ORIE 4580/5580: Simulation Modeling and Analysis

ORIE 5581: Monte Carlo Simulation

unit 3: intro to Monte Carlo simulation

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expectation and variance of sums of rvs

linearity of expectation

for any rvs X and Y, and any constants $a, b \in \mathbb{R}$

$$\mathbb{E}[aX + bY] = a\mathbb{E}[X] + b\mathbb{E}[Y]$$

note: no assumptions! (in particular, does not need independence)

- for general X, Y

$$Var(aX + bY) = a^2 Var(X) + b^2 Var(Y) + 2abCov(XY)$$

- when X and Y are independent

$$Var(aX + bY) = a^2 Var(X) + b^2 Var(Y)$$

law of large numbers

let $X_1, X_2, \ldots$ be a sequence of independent rvs with $\mathbb{E}[X_i] = \mu$ for all i
then, "almost" always

$$\bar{X}_n = \frac{1}{n} \sum_{i=1}^{n} X_i \longrightarrow \mu \quad , \quad \text{as } n \to \infty$$

note: for any finite n, $\bar{X}_n = \frac{1}{n} \sum_{i=1}^{n} X_i$ is still a random variable

central limit theorem

let $X_1, X_2, \ldots$ be a sequence of independent rvs with

$$\mathbb{E}[X_i] = \mu, \, Var(X_i) = \sigma^2 < \infty \text{ for all } i$$

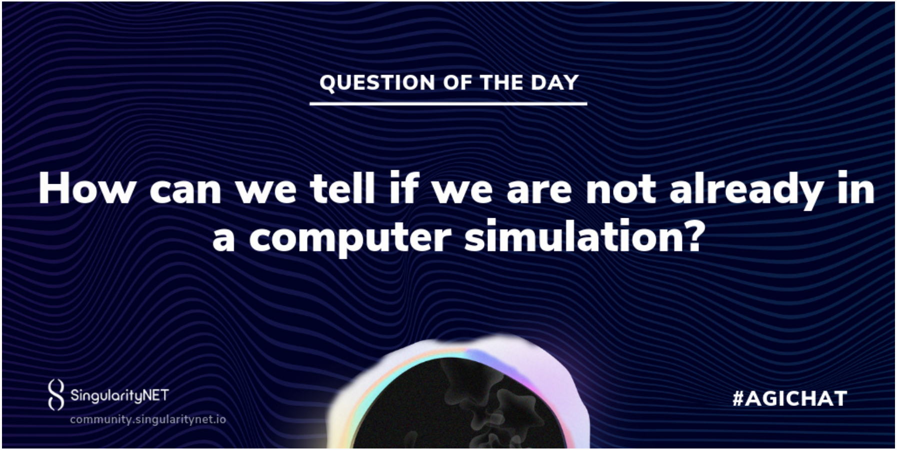
then,

$$\sqrt{n}(\bar{X}_n - \mu) \xrightarrow{D} \sigma\mathcal{N}(0,1) = \mathcal{N}(0,\sigma^2) \quad , \quad \text{as } n \to \infty$$

approximations for large n,

$$\bar{X}_n = \frac{1}{n}\sum_{i=1}^{n} X_i \overset{D}{\approx}$$

$$S_n = \sum_{i=1}^{n} X_i \overset{D}{\approx}$$


QUESTION OF THE DAY
How can we tell if we are not already in a computer simulation?
SingularityNET
community.singularitynet.io
#AGICHAT

staffing a food bank

a food bank depends on volunteers for its labor pool

on any given day, the number of workers who show up is $\mathit{Uniform}(\{1, 2, \ldots, 9\})$,

while the number of donations needed to be collected is $\mathit{Uniform}(\{1, 2, \ldots, 29\})$

assuming the work is equally divided among each worker, what is the average load for each worker?

- let $X =$ number of workers, $Y =$ number of donations
- we have $\frac{\mathbb{E}[Y]}{\mathbb{E}[X]} = \frac{30/2}{10/2} = 3$
- on the other hand, $\mathbb{E}[\mathit{Load}] = \mathbb{E}\left[\frac{Y}{X}\right]$; is this also 3?
- let us simulate and check!

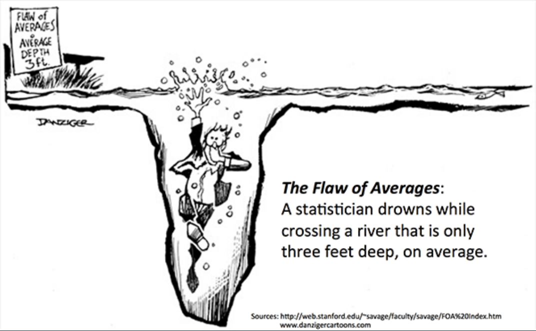
understanding what happened

for random variables X and Y, and function $g(\cdot, \cdot)$,

$$\mathbb{E}[g(X, Y)] \neq g(\mathbb{E}[X], \mathbb{E}[Y])!$$

flaw of averages

moral: in most settings, average inputs don't give average outputs!



