Numerov's Method

Solving the Quantum Harmonic Oscillator

Final Project for the Course
Numerical Methods in Quantum Mechanics
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Numerov's Method

Integrates second-order ordinary differential equations in which the first-order term does not appear:

$$y''(x) = -g(x)y(x) + s(x),$$

given $g(x)$ and $s(x)$ and with the initial conditions $y(x_0) = y_0$ and $y'(x_0) = y'_0$.

The x domain is be **discretized** on a grid of N equispaced points x_i and the solution is provided as the values of $y(x)$ on the grid, i.e. as $y(x_i) = y_i$.

The same subscript notation holds also for the known functions, as g_i and s_i.

Derivation

Let Δx be the discretization step, so that $x_{n-1} = x_n - \Delta x$ and $x_{n+1} = x_n + \Delta x$. Summing the expansions of $y(x)$ up to the fifth order around these points yeilds:

$$y_{n+1} + y_{n-1} = 2y_n + y_n'' \Delta x^2 + \frac{1}{12} y_n'''' \Delta x^4 + O(\Delta x^6).$$

Let $z_n = y_n'' = -g_n y_n + s_n$. Expanding z_n up to the third order, its second derivative is expanded as:

$$z_n'' = y_n'''' = \frac{z_{n+1} + z_{n-1} - 2z_n}{\Delta x^2} + O(\Delta x^2).$$

Numerov's formula is obtained substituting this estimate in the previous formula and making explicit the term y_{n+1}.

Multistep Equation

Numerov's method is a **multistep** method since two initial steps, y_0 and y_1, are required:

$$y_{n+1} = \frac{(12 - 10f_n)y_n - f_{n-1}y_{n-1}}{f_{n+1}} + \frac{t_n}{f_{n+1}} + O(\Delta x^6) \text{ with}$$

$$f_n = 1 + g_n \frac{\Delta x^2}{12} \text{ and } t_n = (s_{n+1} + 10s_n + s_{n-1}) \frac{\Delta x^2}{12}.$$

The f_n and t_n terms are known since $g(x)$ and $s(x)$ are given.

The initial conditions enter through the first two steps y_0 and y_1 and they differ from the standard ones.

Error

A certain attention is needed discussing the method's accuracy:

- Numerov's discretization provides a local error, i.e. at a given discretization step, of the order of $O(\Delta x^6)$.
- The number of grid points is proportional to Δx^{-1}, so it's arguable that the **global** error, after any big number of steps, cumulative result of local errors, is $O(\Delta x^5)$.
- The previous assertion is true only if the local error is constant, but this is not the case and an example is provided in which the global error results $O(\Delta x^4)$.

Example

The problem is $y''(x) = -y(x)$, with $y(0) = 0$ and $y'(0) = 1$.
Since $g(x) = 1$ and $s(x) = 0$, Numerov's method prescribes:

$$y_{n+1} = 2\frac{12 - 5\Delta x^2}{12 + \Delta x^2} y_n - y_{n-1}.$$

The roots $r_\pm$ of the algebric associate to this **difference** equation are such that $r_+ r_- = 1$, so they are written as $r_\pm = \cos\phi \pm i \sin\phi$.

A general solution to the equation is written as $y_n = A r_+^n + B r_-^n$ with arbitrary $A = B^* = (C_1 - iC_2)/2$ and therefore:

$$y_n = C_1 \cos(n\phi) + C_2 \sin(n\phi).$$

Coefficients

The solution is exactly known to be $y(x) = \sin(x)$, so imposing exact initial conditions $y_0 = 0$ and $y_1 = \sin(\Delta x)$ implies:

$$C_1 = 0 \text{ and } C_2 = \frac{\sin(\Delta x)}{\sin(\phi)}.$$

In the limit of $\Delta x \to 0^+$, the angle ϕ is expanded as:

$$\phi = \cos^{-1}\left(\frac{12 - 5\Delta x^2}{12 + \Delta x^2}\right) = \Delta x + \frac{\Delta x^5}{480} + O(\Delta x^6).$$

Using sine and geometric series, the non-zero coefficient results:

$$C_2 = 1 - \frac{\Delta x^4}{480} + O(\Delta x^5).$$

Result

Now, using sine addition formula and trigonometric series, the expression for y_n is rewritten as:

$$y_n = \sin(n\Delta x) - \frac{\Delta x^4}{480}\sin(n\Delta x) + \frac{n\Delta x^5}{480}\cos(n\Delta x) + O(\Delta x^6).$$

Taking $x = n\Delta x$, the global error is defined as the difference between the exact result and estimated one, therefore:

$$\sin(x) - y_n = \frac{\Delta x^4}{480}\big(\sin(x) - x\cos(x)\big) + O(\Delta x^6).$$

This example shows that, in general, Numerov's method provides a global error of order $O(\Delta x^4)$.

