

# Markov Chains and Link Analysis

Shan-Hung Wu  
*shwu@cs.nthu.edu.tw*

Department of Computer Science,  
National Tsing Hua University, Taiwan

NetDB-ML, Spring 2015

## 1 Markov Chains

- Random Processes
- Markov Processes and Markov Chains
- Ergodic Chains
- Reversible Chains

## 2 Link Analysis

- Web as A Graph
- The PageRank
- Personalized PageRank

## 1 Markov Chains

- Random Processes
- Markov Processes and Markov Chains
- Ergodic Chains
- Reversible Chains

## 2 Link Analysis

- Web as A Graph
- The PageRank
- Personalized PageRank

# Random Processes (1/2)

## Definition (Random Process)

Given a probability space  $(\Omega, \mathcal{F}, P)$ , a **random process** (or **stochastic process**), denoted by  $\{X^{(t)} : t \in \mathcal{T}\}$ , is a collection of random variables defined over  $(\Omega, \mathcal{F}, P)$  and indexed by elements  $t$  of a set  $\mathcal{T}$ .

- Typically, we think  $t = 1, 2, \dots$  as **time**
  - $t$  could also be space or position on a DNA string, etc.
- The values of  $X^{(t)}$  are called the **states**
- $X^{(t)}$  is a function of both the outcome  $\omega$  and time  $t$ 
  - Fixing the outcome  $\omega \in \Omega$ ,  $X^{(t)}$  is a deterministic function of  $t$
  - Fixing  $t$ ,  $X^{(t)}$  is a random variable
- The distribution of  $X^{(t)}$ , called **state distribution**, changes with  $t$

## Random Processes (2/2)

- A random process is said to be *discrete* or *continuous in time* depending on whether  $\mathcal{T}$  is discrete (finite or infinitely countable) or continuous
- A random process is *discrete* or *continuous in state* depending on whether  $X$  is discrete or continuous
- Random processes vs graphical models (e.g., Bayesian networks and Markov random fields)?

# Random Processes (2/2)

- A random process is said to be *discrete* or *continuous in time* depending on whether  $\mathcal{T}$  is discrete (finite or infinitely countable) or continuous
- A random process is *discrete* or *continuous in state* depending on whether  $X$  is discrete or continuous
- Random processes vs graphical models (e.g., Bayesian networks and Markov random fields)?
  - A Bayesian network degenerates into a discrete-state-and-time random process when its random variables are indexed by time

# Why Random Process?

- So far, we assume that instances in a dataset are i.i.d.
  - This simplifies the calculation of the likelihood  $P[\mathcal{X}|\theta]$
- However, in practice instances may come in order and successive instances may be dependent
  - E.g., letters in a word, phonemes in speech utterance, page visits in the Web, etc.
- The sequence can be characterized as being generated by a parametric random process
  - We want to estimate the parameter of a random process and then make predictions

## 1 Markov Chains

- Random Processes
- Markov Processes and Markov Chains
- Ergodic Chains
- Reversible Chains

## 2 Link Analysis

- Web as A Graph
- The PageRank
- Personalized PageRank



- A random process is called the *Markov process* if it satisfies the *Markov property*:

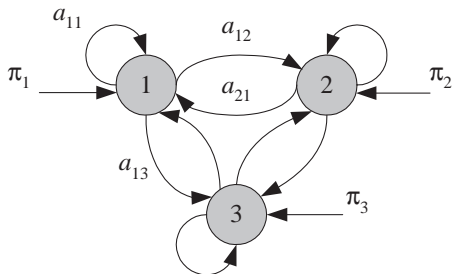
$$P(X^{(t_0+t_1)} \leq x | X^{(t_0)} = x_0, X^{(t)} = x_t, -\infty < t < t_0) =$$

$$P(X^{(t_0+t_1)} \leq x | X^{(t_0)} = x_0)$$

- We can think  $t_0$  and  $t_1$  be the present and future time respectively
- This is a mathematical version of the saying “today is the first day of the rest of your life”

