Numerical evaluation of the roots of orthogonal polynomials

Diego Ruiz Antolín

University of Cantabria

Santander(Spain)

Applications of the zeros of functions:

Applications of the zeros of functions:

- Many scientific problems: resonance, quantum mechanics...

Applications of the zeros of functions:

- Many scientific problems: resonance, quantum mechanics...
- Expansions of other functions.

Applications of the zeros of functions:

- Many scientific problems: resonance, quantum mechanics...
- Expansions of other functions.
- Gaussian quadrature.

Let us define the integral

$$\int_a^b f(x)\omega(x)dx$$

where $\omega(x)$ is a weight function. Let p_n be a polynomial of degree n such that

$$\int_a^b x^k p_n(x)\omega(x)dx = 0, \quad k = 0, 1, ..., n-1.$$

Let $x_1, ..., x_n$ be the zeros of p_n and let ω_i be defined by

$$\omega_i = \int_a^b L_i(x)\omega(x)dx, \quad L_i(x) = \prod_{k=1, k\neq i}^{n} \frac{x - x_k}{x_i - x_k},$$

where $i = 1, 2, ..., n$. Then, the quadrature rule,

$$\int_a^b f(x)\omega(x)dx \approx \sum_{i=1}^{n} \omega_i f(x_i),$$

is a Gaussian quadrature rule.

Some algorithms for the evaluation of the roots of functions:

Some algorithms for the evaluation of the roots of functions:

- G. H. Golub, J. H. Welsch, *Calculation of Gauss quadrature rules*, Math. Comp. 23 (1969), 221-230.

Some algorithms for the evaluation of the roots of functions:

- G. H. Golub, J. H. Welsch, *Calculation of Gauss quadrature rules*, Math. Comp. 23 (1969), 221-230.
- K. Petras, *On the computation of the Gauss-Legendre quadrature formula with a given precision*, J. Comput. Appl. Math., 112 (1999), pp. 253–267.

Some algorithms for the evaluation of the roots of functions:

- G. H. Golub, J. H. Welsch, *Calculation of Gauss quadrature rules*, Math. Comp. 23 (1969), 221-230.
- K. Petras, *On the computation of the Gauss-Legendre quadrature formula with a given precision*, J. Comput. Appl. Math., 112 (1999), pp. 253–267.
- A. Glaser, X. Liu, V. Rokhlin, *A fast algorithm for the calculation of the roots of special functions*, SIAM J. Sci. Comp., 2007, 29: 1420–1438.

Some algorithms for the evaluation of the roots of functions:

- G. H. Golub, J. H. Welsch, *Calculation of Gauss quadrature rules*, Math. Comp. 23 (1969), 221-230.
- K. Petras, *On the computation of the Gauss-Legendre quadrature formula with a given precision*, J. Comput. Appl. Math., 112 (1999), pp. 253–267.
- A. Glaser, X. Liu, V. Rokhlin, *A fast algorithm for the calculation of the roots of special functions*, SIAM J. Sci. Comp., 2007, 29: 1420–1438.
- J. Segura, *Reliable Computation of the Zeros of Solutions of Second Order Linear ODEs Using a Fourth Order Method*, SIAM J. Num. Anal., v.48 n.2, p.452-469, April 2010.

Problems that may arise when computing the zeros of functions:

Problems that may arise when computing the zeros of functions:

- The process may be rather slow.

Let the orthonormal polynomials $\tilde{p}_i(x)$ satisfy the recurrence relation

$$\alpha_1\tilde{p}_1(x) + \beta_0\tilde{p}_0(x) = x\tilde{p}_0(x)$$

$$\alpha_{k+1}\tilde{p}_{k+1}(x) + \beta_k\tilde{p}_k(x) + \alpha_k\tilde{p}_{k-1}(x) = x\tilde{p}_k(x), \quad k = 1, 2, \ldots$$

and let x_j be a zero of the polynomial $\tilde{p}_n$ for a fixed n, then

$$\begin{pmatrix} \beta_0 & \alpha_1 & 0 & \ldots & 0 \\ \alpha_1 & \beta_1 & \alpha_2 & & \\ 0 & \alpha_2 & \beta_2 & & \vdots \\ \vdots & & & \ddots & \alpha_{n-1} \\ 0 & \ldots & & \alpha_{n-1} & \beta_{n-1} \end{pmatrix} \begin{pmatrix} \tilde{p}_0(x_j) \\ \tilde{p}_1(x_j) \\ \vdots \\ \tilde{p}_{n-2}(x_j) \\ \tilde{p}_{n-1}(x_j) \end{pmatrix} = x_j \begin{pmatrix} \tilde{p}_0(x_j) \\ \tilde{p}_1(x_j) \\ \vdots \\ \tilde{p}_{n-2}(x_j) \\ \tilde{p}_{n-1}(x_j) \end{pmatrix}$$

We have that $\tilde{p}_n(x_j) = 0$ if, and only if, x_j is an eigenvalue of the above square matrix.