Schrödinger Equation

Stationary states of a one-dimensional particle of mass m, under a potential $V(x)$, are described by the time-independent Schrödinger equation:

$$\frac{d^2\psi(x)}{dx^2} = -\frac{2m}{\hbar^2}(E - V(x))\psi(x).$$

For the **quantum harmonic oscillator**, $V(x) = x^2k/2$ where k is the force constant. The above equation reads then:

$$\frac{d^2\psi(\xi)}{d\xi^2} = -2(\varepsilon - \xi^2/2)\psi(\xi),$$

using the adimensional units $\xi = x\sqrt{\omega k/\hbar}$ and $\varepsilon = E/(\hbar\omega)$ where $\omega = \sqrt{k/m}$ is the angular frequency.

Exact Solution

The quantum harmonic oscillator can be solved **exactly** and it results that allowed energies are quantized as:

$$\varepsilon_n = n + \frac{1}{2}.$$

The corresponding wave functions are expressed through $H_n(\xi)$, the Hermite polynomials of degree n and the normalization factors $N_n = (2^n n! \sqrt{n})^{-1/2}$ as:

$$\psi_n(\xi) = N_n H_n(\xi) e^{-\xi^2/2}.$$

Hermite polymial $H_n(\xi)$ has n nodes and the same parity of n, so the same is true for $\psi_n(\xi)$. This was expected, since the potential $V(\xi)$ is symmetric.

Numerical Solution

Using adimensional units, for the harmonic oscillator holds:

$$g(\xi) = 2(\xi^2/2 - \varepsilon) \text{ and } s(\xi) = 0.$$

Let $\xi_i = i\Delta\xi$, where $\Delta\xi$ is the discretization step. Numerov's method provides a **direct** numerical integration of the equation:

$$y_{n+1} = \frac{(12 - 10f_n)y_n - f_{n-1}y_{n-1}}{f_{n+1}} + O(\Delta\xi^6).$$

Subscripts denote the point ξ_n in which functions are evaluated.

The above formula can be used also backward, making explicit y_{n-1}, thus needing two ending points as initial conditions.

Numerical Issues

1. A solution to the Schrödinger equation exists for any ε, a priori different from an energy eigenvalue, so it may be unphysical.

2. It is possible to find the particle in classically forbidden regions, where $V(\xi) > E$. Schrödinger equation there reads:

$$\frac{d^2\psi(\xi)}{d\xi^2} = K^2\psi(\xi) \text{ assuming } V(\xi) = V,$$

   implying the behaviour $\psi(\xi) \simeq e^{\pm K\xi}$, the only physical solution being that decreasing as $|\xi| \to +\infty$.

So, **unphysical** but numerically allowed results must be avoided .

Shooting Method

Given n, the extrema of the potential $V(\xi) = \xi^2/2$ on the grid define the interval $[\varepsilon_{min}, \varepsilon_{max}]$, surely containing the eigenevalue ε_n.

1. $\psi_n(\xi)$ is integrated starting from 0 up to ξ_{max} at the trial energy value $\varepsilon = (\varepsilon_{max} + \varepsilon_{min})/2$.
2. The number of nodes found $\overline{n}$ is counted as the number of changes of sign of the integrated wave function.
3. Since ε_n grows with n, if $\overline{n} < n$, then ε is too low and the interval is adjusted to $[\varepsilon_{min} = \varepsilon, \varepsilon_{max}]$ or, otherwise, to the opposite.

Iterating this procedure up to a given tolerance on the **width** of the interval solves the energy eigenvalue issue discussed above.

Symmetry

The integration is performed only for positive values of ξ, because negative ones are obtained through symmetry since:

$$\psi_n(-\xi) = (-1)^n \psi_n(\xi).$$

The first two steps are also determined by the **parity** of n:

- If n is even, $y_0 = 1$ and $y_1 = y_0(12 - 10f_0)/(2f_1)$.
- If n is odd, $y_0 = 0$ and $y_1 = \Delta\xi$.

With these choices, $\psi_n(\xi)$ is integrated correctly up to a global phase of ± 1, having no physical meaning and therefore neglected.

Backward Integration

Let ξ_{cl} be the classical inversion point, such that $V(\xi_{cl}) = \varepsilon$. It is found as the first discrete point for which $V(\xi_{cl}) > \varepsilon$, therefore it is determined with a precision of $O(\Delta\xi)$.

- All the n nodes are located in the interval $[0, \xi_{cl}]$, so $\psi_n(\xi)$ is integrated forward from 0 to ξ_{cl}, counting $\overline{n}$ and adjusting the energy as before.
- Using Numerov's method, explicit for y_{n-1} and with initial points $y_{max} = \Delta\xi$ and $y_{max-1} = y_{max}(12 - 10f_{\max})/(2f_{max-1})$, $\psi_n(\xi)$ is integrated backward from ξ_{max} to ξ_{cl}.

