Lecture 10: Markov Chains

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Outline

Outline

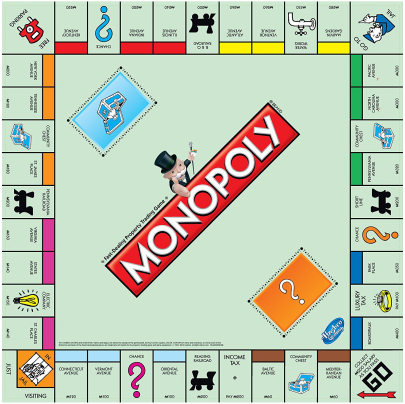
Definition

$I = [0, 5)$

- A stochastic process is a collection of random variables $\{X_t, t \in I\}$. The set I is the *index set* of the process. The random variables are defined on a common state space $\mathcal{S}$.
- I is discrete: discrete-time stochastic processes (sequences of random variables) $X_1, X_2, \ldots X_n$
- I is continuous: continuous-time stochastic processes (uncountable collections of random variables)

Example: Discrete Time & Discrete State Space

- State Space: $\{1, \ldots, 40\}$
- X_k: the player's board position after k dice rollings.
- Stochastic Process for Monopoly: $X_0, X_1, \ldots$



Example: Discrete Time & Continuous State Space

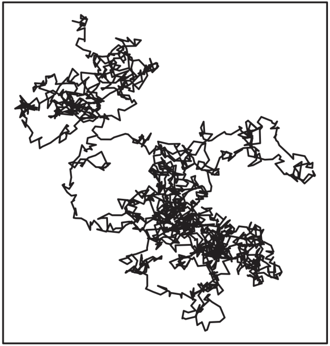
- Air-monitoring with PM2.5 measurements every hour
- State Space: $(0, 2000)$
- X_k: the PM2.5 measurement at the kth hour.
- Stochastic Process for Air-monitoring: $X_0, X_1, \ldots$

Example: Continuous Time & Discrete State Space

- We receive emails at random times day and night.
- State Space: $\{0, 1, 2, \ldots\}$
- $X_t, t \in [0, \infty)$: the number of emails we receive up to time t
- Stochastic Process for Email: $\{X_t\}$

Example: Continuous Time & Continuous State Space

- Two-dimensional Brownian Motion
- State Space: $\mathbb{R}^2$
- $X_t, t \in [0, \infty)$: position of the particle at time t
- Stochastic Process for random motion of particles:$\{X_t\}$



Outline

i.i.d r.v. $X_1, \ldots, X_n$

Model Selection in Stochastic Modeling

- Enough complexity to capture the complexity of the phenomena in question
- Enough structure and simplicity to allow one to compute things of interest

Motivation

- Introduced by Andrey Markov in 1906
- IID sequence of random variables: too restrictive assumption
- Completely dependent among random variables: hard to analysis
- Markov chain: happy medium between complete independence & complete dependence.

Markov Model

$\{X_t\}$ $X_1, X_2, \ldots X_n$

S. $S_1, S_2, \ldots S_n$.

$(S_1, S_2, \ldots S_n)$: Sample path.

Three basic components of Markov model

- A sequence of random variables $\{X_t, t \in \mathcal{T}\}$, where $\mathcal{T}$ is an index set, usually called "**time**".
- All possible sample values of $\{X_t, t \in \mathcal{T}\}$ are called "**states**", which are elements of a sate space $\mathcal{S}$.
- "**Markov property**": given the present value(information) of the process, the future evolution of the process is independent of the past evolution of the process.

Classification of Markov Model

- *Discrete-Time Markov Chain*: Discrete $\mathcal{S}$ & Discrete $\mathcal{T}$
- queue operation *Continuous-Time Markov Chain*: Discrete $\mathcal{S}$ & Continuous $\mathcal{T}$
- *Discrete Markov Process*: Continuous $\mathcal{S}$ & Discrete $\mathcal{T}$
- MCMC *Continuous Markov Process*: Continuous $\mathcal{S}$ & Continuous $\mathcal{T}$

Finite.

Our focus: Discrete-Time Markov Chain with finite state space

Outline

Markov Chain

$P(A|B,C) = P(A|B)$

given B, A and C are independent.

Definition

A sequence of random variables $X_0, X_1, X_2, \dots$ taking values in the *state space* $\{1, 2, \dots, M\}$ is called a *Markov chain* if for all $n \geq 0$,

$$P(X_{n+1} = j | X_n = i, \overset{\text{history}}{X_{n-1} = i_{n-1}, \dots, X_0 = i_0}) = P(X_{n+1} = j | X_n = i).$$

future

current

Time-homogeneous Markov Chains

时齐

Definition

Given a Markov chain $X_0, X_1, X_2, \ldots$ It is called time-homogeneous Markov chain if for all $n \geq 0$,

$$P\left(X_{n+1} = j | X_n = i\right) = q_{i,j}.$$

independent of n

where $q_{i,j}$ is a constant independent of n.

From now on, we focus on time-homogeneous Markov Chains, and we call it Markov chain in brevity.

Transition Matrix

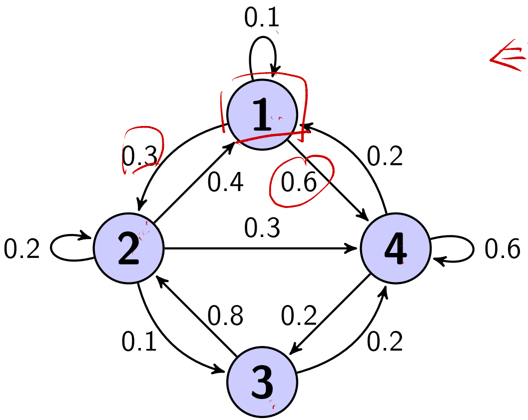
Definition

Let $X_0, X_1, X_2, \ldots$ be a Markov chain with state space $\{1, 2, \ldots, M\}$, and let $q_{i,j} = P(X_{n+1} = j | X_n = i)$ be the transition probability from state i to state j. The $M \times M$ matrix $Q = (q_{i,j})$ is called the *transition matrix* of the chain.

Graphical and Matrix Form of Markov Chain

$\forall i$

State-transition diagram



$$\sum_{j=1}^{M} P(X_{n+1}=j \mid X_n=i) = 1$$

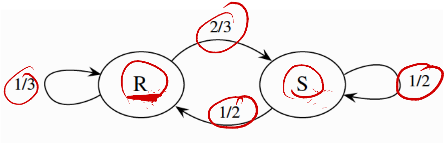
$\Leftrightarrow$

$$\sum_{j=1}^{M} P(X_{n+1}=j, X_n=i) = P(X_n=i)$$

$$Q = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{cccc} 1 & 2 & 3 & 4 \end{array} \\ \begin{bmatrix} 0.1 & 0.3 & 0 & 0.6 \\ 0.4 & 0.2 & 0.1 & 0.3 \\ 0 & 0.8 & 0 & 0.2 \\ 0.2 & 0 & 0.2 & 0.6 \end{bmatrix} \end{array}$$

Row sum $= 1$ in Transition Matrix.