Problems that may arise when computing the zeros of functions:

- The process may be rather slow.

- The convergence is not guaranteed.

Problems that may arise when computing the zeros of functions:

- The process may be rather slow.
- The convergence is not guaranteed.
  - Proximity to singularities.

Problems that may arise when computing the zeros of functions:

- The process may be rather slow.
- The convergence is not guaranteed.
    - Proximity to singularities.
    - Zeros are too close to each other.

Some algorithms for the evaluation of the roots of functions:

- G. H. Golub, J. H. Welsch, *Calculation of Gauss quadrature rules*, Math. Comp. 23 (1969), 221-230.
- K. Petras, *On the computation of the Gauss-Legendre quadrature formula with a given precision*, J. Comput. Appl. Math., 112 (1999), pp. 253–267.
- A. Glaser, X. Liu, V. Rokhlin, *A fast algorithm for the calculation of the roots of special functions*, SIAM J. Sci. Comp., 2007, 29: 1420–1438.
- J. Segura, *Reliable Computation of the Zeros of Solutions of Second Order Linear ODEs Using a Fourth Order Method*, SIAM J. Num. Anal., v.48 n.2, p.452-469, April 2010.

We consider the ODE

$$y''(x) + A(x)y(x) = 0.$$

We consider the ODE

$$y''(x) + A(x)y(x) = 0.$$

Given the function

$$h(x) = \frac{y(x)}{y'(x)},$$

We consider the ODE

$$y''(x) + A(x)y(x) = 0.$$

Given the function

$$h(x) = \frac{y(x)}{y'(x)},$$

we have the Riccati equation

$$h'(x) = 1 + (\omega(x)h(x))^2, \qquad \omega(x) = \sqrt{A(x)}.$$

Let α be such that $y(\alpha) = 0$. We integrate around α

$$\int_{\alpha}^{x} \frac{h'(\zeta)}{1 + (\omega(\zeta)h(\zeta))^2} d\zeta = x - \alpha,$$

Let α be such that $y(\alpha) = 0$. We integrate around α

$$\int_{\alpha}^{x} \frac{h'(\zeta)}{1 + (\omega(\zeta)h(\zeta))^2} d\zeta = x - \alpha,$$

from where we obtain the approximation

$$\alpha \approx x - \frac{1}{\omega(x)} \mathsf{arctan}(\omega(x)h(x)).$$

Let α be such that $y(\alpha)=0$. We integrate around α

$$\int_{\alpha}^{x} \frac{h'(\zeta)}{1+(\omega(\zeta)h(\zeta))^2} d\zeta = x-\alpha,$$

from where we obtain the approximation

$$\alpha \approx x - \frac{1}{\omega(x)} \operatorname{arctan}(\omega(x)h(x)).$$

This leads to the FPM

$$x_{n+1} = g(x_n), \qquad g(x) = x - \frac{1}{\omega(x)} \operatorname{arctan}(\omega(x)h(x))$$

$$\omega(x) = \sqrt{A(x)}, \qquad h(x) = \frac{y(x)}{y'(x)}$$

Advantages of this method:

- It is of fourth order.

Advantages of this method:

- It is of fourth order.
- It is globally convergent.

