Outline

1. Recap
2. Boundary value problems
   - Shooting method
3. Eigenvalue problems
   - The Schrödinger equation
   - Shooting eigenvalues
4. Summary

Last quiz next week!

Recap

An n-th order ODE or n coupled ODEs require n conditions to be specified.

Initial value problems: All conditions are specified at the same point:

$$y(x_1) = y_1, \quad y'(x_1) = v_1, \quad y''(x_1) = a_1 \quad \text{etc.}$$

Boundary value problems: Conditions specified at different points:

$$y(0) = a_0\,; \; y(1) = b_0 \quad \text{or}$$
$$y'(0) = a_1\,; \; b_0 y(1) + b_1 y'(1) = c \quad \text{etc}$$

- Unique solution not guaranteed
- Must usually start with a guess
- Shooting method: Convert to initial value problem by guessing missing initial values, adjust until boundary values are satisfied.
- Relaxation method: Guess solution on entire domain with correct boundary conditions, adjust until ODE is satisfied.

Shooting method

Shoot first, ask questions later!

Shooting method

Shoot first, ask questions later!

1. Guess the unknown initial conditions [load & aim]

Shooting method

Shoot first, ask questions later!

1. Guess the unknown initial conditions [load & aim]
2. Integrate system of odes to final point [shoot]

Shooting method

Shoot first, ask questions later!

1. Guess the unknown initial conditions [load & aim]
2. Integrate system of odes to final point [shoot]
3. Check how close you got [ask questions]

Shooting method

Shoot first, ask questions later!

1. Guess the unknown initial conditions [load & aim]
2. Integrate system of odes to final point [shoot]
3. Check how close you got [ask questions]
4. Adjust your aim, goto 1

Shooting method

Shoot first, ask questions later!

1. Guess the unknown initial conditions [load & aim]
2. Integrate system of odes to final point [shoot]
3. Check how close you got [ask questions]
4. Adjust your aim, goto 1

"Hitting the target" is a question of reducing the discrepancy $\overrightarrow{y}(x_2) - \overrightarrow{b}$ to zero = root finding

For a second-order ode we can use bisection, secant, Ridders',...

Shooting method

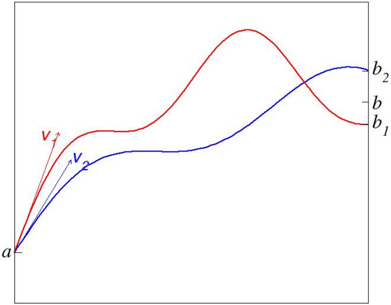
Shoot first, ask questions later!

1. Guess the unknown initial conditions [load & aim]
2. Integrate system of odes to final point [shoot]
3. Check how close you got [ask questions]
4. Adjust your aim, goto 1

"Hitting the target" is a question of reducing the discrepancy $\overrightarrow{y}(x_2) - \overrightarrow{b}$ to zero = root finding

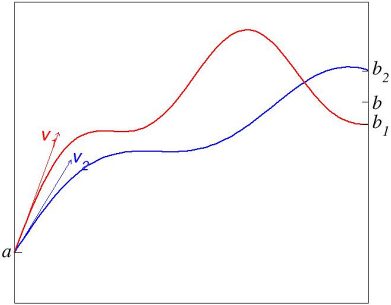
For a second-order ode we can use bisection, secant, Ridders',...
Higher order: Newton–Raphson

Shooting method



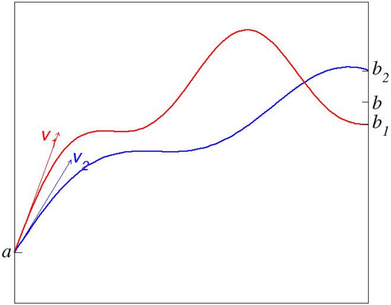
1. We want
   $y(x_1) = a, y(x_2) = b.$

Shooting method



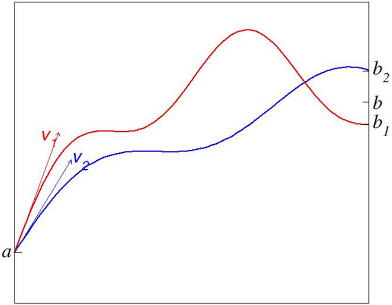
1. We want $y(x_1) = a, y(x_2) = b$.
2. We guess $y'(x_1) = v_1$ and get $y(x_2) = b_1 < b$.

Shooting method



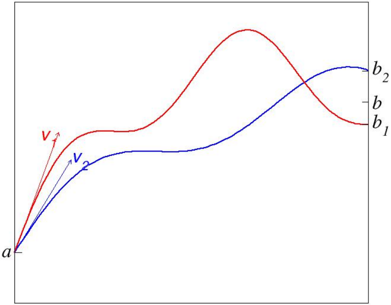
1. We want $y(x_1) = a, y(x_2) = b$.
2. We guess $y'(x_1) = v_1$ and get $y(x_2) = b_1 < b$.
3. We guess $y'(x_1) = v_2$ and get $y(x_2) = b_2 > b$.

Shooting method



1. We want $y(x_1) = a, y(x_2) = b$.
2. We guess $y'(x_1) = v_1$ and get $y(x_2) = b_1 < b$.
3. We guess $y'(x_1) = v_2$ and get $y(x_2) = b_2 > b$.
4. The correct value for $y'(x_1)$ is between v_1 and v_2.

Shooting method



1. We want $y(x_1) = a, y(x_2) = b$.
2. We guess $y'(x_1) = v_1$ and get $y(x_2) = b_1 < b$.
3. We guess $y'(x_1) = v_2$ and get $y(x_2) = b_2 > b$.
4. The correct value for $y'(x_1)$ is between v_1 and v_2.

