

Strong Law of large Numbers and ...

Theorem (Strong Law of Large Number (SLLN))

▷ Let X_k , $k \geq 1$, be a sequence of i.i.d. copies of X such that $\mathbb{E} X$ is well-defined
Then

$$\bar{X}_M := \frac{1}{M} \sum_{k=1}^M X_k \xrightarrow{a.s. \& L^1} m_X = \mathbb{E} X \quad \text{as } M \rightarrow +\infty.$$

▷ More genreally, if $\mathbb{E} \psi(X)$ is well-defined, then

$$\frac{1}{M} \sum_{k=1}^M \psi(X_k) \xrightarrow{a.s. \& L^1} \mathbb{E} \psi(X) \quad \text{as } M \rightarrow +\infty.$$

- Notations: $:=$ stands for a the definition of an object.
- This suggests to go back on the scenario space ω and use **simulation** to approximate $\mathbb{E} X$.
- Physical device...? Not realistic...
- On a computer ? Needs normalization.

- How to work on the scenario space, even if X takes infinitely many values ?
- Write $X = \varphi(U)$, U uniformly distributed over $[0, 1]$ or $[0, 1]^d$ where φ is made explicit, **X can be simulated** and ...
- Note that if $U = (U^1, \dots, U^d)$ has $U([0, 1]^d)$ -distribution $\iff U^1, \dots, U^d$ are independent and $U([0, 1])$ -distributed.
- Why not use **(repeated) simulation?**
- Hence everything relies on simulating **independent realizations** of the simplest continuous law:

$$U([0, 1]) = \mathbf{1}_{[0, 1]}(\xi) d\xi$$

- Once again, how?
- History: the idea goes back to Buffon (Buffon's needle) and for practical implementation to Stanislas Ulam during WW II for atomic and then H -bomb.

Simulation: random (?) numbers

- What should they be: not so clear... Say, **binary digits**
- Physical device to “draw”/“sample” at random sequences of 0 and 1?
- Not reliable and, in any case, **too slow** for computational matter.

Switch to random numbers generated on a computer?

- Little theoretical support.
- Random $\Rightarrow$ algorithm complexity = $O(\text{sample size})$.
- Logic approach: any specified sequence of numbers is not random.

Leads to/suggests a less ambitious **statistical** approach ...

Pseudo-random numbers I

- A sequence $(x_n)_{1 \leq n \leq N}$ of **pseudo-random numbers** is
 - ▶ an as perfect as possible **imitation** of a **generic** sample path of $(U_n(\omega))_{n \geq 1}$, U_n i.i.d. with $\mathcal{U}([0, 1])$ -distribution (defined on $(\Omega, \mathcal{A}, \mathbb{P})$),
 - ▶ generated on a computer
 - ▶ with a **low computational cost**.
- What does **generic** mean ? The scenario ω lies in any event of probability 1 of interest. . .
 - ▶ Not so clear because $N < +\infty$!!
 - ▶ whereas asymptotic statistical frequentist properties are requested (averaging, de-correlation, etc)
 - ▶ In particular, for every not too large d ,

$(x_{d(n-1)+1}, \dots, x_{d(n-1)+d})_{n \leq N/d}$ is a good imitation of i.i.d. copies of $\mathcal{U}([0, 1]^d)$

- ▶ Toolbox **DIEHARD** (Marsaglia, 1998).

Pseudo-random numbers II

- By arithmetic means, one may compute **congruational pseudo-random numbers** of the form

- ▶ $x_n = \frac{y_n}{N}, \quad y_{n+1} = a y_n + b \pmod{N}, \quad a \not\equiv 0 \pmod{N},$

- ▶ $N \text{ prime} \Rightarrow o(a) = N - 1 \text{ in } (\mathbb{Z}/N\mathbb{Z})^*.$

- Needs good choices of (very large) **prime** N , $a \in \{1, \dots, N - 1\}$ and b ,
- N is a **prime Mersenne numbers** (among $2^p - 1$, p prime) e.g.

