Monte Carlo Methods

Juan F. Rubio-Ramírez

Emory University

Motivation

- Solutions of many scientific problems involve intractable high-dimensional integrals.
- Standard deterministic numerical integration deteriorates rapidly with dimension.
- Monte Carlo methods are stochastic numerical methods to approximate high-dimensional integrals.
- Main application in this course: Bayesian statistics.

Computing Integrals in 1D

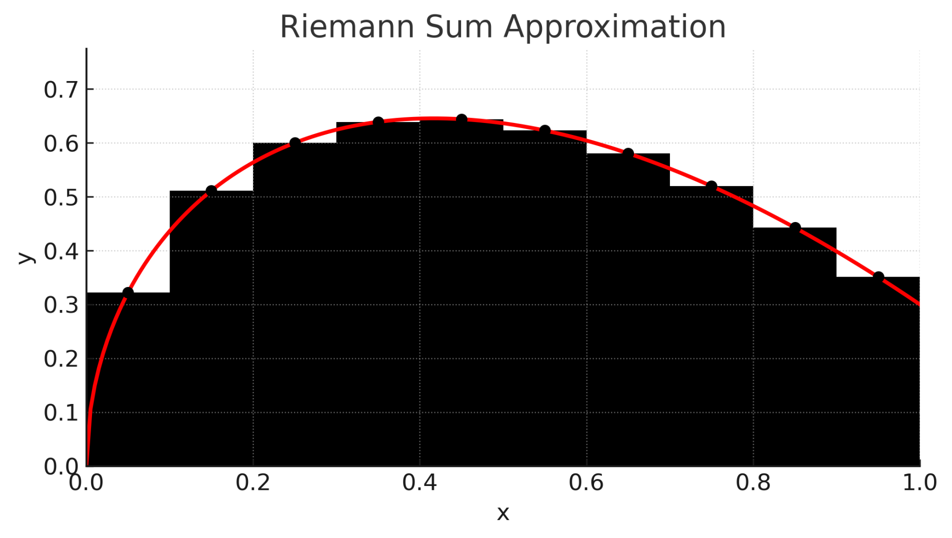
For $f : X \to \mathbb{R}$, let

$$I = \int_X f(x)\, dx.$$

When $X = [0, 1]$, approximate I via the midpoint Riemann sum

$$\hat{I}_n = \frac{1}{n} \sum_{i=0}^{n-1} f\left(\frac{i + \frac{1}{2}}{n} \right).$$

Riemann Sums Figure



Error in 1D

For a small interval $[a, a + \varepsilon]$,

$$\int_a^{a+\varepsilon} f(x)\,dx \approx \varepsilon\, f(a).$$

We want to understand and bound the approximation error:

$$\text{Local error} = \left| \int_a^{a+\varepsilon} f(x)\,dx - \varepsilon f(a) \right|.$$

Then, we will use this local error to compute the global error.

Step 1: Expressing $f(x)$ via its Derivative

By the Fundamental Theorem of Calculus,

$$f(x) = f(a) + \int_a^x f'(y)\,dy.$$

Substitute this expression into the integral:

$$\int_a^{a+\varepsilon} f(x)\,dx = \int_a^{a+\varepsilon} \left[f(a) + \int_a^x f'(y)\,dy \right] dx.$$

Step 2: Representing the Error as a Double Integral

Split the integral into two terms:

$$\int_a^{a+\varepsilon} f(x)\,dx = \underbrace{\int_a^{a+\varepsilon} f(a)\,dx}_{=\varepsilon f(a)} + \int_a^{a+\varepsilon}\int_a^x f'(y)\,dy\,dx.$$

Therefore,

$$\int_a^{a+\varepsilon} f(x)\,dx - \varepsilon f(a) = \int_a^{a+\varepsilon}\int_a^x f'(y)\,dy\,dx.$$

This expresses the integration error as the accumulated effect of the derivative $f'(y)$ over the triangular region $\{(x,y) : a \leq y \leq x \leq a+\varepsilon\}$ in the (x,y)–plane.

Step 3: Bounding the Double Integral

Take absolute values and use the triangle inequality:

$$\left|\int_a^{a+\varepsilon}\int_a^x f'(y)\,dy\,dx\right| \leq \int_a^{a+\varepsilon}\int_a^x |f'(y)|\,dy\,dx.$$

Since $|f'(y)| \leq \sup_{x\in[a,a+\varepsilon]} |f'(x)| =: M$, we obtain

$$\leq M\int_a^{a+\varepsilon}\int_a^x 1\,dy\,dx = M\int_a^{a+\varepsilon}(x-a)\,dx = M\,\frac{\varepsilon^2}{2}.$$

Geometric intuition: the inner integral $\int_a^x 1\,dy = x-a$ represents the width of a growing triangle, and integrating again gives the triangle's area $\varepsilon^2/2$.

