Lecture 11: Markov Chains, Random Walks, Mixing Time, Page Rank

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Overview

- Introduction
  - Why Random Walks & Markov Chains?
  - Basics on Theory of (finite) Markov Chains
- Main Topics
  - Fundamental Theorem of Markov Chains
  - Page Rank
- Conclusion
- Acknowledgements

What is a Random Walk?

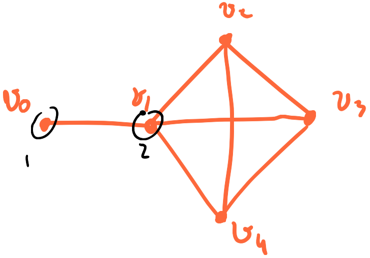
Given a graph $G(V, E)$

1. random walk starts from a vertex v_0
2. at each time step it moves to a *uniformly random neighbor* of the current vertex in the graph

$$v_{t+1} \leftarrow_R N_G(v_t)$$

$v_0 \xrightarrow{1} v_1 \xrightarrow{1/4} v_2$

$v_1 \xrightarrow{1/4} v_0$



$v_0 \xrightarrow{1} v_1 \xrightarrow{1/4} v_0 \xrightarrow{1} v_1 \xrightarrow{1/4} v_2 \xrightarrow{1/3} v_3$

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$p^{(0)} = (1, 0, \ldots, 0)$

$v_0 = 1$

Basic questions involving random walks:

graph G $\quad V = \{1, \ldots, n\}$

at time t $\quad p^{(t)} = (p_1^{(t)}, p_2^{(t)}, \ldots, p_n^{(t)})$

$p_i^{(t)} \leftarrow$ probability of being at i at time t

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- *Stationary distribution:* does the random walk converge to a "stable" distribution? If it does, what is this distribution?

$p^{(t)} = p^{(t+1)}$ "stable"

stationary distribution

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today's lecture

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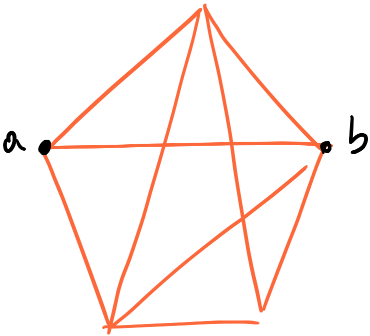
- *Hitting time:* starting from a vertex v_0, what is expected number of steps until it reaches a vertex v_f?
- *Cover time:* how long does it take to reach every vertex of the graph at least once?

Random Walk: Example

- Suppose $G(V, E) = K_n$, the complete graph, $a, b \in V$ two vertices



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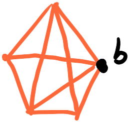
$$x_t = \Pr[\text{reach } b \text{ first time at time } t \text{ starting at } a]$$



$$x_t = \left(\frac{n-2}{n-1}\right)^{t-1} \cdot \underbrace{\frac{1}{n-1}}_{\text{reaching } b \text{ at time } t}$$

$$\mathbb{E}[\text{steps to reach } b] = \sum_{t \geq 1} t \cdot x_t = \sum_{t \geq 1} \frac{t}{n-1} \cdot \left(\frac{n-2}{n-1}\right)^{t-1}$$

$$= \frac{1}{n-1} \sum_{t \geq 1} t \left(\frac{n-2}{n-1}\right)^{t-1} = \frac{1}{n-1}\left(\frac{d}{dx} \underbrace{\sum_{t \geq 1} x^t}_{\frac{x}{1-x}}\right)\Bigg|_{x = \frac{n-2}{n-1}} = \frac{1}{n-1} \cdot \frac{1}{(1-x)^2}\Bigg|_{x = \frac{n-2}{n-1}} = \boxed{n-1}$$

$$\frac{1 \cdot (1-x) - x(-1)}{(1-x)^2} = \frac{1}{(1-x)^2}$$

Random Walk: Example

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  1. What is expected number of steps to reach b in simple random walk starting at a? (i.e., hitting time)
  2. Starting from a, what is expected number of steps to visit all vertices? (i.e, cover time)

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  2. Starting from a, what is expected number of steps to visit all vertices? (i.e, cover time)
  3. Stationary Distribution?

$$\pi = \left(\frac{1}{n}, \frac{1}{n}, \frac{1}{n}, \ldots, \frac{1}{n}\right)$$

$$\Pr[a \text{ in next step}] = \sum_{i=1}^{n} \Pr[\text{currently at } i] \cdot \Pr[i \to a]$$

$$= \sum_{i=1}^{n} \underbrace{\frac{1}{n}}_{\text{because of } \pi} \cdot \frac{1}{n-1}\left(1 - \delta_{ia}\right) = \frac{(n-1)}{n(n-1)} = \frac{1}{n}$$

$$\delta_{ia} = \begin{cases} 1 & \text{if } i = a \\ 0 & \text{otherwise} \end{cases}$$

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- **Practice question:** Compare question 2 to coupon collector problem!

$$(n-1)\underbrace{H_{n-1}}_{\text{harmonic number}}$$

What is a Markov Chain?

