Lecture 11: Markov Chains

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MATH60047/70047 – Stochastic Simulation

November 14, 2022

Imperial College London

Announcements

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- You can now submit your assignments until 16th of November 2022 through the UG office.
- Solutions will be posted after that date.

A brief recap of what happened:

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- Sampling methods: $X_i \sim p_\star$ (from now on we will call it $p_\star$)
  - Direct sampling methods (Inversion, transformation)
  - Rejection sampling

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- Sampling methods: $X_i \sim p_\star$ (from now on we will call it $p_\star$)
  - Direct sampling methods (Inversion, transformation)
  - Rejection sampling
- Integration: $\bar{\varphi} = \int \varphi(x) p_\star(x) \mathrm{d}x$:
  - Using i.i.d samples from $p_\star$:

$$\bar{\varphi} \approx \hat{\varphi}^N_{\mathsf{MC}} = \frac{1}{N} \sum_{i=1}^N \varphi(X_i).$$

  - Using samples from a *proposal* q:

$$\bar{\varphi} \approx \hat{\varphi}^N_{\mathsf{IS}} = \frac{1}{N} \sum_{i=1}^N \bar{\mathsf{w}}_i \varphi(X_i).$$

Today, we will talk about Markov chains.

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- Markov chains have *stationary* distributions
- We design the chain so that the stationary distribution is $p_\star$!

We will first see how to simulate Markov chains.

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- A transition matrix M (discrete case)
- A transition kernel K (continuous case)

Let us denote our state-space with X.

What is a Markov chain?

The discrete case

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A discrete-time Markov chain is a process $(X_n)_{n\in\mathbb{N}}$, when X is finite, satisfies:

$$\mathbb{P}(X_n = j | X_0 = i_0, \ldots, X_{n-1} = i_{n-1}) = \mathbb{P}(X_n = j | X_{n-1} = i_{n-1}).$$

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We note that *transition matrix* is nothing but these transition probabilities:

$$M_{ij} = \mathbb{P}(X_{n+1} = j | X_n = i).$$

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$$X_0 \to X_1 \to X_2 \to \cdots \to X_n$$

We note that we will only consider the time-homogeneous case, i.e. the transition matrix is time-independent:

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A Markov chain therefore can be defined entirely by its:

- Initial state (or initial distribution)
- Transition matrix

Let us denote the initial distribution as p_0. This means,

$$p_0(i) = \mathbb{P}(X_0 = i).$$

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Note that in the continuous-space case, we will use the same notation, but we will consider p_0 as a density function.

The transition matrix M is a matrix of size $d \times d$ where $d = |\mathsf{X}|$.

What is a Markov chain?

The discrete case

The transition matrix M is a matrix of size $d \times d$ where $d = |\mathsf{X}|$.

$$M = \begin{bmatrix} M_{11} & M_{12} & \cdots & M_{1d} \\ M_{21} & M_{22} & \cdots & M_{2d} \\ \vdots & \vdots & \ddots & \vdots \\ M_{d1} & M_{d2} & \cdots & M_{dd} \end{bmatrix}.$$

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We note that this matrix is stochastic, i.e. each row sums to 1:

$$\sum_{j=1}^{d} M_{ij} = 1,$$

since $M_{ij} = \mathbb{P}(X_{n+1} = j | X_n = i)$ and

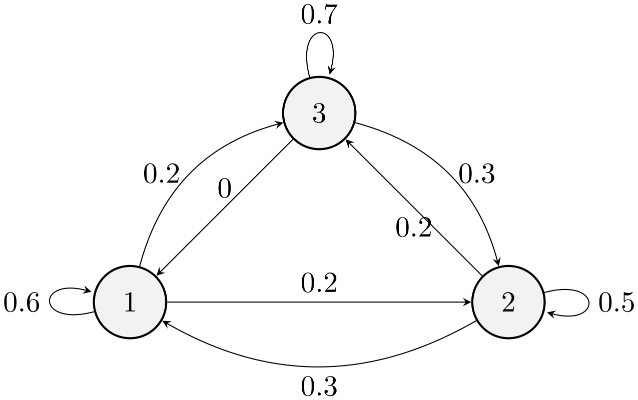
$$\sum_{j=1}^{d} \mathbb{P}(X_{n+1} = j | X_n = i) = 1.$$

What is a Markov chain?

