Numerical Integration and Differentiation

CS 205A:
Mathematical Methods for Robotics, Vision, and Graphics

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Announcements

- HW8
  - Extension: Due on Friday
  - Can use late days until Sunday midnight
  - Solutions out Monday
- Final Exam
  - Tuesday March 20 @ 3:30-6:30pm
  - Room: Gates B3 (this room)
  - Allowed: Two double-sided pages of written notes (can reuse last one)

Today's Task

Last time: Find $f(x)$

Today: Find $\int_a^b f(x)\,dx$ and $f'(x)$

Motivation

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

Some functions are *defined* using integrals!

Sampling from a Distribution

$$p(x) \in \mathrm{Prob}([0,1])$$

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Cumulative distribution function (CDF):

$$F(t) \equiv \int_0^t p(x)\,dx$$

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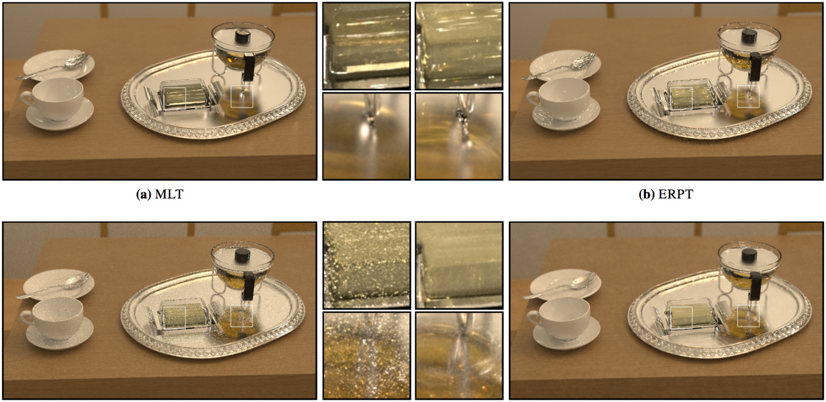
X distributed uniformly in $[0,1] \implies$ $F^{-1}(X)$ distributed according to p

Rendering

"Light leaving a surface is the integral of the light coming in after it is reflected and diffused."

Rendering equation

Rendering



(a) MLT **(b)** ERPT **(c)** PSSMLT **(d)** MEPT

Figure 12: TABLE: *This view of our room scene shows chinaware (using a BRDF with both diffuse and specular components), a teapot containing an absorbing medium, and a butter dish on a glossy silver tray. Illumination comes from the chandelier in Figure 11.*

Jakob, W., Marschner, S. 2012. **Manifold Exploration: A Markov Chain Monte Carlo Technique for Rendering Scenes with Difficult Specular Transport.** *ACM Trans. Graph.* 31 4, Article 58 (July 2012).

Gaussian Blur

http://www.borisfx.com/images/bcc3/gaussian_blur.jpg

$$(I * g)(x, y) = \iint_{\mathbb{R}^2} I(u, v) g(x - u, y - v)\, du\, dv$$

Bayes' Rule

$$P(X|Y) = \frac{P(Y|X)P(X)}{\int P(Y|X)P(X)\,dX}$$

Probability of X given Y

Quadrature

Quadrature

Given a sampling of n values $f(x_1), \ldots, f(x_n)$, find an approximation of $\int_a^b f(x)\,dx$.

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Given a sampling of n values $f(x_1), \ldots, f(x_n)$, find an approximation of $\int_a^b f(x)\,dx$.

1. Endpoints may be fixed, **or** may want to query many (a, b) pairs
2. May be able to query $f(x)$ anywhere, **or** may be given a fixed set of pairs $(x_i, f(x_i))$

Interpolatory Quadrature

$$\int_a^b f(x)\,dx = \int_a^b \left[\sum_i a_i \phi_i(x)\right] dx$$

$$= \sum_i a_i \left[\int_a^b \phi_i(x)\,dx\right]$$

$$= \sum_i c_i a_i \text{ for } c_i \equiv \int_a^b \phi_i(x)\,dx$$

Example 14.6: Monomials x^k on $[0, 1]$.

