Lecture 19

Boundary Value Problems

E.g., the diff. eq. for the height of a ball thrown in the air is

$$\frac{d^2x}{dt^2} = -g$$

Could specify initial conditions in order to fix a solution, e.g., initial height & initial velocity.

Alternatively, we could specify that the ball has initial height $x=0$ @ $t=0$ & final height $x=0$ @ $t=t_1$ where $t_1>0$.

Goal is to find a solution that satisfies these conditions

Shooting method is one way to do so. Idea: just try a number of possibilities until we find a solution.

For the example, just pick an initial velocity, solve the differential equation numerically & then see if final time and height are as desired.

How to modify guesses to assure convergence?

Consider that there is some function f such that

$$x(t_1) = f(v_0)$$

height @ time t_1 is a function of initial velocity & we would like to find v_0 such that $f(v_0)$

So we can just use a root finding method, such as binary search.

For the example, consider that we can rewrite as

$$\frac{dx}{dt} = y \quad \& \quad \frac{dy}{dt} = -g$$

Solve using 4th order Runge-Kutta & perform binary search for initial velocity.

Bring up 1-throw.py

Special kind of boundary value problem occurs for diff. eq's such that every term is linear in the dependent variable. E.g., Schrödinger equation

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

ψ is the wave function, V is the potential energy & E is the total energy of the particle.

Suppose a square well potential

$$V(x) = \begin{cases} 0 & \text{for } 0 < x < L \\ \infty & \text{else} \end{cases}$$

can solve analytically but let's explore numerics.

probability of finding particle @ x where $V(x) = \infty$ is zero, so $\psi(x) = 0$ @ $x = 0$ & $x = L$.

Since equation is 2^{nd} order, rewrite as two 1^{st} order ones

$$\frac{d\psi}{dx} = \phi \qquad \frac{d\phi}{dx} = \frac{2m}{\hbar^2}\left[V(x) - E\right]\psi$$

we need initial conditions

$\psi(x) = 0$ @ $x=0$

but we do not know

$$\phi(0) = \left.\frac{d\psi}{dx}\right|_{x=0}.$$

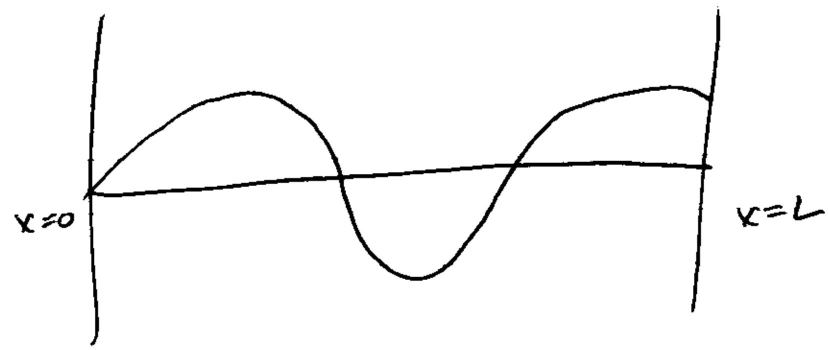
Idea: guess a value & then solve & then check if final @ $x=L$ $\psi(L)=0$ boundary condition is satisfied

upon first guessing, very likely the condition will not be satisfied

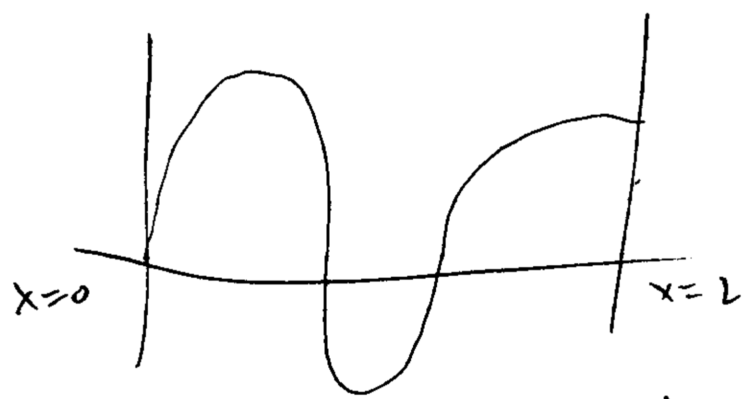
could try to use the shooting method but it won't work in this case.

suppose we change initial value $\left.\frac{d\psi}{dx}\right|_{x=0}$ by doubling it.

