PERIMETER INSTITUTE

Numerical Methods
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Assignment 2: Sniping Schrödinger

Due: Jan 23; Pass-Fail deadline: Jan 30

The ordinary differential equation methods we have discussed in class have all been designed to solve the *Initial Value* (or Cauchy) problem: $d\vec{x}/dt = f(t, \vec{x})$ where $\vec{x}(t_0) = \vec{y}$. However, there is another class of differential equation problem: the *Boundary Value* problem: $d\vec{x}/dt = f(t, \vec{x})$ where $x_i(t_0) = y_i$ and $x_j(t_1) = y_j$ for some (or several) i and j. Typical orbit and trajectory problems tend to be initial value problems. Equilibrium and eigenvalue problems tend to be boundary value problems.

Boundary value problems are harder computationally than initial value problems since they couple information at different values of t. Any solution method must be *global*, adjusting the full numerical solution over the interval $[t_0, t_1]$. In this assignment, we'll explore the *shooting* method which bootstraps a boundary value problem solution by iterating over initial value problems. We'll use this technique to find the energy levels and corresponding wavefunctions for several quantum systems in one dimension.

1 Quantum Mechanics On The Computer

To start, we need to be able to solve the Schrödinger equation at all. For this assignment we're interested in the time-independent Schrödinger equation for a single particle in one spatial dimension:

$$-\frac{1}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x), \tag{1}$$

where for convenience we've set $\hbar = 1$.

a) Write Equation (1) as a system of two first order ODEs.

b) Write an RK4 solver in `python` to solve Equation (1) over the domain $[a, b]$ given $\psi(a)$ and $d\psi/dx(a)$ as initial data.

c) Check your method on some simple test cases, use at least $N = 1000$ steps. Make a plot of your numerical solution and the exact solution for each case.

- A free particle $V(x) = 0$ on [0, 10], with $\psi(0) = 0$ and $d\psi/dx(0) = 1$, and some energy E. The solution should be $\psi(x) \propto \sin(\sqrt{2mE}x)$. Find an energy that makes $\psi(10) \approx 0$.
- A particle in a harmonic oscillator of frequency ω: $V(x) = m\omega^2x^2/2$. This has ground state $\psi_0(x) \propto \exp(-m\omega x^2/2)$ with energy $E_0 = \omega/2$. Using the initial data $\psi(-a) = 0$ and $d\psi/dx(-a) = 1$, find an a that reproduces the ground state over $[-a, a]$ (*Hint*: $a < 10$ is fine). What happens to the solution wave function as you change the energy? What's special about the numerical solutions when the energy is exactly $\omega/2$, $3\omega/2$, etc?

2 The Shooting Method

In a boundary value problem, we do not have enough given data to completely initialize a solution at the beginning of the domain. In a trajectory problem, we may be given desired positions at the beginning and end but not the initial velocity. In the time independent Schrödinger equation for a given potential $V(x)$, we do not know a priori what energy E will lead to a valid solution.

The *shooting* method solves a boundary value problem by guessing the missing initial data and "shooting" a solution out to the end of the domain. It check how close the numerical solution is to the desired boundary value, updates its guess, and tries again. In this way, it rephrases the boundary value problem as a root-finding problem!

As an example, consider the boundary value problem:

$$\ddot{x}(t) = f(t, x) \tag{2}$$
$$x(a) = 0 \tag{3}$$
$$x(b) = y \tag{4}$$

Let $x(t; v)$ denote the solution to the initial value problem of Equation (2) with $x(a) = 0$ and $\dot{x}(a) = v$. This is a problem we can solve numerically with ease. The shooting method defines the function $g(v) = x(b; v) - y$: the difference between the numerical solution and the desired value at b for a given trial v. The value of v that solves the boundary value problem is a root of g, so we can use numerical root-finding to find it! Each iteration of the root finder involves numerically solving the ODE. This is the shooting method, and now we'll use it to find energy levels for quantum systems.

As you saw in Part 1, using the wrong energy in the Schrödinger equation produces a solution that quickly blows up. To simplify our numerical solutions, we will work in a model where *every* potential is contained within an infinite square well. That is, every potential will take the form:

$$V(x) = \begin{cases} U(x) & \text{if } x \in [a, b] \\ \infty & \text{otherwise} \end{cases} \tag{5}$$

As such, *every* wave function will have the boundary conditions $\psi(a) = \psi(b) = 0$. So long as a and b are sufficiently far apart, this has negligible impact on the values of ψ and E for low energy states. Higher energy states can see more of the domain and will eventually resemble the eigenstates of the infinite square well instead of $U(x)$.

a) Write a `python` function that numerically solves Equation (1) for a given energy E over the domain $[a, b]$ and returns $\psi(b)$, we can call this $\psi(b; E)$. Since $\psi(a) = 0$, all $d\psi/dx(a)$ does is control the normalization of ψ: you can set it to 1. Make a plot of $\psi(b; E)$ vs E for $U(x) = m\omega^2 x^2/2$ and $E \in [0, 3\omega]$, using the integration domain from part 1.

b) Our desired boundary condition is $\psi(b) = 0$. Write a `python` function that uses bisection to find a root of $g(E) = \psi(b; E)$ on the test interval $[E_{\text{begin}}, E_{\text{end}}]$. Test your function on the particle-in-a-box $U(x) = 0$, try to find the first few energy levels. You'll have to play with the search bounds, or test many intervals automatically. Make a plot of E_n vs n, does it agree with expectations?

c) Use your shooting method on the harmonic oscillator. Find the first few energy levels, and make a plot of E_n vs n. Find enough energy levels that they diverge from harmonic oscillator behaviour. Plot the wave function for one eigenstate below the divergence and one above, do they agree with expectations?

3 Optional: Not For Credit, Just For Fun

The quantum double-well potential $U(x) = m\lambda(x^2 - a^2)^2$ has a long history in physics and can display many interesting quantum mechanical behaviours: tunnelling and symmetry-breaking just to name a few. It also, very annoyingly, has no closed form solution for $\psi(x)$ or E.

a) Solve the Schrödinger Equation with $U(x) = m\lambda(x^2 - a^2)^2$ for $\psi(x)$ and E using your shooting method for the first few energy levels on a domain $[-b, b]$, with b sufficiently larger than a so that the walls don't interfere too much.

b) Break the symmetry by adding a term $\delta U(x) = mcx$ to the potential. Plot $E_0(c)$ and $E_1(c) - E_0(c)$ versus c. How do they depend on c? What happens as $E_1 - E_0 \to 0$?