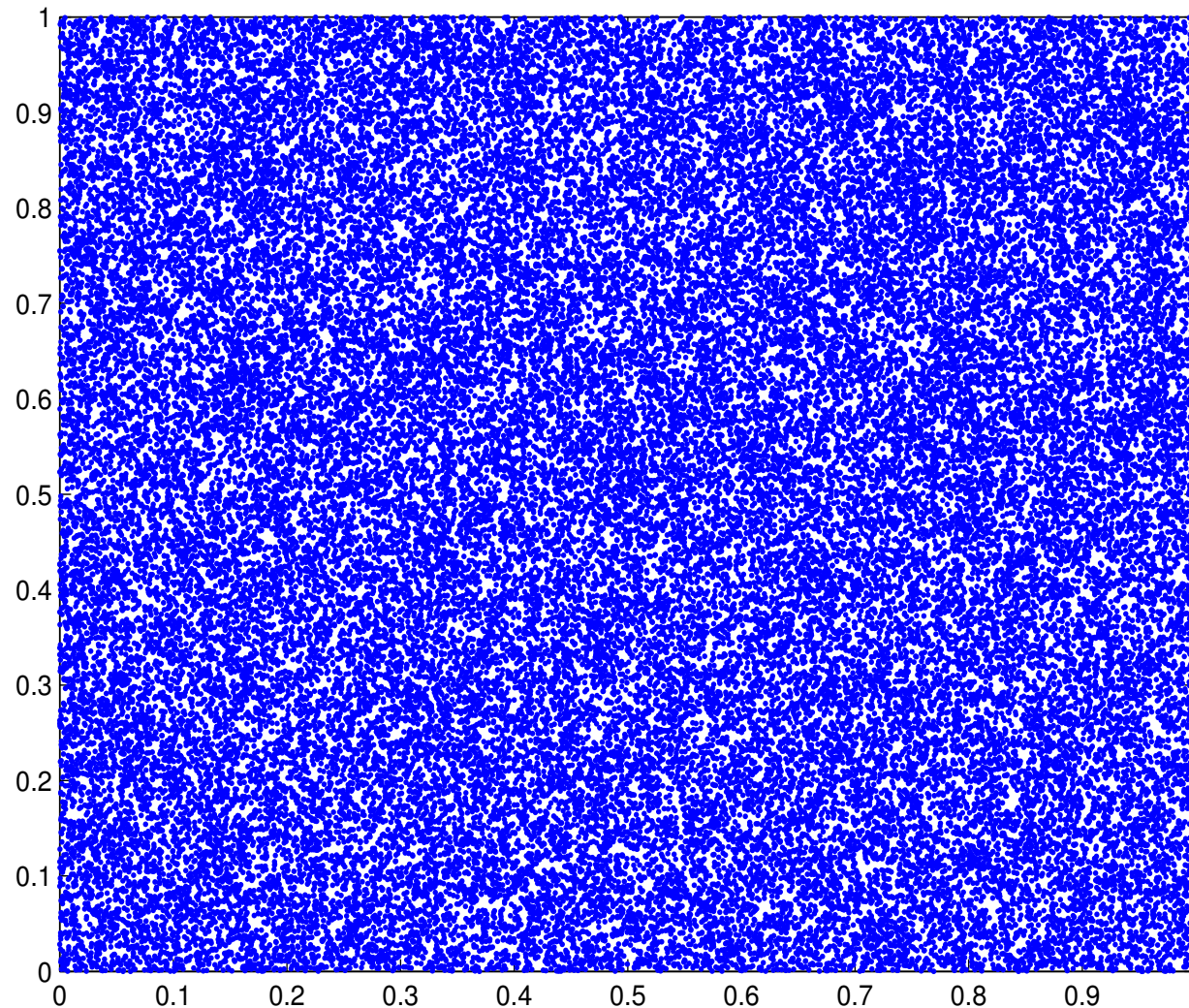
$$N = 2^{19937} - 1.$$

- $\rightsquigarrow$ **Mersenne twister random number generators.**

`www.math.sci.hiroshima-u.ac.jp/~m-mat/MT/emt.html`

- Standard random numbers generators for FORTRAN, C++, Matlab, Python, etc, have improved.

60 000 pseudo-random numbers (texture)



Fundamental theorem of simulation: theory and practice

- Theory:

Theorem (Fundamental theorem of simulation)

Any random variable $X : (\Omega, \mathcal{A}, \mathbb{P}) \rightarrow (E, \mathcal{E})$ Polish space can be written

$$X = \varphi(U), \quad U \stackrel{d}{=} \mathcal{U}([0, 1]) \text{ where } \varphi : [0, 1] \rightarrow (E, \mathcal{E}).$$

- Practice:

- ▶ If $F_X(u) = \mathbb{P}(X \leq u)$, $u \in \mathbb{R}$, cumulative distribution function (c.d.f.),

$$X \stackrel{d}{=} (F_X)_{\text{left}}^{-1}(U), \quad U \stackrel{d}{=} \mathcal{U}([0, 1]).$$

