Simulation Methodology: An Overview

Peter W. Glynn
Stanford University

Theory of RL Bootcamp, Simons Institute
September 4, 2020
Outline:

I. Simulation: Basic Terminology
II. Connection to Numerical Integration
III. The Monte Carlo Method
IV. Dimensional Insensitivity for Monte Carlo
V. Quasi-Random Sequences
VI. Output Analysis
VII. Replication
VIII. Sub-Sampling
IX. Output Analysis in Parallel Computing Context
I. Simulation: Basic Terminology

Simulation:
- Generate trajectories of a dynamical system

\[ x_{n+1} = g(x_n) \]

or

\[ \frac{d}{dt}x(t) = \mu(x(t)) \]

Stochastic Simulation:
- Generate trajectories of a (stochastic) dynamical system

\[ X_{n+1} = g(X_n, \xi_{n+1}) \]

or

\[ \frac{d}{dt}X(t) = \mu(X(t)) + \xi(t) \]
Goal: Compute $\alpha = E[W]$, where $W = f(X_0, X_1, \ldots, X_T)$

Method:
- Generate $n$ iid replications $W_1, W_2, \ldots, W_n$ of $W$
- Estimate $\alpha$ via

$$\alpha_n = \frac{1}{n} \sum_{i=1}^{n} W_i$$
Note that if

\[ X_{i+1} = g(X_i, \xi_{i+1}) \]

\[ s/t \quad X_0 = x \]

then

\[ \alpha = E[W] \]

\[ = E[f(X_0, X_1, \ldots, X_d)] \]

\[ = E[\tilde{f}(\xi_1, \ldots, \xi_d)] \]

\[ = \int_{\mathbb{R}^d} \tilde{f}(z_1, \ldots, z_d) \prod_{i=1}^{d} h_i(z_i) dz_i \]

Such an expectation can be expressed as a \( d \)-dimensional integral

Typically, with \( d \) large
Conversely, if

$$\alpha = \int_{\mathbb{R}^d} q(z_1, \ldots, z_d) dz_1 \ldots dz_d$$

$$= \int_{\mathbb{R}^d} \frac{q(z_1, \ldots, z_d)}{\prod_{i=1}^{d} h_i(z_i)} \prod_{i=1}^{d} h_i(z_i) \, dz_i$$

$$= E \left[ \frac{q(Z_1, \ldots, Z_d)}{\prod_{i=1}^{d} h_i(Z_i)} \right]$$

Every $d$-dimensional integral can be represented as an expectation
Using sampling-based methods to compute (higher dimensional) integrals is known as the *Monte Carlo* method.

Stochastic Simulation $\iff$ *Monte Carlo* Method
III. The Monte Carlo Method

Goal: Compute $\alpha = E[W]$

Method:
- Generate $n$ iid replications $W_1, W_2, \ldots, W_n$ of $W$
- Form

$$\alpha_n = \bar{W}_n = \frac{1}{n} \sum_{i=1}^{n} W_i$$

Proof of validity: Law of Large Numbers (LLN)

$a.s. \Rightarrow \frac{1}{n} \rightarrow E[W] \Rightarrow \alpha_n \rightarrow \alpha$
Goal: Compute $\alpha = E[W]$

Method:

- Generate $n$ iid replications $W_1, W_2, \ldots, W_n$ of $W$
- Form

$$\alpha_n = \bar{W}_n = \frac{1}{n} \sum_{i=1}^{n} W_i$$

Proof of validity: Law of Large Numbers (LLN)

$$\alpha_n \xrightarrow{a.s.} \alpha$$

as $n \to \infty$
Convergence rate analysis:

Central Limit Theorem (CLT): If \( \sigma^2 = \text{Var}(Z_1) < \infty \), then

\[
\sqrt{n}(\alpha_n - \alpha) \Rightarrow \sigma N(0, 1)
\]

as \( n \to \infty \)

Informally,

\[
\alpha_n \overset{D}{\approx} \alpha + \frac{\sigma}{\sqrt{n}} N(0, 1)
\]
Convergence rate analysis:

Central Limit Theorem (CLT): If $\sigma^2 = \text{Var}(X) < \infty$, then

$$\sqrt{n}(\alpha_n - \alpha) \Rightarrow \sigma N(0, 1)$$

as $n \to \infty$

Informally,

$$\alpha_n \overset{D}{\approx} \alpha + \frac{\sigma}{\sqrt{n}} N(0, 1)$$

Implications:

- Slow convergence rate
- Problem hardness characterized by a single constant $\sigma$
- Slow convergence rate suggests error assessment is important
Error assessment via asymptotically valid confidence intervals

\[
P \left( \alpha \in \left[ \alpha_n - z \frac{\sigma}{\sqrt{n}}, \alpha_n + z \frac{\sigma}{\sqrt{n}} \right] \right) \to 1 - \delta
\]

where \( z \) is selected to that \( P(-z \leq N(0, 1) \leq z) = 1 - \delta \)
Error assessment via asymptotically valid confidence intervals

\[ P \left( \alpha \in \left[ \alpha_n - z \frac{\sigma}{\sqrt{n}}, \alpha_n + z \frac{\sigma}{\sqrt{n}} \right] \right) \to 1 - \delta \]

where \( z \) is selected to that \( P(-z \leq N(0, 1) \leq z) = 1 - \delta \)

