights of Gauss-Hermite and Gauss-Laguerre quadratures.

   Stud. Appl. Math. (2018) **A+A+A** Hermite, Laguerre

2. And the Jacobi case is given in

   Non-iterative computation of Gauss-Jacobi quadrature by asymptotic expansions for large degree

   A. Gil, J. Segura, N. M. Temme

Different expansions are given in terms of other functions and zeros for computing accurately all the zeros and and weight for $n \geq 100$:

1. Hermite, in terms of: elementary functions and Airy functions.
2. Laguerre: two approximations in terms of Bessel functions and one with Airy functions.
3. Jacobi, in terms of: elementary functions and Bessel functions.

We only describe one of the simplest expansions (which is new): the elementary expansion for the Jacobi case, which can be used for computing most of the nodes and weights.

Notice: the Bogaert expansion for Gauss-Legendre is in terms of Bessel functions, and our elementary expansion for the more general Jacobi case is simpler but quite powerful.

The starting point

$$P_n^{(\alpha,\beta)}(x) = \frac{(-1)^n}{2^n n!\, w(x)} \frac{1}{2\pi i} \int_C e^{-\kappa\phi(z)} \frac{w(z)(z-x)^{\gamma-1}}{(1-z^2)^\gamma}\, dz,$$

where $\gamma = \frac{1}{2}(\alpha+\beta+1)$, $\kappa = n+\gamma$, and $\phi(z) = \ln(z-x) - \ln(1-z^2)$.

$$y(\theta) = \frac{G_\kappa(\alpha,\beta)}{\sqrt{\pi\kappa}}(\cos\chi\, U(x) - \sin\chi\, V(x)),\ \chi = \kappa\theta + \left(\alpha+\frac{1}{2}\right)\frac{\pi}{2}$$

with expansions

$$U(x) \sim \sum_{m=0}^{\infty} \frac{u_{2m}(x)}{\kappa^{2m}}, \quad V(x) \sim \sum_{m=0}^{\infty} \frac{v_{2m+1}(x)}{\kappa^{2m+1}}.$$

The first coefficients are

$$u_0(x) = 1, \quad v_1(x) = \frac{2\alpha^2 - 2\beta^2 + (2\alpha^2 + 2\beta^2 - 1)x}{8\sin\theta},$$

$$u_2(x) = \frac{1}{384\sin^2\theta}(12(5 - 2\alpha^2 - 2\beta^2)(\alpha^2 - \beta^2)x +$$

$$4(-3(\alpha^2-\beta^2)^2 + 3(\alpha^2+\beta^2) - 6 + 4\alpha(\alpha^2 - 1 + 3\beta^2) +$$

$$(-12(\alpha^2+\beta^2)(\alpha^2+\beta^2-1) - 16\alpha(\alpha^2 - 1 + 3\beta^2) - 3)x^2).$$

For computing the weights we also need $\dot{y}(\theta)$.

Let see how to compute the nodes. Let $W(\theta) = \cos\chi\, U(x) - \sin\chi\, V(x)$,

$$U(x) \sim \sum_{m=0}^{\infty} \frac{u_{2m}(x)}{\kappa^{2m}}, \quad V(x) \sim \sum_{m=0}^{\infty} \frac{v_{2m+1}(x)}{\kappa^{2m+1}}.$$