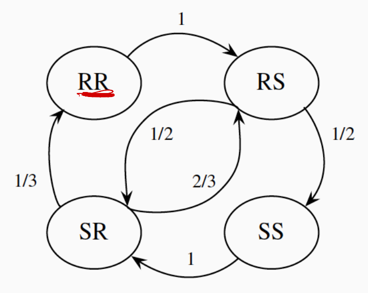
Example: Rainy-sunny Markov Chain



$$\begin{array}{cc} & \begin{array}{cc} R & S \end{array} \\ \begin{array}{c} R \\ S \end{array} & \begin{bmatrix} \frac{1}{3} & \frac{2}{3} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix} \end{array}$$

Example: Rainy-sunny Markov Chain

$$\frac{(X_{n-1}, X_n)}{\text{state}}$$

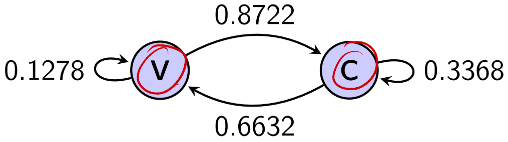


$$\begin{array}{c c}
 & \begin{array}{cccc} RR & RS & SR & SS \end{array} \\
\begin{array}{c} RR \\ RS \\ SR \\ SS \end{array} & \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1/2 & 1/2 \\ 1/3 & 2/3 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}
\end{array}$$

Example: The First Markov Chain in History

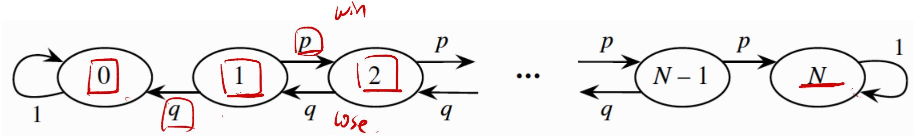
- Andrey Andreyevich Markov was interested in investigating the way the vowels and consonants alternate in Russian literature, e.g., “Eugene Onegin” by Pushkin
- He classified 20,000 consecutive characters: 8638 vowels & 11362 consonants

$$\begin{array}{rc} & \begin{array}{cc}\text{vowel} & \text{consonant}\end{array} \\ \begin{array}{r}\text{vowel}\\ \text{consonant}\end{array} & \begin{bmatrix} 1104/8638 & 7534/8638 \\ 7535/11362 & 3827/11362 \end{bmatrix} \end{array} = \begin{bmatrix} 0.1278 & 0.8722 \\ 0.6632 & 0.3368 \end{bmatrix}$$



Gambler's Ruin As A Markov Chain

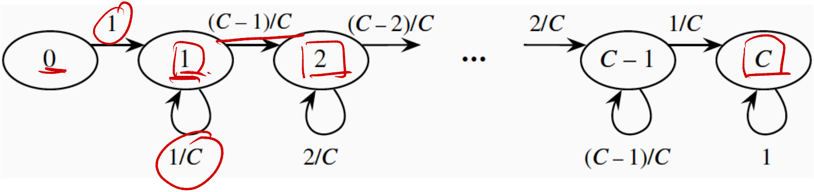
$X_k \in \{0, 1, \ldots N\}$



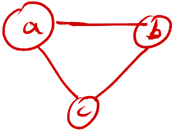
Coupon Collector As A Markov Chain

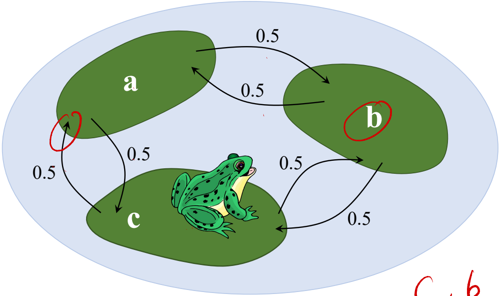
C: # of coupon types.

$X_k \in \{0, 1, \ldots, C\}$



Example: Random Walk on A Graph





Sample path

c, b, c, a, b

c, a, b, a, b.

$$
\begin{array}{c|ccc}
 & a & b & c \\
\hline
a & 0 & 0.5 & 0.5 \\
b & 0.5 & 0 & 0.5 \\
c & 0.5 & 0.5 & 0
\end{array}
$$

Outline

n-step Transition Probability

$q_{a,b} > 0$

$q_{a,c} = 0$

$q_{a,c}^{(2)} > 0$

Definition

Let $X_0, X_1, X_2, \ldots$ be a Markov chain with transition matrix Q. The n-step transition probability from i to j is the probability of being at j exactly n steps after being at i. We denote this by $q_{i,j}^{(n)}$:

$$q_{i,j}^{(n)} = P\left(X_n = j | X_0 = i\right).$$

$$= P\left(X_{m+n} = j \mid X_m = i\right)$$

Example: 2-step Transition Probability

$$P(A,B|C) = \frac{P(A|B,C)}{P(B|C)}$$

$$q_{i,j}^{(2)} = P(X_2=j \mid X_0=i) = \sum_k P(X_2=j, X_1=k \mid X_0=i)$$

$$= \sum_k P(X_2=j \mid X_1=k, X_0=i) \cdot P(X_1=k \mid X_0=i)$$

Markov property

$$= \sum_k P(X_2=j \mid X_1=k) \cdot P(X_1=k \mid X_0=i)$$

$$q_{i,j}^{(2)} = P\left(X_2 = j | X_0 = i\right) = \sum_k q_{i,k} q_{k,j} = \text{(i,j) entry of } Q^2.$$

$Q \times Q$

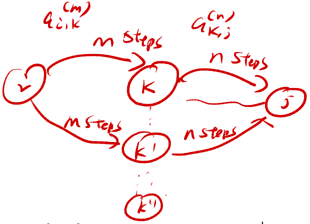
$$= \sum_k q_{k,j} \cdot q_{i,k} = \sum_k q_{i,k} \cdot q_{k,j}$$

$$Q = (q_{i,j})$$

Chapman-Kolmogorov Relationship

① Matrix. $Q^{m+n} = Q^m \cdot Q^n$

$q_{i,j}^{(m+n)} \quad \sum_k \quad q_{i,k}^{(m)} \cdot q_{k,j}^{(n)}$



$$q_{i,j}^{(m+n)} = P\left(X_{m+n} = j | X_0 = i\right) = \sum_k q_{i,k}^{(m)} q_{k,j}^{(n)} = \text{(i,j) entry of } Q^{m+n}.$$

② $q_{i,j}^{(m+n)} = P(X_{m+n} = j \mid X_0 = i) = \sum_k P(X_{m+n} = j, X_m = k \mid X_0 = i)$

$= \sum_k P(X_{m+n} = j \mid X_m = k, X_0 = i) \cdot P(X_m = k \mid X_0 = i)$

⇑ Markov property

$= \sum_k P(X_{m+n} = j \mid X_m = k) \cdot P(X_m = k \mid X_0 = i)$

$= \sum_k q_{k,j}^{(n)} \cdot q_{i,k}^{(m)}$

Proof

Distribution of X_n

$P(X_n = j) = \sum_i P(X_n = j \mid X_0 = i) \cdot P(X_0 = i)$

$= \sum_i q_{i,j}^{(n)} \cdot \alpha_i \quad = (\alpha Q^n)_j$

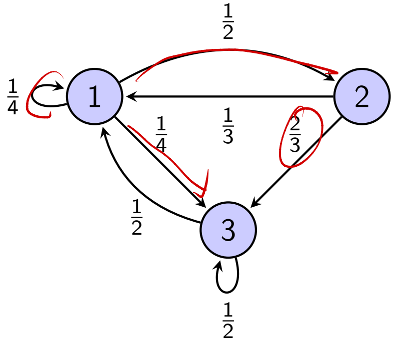
Let X_0, X_1,... be a Markov chain with transition matrix Q and initial distribution $\boldsymbol{\alpha}$, where $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \cdots, \alpha_M)$, $\alpha_i = P(X_0 = i), i = 1, \ldots, M$. For all n $\geq$ 0, the distribution of X_n is $\boldsymbol{\alpha} Q^n$. That is, the j th component of $\boldsymbol{\alpha} Q^n$ is $P(X_n = j)$, denoted as:

$$P(X_n = j) = (\alpha Q^n)_j, \text{ for all } j.$$

$q_{i,j}^{(n)} = (i,j)$ entry of Q^n

Example

Given a Markov chain $X_0, X_1, X_2, \ldots$ with state space $\mathcal{S} = \{1, 2, 3\}$.



$$Q = \begin{array}{c} \\ 1 \\ 2 \\ 3 \end{array} \begin{array}{c} \begin{array}{ccc} 1 & 2 & 3 \end{array} \\ \begin{bmatrix} \frac{1}{4} & \frac{1}{2} & \frac{1}{4} \\ \frac{1}{3} & 0 & \frac{2}{3} \\ \frac{1}{2} & 0 & \frac{1}{2} \end{bmatrix} \end{array}$$

- Find $P(X_3 = 1 | X_2 = 1)$ and $P(X_4 = 3 | X_3 = 2)$.

