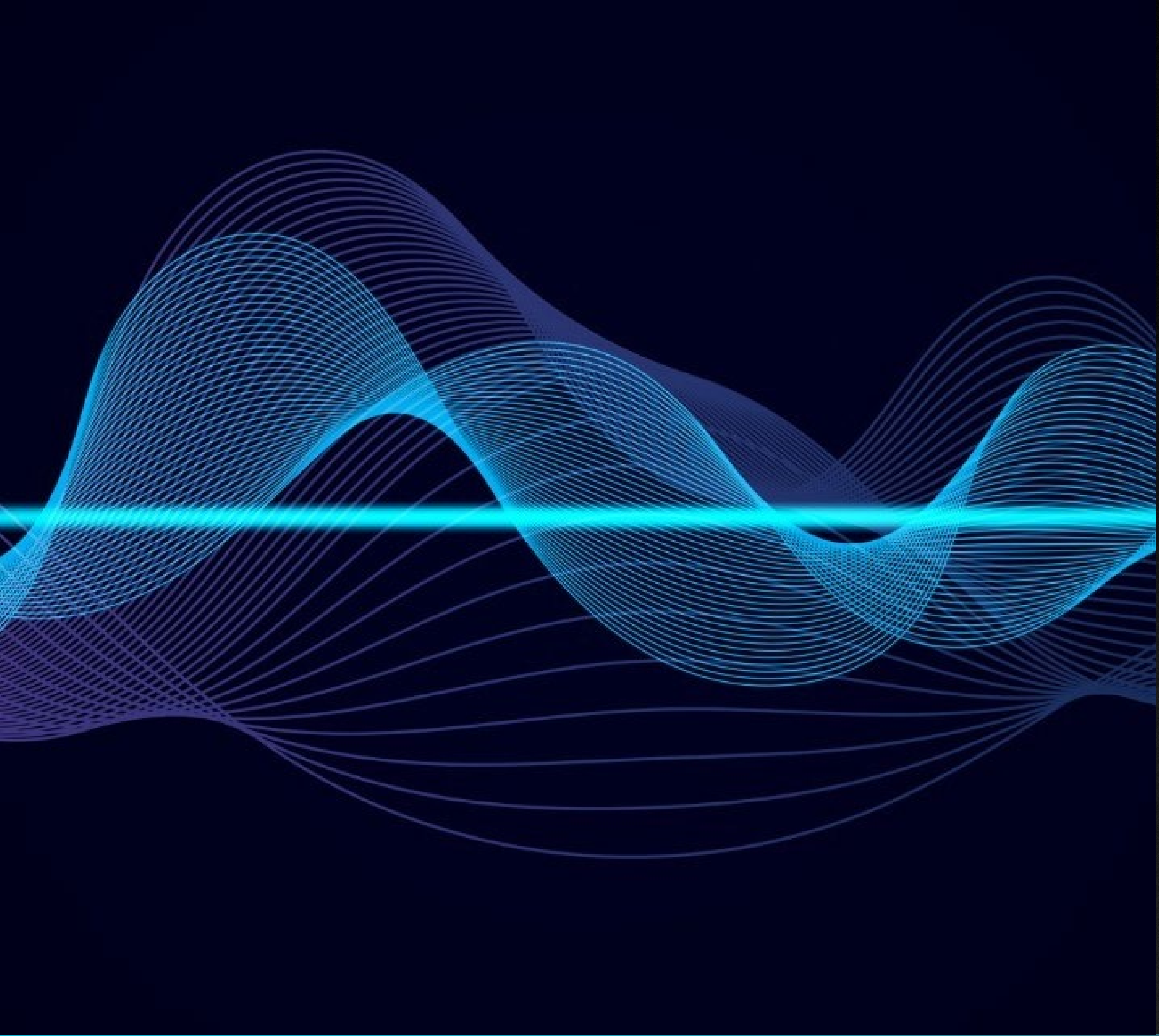


Computational Physics

PHYS 6260

Boundary value problems

Announcements:

- HW2: Due Friday 1/24
- HW3: Due Friday 1/31

Lecture Outline

We will cover these topics

- Shooting method
- Relaxation method
- Eigenvalue problems

Introduction

- So far, we've only looked at initial value problems that are common in physics

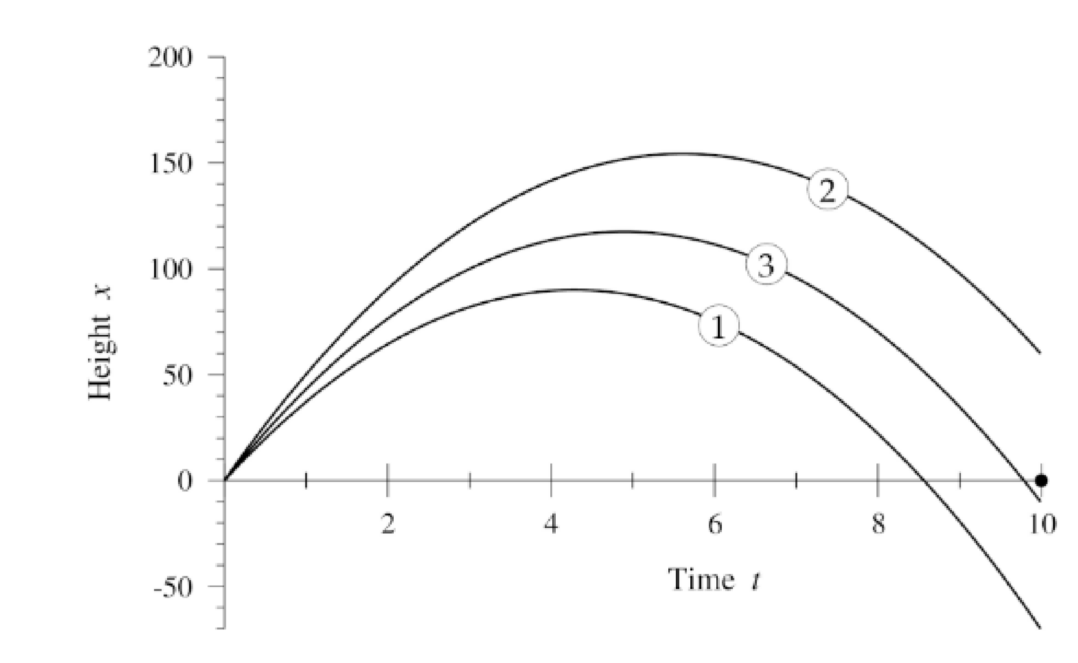
- But there is another class of problems: boundary value problems
- They have constraints on their boundaries

- Simple example: projectile motion with only gravity ($\frac{d^2x}{dt^2} = -g$)
- For an initial value problem, we'd know the initial position and velocity.
- However, *what if we only knew the initial and final position?*
- This is a boundary value problem that is more difficult to solve than initial value problems.