# Markov Chains (1/2)

- A Markov process which is discrete in both time and state is called the first-order **Markov Chain**
- Let  $S_1, \dots, S_K$  be the  $K$  distinct states and  $t = 1, 2, \dots$ , the word “first-order” means:  
$$P(X_{t+1} = S_j | X_t = S_i, X_{t-1} = S_k, \dots) = P(X_{t+1} = S_j | X_t = S_i)$$
- Denote the unconditional **state probability** at time  $t$  by a row vector  $\boldsymbol{\pi}^{(t)} = [\pi_0^{(t)}, \dots, \pi_K^{(t)}]$ , where  $\pi_i^{(t)} = P(X^{(t)} = S_i)$  and  $\sum_{i=1}^K \pi_i^{(t)} = 1$



# Markov Chains (2/2)

- We say a Markov chain is **time homogeneous** iff
$$P(X^{(t+1)} = S_j | X^{(t)} = S_i) = P(X^{(t+m+1)} = S_j | X^{(t+m)} = S_i)$$
  - That is, the **transition probability**  $a_{i,j} = P(X^{(t+1)} = S_j | X^{(t)} = S_i)$  from state  $i$  to  $j$  does not change with time  $t$
  - $\sum_{j=1}^N a_{i,j} = 1$  for any  $i$
- A time homogeneous Markov chain has a fixed **transition matrix**  $\mathbf{A}$ , whose each row sum to 1

# State Probabilities

- Given an initial state probability  $\pi^{(1)}$ , we have  $\pi^{(2)} = \pi^{(1)} \mathbf{A}$ ,  $\pi^{(3)} = \pi^{(2)} \mathbf{A}$ , and so on...
- $\pi^{(t)} = \pi^{(t-1)} \mathbf{A} = \pi^{(1)} \mathbf{A}^{t-1}$  for  $t \geq 2$ 
  - $\pi_i^{(t)}$  is the sum of transition probabilities multiplied along all paths of length  $t-1$  from initial states  $j$  to  $i$  and weighted by the initial state probabilities  $\pi_j^{(1)}$
- In practice, we are often interested in the **steady state probability**  $\pi = \lim_{t \rightarrow \infty} \pi^{(t)}$ 
  - $\pi$  indicates how much chance we see a particular state in the long run
- However, the steady state probability may not exist

## 1 Markov Chains

- Random Processes
- Markov Processes and Markov Chains
- Ergodic Chains
- Reversible Chains

## 2 Link Analysis

- Web as A Graph
- The PageRank
- Personalized PageRank

# Ergodic Markov Chains (1/2)

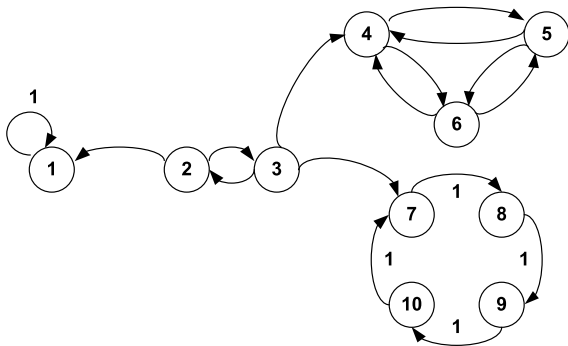
## Definition (Ergodic Markov Chain)

A Markov chain is said to be *ergodic* if there exists a positive integer  $T$  such that for all pairs of states  $i, j$  in the Markov chain, if it is started at time 0 in state  $i$  then for all  $t > T$ , the probability of being in state  $j$  at time  $t$  is greater than 0.

- An ergodic Markov chain cannot have
  - Absorbing state: once entering this state, there is no way to get out
  - Transient state: starting from this state, there is a positive probability that the chain will never return
  - Periodic state: the number of steps required to return to this state are always multiples of some integer larger than 1
- An ergodic chain constitutes of a single set of positive recurrent states
  - Positive recurrent state: starting from this state, the probability of eventual return is 1 and the expected number of steps required is finite (a positive integer)

# Ergodic Markov Chains (2/2)

- Most real world chains are ergodic if we can define proper transition probability between any two states



**Figure :** A non-ergodic Markov chain. Transition probabilities equal to 1 are marked explicitly. States 1 is an absorbing state; states 2 and 3 are transient states; states 7, 8, 9, and 10 are periodic states; states 4, 5, and 6 are positive recurrent states.