$q_{1,1} = \frac{1}{4}$ $\qquad$ $q_{2,3} = \frac{2}{3}$

Example

$P(X_0=1, X_1=2, X_2=3)$

chain's rule $\underline{\underline{\quad}}$ $P(X_0=1)\cdot P(X_1=2 \mid X_0=1)\cdot P(X_2=3 \mid X_1=2, X_0=1)$

Given a Markov chain $X_0, X_1, X_2, \dots$ with state space $\mathcal{S} = \{1, 2, 3\}$.

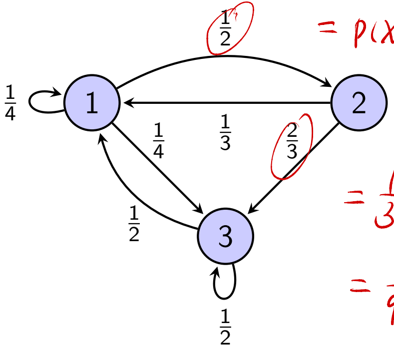
Markov's property

$= P(X_0=1)\cdot q_{1,2}\cdot P(X_2=3 \mid X_1=2)$

$= P(X_0=1)\cdot q_{1,2}\cdot q_{2,3}$

$= \frac{1}{3}\cdot\frac{1}{2}\cdot\frac{2}{3}$

$= \frac{1}{9}$



$$\begin{array}{c|ccc} & 1 & 2 & 3 \\ \hline 1 & & & \\ 2 & & \left[\begin{matrix} \frac{1}{4} & \frac{1}{2} & \frac{1}{4} \\ \frac{1}{3} & 0 & \frac{2}{3} \\ \frac{1}{2} & 0 & \frac{1}{2} \end{matrix}\right] & \\ 3 & & & \end{array}$$

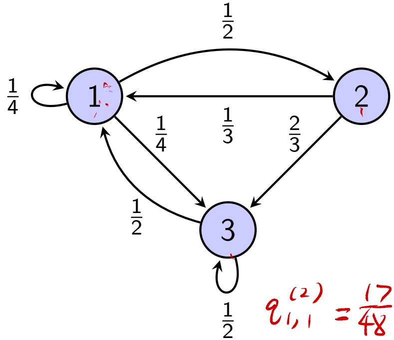
- If $P(X_0=1) = \frac{1}{3}$, find $P(X_0=1, X_1=2, X_2=3)$.

Example

$$Q^2 = \begin{array}{c|ccc} & 1 & 2 & 3 \\ \hline 1 & \frac{17}{48} & \frac{1}{8} & \frac{25}{48} \\ 2 & \frac{5}{12} & \frac{1}{6} & \frac{5}{12} \\ 3 & \frac{3}{8} & \frac{1}{4} & \frac{3}{8} \end{array}$$

$\underline{q^{(2)}_{i,j}}$

Given a Markov chain $X_0, X_1, X_2, \ldots$ with state space $\mathcal{S} = \{1, 2, 3\}$.



$$Q = \begin{array}{c|ccc} & 1 & 2 & 3 \\ \hline 1 & \frac{1}{4} & \frac{1}{2} & \frac{1}{4} \\ 2 & \frac{1}{3} & 0 & \frac{2}{3} \\ 3 & \frac{1}{2} & 0 & \frac{1}{2} \end{array}$$

$q^{(2)}_{1,1} = \frac{17}{48}$; $q^{(2)}_{1,2} = \frac{1}{8}$;

- Find $\underline{P(X_2 = 1 | X_0 = 1)}$, $\underline{P(X_2 = 2 | X_0 = 1)}$, and $\underline{P(X_2 = 3 | X_0 = 1)}$.

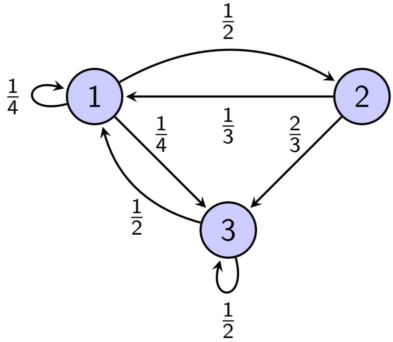
$q^{(2)}_{1,3} = \frac{25}{48}$;

Example

$$E(X_2 \mid X_0=1) = \sum_{j=1}^{3} j \cdot P(X_2=j \mid X_0=1)$$

$$= \sum_{j=1}^{3} j \cdot q_{1,j}^{(2)}$$

Given a Markov chain $X_0, X_1, X_2, \ldots$ with state space $\mathcal{S} = \{1, 2, 3\}$.



$$= 1 \cdot q_{1,1}^{(2)} + 2 \cdot q_{1,2}^{(2)} + 3 \cdot q_{1,3}^{(2)}$$

$$= 1 \cdot \frac{17}{48} + 2 \cdot \frac{1}{8} + 3 \cdot \frac{25}{48}$$

$$\begin{array}{c c} & \begin{array}{ccc} 1 & 2 & 3 \end{array} \\ \begin{array}{c} 1 \\ 2 \\ 3 \end{array} & \begin{bmatrix} \frac{1}{4} & \frac{1}{2} & \frac{1}{4} \\ \frac{1}{3} & 0 & \frac{2}{3} \\ \frac{1}{2} & 0 & \frac{1}{2} \end{bmatrix} \end{array}$$

$$= \frac{104}{48} = \frac{13}{6}.$$

- Find $E(X_2 \mid X_0 = 1)$.

Outline

Recurrent and Transient States

State i is recurrent $\sum_{n=1}^{\infty} P_{i,i}^{(n)} = \infty$

transient $\sum_{n=1}^{\infty} p_{i,i}^{(n)} < \infty$

Definition

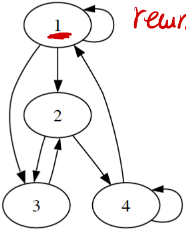
State i of a Markov chain is **recurrent** if starting from i, the probability is 1 that the chain will eventually return to i. Otherwise, the state is **transient**, which means that if the chain starts from i, there is a positive probability of never returning to i.

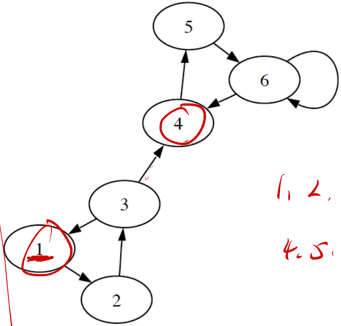
Example

States

1, 2, 3, 4

recurrent.





1, 2, 3 : transient

4, 5, 6 : recurrent.

Irreducible and Reducible Chain

Definition

A Markov chain with transition matrix Q is *irreducible* if for any two states i and j, it is possible to go from i to j in a finite number of steps (with positive probability). That is, for any states i,j there is some positive integer n such that the (i, j) entry of Q^n is positive. A Markov chain that is not irreducible is called *reducible*.

Irreducible Implies All States Recurrent

<1> irreducible. i j.

$\exists$ integer $m>0$, $n>0$.

$P_{j,i}^{(m)}>0$, $P_{i,j}^{(n)}>0$.

1°. $\exists$ at least one recurrent state.

2°. any state $j \neq i$

$i \Leftrightarrow j$

recurrent recurrent

Theorem

In an irreducible Markov chain with a finite state space, all states are recurrent.

$l>0$ integer.

<2> Chapman-Kolmogorov.