Since Schrodinger equation is linear, this doubling leads to doubling of solution $\psi(x)$ which just means that the endpoint $\psi(L)$ will get scaled by, Eg. Suppose initial solution was



then doubling slope leads to



problem here is that there is no solution to the equation for this energy E_1

There are only solutions for particular values of the energy parameter E, which is why energy is quantized.

- So change the goal to find the allowed energies.
- Start w/ some initial conditions & then vary E to find value for which $\psi(0)=0$ & $\psi(L)=0$.
- can think that Schrödinger equation gives a function $f(E)$ equal to wavefunction @ $x=L$ & goal is to find E such that $f(E)=0$ (can use root finding method)
- What about boundary condition $\left.\frac{d\psi}{dx}\right|_{x=0}$? Doesn't matter b/c it will just scale the solution just pick it so that

$$\int |\psi(x)|^2 dx = 1$$ (normalized wavefunction)

Bring up 2-square well.py

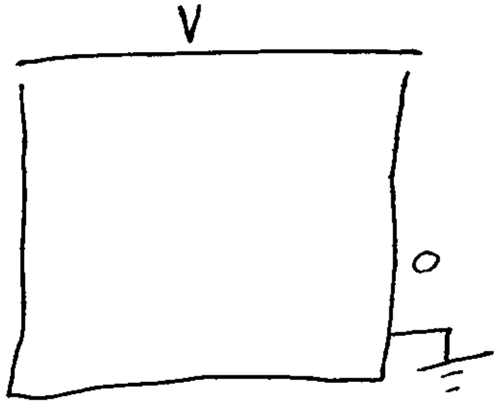
Partial differential equations (Ch. 9)

many examples in physics: wave eqn., diffusion eqn., Laplace, Poisson, Maxwell, Schrödinger.

Begin w/ boundary value problems.

<u>Example:</u> box w/ conducting walls

Goal: Find electrostatic potential inside the box.



three walls are grounded + the top is @ potential V.

potential ϕ is related to vector E-field by

$$\vec{E} = -\vec{\nabla}\phi$$

In absence of charges, Maxwell equation states that $\vec{\nabla} \cdot \vec{E} = 0$

$$\Rightarrow \quad \nabla^2 \phi = 0 \qquad \text{(Laplace's equation)}$$

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} = 0$$

solve this subject to top $= V$ & others $= 0$.

<u>Method of finite differences</u>

just restrict to 2D so that we can easily plot solution.

$$\text{So} \quad \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0$$

divide up space into a grid.
can use a regular square grid

Put points on boundary + inside

↑ where we know sol'n ↑ where we don't know

Let "a" be spacing of grid

Recall central difference approx. to 2nd partial deriv.

$$\frac{\partial^2\phi}{\partial x^2} \approx \frac{\phi(x+a,y)+\phi(x-a,y)-2\phi(x,y)}{a^2}$$

approx. in terms of 3 neighboring points

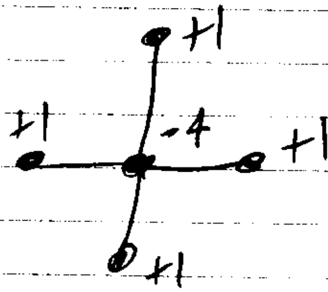
Similar eqn. for $\frac{\partial^2\phi}{\partial y^2}$

$$\frac{\partial^2\phi}{\partial y^2} \approx \frac{\phi(x,y+a)+\phi(x,y-a)-2\phi(x,y)}{a^2}$$

Add these to get

$$\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2} \approx \frac{1}{a^2}\Big[\phi(x+a,y)+\phi(x-a,y)+\phi(x,y+a) + \phi(x,y-a)-4\phi(x,y)\Big]$$

can represent rule visually as



Then rearranging gives

$$\phi(x+a, y) + \phi(x-a, y) + \phi(x, y+a) + \phi(x, y-a) - 4\phi(x,y) = 0$$

this is now a set of simultaneous linear equations which we can solve in principle, using Gaussian elimination e.g.

