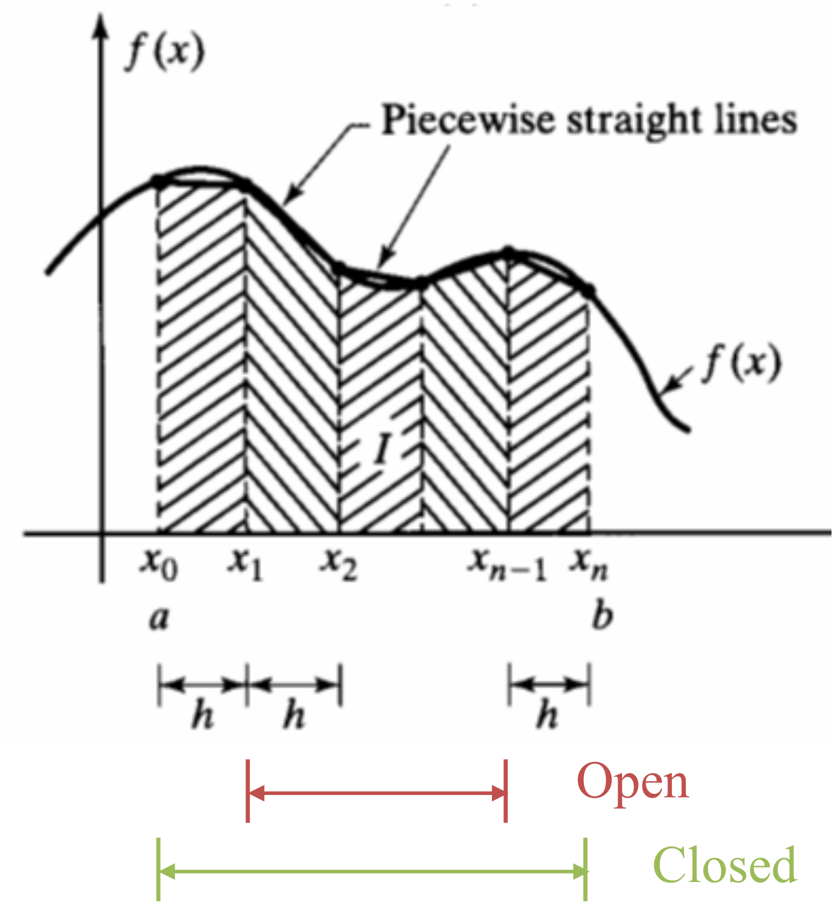
LECTURE 1: Numerical Integration (also called Quadrature)

$$I = \int_a^b f(x)dx$$

Special case of differential equation

$$\frac{dy}{dx} = f(x), \;\; y(a) = 0$$

Simple Trapezoidal Rule



$$x_i = x_0 + ih$$
$$f(x_i) = f_i$$

$$\int_{x_1}^{x_2} f(x)dx =$$
$$\frac{h}{2}(f_1 + f_2) + \mathcal{O}(h^3 f'')$$

- Exact for linear $f(x)$

Image credit: *http://www.unistudyguides.com/wiki/Numerical_Integration*

Simpson's Rule

$$\int_{x_1}^{x_3} f(x)dx = h(\frac{1}{3}f_1 + \frac{4}{3}f_2 + \frac{1}{3}f_3) + \mathcal{O}(h^5 f'''')$$

- Exact for $f(x) = \alpha x + \beta x^2 + \gamma x^3$
- Open if we cannot compute $f(x_0)$ or $f(x_{N+1})$

