Numerical modelling of quantum harmonic oscillator

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Abstract. We present a Python module implementing various ODE solvers, enabling one to do accurate and effective numerical simulations. We investigate it's accuracy investigating a quantum harmonic oscillator in position basis.

Keywords: numerical modelling, Numerov's algorithm, quantum systems, harmonic oscillator

1 Introduction

Numerov's method [1] allows one to solve differential equations of kind:

$$y''(x) = f(x) \cdot y(x) \tag{1}$$

Examples of equation (1) include classical harmonic oscillator:

$$y''(x) = -\omega^2 \cdot y(x) \tag{2}$$

or one-dimensional, time-independent Schrodinger's equation:

$$y''(x) = \frac{2m}{\hbar^2}(E - V(x)) \cdot y(x). \tag{3}$$

Numerov's iterative metod uses an equidistant grid [1,2] $x_n = \delta n$ on which approximates y_i values via equation:

$$\left(1 - \frac{\delta^2}{12} f_{n+2}\right) y_{n+2} = \left(2 + \frac{5}{6}\delta^2 f_{n+1}\right) y_{n+1} - \left(1 - \frac{\delta^2}{12} f_n\right) y_n, \tag{4}$$

where $f_i = f(x_i)$. Equation (4) can be solved for arbitrary n knowing the values y_0 and y_1.

In practice, second-order differential equations are given Cauchy boundary conditions - $y(0) = y_0$ and $y'(0) = v_0$. Therefore, value y_1 is often approximated using Taylor polynomial:

$$y_1 = y(\delta) \approx y(0) + \sum_{n=1}^{4} \frac{\delta^n}{n!} y^{(n)}(0). \tag{5}$$

Differentiating equation (1) and substituting y'' for combinations of y and f one gets the fourth-order approximation in terms of y_0, v_0 and values of different derivatives of f, which can be evaluated symbolically or numerically:

$$y_1 \approx \frac{1}{24}\delta^4 \left(y_0 f''(0) + 2f'(0)v_0 + f_0^2 y_0\right) + \tag{6}$$

$$+\frac{1}{6}\delta^3 \left(y_0 f'(0) + f_0 v_0\right) + \frac{1}{2}\delta^2 f_0 y_0 + \delta v_0 + y_0 \tag{7}$$

2 Quantum harmonic oscillator

Schrodinger equation for quadratic potential $V(x) \propto x^2$ can be rewritten in dimensionless form as:

$$y''(x) = (x^2 - E)y(x). \tag{8}$$

General theory of differential equations allows one to prove [2, 3] that all the square-integrable solutions are given by:

$$y_n(x) = H_n(x) \exp\left(-\frac{x^2}{2}\right), \tag{9}$$

where n is a non-negative integer, and H_n is the n-th Hermite polynomial. Moreover, such solutions exist only for discrete energies $E_n = 2n+1$. We expect that such a solution can be reconstructed using Numerov's method.

We implemented Numerov's method to solve equation (8) using boundary conditions: $y_0 = 0,\ v_0 = 1$ (n odd) or $y_0 = 1,\ v_0 = 0$ (n even) and compared found solutions with analytic one for different energy levels. Figure 1. shows that the method is accurate.

2.1 Determining oscillator energy levels

As we are interested in square-integrable solutions, we require $y(x) \to 0$ for $x \to \infty$. Therefore we can determine energy spectrum basing on the behaviour of found function y. We implemented a gradient descent optimiser [4] that tried to minimise value $y_E(5)^2$, where y_E is the solution of (8) for energy value E and with boundary conditions calculated taking $n = [0.5E]$. Table 2. presents found eigenvalues. While found values are close to exact, analytical, values, for $E = 1$ there is a small discrepancy. It is due to the small noise at $y_E(5)$.

3 Conclusions

We showed that an oscillator quantised in position basis solved numerically confirms the analytical solution. We found wavefunctions corresponding to the different energy levels of the oscillator and confirmed using gradient descent optimisers, that energy spectrum is quantised. Implemented software package can be used to solve other computational physics problems.

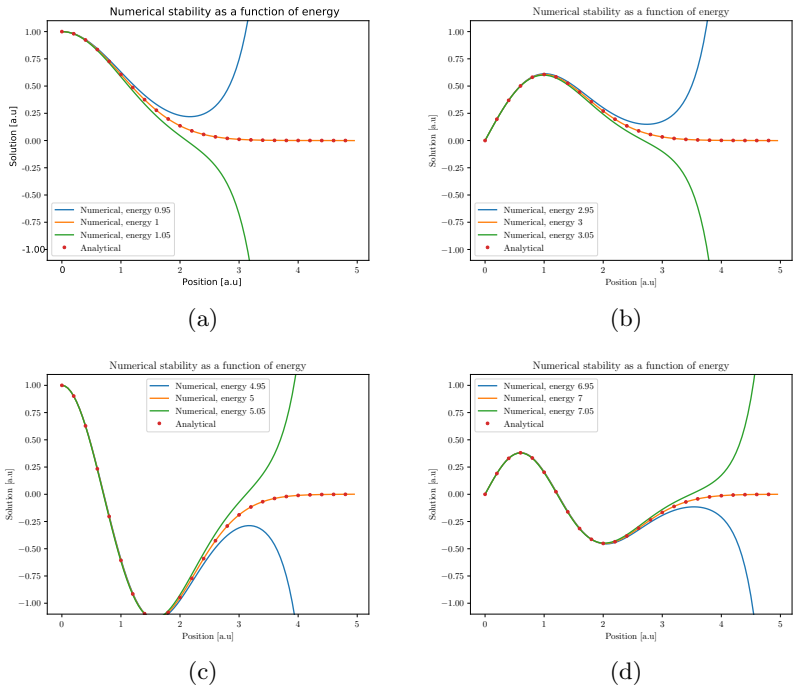

Fig. 1: We compare analytical solution with found numerical solutions for different energy values. We used value $\delta = 0.02$ solving equation on the interval $[0, 5]$. Different n values were used: $n = 0$ for 1a., $n = 1$ for 1b., $n = 2$ for 1c. and $n = 3$ for 1d.

Initial	Found	Exact
0.8	0.98	1
1.2	0.97	1
1.4	0.98	1
3.4	3.00	3
5.7	5.00	5

Fig. 2: The table presents found eigenvalues using gradient descent method starting from inaccurate, but close, guessed energy values.

4 References

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