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

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

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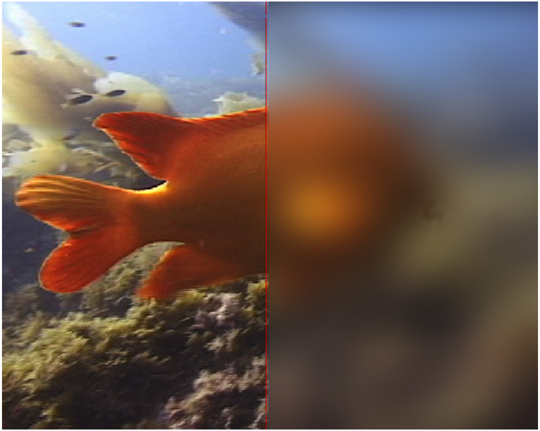
X distributed uniformly in $[0,1] \implies$
$F^{-1}(X)$ distributed according to p

Rendering

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

Rendering equation

Gaussian Blur



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

Bayes' Rule

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

Probability of X given Y

Big Problem

"This leads to a situation where we are trying to minimize an energy function that we cannot evaluate.... If we return to our field metaphor, 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 the feel the gradient of the field under our feet."

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

Quadrature

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

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x_i's may be fixed or may be chosen by the algorithm (depends on context)

Interpolatory Quadrature

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

Riemann Integral

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

Quadrature Rules

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

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w_i describes the contribution of $f(x_i)$

Newton-Cotes Quadrature

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

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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

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

Open; from quadratic interpolation

Composite Rules

Apply rules on subintervals

$$\Delta x \equiv \frac{b-a}{k}, x_i \equiv a + i\Delta x$$

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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?

On a Single Interval

[On the board.]

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

Composite

Width of subinterval is $O(\frac{1}{\Delta x})$

- 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

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

Differentiation

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

Differentiation in Basis

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

ϕ_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:

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

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Forward difference:

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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

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

Choosing h

- **Too big:** Bad approximation of f'

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

Next