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"

$$\frac{\int_{day \in year} s(day) dlength(day)}{length(year)}$$

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"

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

integrals and averages examples

- average snowfall in New Hampshire per day this year
  - domain: New Hampshire $\times$ year - area $\times$ time (3D)
  - integration variables: "location" and "day" in New Hampshire this year
  - function: snowfall of "location" and "day"

$$\frac{\int_{day \in year} \int_{loc \in N.H.} s(loc, day) darea(loc) dlength(day)}{area(loc) length(day)}$$

discreet random variable

- random variable: x
- values: $x_0, x_1, \ldots, x_n$
- probabilities: $p_0, p_1, \ldots, p_n$ $\sum_{j=1}^{n} p_j = 1$
- example: rolling a die
  - values:

    $x_1 = 1, x_2 = 2, x_3 = 3, x_4 = 4, x_5 = 5, x_6 = 6$
  - probabilities:

    $p_1 = \frac{1}{6}, p_2 = \frac{1}{6}, p_3 = \frac{1}{6}, p_4 = \frac{1}{6}, p_5 = \frac{1}{6}, p_6 = \frac{1}{6}$

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: rolling a die
    - expected value:

      $E[x] = (1 + 2 + 3 + 4 + 5 + 6)/6 = 3.5$
    - variance: $\sigma^2[x] = \ldots = 2.917$

estimating expected values

- to estimate the expected value of a variable
  - choose a set of random *values* based on the probability
  - 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: $\{3, 1, 6\} \to E[x] \approx (3 + 1 + 6)/3 = 3.33$
  - roll 9 times: $\{3, 1, 6, 2, 5, 3, 4, 6, 2\} \to E[x] \approx 3.51$

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

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

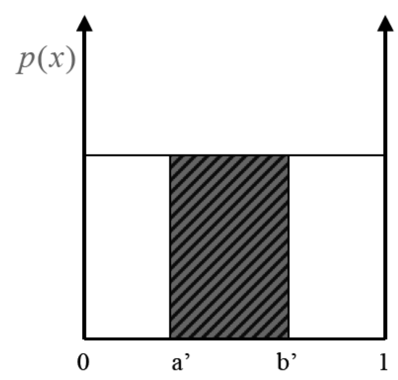
continuous random variable

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

uniformly distributed random variable

- p is the same everywhere in the interval
  - $p(x) = \text{const}$ and $\int_a^b p(x)dx = 1$ implies

$$p(x) = \frac{1}{b - a}$$



[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

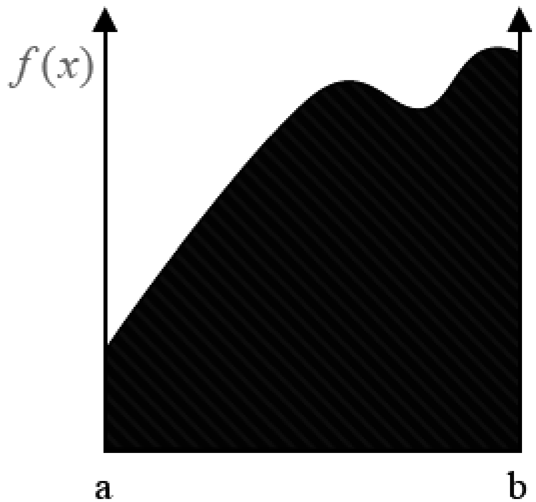
- everything works fine in multiple dimensions
  - but it is often hard to precisely define domain
    - except in simple cases

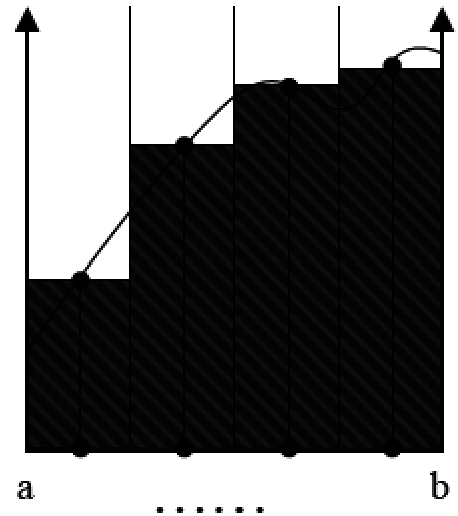
$$E[g(\mathbf{x})] = \int_{\mathbf{x} \in D} g(\mathbf{x}) p(\mathbf{x}) dA_{\mathbf{x}}$$

deterministic numerical integration

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

$$I = \int_a^b f(x)dx \qquad I \approx \sum_j f(x_j)\Delta x$$





[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 substitution: $g(x) = f(x)/p(x)$

