Department of Physics
UMEÅ UNIVERSITY
Claude Dion[1]

January 20, 2015

Numerical Methods in Physics

Numerical solution of Poisson's equation using Numerov's method

PURPOSE: To learn Numerov's method.
To show how unwanted solutions can affect the numerical solution.

LITERATURE:

M. Galassi *et al.*, GNU Scientific Library Reference Manual, 2nd ed. (Network Theory, Bristol, 2006), `http://www.gnu.org/software/gsl/`

[1] Based on work by Sune Pettersson and Anna Jonsson.

1 Introduction

Many physical problems lead to a type of second-order ordinary differential equations which looks like the following

$$\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + k^2(x)y = S(x), \tag{1}$$

where $k^2(x)$ and $S(x)$ are determined from the physical problem. In some cases k and S respectively may be constants and in some cases one of them may be zero. In most standard methods for solving ordinary differential equations we rewrite eq. (1) as two coupled first-order ordinary differential equations. We will not do any such rewriting but we will derive a recursion formula directly from eq. (1).

We will calculate y for a number of points x_j which are defined by

$$x_j = jh + x_0, \tag{2}$$

where x_0 is the starting point of the integration and h is a fixed step size. We also introduce the notation

$$y_{j+1} \equiv y(x_{j+1}) \equiv y(x_j + h). \tag{3}$$

We start by doing two Taylor expansions about y_j:

$$y_{j+1} = y_j + h\left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)_j + \frac{1}{2}h^2\left(\frac{\mathrm{d}^2 y}{\mathrm{d}x^2}\right)_j + \frac{1}{6}h^3\left(\frac{\mathrm{d}^3 y}{\mathrm{d}x^3}\right)_j + \ldots \tag{4}$$

$$y_{j-1} = y_j - h\left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)_j + \frac{1}{2}h^2\left(\frac{\mathrm{d}^2 y}{\mathrm{d}x^2}\right)_j - \frac{1}{6}h^3\left(\frac{\mathrm{d}^3 y}{\mathrm{d}x^3}\right)_j + \ldots \tag{5}$$

If we add these two expansions all terms containing h raised to an odd power disappear, *i.e.*,

$$y_{j+1} + y_{j-1} = 2y_j + h^2\left(\frac{\mathrm{d}^2 y}{\mathrm{d}x^2}\right)_j + \frac{1}{12}h^4\left(\frac{\mathrm{d}^4 y}{\mathrm{d}x^4}\right)_j + \mathcal{O}(h^6). \tag{6}$$

The second derivative is now replaced with the expression given in the original differential equation (1),

$$\left(\frac{\mathrm{d}^2 y}{\mathrm{d}x^2}\right)_j = S(x_j) - k^2(x_j)y_j, \tag{7}$$

which gives

$$y_{j+1} = h^2 S(x_j) + \left[2 - h^2 k^2(x_j)\right] y_j - y_{j-1} + \frac{h^4}{12}\left(\frac{\mathrm{d}^4 y}{\mathrm{d}x^4}\right)_j + \mathcal{O}(h^6). \quad (8)$$

It now is possible to construct a recursion formula by neglecting terms of order h^4 and higher. This method is thus of order 3. Therefore, we have

$$y_{j+1} = h^2 S(x_j) + \left[2 - h^2 k^2(x_j)\right] y_j - y_{j-1}. \quad (9)$$

If you know the solution in two succeeding points (y_{j-1} and y_j) the solution in every other point can be obtained by iteration of Eq. (9).

2 Numerov's method

In many cases we may have to make several hundreds iterations of eq. (9) and the error which is of order h^4 may become significant. By using Numerov's method we can obtain an even better recursion formula than eq. (9) by keeping terms of order h^4 and only neglecting terms of order h^6 and higher. To produce such a recursion formula we define a new function Y,

$$Y_j \equiv y_j + \frac{h^2}{12} k^2(x_j) y_j. \quad (10)$$

We obtain an recursion formula for Y by applying the operator $\left(1 - \frac{h^2}{12}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right)$ on eq. (6),

$$\begin{aligned} y_{j+1} - \frac{h^2}{12}\left(\frac{\mathrm{d}^2 y}{\mathrm{d}x^2}\right)_{j+1} &+ y_{j-1} - \frac{h^2}{12}\left(\frac{\mathrm{d}^2 y}{\mathrm{d}x^2}\right)_{j-1} \\ &= 2y_j - \frac{2h^2}{12}\left(\frac{\mathrm{d}^2 y}{\mathrm{d}x^2}\right)_j + h^2\left(\frac{\mathrm{d}^2 y}{\mathrm{d}x^2}\right)_j \\ &- \frac{h^4}{12}\left(\frac{\mathrm{d}^4 y}{\mathrm{d}x^4}\right)_j + \frac{h^4}{12}\left(\frac{\mathrm{d}^4 y}{\mathrm{d}x^4}\right)_j - \frac{h^6}{144}\left(\frac{\mathrm{d}^6 y}{\mathrm{d}x^6}\right)_j \mathcal{O}(h^6) \end{aligned} \quad (11)$$

Terms of order h^4 will cancel each other and we neglect terms of order h^6 and higher. The second derivatives are rewritten with eq. (7) after which we can introduce the function Y, which gives

$$Y_{j+1} - \frac{h^2}{12} S_{j+1} + Y_{j-1} - \frac{h^2}{12} S_{j-1} = 2Y_j - \frac{2h^2}{12} S_j + h^2 S_j - Y_j \frac{h^2 k_j^2 y_j}{y_j + \frac{h^2}{12} k_j^2 y_j}. \quad (12)$$

This can be rewritten to a recursion formula in Y:

$$Y_{j+1} = Y_j \left(2 - \frac{h^2 k_j^2}{1 + \frac{h^2}{12} k_j^2} \right) - Y_{j-1} + \frac{h^2}{12} \left(S_{j+1} + 10 S_j + S_{j-1} \right). \tag{13}$$

When we have iterated a solution to Y we will obtain the function y from eq. (10).

