Numerical Integration and Differentiation

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

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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 \( p \)
“Light leaving a surface is the integral of the light coming in after it is reflected and diffused.”

Rendering equation
Gaussian Blur

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

Bayes’ Rule

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

Probability of $X$ given $Y$
“This leads to a situation where we are trying to minimize an energy function that we cannot evaluate. We now find ourselves in the field without any light whatsoever... so we cannot establish the height of any point in the field relative to our own. CD effectively gives us a sense of balance, allowing us to feel the gradient of the field under our feet.”

http://www.robots.ox.ac.uk/~ojw/files/NotesOnCD.pdf
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

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

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

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

\( n \) must be odd!

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**CS 205A: Mathematical Methods**
**Numerical Integration and Differentiation**

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Question

Which quadrature rule is best?
Accuracy on a Single Interval

[On the board.]

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

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

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

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

\[ \left| Q[f] - Q[\hat{f}] \right| \leq \left\| \vec{w} \right\|_\infty \]
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
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\( \phi'_i \)'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

**Forward difference:**

\[
f'(x) \approx \frac{f(x + h) - f(x)}{h}
\]
$O(h)$ 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:**

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

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

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

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

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

![Graph showing numerical error and discretization error as a function of $h$]
Choosing $h$

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

Why bother with Richardson?