Lecture 6. Discrete-Time Markov Chains

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Ergodic Problem

Other Topics
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Markov Chains

- Markov process is one of the most important stochastic processes in application. Roughly speaking, A Markov process is independent of the past, knowing the present state.

- In this lecture, we only consider the finite state Markov chain. The readers may be refereed to \(^1\) for further information.

\(^1\)DR. Durrett, Probability: theory and examples (3rd edition), Thomson Learning, 2005.
Example (1D Random Walk)

Let $\xi_i$ are i.i.d. random variables such that $\xi_i = \pm 1$ with probability $\frac{1}{2}$, and let

$$X_n = \xi_1 + \xi_2 + \ldots + \xi_n$$

$\{X_n\}$ represents a unconstrained unbiased random walk on $\mathbb{Z}$, the set of integers.
1D Random Walk

Example (1D Random Walk)

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$$X_n = \xi_1 + \xi_2 + \ldots + \xi_n$$

$$\{X_n\}$$ represents a unconstrained unbiased random walk on $\mathbb{Z}$, the set of integers. Given $X_n = i$, we have

$$\mathbb{P}\{X_{n+1} = i \pm 1| \ X_n = i\} = \frac{1}{2},$$

$$\mathbb{P}\{X_{n+1} = \text{anything else}| \ X_n = i\} = 0.$$

We see that the distribution of $X_{n+1}$ depends only on the value of $X_n$. 
Markov Property

The result above can be restated as the Markov property

\[ P\{X_{n+1} = i_{n+1} \mid \{X_m = i_m\}_{m=1}^n\} = P\{X_{n+1} = i_{n+1} \mid X_n = i_n\}, \]

and the sequence \( \{X_n\}_{n=1}^\infty \) is called a realization of Markov process.
Example (Finite state Markov chain)

Suppose a Markov chain only takes a finite set of possible values, without loss of generality, we let the state space be \( \{1, 2, \ldots, N\} \). Define the \textbf{transition probabilities}

\[
p^{(n)}_{jk} = \mathbb{P}\{X_{n+1} = k | X_n = j\}
\]

This uses the Markov property that the distribution of \( X_{n+1} \) depends only on the value of \( X_n \).
Chapman-Kolmogorov equation

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This uses the Markov property that the distribution of \(X_{n+1}\) depends only on the value of \(X_n\).

Proposition (Chapman-Kolmogorov equation)
We have the relation

\[ \mathbb{P}(X_n = j | X_0 = i) = \sum_k \mathbb{P}(X_n = j | X_m = k) \mathbb{P}(X_m = k | X_0 = i), \]

\[ 1 \leq m \leq n - 1. \]
Definition (Time-stationary, or time homogeneous)

A Markov chain is called stationary if $p_{jk}^{(n)}$ is independent of $n$. 

From now on we will discuss only stationary Markov chains and let $P = (p_{jk})_{j,k=1}^{N}$. 

$P$ is called the transition probability matrix (TPM).
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Time Homogeneity
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Fun: Snake-and-Ladders Game

Connection between games and Markov Chains:
Ehrenfest’s diffusion model

Example (Ehrenfest’s diffusion model)

An urn contains a mixture of white and black balls. At each time 1, 2, ... a ball is picked at random from the urn and replaced by a ball of the other colour. The total number of balls in the urn is therefore a constant $N$, say. Let the state $X_n$ of the system at time $n$ be the number of black balls in the urn.

\[
\begin{pmatrix}
0 & 1 & 0 & 0 & 0 & 0 \\
1 & 0 & \frac{N-1}{N} & 0 & 0 & 0 \\
0 & \frac{2N}{N} & 0 & 0 & 0 & 0 \\
0 & 0 & \frac{2N}{N} & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{2N}{N} & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 \\
\end{pmatrix}
\]
Ehrenfest’s diffusion model

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As will be stated below, the one-step transition matrix can be given as

$$
P = \begin{pmatrix}
0 & 1 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{N} & 0 & \frac{N-1}{N} & 0 & 0 & 0 & 0 \\
0 & \frac{2}{N} & 0 & \frac{N-2}{N} & 0 & 0 & 0 \\
0 & 0 & \ddots & 0 & \ddots & 0 & 0 \\
0 & \cdots & 0 & \frac{N-1}{N} & 0 & \frac{1}{N} & 0 \\
0 & \cdots & 0 & 0 & 1 & 0 & 0
\end{pmatrix}
$$
Implication of Time Homogeneity