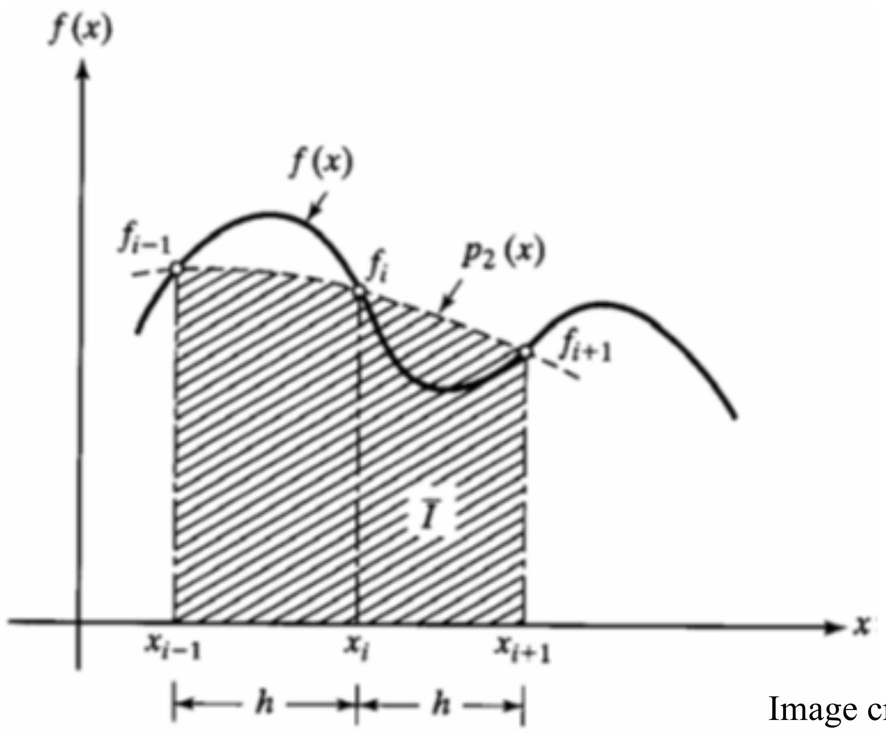


Image credit: *http://www.unistudyguides.com/wiki/Numerical_Integration*

Extended Formula

Trapezoid:

$$\int_{x_1}^{x_N} f(x)dx = h\left[\frac{1}{2}f_1 + f_2 + f_3 + \cdots + f_{N-1} + \frac{1}{2}f_N\right] + O\left(\frac{(b-a)^3 f''}{N^2}\right)$$

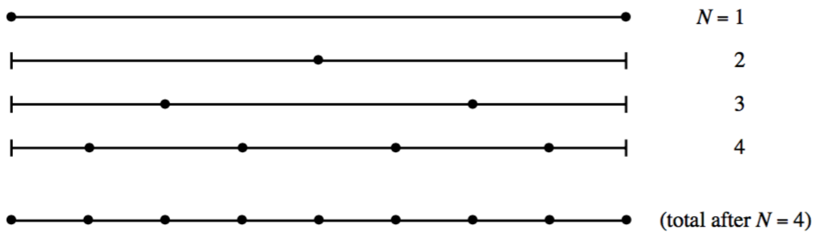
Simpson:

$$\int_{x_1}^{x_N} f(x)dx = h\left[\frac{1}{3}f_1 + \frac{4}{3}f_2 + \frac{2}{3}f_3 + \frac{4}{3}f_4 + \cdots + \frac{2}{3}f_{N-2} + \frac{4}{3}f_{N-1} + \frac{1}{3}f_N\right] + O\left(\frac{1}{N^4}\right)$$

Open Extended Trapezoid:

$$\int_{x_1}^{x_N} f(x)dx = h\left[\frac{3}{2}f_2 + f_3 + f_4 + \cdots + f_{N-2} + \frac{3}{2}f_{N-1}\right] + O\left(\frac{1}{N^2}\right)$$

- How do we achieve a given accuracy?
- We cannot guess *N* ahead of time, so we need to vary it.



- If we double $N \to 2N$, we can reuse function evaluations.

- Error Estimate: Difference between two subsequent steps
- Also need to put a limit to the number of steps:

$$N_{\max} = 2^{\mathrm{JMAX}-1}, \ \mathrm{JMAX} = 20$$

$\to$ QTRAP of NR or QSIMP + TRAPZD

- Final refinement: Extended trapezoidal error is even in $1/N$:

$$\int_{x_1}^{x_N} f(x)dx = h\left[\frac{1}{2}f_1 + f_2 + f_3 + \cdots + f_{N-1} + \frac{1}{2}f_N\right] - \frac{B_2 h^2}{2!}(f'_N - f'_1) - \cdots - \frac{B_{2k}h^{2k}}{(2k)!}(f_N^{(2k-1)} - f_1^{(2k-1)}) - \cdots$$

