Week 5: We survived the midterm!

Amath 301

TA Session

Today's plan

0. Numerical integration
1. Numerical differnetiation
2. Q&A

Numerical integration

Use case:

- PDEs (modeling solutions)
- Integration of many functions is hard/impossible
  - Not all functions are expressed in terms of elementary functions:

$$erf(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$$

- Stochastic/statistical data - writing down f is hard
  - Sometimes impossible: 3-body problem
  - Don't always need the full solution, just behavior in a short interval
- Physical phenomena are expressed in terms of rates
  - Material/energy flux, chemical reactions (directly measure rates)
- Small changes to models can mean big changes in their solution techniques.

Numerical integration Schemes:

Also called "Quadrature" schemes.
Many schemes exist! Methods you've seen before:

- Midpoint/left-point/right-point (bad!)
- Trapezoid: fits a linear function between points
- Simpson's rule: fits a quadratic using 3 points, or adding in a middle point.

Can do very fancy things (not covered in this course):

- Monte carlo integration: really fancy guess & check

Higher order methods aren't used: Issues with precision, cancellation, stability. Usually caps out around 3rd-5th order methods.

Wikipedia is a good place for formulas.

In practice:

1. Write out local formula
2. Perform formula on each interval

$$\int_a^b f(x)dx \approx \sum_{i=0}^{n} w_i f(x_i)$$

Really about how to choose w_i.

- Newton-Coates: (when in doubt, use this)
    - Need evenly spaced points!
    - Weights w_i come from integrating langrange polynomial basis (popular basis for polynomials). Weights vary based on how many points are used.
    - Generates schemes: Trapezoid (linear), Simpson (quadratic), Simpson's 3/8 (cubic), Boole's rule (quatic), rectangle, midpoint, and Milne's rule.

Easy (ish) to derive error bounds if needed.

Gaussian Quadature

(Not on HW, but very, **very cool**)

can evaluate polynomials of degree $\leq 2n-1$ with only n weights!

Computed on $[-1, 1]$. Need to shift/scale for other intervals.

- linear f, $x_0 = 0$, $w = 2$.
- Cubic f, use $x_i = \pm\frac{1}{\sqrt{3}}$, and $w_i = 1$.
- Quintic f, $x_i = 0, \sqrt{\frac{3}{5}}, -\sqrt{\frac{3}{5}}$, and $w_i = \frac{8}{9}, \frac{5}{9}, \frac{5}{9}$.

Rules exist for $n = 4, 5$. Most popular with numerical PDE methods.

Variations for half-infinite (Gauss-Laguerre) and infinite domains (Gauss-Hermite).

Questions?

Numerical Differentiation: Why?

- Compute derivatives from data:
- Derivatives within computers!
- Initial value problems (ODEs)
- Boundary value problems: Solve $\frac{du}{dx} = f(u, x)$ with $u(0) = a$ and $u(L) = b$.
    - A precursor for PDEs - big in physics
    - A step towards PDE solvers
- Initial boundary value problems (PDEs): waves, spatial phenomena:
    - ecology, cancer medicine, radiomedicine, nuclear physics, **everywhere!**

Numerical Differentiation: Schemes

Again, many many schemes out there.

- Primary distinction between schemes is interior vs boundary points.
  - Intetrior regions have neighboring points on both (all) sides
  - Boundary point schemes are usually uni-directional
- Weird stuff happens at the boundaries.
- Two types of problems
  - f to f' - evaluate scheme at each grid point
  - f' to f - Boundary value ODE problem.

Core Numerical Scheme types

Center differences:

- Node x_i plus equally spaced neighbors on both sides
- lower order methods only need 1 neighbor in each side. Higher order methods need more
- Good for interior nodes

Forward differences:

- Start at x_j, use x_{j+1}, x_{j+2}, ... points.
- Good for boundaries/ends of intervals

Backwards differences

- Start at x_j, use x_{j-1}, x_{j-2}, ... points.
- Same as forward differences - but in the other direction.
- Good for boundaries/ends of intervals

Questions?

Let's do something fancy!

Computing derivatives is as simple as matrix multiplication.

This makes solving boundary value problems (a class of ODE problems) as simple as an $Ax = b$ solve.