- Markov property implies that

\[ P\{X_0 = i_0, X_1 = i_1, \ldots, X_n = i_n\} = (\mu_0)_{i_0} p_{i_0 i_1} p_{i_1 i_2} \cdots p_{i_{n-1} i_n} \]

where \((\mu_0)_{i_0}\) is defined by the initial distribution

\((\mu_0)_{i_0} = P\{X_0 = i_0\}\).
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where $(\mu_0)_{i_0}$ is defined by the initial distribution

$$(\mu_0)_{i_0} = \mathbb{P}\{X_0 = i_0\}.$$ 

$P$ is also called a stochastic matrix, in the sense that

$$p_{ij} \geq 0, \quad \sum_{j=1}^{N} p_{ij} = 1.$$
Implication of Time Homogeneity

From this we get

\[ \mathbb{P}\{X_n = i_n | X_0 = i_0\} = \sum_{i_1, \ldots, i_{n-1}} p_{i_0i_1} p_{i_1i_2} \cdots p_{i_{n-1}i_n} \]

\[ = (P^n)_{i_0i_n} \]

The last quantity denotes the \((i_0, i_n)\)-th entry of the matrix \(P^n\).
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\[ \mathbb{P}\{X_n = i_n | X_0 = i_0\} = \sum_{i_1, \ldots, i_{n-1}} p_{i_0i_1}p_{i_1i_2} \cdots p_{i_{n-1}i_n} = (P^n)_{i_0i_n} \]

The last quantity denotes the \((i_0, i_n)\)-th entry of the matrix \(P^n\).

- Given the initial distribution of the Markov chain \(\mu_0\), the distribution of \(X_n\) is then given by

\[ \mu_n = \mu_0 P^n \]
Proposition

\( \mu_n \) satisfies the recurrence relation \( \mu_n = \mu_{n-1}P \). This equation can also be rewritten as

\[
(\mu_n)_i = (\mu_{n-1})_i(1 - \sum_{j \neq i} p_{ij}) + \sum_{j \neq i} (\mu_{n-1})_j p_{ji}.
\]

The interpretation is clear.
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Ergodicity Problem

The following two questions are of special interest.

▶ Is there an invariant distribution? \( \pi \) is called an invariant distribution if

\[
\pi = \pi P
\]

This is equivalent to say that there exists a nonnegative left eigenvector of \( P \) with eigenvalue equal to 1. Notice that 1 is always an eigenvalue of \( P \) since it always has the right eigenvector \((1, \ldots, 1)^T\).
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▶ When is the invariant distribution unique?

To answer these questions, it is useful to recall some general results on nonnegative matrices.
Irreducibility

Definition (Reducibility)

If there exists a permutation matrix $Q$ such that

$$QPQ^T = \begin{pmatrix} A_1 & B \\ 0 & A_2 \end{pmatrix}$$

then $P$ is called reducible. Otherwise $P$ is called irreducible.
Graph representation of Markov chains

Example (Graph representation of Markov chains)
Any Markov chain can be sketched by their graph representation.

Figure: Graph representation of Markov chains. Left panel: chain 1, right panel: chain 2.
The arrows and real numbers show the transition probability of the Markov chain.

- The TPM corresponds to left panel is

\[
P = \begin{bmatrix}
1 & 0 & 0 \\
\frac{1}{2} & 0 & \frac{1}{2} \\
0 & 0 & 1 
\end{bmatrix},
\]

- The TPM corresponds to right panel is

\[
P = \begin{bmatrix}
0 & 1 & 0 \\
1 & 2 & 0 \\
0 & 1 & 0 
\end{bmatrix},
\]
Transition Rules from Graph Representations

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- The reducibility means that there exists a subgroup of the states of the Markov chain, which forms a sub-Markov chain, and subsequently these states do not leave the subgroup, though the other states may have possibility to transition into this group.
- The action of the permutation matrix $Q$ and $Q^T$ is nothing but renaming the label of nodes.
- In the left panel, it is quite clear that $P$ is a reducible matrix, and it has two invariant distributions $\pi_1 = (1, 0, 0)$ and $\pi_2 = (0, 0, 1)$. 
The reducibility means that there exists a subgroup of the states of the Markov chain, which forms a sub-Markov chain, and subsequently these states do not leave the subgroup, though the other states may have possibility to transition into this group.

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In the left panel, it is quite clear that $P$ is a reducible matrix, and it has two invariant distributions $\pi_1 = (1, 0, 0)$ and $\pi_2 = (0, 0, 1)$.