Riemann Integral

$$\int_a^b f(x)\,dx = \lim_{\Delta x_k \to 0} \sum_k f(\tilde{x}_k)(x_{k+1} - x_k)$$
$$\approx \sum_k f(\tilde{x}_k)\Delta x_k$$

Quadrature Rules

$$Q[f] \equiv \sum_i w_i f(x_i)$$

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w_i describes the contribution of $f(x_i)$

Quadrature Rules

Example 14.7:

Method of undetermined coefficients

- Fix quadrature points $x_1,\ x_2, \dots, x_n$.
- Choose n functions $f_1(x),\ f_2(x), \dots, f_n(x)$ where
- $\int_a^b f_i(x)dx$ are known for $i = 1, \dots, n$.
- Solve n-by-n linear system for weights $w_1, \dots, w_n$ such that

$$w_1 f_i(x_1) + \ldots + w_n f_i(x_n) = \int_a^b f_i(x)dx,$$

for $i = 1, \dots, n$.

Newton-Cotes Quadrature

x_i's evenly spaced in $[a, b]$ and symmetric

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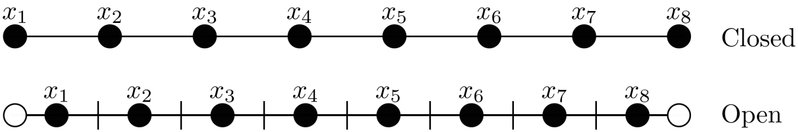
- **Closed:** includes endpoints

$$x_k \equiv a + \frac{(k-1)(b-a)}{n-1}$$

- **Open:** does not include endpoints

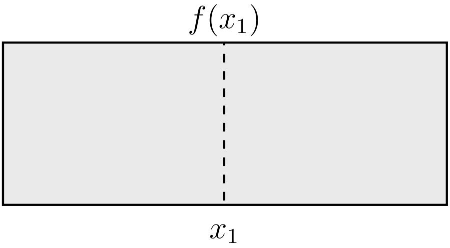
$$x_k \equiv a + \frac{k(b-a)}{n+1}$$



Midpoint Rule

$$\int_a^b f(x)\,dx \approx (b-a) f\left(\frac{a+b}{2}\right)$$

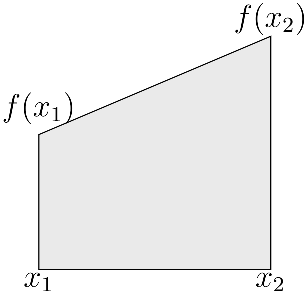
Open



Trapezoidal Rule

$$\int_a^b f(x)\,dx \approx (b-a)\frac{f(a)+f(b)}{2}$$

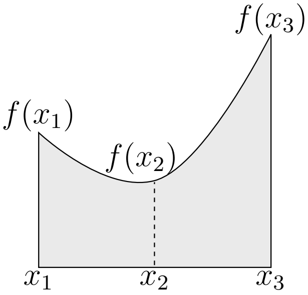
Closed



Simpson's Rule

$$\int_a^b f(x)\,dx \approx \frac{b-a}{6}\left(f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right)$$

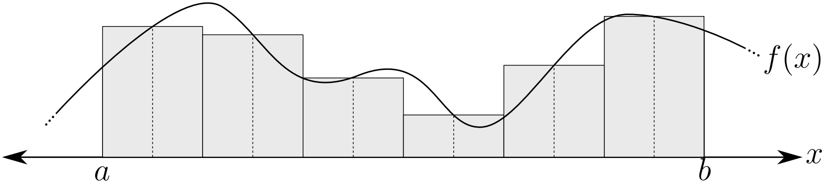
Closed; from quadratic interpolation



Composite Rules

Composite midpoint:

$$\int_a^b f(x)\,dx \approx \sum_{i=1}^{k} f\left(\frac{x_{i+1}+x_i}{2}\right)\Delta x$$

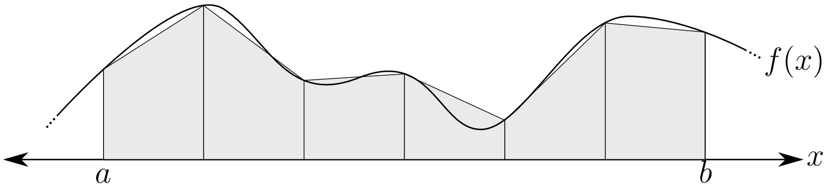


Composite Rules

Composite trapezoid:

$$\int_a^b f(x)\,dx \approx \sum_{i=1}^{k}\left(\frac{f(x_i)+f(x_{i+1})}{2}\right)\Delta x$$

$$= \Delta x\left(\frac{1}{2}f(a)+f(x_1)+\cdots+f(x_{k-1})+\frac{1}{2}f(b)\right)$$