Random walk is a special kind of *stochastic process*:

$$\Pr[X_t = v_t \mid \overbrace{X_0 = v_0, \ldots, X_{t-1} = v_{t-1}}^{\text{history of random walk}}] = \Pr[X_t = v_t \mid \underbrace{X_{t-1} = v_{t-1}]}_{\text{only depend on information at time } t-1}$$

"forgetful stochastic process"

X_t random variable taking values over V

where will the random walk be at time t

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Probability that we are at vertex v_t at time t only depends on the state of our process at time $t-1$.

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Process is "*forgetful*"

Markov chain is characterized by this property.

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Representing Finite Markov Chains

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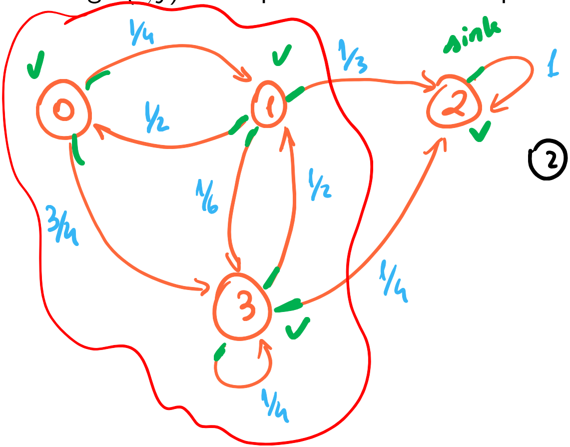
- Vertex is a state of Markov chain
- edge (i, j) corresponds to transition probability from i to j



① weights on edges are ≥ 0

② sum of weights coming out of each node $= 1$ (probability distribution)

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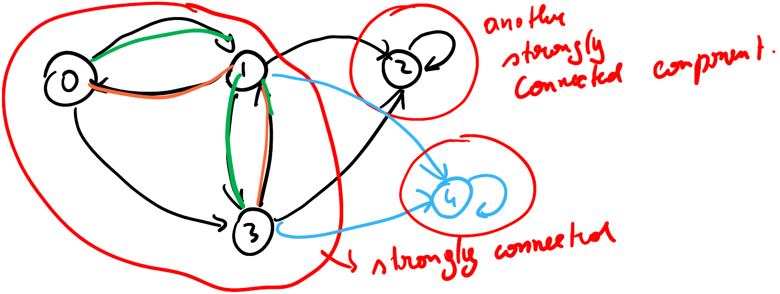

- Markov Chain *irreducible* if underlying directed graph is *strongly connected* (i.e. there is directed path from i to j for any pair $i, j \in V$)

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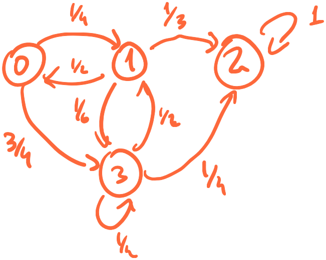


$$P = \begin{array}{c|cccc} & 0 & 1 & 2 & 3 \\ \hline 0 & 0 & 1/4 & 0 & 3/4 \\ 1 & 1/2 & 0 & 1/3 & 1/6 \\ 2 & 0 & 0 & 1 & 0 \\ 3 & 0 & 1/2 & 1/4 & 1/4 \end{array}$$

$p_0 = (1, 0, 0, 0)$

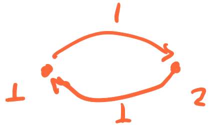
$p_1 = p_0 \cdot P = (\underset{0}{0}, \underset{1}{1/4}, \underset{2}{0}, \underset{3}{3/4})$