In the right panel, it is an irreducible matrix, and the only invariant distribution is $\pi = (\frac{1}{4}, \frac{1}{2}, \frac{1}{4})$. 
we say that $j$ is accessible from $i$, denoted by $i \rightarrow j$ if there is a transition chain from $i \rightarrow k_1 \rightarrow \cdots \rightarrow k_j \rightarrow j$, i.e.

$$p_{ik_1} p_{k_1 k_2} \cdots p_{k_s j} > 0$$

for some $(k_1, k_2, \ldots, k_s)$. 
we say that \( j \) is accessible from \( i \), denoted by \( i \rightarrow j \) if there is a transition chain from \( i \rightarrow k_1 \rightarrow \cdots \rightarrow k_j \rightarrow j \), i.e.

\[
p_{ik_1}p_{k_1k_2}\cdots p_{k_j} > 0
\]

for some \((k_1, k_2, \ldots, k_s)\).

 Irreducibility is equivalent to the property that all nodes on the chain communicate, i.e. given any pair \((i, j)\) we have \(i \rightarrow j\) and \(j \rightarrow i\). So ‘communication’ means that \( i \) and \( j \) are accessible from each other.
The following theorem is a key answer for invariant distribution of a Markov chain.

**Theorem (Perron-Frobenius)**

Let $A$ be an irreducible nonnegative matrix, and let $\rho(A)$ be its spectral radius: $\rho(A) = \max_{\lambda} |\lambda|$, where $\lambda$ is an eigenvalue of $A$. Then,
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**Theorem (Perron-Frobenius)**

Let $A$ be an irreducible nonnegative matrix, and let $\rho(A)$ be its spectral radius: $\rho(A) = \max_{\lambda} |\lambda|$, where $\lambda$ is an eigenvalue of $A$. Then,

1. There exists a positive right eigenvector $x$ of $A$, such that

   $$Ax = \rho(A)x$$

   $$x = (x_1, \ldots, x_N)^T, x_i > 0.$$
Perron-Frobenius Theorem

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   \]

   \[
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   \]

2. \( \lambda = \rho(A) \) is an eigenvalue of multiplicity 1.
Implication on Ergodicity

Coming back to Markov chains, we obtain as a consequence of the Perron-Frobenius Theorem that

- If $P$ is irreducible, then there exists exactly one invariant distribution.

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  - On each component there exists a unique invariant distribution (with zero extension to other states).
  - Arbitrary convex combinations of these invariant distributions on each component are invariant distributions for the whole chain.
  - In this case, the invariant distribution for the whole chain is clearly not unique.

---

Ergodicity: Examples

One typical example may be as follows:

\[ P = \begin{bmatrix}
0 & 1 & 0 & 0 & 0 \\
0.5 & 0.5 & 0 & 0 & 0 \\
0.3 & 0 & 0.4 & 0.3 & 0 \\
0 & 0 & 0 & 0.5 & 0.5 \\
0 & 0 & 0 & 0.5 & 0.5 \\
\end{bmatrix}. \]

In this case, states 1, 2 and 4, 5 form two closed irreducible sub-chains, but \( P \) is reducible. There are infinite many invariant distributions.
But reducibility itself is not a sufficient condition for the non-uniqueness of the invariant distribution, e.g.

\[ P = \begin{bmatrix}
0 & 1 & 0 & 0 & 0 \\
0.3 & 0.4 & 0.3 & 0 & 0 \\
0.3 & 0 & 0.4 & 0.3 & 0 \\
0 & 0 & 0 & 0.5 & 0.5 \\
0 & 0 & 0 & 0.5 & 0.5 \\
\end{bmatrix}. \]

Though the invariant distribution has some zero components which are related to the transience of the states, it is unique.
A stronger assumption is **primitive** which says that there exist an natural number $s$, such that

$$(P^s)_{ij} > 0, \quad \text{for all } i, j$$
A stronger assumption is primitive which says that there exist an natural number $s$, such that

$$(P^s)_{ij} > 0, \quad \text{for all } i, j$$

A critical example is that

$$P = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},$$

which is called a periodic chain. Actually we have primitive $\Leftrightarrow$ irreducible + aperiodic for finite Markov chains.
Theorem

Assume that the Markov chain is primitive. Then for any initial distribution $\mu_0$

$$\mu_n = \mu_0 P^n \to \pi \quad \text{exponentially fast as } n \to \infty,$$

where $\pi$ is the unique invariant distribution.
Theorem
Assume that the Markov chain is primitive. Then for any initial distribution $\mu_0$

$$\mu_n = \mu_0 P^n \to \pi \text{ exponentially fast as } n \to \infty,$$

where $\pi$ is the unique invariant distribution.