- ▶ Thus $X \stackrel{d}{=} \mathcal{E}(\lambda)$, $F_X(x) = (1 - e^{-\lambda x})\mathbf{1}_{\{x \geq 0\}}$, $\lambda > 0$, so that

$$X \stackrel{d}{=} -\frac{\log(1 - U)}{\lambda} \stackrel{d}{=} -\frac{\log(U)}{\lambda}.$$

- Usually, such a φ is not known. More often there exists a computable φ such that

$$X = \varphi(U), \quad U \stackrel{d}{=} \mathcal{U}([0, 1]^d) \quad \text{or} \quad \stackrel{d}{=} U([0, 1]^{\mathbb{N}^*}).$$

Ex: Box-Muller method for bi-variate normal distribution (see later on)

$$\sqrt{-2 \log U_1} (\cos(2\pi U_2), \sin(2\pi U_2)) \stackrel{d}{=} \mathcal{N}(0; I_2).$$

- $[0, 1]^{\mathbb{N}^*} = \bigcup_{d \geq 1} [0, 1]^d$ set of finite $[0, 1]$ -valued sequences.

$$\varphi(u) = \Psi(\tau(u), u^1, \dots, u^{\tau(u)}) \text{ where } \tau^{-1}(k) \in \mathcal{B}or([0, 1]^k)$$

corresponds to Von Neumann Acceptance-Rejection method.

Ex: Polar method (Marsaglia), compete with Box-Muller for $\mathcal{N}(0; I_2)$.

- However, usually, no closed form, no approximation by cubature formula (due to high dimension d).

Definition (Monte Carlo simulation “0”)

Monte Carlo simulation can be “defined” as

- (1) Representation of X as $X = \varphi(U)$, $U \stackrel{d}{=} \mathcal{U}([0, 1]^d)$, $d \in \mathbb{N}^* \cup \{\infty\}$
- (2) Generate M independent copies $X_k = \varphi(U_k)$, $(U_k)_{k \geq 1}$ i.i.d. with distribution $\mathcal{U}([0, 1]^d)$
- (3) Compute $d \times M$ independent copies $u_1, \dots, u_{dM}$ of the uniform distribution over $[0, 1]$ using pseudo-random numbers, packed d by d as follows $(u_{(k-1)d+1:kd})$, $k = 1 : M$. Compute the arithmetic mean

$$m_x \approx \frac{1}{M} \sum_{k=1}^M \varphi(u_{(k-1)d+1:kd})$$

- (4) Forget about “pseudo-” in pseudo-random numbers of step (3) and think about $u_k = U_k(\omega)$ and $\bar{X}_M(\omega)$, for a generic $\omega \dots$

• **Question.** M how large ? (with $M \ll N/d$ of course! Say $\leq 10\%N/d$)

Rates of convergence

- $\bar{X}_M$ as an unbiased estimator of m_X .

$$\mathbb{E} \bar{X}_M = \frac{1}{M} \sum_{k=1}^M \mathbb{E} X_k = m_X.$$

- Quadratic (L^2 -rate of convergence: *MSE* and *RMSE*).

It is a non asymptotic quadratic exact rate due to independence (no correlation is enough)

$$\begin{aligned} \|\bar{X}_M - m_X\|_2^2 &= \|\bar{X}_M - \mathbb{E} \bar{X}_M\|_2^2 = \mathbb{E} (\bar{X}_M - \mathbb{E} \bar{X}_M)^2 \\ &= \text{Var}(\bar{X}_M) \\ &= \frac{1}{M^2} \sum_{k=1}^M \text{Var}(X_k) = \frac{1}{M^2} M \text{Var}(X) \\ \|\bar{X}_M - m_X\|_2^2 &= \frac{\text{Var}(X)}{M}. \end{aligned}$$

or, equivalently,

$$\|\bar{X}_M - m_x\|_2 = \frac{\sigma_x}{\sqrt{M}}$$

with $\underbrace{\sigma_x = \sqrt{\text{Var}(X)}}_{\text{standard deviation}}$ and $\text{Var}(X) = \mathbb{E}(X - \mathbb{E} X)^2 = \mathbb{E} X^2 - (\mathbb{E} X)^2$.

- Weak rate of convergence.

The weak convergence is ruled by the Central Limit Theorem (*CLT*)

$$\sqrt{M} (\bar{X}_M - m_x) \xrightarrow{\mathcal{L}} \mathcal{N}(0; \sigma_x^2) = \sigma_x Z, \quad Z \stackrel{d}{=} \mathcal{N}(0; 1)$$

as $M \rightarrow +\infty$. We will come back on this crucial result.