Step 4: From Local Error to Global Error

The previous bound applies to a single small interval $[a, a+\varepsilon]$:

$$\text{Local error} \leq M\,\frac{\varepsilon^2}{2}, \quad \text{where } M = \sup_{x\in[0,1]} |f'(x)|.$$

If we divide $[0,1]$ into n equal subintervals, then $\varepsilon = 1/n$.

$$\text{Local error} \leq \frac{M}{2n^2}.$$

There are n such intervals, so the total error satisfies

$$\text{Global error} \leq n \times \frac{M}{2n^2} = \frac{M}{2n} = O\left(\frac{1}{n}\right).$$

Thus, the midpoint (or naive) numerical integration rule converges at rate $O(1/n)$.

Computing Integrals in 2D

Partition $[0,1]^2$ into an $m \times m$ uniform grid with mesh $h = 1/m$. For cell midpoints

$$x_i = \frac{i + \frac{1}{2}}{m}, \qquad y_j = \frac{j + \frac{1}{2}}{m}, \qquad i, j = 0, \ldots, m-1,$$

the 2D midpoint estimator with $n = m^2$ evaluations is

$$\widehat{I}_m = \frac{1}{m^2} \sum_{i=0}^{m-1} \sum_{j=0}^{m-1} f(x_i, y_j).$$

We show its error is $O(1/m) = O(n^{-1/2})$.

Step 1: Local Error on One Cell (Analogy with 1D Case)

Consider one rectangular cell

$$R = [a, a+h] \times [b, b+h]$$

By the Fundamental Theorem of Calculus applied in both coordinates,

$$f(x,y) = f(a,b) + \int_a^x f_x(u,b)\,du + \int_b^y f_y(a,v)\,dv + \int_a^x \int_b^y f_{xy}(u,v)\,dv\,du.$$

$$\text{Local Error} = \left| \iint_R f(x,y)dxdy - h^2 f(a,b) \right|$$

We have that Local Error related to this:

$$\iint_R \left(\int_a^x f_x(u,b)\,du + \int_b^y f_y(a,v)\,dv + \int_a^x \int_b^y f_{xy}(u,v)\,dv\,du \right) dx\,dy.$$

Step 2: Bounding the Local Error

Take absolute values and use the sup norm of the derivatives:

$$\text{Local Error} \leq \|f_x\|_\infty \int_a^{a+h}\int_b^{b+h}(x-a)\,dx\,dy + \|f_y\|_\infty \int_a^{a+h}\int_b^{b+h}(y-b)\,dx\,dy$$

$$+\|f_{xy}\|_\infty \int_a^{a+h}\int_b^{b+h}(x-a)(y-b)\,dx\,dy.$$

Each term can be computed explicitly:

$$\int_a^{a+h}\int_b^{b+h}(x-a)\,dx\,dy = \frac{h^3}{2}, \qquad \int_a^{a+h}\int_b^{b+h}(x-a)(y-b)\,dx\,dy = \frac{h^4}{4}.$$

Hence the local error is bounded by

$$\boxed{\text{Local error on } R \ \leq M\,h^3, \quad M = C_1\|f_x\|_\infty + C_2\|f_y\|_\infty + C_3\|f_{xy}\|_\infty.}$$

Step 3: From Local Error to Global Error

There are m^2 cells, each with mesh $h = 1/m$ and local error $\leq Mh^3$. Therefore the *global* error obeys

$$\text{Global error} \ \leq \ m^2 \times Mh^3 = m^2 \times M \left(\frac{1}{m}\right)^3 = \frac{M}{m}.$$

But $n = m^2$, thus

$$O\left(\frac{1}{m}\right) \ = \ O\left(n^{-1/2}\right).$$

Extension to d Dimensions

On $[0,1]^d$ with an m^d grid (mesh $h = 1/m$, $n = m^d$ points):

- The *local* midpoint error on one d-cube is $O(h^{d+1})$ (one power of h from integrating each coordinate; an extra h from the derivative term).
- There are m^d cells.

Therefore

$$\text{Global error} \;\le\; m^d \times O(h^{d+1}) = m^d \times O\big((1/m)^{d+1}\big) = O\left(\frac{1}{m}\right) = O\Big(n^{-1/d}\Big).$$

This is the *curse of dimensionality*: the rate degrades from $O(n^{-1})$ (1D midpoint) to $O(n^{-1/d})$ in d dimensions.

Monte Carlo Integration

Monte Carlo Integration

We are interested in computing

$$I = \int_{\mathcal{X}} \varphi(x)\, \pi(x)\, dx$$

where π is a pdf on $\mathcal{X}$ and $\varphi : \mathcal{X} \to \mathbb{R}$.

Monte Carlo method: draw n i.i.d. samples $X_1, \ldots, X_n \sim \pi$ and compute

$$\widehat{I}_n = \frac{1}{n} \sum_{i=1}^{n} \varphi(X_i).$$

Remark: this corresponds to the empirical measure

$$\widehat{\pi}_n(dx) = \frac{1}{n} \sum_{i=1}^{n} \delta_{X_i}(dx).$$

Law of Large Numbers. If $\mathbb{E}|\varphi(X)| < \infty$, then $\widehat{I}_n \to I$ a.s.

