Lecture 1: Introduction

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MATH60047/70047 – Stochastic Simulation

October 10, 2022

Imperial College London

Stochastic Simulation

What is it about?

This course is about simulating *structured randomness*.

Other names for the course:

- Monte Carlo methods
- Sampling algorithms

Stochastic Simulation

How is it going to work?

The course team:

- Andres Benchimol (Strategic Teaching Fellow)
- Fabio Feser (Graduate TA)
- Antonio Matas-Gil (Graduate TA)

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How is it going to work?

My office hours:

- Monday 11:30-12:30, Huxley 532.

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How is it going to work?

We will have three coursework assignments:

- Assignment 1 (10%)
  - Upload: **26 Oct. 2022** – Deadline: **9 Nov. 2022**
- Assignment 2 (10%)
  - Upload: **16 Nov. 2022** – Deadline: **30 Nov. 2022**
- Assignment 3 (5%)
  - Upload: **30 Nov. 2022** – Deadline: **14 Dec. 2022**
- Final exam (75%)

Assignments and exam will have an extra (or alternative) question for M4R students (will be clarified before the exam).

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How is it going to work?

We will provide:

- Slides (printable, no animations)
- Lecture notes
  - Important for the weeks we cover on whiteboard
- Weekly exercises (with solutions a week later)
- Python code solving coding exercises.

I will run visualization code to demonstrate many algorithms, these can be only accessed through the recording (if visible).

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What is going to (roughly) happen in this course?

This course will teach you how to simulate random numbers that attain certain statistical properties.

This course will also teach you how to estimate certain quantities of interest using these random numbers.

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What is going to (roughly) happen in this course?

The first focus will be on *independent exact sampling* methods.

- We will discuss and design algorithms that sample directly from basic distributions, such as
  - Uniform distribution
  - Gaussian distribution
  - Exponential distribution

  and others.

These random number generation techniques are at the core of many (many!) fields: Simulation (of anything random), statistical inference, generative models, almost all engineering.

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What is going to (roughly) happen in this course?

We will also cover exact sampling of many distributions and stochastic processes:

- Multivariate Gaussian
- Time-dependent processes
- Markov chains

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What is going to (roughly) happen in this course?

Then, we will move on to Monte Carlo integration and Markov chain Monte Carlo methods:

- Importance sampling
- Sampling from intractable distributions by forming Markov chains and targeting them
- Computation of integrals, expectations

Then finally, we will finalize with sequential Monte Carlo (if time permits).

Somewhere in the middle, we will cover Bayesian modelling.

How can this course be useful?

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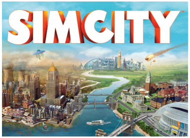
Simulation of anything





It is of great interest in many engineering applications (and even in social sciences) to simulate complex processes.

- A model of how a disease spreads (mechanistic)
- A model of traffic (mechanistic)
- Fluid flows (physical)

Statistical models are *everywhere* (you can imagine).

Simulating (sampling) from such models gives us general ways to ask questions.

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Statistical inference

Simulation from the models are cool but what about data?

In statistics, we are interested in synthesising *the model* and *the data* (among other things).

One very effective way is to use Bayesian statistical methodology (will be introduced in this course).

However, conditioning on data and marginalising out latent variables result in intractable distributions over variables of interest and *sampling* is key to understand their behaviour.

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Statistical inference

A generic probabilistic model:

$$X \sim p(x),$$
$$Y|X = x \sim p(y|x).$$

- X is the phenomenon of interest (unobserved variables, e.g., traffic density, non observed physical states of the system)
- Y is the observed *data* (e.g. coming from sensors, contains noise)

We would be then interested in, *given data*,

$$p(x|y) = \frac{p(y|x)p(x)}{\int p(y|x)p(x)\mathrm{d}x}.$$

This is typically intractable for various reasons (imagine now multiple latent variables, even multiple likelihoods.)

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Generative models

In this case, we have samples $\{Y_i\}_{i=1}^n$ from a dataset. Underlying data distribution $Y_i \sim p_{\text{data}}$ is not accessible in any way.

