Numerical Methods I
Monte Carlo Methods

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Outline

Logistics for Presentations

- This is the last lecture: Dec. 16th is reserved for final presentations and course evaluation forms.
- **We will start at 5pm sharp on Dec. 16th**
- Everyone should attend Dec. 16th as if a regular lecture.
- Each presentation is only 15 minutes including questions: I will strictly enforce this!
- People presenting on the 16th (in alphabetical order): Cohen N., Delong S., Guo S., Li X., Liu Y., Lopes D., Lu. L, Ye. S.
- **Email me PDF/PowerPoint of your presentation at least 1h before the scheduled talk time.**
- If you need to use your own laptop, explain why and still send me the file.

What is Monte Carlo?

- Monte Carlo is any numerical algorithm that uses random numbers to compute a deterministic (non-random) answer: **stochastic** or **randomized algorithm**.
- An important example is **numerical integration in higher dimensions**:

$$J = \int_{\Omega \subseteq \mathbb{R}^n} f(\mathbf{x})\, d\mathbf{x}$$

- Recall that using a **deterministic method** is very accurate and fast for low dimensions.
- But for large dimensions we have to deal with the **curse of dimensionality**:
  The number of quadrature nodes scales like at least 2^n (exponentially). E.g., $2^{20} = 10^6$, but $2^{40} = 10^{12}$!

Probability Theory

- First define a set Ω of possible **outcomes** $\omega \in \Omega$ of an "experiment":
  - A coin toss can end in heads or tails, so two outcomes.
  - A sequence of four coin tosses can end in one of $4^2 = 16$ outcomes, e.g., HHTT or THTH.
- The set Ω can be finite (heads or tails), countably infinite (the number of atoms inside a box), or uncountable (the weight of a person).
- An **event** $A \subseteq \Omega$ is a **set of possible outcomes**: e.g., more tails then heads occur in a sequence of four coin tosses,

$$A = \{HHHH, THHH, HTHH, HHTH, HHHT\}.$$

- Each event has an associated **probability**

$$0 \leq P(A) \leq 1,$$

with $P(\Omega) = 1$ and $P(\emptyset) = 0$.

Conditional Probability

- A basic axiom is that probability is **additive** for disjoint events:

$$P(A \cup B) = P(A \text{ or } B) = P(A) + P(B) \text{ if } A \cap B = \emptyset$$

- Bayes formula gives the **conditional probability** that an outcome belongs to set B if it belongs to set C:

$$P(B|C) = \frac{P(B \cap C)}{P(C)} = \frac{P(B \text{ and } C)}{P(C)}$$

- Two events are said to be **independent** if their probabilities are multiplicative:

$$P(A \cap B) = P(A \text{ and } B) = P(A)\,P(B)$$

- When the set of all outcomes is countable, we can associate with each event a probability, and then

$$P(A) = \sum_{\omega_i \in A} P(\omega_i).$$

Probability Distribution

- If Ω is uncountable, think of outcomes as **random variables**, that is, variables whose value is determined by a random outcome:

$$X = X(\omega) \in \mathbb{R}.$$

- The **probability density function** $f(x) \geq 0$ determines the probability for the outcome to be close to x, in one dimension

$$P(x \leq X \leq x + dx) = f(x)dx,$$

$$P(A) = P(X \in A) = \int_{x \in A} f(x)dx$$

- The concept of a **measure** and the **Lebesque integral** makes this all rigorous and axiomatic, for our purposes the traditional Riemann integral will suffice.

Mean and Variance

- We call the **probability density** or the **probability measure** the **law** or the **distribution** of a random variable X, and write:

$$X \sim f.$$

- The **cummulative distribution function** is

$$F(x) = P(X \leq x) = \int_{-\infty}^{x} f(x')dx',$$

and we will assume that this function is continuous.

