

Monte Carlo Integration

Integrals and Averages

integral of a function
over a domain

$$\int_{\mathbf{x} \in D} f(\mathbf{x}) dA_{\mathbf{x}}$$

“size” of a domain

$$A_D = \int_{\mathbf{x} \in D} dA_{\mathbf{x}}$$

average of a function
over a domain

$$\frac{\int_{\mathbf{x} \in D} f(\mathbf{x}) dA_{\mathbf{x}}}{\int_{\mathbf{x} \in D} dA_{\mathbf{x}}} = \frac{\int_{\mathbf{x} \in D} f(\mathbf{x}) dA_{\mathbf{x}}}{A_D}$$

Integrals and Averages Examples

- average “daily” snowfall in Hanover last year
 - domain: year - time interval (1D)
 - integration variable: “day” of the year
 - function: snowfall of “day”

$$\frac{\int_{\text{day} \in \text{year}} s(\text{day}) d\text{length}(\text{day})}{\text{lenght}(\text{year})}$$

Integrals and Averages Examples

- “today” average snowfall in New Hampshire
 - domain: New Hampshire - surface (2D)
 - integration variable: “location” in New Hampshire
 - function: snowfall of “location”

$$\frac{\int_{\text{location} \in \text{NewHampshire}} s(\text{location}) d\text{area}(\text{location})}{\text{area}(\text{location})}$$

Integrals and Averages Examples

- “today” average snowfall in New Hampshire
 - domain: New Hampshire x year - area x time (3D)
 - integration variables: “location” and “day” in New Hampshire this year
 - function: snowfall of “location” and “day”

$$\frac{\int_{\text{day} \in \text{year}} \int_{\text{loc} \in \text{New Hampshire}} s(\text{loc}, \text{day}) d\text{area}(\text{loc}) d\text{length}(\text{day})}{\text{area}(\text{loc}) \text{length}(\text{day})}$$

Discreet Random Variable

- random variable: x
- values: x_0, x_1, \dots, x_n
- probabilities: p_0, p_1, \dots, p_n $\sum_{j=1}^n p_j = 1$
- example: tossing a die
 - values: $x_1 = 1, x_2 = 2, x_3 = 3, x_4 = 4, x_5 = 5, x_6 = 6$
 - probabilities: $p_1 = 1/6, p_2 = 1/6, p_3 = 1/6, p_4 = 1/6, p_5 = 1/6, p_6 = 1/6$

Expected Value and Variance

- expected value: $E[x] = \sum_{j=1}^n v_j p_j$
 - average value of the variable
- variance: $\sigma^2[x] = E[(x - E[x])^2]$
 - how much different from the average
 - property: $\sigma^2[x] = E[x^2] - E[x]^2$
- example: tossing a die
 - expected value: $E[x] = (1 + 2 + 3 + 4 + 5 + 6) / 6 = 3.5$
 - variance: $\sigma^2[x] = \dots = 0.916$

Estimating Expected Values

- to estimate the expected value of a variable
 - choose a set of random *values* based on the prob.
 - average their results
- $$E[x] \approx \frac{1}{N} \sum_{i=1}^N x_i$$
- larger N give better estimate
 - example: rolling a die
 - roll 3 times:
 - roll 9 times: $\{3,1,6\} \rightarrow E[x] \approx (3+1+6)/3 = 3.33$
 $\{3,1,6,2,5,3,4,6,2\} \rightarrow E[x] \approx 3.51$

Law of Large Numbers

- by taking *infinitely* many samples, the error between the estimate and the expected value is *statistically zero*
 - the estimate will converge to the right value

$$\text{probability} \left[E[x] = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1}^N x_i \right] = 1$$

Continuous Random Variable

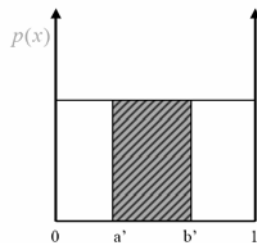
- random variable: x
- values: $x \in [a, b]$
- probability density function: $x \sim p$
 - property: $\int_a^b p(x) dx = 1$
- probability that var. has value x : $p(x) dx$