Proof.
Given two distributions, $\mu_0$ and $\tilde{\mu}_0$, we define the total variation distance by

$$d(\mu_0, \tilde{\mu}_0) = \frac{1}{2} \sum_{i \in S} |\mu_{0,i} - \tilde{\mu}_{0,i}|.$$
Ergodic Theorem: Proof

Since

\[ 0 = \sum_{i \in S} \left( \mu_{0,i} - \tilde{\mu}_{0,i} \right) = \sum_{i \in S} (\mu_{0,i} - \tilde{\mu}_{0,i})^+ - \sum_{i \in S} (\mu_{0,i} - \tilde{\mu}_{0,i})^- , \]

where \( a^+ = \max(a, 0) \) and \( a^- = \max(-a, 0) \). We also have

\[ d(\mu_0, \tilde{\mu}_0) = \frac{1}{2} \sum_{i \in S} (\mu_{0,i} - \tilde{\mu}_{0,i})^+ + \frac{1}{2} \sum_{i \in S} (\mu_{0,i} - \tilde{\mu}_{0,i})^- \]

\[ = \sum_{i \in S} (\mu_{0,i} - \tilde{\mu}_{0,i})^+ \leq 1. \]

Let \( \mu_s = \mu_0 P^s \), \( \tilde{\mu}_s = \tilde{\mu}_0 P^s \) and consider \( d(\mu_s, \tilde{\mu}_s) \).
Ergodic Theorem: Proof

We have

\[ d(\mu_s, \tilde{\mu}_s) = \sum_{i \in S} \left[ \sum_{j \in S} \left( \mu_{0,j}(P^s)_{ji} - \tilde{\mu}_{0,j}(P^s)_{ji} \right) \right]^+ \]

\[ \leq \sum_{j \in S} \left( \mu_{0,j} - \tilde{\mu}_{0,j} \right)^+ \sum_{i \in B_+} (P^s)_{ji}, \]

where \( B_+ \) is the subset of indices where

\( \sum_{j \in S} (\mu_{0,j} - \tilde{\mu}_{0,j}) (P^s)_{ji} > 0. \)

We note that \( B_+ \) cannot contain all the elements of \( S \), otherwise one must have

\( (\mu_0 P^s)_i > (\tilde{\mu}_0 P^s)_i \) for all \( i \), and

\[ \sum_{i \in S} (\mu_0 P^s)_i > \sum_{i \in S} (\tilde{\mu}_0 P^s)_i, \]

which is impossible since both sides sum to 1.
Ergodic Theorem: Proof

Therefore at least one element is missing in $B_+$. By assumption, there exists an $s > 0$ and $\alpha \in (0, 1)$ such that $(P^s)_{ij} \geq \alpha$ for all pairs $(i, j)$. Hence $\sum_{i \in B_+} (P^s)_{ji} \leq (1 - \alpha) < 1$. Therefore

$$d(\mu_s, \tilde{\mu}_s) \leq d(\mu_0, \tilde{\mu}_0)(1 - \alpha),$$

i.e. the Markov chain is contractive after every $s$ steps. Similarly for any $m \geq 0$

$$d(\mu_n, \mu_{n+m}) \leq d(\mu_{n-sk}, \mu_{n+m-sk})(1 - \alpha)^k \leq (1 - \alpha)^k,$$

where $k$ is the largest integer such that $n - sk \geq 0$. 

If \( n \) is sufficiently large the right hand side can be made arbitrarily small. Therefore the sequence \( \{\mu_n\}^\infty_{n=0} \) is a Cauchy sequence. Hence it has to converge to a limit \( \pi \), which satisfies

\[
\pi = \lim_{n \to \infty} \mu_0 P^{n+1} = \lim_{n \to \infty} (\mu_0 P^n) P = \pi P.
\]

Such a \( \pi \) satisfying such a property is also unique. For if there were two such distributions, \( \pi^{(1)} \) and \( \pi^{(2)} \), then

\[
d(\pi^{(1)}, \pi^{(2)}) = d(\pi^{(1)} P^s, \pi^{(2)} P^s) < d(\pi^{(1)}, \pi^{(2)}). \]

This implies

\[
d(\pi^{(1)}, \pi^{(2)}) = 0, \text{ i.e } \pi^{(1)} = \pi^{(2)}. \]
Ergodic Theorem: Time average $=$ Ensemble Average

Remark
We do not discuss the convergence speed here. But in fact it is exponential, which depends on the spectral gap of the transition probability matrix $P$. The readers may be referred to $^3$ $^4$.

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Ergodic Theorem: Time average = Ensemble Average

Remark
We do not discuss the convergence speed here. But in fact it is exponential, which depends on the spectral gap of the transition probability matrix $P$. The readers may be referred to $^3$ $^4$.