- The **mean** or **expectation value** of a random variable X is

$$\mu = \bar{X} = E[X] = \int_{-\infty}^{\infty} xf(x)dx.$$

- The **variance** σ^2 and the **standard deviation** σ measure the **uncertainty** in a random variable

$$\sigma^2 = \text{var}(X) = E[(X-\mu)^2] = \int_{-\infty}^{\infty} (x-\mu)^2 f(x)dx.$$

Multiple Random Variables

- Consider a set of two random variables $Z=(X,Y)$ and the **joint probability distribution** $Z \sim f(x,y)$.
- The **marginal density** for X is the distribution of just X, without regard to Y:

$$g(x)=\int_y f(x,y)dy, \text{ similarly } h(y)=\int_x f(x,y)dx$$

- The **conditional probability distribution** is the distribution of X for a known Y:

$$f(x|y)=\frac{f(x,y)}{h(y)}$$

- Two random variables X and Y are **independent** if

$$f(x,y)=g(x)h(y) \quad \Rightarrow f(x|y)=g(x).$$

Covariance

- The term **i.i.d.**$\equiv$**independent identically-distributed** random variables is used to describe independent **samples** $X_k \sim f,\ k = 1, \ldots$.
- The generalization of variance for two variables is the **covariance**:

$$C_{XY} = \text{cov}(X, Y) = E\left[\left(X - \bar{X}\right)\left(Y - \bar{Y}\right)\right] = E\left(XY\right) - E(X)E(Y).$$

- For independent variables

$$E\left(XY\right) = \int xy\, f(x, y) dxdy = \int xg(x)dx \int yh(y)dy = E(X)E(Y)$$

  and so $C_{XY} = 0$.
- Define the **correlation coefficient** between X and Y as a measure of how correlated two variables are:

$$r_{XY} = \frac{\text{cov}(X, Y)}{\sqrt{\text{var}(X)\text{var}(Y)}} = \frac{C_{XY}}{\sigma_X \sigma_Y}.$$

Law of Large Numbers

- The average of N i.i.d. samples of a random variable $X \sim f$ is itself a random variable:

$$A = \frac{1}{N}\sum_{k=1}^{N} X_k.$$

- A is an **unbiased estimator** of the mean of X, $E(A) = \bar{X}$.
- Numerically we often use a **biased estimate** of the variance:

$$\sigma_X^2 = \lim_{N\to\infty} \frac{1}{N}\sum_{k=1}^{N}\left(X_k - \bar{X}\right)^2 \approx \frac{1}{N}\sum_{k=1}^{N}\left(X_k - A\right)^2.$$

- The weak **law of large numbers** states that the estimator is also **consistent**:

$$\lim_{N\to\infty} A = \bar{X} = E(X) \text{ (almost surely).}$$

Central Limit Theorem

- The central value theorem says that if σ_X is finite, in the limit $N \to \infty$ the random variable A is **normally-distributed**:

$$A \sim f(a) = \left(2\pi\sigma_A^2\right)^{-1/2} \exp\left[-\frac{(a-\bar{X})^2}{2\sigma_A^2}\right]$$

- The **error of the estimator** A decreases as N^{-1}, more specifically,

$$E\left[\left(A-\bar{X}\right)^2\right] = E\left\{\left[\frac{1}{N}\sum_{k=1}^{N}\left(X_k-\bar{X}\right)\right]^2\right\} = \frac{1}{N^2}E\left[\sum_{k=1}^{N}\left(X_k-\bar{X}\right)^2\right]$$

$$\text{var}(A) = \sigma_A^2 = \frac{\sigma_X^2}{N}.$$

- The slow convergence of the error, $\sigma \sim N^{-1/2}$, is a fundamental characteristic of Monte Carlo.

Monte Carlo on a Computer

- In order to compute integrals using Monte Carlo on a computer, we need to be able to generate samples from a distribution, e.g., uniformly distributed inside an interval $I = [a, b]$.
- Almost all randomized software is based on having a **pseudo-random number generator** (PRNG), which is a routine that returns a pseudo-random number $0 \leq u \leq 1$ from the **standard uniform distribution:**

$$f(u) = \begin{cases} 1 & \textbf{if } 0 \leq u \leq 1 \\ 0 & \textbf{otherwise} \end{cases}$$

- Since computers (Turing machines) are deterministic, it is not possible to generate truly random samples (outcomes): Pseudo-random means **as close to random as we can get it**.
- There are well-known good PRNGs that are also efficient: One should **use other-people's PRNGs**, e.g., the **Marsenne Twister**.

