MA3227 Numerical Analysis II

Lecture 22: Monte Carlo Methods

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Monte Carlo Methods

Introduction

Monte Carlo refers to a broad class of algorithms which use randomness to compute a deterministic outcome.

These methods and their name originated from the Manhattan project when the United States developed the first atomic bombs. Since this work was secret, the scientists working on the project required a code name for the methods that they were using. They settled on Monte Carlo in reference to a casino of the same name.

Monte Carlo methods tend to be quite slow, but they are a useful method of last resort when more traditional algorithms break down.

The example on the following slides will help make this clearer.

Monte Carlo Methods

Introductory example

Assume we want to compute the integral

$$I := \int_0^1 \dots \int_0^1 f(y_1, \dots, y_d)\, dy_1 \, \dots \, dy_d.$$

Applying a one-dimensional quadrature rule $(x_k, w_k)_{k=1}^n$ with error $e_n = \mathcal{O}\big(n^{-p}\big)$ repeatedly, we obtain

$$\begin{aligned} I &= \int_0^1 \dots \int_0^1 \left(\sum_{k_1=1}^{n} f(x_{k_1}, y_2, \dots, y_d)\, w_{k_1} + \mathcal{O}\big(n^{-p}\big) \right) dy_2 \, \dots \, dy_d \\ &= \dots \\ &= \sum_{k_d=1}^{n} \dots \sum_{k_1=1}^{n} f(x_{k_1}, \dots, x_{k_d})\, w_{k_1} \, \dots \, w_{k_d} + \mathcal{O}\big(n^{-p}\big). \end{aligned}$$

Observation: we need $N = n^d$ function evaluations (all combinations of $k_1, \dots, k_d \in \{1, \dots, n\}$) to achieve a $\mathcal{O}\big(n^{-p}\big) = \mathcal{O}\big(N^{-p/d}\big)$ error, i.e. the order of convergence in terms of N decreases for increasing d.

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Curse of dimensionality

The observation on the previous slide applies to a vast number of algorithms: the accuracy scales with the "effort per dimension" n, but the overall effort scales with n^d.

This phenomenon is called the curse of dimensionality and often makes it virtually impossible to do computations in dimensions d larger than about 4 or 5.

Problems with dimensions $d > 5$ are more common than one might think. For example, the probability that someone has the corona virus is a function

$$\underbrace{\mathbb{R}}_{\text{body temperature}} \times \underbrace{\{0,1\}}_{\text{cough}} \times \underbrace{\{0,1\}}_{\text{runny nose}} \times \underbrace{\{0,1\}}_{\text{travel history}} \times \underbrace{\{1,\dots,5\}}_{\text{ethnicity}} \times \underbrace{\{1,\dots,193\}}_{\text{nationality}} \to [0,1].$$

Assuming we need 40 points to cover a reasonable range of body temperatures, this means we need to store

$$40 \times 2 \times 2 \times 2 \times 2 \times 193 = 123'520$$

numbers to represent this function. Moreover, each additional variable in our model multiplies the memory requirements.

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Introductory example (continued)

The curse of dimensionality can be overcome by reinterpreting I as the expectation value

$$I = \mathbb{E}[f(X_1, \ldots, X_d)], \qquad X_i \overset{\text{iid}}{\sim} \text{Uniform}[0,1].$$

I will define the precise meaning of $X_i \overset{\text{iid}}{\sim} \text{Uniform}[0,1]$ later.

Expectations can be computed by taking the average of a sufficiently large number of samples $x_i^{(k)}$ of the X_i, i.e.

$$\mathbb{E}[f(X_1, \ldots, X_d)] = \frac{1}{N} \sum_{k=1}^{N} f\left(x_1^{(k)}, \ldots, x_d^{(k)}\right) + \mathcal{O}\left(N^{-1/2}\right).$$

We will discuss the $\mathcal{O}(N^{-1/2})$ error estimate later.

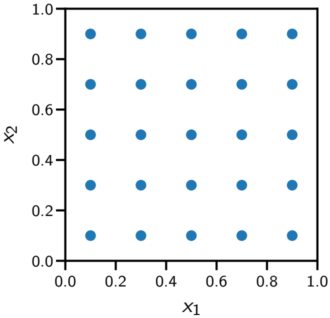
Observation: N evaluations of f lead to $\mathcal{O}\left(N^{-1/2}\right)$ error regardless of d.
In particular, Monte Carlo is better than midpoint rule ($p = 2$) for $d > 4$.

See `convergence()` for numerical demonstration, and see the next slide for a pictorial illustration.

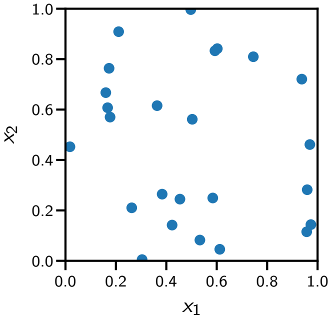
Monte Carlo Methods

Introductory example (continued)

Distribution of the function evaluation points (x_1, x_2).