But we could also use relaxation method.

rewrite as

$$\phi(x,y) = \frac{1}{4}\left[\phi(x+a,y) + \phi(x-a,y) + \phi(x,y+a) + \phi(x,y-a)\right]$$

so $\phi(x,y)$ is just a weighted average of adjacent points.

- this is called the Jacobi method
- can prove that it converges in this scenario.
- stop iterating after a target accuracy is reached.

Bring up 3-laplace.py

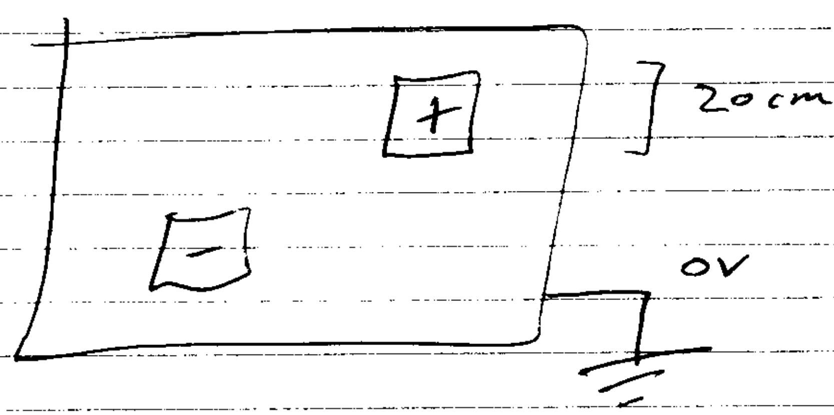
- realize that Jacobi method is just an approximation.
  can increase accuracy by increasing # of grid points or by using higher order derivative approximations

- need to be more clever when boundary conditions are not as simple (pick non uniform spacing of grid points)

Example: Poisson equation of electrostatics

$$\nabla^2 \phi = -\frac{\rho}{\varepsilon_0}$$ ← charge density

Make all the walls have zero potential but put some charges inside the box



charge density $1\,C\,m^{-2}$

can again make use of relaxation method.

write as

$$\frac{1}{a^2}\left[\phi(x+a,y) + \phi(x-a,y) + \phi(x,y+a) + \phi(x,y-a) - 4\phi(x,y)\right] = -\frac{\rho(x,y)}{\varepsilon_0}$$

rewrite as

$$\phi(x,y) = \frac{1}{4}\left[\phi(x+a,y) + \phi(x-a,y) + \phi(x,y+a) + \phi(x,y-a)\right] + \frac{a^2}{4\varepsilon_0}\rho(x,y)$$

Bring up 4-poisson.py

Jacobi is slow. How to speedup?

<u>overrelaxation method.</u>

Idea is to overshoot target value by a little.

Suppose we iterate, beginning w/ $\phi(x,y)$ & next iter. gives $\phi'(x,y)$ then

$$\phi'(x,y) = \phi(x,y) + \Delta\phi(x,y)$$

where Δ is change

For overrelaxation, instead do

$$\phi_\omega(x,y) = \phi(x,y) + (1+\omega)\,\Delta\phi(x,y)$$

where $\omega > 0$.

substituting gives

$$\phi_\omega(x,y) = \phi(x,y) + (1+\omega)\left[\phi'(x,y) - \phi(x,y)\right]$$

$$= (1+\omega)\,\phi'(x,y) - \omega\,\phi(x,y)$$

For the example of Laplace's eqn., we get

$$\phi_\omega(x,y) = \frac{1+\omega}{4}\left\{\phi(x+a,y) + \phi(x-a,y) + \phi(x,y+a) + \phi(x,y-a)\right]$$
$$-\omega\,\phi(x,y)$$

How to choose ω? Pick $\omega < 1$

discuss more next time...