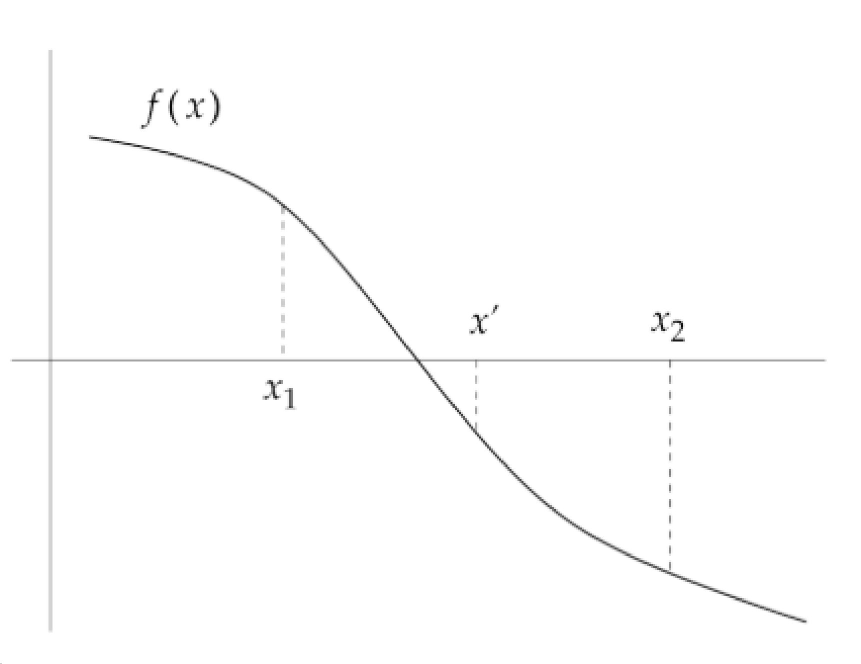
Shooting method

- This is an iterative trial-and-error technique
- Uses standard ODE solvers with guesses at the initial values

- For example, suppose that we know a projectile lands at time t = 10s
- We make an initial guess, solve the ODE
- Compare with the final boundary and change the velocity and repeat
- In essence, this is root finding
- We can use root finding methods (Newton's method, binary, secant) to converge to the answer



Binary search for roots

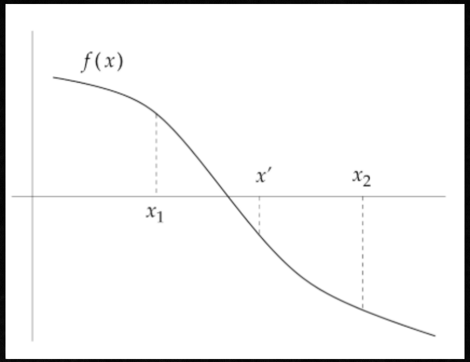


- Rearrange formula into the form: $f(x) = 0$
- Search for roots

1. Select two bounds: x_1 and x_2
   - If one is positive and one is negative, the root must exist within this range
2. Calculate f(x) at the midpoint $x' = (x_1 + x_2)/2$
3. Check whether the sign changed on the left or right
4. Repeat until the root is found to some pre-defined accuracy

- Even in a bad scenario where the range is 10^{10} and the desired accuracy is 10^{-10}, we can converge to a result in 67 steps: $N = \log_2 \left[\frac{x_1 - x_2}{\epsilon}\right] \simeq 66.4$

Binary search



- Disadvantages
  - If the root doesn't exist between the initial bounds, we will never find the root
  - If the function is even and the function has the same sign at the bounds, we may not find the root. For example, think about a parabola with a minimum at y = 0
  - Cannot find multiple roots

- Guidelines to avoid these problems
  - Use known (physical or mathematical) characteristics of the function to bracket the root
  - If an approximate value of the root is known, start with bounds close to that guess. If they aren't positive and negative, double the range and check again. Keep doubling until they bracket the root and then start the binary search.

Shooting method

In-class example

- Let’s solve this projectile problem. Complete the `05_shooting0.py` program on Canvas
- For projectile method, we have two 1st order ODEs

$$\frac{dx}{dt} = y, \qquad \frac{dy}{dt} = -g$$

- Let’s solve this problem with RK4 and binary search
- The binary search uses the following algorithm
  - Starts with an initial bound,
  - Splits the search domain,
  - Determines whether the root exists in the left or right half, and
  - Repeat the splitting until the root is found

Relaxation method

- This method defines a shape for the initial guess, fixing it to the boundary conditions
- The shape is then successively modified to bring it closer to the solution of the ODE

- In a way, this is the opposite of the shooting method
  - Shooting: Starts with a correct solution to the ODE that doesn’t match the boundaries
  - Relaxation: Starts with the correct boundaries but isn’t a correct solution

- We won’t focus on this method to solve ODEs because it’s more useful with PDE solutions, which we’ll start next lecture

Eigenvalue problems

- These are special types of boundary value problems
- Occurs when the equation(s) are linear and homogeneous (every term is linear in the dependent variable)

- The Schrödinger equation is a good example

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

- Here $\psi(x)$ is the wave function, V(x) is the potential energy, and E is the total energy
- Notice how each term is linear in ψ

Eigenvalue problems

- Let’s solve the classic problem of an infinitely deep, square potential well: V(x) = 0 for x = (0,L) and infinitely large elsewhere.
  - This can be easily solved analytically, but let’s solve it numerically