$P_{j,j}^{(n+m+l)} \geq P_{j,i}^{(m)} \cdot P_{i,i}^{(l)} P_{i,j}^{(n)}$

assume i is recurrent

$$\sum_{l=1}^{\infty} P_{i,i}^{(l)} = \infty$$

$$\underbrace{\sum_{l=1}^{\infty} P_{j,j}^{(l)}}_{\infty} \geq \sum_{l=1}^{\infty} P_{j,j}^{(n+m+l)} \geq \underbrace{P_{j,i}^{(m)}}_{>0} \underbrace{P_{i,j}^{(n)}}_{>0} \underbrace{\sum_{l=1}^{\infty} P_{i,i}^{(l)}}_{\infty}$$

$\Rightarrow$ j is recurrent.

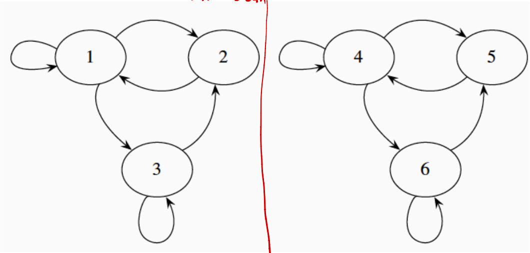
A Reducible Markov Chain with Recurrent States

irreducible

Sub Markov Chain

irreducible

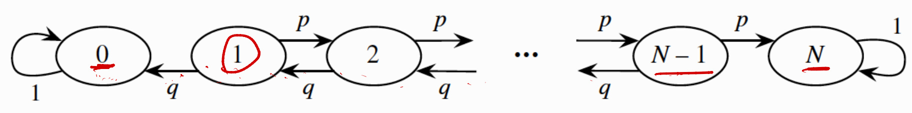
Sub Markov chain



Gambler's Ruin As A Markov Chain

recurrent States : $\{0, N\}$

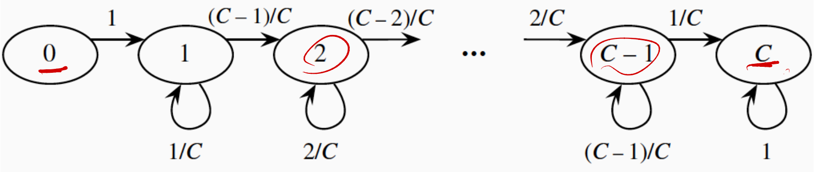
transient States : $\{1, 2, \ldots N-1\}$



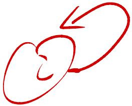
Coupon Collector As A Markov Chain

recurrent states : $\{C\}$

transient states : $\{0, 1, 2, .. C-1\}$



Period



$d(i) = gcd\{1, n_1, n_2\} = 1$

Definition

For a Markov chain with transition matrix Q, the *period* of state i, denoted $d(i)$, is the greatest common divisor of the set of possible return times to i. That is,

$$d(i) = gcd\{n > 0 : Q^n_{i,i} > 0\}.$$

If $d(i) = 1$, state i is said to be *aperiodic*. If the set of return times is empty, set $d(i) = +\infty$.

Periodic, Aperiodic Markov Chain

Definition

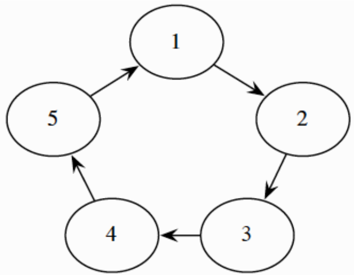
A Markov chain is called *periodic* if it is irreducible and all states have period greater than 1.

A Markov chain is called *aperiodic* if it is irreducible and all states have period equal to 1.

Example: Periodic Chain

$d(1) = d(2) = d(3)$

$= d(4) = d(5) = 5$

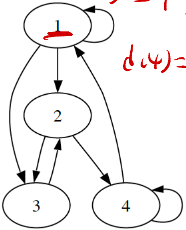


Example

$d(1) = 1$;

$d(2) = 1$;

$d(3) = 1$;



$d(4) = 1$;

irreducible.

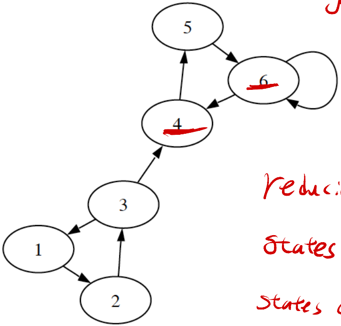
$d(1) = d(2) = d(3) = d(4) = 1$

aperiodic M.C.

$4-5-6-4$ ③

$4-5-6-6-4$ ④.

$\gcd(3, 4, \ldots)$



reducible M.C.

States 1, 2, 3. period 3.

States 4, 5, 6. period 1

Outline

Definition

$\{X_n\}$ π_n :

$\pi_{n+1} = \pi_n Q$.

if at some time n, $\pi_n = s$

$\Rightarrow$ $\pi_{n+1} = sQ = s = \pi_n$;

$k \geq n$; $\pi_k = s$

Definition

A row vector $\mathbf{s} = (s_1, ..., s_M)$ such that $s_i \geq 0$ and $\sum_i s_i = 1$ is a *stationary distribution* for a Markov chain with transition matrix Q if

$$\boxed{\sum_i s_i q_{i,j} = s_j.}$$

for all j, or equivalently,

$$\boxed{\mathbf{s}Q = \mathbf{s}.}$$

Example: Double Stochastic Matrix

Stationary distribution

$\sum_i q_{i,j} \cdot s_i$

$= s_j$

$\sum_i q_{i,j} \cdot \cancel{\frac{1}{M}} \stackrel{?}{=} \cancel{\frac{1}{M}}$ ✓

$\Leftrightarrow \sum_i q_{i,j} = 1$ ✓

$$
\begin{array}{c|c}
 & \begin{array}{ccc} 1 & 2 & 3 \end{array} \\
\begin{array}{c} 1 \\ 2 \\ 3 \end{array} & \begin{bmatrix} \frac{1}{4} & \frac{1}{2} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{2} & \frac{1}{4} \\ \frac{1}{2} & 0 & \frac{1}{2} \end{bmatrix}
\end{array}
$$

Theorem

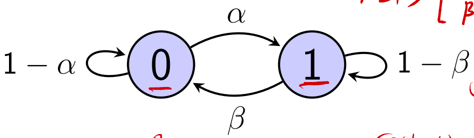
If each column of the transition matrix Q sums to 1, then the uniform distribution over all states, $(1/M, 1/M, \ldots, 1/M)$, is a stationary distribution. (A nonnegative matrix such that the row sums and the column sums are all equal to 1 is called a doubly stochastic matrix.)

Example: Two-State Markov Chain

$$Q = \begin{bmatrix} 1-\alpha & \alpha \\ \beta & 1-\beta \end{bmatrix}$$

$$S = (S_0, S_1) \qquad \underline{SQ = S} \Rightarrow S.$$

$$(S_0, S_1)\begin{bmatrix} 1-\alpha & \alpha \\ \beta & 1-\beta \end{bmatrix} = (S_0, S_1)$$



$$\Downarrow$$

$$S_0 = \frac{\beta}{\alpha+\beta}, \quad S_1 = \frac{\alpha}{\alpha+\beta} \Leftarrow \begin{cases} S_0(1-\alpha) + S_1\beta = S_0 \\ S_0\alpha + S_1(1-\beta) = S_1 \\ S_0 + S_1 = 1 \end{cases}$$

$\Rightarrow$ Stationary distribution $S = \left(\frac{\beta}{\alpha+\beta}, \frac{\alpha}{\alpha+\beta}\right)$

Theorem on Stationary Distribution

Theorem

Given a Markov chain with finite state space.

- *If such Markov chain is irreducible, then it has a unique stationary distribution. In this distribution, every state has positive probability.*
- *If such Markov chain is irreducible and aperiodic, with stationary distribution* $\mathbf{s}$ *and transition matrix* Q*, then* $P(X_n = i)$ *converges to* s_i *as* $n \to \infty$*. In terms of the transition matrix,* Q^n *converges to a matrix in which each row is* $\mathbf{s}$*.*

Example

1°. irreducible, aperiodic.