\( \sigma^2 \) is unknown but can be estimated (internally, from the sample) via

\[ s_n^2 = \frac{1}{n-1} \sum_{i=1}^{n} (W_i - \bar{W}_n)^2 \]

So,

\[ \left[ \alpha_n - z \frac{s_n}{\sqrt{n}}, \alpha_n + z \frac{s_n}{\sqrt{n}} \right] \]

is an approximate \( 100(1 - \alpha)\% \) CI
Asymptotic Validity vs Hard Error Bounds

Asymptotic validity:

- If $\sigma^2 = \text{Var}(Z_1) < \infty$, then

$$P\left(\alpha \in \left[\alpha_n - z\frac{s_n}{\sqrt{n}}, \alpha_n + z\frac{s_n}{\sqrt{n}}\right]\right) \rightarrow 1 - \delta$$

as $n \rightarrow \infty$

- No guarantee for fixed $n$
Asymptotic Validity vs Hard Error Bounds

Asymptotic validity:

- If \( \sigma^2 = \text{Var}(Z) < \infty \), then
  \[
P\left( \alpha \in \left[ \alpha_n - z \frac{s_n}{\sqrt{n}}, \alpha_n + z \frac{s_n}{\sqrt{n}} \right] \right) \to 1 - \delta
  \]
as \( n \to \infty \)

- No guarantee for fixed \( n \)

Hard error bounds:

- Chebyshev’s inequality:
  \[
P\left( \alpha \in \left[ \alpha_n - \frac{\epsilon}{\sqrt{n}}, \alpha_n + \frac{\epsilon}{\sqrt{n}} \right] \right) \geq 1 - \frac{c^2}{\epsilon^2}
  \]
  if \( P(|W| \leq c) = 1 \), so we have a hard error bound
Asymptotic Validity vs Hard Error Bounds

Asymptotic validity:

- If $\sigma^2 = \text{Var}(Z_1) < \infty$, then

$$P \left( \alpha \in \left[ \alpha_n - z \frac{s_n}{\sqrt{n}}, \alpha_n + z \frac{s_n}{\sqrt{n}} \right] \right) \rightarrow 1 - \delta$$

as $n \to \infty$

- No guarantee for fixed $n$

Hard error bounds:

- Chebyshev’s inequality:

$$P \left( \alpha \in \left[ \alpha_n - \frac{\epsilon}{\sqrt{n}}, \alpha_n + \frac{\epsilon}{\sqrt{n}} \right] \right) \geq 1 - \frac{c^2}{\epsilon^2}$$

if $P(|W| \leq c) = 1$, so we have a hard error bound

The great majority of Monte Carlo theory focuses on asymptotic validity (using limit theorems)
Goal: Compute

\[ \alpha(\tilde{f}) = E \left[ \tilde{f}(U_1, \ldots, U_d) \right] \overset{\Delta}{=} E \left[ W(\tilde{f}) \right] \]

where the \( U_i \)'s are iid uniform on \([0, 1]\)

- For any (weighted) integration rule, it is known that

\[ \sup_{\tilde{f} \in C^r(k)} \left| \alpha_c(\tilde{f}) - \alpha(\tilde{f}) \right| = O \left( c^{-r/d} \right) \]

as \( c \to \infty \)

"curse of dimensionality"
- Put $\alpha_n(\tilde{f}) = n^{-1} \sum_{i=1}^{n} W_i(\tilde{f})$
- Chebyshev implies that if $|\tilde{f}| \leq k$, then
  \[
P \left( \left| \alpha_n(\tilde{f}) - \alpha(\tilde{f}) \right| > \frac{\epsilon}{\sqrt{n}} \right) \leq \frac{k^2}{\epsilon^2}
\]
- For a given computational budget $c$, $n \approx c/d$. So,
  \[
P \left( \left| \alpha_c(\tilde{f}) - \alpha(\tilde{f}) \right| > \epsilon \sqrt{\frac{d}{c}} \right) \leq \frac{k^2}{\epsilon^2}
\]
- “Dimensional insensitivity”
V. Quasi-Random Sequences

- These are deterministic sequences $u_1, u_2, \ldots$ in $[0, 1]^d$ that are "equidistributed":

$$\sup_{a \in [0,1]^d} \left| \frac{1}{n} \sum_{i=1}^{n} I(u_i \leq a) - \prod_{i=1}^{d} a_i \right| = O \left( \frac{(\log n)^d}{n} \right)$$

- This implies that

$$\left| \frac{1}{n} \sum_{i=1}^{n} \tilde{f}(u_i) - \alpha(\tilde{f}) \right| = O \left( \frac{(\log n)^d}{n} \right)$$

if $f$ has finite Hardy-Krause variation

- Can be very effective at integration in moderate $d$ settings
Suppose we have a simulation-based algorithm for computing $\alpha$.

How long do we need to run the simulation to get a required accuracy?