Example 1: Simulate a discrete Markov chain

Consider the transition matrix:

$$M = \begin{bmatrix} 0.6 & 0.2 & 0.2 \\ 0.3 & 0.5 & 0.2 \\ 0 & 0.3 & 0.7 \end{bmatrix}, \qquad \text{where } \mathsf{X} = \{1, 2, 3\}.$$



M	$X_t = 1$	$X_t = 2$	$X_t = 3$
$X_{t-1} = 1$	0.6	0.2	0.2
$X_{t-1} = 2$	0.3	0.5	0.2
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Example: Given $X_0 = 1$, how to simulate this chain?

Sample:

$$X_t | X_t = x_{t-1} \sim \text{Discrete}(M_{x_{t-1},\cdot}).$$

What is a Markov chain?

Example 1: Simulate a discrete Markov chain – What does the matrix M mean?

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Simulation!

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$$M^{(n)} = \mathbb{P}(X_n = j | X_0 = i),$$

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where $M^{(n)}$ is a matrix of size $d \times d$. n-step transition matrix:

$$\begin{aligned}
M_{ij}^{(n)} &= \mathbb{P}(X_n = j | X_0 = i) \\
&= \sum_k \mathbb{P}(X_n = j, X_1 = k | X_0 = i) \\
&= \sum_k \mathbb{P}(X_n = j | X_1 = k, X_0 = i)\mathbb{P}(X_1 = k | X_0 = i) \\
&= \sum_k \mathbb{P}(X_n = j | X_1 = k)\mathbb{P}(X_1 = k | X_0 = i) \\
&= \sum_k M_{ik} M_{kj}^{(n-1)}.
\end{aligned}$$

Therefore, $M^{(n)} = M^n$, nth power.

The Chapman-Kolmogorov equation says that we can obtain

$$\mathbb{P}(X_{n+2} = x_{n+2} | X_n = x_n) =$$
$$\sum_{x_{n+1}} \mathbb{P}(X_{n+2} = x_{n+2} | X_{n+1} = x_{n+1}) \mathbb{P}(X_{n+1} = x_{n+1} | X_n = x_n).$$

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This follows from the simple marginalisation rules.

However, this gives us a way to relate M^{m+n} to M^m and M^n:

$$\begin{aligned} M^{(m+n)} &= \mathbb{P}(X_{m+n} = j | X_0 = i) \\ &= \sum_k \mathbb{P}(X_{m+n} = j | X_n = k) \mathbb{P}(X_n = k | X_0 = i) \\ &= \sum_k M_{ik}^{(m)} M_{kj}^{(n)}. \end{aligned}$$

Let $p_0(i) = \mathbb{P}(X_0 = i)$ for $i \in \mathsf{X}$.

What is a Markov chain?

The discrete case: The evolution of the density of the chain

Let $p_0(i) = \mathbb{P}(X_0 = i)$ for $i \in \mathsf{X}$. Then, the density of the chain at time n is given by:

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This implies that

$$p_n = p_{n-1} M.$$

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Simulation.

Properties of Markov chains

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We need Markov chains

- With invariant distributions
- Their convergence is ensured
- Their invariant distribution is unique

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- With invariant distributions
- Their convergence is ensured
- Their invariant distribution is unique

We will now review the properties which ensure these in discrete space case.

For two states, $x, x' \in \mathsf{X}$, we write $x \rightsquigarrow x'$ if there is a path from x to x':

$$\exists n > 0, \text{ s.t. }, \mathbb{P}(X_n = x' | X_0 = x) > 0.$$

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A communication class $C \subset \mathsf{X}$ is a set of states such that $x \in C$ and $x' \in C$ if and only if $x \rightsquigarrow x'$ and $x' \rightsquigarrow x$.

