MAS472/6004 Computational Inference

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Computational Inference

Simple computational tools for solving hard statistical problems.

- Monte Carlo/simulation
- MC and simulation in frequentist inference
- Random number generation/ simulating from probability distributions
- Further Bayesian computation

Methods implemented via simple programs in R.

Chapter 1: Monte Carlo methods

Problem 1: estimating probabilities

A particular site is being considered for a wind farm. At that site, the log of the wind speed in m/s on day t is known to follow an $AR(2)$ process:

$$Y_t = 0.6Y_{t-1} + 0.4Y_{t-2} + \varepsilon_t, \tag{1}$$

with $\varepsilon_t \sim N(0, 0.01)$.

If $Y_1 = Y_2 = 1.5$, what is the **probability** that the wind speed $\exp(Y_t)$ will be below 15 kmh for more than 10 days in a 100 day period?

Problem 2: estimating variances

Given a sample of 5 standard normal random variables $X_1, \ldots, X_5$, what is the **variance** of

$$\max_i\{X_i\} - \min_i\{X_i\}$$

Problem 3: Estimating percentiles

The concentration of pollutant at any point in region following release from point source can be describe by the model

$$C(x,y,z) = \frac{Q}{2\pi u_{10}\sigma_z\sigma_y} \exp\left[-\frac{1}{2}\left\{\frac{y^2}{\sigma_y^2} + \frac{(z-h)^2}{\sigma_z^2}\right\}\right], \quad (2)$$

C: air concentration of pollutant, Q: release rate, u_{10}: wind speed at $10m$ above ground, σ_y, σ_z: diffusion parameters in horizontal and vertical directions, h:release height, (x, y, z): coordinates along wind direction, cross wind and above ground.

Given $Q = 100$, $h = 50$m, but u, σ_z, σ_y uncertain. If

$\log u_{10} \sim N(2, .1)$ $\log \sigma_y^2 \sim N(10, 0.2)$ $\log \sigma_z^2 \sim N(5, 0.05)$

What is the **95th percentile** of $C(100, 100, 40)$?

Problem 4:Estimating expectations

A hospital ward has 8 beds

- The number of patients arriving each day is uniformly distributed between 0 and 5 inclusive.
- The length of stay for each patient is also uniformly distributed between 1 and 3 days inclusive.

If all 8 beds are free initially, what is the **expected** number of days before there are more patients than beds?

Problem 5: Optimal decisions

The Monty Hall Problem

On a game show you are given the choice of three doors.

- Behind one door is a car; behind the others, goats.

The rules of the game are

- After you have chosen a door, the game show host, Monty Hall, opens one of the two remaining doors to reveal a goat.
- You are now asked whether you want to stay with your first choice, or to switch to the other unopened door.

What is the **optimal strategy**? And what is the resulting probability of winning?

These 5 problems are all either hard or impossible to tackle analytically. However, the **Monte Carlo method**, can be used to obtain approximate answers to all of them.

> *Monte Carlo methods are a broad class of computational algorithms relying on repeated random sampling to obtain numerical results. They use randomness to solve problems that might be deterministic in principle.*

Some useful results

Monte Carlo is primarily used to calculate integrals. For example

- Expectation of a random variable $X \sim f(\cdot)$, or a function of it

$$\mathbb{E}g(X) = \int g(x)f(x)\mathrm{dx}$$

- Variance

$$\mathbb{V}\mathrm{ar}(X) = \mathbb{E}(X^2) - \mathbb{E}(X)^2. \tag{3}$$

- Probability $\mathbb{P}(X < a)$ is the expectation of $\mathbb{I}_{X<a}$, the indicator function which is 1 if $X < a$ and otherwise is 0. Then

$$\begin{aligned}\mathbb{P}(X < a) &= 1 \times \mathbb{P}(X < a) + 0 \times \mathbb{P}(X \geq a)\\ &= \mathbb{E}\{\mathbb{I}(X < a)\} = \int \mathbb{I}_{X<a} f(X)\mathrm{dx}\end{aligned}$$

Monte Carlo Integration - I

Suppose we are interested in the integral

$$I = \mathbb{E}(g(X)) = \int g(x)f(x)\mathrm{dx}$$

Let $X_1, X_2, \ldots, X_n$ be independent random variables with pdf $f(x)$. Then a Monte Carlo approximation to I is

$$\hat{I}_n = \frac{1}{n}\sum_{i=1}^{n} g(X_i). \tag{4}$$

Example:

Monte Carlo Integration - II

Some properties of $\hat{I}$.

