

Numerical Methods

Lecture 8-9

Integration Methods

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Ref: Chapt. 4 and Sect. 7.6 of Numerical Recipes

Outline

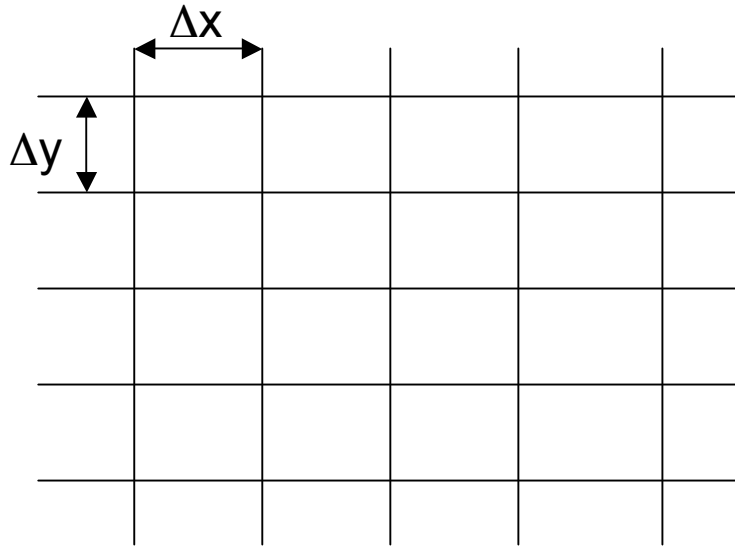
- Grid Integration and Gaussian Quadrature
- Integration of Spherical Harmonics
- Metropolis Method
- Importance Sampling
- Boltzmann Distribution
- Quantum Monte Carlo

General Intuitive Principles

1. Integration of functions is closely related to fitting of functions - the kind of integration depends on the kind of fit
2. If the properties of the function are constrained, use an integration method that reflects this.
e.g. if you know the problem “naturally” represents the function in a Fourier series, use a method that **exactly** integrates the expected dominant terms in the Fourier series.
3. Don't try to fit more parameters (implicitly) than you have known values $f(x_j)$ of your function

Garbage in = Garbage out!

Uniform Grid

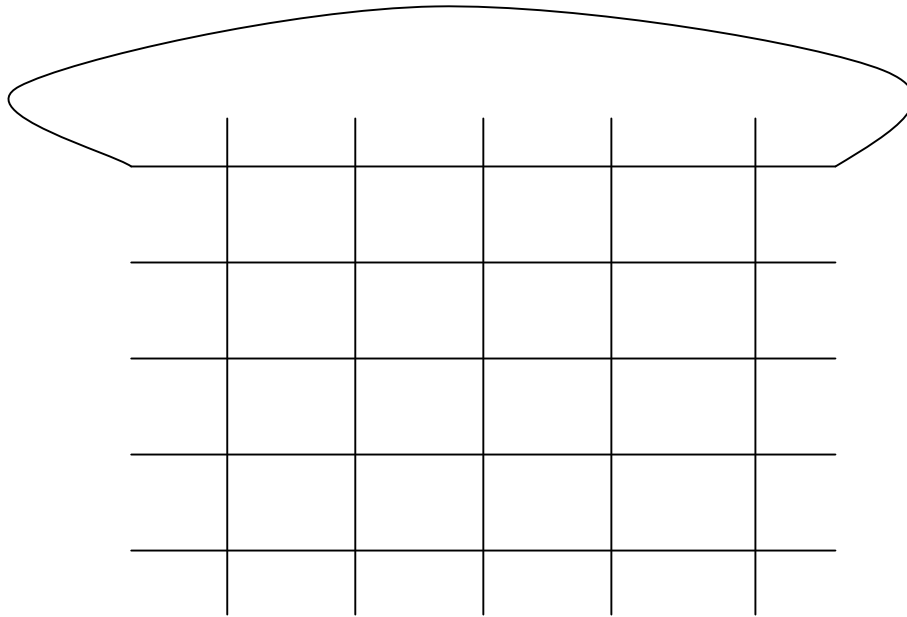


$$\int f(x, y) dx dy$$
$$= \Delta x \Delta y \sum_{i, j} f(i\Delta x, j\Delta y)$$

Implicit fit: $f = \text{constant}$ in each interval

The function should not change much between grid points!