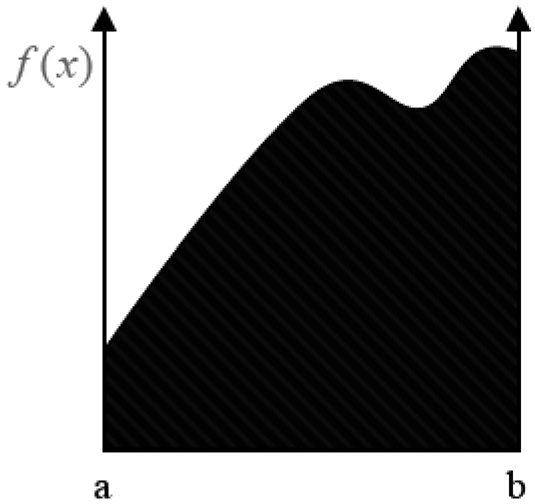
$$I = \int_a^b \frac{f(x)}{p(x)} p(x)dx \approx \frac{1}{N}\sum_{i=1}^{N} \frac{f(x_i)}{p(x_i)}$$

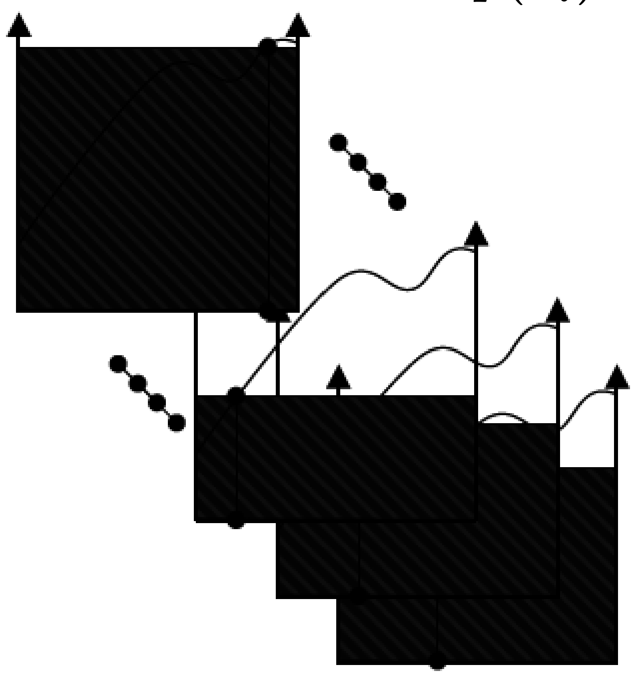
monte carlo numerical integration

- intuition: compute the area randomly and average the results

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

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





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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

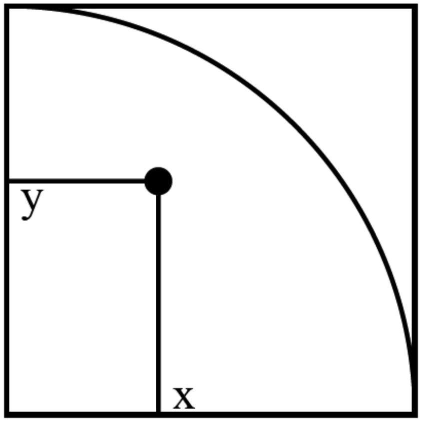
$$I = \int_a^b f(x)dx = \int_a^b k dx = k(b-a)$$

- 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 π

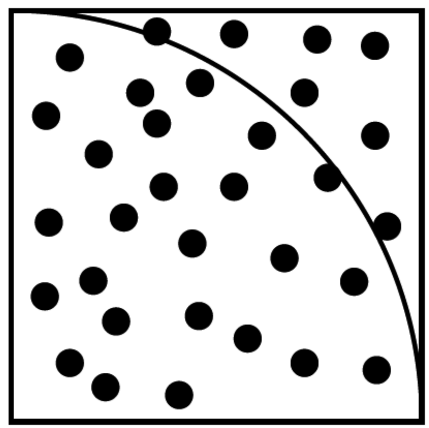
- take the square $[0,1]^2$ with a quarter-circle in it
  - $A_{qcircle} = \int_0^1 \int_0^1 f(x,y) dx dy$
  - $f(x,y) = \begin{cases} 1 & (x,y) \in qcircle \\ 0 & \text{otherwise} \end{cases}$



[MIT OpenCourseware]

example: computing π

- estimating area of quarter-circle by tossing point in the plane and evaluating f
  - $A_{qcircle} \approx \frac{1}{N} \sum_{i=1}^{N} f(x_i, y_i)$