(1) $\hat{I}_n$ is an unbiased estimator of I. **Proof:**

Monte Carlo Integration - III

(2) $\hat{I}_n$ converges to I as $n \to \infty$.

Proof:

Monte Carlo Integration - IV

The SLLN tells us $\hat{I}_n$ converges, but not how fast. It doesn't tell us how large n must be to achieve a certain error.

(3)

$$\mathbb{E}[(\hat{I}_n - I)^2] = \frac{\sigma^2}{n}$$

where $\sigma^2 = \mathbb{V}\text{ar}(g(X))$. Thus the 'root mean square error' (RMSE) of $\hat{I}_n$ is

$$\text{RMSE}(\hat{I}_n) = \frac{\sigma}{\sqrt{n}} = O(n^{-1/2}).$$

Thus, our estimate is more accurate as $n \to \infty$, and is less accurate when σ^2 is large. σ^2 will usually be unknown, but we can estimate it:

$$\hat{\sigma}^2 = \frac{1}{n-1}\sum_{i=1}^{n}(g(X_i) - \hat{I}_n)^2$$

We call $\hat{\sigma}$ the *Monte Carlo standard error*.

Monte Carlo Integration - V

We write[1]

$$\text{RMSE}(\hat{I}_n) = O(n^{-1/2})$$

to emphasise the rate of convergence of the error with n.

To get 1 digit more accuracy requires a 100-fold increase in n. A 3-digit improvement would require us to multiply n by 10^6.

Consequently Monte Carlo is not usually suited for problems where we need a very high accuracy. Although the error rate is low (the RMSE decreases slowly with n), it has the nice properties that the RMSE

- does not depend on $d = \dim(x)$
- does not depend on the smoothness of f

Consequently Monte Carlo is very competitive in high dimensional problems that are not smooth.

Monte Carlo Integration - VI

In addition to the rate of convergence, the central limit theorem tells us the asymptotic[2] distribution of $\hat{I}_n$

(4)

$$\frac{\sqrt{n}(\hat{I}_n - I)}{\sigma} \to N(0,1) \text{ in distribution as } n \to \infty$$

Informally, $\hat{I}_n$ is approximately $N(I, \frac{\sigma^2}{n})$ for large n.

This allows us to calculate confidence intervals for I.

See the R code on MOLE.

- If we require $E\{f(X)\}$, random observations from distribution of $f(X)$ can be generated by generating $X_1, \ldots, X_n$ from distribution of X, and then evaluating $f(X_1), \ldots, f(X_n)$.
- Preceding results can be applied when estimating variances or probabilities of events.
- Percentiles estimated by taking the sample percentile from the generated sample of values $X_1, \ldots, X_n$.
- We expect the estimate to be more accurate as n increases. Determining a percentile is equivalent to inverting a CDF. If wish to know the 95th percentile, we must find ν such that

$$P(X \leq \nu) = 0.95, \tag{5}$$

Monte Carlo solutions to the example problems

Question 1

Define E: the event that in 100 days the wind speed is below 15kmh for more than 10 days.
To estimate $\mathbb{P}(E)$, generate lots of individual time series, and count proportion of series in which E occurs

1. Generate ith realisation of the time series process:
   For $t = 3, 4, \ldots, 100$:
   - Set $Y_t \leftarrow 0.6Y_{t-1} + 0.4Y_{t-2} + N(0, 0.01)$
2. Count number of elements of $\{Y_1, \ldots, Y_{100}\}$ less than $\log 15 = 4.167$:
   - Set $X_i \leftarrow \sum_{t=1}^{100} I\{Y_t < 4.167\}$
3. Determine if event E has occured for time series i:
   - Set $E_i \leftarrow I\{X_i > 10\}$
4. Estimate $\mathbb{P}(E)$ by $\frac{1}{N}\sum_{i=1}^{N} E_i$

Question 2

Define Z to be the difference between max and min of 5 standard normal random variables. Estimate the variance

Question 3

Transformation of a random variable:
Given random variables $X_1, \ldots, X_d$ we want to know the distribution of $Y = f(X_1, \ldots, X_d)$.