PRNGs

- The PRNG is a procedure (function) that takes a collection of m integers called the **state of the generator** $\mathbf{s} = \{i_1, \ldots, i_m\}$, and updates it:
$$\mathbf{s} \leftarrow \Phi(\mathbf{s}),$$
and produces (returns) a number $u = \Psi(\mathbf{s})$ that is a pseudo-random sample from the standard uniform distribution.
- So in pseudo-MATLAB notation, $[u, \mathbf{s}] = rng(\mathbf{s})$, often called a **random stream**.
- Simple built-in generator such as the MATLAB/C function *rand* or the Fortran function *RANDOM_NUMBER* hide the state from the user (but the state is stored somewhere in some global variable).
- All PRNGs provide a routine to **seed the generator**, that is, to set the seed $\mathbf{s}$ to some particular value.
This way one can generate the same sequence of "random" numbers over and over again (e.g., when debugging a program).

Generating Non-Uniform Variates

- Using a uniform (pseudo-)random number generator (**URNG**), it is easy to generate an outcome drawn uniformly in $I = [a, b]$:

$$X = a + (b - a)U,$$

  where $U = rng()$ is a standard uniform variate.
- We often need to generate **(pseudo)random samples** or **variates** drawn from a distribution other than a uniform distribution.
- Almost all **non-uniform samplers are based on a URNG**.
- Sometimes it may be more efficient to replace the URNG with a **random bitstream**, that is, a sequence of random bits, if only a few random bits are needed (e.g., for discrete variables).
- We need a method to convert a uniform variate into a non-uniform variate.

Generating Non-Uniform Variates

- Task: We want to sample a random number with **probability distribution** $f(x)$. For now assume $f(x)$ is a **probability density**:

$$P(x \le X \le x + dx) = f(x)dx,$$

- Tool: We can generate samples from some special distributions, e.g., a sample U from the standard uniform distribution.
- Consider applying a non-linear **differentiable one-to-one** function $g(x)$ to U:

$$X \equiv X(U) = g(U) \quad \Rightarrow \quad dx = g'(U)du$$

- We can find the probability density of X by using the informal differential notation

$$P(u \le U \le u + du) = du = \frac{dx}{g'(u)} = P(x \le X \le x + dx) = f(x)dx$$

$$f[x(u)] = \left[g'(u)\right]^{-1}$$

Inverting the CDF

$$f\left[x(u)\right] = \left[g'(u)\right]^{-1}$$

- Can we find $g(u)$ given the target $f(x)$? It is simpler to see this if we invert $x(u)$:

$$u = F(x).$$

- Repeating the same calculation

$$P\left(u \leq U \leq u + dx\right) = du = F'(x)dx = f(x)dx$$

$$F'(x) = f(x)$$

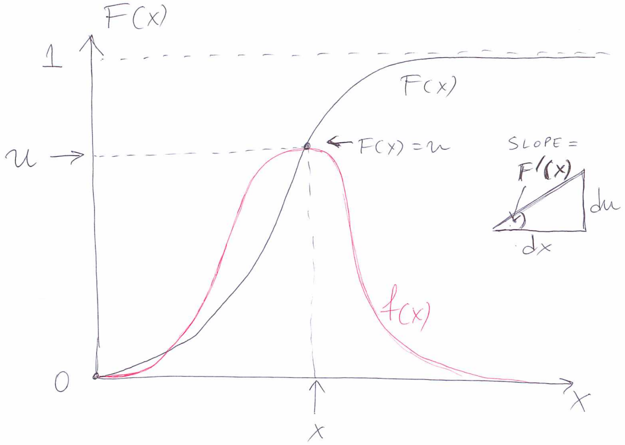
- This shows that $F(x)$ is the **cummulative probability distribution**:

$$F(x) = P(X \leq x) = \int_{-\infty}^{x} f(x')dx'.$$

- Note that $F(x)$ is monotonically non-decreasing because $f(x) \geq 0$. Still it is not always easy to invert the CDF efficiently.