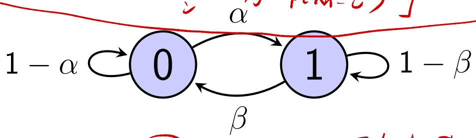
stationary distribution $s = \left(\frac{\beta}{\alpha+\beta}, \frac{\alpha}{\alpha+\beta}\right)$.

$0<\alpha<1$
$0<\beta<1$

2°. $\pi^{(n)} = [P(X_n=0), P(X_n=1)] \Rightarrow \underline{\pi^{(n+1)} = \pi^{(n)} \cdot Q}$.

[$P(X_{n+1}=j) = \sum_i P(X_{n+1}=j \mid X_n=i) \cdot P(X_n=i)$

$= \sum_i q_{i,j} \cdot P(X_n=i)$]



3° $\pi^{(n)} = \pi^{(0)} \cdot \boxed{Q^n}$.   ($Q = \begin{bmatrix} 1-\alpha & \alpha \\ \beta & 1-\beta \end{bmatrix} = \underline{P \Lambda P^{-1}}$

$= \underline{\begin{bmatrix} 1 & -\alpha \\ 1 & \beta \end{bmatrix}} \underline{\begin{bmatrix} 1 & 0 \\ 0 & 1-\alpha-\beta \end{bmatrix}} \underline{\frac{1}{\alpha+\beta} \begin{bmatrix} \beta & \alpha \\ -1 & 1 \end{bmatrix}}$

4°. $Q^n = \underline{P \Lambda^n P^{-1}}$

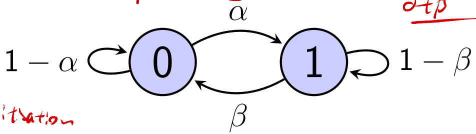
$= \begin{bmatrix} 1 & -\alpha \\ 1 & \beta \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & (1-\alpha-\beta)^n \end{bmatrix} \cdot \frac{1}{\alpha+\beta} \begin{bmatrix} \beta & \alpha \\ -1 & 1 \end{bmatrix}$

Example

$$\Rightarrow Q^n = \frac{1}{\alpha+\beta}\begin{bmatrix} \beta+\alpha(1-\alpha-\beta)^n & \alpha-\alpha(1-\alpha-\beta)^n \\ \beta-\beta(1-\alpha-\beta)^n & \alpha+\beta(1-\alpha-\beta)^n \end{bmatrix}$$

$0<\alpha<1,\ 0<\beta<1,\ |1-\alpha-\beta|<1$

$$\Rightarrow \lim_{n\to\infty} Q^n = \frac{1}{\alpha+\beta}\begin{bmatrix} \beta & \alpha \\ \beta & \alpha \end{bmatrix} = \begin{bmatrix} \frac{\beta}{\alpha+\beta} & \frac{\alpha}{\alpha+\beta} \\ \frac{\beta}{\alpha+\beta} & \frac{\alpha}{\alpha+\beta} \end{bmatrix}$$



initiation

5°. $\pi^{(0)} = (\pi_0^{(0)}, \pi_1^{(0)})$ $\quad \pi^{(n)} = \pi^{(0)} \cdot Q^n$ $\quad \pi_0^{(0)}+\pi_1^{(0)}=1$

$$\Rightarrow \lim_{n\to\infty} \pi^{(n)} = \pi^{(0)} \cdot \lim_{n\to\infty} Q^n = (\pi_0^{(0)}, \pi_1^{(0)}) \cdot \begin{pmatrix} \frac{\beta}{\alpha+\beta} & \frac{\alpha}{\alpha+\beta} \\ \frac{\beta}{\alpha+\beta} & \frac{\alpha}{\alpha+\beta} \end{pmatrix}$$

$$= \frac{1}{\alpha+\beta}(\beta, \alpha) = \left(\frac{\beta}{\alpha+\beta}, \frac{\alpha}{\alpha+\beta}\right) = S$$

Outline

Reversibility

time k: $i \to j$ $k+1$ $q_{i,j}$.

time-Reversibility

time $k+1$: $i \to j$ k $q_{i,j}$

Markov chain enters stationary states. $x^{(n)} = s$, $k \geq n$.

$$P(X_k = j \mid X_{k+1} = i) = \frac{P(X_{k+1} = i \mid X_k = j) \cdot P(X_k = j)}{P(X_{k+1} = i)}$$

Definition

Let $Q = (q_{i,j})$ be the transition matrix of a Markov chain. Suppose there is $\mathbf{s} = (s_1, \ldots, s_M)$ with $s_i \geq 0$, $\sum_i s_i = 1$, such that

$$s_i q_{i,j} = s_j q_{j,i}$$

for all states i and j. This equation is called the *reversibility* or *detailed balance* condition, and we say that the chain is *reversible* with respect to $\mathbf{s}$ if it holds.

$$= \frac{q_{j,i} \cdot s_j}{s_i} = \frac{s_i \cdot q_{i,j}}{s_i} = q_{i,j}$$

Reversible implies Stationary

$$s_i q_{i,j} = s_j q_{j,i}$$

row sum of Q.

$$\Rightarrow \sum_i s_i q_{i,j} = \sum_i s_j q_{j,i} = s_j \sum_i q_{j,i}$$

$$= s_j \cdot 1 = s_j$$

Theorem

Suppose that $Q = (q_{i,j})$ is a transition matrix of a Markov chain that is reversible with respect to a nonnegative vector $\mathbf{s} = (s_1, \ldots, s_M)$ whose components sum to 1. Then $\mathbf{s}$ is a stationary distribution of the chain.

$$\Rightarrow sQ = s$$

Check the Detailed Balance Equation

Given object distribution π

Design M.C $\Leftrightarrow$ Find Q

Theorem

If for an irreducible Markov chain with transition matrix $Q = (q_{i,j})$, there exists a probability solution π to the detailed balance equations

$$\pi_i q_{i,j} = \pi_j q_{j,i}$$

for all pairs of states i, j, then this Markov chain is reversible and the solution π is the unique stationary distribution.

Example: Symmetric Transition Matrix

$\pi_i q_{i,j} = \pi_j q_{j,i}$

$\pi_i = \frac{1}{M}$

$q_{i,j} = q_{j,i} \Rightarrow \pi_i = \pi_j$

$\forall (i,j)$

$$
\begin{array}{c c}
 & \begin{array}{ccc} 1 & 2 & 3 \end{array} \\
\begin{array}{c} 1 \\ 2 \\ 3 \end{array} &
\begin{bmatrix}
\frac{1}{4} & \frac{1}{2} & \frac{1}{4} \\
\frac{1}{2} & \frac{1}{4} & \frac{1}{4} \\
\frac{1}{4} & \frac{1}{4} & \frac{1}{2}
\end{bmatrix}
\end{array}
$$

Theorem

If the transition matrix Q for an irreducible Markov chain is symmetric, then the uniform distribution over all states, $(1/M, 1/M, \ldots, 1/M)$, is the unique stationary distribution.

Example: Random Walk on Undirected Graph

DBE:

$\pi_i q_{i,j} = \pi_j q_{j,i}, \ \forall i, j.$

$\Rightarrow \pi_i \cdot \frac{1}{deg(i)} = \pi_j \cdot \frac{1}{deg(j)}, \ \forall i \sim j$

$\sum_i \pi_i = 1$

$\Rightarrow \pi_i = \frac{deg(i)}{\sum_j deg(j)}$

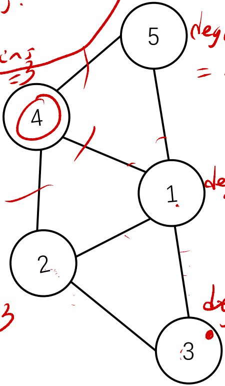
$\forall i \in \{1, 2, \dots, n\}$

$(i \sim j)$

$i, \ \frac{1}{deg(i)} \rightarrow j$

$X_0, X_1, X_2, \dots$

$q_{i,j} = \frac{1}{deg(i)} \cdot \frac{(i \sim j)}{j}$



$\vec{deg} = (4, 3, 2, 3, 2)$

$\Rightarrow \pi = \left(\frac{2}{7}, \frac{3}{14}, \frac{1}{7}, \frac{3}{14}, \frac{1}{7}\right)$

Example: Random Walk on Undirected Graph

Outline

How to Organize the Web?