- The Monte Carlo method can be used
  - Sample unknown inputs from their distributions,
  - evaluate the function to obtain output value from its distribution.
- Given suitably large sample, 95th percentile from distribution of $C(100, 100, 40)$ can be estimated by the 95th percentile from sample of simulated values of $C(100, 100, 40)$.

For $i = 1, 2, \ldots, N$:

1. Sample a set of input values:
   - Sample $u_{10,i}$ from $\log N(2, .1)$
   - Sample $\sigma^2_{y,i}$ from $\log N(10, 0.2)$
   - Sample $\sigma^2_{z,i}$ from $\log N(5, 0.05)$
2. Evaluate the model output C_i:
   - Set $C_i \leftarrow \frac{100}{2\pi u_{10,i}\sigma_{z,i}\sigma_{y,i}} \exp\left[-\frac{1}{2}\left\{\frac{40^2}{\sigma^2_{y,i}} + \frac{100}{\sigma^2_{z,i}}\right\}\right]$
3. Return the 95th percentile of $C_1, C_2, \ldots, C_N$.

Question 4

- Define W to be the number of days before the first patient arrives to find no available beds.
- The question has asked us to give $E(W)$.
- If we can generate $W_1, \ldots, W_n$ from the distribution of W, we can then estimate $E(W)$ by $\bar{W}$.

See the R code on MOLE for a way to simulate this process.

The Monty Hall Problem

- Simulate N separate games by randomly letting x take values in $\{1, 2, 3\}$ with equal probability. x represents which door the car is behind.
- Simulate the contestant randomly picking a door by choosing a value y in $\{1, 2, 3\}$ (it doesn't matter how we do this, we can always choose 1 if you like, the results are the same).
- Now the game show host will open the door which hasn't been picked that contains a goat. For each of the N games, record the success of the two strategies
  1. stick with choice y
  2. change to the unopened door.
- Calculate the success rate for each strategy.

Example 1

Consider the probability p that a standard normal random variable will lie in the interval $[0, 1]$. This can be written as an integral

$$p = \int_0^1 \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right) dx. \tag{6}$$

Two methods for estimating/evaluating this probability are

1. numerical integration/quadrature, e.g., trapezium rule, Simpson's rule etc
2. given a sample of standard normal random variables $Z_1, \ldots, Z_n$, look at the proportion of Z_is occurring in the interval $[0, 1]$.

Example 1: An alternative method

1. Y is a RV with $f(Y)$ any function of Y. To generate a random value from the distribution of $f(Y)$, generate a random Y from the distribution of Y, and then evaluate $f(Y)$.
2. Providing $\mathbb{E}\{f(Y)\}$ exists, given a sample $f(Y_1), \ldots, f(Y_n)$,

$$\frac{1}{n}\sum_{i=1}^{n} f(Y_i)$$

   is an unbiased estimator of $\mathbb{E}\{f(Y)\}$.
3. Let X be a random variable with a $U[0, 1]$ distribution. For an arbitrary function $f(X)$, what is the expectation of $f(X)$?

4 Now choose f to be the function $f(X) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{X^2}{2}\right)$. Then if $X \sim U[0,1]$

$$\mathbb{E}\{f(X)\} = \int_0^1 \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right) 1 \mathrm{d}x \tag{8}$$

Given a sample $f(X_1), \ldots, f(X_n)$ from the distribution of $f(X)$, we can estimate $E\{f(X)\}$ by the *unbiased* **Monte Carlo** estimator $\hat{p}$

$$\hat{p} = \frac{1}{n} \sum_{i=1}^{n} f(X_i), \tag{9}$$

where X_i is drawn randomly from the $U[0,1]$ distribution.