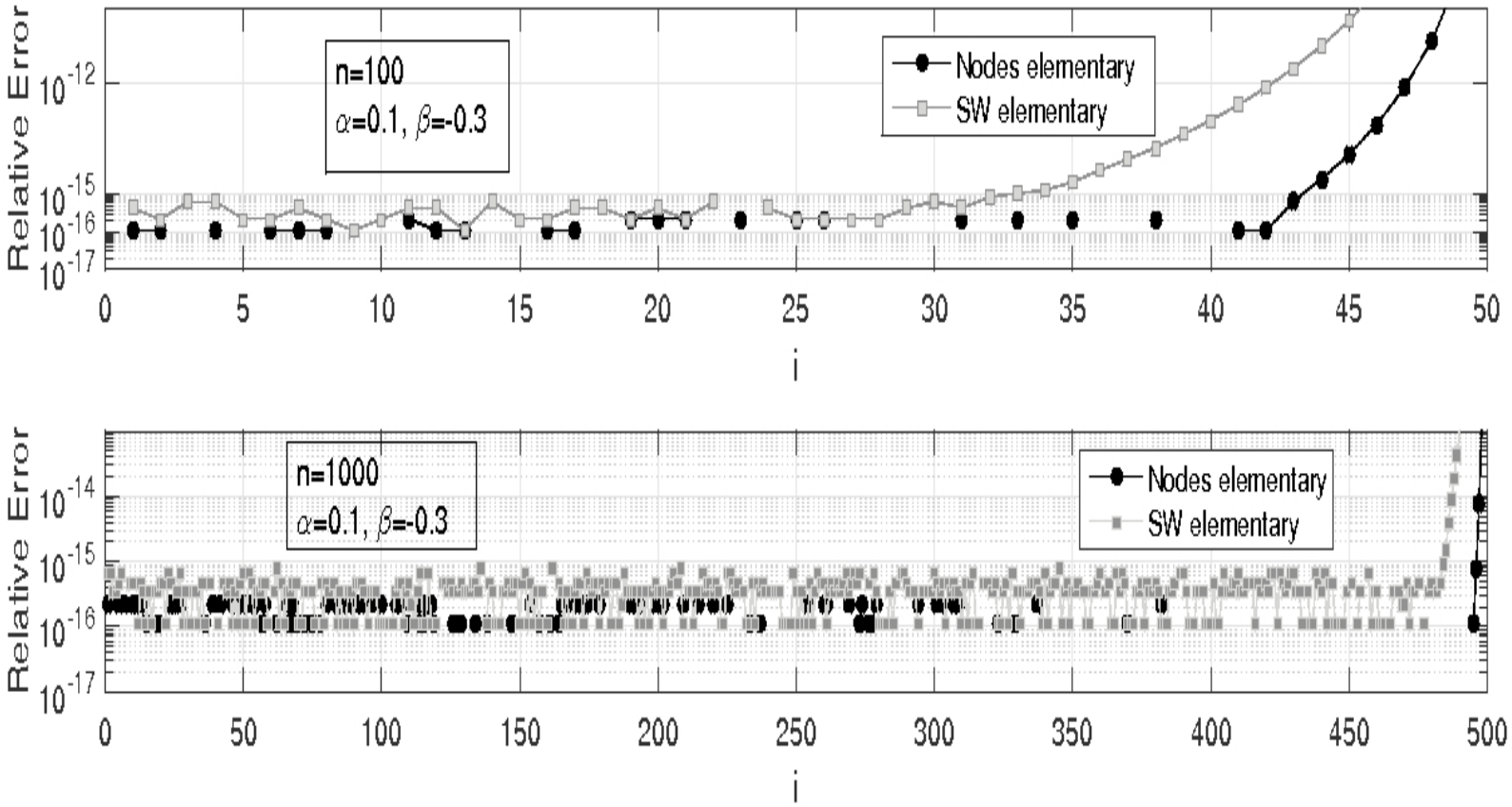
A first approximation is $\cos\chi = 0 \to \theta = \theta_0 = \left(n - k + \frac{3}{4} + \frac{\alpha}{2}\right)\frac{\pi}{\kappa}$.