- First Try: Web Directories
- Yahoo, DMOZ, LookSmart

Yahoo


YAHOO!
New
Cool
Today's News
More Yahoos
Exploring Mars
The New York Times
Win a $20,000 Trip!
CLICK HERE!
Looking for a Car? Job? Date?
Search
options
Yellow Pages - People Search - Maps - Classifieds - News - Stock Quotes - Sports Scores
Arts and Humanities
Architecture, Photography, Literature...
News and Media [Xtra!]
Current Events, Magazines, TV, Newspapers...
Business and Economy [Xtra!]
Companies, Investing, Employment...
Recreation and Sports [Xtra!]
Sports, Games, Travel, Autos, Outdoors...
Computers and Internet [Xtra!]
Internet, WWW, Software, Multimedia...
Reference
Libraries, Dictionaries, Phone Numbers...
Education
Universities, K-12, College Entrance...
Regional
Countries, Regions, U.S. States...
Entertainment [Xtra!]
Cool Links, Movies, Music, Humor...
Science
CS, Biology, Astronomy, Engineering...
Government
Military, Politics [Xtra!], Law, Taxes...
Social Science
Anthropology, Sociology, Economics...
Health [Xtra!]
Medicine, Drugs, Diseases, Fitness...
Society and Culture
People, Environment, Religion...
My Yahoo! - Yahooligans! for Kids - Beatrice's Web Guide - Yahoo! Internet Life
Weekly Picks - Today's Web Events - Chat - Weather Forecasts
Random Yahoo! Link - Yahoo! Shop
National Yahoos Canada - France - Germany - Japan - U.K. & Ireland
Yahoo! Metros Atlanta - Austin - Boston - Chicago - Dallas / Fort Worth - Los Angeles
Get Local Minneapolis / St. Paul - New York - S.F. Bay - Seattle - Washington D.C.
How to Include Your Site - Company Information - Contributors - Yahoo! to Go

How to Organize the Web?

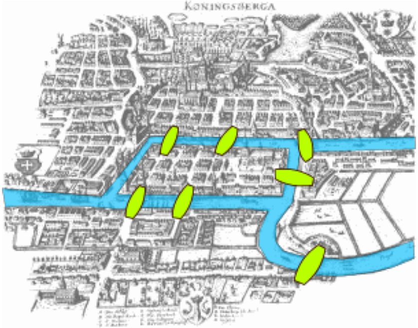
- Second Try: Web Search
- Information Retrieval:
  - find relevant docs in a small and trusted set
  - newspaper articles, patents, etc
- Hardness: web is huge, full of untrusted documents, random things, web spam, etc.

Challenges for Web Search

- Web contains many sources of information. Who to trust?
  - **Trick**: Trustworthy pages may point to each other!
- What is the best answer to query keywords?
  - Webpages are not equally important (www.nothing.com vs.www.stanford.edu)
  - **Trick**: rank pages containing keywords according to their importances (popularity)
  - Find the page with the highest rank
  - How to rank?

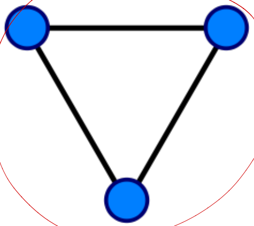
Modeling Language: Graph Theory

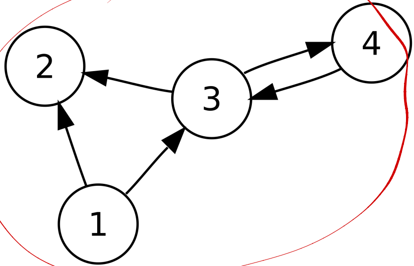
- Origin: 1735 Euler for Seven Bridges of Königsberg



Key Elements of A Graph

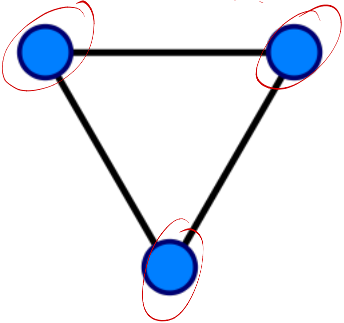
- A graph is an ordered pair $G = (V, E)$
- V: a set of vertices or nodes
- E: a set of edges or links between nodes
- Edge: undirected/directed





Undirected Graph

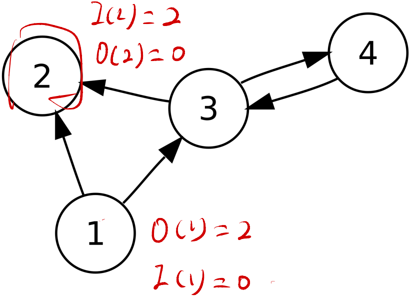
- Degree of vertex v: metric for connectivity of vertex v.
- $deg(v)$: the number of edges with v as an end vertex



2

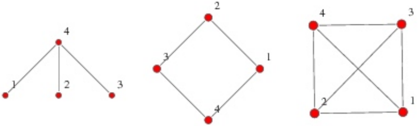
Directed Graph

- Indegree of vertex v: the number of incoming edges ends at v.
- Outdegree of vertex v: the number of outgoing edges starting from v.
- $I(v)$: indegree of v
- $O(v)$: outdegree of v



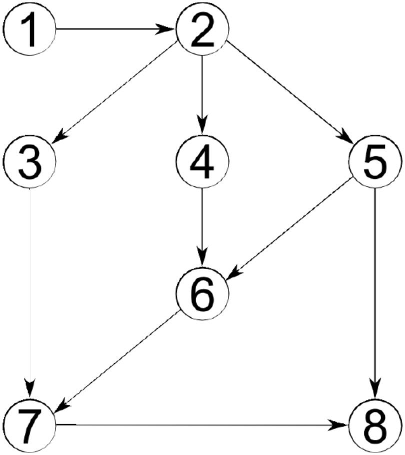
Adjacency Matrix

- A square $(0,1)-$matrix to represent a finite graph
- Matrix elements: pairs of vertices are adjacent or not
- Symmetric matrix: for undirected graph



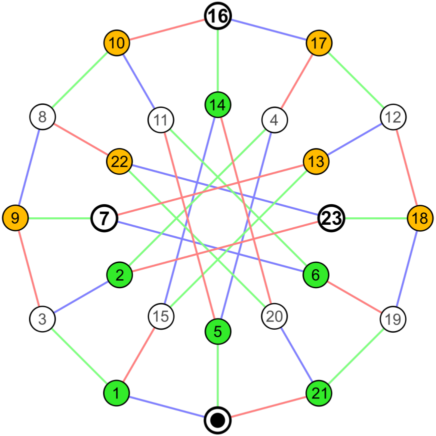
$$\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}$$

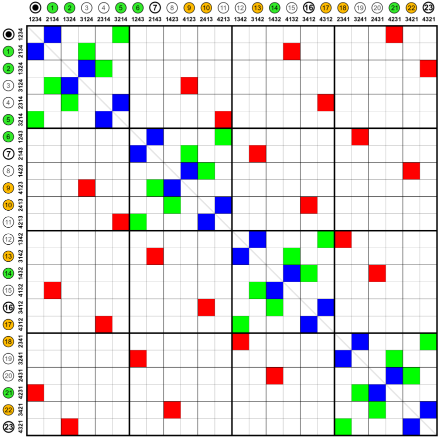
Adjacency Matrix: Directed Graph



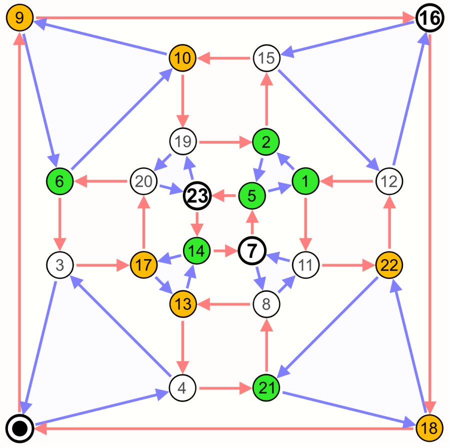
	1	2	3	4	5	6	7	8
1		1						
2			1	1	1			
3							1	
4						1		
5						1		1
6							1	
7								1
8								

