Monte Carlo Methods

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Preliminary note

The material in these slides is strongly based on [1]. When other materials are used, they are cited accordingly.
Mathematical notation follows as good as it can a good practices proposal from the Beijing Academy of Artificial Intelligence.

What to expect?

In this session we will discuss:

- Crude Monte Carlo.
- Average Value theorem.
- Monte Carlo Integration.

Estimating expectation

Suppose we want to compute the expectation for a random variable Y:

$$\mathbb{E}Y = \mu = \begin{cases} \int yf(y)\,\mathrm{d}y & \text{(continuouscase)} \\ \sum yf(y) & \text{(discretecase)} \end{cases}$$

Many time knowing $f(y)$ is not possible (Y may be a function of several other random variables).

ith Crude Monte Carlo (CMC) you can approximate μ by simulating many independent copies $Y_i, \ldots, Y_N$ of Y and then take their sample mean as an estimator of μ.

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First integration with CMC I

Imagine we want to estimate the value of a given integral $I = \int_{-\pi}^{\pi} \cos x \, \mathrm{d}x$. By the Average Value Theorem, we know that:

$$< f(x) >= \frac{1}{b-a} \int_a^b f(x) \, \mathrm{d}x$$

from which we obtain

$$\int_a^b f(x) \, \mathrm{d}x = (b-a) < f(x) >$$

Certainly:

First integration with CMC II

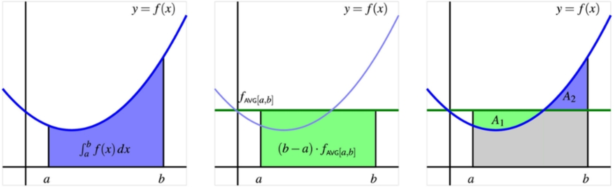

Figure 1: Visual inspection of the Average Value Theorem.

So, we can device an algorithm that takes values of the function and obtain their average to estimate the value of the requested integral.

First integration with CMC III

```
from scipy import random
import numpy as np

a = -np.pi
b = np.pi
N = 1000

ar = np.zeros(N)

for i in range (len(ar)):
    ar[i] = random.uniform(a,b)

integral = 0.0

def f(x):
```

First integration with CMC IV

```
    return np.cos(x)

for i in ar:
    integral += f(i)

ans = (b-a)/float(N)*integral

print ("Approx to the integral by CMC: {}.".format(ans
```

Exercise 1 Integration

Evaluate with CMC the integral of $f(x) = x^2$ from -2 to 2 and compare the result with the corresponding analytical one. Now try to do the same for a multivariate function $f(x, y) = x^2 + 3y^2 + 1$ between $-2 < x < 3$ and $-1 < y < 0.5$.

Central limit theorem

In many situations, for independent and identically distributed (iid) random variables, the sampling distribution of the standardized sample mean tends towards the standard normal distribution even if the original variables themselves are not normally distributed.

Thus, $\bar{Y}$ approximately has a $\mathcal{N}(\mu, \sigma^2/N)$ distribution for large N, provided that $\mathrm{Var} Y < \infty$.

Thus we can construct an approximate $(1-\alpha)$ confidence interval for μ:

$$\left(\bar{Y} - z_{1-\alpha/2}\frac{S}{\sqrt{N}}, \bar{Y} + z_{1-\alpha/2}\frac{S}{\sqrt{N}}\right)$$

where S is the sample standard deviation of Y_i and z_γ is the γ-quantile of the $\mathcal{N}(0,1)$ distribution. Estimated standard error: $S/\sqrt{N}$; estimated relative error: $S/(\bar{Y}\sqrt{N})$.

Algorithm for CMC

Algorithm 1: CMC for iid

Input: Random variable $Y \sim f$, sample size N, confidence level $1-\alpha$.

Output: Point estimate and approximate $(1-\alpha)$ confidence interval for $\mu = \mathbb{E}Y$.

Simulate $Y_1, \dots, Y_N \overset{iid}{\sim} f$

$\bar{Y} \leftarrow \frac{1}{N}\sum_{i=1}^{N} Y_i$

$S^2 \leftarrow \frac{1}{N-1}\sum_{i=1}^{N}(Y_i - \bar{Y})^2$

return $\bar{Y}$ *and conf. interval* $\left(\bar{Y} - z_{1-\alpha/2}\frac{S}{\sqrt{N}}, \bar{Y} + z_{1-\alpha/2}\frac{S}{\sqrt{N}}\right)$

Monte Carlo integration

Consider the complicated integral

$$\mu = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \sqrt{|x_1 + x_2 + x_3|} e^{-(x_1^2+x_2^2+x_3^2)/2} \, \mathrm{d}x_1 \, \mathrm{d}x_2 \, \mathrm{d}x_3$$

Defining $Y = |X_1 + X_2 + X_3|^{1/2}(2\pi)^{3/2}$ with $X_1, X_2, X_3 \overset{iid}{\sim} \mathcal{N}(0,1)$, we can write $\mu = \mathbb{E}Y$. Use the code here to test the calculation. If you want to learn more about CLT and confidence intervals, a good start can be found here.

Polynomial regression. Original data.

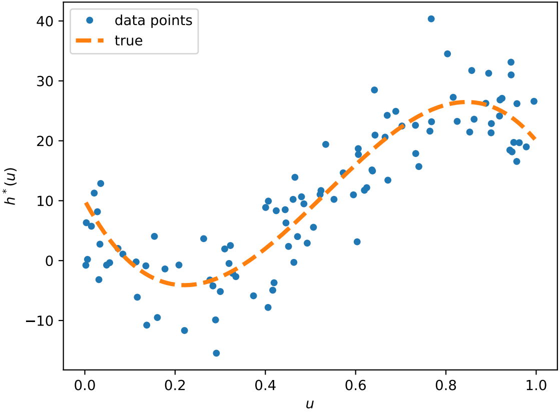

Figure 2: Training data and the optimal polynomial prediction function h^*[1]

Polynomial regression. Estimating the generalization risk

The code here shows how to estimate how good is the graph below.

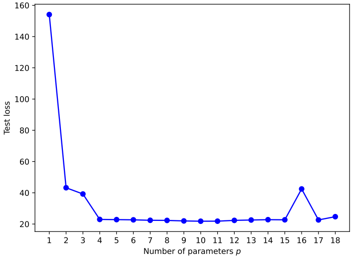

Figure 3: Fitted models for different orders of polynomial regressions[1].

Dirk P. Kroese, Zdravko Botev, Thomas Taimre, and Radislav: Vaisman.
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Machine Learning & Pattern Recognition. Chapman & Hall/CRC, 2020.