- We can write Schrödinger’s equation as two 1st order ODEs

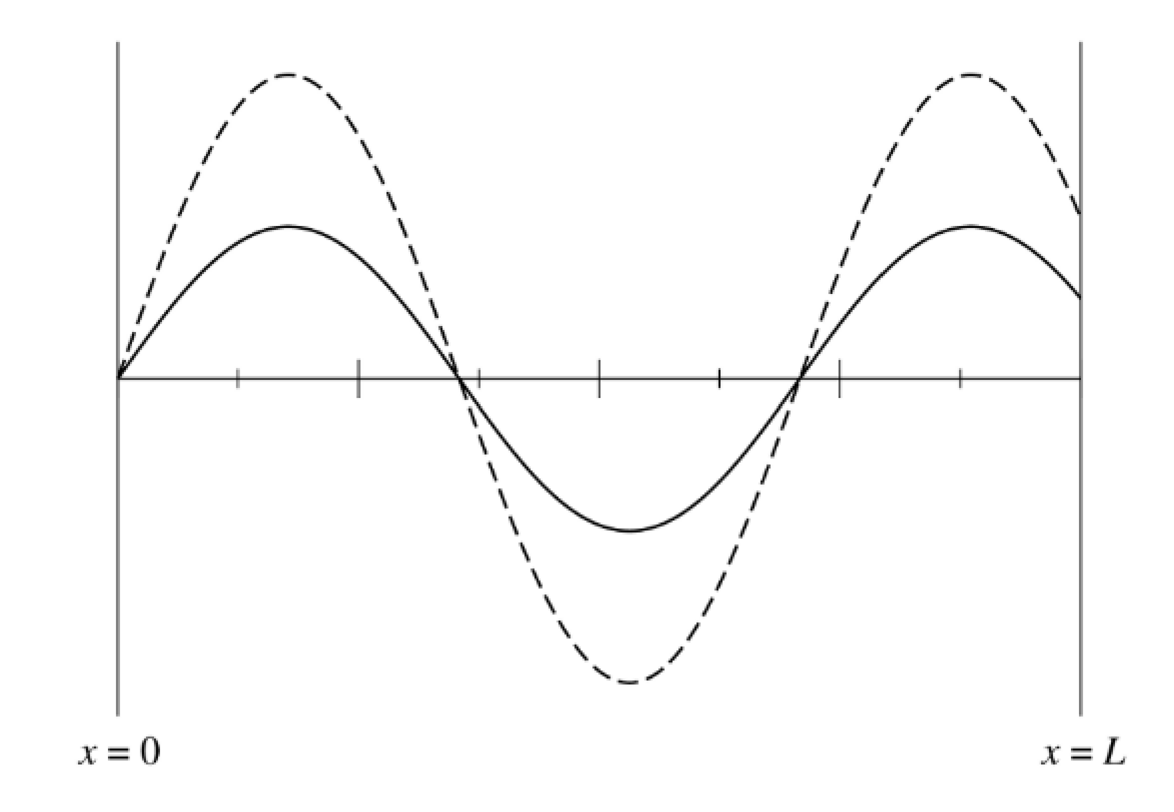
$$\frac{d\psi}{dx} = \phi, \qquad \frac{d\phi}{dx} = \frac{2m}{\hbar^2}[V(x) - E]\psi$$

- We know that $\psi = 0$ at x = 0 and L.
- Its derivative is unknown at the boundaries, so we have to make an initial guess.

Eigenvalue problems

- In linear & homogeneous equations, the shooting method (adjusting $d\psi/dx$) doesn't work
- Because it's linear, if we double the initial guess the whole solution is double ($\psi \to 2\psi$)
- In other words, it retains the shape, no matter how much we adjust the initial value, it will never match the boundary conditions