Key idea

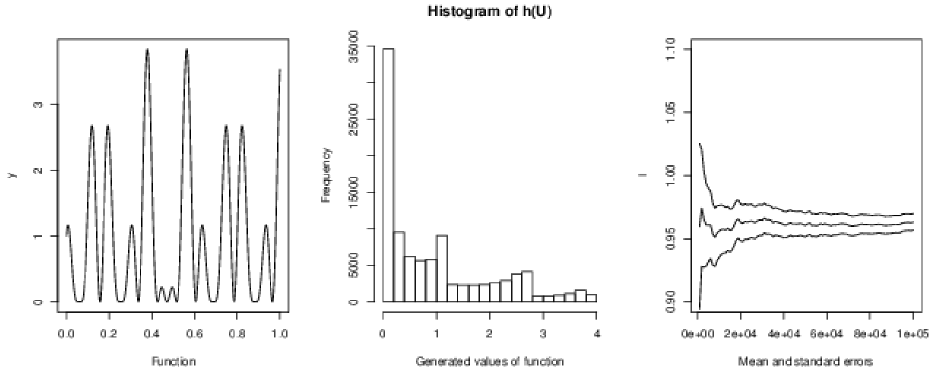
re-express the integral of interest (6) as an *expectation*.

Example 2

Consider the integral $\int_0^1 h(x)\mathrm{d}x$ where

$$h(x) = [\cos(50x) + \sin(20x)]^2$$

Generate $X_1, \ldots, X_n$ from $U[0,1]$ and estimate with $\hat{I}_n = \frac{1}{n} \sum h(X_i)$.



The general framework

$$R = \int f(x)dx \tag{10}$$

Let $g(x)$ be some density function that is easy to sample from. How do we re-write (10) as the expectation of a function of a random variable X with density function $g(x)$?

So we now have $R = E\{h(X)\}$, where X has the density function $g(x)$. If we now sample $X_1, \ldots, X_n$ from $g(x)$, then evaluate $h(X_1), \ldots, h(X_n)$,

$$\hat{R} = \frac{1}{n} \sum_{i=1}^{n} h(X_i) \tag{12}$$

is an unbiased estimator of R.

Example 3

Use Monte Carlo integration to estimate

$$R = \int_{-1}^{1} \exp(-x^2) dx. \tag{13}$$

We'll consider two different choices for $g(x)$.

1. A uniform density on $[-1,1]$: $g(x) = 0.5$ for $x \in [-1,1]$. We sample $X_1, \ldots, X_n$ from $U[-1,1]$, and estimate R by

$$\hat{R} = \frac{1}{n} \sum_{i=1}^{n} \frac{\exp(-X_i^2)}{g(X_i)} = \frac{1}{n} \sum_{i=1}^{n} 2\exp(-X_i^2). \tag{14}$$

2 A normal density function $N(0, 0.5)$.
Note: sampled value X from $g(x)$ not constrained to lie in $[-1, 1]$.
Re-write R as

$$R = \int_{-\infty}^{\infty} I\{-1 \leq x \leq 1\} \exp(-x^2) dx, \tag{15}$$

where $I\{\}$ denotes the indicator function.
We now sample $X_1, \ldots, X_n$ from $N(0, 0.5)$ and estimate R by

$$\hat{R} = \frac{1}{n} \sum_{i=1}^{n} \frac{I\{-1 \leq X_i \leq 1\} \exp(-X_i^2)}{g(X_i)} = \frac{1}{n} \sum_{i=1}^{n} \pi^{1/2} I\{-1 \leq X_i \leq \tag{16}$$

Key idea

$g(x)$ needs to mimic $f(x)$ as closely as possible. Consider again $R = \int_{-1}^{1} \exp(-x^2)\mathrm{dx}$.