Since the potential is finite, the two computed wave functions $\psi^L(\xi)$ and $\psi^R(\xi)$ should **match** at ξ_{cl} with continuous derivative.

Matching

Continuity at ξ_{cl} is obtained rescaling $\psi^R(\xi)$ by $\psi^L(\xi_{cl})/\psi^R(\xi_{cl})$.

Normalization of the whole computed wave function is obtained rescaling it by $(\sum_{i=0}^{+\xi_{max}} 2|y_i|^2 - |y_0|^2)\Delta\xi$.

Let i be the such that $\xi_{cl} = i\Delta\xi$ and expand y_{i-1}^L and y_{i-1}^R around y_i up to the second order. Rewriting their sum holds:

$$y_i'^R - y_i'^L = \frac{y_{i+1}^R + y_{i-1}^L - (14 - 12f_i)y_i}{\Delta\xi} + O(\Delta\xi^2),$$

since $y_i^L = y_i^R = y_i$ for continuity and $y_i''^L = y_i''^R = -g_i y_i$ for the Schrödinger equation of the harmonic oscillator.

Derivative Discontinuity

At the eigenvalue ε_n, the difference $\psi'^R(\xi_{cl}) - \psi'^L(\xi_{cl})$ should be zero, but in general it is not since $\varepsilon \neq \varepsilon_n$. Integrating Schrödinger equation holds:

$$\int_{\xi_{cl}-\delta}^{\xi_{cl}+\delta} \frac{d^2\psi_n(\xi)}{d\xi^2} = -2 \int_{\xi_{cl}-\delta}^{\xi_{cl}+\delta} (\varepsilon_n - V(\xi))\psi_n(\xi).$$

Here δ is a positive quantity and in the limit of $\delta \to 0$, since $V(\xi_{cl}) = \varepsilon$, the above expression results:

$$\psi_n'^R(\xi_{cl}) - \psi_n'^L(\xi_{cl}) = -2(\varepsilon_n - \varepsilon)\psi_n(\xi_{cl}).$$

The left-hand side is **evaluated** through the previous estimate to the order $O(\Delta\xi^2)$.

Adjusting

The energy interval is adjusted according to the evaluation of the discontinuity in the first derivative:

- If $(y_i'^R - y_i'^L)y_i > 0$, then ε is too high and the energy range is set to $[\varepsilon_{min}, \varepsilon_{max} = (\varepsilon_{min} + \varepsilon_{max})/2]$.
- If $(y_i'^R - y_i'^L)y_i < 0$, then ε is too low and the energy range is set to $[\varepsilon_{min} = (\varepsilon_{min} + \varepsilon_{max})/2, \varepsilon_{max}]$.

This procedure is iterated up to a given tolerance on the width of the interval and it ensures finding **only** physically acceptable solutions.

This backward integration approach, modifying the shooting method, completely solves the two issues discussed above.

Repository

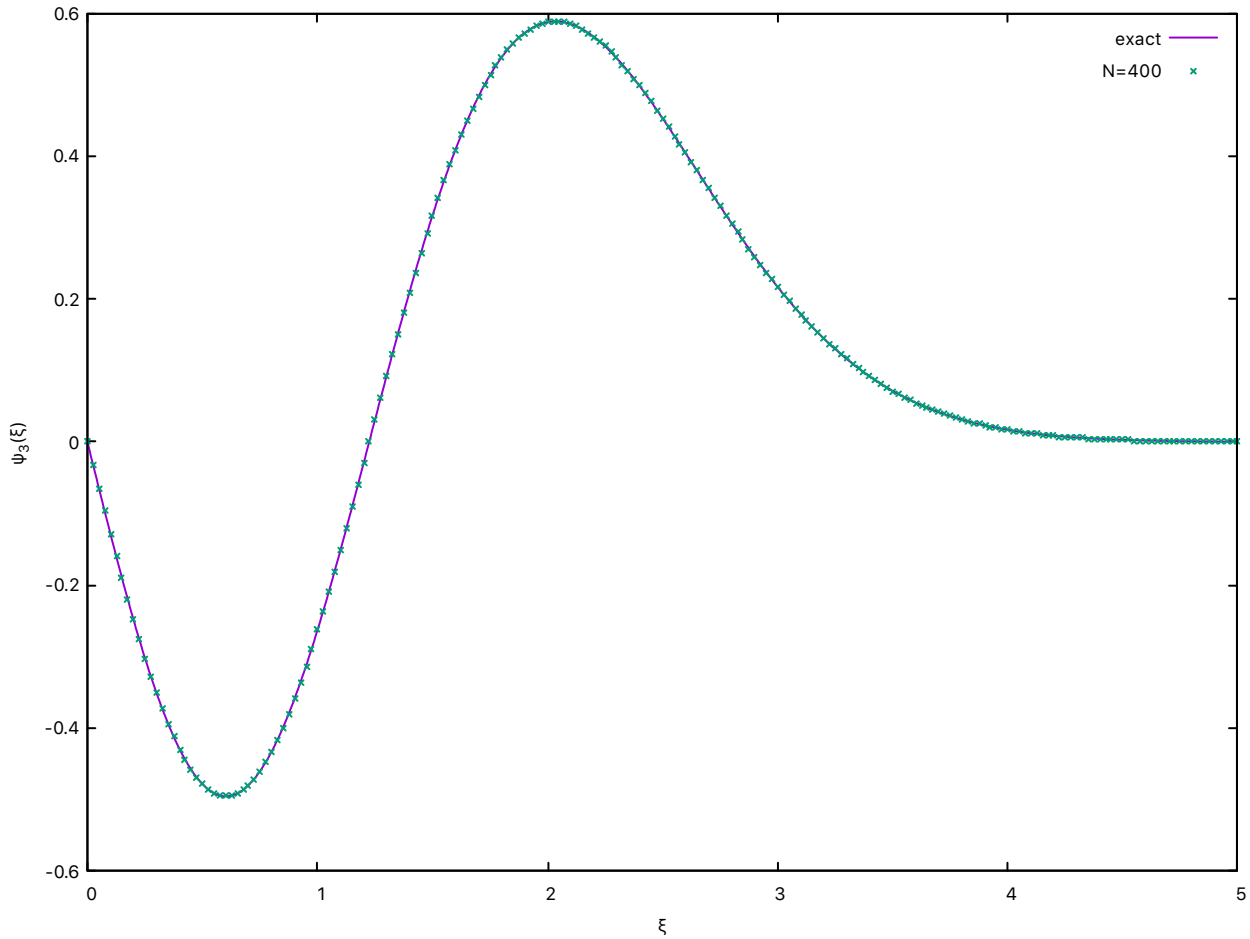
All the reported results are **reproducible** with the material available at this GitHub repository.