- $P \in \mathbb{R}^{n \times n}$ transition matrix
- entry $P_{i,j}$ corresponds to transition probability from i to j
- $\boxed{p_t \in \mathbb{R}^n}$ probability vector: $p_t(i) :=$ Pr[being at *state i* at *time t*]
- Transition given by

row vector

$$\boxed{p_{t+1} = p_t \cdot P}$$

Properties of Markov Chains



- *Period* of a state i is:

$$\gcd\{t \in \mathbb{N} \mid P^t_{i,i} > 0\}$$

That is, gcd of all times t such that the probability of starting at state i and being back at i at time t is positive

$P^t_{i,i}$ = Pr [back at state i after t steps if started at i]

$P^1_{i,i}$ = Pr. stay at state i

$P^2_{i,i}$ = Pr $[\, i \to v \to i \,]$

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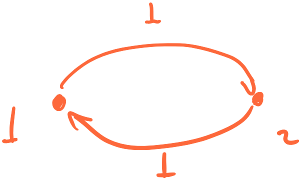

in periodic Markov chain we may never reach stationary distribution!

$\pi = (\frac{1}{2}, \frac{1}{2})$

$p_0 = (1, 0)$

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Lemma

For any finite, irreducible and aperiodic Markov Chain, there exists $T < \infty$ such that

$$P^t_{i,j} > 0 \quad \textit{for any } i, j \in V \textit{ and } t \geq T.$$

at some point we will reach every vertex with > 0 probability if we take enough steps

Stationary Distributions

Definition (Stationary Distribution)

A stationary distribution of a Markov Chain is a probability distribution $\pi \in \mathbb{R}^n$ such that

$$\pi P = \pi.$$

transition matrix

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$$\pi P^2 = (\pi P) \cdot P = \pi P = \pi$$

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- Given two distributions $p, q \in \mathbb{R}^n$, their *total variational distance* is

$$\Delta_{TV}(p,q) = \frac{1}{2}\sum_{i=1}^{n} |p_i - q_i| = \frac{1}{2} \cdot \cancel{\|p - q\|_1}$$

$\|p-q\|_1$

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$$\Delta_{TV}(p, q) = \frac{1}{2} \sum_{i=1}^{n} |p_i - q_i| = \frac{1}{2} \cdot \|p, q\|_1$$

- p_t *converges* to q iff $\lim_{t \to \infty} \Delta_{TV}(p_t, q) = 0$

Mixing Time of Markov Chains

Definition (Mixing Time)

The ε-mixing time of a Markov Chain is the smallest t such that

$$\Delta_{TV}(p_t, \pi) \leq \varepsilon$$

regardless of the initial starting distribution p_0.

Practice problem: For complete graph K_n compute its ε-mixing time.

Hint: look at eigenvalues and eigenvectors of transition matrix $P = \begin{pmatrix} 0 & & 1 \\ & \ddots & \\ 1 & & 0 \end{pmatrix} \cdot \frac{1}{n-1}$

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- Eigenvalues $\lambda_1 = 1, \lambda_2 = \cdots = \lambda_n = -1/(n-1)$, corresponding eigenvectors $v_1, \ldots, v_n$ (orthonormal)

K_n complete graph

all one's matrix

$$P = \begin{pmatrix} 0 & & \frac{1}{n-1} \\ & \ddots & \\ \frac{1}{n-1} & & 0 \end{pmatrix} = -\frac{I}{n-1} + \frac{J}{n-1}$$

$$P = \frac{1}{n-1}\begin{pmatrix} 0 & & 1 \\ & \ddots & \\ 1 & & 0 \end{pmatrix} = \underbrace{\frac{1}{n-1} J}_{\text{rank } 1} - \frac{1}{n-1} I$$

$$J = \vec{1} \cdot \vec{1}^T$$

$$\begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} (1 \ 1 \cdots 1)$$

eigenvectors

$$v_1 = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \cdot \frac{1}{\sqrt{n}}$$

$$v_2$$

$$\vdots$$

$$\underbrace{v_n}_{\text{orthonormal}}$$

orthonormal (l_2-norm $=1$)

eigenvalues

$$\lambda_1 = 1$$

$$\lambda_2 = -1/n-1$$

$$\lambda_3 = -1/n-1$$

$$\vdots$$

$$\lambda_n = -1/n-1$$

eigenvectors of P:

$i > 1$

$$J \cdot v_i = 0$$

$$v_i \perp \vec{1}$$

$$P v_i = -\frac{1}{n-1} I \cdot v_i$$

$$= -\frac{1}{n-1} \cdot v_i$$

$$P = \lambda_1 v_1 v_1^T + \sum_{i=2}^{n} \lambda_i v_i v_i^T$$

$$\lambda_1 = 1 \qquad \lambda_2 = \dots = \lambda_n = -\frac{1}{n-1}$$

$$P^t = \lambda_1^t v_1 v_1^T + \sum_{i=2}^{n} \lambda_i^t v_i v_i^T$$

$$= v_1 v_1^T + \underbrace{\sum_{i=2}^{n} \lambda_i^t v_i v_i^T}_{\text{if } t \text{ large then}}$$

$$\lambda_i \longmapsto 0$$

$$\lambda_i^t = \left(-\frac{1}{n-1}\right)^t \qquad \text{if } t = \log_{n-1}(1/\epsilon)$$

$$\lambda_i^t = \left(-\frac{1}{n-1}\right)^t$$

$$\boxed{t = \log_{n-1}\left(\frac{n}{\epsilon}\right)}$$ then

$$|\lambda_i^t| = \frac{\epsilon}{n}$$

$$P^t = \underbrace{v_1 v_1^T}_{\text{stationary distribution}} + \frac{\epsilon}{n} \cdot (-1)^t \underbrace{\sum_{i=2}^{n} v_i v_i^T}_{\text{everything } \perp \text{ to stationary}}$$

$\vec{q} \in \mathbb{R}^n$ initial probability distribution

$$\vec{q} = \alpha_1 v_1 + \alpha_2 v_2 + \dots + \alpha_n v_n$$

$$\boxed{P^t \vec{q} = \lambda_1^t \alpha_1 v_1 + \lambda_2^t \alpha_2 v_2 + \dots + \lambda_n^t \alpha_n v_n}$$

$$\|P^{(t)} q - v_1\|_1 = \underbrace{\left|\left(\lambda_1^t \alpha_1 - 1\right)\right|}_{\leq \epsilon} + \underbrace{\sum_{j=2}^{n} \underbrace{|\lambda_j^t|}_{\leq \frac{\epsilon}{n}}}_{\leq \epsilon}$$

$$\sum_{i=1}^{n} \lambda_i^t \alpha_i = 1$$

Template:

- find stationary distribution
- get eigenvalues of the transition matrix of Markov chain

  $\lambda_1 = 1 \quad \lambda_2 = \dots = \lambda_n = -1/n-1$
- need to compute t such that

  $$|\lambda_j^t| < \frac{\epsilon}{n} \text{ for all } j > 1 .$$
- t is your mixing time

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Fundamental Theorem of Markov Chains

- The *return time* from state i to itself is defined as

$$H_{i,i} := \underbrace{\min\{t \geq 1 \mid \underbrace{X_t = i}_{\text{at } i \text{ in time } t}, \underbrace{X_0 = i}_{\text{started at } i}\}}_{\text{first time}}$$

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- *Expected return time:* defined as $h_{i,i} := \mathbb{E}[H_{i,i}]$.

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- *Expected return time:* defined as $h_{i,i} := \mathbb{E}[H_{i,i}]$.

Theorem (Fundamental Theorem of Markov Chains)

Any finite, irreducible and aperiodic Markov Chain has the following properties:

1. *There exists a unique stationary distribution* π*, where* $\boxed{\pi_i > 0}$ *for all* $i \in [n]$
2. *The sequence of distributions* $\{p_t\}_{t \geq 0}$ *will converge to* π*, no matter what the initial distribution is*
3. $$\boxed{\pi_i = \lim_{t \to \infty} P^t_{i,i} = \frac{1}{h_{i,i}}}$$

Fundamental Theorem of Markov Chains

Theorem (Fundamental Theorem of Markov Chains)

Any finite, irreducible and aperiodic Markov Chain has the following properties:

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2. *For every distribution* $p_0 \in \mathbb{R}^n_{\geq 0}$, $\lim_{t \to \infty} \underbrace{p_0 \cdot P^t}_{p_t} = \pi$
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Intuition for proof of this theorem:

- two random walks are "indistinguishable" after they "meet" at the *same vertex v* at a particular *time t*
- By finiteness, irreducibility and aperiodicity, two walks will meet with positive probability (and thus by Markov property) become *same distribution*

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If our underlying graph is undirected:

- If A_G adjacency matrix of $G(V,E)$ and $D = diag(d_1, d_2, \ldots, d_n)$, transition matrix:

$$\boxed{P = D^{-1} \cdot A_G}$$

$$D = \begin{pmatrix} d_1 & & & \\ & d_2 & & \\ & & \ddots & \\ & & & d_n \end{pmatrix}$$

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- Note that in this case, easy to guess stationary distribution: $\boxed{\pi \cdot P = \pi}$

Practice problem: prove this!

$$\pi_i = \frac{d_i}{2m}, \quad m = |E|$$

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  - P and P' has $\underbrace{\textit{same eigenvalues}}_{\text{similarity (conjugation)}}$! And P' has only $\underbrace{\textit{real eigenvalues}}_{\text{symmetric matrices} \Rightarrow \text{real eigenvalues (spectral thm)}}$!