Central Limit Theorem. If $\sigma^2 = \mathrm{Var}(\varphi(X)) = \int_{\mathcal{X}} [\varphi(x) - I]^2 \pi(x)\, dx < \infty$, then

$$\mathrm{Var}(\widehat{I}_n) = \mathbb{E}[(\widehat{I}_n - I)^2] = \frac{\sigma^2}{n} \text{ and, hence } \sqrt{n}\frac{\widehat{I}_n - I}{\sigma} \Rightarrow \mathcal{N}(0,1).$$

Variance Estimation

Proposition. If $\sigma^2 = \mathrm{Var}(\varphi(X)) < \infty$, then

$$S_n^2 = \frac{1}{n-1}\sum_{i=1}^{n}(\varphi(X_i) - \widehat{I}_n)^2$$

is an unbiased estimator of σ^2.

Variance Estimation — Proof

Let $Y_i = \varphi(X_i)$, $i = 1, \ldots, n$, be i.i.d. with

$$\mu = \mathbb{E}[Y], \qquad \sigma^2 = \mathrm{Var}(Y) < \infty, \qquad \overline{Y} = \frac{1}{n}\sum_{i=1}^{n} Y_i.$$

The sample variance is

$$S_n^2 = \frac{1}{n-1}\sum_{i=1}^{n}(Y_i - \overline{Y})^2.$$

Goal: show that $\mathbb{E}[S_n^2] = \mathrm{Var}(Y) = \sigma^2$.

Step 1. Algebraic Identity

Expand the deviations:

$$\sum_{i=1}^{n}(Y_i - \overline{Y})^2 = \sum_i \left(Y_i^2 - 2Y_i\overline{Y} + \overline{Y}^2\right)$$
$$= \sum_i Y_i^2 - 2\overline{Y}\sum_i Y_i + n\,\overline{Y}^2.$$

Since $\sum_i Y_i = n\overline{Y}$,

$$\boxed{\sum_{i=1}^{n}(Y_i - \overline{Y})^2 = \sum_{i=1}^{n} Y_i^2 - n\,\overline{Y}^2.}$$

This identity will let us compute $\mathbb{E}[S_n^2]$ directly.

Step 2. Take Expectations

By definition and linearity of expectation,

$$\begin{aligned}\mathbb{E}[S_n^2] &= \frac{1}{n-1}\mathbb{E}\left[\sum_i (Y_i - \overline{Y})^2\right] \\ &= \frac{1}{n-1}\left(\mathbb{E}\left[\sum_i Y_i^2\right] - n\,\mathbb{E}[\overline{Y}^2]\right).\end{aligned}$$

Because the Y_i are i.i.d.,

$$\mathbb{E}\left[\sum_i Y_i^2\right] = n\,\mathbb{E}[Y^2],$$

so

$$\boxed{\mathbb{E}[S_n^2] = \frac{1}{n-1}\left(n\,\mathbb{E}[Y^2] - n\,\mathbb{E}[\overline{Y}^2]\right).}$$

Step 3. Evaluate $\mathbb{E}[\overline{Y}^2]$

Use $\mathbb{E}[Z^2] = \mathrm{Var}(Z) + (\mathbb{E}Z)^2$ with $Z = \overline{Y}$:

$$\mathbb{E}[\overline{Y}^2] = \mathrm{Var}(\overline{Y}) + (\mathbb{E}[\overline{Y}])^2.$$

Since $\mathbb{E}[\overline{Y}] = \mu$ and, for i.i.d. draws,

$$\mathrm{Var}(\overline{Y}) = \mathrm{Var}\left(\frac{1}{n}\sum_i Y_i\right) = \frac{1}{n^2}\sum_i \mathrm{Var}(Y_i) = \frac{\sigma^2}{n},$$

we obtain

$$\boxed{\mathbb{E}[\overline{Y}^2] = \frac{\sigma^2}{n} + \mu^2.}$$

Step 4. Substitute and Simplify

Plug $\mathbb{E}[Y^2] = \sigma^2 + \mu^2$ and $\mathbb{E}[\overline{Y}^2] = \frac{\sigma^2}{n} + \mu^2$ into

$$\mathbb{E}[S_n^2] = \frac{1}{n-1}\left(n\,\mathbb{E}[Y^2] - n\,\mathbb{E}[\overline{Y}^2]\right):$$

$$\begin{aligned}
\mathbb{E}[S_n^2] &= \tfrac{1}{n-1}\left[n(\sigma^2+\mu^2) - n\left(\tfrac{\sigma^2}{n}+\mu^2\right)\right] \\
&= \tfrac{1}{n-1}\left((n-1)\sigma^2\right) = \boxed{\sigma^2 = \mathrm{Var}(Y) = \mathrm{Var}(\varphi(X)).}
\end{aligned}$$

Thus S_n^2 is an *unbiased* estimator of the population variance.

Error Estimates $|\widehat{I}_n - I|$

Chebyshev Inequality:

$$\mathbb{P}\left(|\widehat{I}_n - I| > c\,\frac{\sigma}{\sqrt{n}}\right) \leq \frac{1}{c^2}.$$

Central Limit Theorem Approximation:

$$\mathbb{P}\left(|\widehat{I}_n - I| > c\,\frac{\sigma}{\sqrt{n}}\right) \approx 2(1 - \Phi(c)).$$

Confidence Interval:

$$\widehat{I}_n \pm c_\alpha \frac{S_n}{\sqrt{n}}, \qquad 2(1 - \Phi(c_\alpha)) = \alpha.$$

Rate of convergence: $\mathcal{O}(n^{-1/2})$.

