Tutorial Introduction to Computational Physics SS2011

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1 Numerov algorithm for the Schrödinger equation

The Numerov algorithm is a high accuracy discretisation method used for special differential equations of the type

$$y''(x) + k(x)y(x) = 0 \ .$$

It is given by

$$\left(1 + \frac{1}{12}h^2 k_{n+1}\right) y_{n+1} = 2 \ \left(1 - \frac{5}{12}h^2 k_n\right) y_n - \left(1 + \frac{1}{12}h^2 k_{n-1}\right) y_{n-1} + \mathcal{O}(h^6)$$

and provides 6th order accuracy by using the three values y_n, y_{n-1}, y_{n+1} only, with $k_i := k(x_i)$ and $y_i = y(x_i)$. Its proof is given in our script chapter 6.6. and will also be discussed in the tutorials. The Numerov algorithm has historically been used first for solving Newton's equation of motion for gravitating bodies, but it is also a fine algorithm to solve numerically the time independent Schrödinger equation. It reads:

$$\Psi\text{''}(z) + \frac{2m}{\hbar^2}(E - V(z))\Psi(z) = 0 \tag{1.1}$$

For the harmonic oscillator problem one has $V(z) = mz^2/2$.

- The dimensionless form of this equation is obtained from $x = z/z_0$, with a suitable z_0, and looks as follows:

$$\psi\text{''}(x) + (2\varepsilon - x^2)\psi(x) = 0 \tag{1.2}$$

- Write a computer program that uses the Numerov algorithm to solve this equation. Test it against the known analytic solution:

$$\psi(x) = \frac{H_n(x)}{(2^n n! \sqrt{\pi})^{1/2}} \exp\left(-\frac{x^2}{2}\right) \tag{1.3}$$

  in which $H_n(x)$ are the Hermite polynomials. These are the solutions for the energy Eigenvalues $\varepsilon = n + 1/2$. One should use choose $\psi(0) \neq 0$ for the symmetric Eigenfunctions, and $\psi(0) = 0$ and $\psi(h) \neq 0$ for the antisymmetric Eigenfunctions. Note that the norm of these Eigenfunctions is irrelevant. A definition of $H_n(x)$ can be found for example in `http://mathworld.wolfram.com/HermitePolynomial.html`. For practical, computational purposes the most efficient way to compute $H_n(x)$ is to start with $H_0(x) = 1$, $H_1(x) = 2x$ and then use the recurrence relation

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)$$

  to define the higher order polynomials.

2 Neutrons in a gravity field (homework)

Another possible application of the Numerov algorithm is the calculation of stationary states $\Psi(z)$ of neutrons in the gravity field of the Earth[1]. The gravity of the Earth is given by $V(z) = mgz$ for $z \geq 0$. At $z = 0$ a horizontal perfectly reflecting mirror reflects the neutrons so that one can take $V(z) = \infty$ for $z < 0$. We seek solutions for $z \geq 0$, since $\Psi(z) = 0$ for $z < 0$. After a proper choice of length and energy units (please specify!) the above equation can be rewritten as

$$\psi"(x) + (\varepsilon - x)\psi(x) = 0 \tag{2.4}$$

1. (10 points) Use your Numerov program to solve this differential equation. Choose some values of ε and plot the solution from $x = 0$ to $x \gg \varepsilon$ (i.e. well into the classically forbidden zone). We are interested in the asymptotic behaviour of the solution for large x, i.e. whether it goes to positive infinity or negative. Show (plot) two solutions obtained from your program (for two values of ε), one with positive and one with negative asymptotic behaviour.

2. (10 points) The Eigenvalues ε_n of Schr"odinger's equation belong to normalizable eigenfunctions, for which it is $\psi(x) \to 0$ for $x \to \infty$. It means that while varying ε_n from smaller to larger values, the function $\psi(x)$ for $x \to \infty$ changes sign. Use this property to determine the Eigenvalues ε_n of the first three bound states to 2 decimals behind the comma.

[1] See `http://www.uni-heidelberg.de/presse/news/2201abele.html`