The Flaw of Averages: A statistician drowns while crossing a river that is only three feet deep, on average.

Sources: http://web.stanford.edu/~savage/faculty/savage/FOA%20Index.htm
www.danzigercartoons.com

what can go wrong?

- non-linearities
- correlations between rvs
- 'inspection paradox' (buses take longer to arrive than they should!)
- ...

simulation allows us to avoid such problems!

confidence intervals

how many replications?

simulating food bank for many days (samples/replications) = distribution of loads

as number of replications increases, sample average $\rightarrow$ average load (by LLN)

question: every time we run the simulation model with some fixed number of replications, our estimate of $\mathbb{E}[\mathit{load}]$ changes.
how 'confident' can we be in our estimate?

- *answer*: use CLT to build a confidence interval!

confidence intervals

let $X_1, X_2, \ldots$ be a sequence of i.i.d. random variables with mean $\mathbb{E}[X_1] = \mu$ and variance $Var(X_1) = \sigma^2 < \infty$

want to measure μ from simulations

confidence interval: attempt 1...

an interval $[a, b]$ is called a 95% confidence interval for $\mathbb{E}[X_1]$ if

$$\mathbb{P}[a \leq \mathbb{E}[X_1] \leq b] \geq 0.95$$

what is wrong with this?

confidence intervals: definition

an random interval $[A, B]$ (computed from data/experiments) is called a 95% confidence interval for some (deterministic) quantity μ if

$$\mathbb{P}[A \leq \mu \leq B] \geq 0.95$$

confidence intervals for population mean

$X_1, X_2, \ldots$ are i.i.d. rvs with $\mathbb{E}[X_1] = \mu$ and $Var(X_1) = \sigma^2 < \infty$; $\bar{X}_n = \frac{1}{n}\sum_{i=1}^{n} X_i$

- from the central limit theorem:

$$\sqrt{n}(\bar{X}_n - \mu) \stackrel{D}{\approx} \sigma\mathcal{N}(0,1) = \mathcal{N}\left(0, \sigma^2\right)$$

- from the inverse cdf of $\mathcal{N}(0,1)$, we can compute

$$\mathbb{P}[\qquad\qquad \leq \mathcal{N}(0,1) \leq \qquad\qquad] \geq 0.95.$$

confidence intervals

want to measure $\mu = \mathbb{E}[X_1]$ from simulations

- from the central limit theorem: $\sqrt{n}(\bar{X}_n - \mu) \overset{D}{\approx} \sigma\mathcal{N}(0,1)$
- from the cdf of $\mathcal{N}(0,1)$, we have $\mathbb{P}[-1.96 \leq \mathcal{N}(0,1) \leq 1.96] \geq 0.95$

putting these together, we have:

confidence intervals: problems

- the confidence interval is approximate because

- the confidence interval is ‘exact’ when

- the confidence interval above requires knowledge of σ^2

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- the confidence interval above requires knowledge of σ^2

can replace σ^2 with its sample estimator

$$s_n^2 = \frac{1}{n-1} \sum_{i=1}^{n} (X_i - \bar{X}_n)^2 .$$

fixed sample-size: recipe for CI

approximate $100(1-\alpha)\%$ Gaussian CI for $\mathbb{E}X$

1. select a sample size N
2. generate N i.i.d. samples $X_1, X_2, \ldots, X_N$ of X
3. compute the estimators $\bar{X}_N, s_N^2$

$$\bar{X}_N = \frac{1}{N}\sum_{n=1}^{N} X_n, \qquad s_N^2 = \frac{1}{N-1}\sum_{n=1}^{N}\left(X_n - \bar{X}_N\right)^2$$

4. look up the value of $z_{\alpha/2}$ such that

$$\mathbb{P}[-z_{\alpha/2} \le N(0,1) \le z_{\alpha/2}] = 1-\alpha$$

5. the approximate $100(1-\alpha)\%$ CI for $\mathbb{E}X$ is given by

$$\bar{X}_N \mp z_{\alpha/2}\,\frac{s_N}{\sqrt{N}}$$

selecting the sample size

how large should N be so that the resulting $100(1-\alpha)\%$ confidence interval will have a pre-specified width?