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A communication class $C \subset \mathsf{X}$ is a set of states such that $x \in C$ and $x' \in C$ if and only if $x \rightsquigarrow x'$ and $x' \rightsquigarrow x$.

A chain is irreducible if X is a single communication class.

A Markov chain is recurrent if every state is to be visited infinitely often.

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Define the return time:

$$\tau_i = \inf\{n \geq 0 : X_n = i\}.$$

We say that the state is recurrent if

$$\mathbb{P}(\tau_i < \infty | X_1 = i) = 1.$$

If a state is not recurrent, it is transient.

We say that a state i is positively recurrent if

$$\mathbb{E}[\tau_i | X_1 = i] < \infty.$$

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If a recurrent state is not positive recurrent, it is null recurrent.

A probability mass function $p_\star$ is called M-invariant if

$$p_\star(i) = \sum_j M_{ij} p_\star(j).$$

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Equivalently

$$p_\star = p_\star M.$$

Theorem 1

If M is irreducible, then M has a unique invariant distribution if and only if it is positive recurrent.

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This is existence, we do not talk about convergence yet.

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A Markov transition matrix M is reversible w.r.t. $p_\star$ if and only if for all $i, j \in \mathsf{X}$,

$$p_\star(i) M_{ij} = p_\star(j) M_{ji}.$$

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A Markov transition matrix M is reversible w.r.t. $p_\star$ if and only if for all $i, j \in \mathsf{X}$,

$$p_\star(i) M_{ij} = p_\star(j) M_{ji}.$$

This is called the detailed balance condition (we will discuss the continuous version)

Constructing a chain with stationary distribution $p_\star$ is ensured if detailed balance is satisfied since it implies $p_\star = p_\star M$.

We have seen how to construct chains with invariant distributions $p_\star$.

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For this, we need a final ingredient: aperiodicity.

A state i is called aperiodic if

$$\{n > 0 : \mathbb{P}(X_{n+1} = i | X_1 = i) > 0\}$$

has no common divisor other than 1.

Definition 2

An irreducible Markov chain is called ergodic if it is positive recurrent and aperiodic.

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Ergodicity brings us the missing ingredient for the convergence: We can now ensure p_n to converge to $p_\star$.

If $(X_n)_{n\in\mathbb{N}}$ is an ergodic Markov chain with any initial p_0 and a Markov transition matrix M with $p_\star$ as its invariant distribution, then

$$\lim_{n\to\infty} p_n(i) = p_\star(i).$$

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$$\lim_{n \to \infty} p_n(i) = p_\star(i).$$

Moreover, for $i, j \in \mathsf{X}$

$$\lim_{n \to \infty} \mathbb{P}(X_n = i | X_1 = j) = p_\star(i).$$

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We will be mainly interested in the continuous case, however, the analogous concepts are defined in a much more complicated way.

We will not go into the details here, we will just now introduce the continuous state-space notation.

We assume now our state-space is uncountable, e.g., $\mathsf{X} = \mathbb{R}$.

What is a Markov chain?

The continuous case case

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We denote the initial *density* of the chain by $p_0(x)$.

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We denote the initial *density* of the chain by $p_0(x)$.

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The density of the chain at time n is denoted by $p_n(x_n)$.

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The continuous case

A discrete-time Markov chain is a process $(X_n)_{n\in\mathbb{N}}$, when X is uncountable, satisfies:

$$p(x_n|x_{1:n-1}) = p(x_n|x_{n-1}) = K(x_n|x_{n-1}).$$

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A discrete-time Markov chain is a process $(X_n)_{n \in \mathbb{N}}$, when X is uncountable, satisfies:

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$$X_0 \longrightarrow X_1 \longrightarrow X_2 \longrightarrow \cdots \longrightarrow X_n$$

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- Initial state (or initial distribution)
- Transition kernel

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The transition kernel is a density function $K(x_n|x_{n-1})$ for fixed x_{n-1}, i.e.,

$$\int_{\mathsf{X}} K(x_n|x_{n-1})\,\mathrm{d}x_n = 1.$$

Otherwise, it is a function of (x_n, x_{n-1}).