Chebyshev Inequality — Step by Step

We know that

$$\mathrm{Var}(\widehat{I}_n) = \mathbb{E}\big[(\widehat{I}_n - I)^2\big] = \frac{\sigma^2}{n}.$$

Chebyshev's inequality states:

$$\mathbb{P}(|Z| > c) \leq \frac{\mathrm{Var}(Z)}{c^2}.$$

Apply it to $Z = \widehat{I}_n - I$:

$$\mathbb{P}(|\widehat{I}_n - I| > t) \leq \frac{\mathrm{Var}(\widehat{I}_n)}{t^2} = \frac{\sigma^2/n}{t^2}.$$

Choose $t = c\sigma/\sqrt{n}$:

$$\boxed{\mathbb{P}\left(|\widehat{I}_n - I| > c\,\frac{\sigma}{\sqrt{n}}\right) \leq \frac{1}{c^2}.}$$

Valid for all n, though conservative since it only uses the variance.

Central Limit Theorem Approximation — From Inequality to Probability

From the Central Limit Theorem,

$$\frac{\sqrt{n}(\widehat{I}_n - I)}{\sigma} \xrightarrow{D} \mathcal{N}(0,1).$$

Hence, for large n,

$$\mathbb{P}\left(|\widehat{I}_n - I| > c\,\frac{\sigma}{\sqrt{n}}\right) = \mathbb{P}(|Z| > c) = 2(1 - \Phi(c)).$$

- $\Phi(c)$: CDF of the standard normal.
- Example values: $c{=}1.96 \Rightarrow 95\%$ coverage; $c{=}2.58 \Rightarrow 99\%$.
- Much tighter than Chebyshev's bound.

Building a Confidence Interval

From the Central Limit Theorem approximation and unbiased estimator of σ^2,

$$\frac{\widehat{I}_n - I}{S_n/\sqrt{n}} \approx Z \sim \mathcal{N}(0,1).$$

Let c_α satisfy $2(1-\Phi(c_\alpha)) = \alpha$. Then

$$\mathbb{P}\left(-c_\alpha < \frac{\widehat{I}_n - I}{S_n/\sqrt{n}} < c_\alpha\right) \approx 1-\alpha.$$

Rearranging gives the $(1-\alpha)$ confidence interval for I:

$$\boxed{I \in \left[\widehat{I}_n - c_\alpha \tfrac{S_n}{\sqrt{n}},\ \widehat{I}_n + c_\alpha \tfrac{S_n}{\sqrt{n}}\right].}$$

Comparing Chebyshev and Central Limit Theorem Bounds

Chebyshev (exact, loose):

$$\mathbb{P}(|\widehat{I}_n - I| > c\sigma/\sqrt{n}) \leq \frac{1}{c^2}.$$

Central Limit Theorem (approx., tight):

$$\mathbb{P}(|\widehat{I}_n - I| > c\sigma/\sqrt{n}) \approx 2(1 - \Phi(c)).$$

c	Chebyshev	Central Limit Theorem (Normal)
1	1.00	0.317
2	0.25	0.0455
3	0.111	0.0027

$\Rightarrow$ Central Limit Theorem gives realistic probabilities; Chebyshev is universally valid but overly conservative.

Monte Carlo Error Rate

Because $\mathrm{Var}(\widehat{I}_n) = \sigma^2/n$,

$$\text{RMSE} = \sqrt{\mathrm{Var}(\widehat{I}_n)} = \frac{\sigma}{\sqrt{n}}.$$

Hence the typical estimation error decreases at rate

$$\boxed{\mathcal{O}(n^{-1/2})}.$$

Implications:

- Doubling the precision (halving the error) requires $4\times$ as many samples.
- This $n^{-1/2}$ rate is fundamental—independent of the dimension of X.

Monte Carlo Integration

Often the integral is $I = \mathbb{E}_\pi[\varphi(X)]$ for a specific φ and target distribution π.

Monte Carlo approach relies on independent copies of $X \sim \pi$.

$$\text{MC to approximate } \mathbb{E}_\pi[\varphi(X)] \quad \Longleftrightarrow \quad \text{simulate from } \pi.$$

Thus “Monte Carlo” sometimes refers broadly to simulation methods.

Why Monte Carlo in our Case?

From previous chapter, we want to compute moments associated with: Posterior distribution:

$$\pi(\theta \mid Y^T, i) = \frac{f(Y^T \mid \theta, i)\,\pi(\theta \mid i)}{\int_{\Theta_i} f(Y^T \mid \theta, i)\,\pi(\theta \mid i)\,d\theta}$$

The dimension of θ can be large.

A Bit of Historical Background and Intuition

Metropolis and Ulam (1949) and von Neumann (1951). Why the name "Monte Carlo"?