# Steady State Probability and Random Walk

## Theorem

*For any ergodic Markov chain, there is a unique steady state probability vector  $\pi$  such that if  $\eta(i, t)$  is the number of visits to state  $i$  in  $t$  steps, then  $\lim_{t \rightarrow \infty} \frac{\eta(i, t)}{t} = \pi_i$ .*

- If a Markov chain is ergodic, the steady state  $\pi$  exists, and its value is independent with the initial state
- But how to find  $\pi$ ?



# Steady State Probability and Random Walk

## Theorem

For any ergodic Markov chain, there is a unique steady state probability vector  $\pi$  such that if  $\eta(i, t)$  is the number of visits to state  $i$  in  $t$  steps, then  $\lim_{t \rightarrow \infty} \frac{\eta(i, t)}{t} = \pi_i$ .

- If a Markov chain is ergodic, the steady state  $\pi$  exists, and its value is independent with the initial state
- But how to find  $\pi$ ?
  - Since  $\pi \mathbf{A} = \pi$ ,  $\pi$  is the (left) eigenvector of  $\mathbf{A}$  corresponding to the eigenvalue 1
  - Or we can multiply  $\pi^{(1)}$  enough times by  $\mathbf{A}$  to get an approximation
- The steady state probability  $\pi$  also implies the (probability of the) final stop of a *random walk*
  - Insensitive to the initial state where the walk begins

## 1 Markov Chains

- Random Processes
- Markov Processes and Markov Chains
- Ergodic Chains
- Reversible Chains

## 2 Link Analysis

- Web as A Graph
- The PageRank
- Personalized PageRank

# Reversible Markov Chains (1)

## Definition (Reversible Markov Chain)

A Markov chain is said to be *reversible* if there exists a probability distribution over states,  $\pi$ , such that the *detailed balanced equation*

$$\pi_i P(X^{(t+1)} = S_j | X^{(t)} = S_i) = \pi_j P(X^{(t+1)} = S_i | X^{(t)} = S_j)$$

holds for all times  $t$  and states  $i$  and  $j$ .

- If the Markov chain has finite states and is time-homogeneous, we have  $\pi_i A_{i,j} = \pi_j A_{j,i}$

## Reversible Markov Chains (2)

- Summing the detailed balanced equations over all states gives
$$\sum_i \pi_i A_{i,j} = \sum_i \pi_j A_{j,i} = \pi_j \sum_i A_{j,i} = \pi_j$$
  - Valid for all  $j$ , which implies  $\pi \mathbf{A} = \pi$
- So, for reversible Markov chains,  *$\pi$  is always the steady state probability vector*
- If, the chain begins with the steady state distribution (i.e.,  $\pi_i^{(1)} = P(X^{(1)} = S_i) = \pi_i$ ), then we have  $\pi_i^{(t)} = P(X^{(t)} = S_i) = \pi_i$  for all  $t$ , and the detailed balanced equation be written as
$$P(X^{(t+1)} = S_j, X^{(t)} = S_i) = P(X^{(t+1)} = S_i, X^{(t)} = S_j)$$

## 1 Markov Chains

- Random Processes
- Markov Processes and Markov Chains
- Ergodic Chains
- Reversible Chains

## 2 Link Analysis

- Web as A Graph
- The PageRank
- Personalized PageRank

# Web as A Graph

- Nodes (vertexes): web pages
- Links: hyperlinks (e.g., `<a href="http://www.ibm.com">A computer service company</a>`)
  - Directed
  - Annotated by anchor text
- How can this structure help in, for example, searching a web page?

# Web as A Graph

- Nodes (vertexes): web pages
- Links: hyperlinks (e.g., `<a href="http://www.ibm.com">A computer service company</a>`)
  - Directed
  - Annotated by anchor text
- How can this structure help in, for example, searching a web page?
  - When scoring a page for a term query, a search engine can additionally calculate the (cosine) similarity between the query terms and the the tokens in the anchor text pointing to that page
- Idea: descriptions to a website from others are usually more precise than those from site holders themselves
  - Evidence: despite that everyone knows IBM is a computer company, we seldom see the word “computer” in its homepage

## 1 Markov Chains

- Random Processes
- Markov Processes and Markov Chains
- Ergodic Chains
- Reversible Chains