We redefine the arctangent as follows,

$$\mathrm{arctan}_j(\zeta) = \begin{cases} \mathrm{arctan}(\zeta) & if \quad j\zeta > 0 \\ \\ \mathrm{arctan}(\zeta) + j\pi & if \quad j\zeta \le 0 \end{cases}, \quad j = \pm 1$$

We redefine the arctangent as follows,

$$\mathrm{arctan}_j(\zeta) = \begin{cases} \arctan(\zeta) & if \quad j\zeta > 0 \\ \\ \arctan(\zeta) + j\pi & if \quad j\zeta \leq 0 \end{cases} , \quad j = \pm 1$$

obtaining the FPM

$$T_j(x) = \begin{cases} x - \frac{1}{\omega(x)} \mathrm{arctan}_j(\omega(x)h(x)) & if \quad y'(x) \neq 0 \\ \\ x - \frac{1}{\omega(x)} j \frac{\pi}{2} & if \quad y'(x) = 0 \end{cases} , \quad j = \pm 1$$

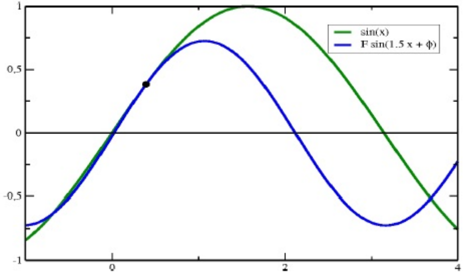
$$x_{n+1} = T_j(x_n), \qquad j = sign(A'(x))$$

Let $y(x)$ be a solution of $y''(x) + A(x)y(x) = 0$ with two consecutive zeros α_1 and α_2 such that $A(x) > 0$ in $[\alpha_1, \alpha_2]$. Then the following hold:

1. If $A'(x) > 0$ in (α_1, α_2), then the FPM converges monotonically to α_1 for any $x_0 \in (\alpha_1, \alpha_2]$.
2. If $A'(x) < 0$ in (α_1, α_2), then the FPM converges monotonically to α_2 for any $x_0 \in [\alpha_1, \alpha_2)$.

The order of convergence is 4.

Graphically, the behaviour of the method is as follows,



y''(x)+y(x)=0,y''(x)+2.25 y(x)=0

If $A(x) < 0$, we consider

$$h(x) = \frac{y(x)}{y'(x)}$$

If $A(x) < 0$, we consider

$$h(x) = \frac{y(x)}{y'(x)}$$

then we have the Riccati equation

$$h'(x) = 1 - (\omega(x)h(x))^2, \qquad \omega(x) = \sqrt{-A(x)}.$$

If $A(x) < 0$, we consider

$$h(x) = \frac{y(x)}{y'(x)}$$

then we have the Riccati equation

$$h'(x) = 1 - (\omega(x)h(x))^2, \qquad \omega(x) = \sqrt{-A(x)}.$$

This leads to the FPM,

$$x_{n+1} = g(x_n), \qquad g(x) = x - \frac{1}{\omega(x)} tanh^{-1}(\omega(x)h(x))$$

Let us consider the EDO

$$y''(x) + (2n + 1 - x^2)y(x) = 0,$$

Let us consider the EDO

$$y''(x) + (2n + 1 - x^2)y(x) = 0,$$

which has the solution

$$\tilde{H}_n(x) = \frac{e^{-\frac{x^2}{2}}}{\pi^{\frac{1}{4}} 2^{\frac{n}{2}} \sqrt{n!}} H_n(x),$$

being $H_n(x)$ the Hermite polynomial of order n.

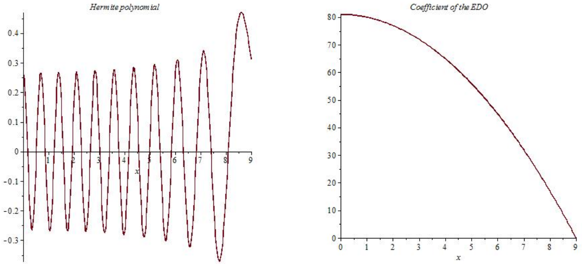
Let us consider the EDO

$$y''(x) + (2n + 1 - x^2)y(x) = 0,$$

which has the solution

$$\tilde{H}_n(x) = \frac{e^{-\frac{x^2}{2}}}{\pi^{\frac{1}{4}} 2^{\frac{n}{2}} \sqrt{n!}} H_n(x),$$

being $H_n(x)$ the Hermite polynomial of order n.We see that



Let us consider the EDO

$$y''(x) + (2n + 1 - x^2)y(x) = 0,$$

which has the solution

$$\tilde{H}_n(x) = \frac{e^{-\frac{x^2}{2}}}{\pi^{\frac{1}{4}} 2^{\frac{n}{2}} \sqrt{n!}} H_n(x),$$

being $H_n(x)$ the Hermite polynomial of order n. We see that

Number of zeros	CPU time
1000	0.004
10000	0.047
100000	0.468
1000000	4.68

Thank you for your attention