[MIT OpenCourseWare]

example: computing π

- by definition: $A_{qcircle} = \pi/4$
- numerical estimation of π

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

monte carlo numerical integration

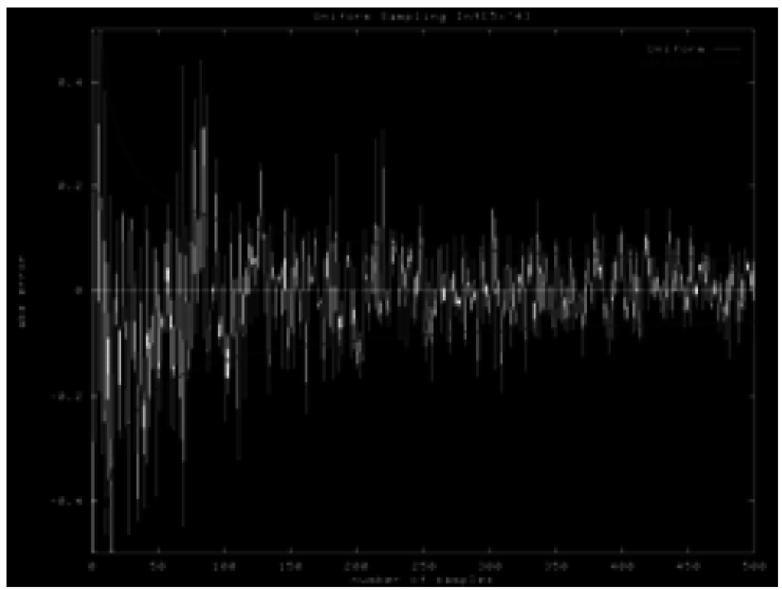
- works in any dimension!
  - need to carefully pick the points
  - need to properly define the pdf
    - hard for complex domain shapes
    - e.g., how to uniformly sample a sphere?

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

- works for badly-behaving functions!

monte carlo numerical integration

- expected value of te 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

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

1d interval - uniform sampling

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

$$r = rand() \Rightarrow x = r$$

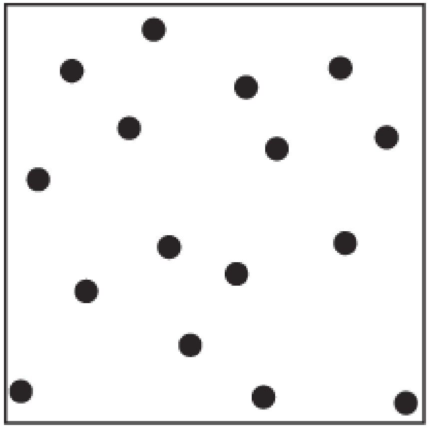
- pick a distribution similar to the function

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

2d square - uniform sampling

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

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

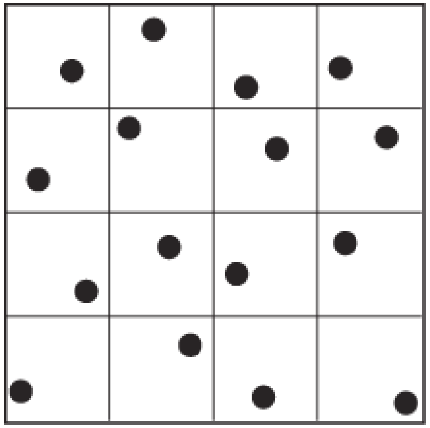


[Shirley]

2d square - stratified sampling

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

$$\mathbf{x} = \begin{bmatrix} \frac{i + r_x}{n_i} & \frac{j + r_y}{n_j} \end{bmatrix}^T$$

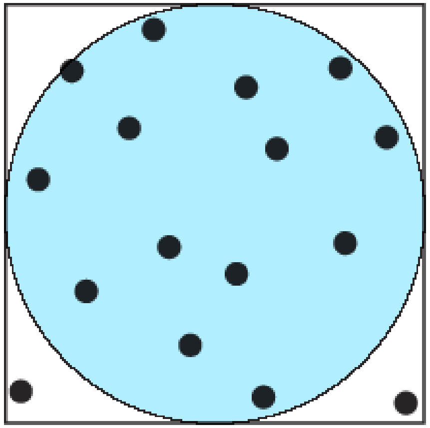


[Shirley]

2d circle - rejection sampling

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

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



[Shirley]