- Apply to N and $2N$: $I = \frac{4}{3}I_{2N} - \frac{1}{3}I_N$ cancels out leading error.

$$I_{\text{true}} = I_N + E_t$$

$$E_t(N) = \frac{C}{N^2} = I_{\text{true}} - I_N \qquad E_t(2N) = \frac{C}{4N^2} = I_{\text{true}} - I_{2N}$$

$$I_{\text{true}} = I_{2N} - \frac{I_{2N} - I_N}{3} = \frac{4}{3}I_{2N} - \frac{1}{3}I_N$$

→ We get Simpson's Rule

Romberg Integration

- Use N, $2N$, $4N$, … to cancel out higher orders $O(N^{-2k})$ using polynomial extrapolation

Romberg Integration
$\rightarrow$ Romberg is the best routine for uniform interval sampling

Doubling N from I_1 to I_2,

$$I_1 + ch_1^2 = I_2 + ch_2^2,$$

$$I_2 - I_1 = ch_1^2 - ch_2^2 = 3ch_2^2,$$

$$\epsilon_2 = ch_2^2 = \tfrac{1}{3}(I_2 - I_1).$$

$$R_{i,1} = I_i\,,$$

$$R_{i,2} = I_i + \tfrac{1}{3}(I_i - I_{i-1}) = R_{i,1} + \tfrac{1}{3}(R_{i,1} - R_{i-1,1}).$$

$$\begin{array}{ccccccccc}
I_1 \equiv R_{1,1} & & & & & & & & \\
& \searrow & & & & & & & \\
I_2 \equiv R_{2,1} & \rightarrow & R_{2,2} & & & & & & \\
& \searrow & & \searrow & & & & & \\
I_3 \equiv R_{3,1} & \rightarrow & R_{3,2} & \rightarrow & R_{3,3} & & & & \\
& \searrow & & \searrow & & \searrow & & & \\
I_4 \equiv R_{4,1} & \rightarrow & R_{4,2} & \rightarrow & R_{4,3} & \rightarrow & R_{4,4} & & \\
& \searrow & & \searrow & & \searrow & & \searrow &
\end{array}$$

Improper Integrals

- Cannot be evaluated Ex) $\left.\frac{\sin(x)}{x}\right|_{x=0}$

Use open formula: Extended Midpoint Rule

- Infinite boundaryc Ex) $\int_{-\infty}^{\infty} f(x)dx$
- Integrable singularity Ex) $\int_0^{x_0} x^{-\frac{1}{2}}dx$

Change of variables

$$\int_a^b f(x)dx = \int_{1/b}^{1/a} \frac{1}{t^2} \cdot f(1/t)dt$$

$ab > 0$

$b \to \infty, a > 0$

$a \to -\infty, b < 0$

Examples: Change of variables

- Integrable singularity

If the integrand diverges as $(x-a)^{-\gamma}$,
$0 \le \gamma < 1$, near $x = a$,

$$\int_a^b f(x)dx = \frac{1}{1-\gamma}\int_0^{(b-a)^{1-\gamma}} t^{\frac{\gamma}{1-\gamma}} f(t^{\frac{1}{1-\gamma}} + a)dt \qquad (b > a)$$

- Exponential fall-off

$$t = e^{-x} \qquad \text{or} \qquad x = -\log t$$

$$\int_{x=a}^{x=\infty} f(x)dx = \int_{t=0}^{t=e^{-a}} f(-\log t)\frac{dt}{t}$$

Gaussian Quadratures

- Move beyond equally spaced points
- Choose abscissas and weights, achieving twice the order of accuracy
- Higher order $\neq$ Higher accuracy!
- We can choose to be high accuracy for polynomial times a function *W(x)*

$$\int_a^b W(x) f(x) dx \approx \sum_{j=1}^{N} w_j f(x_j)$$

Weights & Abscissas tabulated for several cases

Read about orthogonal polynomials
construction of weights & abscissas in NR

- Commonly used cases:

Rescale for other intervals

Gauss-Legendre:

$$W(x) = 1 \qquad -1 < x < 1$$

Gauss-Chebyshev:

$$W(x) = (1 - x^2)^{-1/2} \qquad -1 < x < 1$$

Gauss-Laguerre:

$$W(x) = x^\alpha e^{-x} \qquad 0 < x < \infty$$

Gauss-Hermite:

$$W(x) = e^{-x^2} \qquad -\infty < x < \infty$$

Gauss-Jacobi:

$$W(x) = (1 - x)^\alpha (1 + x)^\beta \qquad -1 < x < 1$$

Multidimensional Integrals

are HARD!