Sampling by Inversion

Generate a standard uniform variate u and then solve the **non-linear equation** $F(x) = u$. If $F(x)$ has finite jumps just think of u as the independent variable instead of x.



Exponentially-Distributed Number

- As an example, consider generating a sample from the **exponential distribution with rate** λ:

$$f_\lambda(t) = \begin{cases} \lambda e^{-\lambda t} & \text{if } t \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

- Related to the **Poisson process** of events whose rate of occurence is λ and whose occurence does not depend on the past (history):

$$P(t \leq T \leq t + dt \mid T \geq t) = P(T < dt) = \lambda dt.$$

- Using the **inversion technique** we get

$$F(t) = P(T \leq t) = \int_{t'=0}^{t} \lambda e^{-\lambda t} dt = 1 - e^{-\lambda t} = u' \equiv 1 - u$$

$$T = -\lambda^{-1} \ln(U),$$

where numerical care must be taken to ensure the log does not overflow or underflow.

Rejection Sampling

- An alternative method is to use **rejection sampling**:
  Generate a sample X from some other distribution $g(x)$ and accept them with **acceptance probability** $p(X)$, otherwise **reject** and try again.
- The rejection requires sampling a standard uniform variate U:
  Accept if $U \leq p(X)$, reject otherwise.
- It is easy to see that

$$f(x) \sim g(x)p(x) \quad \Rightarrow p(x) = Z\frac{f(x)}{g(x)},$$

where Z is determined from the **normalization condition**:

$$\int f(x)dx = 1 \quad \Rightarrow \quad \int p(x)g(x) = Z$$

Envelope Function

$$p(x) = \frac{f(x)}{Z^{-1}g(x)} = \frac{f(x)}{\tilde{g}(x)}$$

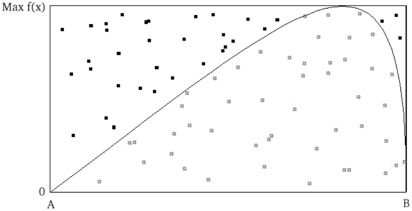
- Since $0 \leq p(x) \leq 1$, we see that $\tilde{g}(x) = Z^{-1}g(x)$ must be a **bounding** or **envelope** function:

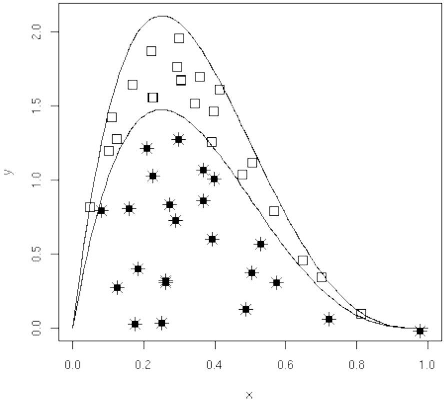
$$\tilde{g}(x) \geq f(x), \text{ for example, } \tilde{g}(x) = \max f(x) = \text{const.}$$

- Rejection sampling is very simple:
  Generate a sample X from $g(x)$ and a standard uniform variate U and accept X if $U\tilde{g}(x) \leq f(x)$, reject otherwise and try again.
- For efficiency, we want to have the **highest possible acceptance probability**, that is

$$P_{acc} = \frac{\int f(x)dx}{\int \tilde{g}(x)dx} = Z\frac{\int f(x)dx}{\int g(x)dx} = Z.$$

Rejection Sampling Illustrated





Normally-Distributed Numbers

- The **standard normal distribution** is a Gaussian "bell-curve":

$$f(x) = \left(2\pi\sigma^2\right)^{-1/2} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right),$$

where μ is the **mean** and σ is the **standard deviation**.

