12. Numerical derivatives

Last time

- Julia for mathematics
- Anonymous functions
- Generic functions and methods
- Vectors: mathematics vs containers

Goals for today

- Finite differences
- Taylor series
- Interpolation
- Matrices

Approximating derivatives

- Recall definition of derivative of $f : \mathbb{R} \to \mathbb{R}$:

$$f'(a) := \lim_{h \to 0} \left[\frac{f(a+h) - f(a)}{h} \right]$$

Approximating derivatives

- Recall definition of derivative of $f : \mathbb{R} \to \mathbb{R}$:

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- Simplest numerical method: **ignore limit**:

$$f'(a) \simeq \frac{f(a+h) - f(a)}{h}$$

  for fixed, small h

- **Finite difference** approximation (“finite” vs. infinitesimal)

Finite differences

- Immediate questions arise:
  - Is approximation good? How large is error from true $f'(a)$?
  - How make better approximation?
  - Is this well conditioned?

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- Use Lagrange remainder: $R_1 = \frac{1}{2}h^2 f''(\xi)$
- So $f(a+h) = f(a) + hf'(a) + \mathcal{O}(h^2)$ assuming f'' bounded
- So error in $f'(a)$ is $\mathcal{O}(h)$ – **order 1**

Numerical calculation of error

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- Why?
- $\delta(h)$ is **ill-conditioned** for h near 0

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- How can we reduce error in finite differences?
- Find approximation to $f'(a)$ of **higher order** – how?

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- Find approximation to $f'(a)$ of **higher order** – how?
- Write out Taylor series:

$$f(a+h) = f(a)+hf'(a)+\frac{1}{2!}h^2f''(a)+\frac{1}{3!}h^3f'''(a)+\cdots$$

$$f(a-h) = f(a)-hf'(a)+\frac{1}{2!}h^2f''(a)-\frac{1}{3!}h^3f'''(a)+\cdots$$

Higher-order finite difference approximations II

$$f(a+h) = f(a) + hf'(a) + \frac{1}{2!}h^2 f''(a) + \frac{1}{3!}h^3 f'''(a) + \cdots$$

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- Subtract:
- $f(a+h) - f(a) = 2hf'(a) + \mathcal{O}(h^3)$

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- Subtract:
- $f(a+h) - f(a) = 2hf'(a) + \mathcal{O}(h^3)$
- Get **centered difference** approximation:

$$f'(a) = \frac{f(a+h) - f(a-h)}{2h} + \mathcal{O}(h^2)$$

- Order 2 – compare numerically

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- So $f''(a) = \frac{f(a+h) - 2f(a) + f(a-h)}{h^2} + \mathcal{O}(h^2)$

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- How interpret geometrically?

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Alternative derivation: Interpolation II

- We are looking for **linear combination**

$$f'(t_k) \simeq \sum_i \delta_i t_i$$

- **Fornberg algorithm** generates these recursively from interpolant
- Also for higher derivatives

Multivariable functions

- What happens for multivariable functions $f(x, y)$?
- Finite difference formulae give partial derivatives
- e.g. $\frac{\partial f}{\partial y}(a, b) \simeq \frac{f(a,b+h)-f(a,b)}{h}$

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- Finite difference formulae give partial derivatives
- e.g. $\frac{\partial f}{\partial y}(a, b) \simeq \frac{f(a,b+h)-f(a,b)}{h}$
- Build more complicated expressions, e.g.

$$\nabla^2 f(a, b) \simeq \frac{f(a+h, b) + f(a-h, b) + f(a, b+h) + f(}{h^2}$$

Derivatives as matrices

- Suspose represent polynomial $p(x) = a_n x^n + \cdots + a_1 x + a_0$ via its coefficients
- Vector of coefficients **a** $:= (a_0, a_1, \ldots, a_n)$
- Differentiation gives new polynomial with coefficients $(a_1, 2a_2, 3a_3, \ldots n a_n)$
- It maps original vector to new vector and is **linear**
- So can represent by a matrix!

Derivatives as matrices II

- Different approach: Suppose have samples f_i at equally-spaced points t_i
- How calculate 2nd derivative?
- Finite difference at each point: tridiagonal **Strang matrix**

$$M = \begin{pmatrix} 1 & -2 & 1 & 0 & \cdots 0 & \\ 0 & 1 & -2 & 1 & \cdots 0 & \\ \vdots & \vdots & \vdots & & & \\ 0 & 0 & 0 & \cdots 1 & -2 & 1 \end{pmatrix}$$

Summary

- Finite-difference approximations for derivatives
- Calculate order of error using Taylor expansions
- Or via interpolation