- Strong *a.s.* rate of convergence.

The Law of the Iterated Logarithm (*LIL*) provides an *a.s.* rate of convergence, namely

$$\overline{\lim}_M \sqrt{\frac{M}{2 \log(\log M)}} (\bar{X}_M - m_x) = \pm \sigma_x \quad a.s.$$

Weak convergence (very short background)

- Definition: $(Y_M)_{M \geq 1}$ sequence of random variables.

$$Y_M \xrightarrow{\mathcal{L}} Y_\infty \quad \text{as} \quad M \rightarrow +\infty$$

if $\forall f \in \mathcal{C}_{\text{bounded}}(\mathbb{R}, \mathbb{R}), \quad \mathbb{E} f(Y_M) \rightarrow \mathbb{E} f(Y_\infty)$

- Extension: Let

$$\text{Disc}(f) = \{x \in \mathbb{R} : f \text{ is discontinuous at } x\}.$$

Proposition

(a) If $Y_M \xrightarrow{\mathcal{L}} Y_\infty$, $f : \mathbb{R} \rightarrow \mathbb{R}$ is bounded and $\mathbb{P}(Y_\infty \in \text{Disc}(f)) = 0$, then

$$\mathbb{E} f(Y_M) \rightarrow \mathbb{E} f(Y_\infty).$$

(b) Thus, if $f = \mathbf{1}_{[K, K']}$ and $\mathbb{P}(Y_\infty = y) = 0, \forall y \in \mathbb{R}$, then $\text{Disc}(f) = \{K, K'\}$ so that $\mathbb{P}(Y_\infty \in \text{Disc}(f)) = 0$. Hence, as $M \rightarrow +\infty$,

$$\mathbb{P}(Y_M \in [K, K']) = \mathbb{E} \mathbf{1}_{[K, K']}(Y_M) \longrightarrow \mathbb{E} \mathbf{1}_{[K, K']}(Y_\infty) = \mathbb{P}(Y_\infty \in [K, K']).$$

Application to CLT

- How to use the CLT ?

$$\sqrt{M} (\bar{X}_M - m) \xrightarrow{\mathcal{L}} \mathcal{N}(0; \sigma_x^2) = \sigma_x Z, \quad Z \stackrel{d}{=} \mathcal{N}(0; 1)$$

- Assume $\sigma = \sigma_x > 0$. For every $z \in \mathbb{R}$,

$$\mathbb{P}(\sigma Z = z) = \mathbb{P}(Z = z/\sigma) = \int_{\{z/\sigma\}} e^{-\frac{\xi^2}{2}} \frac{d\xi}{\sqrt{2\pi}} = 0. \quad \text{Hence}$$

$$\begin{aligned} \mathbb{P} \left(\sqrt{M} \frac{\bar{X}_M - m_x}{\sigma} \in [b, a] \right) &= \mathbb{P}(\sqrt{M}(\bar{X}_M - m_x) \in [\sigma b, \sigma a]) \\ &\xrightarrow{CLT \& (b)} \mathbb{P}(\sigma Z \in [\sigma b, \sigma a]) \quad \text{as } M \rightarrow +\infty \\ &= \mathbb{P}(Z \in [b, a]). \end{aligned}$$

Confidence intervals I

- The convergence in distribution of the *CLT* means that for every real numbers $b < a$,

$$\lim_M \mathbb{P} \left(\sqrt{M} \frac{\bar{X}_M - m_x}{\sigma_x} \in [b, a] \right) \xrightarrow{M \rightarrow +\infty} \mathbb{P}(\mathcal{N}(0; 1) \in [b, a]) \\ = \Phi_0(a) - \Phi_0(b)$$

where $\Phi_0(x) = \int_{-\infty}^x e^{-\frac{\xi^2}{2}} \frac{d\xi}{\sqrt{2\pi}}$ denotes the c.d.f. of $\mathcal{N}(0; 1)$.

