Thomas Waterman
Dr. Dallas
Numerical Analysis
May 8, 2025

Numerov's Method

Abstract:

This project sought to implement the Numerov Method to solve Differential equations of the form $Y'' + g(x)Y = 0$. This was completed using a python script in which a user may input the range of the function to be graphed, any function $g(x)$, the two initial values of the function Y, and the spacing between nodes. A smaller spacing between nodes will give a more accurate result. Overall, the code works very well, though one must be careful around Y = 0 because of dividing by 0 issues.

Introduction:

Differential equations work extremely well to explain the world that humanity experiences. Since Newton first postulated his famous laws, which may be written as differential equations, solving differential equations became essential to modeling reality.

In light of quantum mechanics, solving the Schrödinger Equation is of great interest to physicists. Additionally, solving the equation efficiently is also desirable. In general the Schrödinger Equation is as follows:

$$\frac{\hbar}{2m}\nabla^2\Psi + V(r)\Psi = E\Psi$$

By reducing the Schrödinger equation to the one-dimensional case, this equation may be manipulated into the following form:

$$\frac{d^2\psi}{dx^2} + (V(x) - E)\psi = 0$$

Leaving the Schrödinger Equation behind, one may see that the family of differential equation that it falls into is:

$$Y'' + g(x)Y = 0$$

While many differential equations have nice, closed form solutions, the general solution to this differential equation is not able to be written in a closed form. Depending on $g(x)$, the solution may have a closed form representation. A closed form solution is a solution that may be written without an infinite sum. Regardless, solving a differential equation that does not have a closed form solution is extremely tedious and prone to algebraic errors. To solve this type of differential equation one begins by assuming that the solution will look as follows:

$$y = \sum_{n=1}^{\infty} a_n x^n$$

By plugging into the differential equation and reindexing the power series one may obtain a recurrence relation between the different a_n values. Finally, with boundary conditions, one may determine what a few of the a_n values should be and may then calculate the rest from them. As it is impossible to graph a summation to infinity, one will be forced to stop the summation at some finite number and thus introduce error. As directly solving this ordinary differential equation (ODE) is tedious, and any attempt to plot the solution will result in some error, solving the differential equation numerically becomes very appealing.

Method:

Of the many methods available, Numerov's method appears to be ideal for this type of problem. Numerov's method was designed to solve the following ODE:

$$Y'' + g(x)Y = s(x)$$

If one is to set the function $s(x) = 0$, then the Numerov method can effortlessly be reduced into the ODE of concern. The derivation of the Numerov method begins with a Taylor series expansion. A detailed derivation may be found at the following link from Drexel University: Numerov derivation (McMillan). The final, simplified form of the method relies on knowing y_{n-1} and y_n. The $O(h^4)$ term is the error term. The spacing between nodes is given by h.

$$y_{n+1} = \frac{2y_n\left(1+\frac{5h^2}{12}g_n\right)-y_{n-1}\left(1+\frac{h^2}{12}g_{n-1}\right)}{1+\frac{h^2}{12}g_{n+1}} + O(h^4)$$

Result:

To test the method, and to ensure that the coding was correctly performed, several simple functions were chosen for g(x).

Test 1:

First g(x) was set to 0. This simplifies the differential equation to: $Y'' + 0Y = 0$. The solution to this ODE is a straight line. The results of the code agree with this.

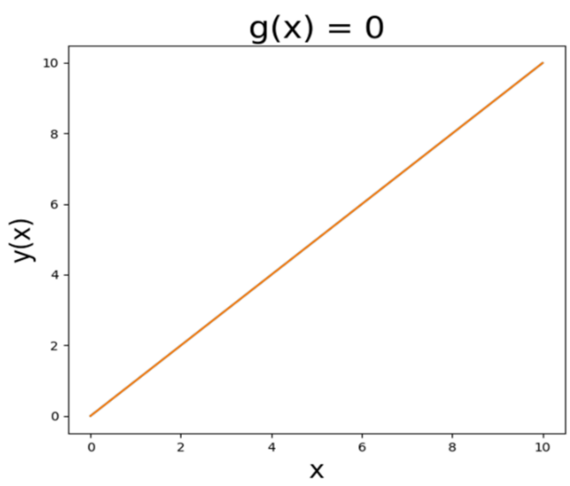

Figure 1: Output of Code for Test 1

Test 2:

Then g(x) was set to -1. This simplifies the differential equation to: $Y'' - Y = 0$. The solution to this ODE is a sin function. The results of the code agree with this.

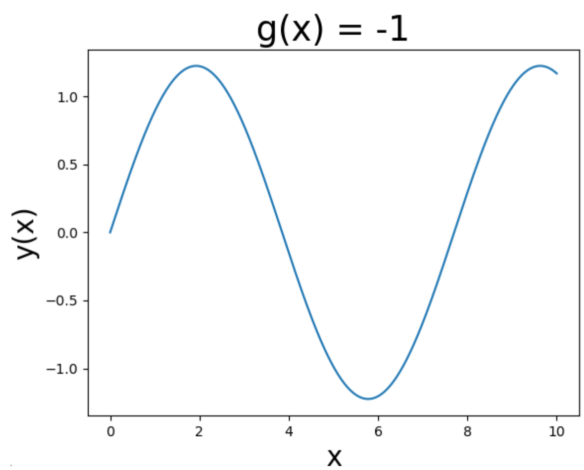

Figure 2: Output of Code for Test 2

Test 3:

Finally, g(x) was set to $1/x^2$. This simplifies the differential equation to: $x^2Y'' - Y = 0$. The solution to this ODE is $Ax^n + Bx^{-n}$. I selected values for y_{n-1} and y_n so that B = 0. The results of the code agree with these parameters.

