Numerical Integration and Differentiation


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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

\[ \text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_{0}^{x} e^{-t^2} \, dt \]

Some functions are *defined* using integrals!
Sampling from a Distribution

\[ p(x) \in \text{Prob}([0, 1]) \]
Sampling from a Distribution

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Cumulative distribution function (CDF):

\[ F(t) \equiv \int_0^t p(x) \, dx \]
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Cumulative distribution function (CDF):

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

\( X \) 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
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.

Gaussian Blur

\[(I \ast g)(x, y) = \iiint_{\mathbb{R}^2} I(u, v) g(x - u, y - v) \, du \, dv\]
Bayes’ Rule

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

*Probability of \( X \) given \( Y \)*
Quadrature

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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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

\[
\int_a^b f(x) \, dx = \int_a^b \left[ \sum_i a_i \phi_i(x) \right] \, dx = \sum_i a_i \left[ \int_a^b \phi_i(x) \, dx \right] = \sum_i c_i a_i \quad \text{for} \quad c_i \equiv \int_a^b \phi_i(x) \, dx
\]

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

\[ Q[f] \equiv \sum_i w_i f(x_i) \]
Quadrature Rules

\[ Q[f] \equiv \sum_{i} w_i f(x_i) \]

\( w_i \) describes the contribution of \( f(x_i) \).
Quadrature Rules

Example 14.7: Method of undetermined coefficients

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

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

for $i = 1, \ldots, n$. 
Newton-Cotes Quadrature

$x_i$’s evenly spaced in $[a, b]$ and symmetric
Newton-Cotes Quadrature

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

- **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

\[ f(x_1) \]

\[ x_1 \]
Trapezoidal Rule

\[
\int_{a}^{b} f(x) \, dx \approx (b - a) \frac{f(a) + f(b)}{2}
\]

Closed
Simpson’s’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 Simpson:

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

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

\(n\) 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 \( \approx O\left(\frac{1}{\Delta x}\right) \)

- 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”

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

- **Iterated integral**: Apply one-dimensional strategy
- **Subdivision**: Fill with triangles/rectangles, tetrahedra/boxes, etc.
Monte Carlo: Randomly draw points in $\Omega$ and average $f(\vec{x})$; converges like $\frac{1}{\sqrt{k}}$ 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. $f : \mathbb{R} \rightarrow \mathbb{R}$
Differentiation in Basis

\[ f'(x) = \sum a_i \phi_i'(x) \]

\( \phi_i'' \)'s basis for derivatives
Differentiation in Basis

\[ f'(x) = \sum a_i \phi'_i(x) \]

\( \phi'_i \)'s basis for derivatives

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

\[
\begin{align*}
\text{Forward difference:} \\
f'(x) &\approx \frac{f(x + h) - f(x)}{h}
\end{align*}
\]
\( O(h) \) Approximations

**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:

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


\[ O(h) \text{ Approximation of } f'' \]

Centered difference:

\[
f''(x) \approx \frac{f(x + h) - 2f(x) + f(x - h)}{h^2}
\]

\[
= \frac{f(x + h) - f(x)}{h} - \frac{f(x) - f(x - h)}{h}
\]
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:

\[ \sum_{i=1}^{n} c_i f(x_i) \approx \left( \sum_{i} c_i \right) f(0) + \left( \sum_{i} c_i x_i \right) f'(0) + \left( \frac{1}{2!} \sum_{i} c_i (x_i)^2 \right) f''(0) + \ldots \]

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

\[ D(h) \equiv \frac{f(x + h) - f(x)}{h} = f'(x) + \frac{1}{2}f''(x)h + O(h^2) \]
Richardson Extrapolation

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

\[ D(\alpha h) = f'(x) + \frac{1}{2} f''(x) \alpha h + O(h^2) \]
Richardson Extrapolation

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

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

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

Extrapolation for integration: Romberg Integration