Monte Carlo Integration
Lecture 3

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01/16/2024

Numerical intergration

Why do we care?

Numerical intergration

Why do we care?

Application in Quantum Chemistry:

$$v_{p,q,r,s} = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\chi_p(\mathbf{r}_1)\chi_r(\mathbf{r}_1)\chi_q(\mathbf{r}_2)\chi_s(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|} d\mathbf{r}_1 d\mathbf{r}_2$$

Numerical intergration

Why do we care?

Discretization of continuous operators:

$$[\mathbf{D}]_{i,j} = \int_X \phi_i(\mathbf{x})\, \mathcal{D}\, \phi_j(\mathbf{x}) d\mathbf{x}$$

Numerical intergration

Why do we care?

Numerically solving differential equations:

- Left Riemann sum $\rightarrow$ explicit Euler
- Right Riemann sum $\rightarrow$ implicit Euler
- Trapezoidal rule $\rightarrow$ Crank-Nicolson

  $\vdots$

Numerical integration

We are interested in computing

$$F = \int_a^b f(x) \, dx$$

Numerical integration

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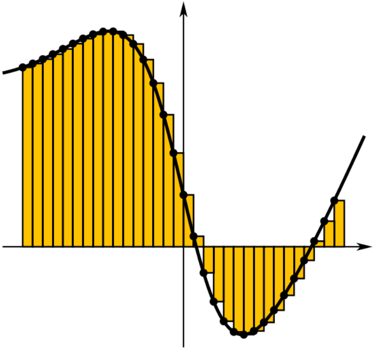
$$F = \int_a^b f(x)\; dx$$

Riemann sum (Left):



Numerical integration

We are interested in computing

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

Let $f : [a, b] \to \mathbb{R}$ be a function defines on a closed interval $[a, b] \subset \mathbb{R}$ and let $\{x_0, ..., x_n\}$ be a partition of $[a, b]$, i.e.,

$$a = x_0 < x_1 < ... < x_n = b.$$

Then

$$R_{\text{left}}(f, n) = \sum_{i=1}^{n} f(x_{i-1}) \Delta x_i$$

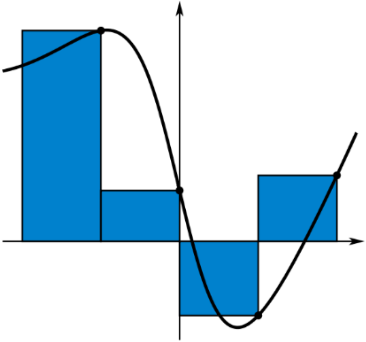
where $\Delta x_i = x_i - x_{i-1}$

Numerical integration

We are interested in computing

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

Riemann sum (Right):

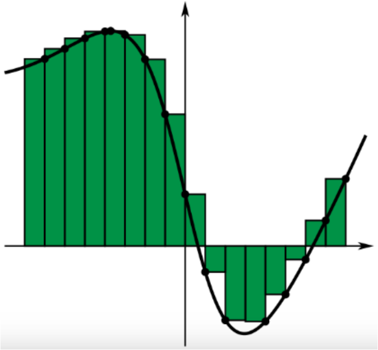


Numerical integration

We are interested in computing

$$F = \int_a^b f(x)\, dx$$

Riemann sum (Upper):

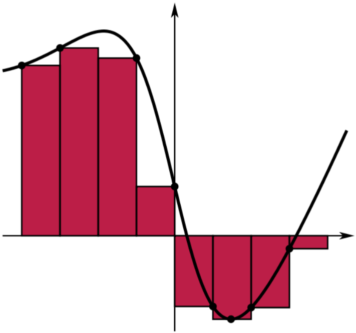


Numerical integration

We are interested in computing

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

Riemann sum (Lower):



Riemann Sums

Let $f : [a, b] \to \mathbb{R}$ be a function defines on a closed interval $[a, b] \subset \mathbb{R}$ and let $\{x_0, ..., x_n\}$ be a partition of $[a, b]$, i.e.,

$$a = x_0 < x_1 < ... < x_n = b.$$

Then

$$R(f, n) = \sum_{i=1}^{n} f(\tilde{x}_i)\Delta x_i$$

where $\Delta x_i = x_i - x_{i-1}$ and $\tilde{x}_i \in [x_{i-1}, x_i]$.