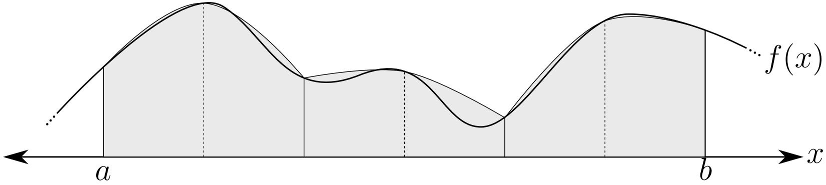
Composite Rules

Composite Simpson:

$$\int_a^b f(x)\,dx \approx \frac{\Delta x}{3}\left[f(a) + 2\sum_{i=1}^{n-2-1} f(x_{2i}) + 4\sum_{i=1}^{n/2} f(x_{2i-1}) + f(b)\right]$$

$$= \frac{\Delta x}{3}\left[f(a) + 4f(x_1) + 2f(x_2) + \cdots + 4f(x_{n-1}) + f(b)\right]$$

n *must be odd!*



Question

Which quadrature rule is best?

Accuracy on a Single Interval

- Midpoint *and* trapezoid: $O(\Delta x^3)$
- Simpson: $O(\Delta x^5)$

[See Mathematica notebook.]

Composite Accuracy

Number of subintervals $\approx O(\frac{1}{\Delta x})$

- Midpoint *and* trapezoid: $O(\Delta x^2)$
- Simpson: $O(\Delta x^4)$

Other Strategies

- **Gaussian quadrature:** Optimize both w_i's *and* x_i's; gets two times the accuracy (but harder to use!)
- **Adaptive quadrature:** Choose x_i's where information is needed (e.g. when quadrature strategies do not agree)

Multivariable Integrals I

"Curse of dimensionality"

$$\int_{\Omega} f(\vec{x})\, d\vec{x}, \Omega \subseteq \mathbb{R}^n$$

- **Iterated integral:** Apply one-dimensional strategy
- **Subdivision:** Fill with triangles/rectangles, tetrahedra/boxes, etc.

Multivariable Integrals II

- **Monte Carlo:** Randomly draw points in Ω and average $f(\vec{x})$; converges like $1/\sqrt{k}$ regardless of dimension

Conditioning

Given quadrature scheme

$$Q[f] = \sum_{i=1}^{n} w_i f(x_i)$$

and perturbed function $\hat{f}$, then

$$\frac{|Q[f] - Q[\hat{f}]|}{\|f - \hat{f}\|_\infty} \leq \|\vec{w}\|_1 \leq n\|\vec{w}\|_\infty$$

Note: Norm typo in book.

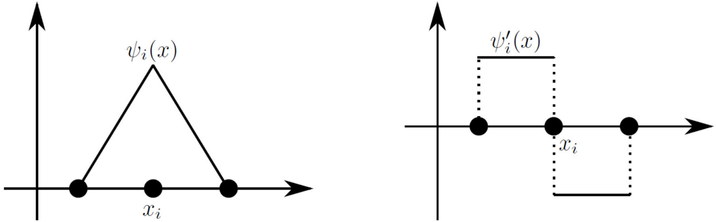
Differentiation

- Lack of stability
- Jacobians vs. $f : \mathbb{R} \to \mathbb{R}$

Differentiation in Basis

$$f'(x) = \sum a_i \phi_i'(x)$$

ϕ_i''s basis for derivatives



Differentiation in Basis

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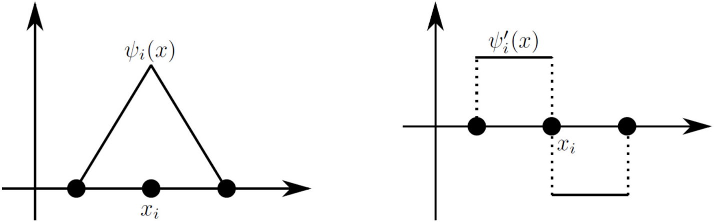

Important for finite element method!