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  - Eigenvectors of P are $D^{-1/2} v_i$ where v_i are eigenvectors of P'. And v_i can be taken to form *orthonormal basis*.

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    - eigenvector has *all positive coordinates*
    - eigenvalue is *positive*

$\lambda_1, \ldots, \lambda_n$

$|\lambda_1| > |\lambda_j|$

$\lambda_1 > 0$

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  - This eigenvector is π!
  - All random walks converge to π, as we wanted to show.

$\pi P = \pi$ max eigenvalue = all other eigenvalues are <1

$$q P^t = q \cdot \left(\sum_{i=1}^{n} \lambda_i^t \cdot v_i v_i^T \right) \xrightarrow{t \to \infty} \pi \quad \xrightarrow{t\to\infty} 0.$$

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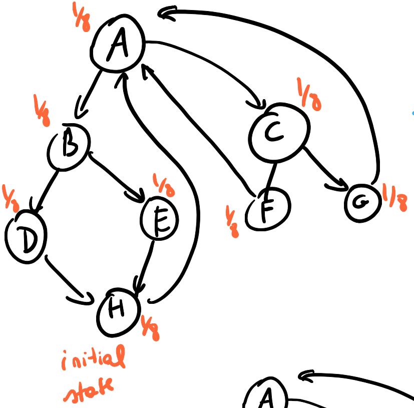
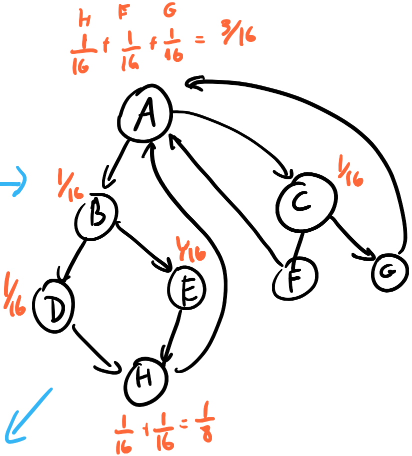
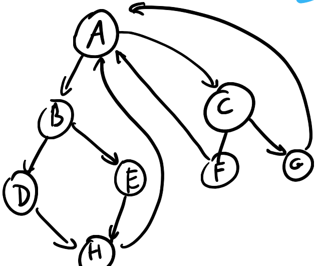
Page Rank - Example







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Practice problem! check this!

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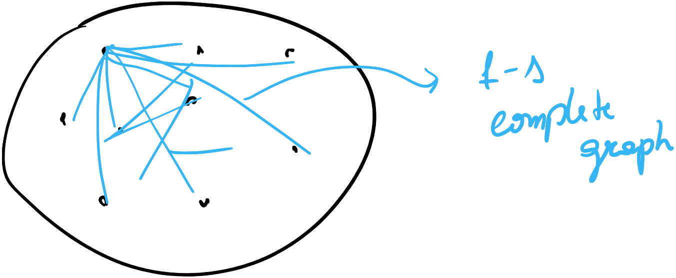

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- This modification does not change "relative importance" of vertices

Conclusion

Markov Chains and Random Walks are ubiquitous in randomized algorithms.

- Page Rank algorithm (today's lecture)
- Approximation algorithms for counting problems [Karp, Luby & Madras]
  - Permanent of non-negative matrices [Jerrum, Vigoda & Sinclair]
- Sampling Problems
  - Gibbs sampling in statistical physics
  - many more places
- Probability amplification without too much randomness (efficient)
  - Random walks on expander graphs
- many more

Acknowledgement

- Lecture based largely on:
  - Lap Chi's notes
  - [Motwani & Raghavan 2007, Chapter 6]
- See Lap Chi's notes at `https://cs.uwaterloo.ca/~lapchi/cs466/notes/L11.pdf`
- Also see Lap Chi's notes `https://cs.uwaterloo.ca/~lapchi/cs466/notes/L14.pdf` for a proof of fundamental theorem of Markov chains for undirected graphs.

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