CS5016: Computational Methods and Applications

Monte Carlo Methods

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We will use Python for all coding assignments.

You can brush up your Python skills by going to `https://realpython.com/start-here/`

Matplotlib is a Python 2D plotting library that can produce publication quality figures in a variety of formats and interactive environments across platforms.

It allows you to create awesome plots very easily. So, **master it!!!**

To learn more, visit: `https://matplotlib.org/stable/index.html`

Discrete Distributions

A discrete distribution describes the probability of occurrence of each value of a **discrete random variable**.

E.g., Throw a 6-faced dice; what is probability/chance that the top side shows 3 dots?

Discrete distributions are very common. Can you think of a few discrete distributions?

To know more about random variables, visit
`https://en.wikipedia.org/wiki/Random_variable`

Sampling From a Discrete Distribution

Consider an experiment in which you throw a 6-faced dice. If the probability of the top-facing side being $\{1, 2, 3, 4, 5, 6\}$ is given by the discrete probability distribution $\{1/12, 3/12, 4/12, 1/12, 2/12, 2/12\}$, respectively. How would you simulate this experiment?

Let us say Python has a function that samples a *continuous random variable uniformly distributed* in the interval [0,1]. Can this help?

How is such a function implemented?

To learn more about continuous random variables, visit `https://www.colorado.edu/amath/sites/default/files/attached-files/ch4.pdf`

The Trick

Let X be a discrete random variable taking values in set $\mathcal{X} = \{x_1, x_2, \ldots, x_k\}$

Let $p(x) = P[X = x]$ for any $x \in \mathcal{X}$; $p(\cdot)$ is know as the **probability mass function**.

The cumulative distribution function (CDF) of X can then be defined as

$$F(x_j) = P[X \leq x_j] = \sum_{i \leq j} p(x_i)$$

Now, consider the following *partition* of the interval $(0, 1)$

$$((0, F(x_1)), (F(x_1), F(x_2)), \ldots, (F(x_{k-1}), 1)])$$

Let U be a uniformly distributed random variables in the interval $(0, 1)$. Then, for any $a, b \in (0, 1)$, we have

$$P[a \leq U \leq b] = b - a$$

Let $I_j \in \{0, 1\}$ take the value 1 only if $U \in (F(x_j), F(x_{j+1}))$. Then, we have

$$\begin{aligned} P[I_j = 1] &= P[F(x_j) \leq U \leq F(x_{j+1})] \\ &= F(x_{j+1}) - F(x_j) \\ &= p(x_j) = P[X = x_j] \end{aligned}$$

where $F(x_0)$ is defined to be 0.

Probability that $I_j = 1$ is same as the probability that $X = x_j$, and this can be used to generate from the distribution of X.

Would the same result hold if the partitions are shuffled?

What is Monte Carlo Method?

- Monte Carlo methods, or Monte Carlo experiments, are a broad class of **computational algorithms** that rely on repeated random sampling to obtain numerical results[1].
- The underlying concept is to use randomness to solve problems that might be deterministic in principle.
- They are often used in **physical and mathematical problems** and are most useful when it is difficult or impossible to use other approaches.

[1] `https://en.wikipedia.org/wiki/Monte_Carlo_method`

Estimating π

- π appears in many formulas in all areas of mathematics and physics.
- What is its value? $22/7$, $333/106$, $355/113 \ldots$; none of the above. In fact, π is an irrational number.
- Among other definitions, π can be defined as the ratio of a circle's area to the square of its radius.
- **Can we create a simple Monte Carlo experiment to estimate the value of π using the above definition?**

Estimating π

- Consider a unit square centered at the origin of a 2-D plane.
- Inscribe a circle within this square.
- Generate points of type (x, y), where x and y are uniformly and independently sampled from the interval $[-0.5, 0.5]$, and place them on the 2-D plane.
- Then, for a large number points, we have

$$\frac{\text{no. points within the circle}}{\text{no. points within the square}} \stackrel{(a)}{=} \frac{\text{area of circle}}{\text{area of square}} = \frac{\pi}{4}$$

Or, equivalently,

$$\pi = \frac{4 \times \text{no. points within the circle}}{\text{no. points within the square}}$$

Why does equality (a) hold? Are there other Monte Carlo methods to generate π?

Python's scipy.stats module

This module contains a large number of probability distributions as well as a growing library of statistical functions.

Have a look at the various function of this module by visiting `https://docs.scipy.org/doc/scipy/reference/stats.html`

Thank You