- CI $\implies \bar{X}_N \mp z_{\alpha/2}\left(\sigma/\sqrt{N}\right)$
- half-width $\implies z_{\alpha/2}\dfrac{\sigma}{\sqrt{N}}$
- ℓ be the desired half-width
- Set $N =$

selecting the sample size

- problem: σ^2 is unknown!
- estimating σ^2 through s_N^2 requires simulation!
- solution: 'pilot runs'

  perform k simulation runs to get $[X'_n : n = 1, \ldots, k]$ as outcomes

  compute

$$\tilde{X}_k = \frac{1}{k} \sum_{n=1}^{k} X'_n, \qquad \tilde{s}_k^2 = \frac{1}{k-1} \sum_{n=1}^{k} \left(X'_n - \tilde{X}_k \right)^2$$

  use $\tilde{s}_k^2$ to estimate σ^2

for confidence level α, half-width ℓ, set

$$N = \left\lceil \frac{z_{\alpha/2}^2 \tilde{s}_k^2}{\ell^2} \right\rceil$$

basic simulation workflow

- perform pilot run of k simulations (sufficient but not large k)
- compute required sample-size N for desired confidence interval
- run N additional simulations $\Longrightarrow$ production runs
- form fixed-sample confidence intervals from these N samples
- note: final CI may be different than desired, because it is constructed by using s_N^2 (may be larger/smaller than $\tilde{s}_k^2$)
- for the final confidence interval, discard the information from the trial runs not a problem, since $N \gg k$ usually

confidence intervals as a social contract

a random interval $[A, B]$ (computed from data/experiments) is a 95% confidence interval for some unknown μ if before the experiment is done

$$\mathbb{P}[A \leq \mu \leq B] \geq 0.95$$

confidence intervals vs quantiles

the CI for the mean is NOT the same as the quantiles of a random variable.

- suppose that X is a rv with probability density function

- we can select q_1 and q_2 so that

$$\mathbb{P}[q_1 \leq X \leq q_2] = 0.95,$$

but $[q_1, q_2]$ is not a 95% confidence interval for $\mathbb{E}X$.

three advanced probability tools

tool 1: Jensen's inequality

Q: can we say something about $\mathbb{E}[f(X)]$ vs $f(\mathbb{E}[X])$ (in particular, $\geq$ or $\leq$) without simulating?

Jensen's inequality

if X is a random variable and f is a convex function, then

$$\mathbb{E}[f(X)] \geq f(\mathbb{E}[X])$$

example – in our food-bank staffing problem, since $f(x) = \frac{1}{x}$, $x > 0$ is convex:

$$\mathbb{E}[Y]\mathbb{E}\left[\frac{1}{X}\right] \geq \frac{\mathbb{E}[Y]}{\mathbb{E}[X]}$$

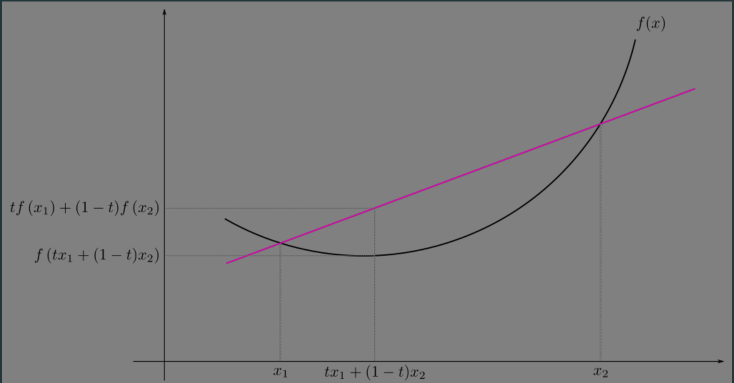
tool 1: Jensen's inequality

Jensen's inequality

if X is a random variable and f is a convex function, then

$$\mathbb{E}[f(X)] \geq f(\mathbb{E}[X])$$

proof sketch (plus way to remember)



tool 2: Chebyshev's Inequality

Q: since the CLT convergence is faster/slower for different rvs, can we be sure that CIs based on variance always make sense?