Two simple examples:

1. Probability of getting a total of six points when rolling two fair dice.
2. Throwing darts at a graph.

Classical Monte Carlo Integration

Assume we know how to generate draws from $\pi(\theta \mid Y^T, i)$. What does it mean to draw from it? Two basic questions:

1. Why do we want to do it?
2. How do we do it?

How Do We Do It? Random Number Generators

Large literature. Two good surveys:

- Devroye (1986) *Non-Uniform Random Variate Generation*.
- Robert & Casella (2004) *Monte Carlo Statistical Methods*.

Random Draws?

Natural sources of randomness are hard to use. A computer is deterministic! von Neumann (1951): "Anyone who considers arithmetical methods of producing random digits is, of course, in a state of sin."

Basic Building Block

- Pseudo-random number generators are highly non-linear iterative algorithms that “look random”.
- We focus on $U(0,1)$ draws.
- In general, other distributions arise from transforming uniforms.

Goal

Design iterative algorithms (Lehmer, 1951) that:

1. Are unpredictable for the uninitiated (relation to chaotic dynamical systems).
2. Pass standard statistical tests (K–S, ARMA(p, q), etc.).

Basic Component: Congruential Generators

Multiplicative congruential generator:

$$x_i = (ax_{i-1} + b) \bmod (M + 1) \text{ and } x_0 \text{ is the seed.}$$

Then:

$$u_i = x_i/(M + 1) \text{ is an } U(0, 1)$$

Example: Generating Integers and Uniforms

Parameters: $a = 5$, $b = 3$, $M = 16$, seed $x_0 = 7$.

$$x_i = (ax_{i-1} + b) \bmod (M+1) \quad \Rightarrow \quad x_i \in \{0, \ldots, M\}.$$

i	Computation	x_i	$u_i = x_i/(M+1)$
0	seed	7	0.412
1	$(57 + 3) \bmod 17 = 4$	4	0.235
2	$(54 + 3) \bmod 17 = 6$	6	0.353
3	$(56 + 3) \bmod 17 = 16$	16	0.941
4	$(516 + 3) \bmod 17 = 15$	15	0.882

Choices of Parameters

Period/performance hinge on a, b, M. Bad choice example: $a = 13$, $c = 0$, $M = 31$, $x_0 = 1$ (historical bad examples: IBM RND, 1960s).

A Good Choice

Traditional: $a = 7^5 = 16807$, $c = 0$, $m = 2^{31} - 1$. Period bounded by M. 32 vs 64 bit hardware matters. Beware IEEE floating-point standard. Alternatives exist.

Real Life

Don't code your own RNG. MATLAB implements state-of-the-art (e.g., KISS by Marsaglia & Zaman, 1991). For Fortran/C++: see DIEHARD battery.

Nonuniform Distributions

We often need non-uniform draws. Basic approach, move from uniforms via:

- Transformations (standard tricks).
- Inverse cdf method.

These underpin commercial software.

Transformations Example: Normal via Box–Muller

Let $U_1, U_2 \sim U(0,1)$. Then

$$x = \cos(2\pi U_1)\sqrt{-2\log U_2}, \quad y = \sin(2\pi U_1)\sqrt{-2\log U_2}$$

are i.i.d. $N(0,1)$ (points lie on a spiral in (x,y)).

Transformations Example: Multivariate Normal

If $x \sim N(0, I)$ and $\Sigma\Sigma^\top$ is the covariance, then

$$y = \mu + \Sigma x \sim N(\mu, \Sigma\Sigma^\top).$$

Use Cholesky for Σ.

The Inverse Transform Method

Goal: Generate a random variable X with a known CDF using uniform draws.

- Let:

$$X = F^{-1}(U) \text{ and } U \sim U(0,1)$$

- Then

$$P(X \leq x) = P(F^{-1}(U) \leq x) = P(U \leq F(x)) = F(x).$$

- Hence X has distribution F.

Example Inverse 1: Exponential Distribution

Let $X \sim \text{Exp}(\lambda)$ with

$$F(x) = 1 - e^{-\lambda x}, \qquad x \geq 0.$$

Solve for x in terms of $u = F(x)$:

$$u = 1 - e^{-\lambda x} \quad \Rightarrow \quad x = -\frac{1}{\lambda} \ln(1-u).$$

Algorithm

1. Draw $U \sim U(0,1)$.
2. Set $X = -\frac{1}{\lambda} \ln U$.

Then X follows $\text{Exp}(\lambda)$. Simple and exact.

Example Inverse 2: Discrete Case (Bernoulli)

Let $X \in \{0,1\}$ with $P(X=1)=p$. CDF:

$$F(x) = \begin{cases} 0, & x < 0, \\ 1-p, & 0 \le x < 1, \\ 1, & x \ge 1. \end{cases}$$

Algorithm:

$$X = \begin{cases} 1, & \text{if } U < p, \\ 0, & \text{otherwise.} \end{cases}$$

Comment: works for any discrete distribution by comparing U with cumulative probabilities.

Fundamental Theorem of Simulation

- Transformations and Inverse Method very limited set of distributions.
- We now present a general approach
- Suppose $f(x)$ is a probability density on a measurable space $\mathcal{X} \subseteq \mathbb{R}^d$.
- Imagine the set under its graph:

$$A = \{(x, y) \in \mathcal{X} \times [0, \infty) : 0 \leq y \leq f(x)\}.$$

- If we draw points uniformly in A, the projection of these points onto the x-axis follows exactly the distribution with density $f(x)$.
- Intuitively, higher parts of the curve receive proportionally more projected points.