- The **standard normal distribution** has $\sigma = 1$ and $\mu = 0$.
- If we have a sample X_s from the standard distribution we can generate a sample X from $f(x)$ using:

$$X = \mu + \sigma X_s$$

- Consider sampling the positive half of the standard normal, that is, sampling:

$$f(x) = \sqrt{\frac{2}{\pi}} e^{-x^2/2} \text{ for } x \geq 0$$

Optimizing Rejection Sampling

- We want the **tighest possible** (especially where $f(x)$ is large) **easy-to-sample** $g(x) \approx f(x)$.
- We already know how to sample an exponential:

$$g(x) = e^{-x}$$

- We want the tightest possible $\tilde{g}(x)$:

$$\min\left[\tilde{g}(x) - f(x)\right] = \min\left[Z^{-1}e^{-x} - \sqrt{\frac{2}{\pi}}e^{-x^2/2}\right] = 0$$

$$\tilde{g}'(x^{\star}) = f'(x^{\star}) \text{ and } \tilde{g}(x^{\star}) = f(x^{\star})$$

- Solving this system of two equations gives $x^{\star} = 1$ and

$$Z = P_{acc} = \sqrt{\frac{\pi}{2}}e^{-1/2} \approx 76\%$$

Histogram Validation

- We need some way to test that a sampler is correct, that is, that the generated sequence of random numbers really comes from the specified distribution $f(x)$. One easy way to do that is by computing the **histogram** of the samples.
- Count how many N_x samples of the N samples are inside a **bin of width** h centered at x:

$$f(x) \approx P_x = \frac{1}{h} P(x - h/2 \leq X \leq x + h/2) \approx \frac{1}{h} \frac{N_x}{N}.$$

- If we make the bins smaller, the **truncation error** will be reduced:

$$P_x - f(x) = \frac{1}{h} \int_{x-h/2}^{x+h/2} f(x') dx' - f(x) = \alpha h^2 + O(h^4)$$

- But, this means there will be fewer points per bin, i.e., **statistical errors** will grow. As usual, we want to find the optimal tradeoff between the the two types of error.

Statistical Error in Histogramming

- For every sample point X, define the **indicator** random variable Y:

$$Y = \mathbb{I}_x(X) = \begin{cases} 1 & \text{if } x - h/2 \leq X \leq x + h/2 \\ 0 & \text{otherwise} \end{cases}$$

- The mean and variance of this **Bernoulli random variable** are:

$$E(Y) = \bar{Y} = hP_x \approx hf(x)$$

$$\sigma_Y^2 = \int (y - \bar{Y})^2 f(y) dy = \bar{Y} \cdot (1 - \bar{Y}) \approx \bar{Y} \approx hf(x)$$

- The number N_x out of N trials inside the bin is a sum of N random Bernoulli variables Y_i:

$$f(x) \approx \frac{1}{h} \frac{N_x}{N} = h^{-1} \left(\frac{1}{N} \sum_{i=1}^{N} Y_i \right) = \tilde{P}_x$$

Optimal Bin Width

- The central limit theorem says

$$\sigma(\tilde{P}_x) \approx h^{-1}\frac{\sigma_Y}{\sqrt{N}} = \sqrt{\frac{f(x)}{hN}}$$

- The optimal bin width is when the truncation and statistical errors are equal:

$$h^2 \sim \sqrt{\frac{1}{hN}} \quad \Rightarrow \quad h \sim N^{-1/5},$$

  with total error $\varepsilon \sim (hN)^{-1/2} \sim N^{-2/5}$.

- This is because statistical errors dominate and so **using a larger bin is better**...unless there are small-scale features in $f(x)$ that need to be resolved.

Integration via Monte Carlo

- Define the random variable $Y = f(\mathbf{X})$, and generate a sequence of N **independent uniform samples** $\mathbf{X}_k \in \Omega$, i.e., N random variables distributed uniformly inside Ω:

$$\mathbf{X} \sim g(\mathbf{x}) = \begin{cases} |\Omega|^{-1} & \text{for } \mathbf{x} \in \Omega \\ 0 & \text{otherwise} \end{cases}$$

  and calculate the mean

$$\hat{Y} = \frac{1}{N} \sum_{k=1}^{N} Y_k = \frac{1}{N} \sum_{k=1}^{N} f(\mathbf{X}_k)$$

- According to the weak law of large numbers,

$$\lim_{N \to \infty} \hat{Y} = E(Y) = \bar{Y} = \int f(\mathbf{x}) g(\mathbf{x}) dx = |\Omega|^{-1} \int_{\Omega} f(\mathbf{x})\, d\mathbf{x}$$