3 Poisson's equation

We will use Numerov's method to solve Poisson's equation,

$$\nabla^2 \Phi = -4\pi\rho \tag{14}$$

which here is written in Gaussian units, *i.e.*, the charge is measured in esu (1 esu = 0.1 A m/$c \approx 3.33564 \times 10^{-10}$ C), distance is measured in cm and the potential is measured in statvolt = erg/esu $\approx$ 299.79 V. If we use spherical coordinates we can write

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial \Phi}{\partial r} \right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial \Phi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2 \Phi}{\partial \Psi^2} = -4\pi\rho \tag{15}$$

As an example we will take a spherically symmetric charge distribution ρ and electrostatic potential Φ.

Exercise 1

Simplify Eq. (15) provided that ρ and Φ is spherically symmetric, and introduce the function φ through the substitution $\Phi(r) = r^{-1}\varphi(r)$. Write down Numerov's recursion formula for your simplified Poisson equation.

The charge distribution we will examine is

$$\rho(r) = \frac{1}{8\pi} \mathrm{e}^{-r} \tag{16}$$

which total charge is

$$Q = \int \rho(r) \mathrm{d}^3 r = \int_0^\infty \rho(r) 4\pi r^2 \mathrm{d}r = 1. \tag{17}$$

The exact solution to the problem is

$$\varphi(r) = 1 - \frac{1}{2}(r+2)\mathrm{e}^{-r}. \tag{18}$$

This solution has the expected behavior for large r where

$$\Phi(r) = \frac{\varphi(r)}{r} \longrightarrow \frac{1}{r} \tag{19}$$

which is the Coulomb potential from a unit charge.

4 Initial values

To be able to start our recursion formula we must know φ_0 and φ_1. To make the electrostatic potential Φ finite in $r = 0$ we must have $\varphi(0) = 0$. This is also in agreement with the exact solution. φ_1 can be determined in two ways:

1. Since we know the exact solution we can calculate $\varphi_1 = \varphi(h)$. This is of course only possible if we know the analytical solution.

2. In the general case we do not know the solution in advance. Then we can calculate φ_1 by taking an Euler step from $r = 0$ to $r = h$.

$$\begin{aligned} \varphi_1 &= \left(\frac{\partial \varphi}{\partial r}\right)_{r=0} h \\ &= \Phi(0)h \end{aligned} \tag{20}$$

   $\Phi(0)$ can be obtained by solving the Coulomb integral numerically.

$$\Phi(0) = \int \frac{\rho(r)}{r} \mathrm{d}^3 r = 4\pi \int_0^\infty \rho r \mathrm{d}r \tag{21}$$

Exercise 2

Write a computer program which implements the recursion formula you derived in exercise 1. Run the program with step size $h = 0.1$ and $\varphi_0 = 0$. Try three different choices of φ_1:

1. φ_1 is taken from the analytical solution.

2. $\varphi_1 = \Phi(0)h$, where $\Phi(0)$ has been obtained from numerical integration.

3. $\varphi_1 = 95\%$ of the analytical value.

The last case is there to show the effect of an uncertain determination of $\Phi(0)$.

Present the results in a table with 5 columns which contains: r ($r = 2, 4, 6, \ldots, 20$), the exact solution $\varphi(r)$, the errors in the three numerical solutions. The errors are calculated as $\varphi_{\text{exact}}(r) - \varphi_{\text{num}}(r)$.

5 Unwanted solutions

When the initial value for φ_1 was 5% too small (choice 3 above) it resulted in a 50% error for large r. The explanation of this is that for large r unwanted solutions influence the result.

A good approximation to Poisson's equation for very large values of r is

$$\frac{\partial^2 \varphi}{\partial r^2} = 0 \tag{22}$$

This equation has two possible solutions:

$$\begin{aligned} &\varphi \sim r; && \Phi \sim \text{constant} \\ &\varphi \sim \text{constant}; && \Phi \sim r^{-1}. \end{aligned}$$

We know that the potential at large distance from a charge distribution shall be $\Phi \sim r^{-1}$, which means that $\varphi \approx$ constant for large r. Due to numerical round offs also the solution with $\varphi \sim r$ can appear and for large r this solution will dominate.

The numerical solution for large r can then be written as

$$\varphi = mr + b. \tag{23}$$

We assume that this linear relation is valid for the last ten points determined in exercise 2.

Exercise 3

Use your results for choice 3 in exercise 2. Fit a straight line between the last and the tenth point from the end and determine the constants m and b. Subtract mr from your earlier solution for φ.

Add to your earlier table a column which contains the error after the unwanted solution has been subtracted.

6 Bonus exercise

The 1D time-independent Schrödinger equation for a harmonic oscillator reads

$$\left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{m\omega^2}{2}x^2\right)\psi(x) = E\psi(x), \tag{24}$$

where m is the mass of the particle, ω the angular frequency of the harmonic potential, and E the energy (eigenvalue) of the wave function (eigenvector) ψ. Write Numerov's recursion formula for this Schrödinger equation.

7 Presentation of results

Present your results in a **brief** report where you also include the path to your code and instructions for compiling and running. Do not supply listings of your programs, but give the path where they can be found.