Fundamental Theorem of Simulation

Theorem. Let $f : \mathbb{R}^d \to [0, \infty)$ satisfy $\int f(x)\,dx = 1$. Define

$$A = \{(x, y) \in \mathbb{R}^d \times [0, \infty) : \ 0 \leq y \leq f(x)\}.$$

If (X, Y) is uniformly distributed on A, marginal distribution of X has density $f(x)$.

Idea: Uniform sampling under the density surface produces samples distributed according to that density.

Proof

- Since $\int f(x)\,dx = 1$, the total volume of A is one:

$$|A| = \int_{\mathbb{R}^d}\int_0^{f(x)} dy\,dx = 1.$$

- The joint density of (X, Y) is therefore

$$p_{X,Y}(x, y) = \mathbf{1}\{0 \le y \le f(x)\}.$$

- Integrating out y,

$$p_X(x) = \int_0^{f(x)} 1\,dy = f(x).$$

- Hence the marginal of X has density $f(x)$. $\square$

Acceptance Sampling: Motivation

We cannot easily draw points uniformly under $f(x)$.

- Introduce a simpler density $g(x)$ such that we can draw from it.
- Find a constant $a > 0$ such that:

$$f(x) \leq a\, g(x) \quad \forall x.$$

- The function $a\, g(x)$ is called an **envelope** of $f(x)$.

Idea: sample uniformly under $a\, g(x)$ and keep only points under $f(x)$.

1. Draw $X \sim g(x)$.
2. Draw $U \sim U(0,1)$.
3. Accept X if $U \leq \frac{f(X)}{a\,g(X)}$.

Interpretation:

- The pair $(X, Uag(X))$ is uniformly distributed under the curve $ag(x)$.
- Accepted draws correspond to points that lie under $f(x)$.
- Hence accepted X follow the target density $f(x)$.

Choice of a

Let $f, g \geq 0$ and assume $\mathrm{supp}(f) \subseteq \mathrm{supp}(g)$ (i.e., $g(x) = 0 \Rightarrow f(x) = 0$). Define

$$a \;=\; \sup_x \frac{f(x)}{g(x)}.$$

Claim: $f(x) \leq a\, g(x)$ for all x.

Is $a \geq 1$ Always?

Let f, g be densities with $\operatorname{supp}(f) \subseteq \operatorname{supp}(g)$ and

$$a = \sup_x \frac{f(x)}{g(x)}.$$

Claim. $a \geq 1$, with $a = 1$ iff $f = g$ almost everywhere (w.r.t. g). Hence $a > 1$ whenever $f \neq g$ on a set of positive g-measure.

Proof

Let $R(x) = \frac{f(x)}{g(x)}$ where $g(x) > 0$ (define $R = 0$ when $g = 0$; then $f = 0$ there). Since f, g are densities,

$$\mathbb{E}_g[R(X)] \;=\; \int \frac{f(x)}{g(x)}\, g(x)\, dx \;=\; \int f(x)\, dx \;=\; 1.$$

If $R(x) < 1$ for all x with $g(x) > 0$, then $\mathbb{E}_g[R(X)] < 1$, a contradiction. Thus $\sup_x R(x) \geq 1$, i.e. $a \geq 1$.

Moreover, $a = 1$ iff $R(x) \leq 1$ a.e. and $\mathbb{E}_g[R] = 1$, which forces $R(x) = 1$ a.e., i.e. $f(x) = g(x)$ a.e. $\square$

Quality of the Envelope

- The acceptance rate is $P(\text{accept}) = \frac{1}{a}$.
- A tight envelope (a close to 1) $\Rightarrow$ more efficient sampling.
- A loose envelope (a large) $\Rightarrow$ many rejections.
- Ideally, $g(x)$ resembles $f(x)$ in shape and tails.

Proof $P(\text{accept}) = \frac{1}{a}$

Let $A = \{U \leq f(X)/(ag(X))\}$. Then

$$\mathbb{P}(A) = \mathbb{E}[\mathbf{1}_A] = \mathbb{E}\Big[\mathbf{1}\Big\{U \leq \frac{f(X)}{ag(X)}\Big\}\Big] = \mathbb{E}\Big[\mathbb{E}\Big(\mathbf{1}\Big\{U \leq \frac{f(X)}{ag(X)}\Big\} \;\Big|\; X\Big)\Big].$$

Independence $\Rightarrow$ given $X = x$, $U \sim U(0,1)$ so

$$\mathbb{P}\Big(U \leq \frac{f(X)}{ag(X)} \;\Big|\; X\Big) = \frac{f(X)}{ag(X)}.$$

Hence

$$\mathbb{P}(A) = \mathbb{E}\Big[\frac{f(X)}{ag(X)}\Big] = \int \frac{f(x)}{ag(x)}\, g(x)\, dx = \frac{1}{a}\int f(x)\, dx = \frac{1}{a}.$$

Proof (One Line with the Supremum Property)

