Numerical shooting

Solving boundary value problems

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Numerical shooting

Many differential equation problems are posed in terms of
Boundary Value Problems (BVPs)

Simple example, consider heat diffusion between two hot objects, one at $x = 0$ and one at $x = 1$

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}, \qquad u(0, t) = A, \qquad u(1, t) = B$$

Steady-state heat diffusion is an ODE

$$0 = D\frac{\partial^2 u}{\partial x^2}, \qquad u(0) = A, \qquad u(1) = B$$

How do we solve numerically?

Initial value problems

Have plenty of numerical integrators (Euler's method, Runge-Kutta, etc) – how can we use them?

Rewrite the initial value problem as first-order system

$$\frac{du_1}{dx} = u_2, \qquad \frac{du_2}{dx} = 0, \qquad \boxed{u_1(0) = A, \qquad u_2(0) = \alpha}$$

Need to find the unknown α such that $u_1(1) = B$

This is a root-finding problem!

Root finding

Root finding is (generally) finding solutions u such that $f(u) = 0$

Here, f is given by the boundary conditions

could be removed

$$f(u) = \begin{bmatrix} u_1(0) - A \\ u_1(1) - B \end{bmatrix} = 0$$

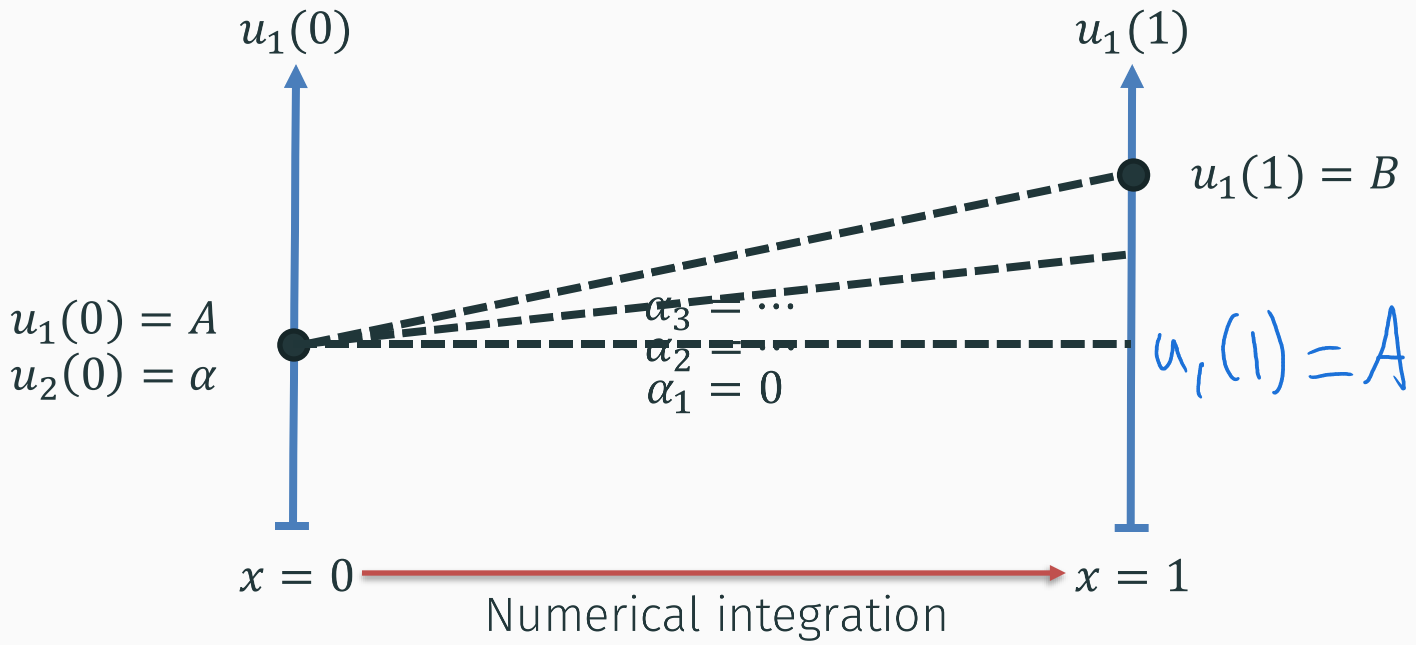
Value of $u_1(1)$ is found by numerical integration

A α

Start with a guess for $u(0) = [u_1(0), u_2(0)]$ then use Newton's method to iterate to a solution

Number of unknowns = number of equations!

Root finding – graphically



A common hang-up

How can you put an ODE integrator inside a root finder? Don't you need derivatives for a Newton iteration?

- You need derivatives to exist for a Newton iteration (which they do)
- Derivatives can be approximated with finite differences
  - Doesn't always have to be a good approximation…
- Or computed directly with differentiable programming
  - A trendy topic – https://arxiv.org/abs/1907.07587

Automatic Differentiation

Benefits

- Simple to implement
  - Doesn't require special formulations or rewriting of equations
- Memory costs are low compared with other approaches
  - Important for high dimensional systems
- Makes use of existing (robust) numerical solvers

Drawbacks

- Can have convergence issues for stiff or (very) unstable problems
  - Can be mitigated with multiple shooting – break the interval into segments
- Adaptive step sizes in the ODE integrator can cause convergence issues

Summary

- Boundary value problems can be rewritten as a root-finding problem
- The boundary conditions provide the zero problem (the function to be set to zero)
- The zero problem implicitly contains a numerical integration step
- Can be an easy but not necessarily robust approach to solve BVPs