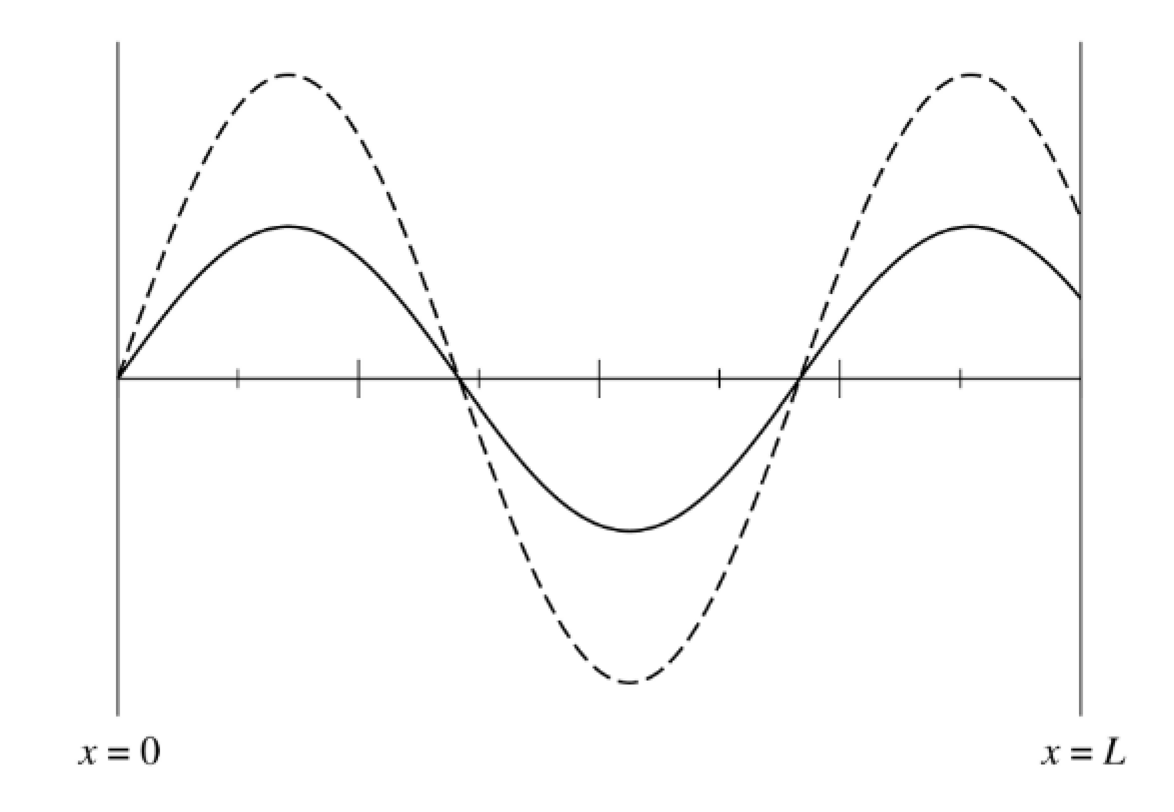
- The fundamental problem is that there is no general solution
- There are only solutions for special values of E, the eigenvalues



Eigenvalue problems

- Therefore, we vary the energy E with the shooting method to find where the solution equals zero at x = L

- We haven't addressed the initial value of $\phi = \frac{d\psi}{dt}$ yet
- But it doesn't matter because, the solution is always normalized in the end