Midpoint



Monte Carlo

Monte Carlo Methods

Monte Carlo methods

In abstract terms, Monte Carlo corresponds to the approximation

$$\mathbb{E}[F] \approx \frac{1}{N} \sum_{k=1}^{N} F_k \qquad \text{where} \qquad F, F_k \overset{\text{iid}}{\sim} \mathcal{F}, \tag{1}$$

i.e. it amounts to estimating expectations by taking the mean of a sufficiently large number of samples as illustrated on the previous slide.

Outlook

Our next aim will be to clarify what we mean by $\overset{\text{iid}}{\sim}$ and $\approx$ in (1). This will require us to revisit some key definitions and results from probability theory.

Disclaimer

As usual in this module, I will take an engineer's approach to mathematics, i.e. I will ignore many technical details like measurability or σ-algebras since they are hardly ever relevant in applications.

Monte Carlo Methods

Def: Measure on a set Ω

Function P mapping subsets of Ω to nonnegative real numbers such that

$$P(\{\}) = 0 \quad \text{and} \quad P(A \cup B) = P(A) + P(B) \text{ if } A, B \subset \Omega \text{ are disjoint.}$$

Def: Probability measure on a set Ω

A measure P such that $P(\Omega) = 1$.

Def: Probability space

A pair (Ω, P) where P is a probability measure on Ω

Def: Random variables

Any function $X : \Omega \to \Xi$ defined on a probability space (Ω, P).

Def: Distribution of a random variable $X : \Omega \to \Xi$

The probability measure $\hat{P}$ on Ξ given by $\hat{P}(A) = P\big(X^{-1}(A)\big)$.

It is common practice to write $P(X \in A)$ instead of $P(X^{-1}(A))$, and $P(X_1 \in A_1, X_2 \in A_2)$ instead of $P\big(X_1^{-1}(A_1) \cap X_2^{-1}(A_2)\big)$.

This can be confusing if we forget that $P(X \in A)$ is just a shorthand for $P(X^{-1}(A))$, so try your best not to forget this.

Monte Carlo Methods

Discussion

It is possible and common practise to talk about random variables and their distributions without ever specifying what the underlying probability space is.

For example, when we say $X \sim \text{Uniform}[0,1]$ ("X is uniformly distributed in $[0,1]$"), we mean that $X : \Omega \to [0,1]$ is a function defined on some unspecified probability space Ω such that

$$\begin{aligned} P(X \in [a,b]) &= P\big(X^{-1}([a,b])\big) \\ &= P\big(\{\omega \in \Omega \mid X(\omega) \in [a,b]\}\big) \\ &= b - a \end{aligned}$$

for all a, b such that $0 \leq a \leq b \leq 1$.

There are countless ways how we could construct such an X. The simplest construction is to choose $\Omega = [0,1]$, $P([a,b]) = b - a$ and $X(\omega) = \omega$, but equally well we could also set $X(\omega) = 1 - \omega$, or $\Omega = [0,2]$, $P([a,b]) = \frac{b-a}{2}$, $X(\omega) = \frac{\omega}{2}$, or an even more complicated construction. The point is that when we say $X \sim \text{Uniform}[0,1]$, we do not care how X comes about as long as $P(X \in [a,b]) = b - a$.

Representations of distributions

Recall that " distribution of a random variable $X : \Omega \to \Xi$ " refers to the probability measure $\hat{P}(A) = P(X^{-1}(A)) = P(X \in A)$ on Ξ.

Furthermore, recall that a measure on Ξ is just a function mapping subsets of Ξ to nonnegative real numbers.

There are many ways to represent measures, and correspondingly there are many ways to represent distributions.

The three most common ways to represent distributions are listed on the next slide.

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Representations of distributions (continued)

- Probability density function (PDF) of $X : \Omega \to \Xi$ where Ξ is discrete: a function $p : \Xi \to [0, \infty)$ such that for all $A \subset X$

$$P(X \in A) = \sum_{x \in A} p(x).$$

- Probability density function (PDF) of $X : \Omega \to \mathbb{R}^n$: a function $f : \mathbb{R}^n \to [0, \infty)$ such that for all $A \subset \mathbb{R}^n$

$$P(X \in A) = \int_A f(x)\, dx.$$

- Cumulative distribution function (CDF) of $X : \Omega \to \mathbb{R}$: a function $F : \mathbb{R} \to [0, 1]$ such that for all $a \in \mathbb{R}$

$$P(X \leq a) = F(a).$$

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Example

	Uniform$[0,1]$	$\mathcal{N}(\mu,\sigma^2)$
Name	Uniform distribution on $[0,1]$.	Normal distribution with mean μ and standard deviation σ
PDF	$f(x) = \begin{cases} 1 & \text{if } 0 \le x \le 1, \\ 0 & \text{otherwise.} \end{cases}$	$f(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$
CDF	$F(x) = \begin{cases} 0 & \text{if } x < 0, \\ x & \text{if } 0 \le x \le 1, \\ 1 & \text{if } x > 1. \end{cases}$	$F(x) = \int_{-\infty}^{x} f(x)\,dx$ (No explicit formula available)