Accuracy of Monte Carlo Integration

- This gives a Monte Carlo approximation to the integral:

$$J=\int_{\Omega\in\mathbb{R}^n} f(\mathbf{x})\,d\mathbf{x}=|\Omega|\,\bar{Y}\approx|\Omega|\,\hat{Y}=|\Omega|\,\frac{1}{N}\sum_{k=1}^{N} f\left(\mathbf{X}_k\right).$$

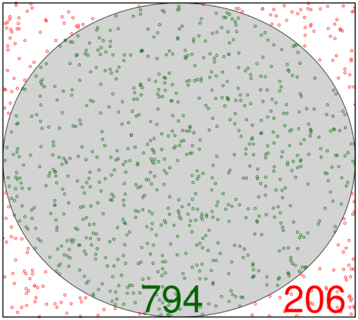
- Recalling the central limit theorem, for large N we get an **error estimate** by evaluating the standard deviation of the estimate $\hat{Y}$:

$$\sigma^2\left(\hat{Y}\right)\approx\frac{\sigma_Y^2}{N}=N^{-1}\int_{\Omega}\left[f(\mathbf{x})-|\Omega|^{-1}J\right]^2 d\mathbf{x}$$

$$\sigma\left(\hat{Y}\right)\approx\frac{1}{\sqrt{N}}\left[\int_{\Omega}\left[f(\mathbf{x})-\overline{f(\mathbf{x})}\right]^2 d\mathbf{x}\right]^{1/2}$$

- Note that this error goes like $N^{-1/2}$, which is order of convergence $1/2$: **Worse than any deterministic quadrature**.
- But, the same number of points are needed to get a certain accuracy **independent of the dimension**.

Integration by Rejection



Note how this becomes **less efficient as dimension grows** (most points are outside the sphere).

- Integration requires $|\Omega|$:

$$\int_{\Omega \in \mathbb{R}^n} f(\mathbf{x})\, d\mathbf{x} \approx |\Omega| \frac{1}{N} \sum_{k=1}^{N} f(\mathbf{X}_k)$$

- Consider Ω being the unit circle of radius 1.
- Rejection: Integrate by sampling points inside an **enclosing region**, e.g, a square of area $|\Omega_{encl}| = 4$, and rejecting any points outside of Ω:

$$\int_{\Omega \in \mathbb{R}^n} f(\mathbf{x})\, d\mathbf{x} \approx |\Omega_{encl}| \frac{1}{N} \sum_{\mathbf{X}_k \in \Omega} f(\mathbf{X}_k)$$

Example of Integration

- Consider computing the integral for $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$:

$$J = \int_{\|\mathbf{x}\|<1} \int_{\|\mathbf{y}\|<1} \frac{e^{-\lambda\|\mathbf{x}-\mathbf{y}\|}}{\|\mathbf{x}-\mathbf{y}\|} d\mathbf{x} d\mathbf{y}.$$

- The integral is related to the expectation value of the random variable

$$Z = Z(\mathbf{X}, \mathbf{Y}) = \frac{e^{-\lambda\|\mathbf{X}-\mathbf{Y}\|}}{\|\mathbf{X}-\mathbf{Y}\|},$$

  where $\mathbf{X}$ and $\mathbf{Y}$ are random variables uniformly sampled from the unit sphere in $\mathbb{R}^n$.

- Specifically, in three dimensions, $n = 3$,

$$J = |\Omega|\, \bar{Z} \approx \left(\frac{4\pi}{3}\right)^2 \left[\frac{1}{N} \sum_{k=1}^{N} Z(\mathbf{X}_k, \mathbf{Y}_k)\right]$$

Variance Reduction

- Recall that the standard deviation of the Monte Carlo estimate for the integral is:

$$\sigma\left(\hat{Y}\right) \approx \frac{1}{\sqrt{N}}\left[\int_\Omega \left[f(\mathbf{x}) - \overline{f(\mathbf{x})}\right]^2 d\mathbf{x}\right]^{1/2}$$

- Since the answer is approximately normally-distributed, we have the well-known **confidence intervals**:

$$P\left(\frac{J}{|\Omega|} \in \left[\hat{Y} - \sigma, \hat{Y} + \sigma\right]\right) \approx 66\%$$

$$P\left(\frac{J}{|\Omega|} \in \left[\hat{Y} - 2\sigma, \hat{Y} + 2\sigma\right]\right) \approx 95\%$$

- The most important thing in Monte Carlo is **variance reduction**, i.e., finding methods that give the same answers in the limit $N \to \infty$ but have a much smaller σ.