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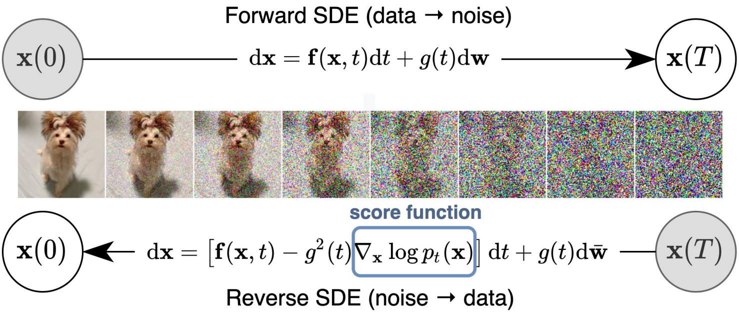
Generative models

The standard way to do it is to run forward and backward stochastic differential equations[1]



[1] Figure from: `https://yang-song.net/blog/2021/score/`

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Generative models

The standard way to do it is to run forward and backward stochastic differential equations[2] (Animation removed)

[2]Figure from: `https://yang-song.net/blog/2021/score/`

In summary, this course can be immensely useful for you to go into any of these areas.

We will balance computation and theory for practical and conceptual understanding.

Estimating π

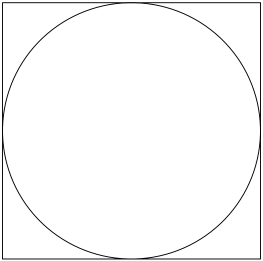
In this course, a core focus will be estimating certain quantities (probabilities, expectations, etc.) using *sampling*.

Sampling here means *random variate generation*.

Let's try to solve a simple problem to illustrate the methodology: Estimating π.

Can we estimate π using sampling? Any ideas?

Estimating π



Given the knowledge that:

$$\frac{\text{area of circle}}{\text{area of square}} = \frac{\pi r^2}{4r^2} = \frac{\pi}{4}.$$

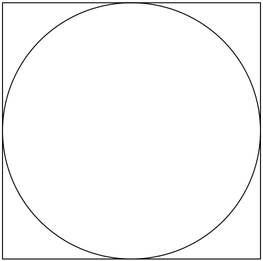
Estimating π

What does this mean?

- Write down the estimation problem as
  - a probability (of a set)
  - an expectation

Most of the time, expectation is the most general way.

Estimating π



Consider a 2D uniform distribution on $[-1, 1] \times [-1, 1]$.

- The 'probability' of the square (whole space) is 1.
- The 'probability of the circle' (set) is precisely the ratio of areas.

$$\mathbb{P}(\text{Circle}) = \frac{\pi}{4}.$$

Estimating π

Last question:

Can we estimate the probability of this set, if we had access to samples from Unif$([-1,1] \times [-1,1])$?

Estimating π

(Animation removed)

Estimating π

Proof: What you will be understand by the end of the course

For probabilists, let $\mathsf{X} = [-1, 1] \times [-1, 1]$ and define the uniform measure such that $\mathbb{P}(\mathsf{X}) = 1$.

Let A be the "circle" s.t. $A \subset \mathsf{X}$. Now, the probability of A is given

$$\begin{aligned}
\mathbb{P}(A) &= \int_A \mathbb{P}(\mathrm{d}x) \\
&= \int \mathbf{1}_A(x)\mathbb{P}(\mathrm{d}x), \\
&\approx \frac{1}{N}\sum_{i=1}^{N} \mathbf{1}_A(x_i) \to \frac{\pi}{4} \qquad \text{as } N \to \infty.
\end{aligned}$$

where $x_i \sim \mathbb{P}$.

Monte Carlo method: A brief history

The first thoughts and attempts I made to practice [the Monte Carlo Method] were suggested by a question which occurred to me in 1946 as I was convalescing from an illness and playing solitaires. The question was what are the chances that a Canfield solitaire laid out with 52 cards will come out successfully? After spending a lot of time trying to estimate them by pure combinatorial calculations, I wondered whether a more practical method than "abstract thinking" might not be to lay it out say one hundred times and simply observe and count the number of successful plays. This was already possible to envisage with the beginning of the new era of fast computers, and I immediately thought of problems of neutron diffusion and other questions of mathematical physics, and more generally how to change processes described by certain differential equations into an equivalent form interpretable as a succession of random operations. Later [in 1946], I described the idea to John von Neumann, and we began to plan actual calculations.[3]

[3] Eckhardt, Roger. "Stan Ulam, John von Neumann, and the Monte Carlo method." *Los Alamos Science* 15.131-136 (1987): 30.

Monte Carlo method: A brief history

Ulam was a physicist working at Los Alamos on nuclear weapons.

- Monte Carlo was the code name they chose for their project.
- Simulations were used for the Manhattan Project to compute intractable quantities
- After these, Monte Carlo methods become widely popular in physics, then everywhere else too

See you tomorrow!