- Left Riemann sum: If $\tilde{x}_i = x_{i-1}$
- Right Riemann sum: If $\tilde{x}_i = x_i$
- Upper Riemann sum: If $\tilde{x}_i = \sup(f([x_{i-1}, x_i])$
- Lower Riemann sum: If $\tilde{x}_i = \inf(f([x_{i-1}, x_i])$
- Middle Riemann sum: If $\tilde{x}_i = (x_i + x_{i-1})/2$

Middle Riemann sum error

Middle Riemann sum error

- Let $f : [a, b] \to \mathbb{R}$ be a twice continuous differentiable function and

$$M = \sup_{x \in [a,b]} |f''(x)|$$

Then

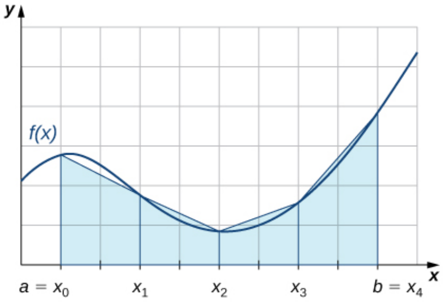
$$|R_{\text{mid}}(f, n) - F| \leq \frac{M(b-a)^3}{24n^2} \sim \mathcal{O}\left(\frac{1}{n^2}\right)$$

Trapezoidal rule

We are interested in computing

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

Trapezoidal rule:



Trapezoidal rule

We are interested in computing

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

Trapezoidal rule:

Let $f : [a, b] \to \mathbb{R}$ be a function defines on a closed interval $[a, b] \subset \mathbb{R}$ and let $\{x_0, ..., x_n\}$ be a partition of $[a, b]$, i.e.,

$$a = x_0 < x_1 < ... < x_n = b.$$

Then

$$T(f, n) = \frac{\Delta x}{2}\left(f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)\right)$$

Trapezoidal rule error

- Let $f : [a, b] \to \mathbb{R}$ be a twice continuous differentiable function and

  $$M = \sup_{x \in [a,b]} |f''(x)|$$

  Then

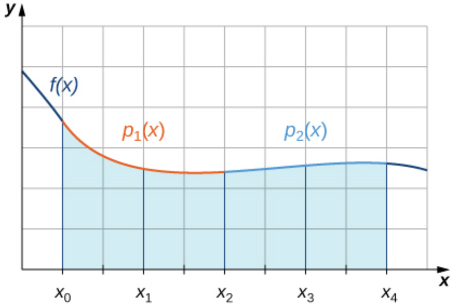
  $$|T(f, n) - F| \leq \frac{M(b-a)^3}{12n^2} \sim \mathcal{O}\left(\frac{1}{n^2}\right)$$

Simpson's rule

We are interested in computing

$$F = \int_a^b f(x)\; dx$$

Simpson's rule:



Simpson's rule

We are interested in computing

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

Simpson's rule:
Let $f : [a, b] \to \mathbb{R}$ be a function defines on a closed interval $[a, b] \subset \mathbb{R}$ and let $\{x_0, ..., x_n\}$ be a partition of $[a, b]$ with n even, i.e.,

$$a = x_0 < x_1 < ... < x_n = b.$$

Then

$$S(f, n) = \frac{\Delta x}{3}\left(f(x_0) + 4\sum_{i=0}^{n/2-1} f(x_{2i+1}) + 2\sum_{i=1}^{n/2-1} f(x_{2i}) + f(x_n)\right)$$

Simpson's rule error

- Let $f : [a, b] \to \mathbb{R}$ be a four-times continuously differentiable function and
$$M = \sup_{x \in [a,b]} |f''(x)|$$
Then
$$|S(f, n) - F| \leq \frac{M(b-a)^5}{180n^4} \sim \mathcal{O}\left(\frac{1}{n^4}\right)$$

Other classical techniques

Gaussian quadrature:

$$F = \sum_{i=1}^{n} w_i f(x_i)$$

- Gauss–Legendre quadrature
- Gauss–Jacobi quadrature
- Chebyshev–Gauss quadrature
- Gauss–Laguerre quadrature
- Gauss–Hermite quadrature

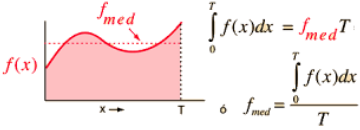
How does randomness come into play?