Uniformly Distributed Random Variable

- p is the same everywhere in the interval

$$p(x) = \text{const} \quad \text{and} \quad \int_a^b p(x) dx = 1 \quad \text{implies}$$

$$p(x) = 1/(b-a)$$



[Bala]

Expected Value and Variance

- expected value: $E[x] = \int_a^b xp(x) dx$
 $E[g(x)] = \int_a^b g(x)p(x) dx$
- variance: $\sigma^2[x] = \int_a^b (x - E[x])^2 p(x) dx$
 $\sigma^2[g(x)] = \int_a^b (g(x) - E[g(x)])^2 p(x) dx$
- estimating expected values: $E[g(x)] \approx \frac{1}{N} \sum_{i=1}^N g(x_i)$

Multidimensional Random Variables

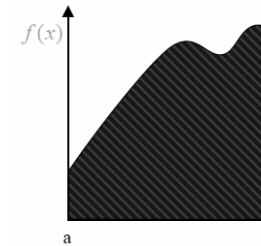
- everything works fine in multiple dimensions
 - but it is often hard to precisely define domain
 - except in simple cases

$$E[g(\mathbf{x})] = \int_{\mathbf{x} \in D} g(\mathbf{x}) p(\mathbf{x}) dA_{\mathbf{x}}$$

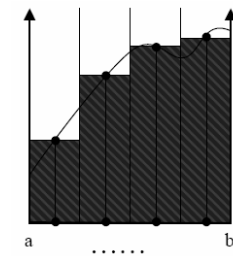
Deterministic Numerical Integration

- split domain in set of fixed segments
- sum function values times size of segments

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



$$I \approx \sum_j f(x_j) \Delta x$$



[Bala]

Monte Carlo Numerical Integration

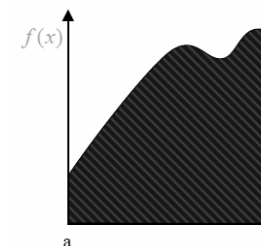
- need to evaluate $I = \int_a^b f(x) dx$
- by definition $E[g(x)] = \int_a^b g(x) p(x) dx$
- can be estimated as $E[g(x)] \approx \frac{1}{N} \sum_{i=1}^N g(x_i)$
- by substituting $g(x) = f(x) / p(x)$

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

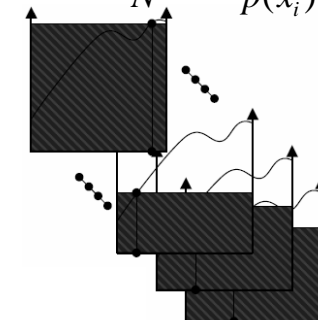
Monte Carlo Numerical Integration

- intuition: compute the area randomly and average the results

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



$$I \approx \frac{1}{N} \sum_{i=1}^N \frac{f(x_i)}{p(x_i)}$$



[Bala]

Monte Carlo Numerical Integration

- formally, we can prove that

$$\bar{I} = \frac{1}{N} \sum_{i=1}^N \frac{f(x_i)}{p(x_i)} \Rightarrow E[\bar{I}] = E[g(x)]$$

- meaning that if we were to try multiple times to evaluate the integral using our new procedure, we would get, on average, the same result
- variance of the estimate: $\sigma^2[\bar{I}] = \frac{1}{N} \sigma^2[g(x)]$

Example: Integral of Constant Function

- analytic integration

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

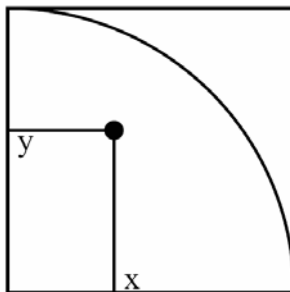
- Monte Carlo integration

$$\begin{aligned} I &= \int_a^b f(x) dx = \int_a^b k dx \approx \\ &\approx \frac{1}{N} \sum_{i=1}^N \frac{f(x_i)}{p(x_i)} = \frac{1}{N} \sum_{i=1}^N k(b-a) = \\ &= \frac{N}{N} k(b-a) = k(b-a) \end{aligned}$$

Example: Computing Pi

- take the square $[0,1]^2$, with a quarter-circle in it

$$A_{circle} = \int_0^1 \int_0^1 f(x,y) dx dy \quad f(x,y) = \begin{cases} 1 & (x,y) \in circle \\ 0 & otherwise \end{cases}$$