Define $r(x) = \frac{f(x)}{g(x)}$ for $g(x) > 0$ and set $r(x) = 0$ when $g(x) = 0$ (using $g(x) = 0 \Rightarrow f(x) = 0$). By definition of the supremum,

$$r(x) \;\leq\; \sup_z r(z) \;=\; a \quad \text{for every } x.$$

Multiplying by $g(x) \geq 0$ yields

$$f(x) \;=\; r(x)\, g(x) \;\leq\; a\, g(x) \qquad \forall x.$$

□

Truncated Densities and Accept-reject

- Suppose the target is a **truncated version** of an easy distribution $g(x)$:

$$f(x) = \frac{g(x)\,\mathbf{1}\{x \in A\}}{P_g(A)}, \qquad A = \text{allowed region.}$$

- We can draw $X \sim g$ easily, but we only want $X \in A$.
- Accept–Reject Sampling fits perfectly:
  1. Draw $X \sim g$.
  2. If $X \in A$, accept; otherwise, reject.

Why It Works So Well

- Because $a = \frac{1}{P_g(A)}$, the acceptance probability is simply

$$P(\text{accept}) = P_g(X \in A).$$

- Efficiency depends only on how much mass of g lies inside A.
- If truncation is mild (e.g. 80–90% of the mass kept), then the acceptance rate is high and the algorithm is almost costless.
- Even for more severe truncation, the method is simple, exact, and needs no renormalization.

Key idea: For truncated densities, Accept–Reject $\Rightarrow$ "Draw from the full g and keep what's valid." No extra math—just logical filtering.

Truncated Distributions and the Accept–Reject Rule

Target density: truncated version of an easy $g(x)$,

$$f(x) = \frac{g(x)\,\mathbf{1}\{x \in A\}}{P_g(A)}, \qquad P_g(A) = \int_A g(x)\,dx.$$

Hence

$$\frac{f(x)}{g(x)} = \begin{cases} \dfrac{1}{P_g(A)}, & x \in A, \\ 0, & x \notin A. \end{cases}$$

To satisfy $f(x) \leq a\,g(x)$ for all x, choose

$$a = \sup_x \frac{f(x)}{g(x)} = \frac{1}{P_g(A)}.$$

Substitute into the Acceptance Condition

The generic rule:

$$U \leq \frac{f(X)}{a\, g(X)}.$$

Substitute the truncated expressions:

$$\frac{f(X)}{a\, g(X)} = \begin{cases} \dfrac{1/P_g(A)}{1/P_g(A)} = 1, & X \in A, \\ 0, & X \notin A. \end{cases}$$

Therefore

$$U \leq \begin{cases} 1, & X \in A, \\ 0, & X \notin A. \end{cases}$$

Interpretation:

- If $X \in A$: $U \leq 1$ always true $\Rightarrow$ accept.

Conclusion: Why It Simplifies Perfectly

- For truncated densities, the acceptance test reduces to a simple membership check:

$$U \leq \frac{f(X)}{a\, g(X)} \iff X \in A.$$

- Inside A, f and g have the same shape—just rescaled by $1/P_g(A)$.
- The acceptance rate is $P_g(A)$: the mass of g inside A.
- Hence the algorithm is extremely efficient:
  1. Draw $X \sim g$,
  2. Accept if $X \in A$.

Summary: In the truncated case, Accept–Reject becomes "keep draws that lie in the truncation region."

Acceptance Pitfalls

1. Many rejections: minimize a.
2. Need π/g bounded $\Rightarrow$ g must have thicker tails.
3. Computing a can be hard.

Can we do better? Yes—importance sampling.

Importance Sampling I

Same setup. For any integrable h,

$$\mathbb{E}_\pi[h(\theta)] = \int h(\theta) \frac{\pi(\theta)}{g(\theta)} g(\theta)\, d\theta.$$

Importance Sampling II

With draws $\{\theta_j\}_{j=1}^{m}$ from g,

$$h_m^{IS} := \frac{1}{m}\sum_{j=1}^{m} h(\theta_j)\,\frac{\pi(\theta_j)}{g(\theta_j)} \;\rightarrow\; \mathbb{E}_\pi[h(\theta)].$$

Importance Sampling III (CLT)

If $\mathbb{E}_\pi[\frac{\pi(\theta)}{g(\theta)}]$ exists, then

$$m^{1/2}\big(h_m^{IS} - \mathbb{E}_\pi[h(\theta)]\big) \;\Rightarrow\; N(0,\sigma^2),$$

with

$$\sigma^2 \approx \frac{1}{m}\sum_{j=1}^{m}\big(h(\theta_j) - h_m^{IS}\big)^2 \left(\frac{\pi(\theta_j)}{g(\theta_j)}\right)^2.$$

Importance Sampling IV: Variance Intuition

We want the weight ratio $\pi(\theta)/g(\theta)$ to be as flat as possible. Ideally $g = \pi$.

Importance Sampling V: Picking g

Use a local (e.g., Taylor) approximation to π as g. Question: how to compute the Taylor approximation?

Existence Condition

A simple sufficient condition: $\pi(\theta)/g(\theta)$ bounded. Denote $\omega(\theta) = \pi(\theta)/g(\theta)$.