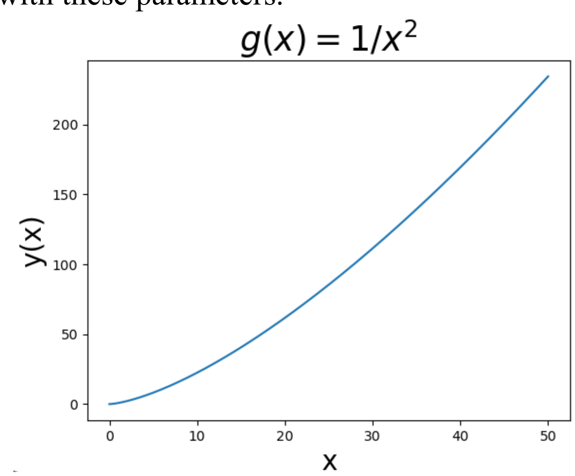

Figure 3: Output of Code for Test 3

Schrödinger Equation:

Unfortunately, this method alone is not enough to solve the Schrödinger Equation. The Schrödinger Equation has a value of energy that is unknown when the problem is being attempted. If one is to truly solve the Schrödinger equation, one must also implement a method of determining what the Energy value should be. Several different papers have been published that have done just this (Berghe, 1989) (Caruso, 2022) (Numerov's Method, 2022). As a method for fine-tuning the Energy value was not implemented, one can observe the “explosions” that occur when one chooses the energy value incorrectly. Two different values of energy were chosen: 0.2 and 0.23. In the figures below one can observe the need for an algorithm to determine a precise value for the energy in the Schrödinger Equation.

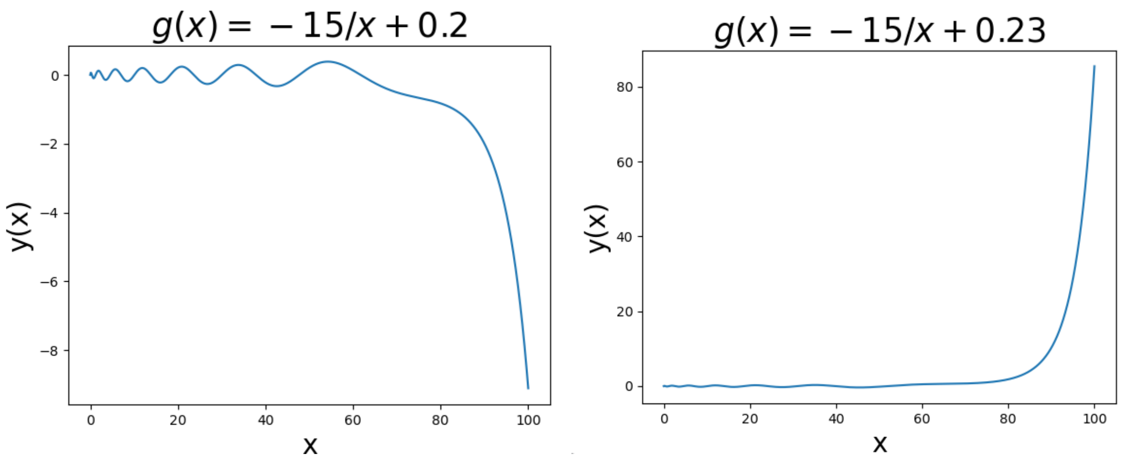

Figure 4: Observing how a small change in energy has a drastic result on the solution.

Conclusion:

Overall, this project successfully implemented the Numerov Method to allow a user to easily solve a differential equation of the form: $Y'' + g(x)Y = 0$. With more work, this method, along with adequate knowledge of boundary conditions, could be used with another method, such as the shooting method, to solve the Schrödinger Equation numerically for any one system that could be reduced to one dimension.

Works Cited

Berghe, G. V. (1989). Numerical methods for solving radial Schrodinger equations. *Journal of Computational and Applied Mathematics, 28*.

Caruso, F. (2022). Applications of the Numerov method to simple quantum systems using Python. *Rev. Bras. Ensino Fís.* Retrieved from https://www.scielo.br/j/rbef/a/Wn6byfBVypcgn8jnZTpfJsg/?lang=en

McMillan, S. (n.d.). Numerov Method. *Drexel University: Computational Physics*. Retrieved from https://www.physics.drexel.edu/~steve/Courses/Comp_Phys/Physics-305/numerov.pdf

Numerov's Method. (2022, October 23). Retrieved from Wikipedia: https://en.wikipedia.org/wiki/Numerov%27s_method