Consider the following Markov chain: $X_0 = 0$ and

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$$K(x_n|x_{n-1}) = \mathcal{N}(x_n; ax_{n-1}, 1),$$

where $0 < a < 1$.
We can simulate this chain by:

$$\begin{aligned}
X_1 &\sim \mathcal{N}(0, 1) \\
X_2 &\sim \mathcal{N}(aX_1, 1) \\
X_3 &\sim \mathcal{N}(aX_2, 1) \\
&\vdots \\
X_n &\sim \mathcal{N}(aX_{n-1}, 1).
\end{aligned}$$

Simulation.

The Chapman-Kolmogorov equation for the continuous case

$$p(x_n|x_{n-k}) = \int_{\mathsf{X}} K(x_n|x_{n-1}) p(x_{n-1}|x_{n-k}) \, \mathrm{d}x_{n-1},$$

for $k > 1$.

Let $p_0(x)$ be the initial density such that $X_0 \sim p_0(x)$.

Then, the density of the chain at time n is given by

$$p_n(x_n) = \int_{\mathsf{X}} K(x_n|x_{n-1}) p_{n-1}(x_{n-1})\, \mathrm{d}x_{n-1}.$$

What is a Markov chain?

The continuous case: m-step transition kernel

It is useful for us to define the m-step transition kernel:

$$
\begin{aligned}
p(x_{m+n}|x_n) &= K^m(x_{m+n}|x_n), \\
&= \int_{\mathsf{X}} K(x_{m+n}|x_{m+n-1}) \cdots K(x_{n+1}|x_n)\, \mathrm{d}x_{m+n-1} \cdots \mathrm{d}x_{n+1}.
\end{aligned}
$$

What is a Markov chain?

Properties

We have the similar conditions of aperiodicity and irreducibility as in the discrete case, but,

- These are defined over *sets* rather than states.
- irreducibility is replaced by ϕ-irreducibility.
- aperiodicity is defined for sets

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- These are defined over *sets* rather than states.
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We will not go into the details of these conditions for continuous space case.

A probability distribution $p_\star$ is called K-invariant if

$$p_\star(x) = \int_{\mathsf{X}} p_\star(x')K(x|x')\,\mathrm{d}x'.$$

Similar to the discrete case.

The detailed balance condition for the continuous case takes a similar form:

$$p_\star(x)K(x'|x) = p_\star(x')K(x|x').$$

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Note that this is a sufficient condition for stationarity of $p_\star$:

$$\begin{aligned}\int p_\star(x)K(x'|x)\mathrm{d}y &= \int p_\star(x')K(x|x')\mathrm{d}x', \\ \implies p_\star(x) &= \int K(x|x')p_\star(x')\mathrm{d}x',\end{aligned}$$

which implies $p_\star$ is K-invariant.

Consider the following Markov chain: $X_0 = 0$ and

$$K(x_n|x_{n-1}) = \mathcal{N}(x_n; ax_{n-1}, 1),$$

where $0 < a < 1$.

Consider the following Markov chain: $X_0 = 0$ and

$$K(x_n|x_{n-1}) = \mathcal{N}(x_n; ax_{n-1}, 1),$$

where $0 < a < 1$. Note that we can also write this as

$$X_n = aX_{n-1} + \epsilon_n,$$

where $\epsilon_n \sim \mathcal{N}(0, 1)$.

What is a Markov chain?

Example: Go back to Gaussian model

Prove that for

$$p_\star(x) = \mathcal{N}\left(x; 0, \frac{1}{1 - a^2}\right),$$

the detailed balance condition is satisfied for the kernel

$$K(x_n | x_{n-1}) = \mathcal{N}(x_n; a x_{n-1}, 1),$$

where $0 < a < 1$.

Prove that $K^m(x_{m+n}|x_n)$ is given by

$$K^m(x_{m+n}|x_n) = \mathcal{N}\left(x_{m+n}; a^m x_n, \frac{1-a^{2m}}{1-a^2}\right).$$

Then prove that

$$p_\star(x) = \lim_{m\to\infty} K^m(x|x'),$$

independent of x'.

See you tomorrow!