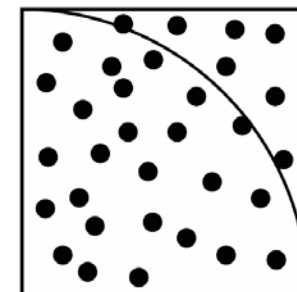


[MIT OpenCourseWare]

Example: Computing Pi

- estimate area of circle by tossing point in the plane and evaluating f

$$A_{circle} \approx \frac{1}{N} \sum_{i=1}^N f(x_i, y_i)$$



[MIT OpenCourseWare]

Example: Computing Pi

- by definition $A_{circle} = \pi / 4$

- numerical estimation of pi

$$\pi \approx \frac{4}{N} \sum_{i=1}^N f(x_i, y_i)$$

Monte Carlo Numerical Integration

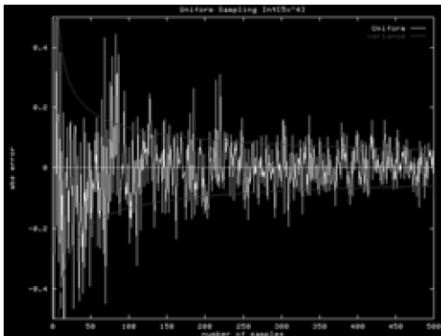
- works in any dimension!
 - need to carefully pick the points
 - need to properly define the pdf
 - hard for complex domain shapes
 - e.g. how to uniformly sample a sphere?

$$I = \int_{\mathbf{x} \in D} f(\mathbf{x}) dA_{\mathbf{x}} \approx \frac{1}{N} \sum_{i=1}^N \frac{f(\mathbf{x}_i)}{p(\mathbf{x}_i)}$$

- works for badly-behaving functions!

Monte Carlo Numerical Integration

- expected value of the error is $O(1/\sqrt{N})$
 - convergence does not depend on dimensionality
 - deterministic integration is hard in high dimensions



[Bala]

Importance Sampling Principle

- how to minimize the noise?
- pick samples in area where function is large

$$I \approx \frac{1}{N} \sum_{i=1}^N \frac{f(\mathbf{x}_i)}{p(\mathbf{x}_i)}$$

- pick a distribution similar to the function

$$p_{\text{optimal}} \propto f(\mathbf{x})$$

1D Interval - Uniform Sampling

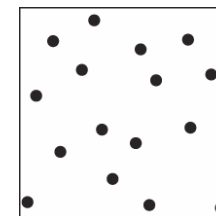
- call random function in $[0,1)$, rescale if necessary
 - in reality only pseudorandom
 - relies on good generator

$$r = \text{rand}() \Rightarrow x = r$$

2D Square - Uniform Sampling

- pick two *independent* random values in $[0,1)$

$$\mathbf{r} = [\text{rand}() \text{ rand}()]^T \Rightarrow \mathbf{x} = \mathbf{r}$$

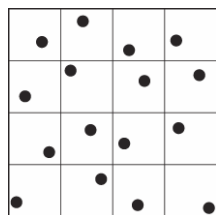


[Shirley]

2D Square - Stratified Sampling

- divide domain in smaller domains, then pick random points in each
 - better variance than normal sampling

$$\mathbf{x} = \left[\begin{array}{cc} \frac{i + r_x}{n_i} & \frac{j + r_y}{n_j} \end{array} \right]^T$$

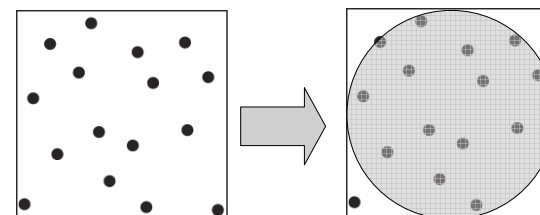


[Shirley]

2D Circle - Rejection Sampling

- pick random points in the uniform square and discard the ones outside the domain

$$\begin{cases} \mathbf{r} \in [0,1]^2 \\ \mathbf{r} \sim 1 \end{cases} \Rightarrow \mathbf{x} = \begin{cases} 2\mathbf{r} - 1 & |2\mathbf{r} - 1| \leq 1 \\ \text{discard} & \text{otherwise} \end{cases}$$