- Keeping in mind $\Phi_0(x) + \Phi_0(-x) = 1$, $a > 0$, $b = -a$.

$$\lim_M \mathbb{P} \left(\sqrt{M} \frac{\bar{X}_M - m_x}{\sigma_x} \in [-a, a] \right) \xrightarrow{M \rightarrow +\infty} 2\Phi_0(a) - 1 = \mathbb{P}(|\mathcal{N}(0; 1)| \leq a).$$

- Confidence level α . Let q_α be the two-sided quantile

$$\mathbb{P}(|\mathcal{N}(0; 1)| \leq q_\alpha) = \alpha \quad \text{i.e.} \quad 2\Phi_0(q_\alpha) - 1 = \alpha.$$

- Define the **random interval**

$$J_{\alpha,M}(\omega) := \left[\bar{X}_M(\omega) - q_\alpha \frac{\sigma_x}{\sqrt{M}}, \bar{X}_M(\omega) + q_\alpha \frac{\sigma_x}{\sqrt{M}} \right],$$

$$\begin{aligned} \text{then } \mathbb{P}\{\omega : m_x \in J_{\alpha,M}(\omega)\} &= \mathbb{P}\left(\sqrt{M} \frac{|\bar{X}_M - m_x|}{\sigma_x} \leq q_\alpha\right) \\ &\xrightarrow{M \rightarrow \infty} \mathbb{P}(|\mathcal{N}(0;1)| \leq q_\alpha) = \alpha. \end{aligned}$$

- $J_{\alpha,M}$ is asymptotically a **confidence interval** for $\bar{X}_M$ at level α .
- Rate of convergence in the CLT**

Theorem (Berry-Essen (and Shiryaev))

If $X_1 \in L^3(\mathbb{P})$, $\sigma_x > 0$, the rate in the **CLT** is ruled by $\forall n \geq 1, \forall x \in \mathbb{R}$,

$$\left| \mathbb{P}(\sqrt{M}(\bar{X}_M - m_x) \leq x\sigma_x) - \Phi_0(x) \right| \leq \frac{C \mathbb{E}|X_1 - \mathbb{E}X_1|^3}{\sigma_x^3 \sqrt{M}} \frac{1}{1 + |x|^3}.$$

- It turns out to be again $1/\sqrt{M}$.

Confidence interval II

- In practice the standard deviation σ_X is unknown. But

$$\begin{aligned}\bar{V}_M &= \frac{1}{M-1} \sum_{k=1}^M (X_k - \bar{X}_M)^2 \\ &= \frac{1}{M-1} \sum_{k=1}^M X_k^2 - \frac{M}{M-1} \bar{X}_M^2 \\ &\xrightarrow{M \rightarrow +\infty} \mathbb{E} X^2 - (\mathbb{E} X)^2 = \text{Var}(X) = \sigma_X^2\end{aligned}$$

by applying twice the *SLLN*.

- Why $M-1$ and not M ? To be unbiased *i.e.* $\mathbb{E} V_M = \sigma_X^2$! We don't care in Numerical Probability.
- Confidence interval:

$$I_{\alpha,M} := \left[\bar{X}_M(\omega) - q_\alpha \sqrt{\frac{\bar{V}_M}{M}}, \bar{X}_M(\omega) + q_\alpha \sqrt{\frac{\bar{V}_M}{M}} \right] \simeq J_{\alpha,M}.$$

Monte Carlo simulation I

Definition (Monte Carlo simulation I)

Simulate $X_1, \dots, X_M$.

- Define a confidence level $\alpha \in (0, 1)$,
- Compute $\bar{X}_M$,
- Compute $\bar{V}_M$,
- Design the (empirical) confidence interval

$$I_{\alpha, M} = \left[\bar{X}_M(\omega) - q_\alpha \sqrt{\frac{\bar{V}_M}{M}}, \bar{X}_M(\omega) + q_\alpha \sqrt{\frac{\bar{V}_M}{M}} \right] \dots$$

In fact one also has that

$$\mathbb{P}(\{\omega : m_X \in I_{\alpha, M}(\omega)\}) \xrightarrow{M \rightarrow +\infty} \mathbb{P}(|\mathcal{N}(0; 1)| \leq q_\alpha) = \alpha.$$

Monte Carlo simulation II

- It is just another point of view
- Starting from the obvious

$$q_\alpha \sqrt{\frac{\overline{V}_M}{M}} = \varepsilon \iff M = q_\alpha^2 \frac{\overline{V}_M}{\varepsilon^2} \simeq q_\alpha^2 \frac{\sigma_X^2}{\varepsilon^2}$$

Definition (Monte Carlo simulation II)

- ▶ Define an *RMSE* $\varepsilon > 0$ (quadratic error).
- ▶ Define a confidence level α .
- ▶ Simulate $X_1, \dots, X_M$ and compute $\overline{X}_M$ and $\overline{V}_M$ until $\frac{\overline{V}_M}{M} = \frac{\varepsilon^2}{q_\alpha^2}$.
- ▶ Compute the confidence interval.

$$I_{\alpha, M} = [\overline{X}_M - \varepsilon, \overline{X}_M + \varepsilon].$$