Chebyshev's inequality

let X be any rv with finite mean μ and finite variance $\sigma^2 > 0$

then for any $k > 0$,

$$\mathbb{P}\left[|X - \mu| \geq k\sigma\right] \leq \frac{1}{k^2}$$

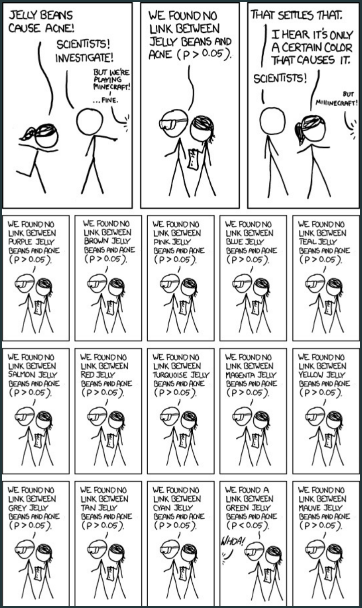
‘always-valid’ confidence intervals

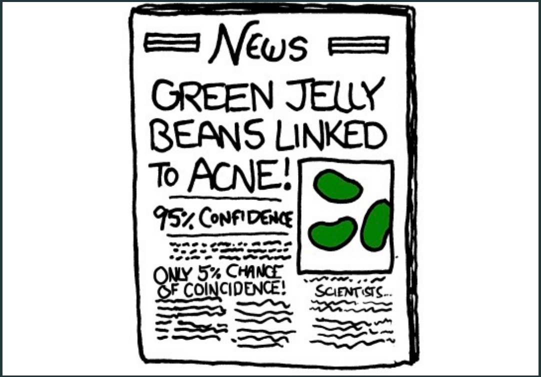
Chebyshev’s inequality

let X be any rv with finite mean μ and finite variance $\sigma^2 > 0$
then for any $k > 0$,

$$\mathbb{P}\left[|X - \mu| \geq k\sigma\right] \leq \frac{1}{k^2}$$

worst-case CI: if we choose $k = 2$, then we always have 75% confidence intervals


JELLY BEANS CAUSE ACNE!
SCIENTISTS! INVESTIGATE!
BUT WE'RE PLAYING MINECRAFT!
... FINE.
WE FOUND NO LINK BETWEEN JELLY BEANS AND ACNE (P > 0.05).
THAT SETTLES THAT.
I HEAR IT'S ONLY A CERTAIN COLOR THAT CAUSES IT.
SCIENTISTS!
BUT MIIIINECRAFT!
WE FOUND NO LINK BETWEEN PURPLE JELLY BEANS AND ACNE (P > 0.05).
WE FOUND NO LINK BETWEEN BROWN JELLY BEANS AND ACNE (P > 0.05).
WE FOUND NO LINK BETWEEN PINK JELLY BEANS AND ACNE (P > 0.05).
WE FOUND NO LINK BETWEEN BLUE JELLY BEANS AND ACNE (P > 0.05).
WE FOUND NO LINK BETWEEN TEAL JELLY BEANS AND ACNE (P > 0.05).
WE FOUND NO LINK BETWEEN SALMON JELLY BEANS AND ACNE (P > 0.05).
WE FOUND NO LINK BETWEEN RED JELLY BEANS AND ACNE (P > 0.05).
WE FOUND NO LINK BETWEEN TURQUOISE JELLY BEANS AND ACNE (P > 0.05).
WE FOUND NO LINK BETWEEN MAGENTA JELLY BEANS AND ACNE (P > 0.05).
WE FOUND NO LINK BETWEEN YELLOW JELLY BEANS AND ACNE (P > 0.05).
WE FOUND NO LINK BETWEEN GREY JELLY BEANS AND ACNE (P > 0.05).
WE FOUND NO LINK BETWEEN TAN JELLY BEANS AND ACNE (P > 0.05).
WE FOUND NO LINK BETWEEN CYAN JELLY BEANS AND ACNE (P > 0.05).
WE FOUND A LINK BETWEEN GREEN JELLY BEANS AND ACNE (P < 0.05).
WHOA!
WE FOUND NO LINK BETWEEN MAUVE JELLY BEANS AND ACNE (P > 0.05).


NEWS
GREEN JELLY BEANS LINKED TO ACNE!
95% CONFIDENCE
ONLY 5% CHANCE OF COINCIDENCE!
SCIENTISTS...

tool 3: the union bound

Q: how can we get simultaneous confidence intervals for multiple hypothesis?

• e.g. I give you five 95% confidence intervals; do they simultaneously contain their respective means 95% of the time?

tool 3: the union bound

Q: how can we get simultaneous confidence intervals for multiple hypothesis?

the union bound

let $A_1, A_2, \ldots, A_k$ be events; then

$$\begin{aligned} P(A_1 \cap A_2 \cap \cdots \cap A_k) &= 1 - P(A_1^c \cup A_2^c \cup \cdots \cup A_k^c) \\ &\geq 1 - (P(A_1^c) + P(A_2^c) + \cdots + P(A_k^c)) \end{aligned}$$

let A_i = event that the ith CI contains its true mean...