- The main code, implementing Numerov's method, is written in Fortran 90. A `readme` file describes in detail input parameters and output.
- Some Bash scripts are created to ease and automatize testing, setting $n = 3$.
- Also some Gnuplot scripts were used to produce the plots.

The main input parameters are the integration extreme ξ_{max}, set to 10, such that the whole system is contained in $[-\xi_{max}, +\xi_{\mathrm{max}}]$, the number of discretization points and the number of nodes n.

Wave Function

With 400 sample points in $[-10 : +10]$, the integrated wave function perfectly **matches** the exact $\psi_3(\xi)$.



Probability Density

The following plot shows the quantum probability density as the square modulus of the computed wave function. The classical inversion points are obtained as:

$$V(\xi_{cl}) = \frac{\xi_{cl}^2}{2} = \varepsilon_n = n + \frac{1}{2}, \text{ so } \xi_{cl} = \pm\sqrt{2n+1}.$$

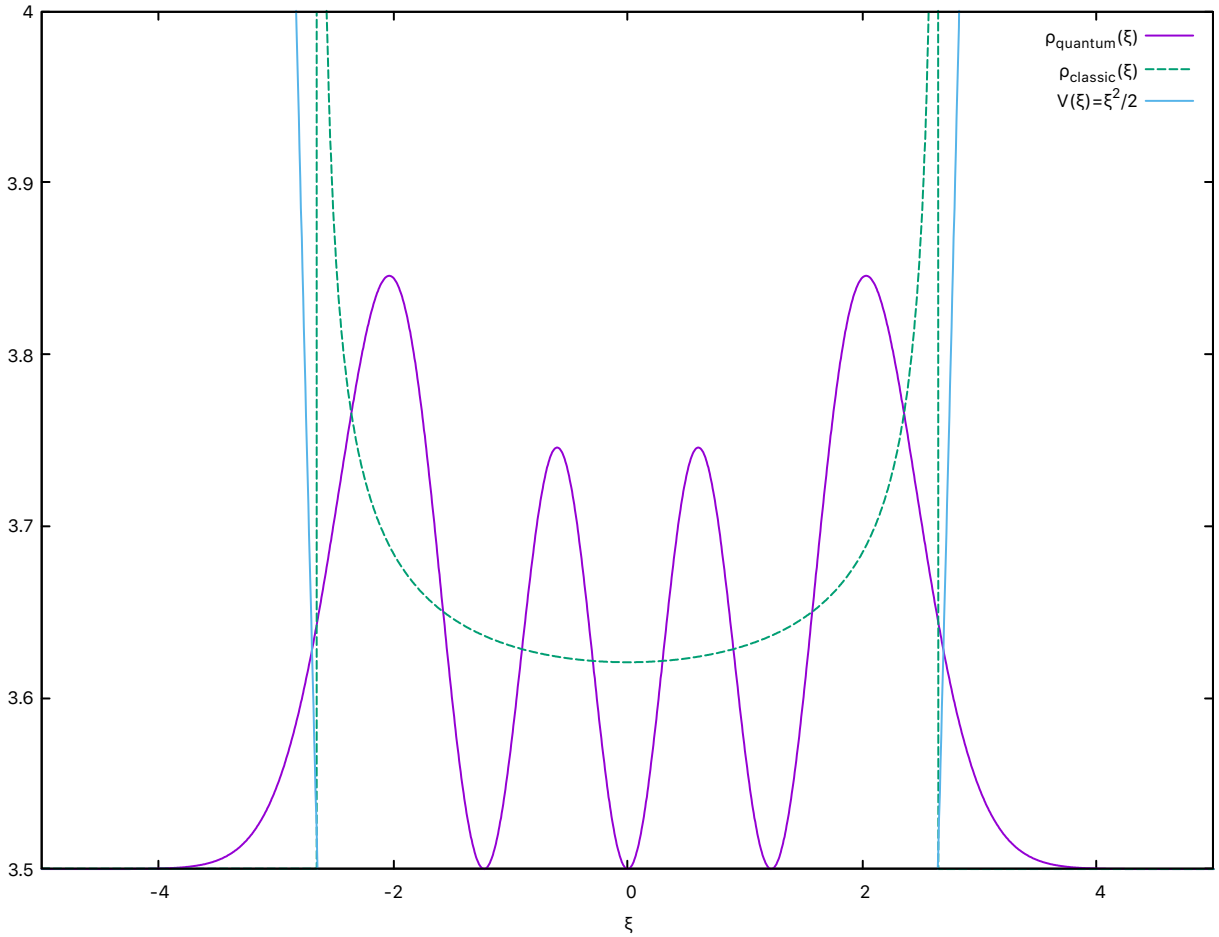
For $n = 3$, outside $[-\sqrt{7} \approx -2.65, +\sqrt{7} \approx +2.65]$, the quantum probability decays **exponentially**.