Importance Sampling

- As an example of variance reduction, consider rewriting:

$$\int f(\mathbf{x})\,d\mathbf{x} = \int \frac{f(\mathbf{x})}{g(\mathbf{x})}\,g(\mathbf{x})d\mathbf{x} = E\left[\frac{f(\mathbf{X})}{g(\mathbf{X})}\right] \text{ where } \mathbf{X} \sim g.$$

- This now corresponds to taking samples not uniformly inside Ω, but rather, taking **samples from importance function** $g(\mathbf{x})$:

$$\int f(\mathbf{x})\,d\mathbf{x} \approx \frac{1}{N}\sum_{k=1}^{N}\frac{f(\mathbf{X}_k)}{g(\mathbf{X}_k)} \text{ where } \mathbf{X} \sim g$$

- Note that $|\Omega|$ does not appear since it is implicitly included in the normalization of $g(\mathbf{x})$.
- The previous uniform sampling algorithm corresponds to $g(\mathbf{x}) = |\Omega|^{-1}$ for $\mathbf{x} \in \Omega$.

Variance Reduction via Importance Sampling

- Repeating the variance calculation for

$$Y(\mathbf{X}) = \frac{f(\mathbf{X})}{g(\mathbf{X})}$$

- The variance is now

$$\sigma^2\left(\hat{Y}\right) \approx \frac{\sigma_Y^2}{N} = N^{-1}\int \left[Y(\mathbf{x}) - \overline{Y}\right]^2 g(\mathbf{x})d\mathbf{x}$$

$$\sigma\left(\hat{Y}\right) \approx \frac{1}{\sqrt{N}}\left[\int \left[\frac{f(\mathbf{x})}{g(\mathbf{x})} - \overline{Y}\right]^2 g(\mathbf{x})d\mathbf{x}\right]^{1/2}.$$

- We therefore want $f(\mathbf{x})/g(\mathbf{x})$ to be as close as possible to a constant, ideally

$$g_{ideal}(\mathbf{x}) = \frac{f(\mathbf{x})}{\int f(\mathbf{x})dx}$$

  but this requires being able to create independent samples from $f(\mathbf{x})$, which is rarely the case.

Importance Sampling Example

- Consider again computing:

$$J = \int_{\|\mathbf{x}\|<1} \int_{\|\mathbf{y}\|<1} \frac{e^{-\lambda\|\mathbf{x}-\mathbf{y}\|}}{\|\mathbf{x}-\mathbf{y}\|} d\mathbf{x} d\mathbf{y}.$$

- The standard Monte Carlo will have a large variance because of the singularity when $\mathbf{x} = \mathbf{y}$:
  The integrand is very non-uniform around the singularity.
- If one could sample from the distribution

$$g(\mathbf{x}, \mathbf{y}) \sim \frac{1}{\|\mathbf{x}-\mathbf{y}\|} \text{ when } \mathbf{x} \approx \mathbf{y},$$

  then the importance function will capture the singularity and the variance will be greatly reduced.

Conclusions/Summary

- Monte Carlo is an umbrella term for **stochastic computation** of deterministic answers.
- Monte Carlo answers are random, and their accuracy is measured by the **variance** or uncertaintly of the estimate, which typically scales like $\sigma \sim N^{-1/2}$, where N is the number of **samples**.
- Implementing Monte Carlo algorithms on a computer requires a PRNG, almost always a **uniform pseudo-random number generator** (URNG).
- One often needs to convert a sample from a URNG to a sample from an arbitrary distribution $f(x)$, including inverting the cummulative distribution and rejection sampling.
- Monte Carlo can be used to perform **integration in high dimensions** by simply evaluating the function at random points.
- **Variance reduction** is the search for algorithms that give the same answer but with less statistical error. One example is **importance sampling**.