2d circle - remapping from square

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

$$\mathbf{r} \in [0,1]^2,\ \mathbf{r} \sim 1$$

$$\varphi = 2\pi r_x,\ r = r_y$$

$$\mathbf{x} = \left(r_y \cos(2\pi r_x), r_y \sin(2\pi r_x)\right)$$

$$\mathbf{x} \sim \text{non-uniform}$$

2d circle - remapping from square

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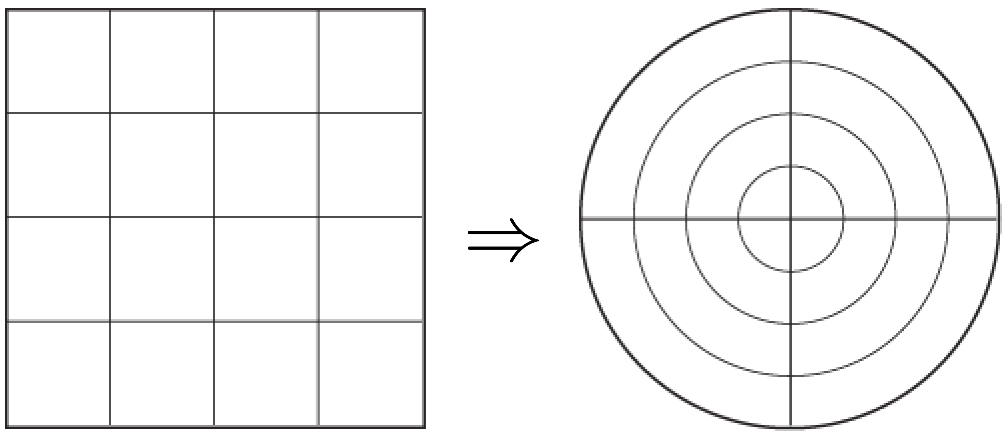
$$\mathbf{x} \sim \text{non-uniform}$$



[Shirley]

2d circle - remapping from square

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

$$\mathbf{r} \in [0,1]^2,\ \mathbf{r} \sim 1$$

$$\varphi = 2\pi r_x,\ r = \sqrt{r_y}$$

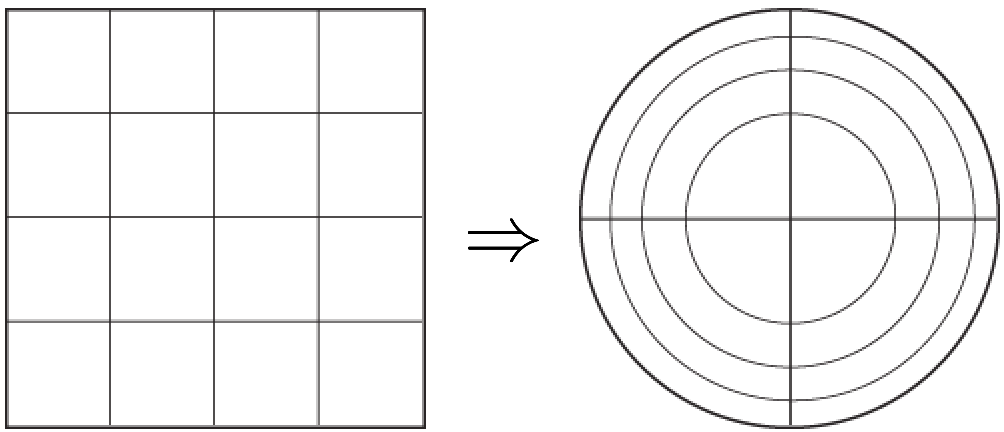
$$\mathbf{x} = \left(\sqrt{r_y}\cos(2\pi r_x), \sqrt{r_y}\sin(2\pi r_x)\right)$$

$$\mathbf{x} \sim 1/\pi$$

2d circle - remapping from square

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

$$\mathbf{x} \sim 1/\pi$$



[Shirley]

3d direction - uniform distribution

- uniform distribution with respect to solid angle

$$\mathbf{r} \in [0,1]^2,\ \mathbf{r} \sim 1$$

$$\varphi = 2\pi r_x,\ \theta = \arccos(r_y)$$

$$\mathbf{d} = \left(\sqrt{1-r_y^2}\cos(2\pi r_x), \sqrt{1-r_y^2}\sin(2\pi r_x), r_y\right)$$

$$\mathbf{d} \sim \frac{1}{2\pi}$$

3d direction - cosine distribution

- cosine distribution wrt solid angle

$$\mathbf{r} \in [0,1]^2,\ \mathbf{r} \sim 1$$

$$\varphi = 2\pi r_x,\ \theta = \arccos(\sqrt{r_y})$$

$$\mathbf{d} = \left(\sqrt{1-r_y}\cos(2\pi r_x), \sqrt{1-r_y}\sin(2\pi r_x), \sqrt{r_y}\right)$$

$$\mathbf{d} \sim \frac{\cos(\theta)}{\pi}$$

3d direction - cosine power distribution

- cosine power distribution wrt solid angle

$$r \in [0,1]^2,\ r \sim 1$$

$$\varphi = 2\pi r_x,\ \theta = \arccos\left(r_y^{1/(n+1)}\right)$$

$$\mathbf{d} = \left(\sqrt{1 - r_y^{\frac{2}{n+1}}}\cos(2\pi r_x), \sqrt{1 - r_y^{\frac{2}{n+1}}}\sin(2\pi r_x), r_y^{\frac{1}{n+1}}\right)$$

$$\mathbf{d} \sim \frac{n+1}{2\pi}\cos^n(\theta)$$