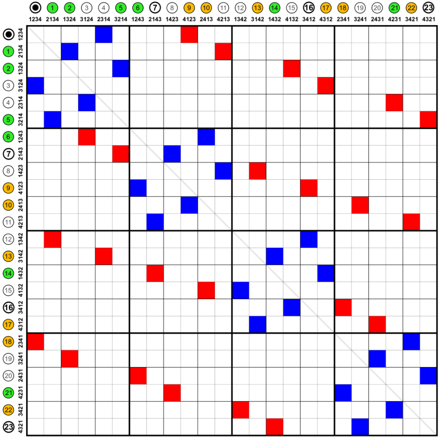
Adjacency Matrix of Nauru Graph





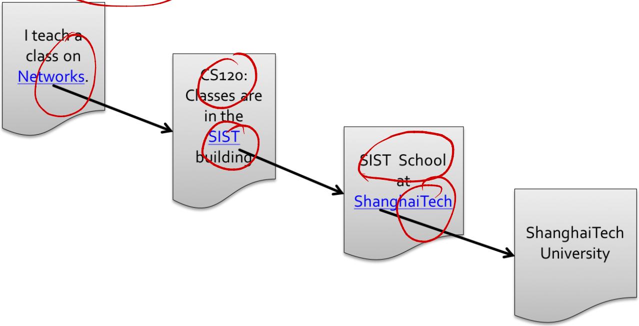
Adjacency Matrix of Cayley Graph



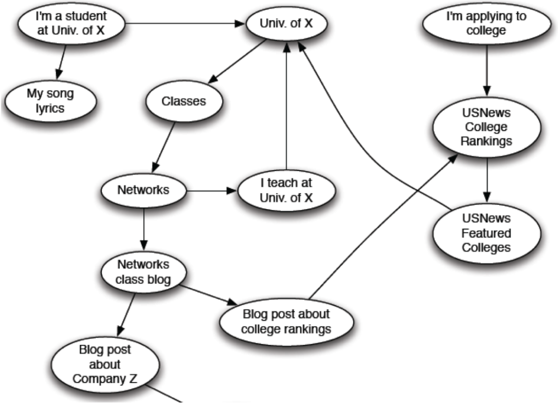


World Wide Web as A Graph

- Web as a directed graph
- Nodes: webpages
- Edges: hyperlinks

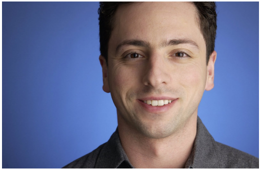


Web as A Directed Graph



Milestones in Networking

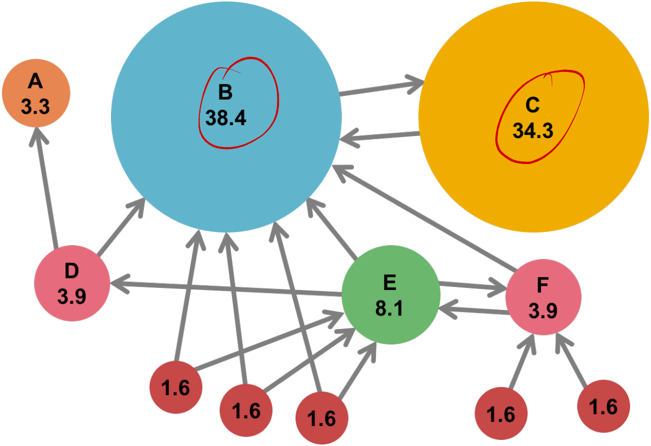
- 1998: Larry Page (1973-) and Sergey Brin (1973-) invented PageRank algorithm and then founded Google.
- 1998: Jon Kleinberg (1971-) invented Hyperlink-Induced Topic Search (HITS) algorithm.



Links as Votes

- Page is more important if it has more links
- Incoming links or outgoing links?
- Think of incoming links as votes:
  - www.stanford.edu has 23400 incoming links
  - www.nothing.com has 1 incoming link
- Are all in-links are equal?
  - Links from important pages count more
  - Recursive question!

Example: PageRank Scores

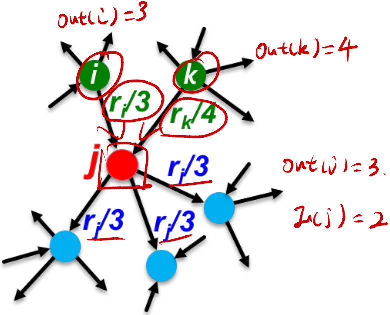


Simple Recursive Formulation

- Each link's vote is proportional to the importance of its source page.
- If page j with importance r_j has n out-links, each link gets r_j/n votes
- Page j's own importance is the sum of the votes on its in-links

Example

- $r_j = r_i/3 + r_k/4.$



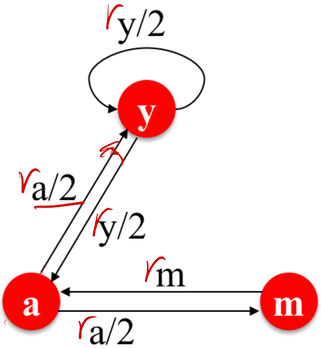
PageRank: The "Flow" Model

- A "vote" from an important page is worth more
- A page is important if it is pointed to by other important pages
- Define a rank r_j for page j:

$$r_j = \sum_{i \to j} \frac{r_i}{O_i}$$

where O_i is the outdegree of i.

Example: Flow Equation



$$r_y = r_y/2 + r_a/2$$
$$r_a = r_y/2 + r_m$$
$$r_m = r_a/2$$

Solving the Flow Equations

- Additional constraint forces uniqueness:
  - $r_y + r_a + r_m = 1$.
  - solution: $r_y = 2/5, r_a = 2/5, r_m = 1/5$.
- Gaussian elimination method works for small examples
- We need a better method for large web-size graphs

PageRank: Matrix Formulation

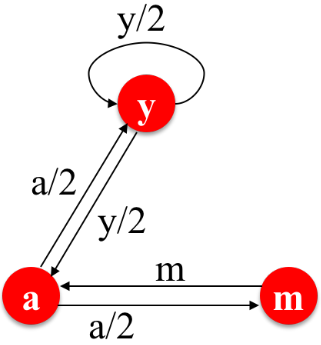
- Adjacency matrix Q
  - Each page i has O_i out-links
  - If $i \to j$, then $Q_{i,j} = \frac{1}{O_i}$, else $Q_{i,j} = 0$.
- Q is a stochastic matrix
- Row sum to 1.

PageRank: Matrix Formulation

- Rank vector $\mathbf{r}$
  - Vector with an entry per page
  - r_i is the importance score of page i
  - $\sum_i r_i = 1$
- The flow equations can be written

$$\mathbf{r} = \mathbf{r} \cdot Q$$

Example



$$r_y = r_y/2 + r_a/2$$
$$r_a = r_y/2 + r_m$$
$$r_m = r_a/2$$

$$Q = \begin{array}{c c} & \begin{array}{ccc} y & a & m \end{array} \\ \begin{array}{c} y \\ a \\ m \end{array} & \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 1 & 0 \end{pmatrix} \end{array}$$

Random Walk Interpretation

transition Matrix.

- Random Walk on Directed Graphs
- $\mathbf{r} \cdot Q = \mathbf{r}$
- $\mathbf{r}$: stationary distribution

Power Iteration Method

Markov chain.

irreducible / aperiodic.