Two terrible choices of g:

1. A uniform density on $[0, 1]$: $g(x) = 1$ for $x \in [0, 1]$.

$$R = \int_{-\infty}^{\infty} I\{-1 \leq x \leq 1\} \exp(-x^2) dx, \tag{17}$$

For $x \in [-1, 0)$, we have $f(x) > 0$ and $g(x) = 0$. Must have $g(x) > 0$ for all x where $f(x) > 0$.

2. A normal density $N(0, 0.09)$.
In this case, we have $g(x) > 0$ for $x \in [-1, 1]$, but we when we sample x from g, we expect around 95% of the values to lie in the range $(-0.6, 6)$.
The Monte Carlo estimate of R is given by

$$\hat{R} = \frac{1}{n} \sum_{i=1}^{n} I\{-1 \leq X_i \leq 1\} \frac{\exp(-X_i^2)\sqrt{0.18\pi}}{\exp(-5.56X_i^2)}. \tag{18}$$

Convergence

- Provided $f(x) > 0 \Rightarrow g(x) > 0$, $\hat{R}$ will converge to R as $n \to \infty$.
- Use the central limit theorem to derive a confidence interval for $\hat{R}$:

$$\hat{R} \sim N\left(R, \frac{\sigma^2}{n}\right), \tag{19}$$

where we estimate σ^2 by

$$\hat{\sigma}^2 = \frac{1}{n-1} \sum_{i=1}^{n} \left\{h(X_i) - \hat{R}\right\}^2 \tag{20}$$

- We can then report the confidence interval as

$$\hat{R} \pm Z_{1-\alpha/2}\sqrt{\hat{\sigma}^2/n}, \tag{21}$$

- Estimates of σ^2 in the example: $U[-1, 1] : 0.16$, $N(0, 0.5) : 0.42$, $N(0, 0.09) : 6.81$.

Comparison of Monte Carlo with numerical integration

Mid-ordinate rule

Consider finding $I = \displaystyle\int_0^1 f(x)\ \mathrm{dx}$. There are many different numerical integration schemes we might use.
For example, the mid-ordinate rule is one of the simplest methods, and approximates I by a sum

$$\tilde{I}_n = \frac{1}{n} \sum_{i=1}^{n} f(x_i),$$

The points $x_i = (i - \frac{1}{2})h$ are equally spaced at intervals of $h = 1/n$.

Comparison of MC with numerical integration II

Mid-ordinate rule error analysis

For smooth 1-d functions the error rates for quadrature rules can be much better than Monte Carlo

For example, if $f:[0,1]\to\mathbb{R}$ and $f''(x)$ is continuous, then

$$|I-\tilde{I}_n| \leq \frac{1}{24n^2}\max_{0\leq x\leq 1}|f''(x)|$$

So

$$\mathrm{RMSE}(\tilde{I}) = O(n^{-2})$$

i.e., it is a second order method. Other rules achieve higher errror rates. For example, Simpson's rule is a fourth order method.

This is much faster than Monte Carlo: to get an extra digit of accuracy we only need multiply n by a factor of $\sqrt{10}=3.2$

Comparison of MC with numerical integration III

Curse of dimensionality

Classial quadrature methods work well for smooth 1d problems. But for d-dimensional integrals we have a problem. Suppose

$$I=\int_0^1\int_0^1\dots\int_0^1 f(x_1,\dots,x_d)\mathrm{d}x_1\dots\mathrm{d}x_d$$

We can use the same N point 1-d quadrature rules on each of the d integrals.

This uses $n=N^d$ evaluations of f. The 1d mid-ordinate rule has error $O(N^{-2})$, so the d-dimensional mid-ordinate rule has error

$$|I-\tilde{I}| = O(N^{-2}) = O(n^{-2/d})$$

For $d=4$ this is the same as Monte Carlo. For larger d it is worse.

In addition, we require f to be smooth ($f''(x)$ to be continuous) for the method to work well.

Monte Carlo has the same $O(n^{-1/2})$ error rate regardless of $\dim(x)$ or $f''(x)$