Classical probability density is instead defined only inside the above interval and diverges at ξ_{cl} as:

$$\rho(\xi) \propto \frac{1}{\sqrt{\varepsilon_n - \xi^2/2}}.$$

Comparison

Quantum and classical probability densities, shifted by the eigenvalue ε_3, are plotted together with the potential $V(\xi)$.



Global Error

The absolute value **difference** between the exact eigenvalue and the computed energy is taken as a measure of global error:

$$E(\Delta\xi) = |\varepsilon_n - \varepsilon_{computed}(\Delta\xi)|.$$

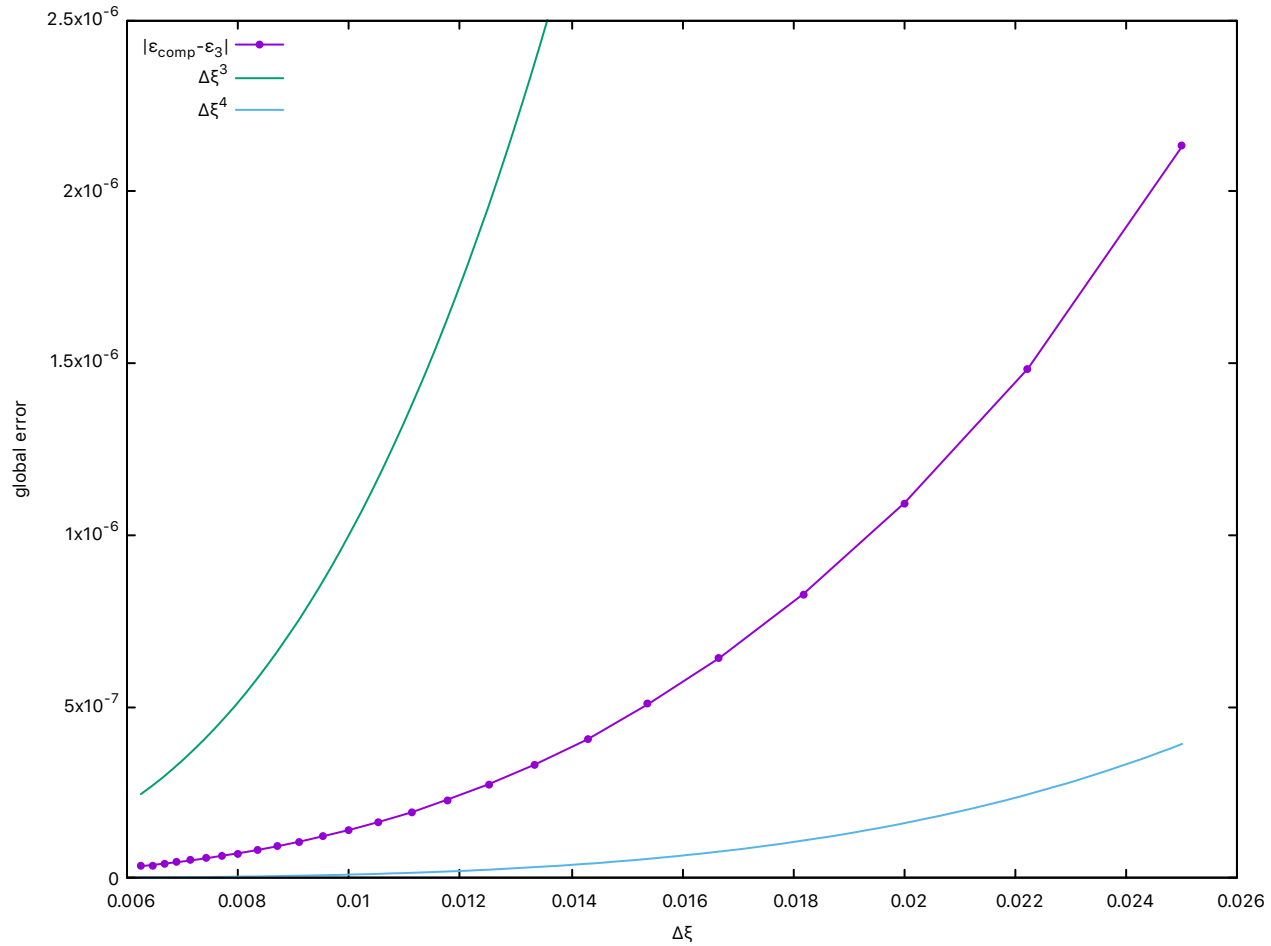
As discussed in general for Numerov's method, this is expected to go to zero no faster than $\Delta\xi^4$. An estimate of this order of convergence is given by:

$$p = \lim_{\Delta\xi \to 0^+} \log_2 \frac{E(\Delta\xi) - E(\Delta\xi/2)}{E(\Delta\xi/2) - E(\Delta\xi/4)}.$$

For the three values of $\Delta\xi \in \{10/1600, 10/800, 10/400\}$, the above expression results $p \approx 2.96$.

Error Order

Also this plot confirms that the order of the error is $O(\Delta\xi^3)$, instead of the lower **bound** $O(\Delta\xi^4)$.



Lower Order

The reason behind a performance worse than the lower bound of Numerov's method is that, somewhere in the code, a lower order error is introduced.

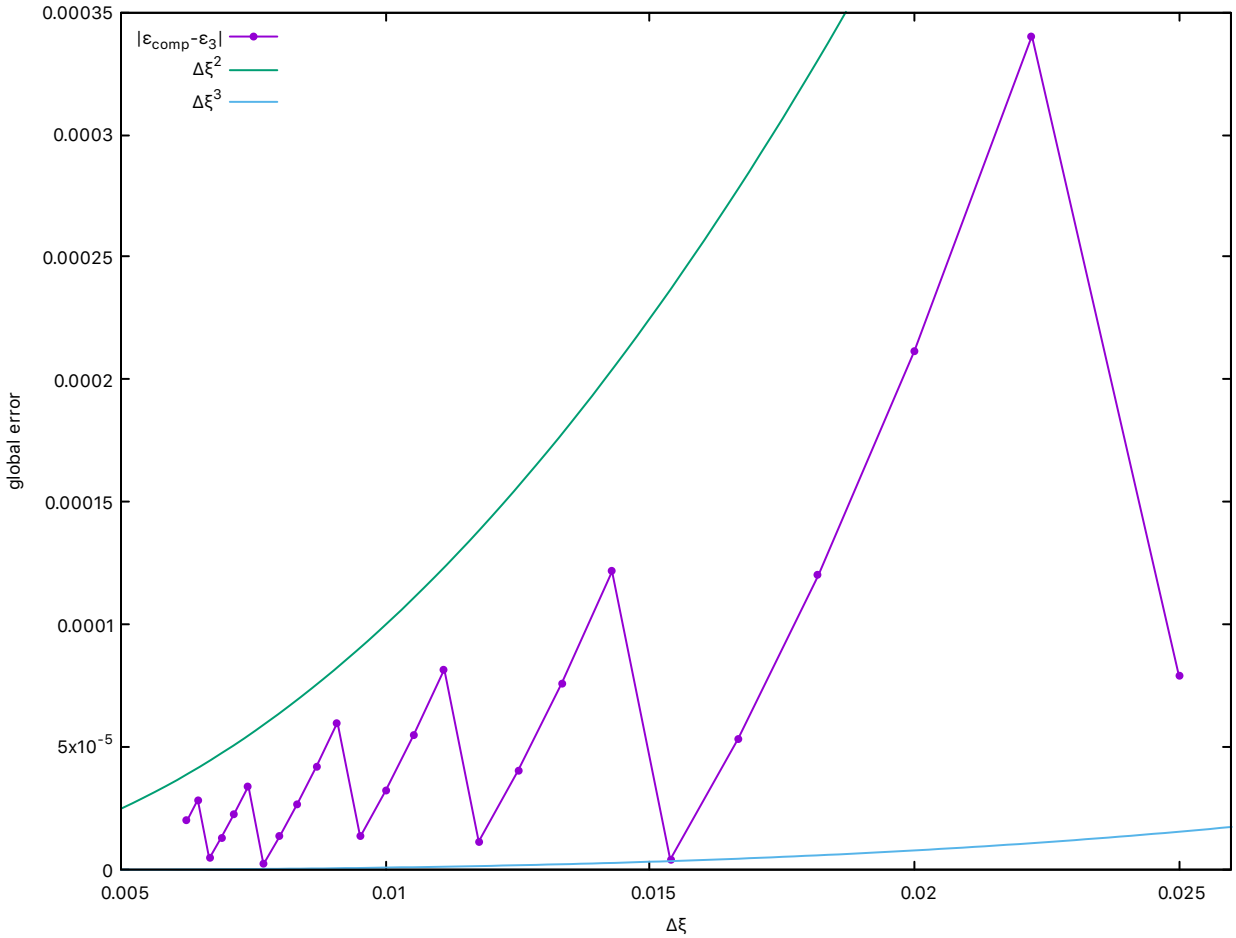
If the expansion of y_i^L and y_i^R around y_i is truncated to the second instead of the third order, the derivative discontinuity is evaluated as:

$$y_i'^R - y_i'^L = \frac{y_{i+1}^R + y_{i-1}^L - 2y_i}{\Delta\xi} + O(\Delta\xi).$$

This estimate is one order of error **worse** than the previous one. The following plot shows that one order of convergence is lost using this estimate.

Slower Convergence

Since the overall scaling gets worse, it means that the above poor estimate becomes the new **bottleneck** of the algorithm.



Higher Order

If the expansion of y_i^L and y_i^R around y_i is truncated instead to the fourth order, with the purpose of getting a more accurate estimate, the derivative discontinuity is evaluated as:

$$y_i'^R - y_i'^L = \frac{y_{i+1}^R + y_{i-1}^L - (14 - 12f_i)y_i}{\Delta\xi(3 - 2f_i)} + O(\Delta\xi^3),$$

since $y_i'''^R - y_i'''^L = -g_i(y_i'^R - y_i'^L)$, as derived from the Schrödinger equation of the harmonic oscillator.

The fact that **no** global error improvement is found means that the bottleneck, preventing obtaining Numerov's order of error of $O(\Delta\xi^4)$, is not due to the derivative discontinuity estimate.

Cusp

Let again i be such that $\xi_{cl} = i\Delta\xi$ and let y_i be the prediction obtained using forward Numerov's formula centered in y_{i-1}.

After backward integrating and matching, the issue is that Numerov's prediction for y_i, centered in the same y_i, generally differs from y_i:

$$y_{cusp} = \frac{y_{i+1}f_{i+1} + y_{i-1}f_{i-1} + 10f_i y_i}{12} \neq y_i.$$

This inexact result is the exact one of **another** problem, in which a Dirac delta function $v\delta(\xi - \xi_{cl})$ is superimposed at ξ_{cl}.

For the same argument of derivate continuity, a diverging potential produces a derivative discontinuity: a cusp.

Dirac Delta Coefficient

To get coherent results from Numerov's formula also in y_i, it must be allowed to have $f_{cusp} \neq f_i$ since:

$$y_{cusp} f_{cusp} = y_i f_i \text{ so } \delta f = f_{cusp} - f_i = f_i \left(\frac{y_i}{y_{cusp}} - 1 \right).$$

Differentiating $g(\xi) = -2(\varepsilon - V(\xi))$, it follows that $\delta g = 2\delta V$ and from the definition of $f(\xi)$, it is that $\delta g = 12\delta f / \Delta\xi^2$. Therefore:

$$\delta V = \delta f \frac{6}{\Delta\xi^2} = v.$$

Then, the above estimate of δf allows to compute the **coefficient** v of the Dirac delta function centered in ξ_{cl}.

Perturbation Theory

The first order **correction** to the energy eigenvalue ε_n is given by the expectation value of $\delta H = \delta V \delta(\xi - \xi_{cl})$, the perturbation Hamiltonian, on the unperturbed eigenstate ψ_n:

$$\delta\varepsilon_n = \langle\psi_n|\delta H|\psi_n\rangle = \int \delta f \frac{6}{\Delta\xi^2}\delta(\xi - \xi_{cl})|\psi_n|^2 d\xi.$$