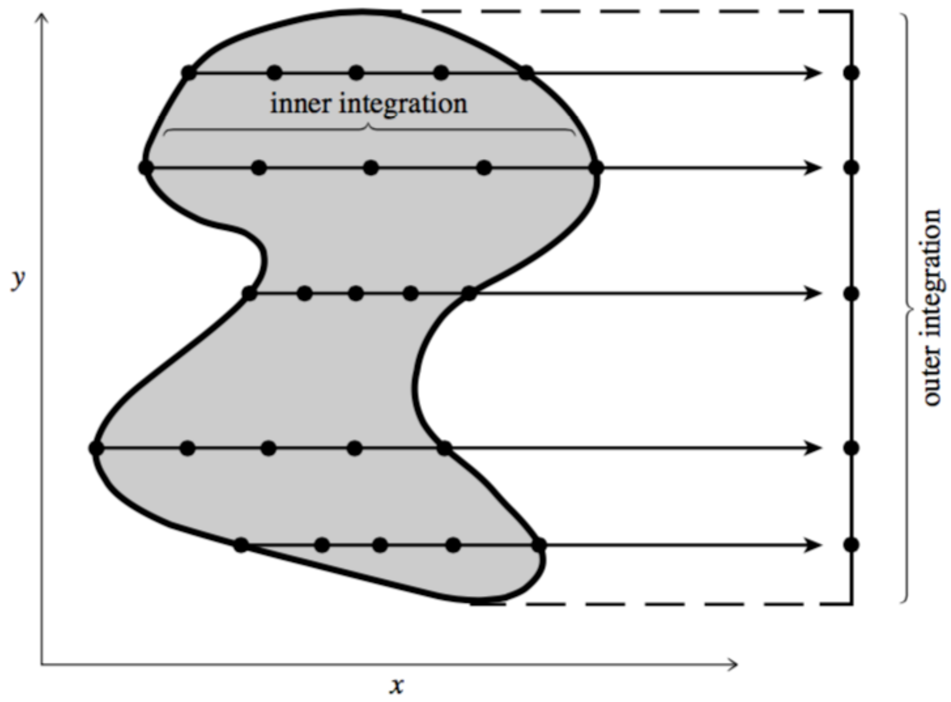
- Number of points scales as N^M, where M: # of dimensions
- Boundary can be complicated

Can dimension be reduced?

$$\int_0^x dt_n \int_0^{t_n} dt_{n-1} \cdots \int_0^{t_3} dt_2 \int_0^{t_2} f(t_1) dt_1 = \frac{1}{(n-1)!} \int_0^x (x-t)^{n-1} f(t) dt$$

If complicated boundary, low res, not strongly peaked integrand
→ Monte Carlo Integration (to be discussed later)

If boundary is simple and function is smooth
→ Repeated 1-D integrals



$$I = \int\int dxdy f(x,y)$$

$$H(x) = \int_{y_1}^{y_2} f(x,y)dy$$

$$I = \int_{x_1}^{x_2} H(x)dx$$

Best to use Gaussian Quadratures for high precision

Image credit: Press et al., *Numerical Recipes,* 3rd ed. (pg. 198)

Summary

- Workhorse for 1-D integrals is:
  Romberg: simple, nested error estimate
- Input: EPS (Error), Max # of iterations
- If evaluations expensive, use Gaussian Quadratures
- If many dimensions, use 1-D repeated integrals,
  with Gauss Q. preferred
- Complicated boundary + many dim integrals
  $\rightarrow$ Use Monte Carlo

Literature

- *Numerical Recipes*, Press et al., Chapter 4
  (http://apps.nrbook.com/c/index.html)
- *Computational Physics*, Mark Newman, Chapter 5
  (http://www-personal.umich.edu/~mejn/cp/chapters/int.pdf)