Uniform Grid - Periodic Functions



$$f(x + L, y) = f(x, y)$$

$$f(x, y + L) = f(x, y)$$

$$\int f(x, y) dx dy$$
$$= \Delta x \Delta y \sum_{i, j} f(i\Delta x, j\Delta y)$$

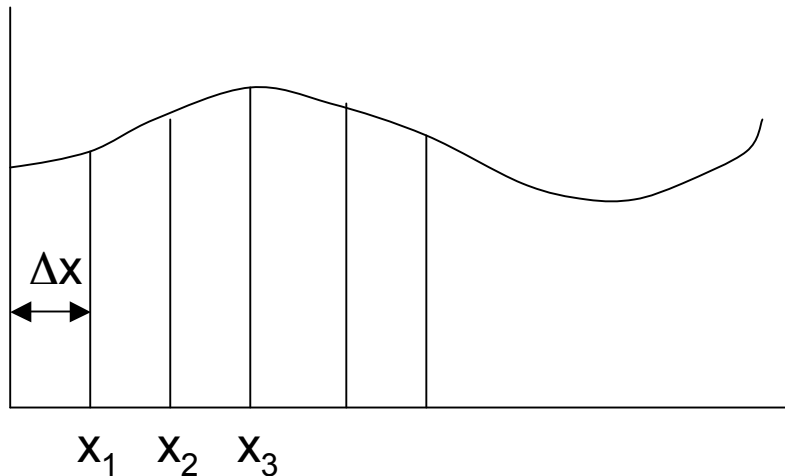
Uniform grid integrates Fourier series
exactly for $\lambda > 2\Delta x$

Examples: general FFT,

Band structure integration of fns. in Brillouin Zone (Pack-Monkhorst)

Higher Order (Newton-Cotes Formulae)

(Polynomial Fitting)



Trapezoidal Rule: $\int_{x_1}^{x_2} f(x) dx = \Delta x \left[\frac{1}{2} f_1 + \frac{1}{2} f_2 \right]$

Linear fit of f
in $[x_1, x_2]$

Simpson's Rule: $\int_{x_1}^{x_3} f(x) dx = \Delta x \left[\frac{1}{3} f_1 + \frac{4}{3} f_2 + \frac{1}{3} f_3 \right]$

Cubic fit of f
in $[x_1, x_3]$

Error: $O[(\Delta x)^5 d^4f/dx^4]$ - !! requires smooth function !!
Higher order is not always better!

Gaussian Quadrature

(Fitting with General Orthogonal Fns.)

$$\int_a^b f(x)W(x)dx \approx \sum_{i=1}^N w_i f(x_i) \quad x_i \text{ and } w_i \text{ arbitrary}$$

Example: integration on a sphere

$$\int f(\theta)d\Omega = 2\pi \int_0^\pi f(\theta)\sin\theta d\theta = 2\pi \int_{-1}^1 f(\theta)dx, \quad x = \cos\theta$$

Fit f with Legendre Polynomials in $\cos(\theta)$ [Spherical Harmonics]

$$f(x) \approx \sum_{i=1}^N c_i P_i(x), \quad \int_a^b P_i(x)P_j(x)W(x)dx = \delta_{ij}$$

“natural” weight function

Gaussian Quadrature

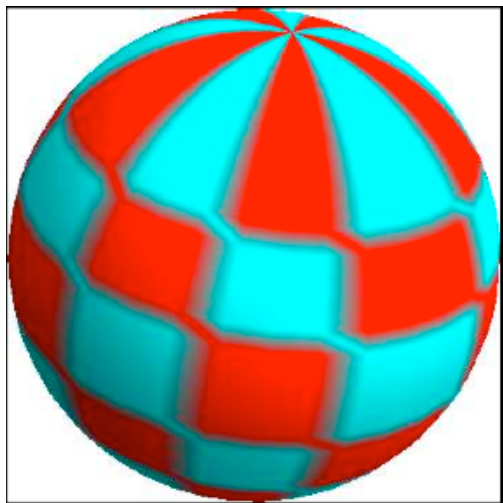
$$\int_a^b P_j(x)W(x)dx = \sum_{i=1}^N w_i P_j(x_i)$$

Choose x_i and w_i to integrate P_i exactly for $i < N$

Choose x_i so that $P_N(x_i)=0$ and solve for $j=0, \dots, N-1$ to find w_i [see Numerical Recipes, Sect. 4.5]

This often allows us to match the integration to the physical problem at hand by using the appropriate orthogonal functions (usually eigenfunctions associated with the problem)