Unknown Normalizing Constants

If only unnormalized densities $\tilde{\pi}, \tilde{g}$ are available, then

$$\mathbb{E}_\pi[h(\theta)] = \frac{\displaystyle\int h(\theta)\,\frac{\tilde{\pi}(\theta)}{\tilde{g}(\theta)}\,\tilde{g}(\theta)\,d\theta}{\displaystyle\int \frac{\tilde{\pi}(\theta)}{\tilde{g}(\theta)}\,\tilde{g}(\theta)\,d\theta}.$$

Self-Normalized IS Estimator

$$h_m^{SN} = \frac{\sum_{j=1}^{m} h(\theta_j)\,\omega(\theta_j)}{\sum_{j=1}^{m} \omega(\theta_j)}, \quad \sigma^2 \approx \frac{m \sum_{j=1}^{m} \left(h(\theta_j) - h_m^{SN}\right)^2 \omega(\theta_j)^2}{\left(\sum_{j=1}^{m} \omega(\theta_j)\right)^2}.$$

Example I: Bad g (Heavy Tails Target)

Suppose π is t_ν but we sample from $g = N(0,1)$. Estimate $\mathbb{E}[X]$ of t_ν using IS weights $\omega(\theta) = t_\nu(\theta)/\phi(\theta)$.

Computation Sketch

Draw $\theta_j \sim N(0,1)$, then

$$\widehat{\text{mean}} = \frac{1}{m}\sum_{j=1}^{m} \theta_j \, \omega(\theta_j), \quad \widehat{\text{Var}}(\widehat{\text{mean}}) = \frac{1}{m}\sum_{j=1}^{m} (\theta_j - \widehat{\text{mean}})^2 \, \omega(\theta_j)^2.$$

Illustration (Reported in Slides)

As $\nu = 3, 4, 10, 100$, the estimated variance of the mean falls, but can be extremely large for small ν under normal g.

Table (Example I)

ν	3	4	10	100
Est. Mean	0.1026	0.0738	0.0198	0.0000
Est. Var(Est. Mean)	684.52	365.66	36.82	3.59

Example II: Heavy-Tailed g for Light-Tailed Target

Now $\pi = N(0,1)$, but draw from $g = t_\nu$. Variance of the IS estimator is moderate across ν.

Table (Example II)

t_ν	3	4	10	100
Est. Mean	-0.0104	-0.0075	0.0035	-0.0029
Est. Var(Est. Mean)	2.0404	2.1200	2.2477	2.7444

Relative Numerical Efficiency (RNE)

If $g = \pi$, then

$$\sigma^2 \approx \frac{1}{m} \sum_{j=1}^{m} \left(h(\theta_j) - h_m^{IS}\right)^2 \approx \mathrm{Var}_\pi[h(\theta)].$$

Define

$$\mathrm{RNE} = \frac{\mathrm{Var}_\pi[h(\theta)]}{\sigma^2}.$$

RNE close to 1: good IS; near 0: poor IS.

RNE Tables

Target t_ν, $g = N(0,1)$:

$$\text{RNE} = \{0.0134,\ 0.0200,\ 0.0788,\ 0.2910\} \text{ for } \nu = \{3, 4, 10, 100\}.$$

Target $N(0,1)$, $g = t_\nu$:

$$\text{RNE} = \{0.4777,\ 0.4697,\ 0.4304,\ 0.3471\}.$$

Two researchers share the likelihood $f(Y^T \mid \theta)$ but have priors $\pi_1(\theta) \neq \pi_2(\theta)$. If researcher 1 has draws $\theta^{(j)} \sim \pi(\theta \mid Y^T, \pi_1)$, then for any h,

$$\int h(\theta)\, \pi(\theta \mid Y^T, \pi_2)\, d\theta \approx \frac{\sum_{j=1}^m h(\theta^{(j)})\, \dfrac{\pi_2(\theta^{(j)})}{\pi_1(\theta^{(j)})}}{\sum_{j=1}^m \dfrac{\pi_2(\theta^{(j)})}{\pi_1(\theta^{(j)})}}.$$

Derivation for Prior Robustness

$$\int h(\theta)\pi(\theta \mid Y^T, \pi_2)\, d\theta = \frac{\int h(\theta)\, f(Y^T \mid \theta)\pi_2(\theta)\, d\theta}{\int f(Y^T \mid \theta)\pi_2(\theta)\, d\theta} = \frac{\int h(\theta)\, \frac{\pi_2(\theta)}{\pi_1(\theta)}\, \pi(\theta \mid Y^T, \pi_1)\, d\theta}{\int \frac{\pi_2(\theta)}{\pi_1(\theta)}\, \pi(\theta \mid Y^T, \pi_1)\, d\theta}.$$

Importance Sampling Summary

- Choose g close to π (match location, scale, tails).
- Use self-normalized IS if normalizing constants unknown.
- Diagnose with RNE; respecify g if RNE is low.

Takeaways

- Simulation approximates expectations under complex posteriors/marginals.
- RNG quality matters; use proven libraries.
- Acceptance sampling is simple but can be inefficient.
- Importance sampling is powerful; success hinges on a good proposal.