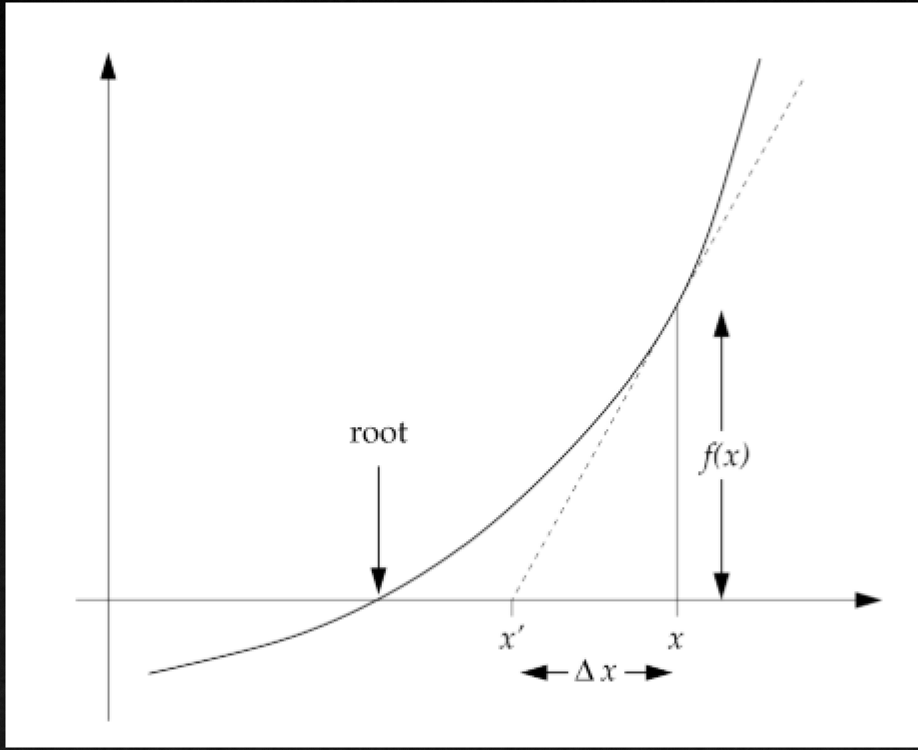
Newton’s method

- Probably have heard about this method in other classes
- Use the derivative to iterate to the root
  - Only works for problems with known functions and their derivatives

- Make an initial guess of the root: x
- Use the derivative f’(x) to extrapolate to y = 0, resulting in another guess x’

$$x' = x - \Delta x = x - \frac{f(x)}{f'(x)}$$

- Iterative until Δx becomes smaller than some tolerance

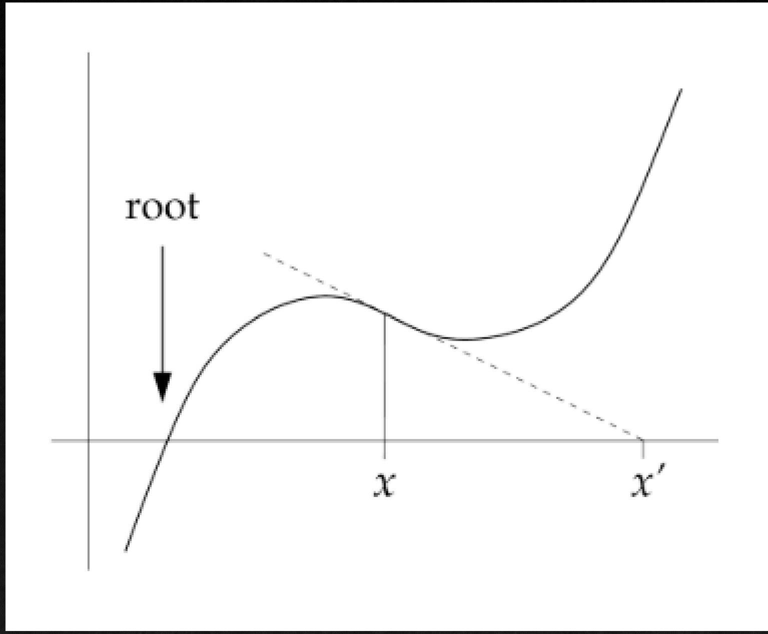


Newton’s method

Disadvantages

- First and already mentioned, the derivative must be known

- But more seriously, the method can diverge in two cases
  - The absolute value of the derivative is very small
  - The slope “points” in the opposite direction of the root, as the cubic function shown to the right



Eigenvalue problems

In-class problem

- Consider an infinitely deep, square potential well. Start with the code `05_eigen0.py`
- V(x) = 0 for x = (0,L) and infinitely large elsewhere

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

- Boundary conditions: $\psi = 0$ at x = 0 and L
- Calculate the ground state energy E of an electron in the square well but with L = 0.5292 Ångstroms
- Use the secant method to find the energy, which is Newton's method but using numerical derivatives

$$x_{new} = x_{old} - f(x_{old}) * (x_{old} - x_1) \,/\, [f(x_{old}) - f(x_1)]$$

  - Here x_1 is a nearby x-value to the previous guess x_{old}