Theorem (Ergodic theorem)

let $X_n$ be an irreducible, positive recurrent Markov chain with invariant distribution $\pi(x)$, and $f$ be a bounded function, then

$$ \frac{1}{N} \sum_{n=1}^{N} f(X_n) \rightarrow \langle f \rangle_{\pi}, \ a.s. $$

---


Theorem
Assume that the Markov chain \( \{X_n\}_{n \geq 0} \) admits a unique invariant distribution \( \pi \) and is also initially distributed according to \( \pi \). Denote by \( P \) its transition probability matrix. Define a new Markov chain \( \{Y_n\}_{0 \leq n \leq N} \) by \( Y_n = X_{N-n} \) where \( N \in \mathbb{N} \) is fixed.
**Time Reversal**

**Theorem**
Assume that the Markov chain \( \{X_n\}_{n \geq 0} \) admits a unique invariant distribution \( \pi \) and is also initially distributed according to \( \pi \). Denote by \( P \) its transition probability matrix. Define a new Markov chain \( \{Y_n\}_{0 \leq n \leq N} \) by \( Y_n = X_{N-n} \) where \( N \in \mathbb{N} \) is fixed. Then \( \{Y_n\}_{0 \leq n \leq N} \) is also a Markov chain with invariant distribution \( \pi \). Its transition probability matrix \( \hat{P} \) is given by

\[
\hat{p}_{ij} = \frac{\pi_j}{\pi_i} p_{ji}.
\]
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Proof.
It is straightforward to check that \( \hat{P} \) is a stochastic matrix with an invariant distribution \( \pi \). To prove that \( \{Y_n\} \) is Markov with transition probability matrix \( \hat{P} \), it is enough to observe that

\[
\Pr(Y_0 = i_0, Y_1 = i_1, \ldots, Y_N = i_N) = \Pr(X_N = i_0, X_{N-1} = i_1, \ldots, X_0 = i_N)
= \pi_{i_N} p_{i_N i_{N-1}} \cdots p_{i_1 i_0} = \pi_{i_0} \hat{p}_{i_0 i_1} \cdots \hat{p}_{i_{N-1} i_N}
\]

for any \( i_0, i_1, \ldots, i_N \). \( \square \)
A particularly important class of Markov chains are those that satisfy the condition of *detailed balance*

\[ \pi_i p_{ij} = \pi_j p_{ji} \]

In this case, we have \( \hat{p}_{ij} = p_{ij} \). We call the chain *reversible*. The reversible chain can be equipped with variational structure and has nice spectral properties. Define the *graph Laplacian matrix*

\[ L = P - I \]

and correspondingly its action on any function \( f \)

\[ (Lf)(i) = \sum_{j \in S} p_{ij} (f(j) - f(i)). \]
Dirichlet form

Let $L^2_\pi$ be the space of square summable functions $f$ endowed with the $\pi$-weighted scalar product

$$(f, g)_\pi = \sum_{i \in S} \pi_i f(i) g(i).$$

Denote the Dirichlet form or energy of a function $f$ by

$$D(f) = \frac{1}{2} \sum_{i,j \in S} \pi_i p_{ij} (f(j) - f(i))^2.$$

One can show that $D(f) = (f, -L f)_\pi$. These formulations are particularly useful in potential theory for Markov chains.
Example (Hitting time distribution of a Markov chain)

Consider TPM of a 4-state Markov chain (1, 2, 3, 4):

\[
P = \begin{bmatrix}
\frac{1}{4} & \frac{1}{2} & \frac{1}{4} & 0 \\
\frac{1}{3} & 0 & \frac{1}{3} & \frac{1}{3} \\
\frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\
0 & \frac{1}{3} & \frac{1}{3} & \frac{1}{3}
\end{bmatrix}.
\]

Define the first hitting time \( n_\ast = \inf \{ n \mid X_n = 3 \text{ or } 4 \} \) and the hitting time probability \( q(m) = \text{Prob}\{n_\ast = m\} \), an interesting question is to ask how to obtain \( q(m) \).
Hitting time distribution

The idea is to modify the chain to a 3-state chain

$$\tilde{P} = \begin{bmatrix} \frac{1}{4} & \frac{1}{2} & \frac{1}{4} \\ \frac{1}{3} & 0 & \frac{2}{3} \\ 0 & 0 & 1 \end{bmatrix}.$$ 

then

$$1 - (\mu_n)_3 = \sum_{m=n+1}^{\infty} q(m),$$

hence

$$q(n) = (\mu_n)_3 - (\mu_{n-1})_3 = \mu_0 \cdot (\tilde{P}^n - \tilde{P}^{n-1}) \cdot \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$