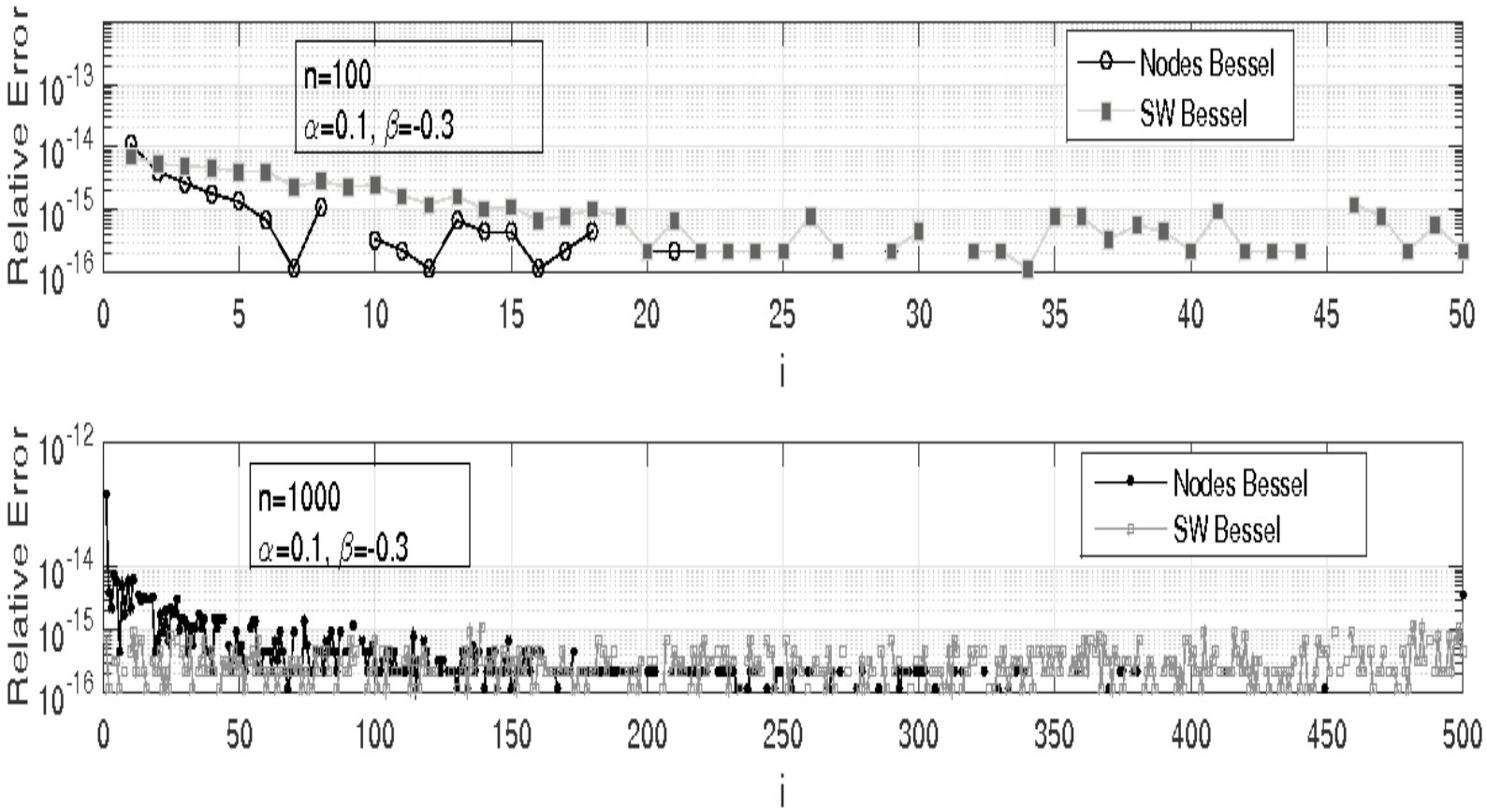
Now we write $W(\theta) = W(\theta+\epsilon) = W(\theta_0) + \epsilon\dot{W}(\theta_0) + \frac{\epsilon^2}{2}\ddot{W}(\theta) + \ldots = 0$, we assume the expansion $\epsilon = \frac{\theta_1}{\kappa^2} + \frac{\theta_2}{\kappa^3} + \frac{\theta_3}{\kappa^4} + \ldots$, and using the expansions of U and V and comparing equal powers of κ we determine the coefficients θ_i, $i \geq 1$, (depending on θ_0). The first two cofficients are:

$$\theta_1 = -\frac{1}{8\sin\theta_0}\left(2\beta^2 x + 2\alpha^2 x - x - 2\beta^2 + 2\alpha^2\right),$$