## 2 Link Analysis

- Web as A Graph
- The PageRank
- Personalized PageRank



# The PageRank Algorithm (1/2)

- In addition to the anchor text, the structure of the graph also helps in scoring a page
- PageRank is a score derived from the structure of the graph
- The idea is to model the graph as a Markov chain
  - Pages as the states; hyperlinks as the transitions
- In the simplest form, the *random walk model* can be used to calculate the transition matrix  $\mathbf{A}$ 
  - If a page  $p_i$  has two links to  $p_j$  and  $p_k$ , then  $a_{i,j} = a_{i,k} = 1/2$
- The state probability  $\pi_i^{(t)}$  denotes the probability that a random walking user stay at the page  $i$  at time  $t$
- If the chain is ergodic, then the PageRank of page  $i$  can be simply the steady state probability  $\pi_i$  denoting the “popularity”

# The PageRank Algorithm (2/2)

- What if a page has no outward link?
  - It becomes an absorbing state and prevents the chain from being ergodic
- Solution?

# The PageRank Algorithm (2/2)

- What if a page has no outward link?
  - It becomes an absorbing state and prevents the chain from being ergodic
- Solution? Observe that users may teleport between pages (e.g., enter URLs directly in the browser)
- We can associate each  $a_{i,j}$  with a teleport probability:
  - $a_{i,j} = 1/K$  if page  $i$  has no outward link;
  - $a_{i,j} = (1 - \alpha)/o_i + \alpha/K$  otherwise, where  $o_i$  is number of outward links from page  $i$  and  $\alpha$  is a user-specified parameter

# Remarks

- PageRank is one of the commonly used scoring functions in major search engines today
  - Often contributes to a portion of the final score of a page
- Why is PageRank so popular?

# Remarks

- PageRank is one of the commonly used scoring functions in major search engines today
  - Often contributes to a portion of the final score of a page
- Why is PageRank so popular?
- It is language independent
  - Exploits the link structure and provides an alternative view to the content-based scores (e.g., cosine similarity)
  - Agnostic to queries (i.e., the PageRank of page remains the same for all queries)
- It can be computed in a scalable manner
  - We can multiply  $\pi^{(1)}$  enough times by  $\mathbf{A}$  to get an approximation of the steady state  $\pi$
  - Each multiplication task can be divided into parts and done in parallel (e.g., using the MapReduce framework)
- It is spam-resistant
  - You need to fake “inward links” from others' pages to increase the visibility of your site

## 1 Markov Chains

- Random Processes
- Markov Processes and Markov Chains
- Ergodic Chains
- Reversible Chains

## 2 Link Analysis

- Web as A Graph
- The PageRank
- Personalized PageRank

# Personalized PageRank (1/2)

- The PageRank is static to different users
- Can we personalize PageRank based a particular user's interests?

# Personalized PageRank (1/2)

- The PageRank is static to different users
- Can we personalize PageRank based a particular user's interests?
- Recall the random walk model assumes that all links of a page are clicked with the equal probability
- We can instead estimate the  $\pi^{(1)}$  and  $\mathbf{A}$  by tracing the sequence of page visits from a user



# Personalized PageRank (2/2)

- Given  $N$  sample sequences of length  $T$ , where  $X^{(n,t)}$  is the state at time  $t$  in sequence  $n$
- If we assume that  $\pi_i^{(1)}$  and  $a_{i,j}$  are with Binomial distributions (or Multinomial distributions with constrains), we can easily obtain their ML estimators:

- $\hat{\pi}_i^{(1)} = \frac{\sum_{n=1}^N \zeta(X^{(n,1)}=s_i)}{N}$ , where  $\zeta(x)$  equals 1 if  $x$  is true and 0 otherwise
- $\hat{a}_{i,j} = \frac{\sum_{n=1}^N \sum_{t=1}^{T-1} \zeta(X^{(n,t)}=s_i \text{ and } X^{(n,t+1)}=s_j)}{\sum_{n=1}^N \sum_{t=1}^{T-1} \zeta(X^{(n,t)}=s_i)}$  [Proof]

- To ensure an ergodic chain, we still assume the teleport probabilities
  - We can further estimate the teleport probabilities of a particular user

# What's Next?

- Markov chains are the most simple type of Markov processes
  - Lay out the fundamentals for other processes commonly used in machine learning:

	<b>States are fully observable</b>	<b>States are partially observable</b>
<b>Transition is autonomous</b>	Markov chains	Hidden Markov models
<b>Transition is controlled</b>	Markov decision processes	Partially observable Markov decision processes