Example

$$X \sim \text{Bernoulli}(p) \qquad \Longleftrightarrow \qquad P(X=0) = 1-p, \quad P(X=1) = p.$$

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Def: Expectation and variance

Given a random variable $X : \Omega \to \Xi$, we define

$$\mathbb{E}[X] = \int X(\omega)\, d\omega, \qquad \mathrm{Var}[X] = \mathbb{E}\big[(X - \mathbb{E}[X])^2\big]$$

where $\int d\omega$ denotes the integral with respect to the probability measure P of the underlying probability space.

Integration with respect to a measure may not have been introduced to you yet. If so, ignore the above and study the below special cases instead.

Again, it is possible and common practice to work with expectations without referring to the underlying probability space (Ω, P).

For example, one can show that if $X : \Omega \to \Xi$ with Ξ discrete or $\Xi = \mathbb{R}^n$ has probability density $p(x)$, then

$$\mathbb{E}[X] = \sum_{x \in \Xi} x\, p(x) \qquad \text{or} \qquad \mathbb{E}[X] = \int_{\mathbb{R}^n} x\, p(x)\, dx,$$

and similarly for any function f on Ξ we have

$$\mathbb{E}[f(X)] = \sum_{x \in \Xi} f(x)\, p(x) \qquad \text{or} \qquad \mathbb{E}[X] = \int_{\mathbb{R}^n} f(x)\, p(x)\, dx.$$

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Def: Independence

A collection of random variables $(X_i : \Omega \to \Xi_i)_{i=1}^n$ are called independent if for all $(A_i \subset \Xi_i)_{i=1}^n$ it holds

$$P\big(X_1 \in A_1, \ldots, X_n \in A_n\big) = \prod_{i=1}^n P(X_i \in A_i).$$

One can show that $(X_i)_{i=1}^n$ are independent if and only if

- $f(x_1, \ldots, x_n) = f_1(x_1) \ldots f_n(x_n)$ for all $(x_i)_{i=1}^n$, where f, f_i are the PDFs of $(X_i)_{i=1}^n$ and X_i, respectively.
- $F(x_1, \ldots, x_n) = F_1(x_1) \ldots F_n(x_n)$ for all $(x_i)_{i=1}^n$, where F, F_i are the CDFs of $(X_i)_{i=1}^n$ and X_i, respectively.

Moreover, if $(X_i)_{i=1}^n$ are independent then

- $\mathbb{E}(X_1 \ldots X_n) = \prod_{i=1}^n \mathbb{E}(X_i)$.
- $(f_i(X_i))_{i=1}^n$ are independent for any collcetion of functions f_i.

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Def: Independently and identically distributed

We say a collection of random variables $X_1, \ldots, X_n$ is identically and independently distributed according to a distribution $\mathcal{D}$, or $X_1, \ldots, X_n \overset{\text{iid}}{\sim} \mathcal{D}$, if the X_i are independent and each $X_i \sim \mathcal{D}$.

Discussion

We have now clarified what we mean by $F, F_k \overset{\text{iid}}{\sim} \mathcal{F}$ in the Monte Carlo formula

$$\mathbb{E}[F] \approx \frac{1}{N} \sum_{k=1}^{N} F_k \qquad \text{where} \qquad F, F_k \overset{\text{iid}}{\sim} \mathcal{F}.$$

The central limit theorem presented on the next slide will allow us to clarify what we mean by $\approx$.

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Central limit theorem

Assume $F, F_1, \dots, F_N \overset{\text{iid}}{\sim} \mathcal{F}$. Then,

$$\frac{1}{N}\sum_{k=1}^{N} F_k \quad \xrightarrow{d} \quad \mathcal{N}\Big(\mathbb{E}[F], \tfrac{1}{N}\mathrm{Var}[F]\Big) \qquad \text{for } N \to \infty.$$

Here, $\xrightarrow{d}$ stands for convergence in distribution. This means that the distribution of the random variable on the left becomes increasingly indistinguishable from a normal distribution with mean and standard deviation as indicated on the right.

In this module, we will mostly ignore the convergence part and simply assume that

$$\frac{1}{N}\sum_{k=1}^{N} F_k \quad \sim \quad \mathcal{N}\Big(\mathbb{E}[F], \tfrac{1}{N}\mathrm{Var}[F]\Big) \qquad \text{if } N \gtrsim 100.$$

Interpretation of the central limit theorem

TODO