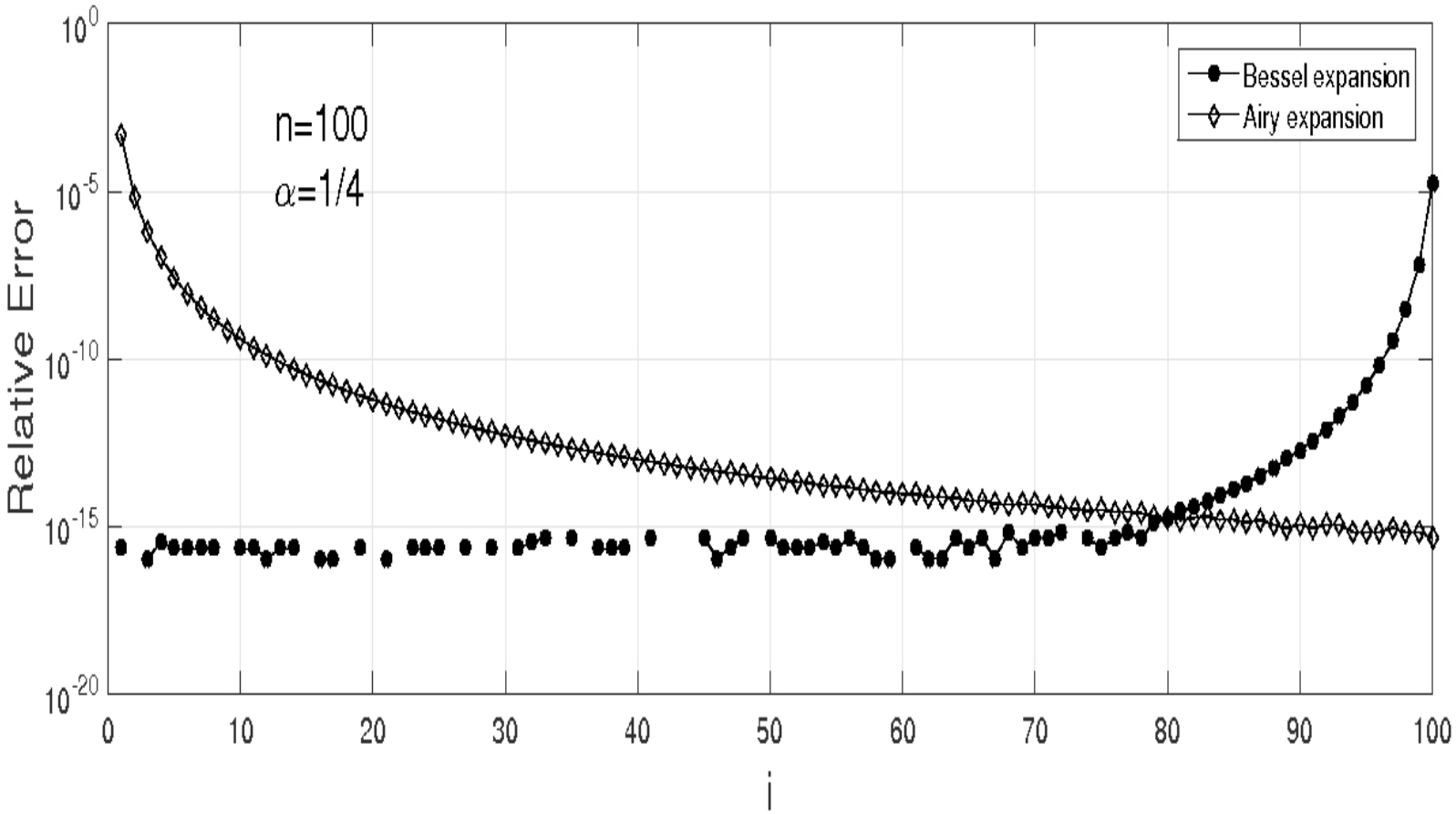
$$\begin{aligned}\theta_2 = \frac{1}{384\sin^3\theta_0}(&-33x - 36\beta^2x^2 + 36\alpha^2x^2 + 24\beta^4x^2 - 24\alpha^4x^2 + 2x^3 + \\ &84\beta^2x - 60\alpha^4x - 60\beta^4x + 84\alpha^2x + 4\beta^4x^3 + 4\alpha^4x^3 - 8\beta^2x^3 + \\ &40\alpha^2 - 8\alpha^2x^3 - 40\beta^2 + 32\beta^4 - 32\alpha^4 + 24\alpha^2\beta^2x^3 - 24\alpha^2\beta^2x),\end{aligned}$$

where $x = \cos\theta_0$.
With this we compute $\theta = \theta_0 + \epsilon$ and then $x_k \sim \cos\theta$