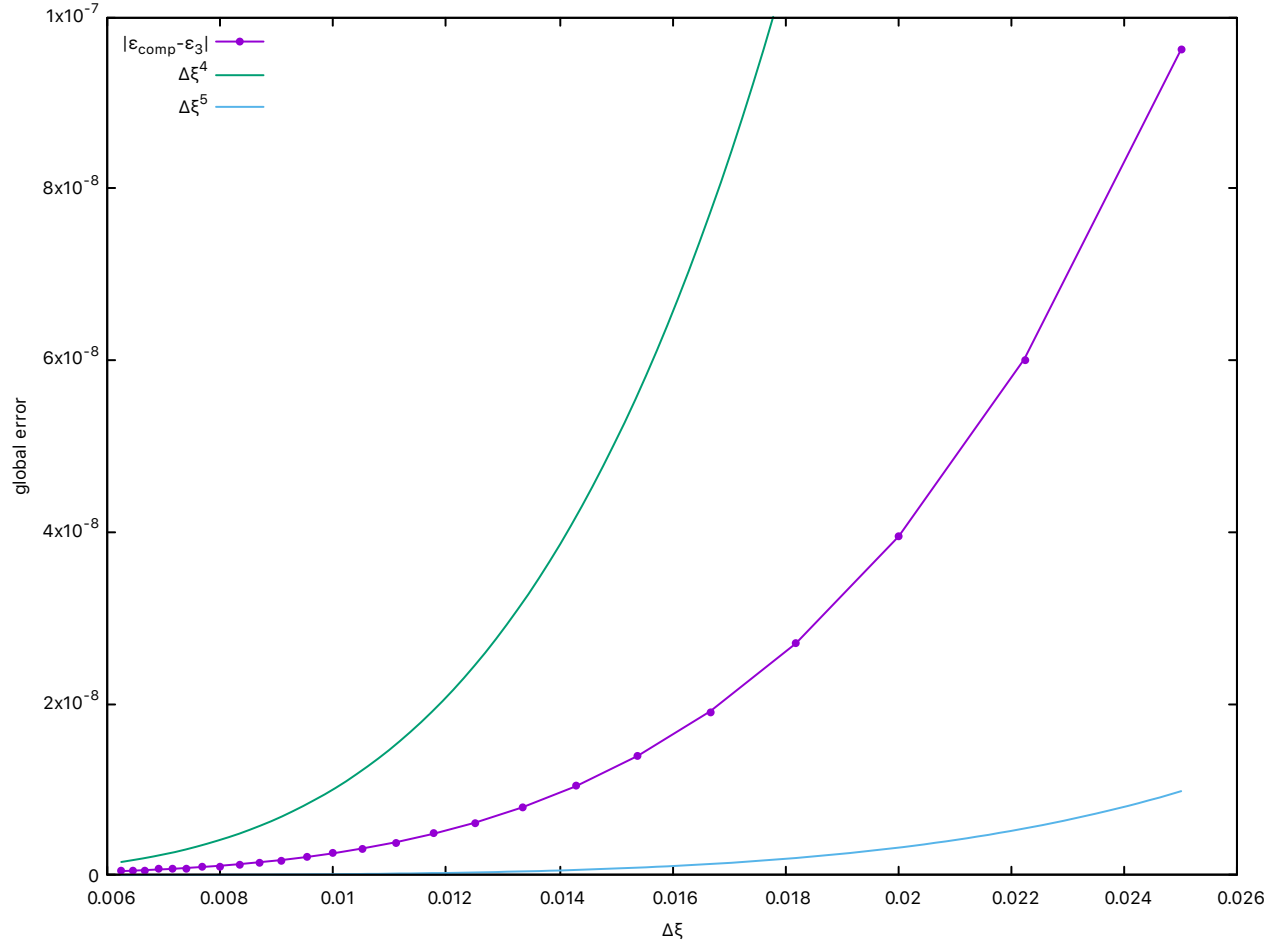
The integral is written as a sum on the grid and its only non-zero contribution comes from the interval of width $\Delta\xi$ around ξ_{cl}, so:

$$\delta\varepsilon_n = \delta f \frac{6}{\Delta\xi}|y_i|^2.$$

This first order estimate of the difference between the eigenvalue of the inexact problem and ε_n is used to adjust the trial energy ε.

Error Order Improvement

A tolerance is set also on $|\delta\varepsilon_n|$. With this adjustment, the algorithm reaches Numerov's method error order lower bound of $O(\Delta\xi^4)$.



Conclusion

The threshold on the size of $|\delta\varepsilon_n|$ substitutes the previous one on the width of the $[\varepsilon_{\text{min}}, \varepsilon_{\text{max}}]$ interval, so both are set to 10^{-10} in units of $\hbar\omega$.

For the same three values of $\Delta\xi \in \{10/1600, 10/800, 10/400\}$, the order error estimate correctly results $p \approx 4.00$.

- The above result shows that the bottleneck in the original code was in the process of halving the energy interval while backward integrating and looking for the eigenvalue ε_n.
- The code reaches now the error order lower **bound** admitted using Numerov's integration method and no further improvement can be obtained using this algorithm.