We can find the value for $y'(x_1)$ using bisection!
This will give us the solution of the boundary value problem.

Eigenvalue problems

Consider 1-dimensional Schrödinger equation:

$$H\Psi = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi = i\hbar\frac{\partial\Psi}{\partial t} = E\Psi$$

with boundary conditions $\Psi(-\infty) = \Psi(\infty) = 0$

Eigenvalue problems

Consider 1-dimensional Schrödinger equation:

$$H\Psi = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi = i\hbar\frac{\partial\Psi}{\partial t} = E\Psi$$

with boundary conditions $\Psi(-\infty) = \Psi(\infty) = 0$

Solutions

1. $\Psi \equiv 0$ (for any E)
2. $\Psi_n \neq 0$ for some $E = E_n$

The set of E_n is the spectrum

Eigenvalue problems

Consider 1-dimensional Schrödinger equation:

$$H\Psi = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi = i\hbar\frac{\partial\Psi}{\partial t} = E\Psi$$

with boundary conditions $\Psi(-\infty) = \Psi(\infty) = 0$

Solutions

1. $\Psi \equiv 0 \quad$ (for any E)
2. $\Psi_n \neq 0 \quad$ for some $E = E_n$

The set of E_n is the spectrum

The spectral problem: Find all E_n, Ψ_n

Eigenvalue problems

Consider 1-dimensional Schrödinger equation:

$$H\Psi = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi = i\hbar\frac{\partial \Psi}{\partial t} = E\Psi$$

with boundary conditions $\Psi(-\infty) = \Psi(\infty) = 0$

Solutions

1. $\Psi \equiv 0$ (for any E)
2. $\Psi_n \neq 0$ for some $E = E_n$

The set of E_n is the spectrum

The spectral problem: Find all E_n, Ψ_n

Possible solution: Treat E_n as additional variable, shoot!

Exploiting symmetry

Problem is greatly simplified if $V(x) = V(-x)$

$$\Longrightarrow \quad \begin{cases} \Psi_n(-x) = \Psi_n(x) & \text{even} \\ \Psi_n(-x) = -\Psi_n(x) & \text{odd} \end{cases}$$

Exploiting symmetry

Problem is greatly simplified if $V(x) = V(-x)$

$$\Longrightarrow \quad \begin{cases} \Psi_n(-x) = \Psi_n(x) & \text{even} \\ \Psi_n(-x) = -\Psi_n(x) & \text{odd} \end{cases}$$

But $\Psi(0) = \Psi(-0)$

$$\Longrightarrow \quad \begin{cases} \Psi_n(0) \neq 0\,, \quad \Psi_n'(0) = 0 & \text{even} \\ \Psi_n(0) = 0\,, \quad \Psi_n'(0) \neq 0 & \text{odd} \end{cases}$$

So we can start at $x = 0$, not $x = -\infty$

Exploiting symmetry

Problem is greatly simplified if $V(x) = V(-x)$

$$\Longrightarrow \quad \begin{cases} \Psi_n(-x) = \Psi_n(x) & \text{even} \\ \Psi_n(-x) = -\Psi_n(x) & \text{odd} \end{cases}$$

But $\Psi(0) = \Psi(-0)$

$$\Longrightarrow \quad \begin{cases} \Psi_n(0) \neq 0\,, \quad \Psi'_n(0) = 0 & \text{even} \\ \Psi_n(0) = 0\,, \quad \Psi'_n(0) \neq 0 & \text{odd} \end{cases}$$

So we can start at $x = 0$, not $x = -\infty$

We can also set $\Psi(0) = 1$ or $\Psi'(0) = 1$ since the value is irrelevant (will normalise solution at end)

Shooting eigenvalues

1. Set $\Psi(0) = 1, \Psi'(0) = 0$ (even) or $\Psi(0) = 0, \Psi'(0) = 1$ (odd)

Shooting eigenvalues

1. Set $\Psi(0) = 1, \Psi'(0) = 0$ (even) or $\Psi(0) = 0, \Psi'(0) = 1$ (odd)
2. Choose some E

Shooting eigenvalues

1. Set $\Psi(0) = 1, \Psi'(0) = 0$ (even) or $\Psi(0) = 0, \Psi'(0) = 1$ (odd)
2. Choose some E
3. Integrate ODE for $\Psi(x), x \in [0, \infty\rangle$
   In practice: $x \in [0, L], L \sim 10$ depending on problem

Shooting eigenvalues

1. Set $\Psi(0) = 1, \Psi'(0) = 0$ (even) or $\Psi(0) = 0, \Psi'(0) = 1$ (odd)
2. Choose some E
3. Integrate ODE for $\Psi(x), x \in [0, \infty\rangle$
   In practice: $x \in [0, L], L \sim 10$ depending on problem
4. Use root finding algorithm to solve $\Psi(x = L; E) = 0$ for E

Summary

- Boundary value problems much harder than inital value
- Must (usually) start by guessing a solution!

Summary

- Boundary value problems much harder than inital value
- Must (usually) start by guessing a solution!
- Shooting method:
  1. Guess unknown initial values v_i
  2. Solve ODE with these values: $f(x|v_i)$
  3. Find solution at final point x_f
  4. Solve $f(x_f|v_i) - v_f = 0$ — root finding!

Summary

- Boundary value problems much harder than inital value
- Must (usually) start by guessing a solution!
- Shooting method:
  1. Guess unknown initial values v_i
  2. Solve ODE with these values: $f(x|v_i)$
  3. Find solution at final point x_f
  4. Solve $f(x_f|v_i) - v_f = 0$ — root finding!
- Eigenvalue problems
  - May be made into boundary value problem by treating eigenvalue as additional variable.