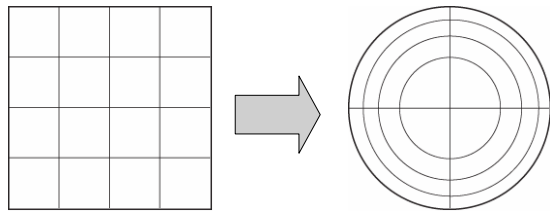


[Shirley]

2D Circle - Remapping from Square

- pick random points in the uniform square and remap them on the circle using polar coords.

$$\begin{cases} \mathbf{r} \in [0,1]^2 \\ \mathbf{r} \sim 1 \end{cases} \Rightarrow \begin{cases} \varphi = 2\pi r_x \\ r = r_y \end{cases} \Rightarrow \begin{cases} \mathbf{x} = (r_y \cos(2\pi r_x), r_y \sin(2\pi r_x)) \\ \mathbf{x} \sim \text{non uniform} \end{cases}$$

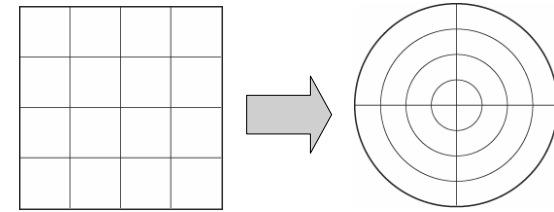


[Shirley]

2D Circle - Remapping from Square

- make sampling uniform by computing proper pdf
 - Sh. 14.4.1

$$\begin{cases} \mathbf{r} \in [0,1]^2 \\ \mathbf{r} \sim 1 \end{cases} \Rightarrow \begin{cases} \varphi = 2\pi r_x \\ r = \sqrt{r_y} \end{cases} \Rightarrow \begin{cases} \mathbf{x} = (\sqrt{r_y} \cos(2\pi r_x), \sqrt{r_y} \sin(2\pi r_x)) \\ \mathbf{x} \sim 1/\pi \end{cases}$$



[Shirley]

3D Direction - Uniform Distribution

- uniformly distribution with respect to solid angle

$$\begin{cases} \mathbf{r} \in [0,1]^2 \\ \mathbf{r} \sim 1 \end{cases} \Rightarrow \begin{cases} \varphi = 2\pi r_x \\ \theta = \arccos(r_y) \end{cases} \Rightarrow \begin{cases} \mathbf{d} = (\sqrt{1-r_y^2} \cos(2\pi r_x), \sqrt{1-r_y^2} \sin(2\pi r_x), r_y) \\ \mathbf{d} \sim \frac{1}{2\pi} \end{cases}$$

3D Direction - Cosine Distribution

- cosine distribution with respect to solid angle

$$\begin{cases} \mathbf{r} \in [0,1]^2 \\ \mathbf{r} \sim 1 \end{cases} \Rightarrow \begin{cases} \varphi = 2\pi r_x \\ \theta = \arccos(\sqrt{r_y}) \end{cases} \Rightarrow \begin{cases} \mathbf{d} = (\sqrt{1-r_y} \cos(2\pi r_x), \sqrt{1-r_y} \sin(2\pi r_x), \sqrt{r_y}) \\ \mathbf{d} \sim \frac{\cos(\theta)}{\pi} \end{cases}$$

3D Direction - Cosine Power Distribution

- cosine power distribution wrt solid angle

$$\begin{cases} \mathbf{r} \in [0,1]^2 \\ \mathbf{r} \sim 1 \end{cases} \Rightarrow \begin{cases} \varphi = 2\pi r_x \\ \theta = \arccos(r_y^{1/(n+1)}) \end{cases} \Rightarrow$$
$$\Rightarrow \begin{cases} \mathbf{d} = \left(\sqrt{1 - r_y^{\frac{2}{n+1}}} \cos(2\pi r_x), \sqrt{1 - r_y^{\frac{2}{n+1}}} \sin(2\pi r_x), r_y^{\frac{1}{n+1}} \right) \\ \mathbf{d} \sim \frac{n+1}{2\pi} \cos^n(\theta) \end{cases}$$