Output Analysis
Setting 1: IID Replications

Goal: Compute $\alpha = E[W]$

Method: Generate iid copies $W_1, \ldots, W_n$ and estimate via $\alpha_n = \bar{W}_n$

Two types of procedures:
- Fixed sample size:
  Choose $n$ and construct confidence interval of unknown size
- Sequential procedures:
  Choose error tolerance $\epsilon$ and generate samples until confidence interval is of required size
  - Chow-Robbins (1965)
  - G-Whitt (1992)
Setting 2: Smooth Functions of Expectations

- **Goal:** Compute $\alpha = g(E[Z])$
- **Estimator:** $\alpha_n = g(\overline{Z}_n)$
- **Central Limit Theorem:**

$$\alpha_n - \alpha = \nabla g(E[Z]) \left( \overline{Z}_n - E[Z] \right) + o_P(n^{-1/2})$$

$$\frac{n^{1/2}(\alpha_n - \alpha)}{s_n} \Rightarrow N(0, 1)$$

as $n \to \infty$, where $s_n^2 \Rightarrow \sigma^2$ and $\sigma^2 = \text{Var}(\nabla g(E[Z])(Z - E[Z]))$
Application

Goal: Compute

\[
\alpha = E_x \left[ \sum_{i=0}^{\infty} e^{-c_i r(X_i)} \right]
\]

Note that

\[
\alpha = E_x \left[ \sum_{i=0}^{\tau(x)-1} e^{-c_i r(X_i)} \right] + E_x \left[ e^{-c_{\tau(x)}} \right] \cdot \alpha
\]

So,

\[
\alpha = \frac{E_x \left[ \sum_{i=0}^{\tau(x)-1} e^{-c_i r(X_i)} \right]}{1 - E_x \left[ e^{-c_{\tau(x)}} \right]} = g(E[Z]),
\]

where \( g(z_1, z_2) = z_1/(1 - z_2) \)
Setting 3: Steady-State Simulation

- Markov chain $X = (X_n : n \geq 0)$ with unique equilibrium distribution $\pi(\cdot)$
- Goal: Compute

$$\alpha = \int_S r(x)\pi(dx) \quad (= E[r(X_\infty)])$$

Estimator:

$$\alpha_n = \frac{1}{n} \sum_{i=0}^{n-1} r(X_i)$$

$$n^{1/2}(\alpha_n - \alpha) \Rightarrow \sigma N(0, 1)$$

where

$$\sigma^2 = \text{Var}_\pi(r(X_0)) + 2 \sum_{j=1}^{\infty} \text{Cov}_\pi(r(X_0), r(X_j))$$

The time-average variance constant (TAVC) $\sigma^2$ is $2\pi f(0)$, where $f(\cdot)$ is the spectral density of $X$. 
There are many simulation settings in which the variance is difficult to estimate:

- Smooth functions of expectations
- Steady-state simulation
- Stochastic gradient descent
- Quantiles
- etc.
There are many simulation settings in which the variance is difficult to estimate:

- **Goal:** Compute $\alpha$
- **Algorithm:** An estimator $\alpha_n$
- **A limit theorem:**
  \[ a_n(\alpha_n - \alpha) \Rightarrow \sigma N(0, 1) \]
  Now, repeat the algorithm $m$ iid times (m “replications”): $\alpha_n^1, \alpha_n^2, \ldots, \alpha_n^m$
- **Note that**
  \[ \alpha_n^i \overset{D}{\approx} N(\alpha, \sigma^2/a_n^2) \]
- $m$ approximately normal rv’s with unknown mean and unknown variance
- **Confidence interval:** Student-t with $m - 1$ degrees of freedom
Suppose that we wish to compute $\alpha$ using a Monte Carlo algorithm $\alpha_n$ for which

$$n^a(\alpha_n - \alpha) \Rightarrow W$$

where $W$ is a continuous rv. (It can be non-Gaussian and include “nuisance parameters”)

- If $m \ll n$,
  $$m^a(\alpha_m - \alpha) \overset{D}{=} m^a(\alpha_m - \alpha_n) \overset{D}{=} W$$

- So, construct multiple sub-samples of size $m$ from our $n$-sample, and use empirical of
  $$m^a(\alpha^i_m - \alpha_n), \quad 1 \leq i \leq r$$

to estimate $w_1, w_2$ such that

$$P(w_1 \leq W \leq w_2) \approx 1 - \delta$$

- Then,

$$P\left(\alpha \in \left[\alpha_n - \frac{w_2}{n^a}, \alpha_n - \frac{w_1}{n^a}\right]\right) \approx 1 - \delta$$
Goal: Compute $\alpha = E[W]$

- $p$ parallel processors available
- $c$ units of compute time
- Run simulations independently on each processor

$$\overline{W}_i(c) = \frac{\sum_{j=1}^{N_i(c)} W_{ij}}{N_i(c)}$$

- Biased estimator

$$\frac{1}{p} \sum_{i=1}^{p} \overline{W}_i(c) \xrightarrow{D} E[\overline{W}(c)] + \frac{\eta}{\sqrt{pc}} N(0, 1)$$

Bias can dominate if $p$ is large

G + Heidelberger (1990’s)