Gaussian Quadrature



Spherical problems:

Grid points = zeros of (real)
spherical harmonics

See Numerical Recipes 4.5 for w_i

Periodic problems: Fourier Series, uniform grid ($\sin(x)=0$)

Integration with $W(x) = e^{-x^2}$ on $[-\infty, +\infty]$:
Hermite Polynomials (SHO eigenfunctions)

Monte Carlo Integration

$$\int_a^b f(x)W(x)dx \approx \frac{1}{N} \sum_{i=1}^N f(x_i)$$

Choose x_i at random
from distribution W
($W > 0$ is normalized)

This gives a unbiased random estimate of the integral

Random error
in integral

$$\langle \delta I^2 \rangle = \frac{1}{N} \langle \delta f^2 \rangle$$

NB: assumes x_i are independent

Error $\sim 1/\text{sqrt}(N)$

very slow
convergence!

In general, only use Monte Carlo integration for very high-dimensional integrals, where grid methods are impossible ($n > 5$)

Monte Carlo Integration - Importance Sampling

$$\int_a^b f(x)W(x)dx \approx \frac{1}{N} \sum_{i=1}^N f(x_i)$$

$$\langle \delta I^2 \rangle = \frac{1}{N} \langle \delta f^2 \rangle$$

The division of f and W is often adjustable (but $W > 0$).
The ideal is $f = \text{constant}$ (you get the integral exactly)

Points are sampled according to their weight
(or “importance”) in the integrand

Metropolis Method

How do we “choose x_i at random from distribution W ”?

Random Walk:

Trial move: $x_{i+1} = x_i + \Delta$, Δ random on $[-1,+1]$

Accept/reject move with probability

$$P_a(x_i \rightarrow x_{i+1}) = \min\left[1, \frac{W(x_{i+1})}{W(x_i)}\right]$$

If move is rejected, stay at x_i and try new move

After many steps, the distribution of x_i is W (normalized)

Metropolis Method - Detailed Balance

Consider many “walkers”, each following random walk

Steady-state distribution occurs if:

$$P(x)P_a(x \rightarrow x') = P(x')P_a(x' \rightarrow x)$$

Detailed
Balance

If $W(x') > W(x)$

$$\Rightarrow P_a(x \rightarrow x') = 1 \text{ and } P_a(x' \rightarrow x) = \frac{W(x)}{W(x')}$$

$$\Rightarrow P(x) = \frac{W(x)}{Z} \quad \text{where } Z \text{ is a normalization factor}$$

Random Walks - Critical Slowing Down

Random error
in integral

$$\langle \delta I^2 \rangle = \frac{1}{N} \langle \delta f^2 \rangle$$

NB: assumes x_i are independent

If walk cannot effectively move to sample all values of f , the the samples of f_i are very strongly correlated

Effective N is much smaller than the number of steps

When numerical “walk” simulates physical dynamics, this is often associated with a phase transition

* But Metropolis dynamics can deliberately be made different from physical dynamics to avoid this

Classical Statistical Mechanics - Boltzmann Distribution

$$W(x) = \frac{1}{Z} \exp[-U(x)/kT]$$

x gives coordinates of all dynamical variables (usually high-dimensional for interacting system)

We do not need to know the partition function, Z , since Metropolis only uses ratios (self-normalizing)

Monte Carlo sampling of x (ensemble averaging) is an alternative to direct simulation of the dynamics (time averaging)

Quantum Monte Carlo - Quantum Distribution

$$W(x) = \frac{1}{\langle \psi | \psi \rangle} |\psi(x)|^2$$

$$E = \int \frac{H\psi}{\psi} W(x) dx = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle}$$

Variational Quantum Monte Carlo:

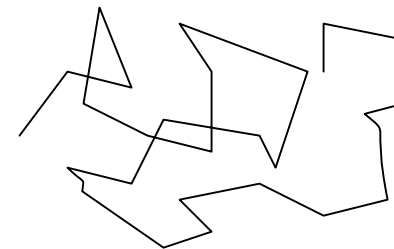
- * Use a general parametric form of many-body wave function
- * Minimize E with respect to the parameters

Summary

- Grid Integration
- Gaussian Quadrature
- Monte Carlo Integration
- Metropolis Method
- Importance Sampling
- Classical Monte Carlo
- Quantum Monte Carlo

Integration \leftrightarrow Fitting

$$\langle \delta I^2 \rangle = \frac{1}{N} \langle \delta f^2 \rangle$$



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