Definition of Derivative

$$f'(x) \equiv \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

$O(h)$ Approximations

Forward difference:

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

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Forward difference:

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

Backward difference:

$$f'(x) \approx \frac{f(x) - f(x-h)}{h}$$

$O(h^2)$ Approximation

Centered difference:

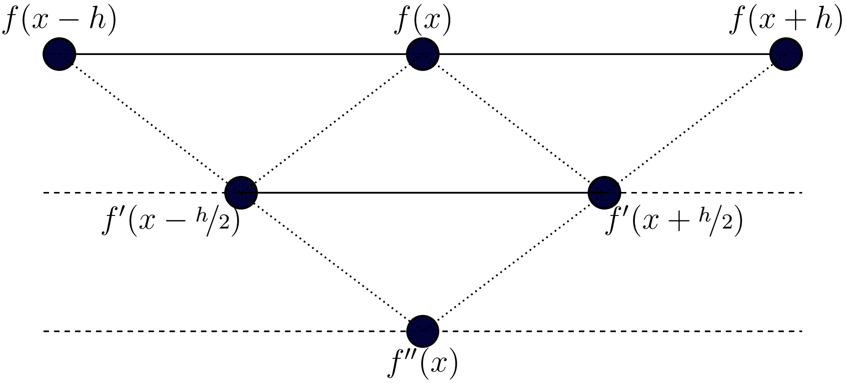
$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

$O(h)$ Approximation of f''

Centered difference:

$$f''(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$
$$= \frac{\frac{f(x+h)-f(x)}{h} - \frac{f(x)-f(x-h)}{h}}{h}$$

Geometric Interpretation for f''



Deriving Finite Differences Schemes

General case: Want $f^{(k)}(0)$ using an n-sample FD scheme

$$f^{(k)}(0) \approx \sum_{i=1}^{n} c_i f(x_i).$$

Approach: Consider Taylor Series expansions, and solve a linear system (symbolically) to find the coefficients:

$$\sum_{i=1}^{n} c_i f(x_i) \approx \left(\sum_i c_i\right) f(0) + \left(\sum_i c_i x_i\right) f'(0) + \left(\frac{1}{2!}\sum_i c_i (x_i)^2\right) f''(0) + \dots$$

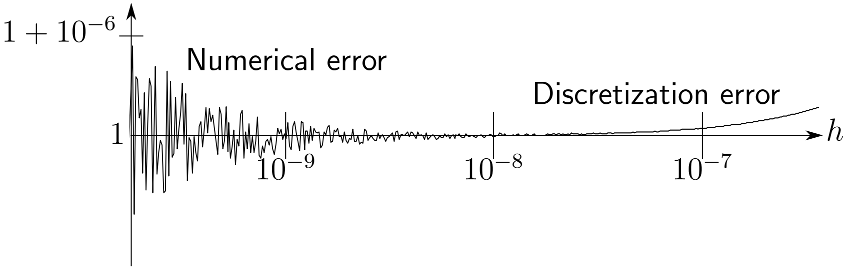
So we have $A\vec{c} = \hat{e}_k \implies \vec{c} = A^{-1}\hat{e}_k$ for the k^{th} derivative finite-difference scheme.

See Mathematica notes.

`https://en.wikipedia.org/wiki/Finite_difference_coefficient`

Choosing h

- **Too big:** Bad approximation of f'
- **Too small:** Numerical issues
  (h small, $f(x) \approx f(x+h)$)



Richardson Extrapolation

$$D(h) \equiv \frac{f(x+h) - f(x)}{h} = f'(x) + \frac{1}{2}f''(x)h + O(h^2)$$

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$$D(\alpha h) = f'(x) + \frac{1}{2} f''(x) \alpha h + O(h^2)$$

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$$D(\alpha h) = f'(x) + \frac{1}{2}f''(x)\alpha h + O(h^2)$$

$$\begin{pmatrix} f'(x) \\ f''(x) \end{pmatrix} = \begin{pmatrix} 1 & \frac{1}{2}h \\ 1 & \frac{1}{2}\alpha h \end{pmatrix}^{-1} \begin{pmatrix} D(h) \\ D(\alpha h) \end{pmatrix} + O(h^2)$$

Extrapolation for integration: **Romberg Integration**