Monte Carlo Estimator

We are interested in computing

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

Idea:



Monte Carlo Estimator

We are interested in computing

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

Idea:
We approximate F by averaging samples of the function f at uniform random points in $[a, b]$.

Formally: Given N uniform random variables $X_i \sim \mathcal{U}(a, b)$, its PDF is

$$\rho(x) = \frac{1}{b-a} \mathbb{1}_{[a,b]}(x)$$

and define the Monte Carlo estimator as

$$\left\langle F^N \right\rangle = (b-a) \frac{1}{N} \sum_{i=1}^{N} f(X_i)$$

Expectation value and convergence

Note:
The MC estimator is a random variable itself.
What is its expectation value?

Expectation value and convergence

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The MC estimator is a random variable itself.
What is its expectation value?

Expectation value of the MC estimator

$$\mathbb{E}(\langle F^N \rangle) = \mathbb{E}\left((b-a)\frac{1}{N}\sum_{i=1}^{N} f(X_i)\right) = (b-a)\frac{1}{N}\sum_{i=1}^{N}\mathbb{E}\left(f(X_i)\right)$$
$$= (b-a)\frac{1}{N}\sum_{i=1}^{N}\int_{-\infty}^{\infty} f(x)\rho(x)\ dx = \frac{1}{N}\sum_{i=1}^{N}\int_a^b f(x)\ dx$$
$$= \int_a^b f(x)\ dx = F$$

What does $N \to \infty$ mean?

Law of large numbers

Let $X_1, X_2, \ldots$ be an infinite sequence of i.i.d. random variables with

$$\mathbb{E}(X_1) = \mathbb{E}(X_2) = \ldots = \mu$$

and

$$\mathbb{V}(X_1) = \mathbb{V}(X_2) = \ldots = \sigma^2.$$

Then

1. Weak law of large numbers:
   For any $\varepsilon > 0$
   $$\lim_{N\to\infty} \mathbb{P}\left(|\bar{X}_N - \mu| < \varepsilon\right) = 1$$
   (convergence in probability)
2. Strong law of large numbers:
   $$\mathbb{P}\left(\lim_{N\to\infty} \bar{X}_N = \mu\right) = 1$$
   (converges almost surely)

Convergence of Monte-Carlo estimator

The random variables

$$Y_i = (b-a)f(X_i)$$

are i.i.d. with

$$\mathbb{E}(Y_i) = \mathbb{E}((b-a)f(X_i)) = (b-a)\int_{-\infty}^{\infty} f(x)\rho(x)dx = \frac{b-a}{(b-a)}\int_a^b f(x)dx$$
$$= F$$

Strong Law of Large Numbers:

$$\mathbb{P}\left(\lim_{N\to\infty}\langle F^N\rangle = F\right) = \mathbb{P}\left(\lim_{N\to\infty}\frac{1}{N}\sum_{i=1}^{N} Y_i = F\right) = 1$$

The MC estimator converges almost surely to the integral F.

Rate of convergence

How quickly does this estimate converge? → standard deviation

$$\mathbb{V}(\langle F^N \rangle) = \mathbb{V}\left((b-a)\frac{1}{N}\sum_{i=1}^{N} f(X_i)\right) = \frac{(b-a)^2}{N^2}\sum_{i=1}^{N} \underbrace{\mathbb{V}\left(f(X_i)\right)}_{=:s^2}$$

$$= \frac{(b-a)^2 s^2}{N}$$

Hence

$$\sigma = \sqrt{\mathbb{V}(\langle F^N \rangle)} = \frac{(b-a)s}{\sqrt{N}} \sim \mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$$

We must quadruple the number of samples in order to reduce the error by half!

What happens in higher dimensions?