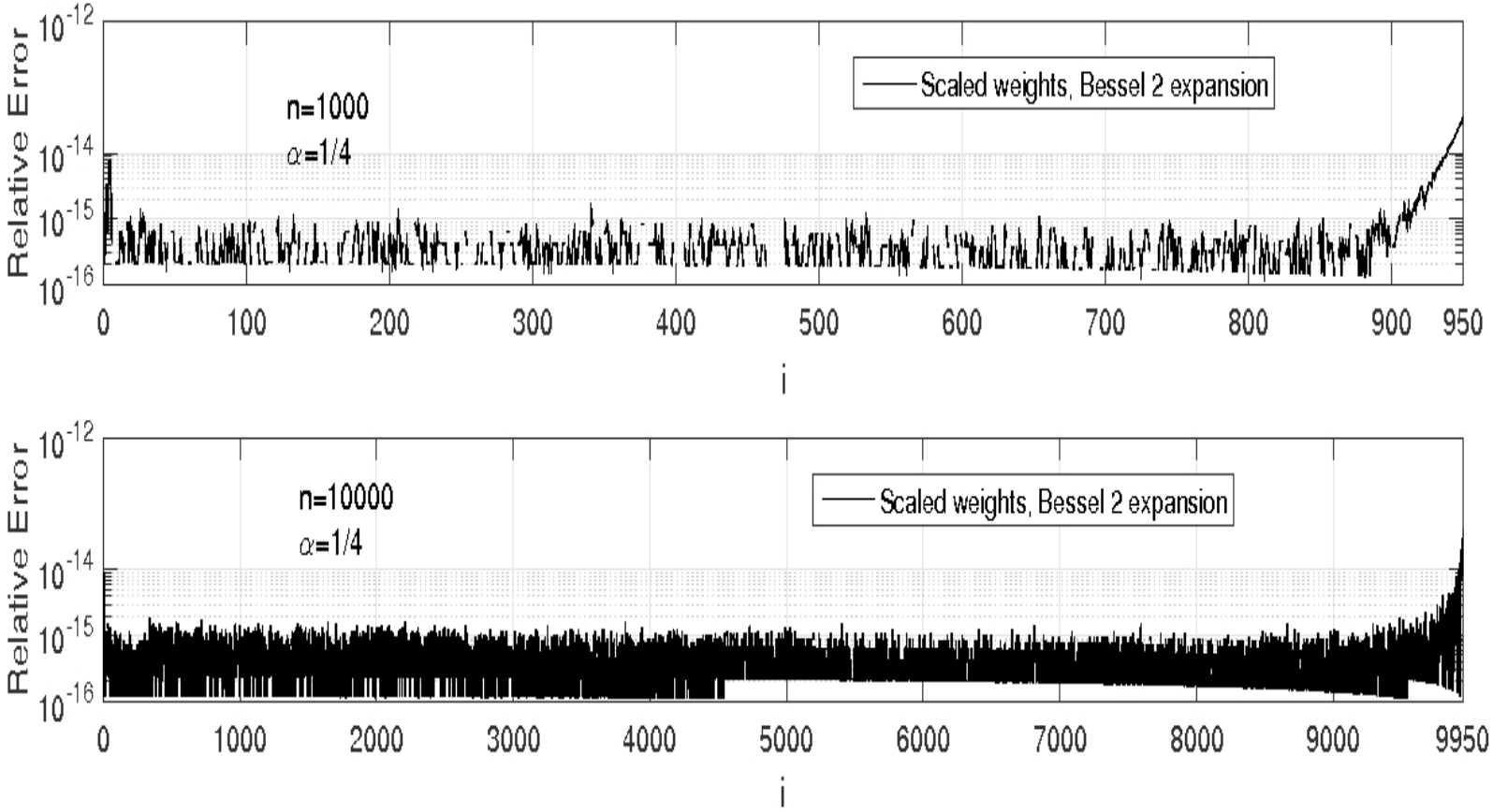

Relative Error
n=100
α=0.1, β=-0.3
Nodes elementary
SW elementary
i
Relative Error
n=1000
α=0.1, β=-0.3
Nodes elementary
SW elementary
i


Relative Error
n=100
α=0.1, β=-0.3
Nodes Bessel
SW Bessel
i
Relative Error
n=1000
α=0.1, β=-0.3
Nodes Bessel
SW Bessel
i

We finish with two more plots (now for Gauss-Laguerre).



Relative accuracy for computing the zeros of $L_n^{(1/4)}(x)$ for $n = 100$ with two different asymptotic expansions. The points not shown in the plot correspond to values with all digits correct in double precision accuracy.



Relative accuracy obtained for the computation of the Laguerre doubly-scaled weights for $n = 1000$, 10000 (with $\alpha = 1/4$) using an asymptotic expansion in terms of Bessel functions.

THANK YOU!