$\lim_{n\to\infty} \pi^{(n)} = \lim_{t\to\infty} \pi^{(t)} = r$

- Given a web graph with n nodes, where the nodes are pages and edges are hyperlinks.

Stationary distribution

$\pi^{(n)} = \pi^{(n-1)} \cdot Q$

- Power iteration: a simple iterative scheme
  - Suppose there are N web pages
  - Initialize: $\mathbf{r}(0) = [\frac{1}{N}, \ldots, \frac{1}{N}]$.
  - Iterate: $\mathbf{r}(t+1) = \mathbf{r}(t) \cdot Q$.
  - Stop when $|\mathbf{r}(t+1) - \mathbf{r}(t)|_1 < \epsilon$

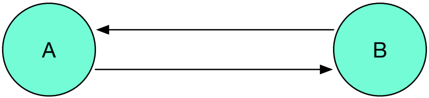
$\sum_i |r_i(t+1) - r_i(t)| < \varepsilon$

The Google Formulation

$$r_j^{(t+1)} = \sum_{i \to j} \frac{r_i^{(t)}}{O_i} \implies \mathbf{r}^{(t+1)} = \mathbf{r}^{(t)} \cdot Q$$

$$\begin{cases} \text{Does this converge?} \\ \text{Converge to what we want?} \\ \text{Result reasonable?} \end{cases}$$

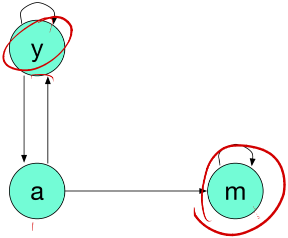
Example: Spider Traps with Two Nodes



$$r_A^{(t+1)} = r_B^{(t)}$$
$$r_B^{(t+1)} = r_A^{(t)}$$

$$\begin{array}{lcccccc} r_A & \rightarrow & 1 & 0 & 1 & 0 & \ldots \\ r_B & \rightarrow & 0 & 1 & 0 & 1 & \ldots \end{array}$$

Example: Spider Traps with One Node

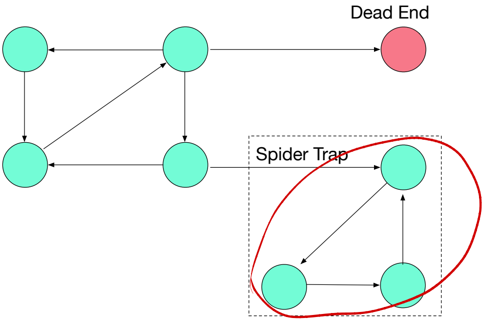


$$\begin{array}{c|ccc} & y & a & m \\ \hline y & 1/2 & 1/2 & 0 \\ a & 1/2 & 0 & 1/2 \\ m & 0 & 0 & 1 \end{array} \Longrightarrow \begin{array}{cccccc} r_y \rightarrow & 1/3 & 2/6 & 3/12 & \dots & 0 \\ r_a \rightarrow & 1/3 & 1/6 & 2/12 & \dots & 0 \\ r_m \rightarrow & 1/3 & 3/6 & 7/12 & \dots & 1 \end{array}$$

Example: Dead End

$$\begin{array}{llccccc} r_A & \rightarrow & 1 & 0 & 0 & 0 & \dots \\ r_B & \rightarrow & 0 & 1 & 0 & 0 & \dots \end{array}$$

Observations



- Some pages are dead ends (no out-links)
- Spider traps (all out-links are within the group)

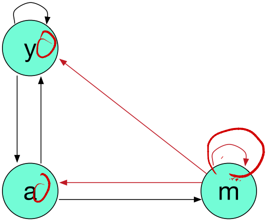
Google's Solution

- Idea: irreducibility leads to unique stationary distribution
- Random Teleports: create virtual links between any two pages
- Given the WWW graph $G = (V, E)$ and $N = |V|$.
- At each time, walker at page i has the following operations:
- If $O_i = 0$ (dead-end), then select any page j with equal probability $1/N$.
- Otherwise, walker has two options

$$\begin{cases} \text{w.p. } \beta & \text{Follow an out-link at random } \frac{1}{O_i} \\ \text{w.p. } 1-\beta & \text{Jump to some random pages} \end{cases} \tag{1}$$

- $\beta = (0.8, 0.9)$

Example: Google's Solution for Spider Traps



$$\begin{array}{c|ccc} & y & a & m \\ y & 1/2 & 1/2 & \mathbf{0} \\ a & 1/2 & 0 & \mathbf{1/2} \\ m & 0 & 0 & \mathbf{1} \end{array} \quad \Longrightarrow \quad \begin{array}{c|ccc} & y & a & m \\ y & 1/2 & 1/2 & 0 \\ a & 1/2 & 0 & 1/2 \\ m & 1/3 & 1/3 & 1/3 \end{array}$$

General Solution

- Assume no Dead Ends
- Pagerank Equation:

$$r_j = \sum_{i \to j} \beta \cdot \frac{r_i}{O_i} + (1 - \beta) \cdot \frac{1}{N}$$

- Google Matrix

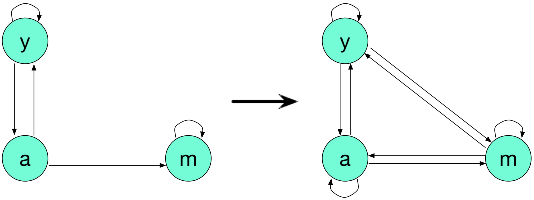
$$G = \beta \cdot Q + (1 - \beta) \left[\frac{1}{N} \right]_{N \times N}$$

$$\mathbf{r} = \mathbf{r} \cdot G$$

Random Teleports

- Google Matrix

$$Q \to G = \beta \cdot Q + (1-\beta)\left[\frac{1}{N}\right]_{N\times N}$$



Do Some Calculation

Let $\beta = 0.8$.

$$Q = 0.8 \cdot \begin{pmatrix} 1/2 & 1/2 & 0 \\ 1/2 & 0 & 1/2 \\ 0 & 0 & 1 \end{pmatrix} + 0.2 \cdot \begin{pmatrix} 1/3 & 1/3 & 1/3 \\ 1/3 & 1/3 & 1/3 \\ 1/3 & 1/3 & 1/3 \end{pmatrix}$$

As a result,

$$G = \begin{pmatrix} 7/15 & 7/15 & 1/15 \\ 7/15 & 1/15 & 7/15 \\ 1/15 & 1/15 & 13/15 \end{pmatrix}$$

Implementation of PageRank in Practice

- BigTable: distributed storage system
- GFS (Google File System): distributed file system
- Mapreduce: distributed computing system (followed by Hadoop & Spark)

Outline

Markov Chain Monte Carlo (MCMC)

- Revolutionized statistics and scientific computation
- Expanding the range of possible distributions that we can simulate from, including joint distributions in high dimensions
- Basic idea: build your own Markov chain $(X_0, X_1, \ldots)$ so that the desired distribution π is the stationary distribution of the chain.
- Sampling from distribution π (running the chain for a long time and then sampling)
- Further do sample mean & sample variance & other sample functions

MCMC Method

- Forward engineering: given the transition matrix Q, find the stationary distribution of Markov chain.
- Reverse engineering: given a distribution π that we want to simulate, we will engineer a Markov chain whose stationary distribution is π. Then run this engineered Markov chain for a long time, the distribution of the chain will approach π.

MCMC Method

- Markov Chain Monte Carlo (MCMC) is a remarkable methodology, which utilizes Markov sequences to effectively simulate from what would otherwise be intractable distributions.
- All MCMC algorithms construct reversible (time-reversible) Markov chain: detailed balance equations help us.
- Two most widely used algorithms: Metropolis-Hastings & Gibbs Sampling

Theory Justification: Strong Law of Large Numbers for Markov Chains

Theorem

Assume that $X_0, X_1, \cdots$ *is an irreducible and aperiodic Markov chain with stationary distribution* π*. Let* g *be a bounded, real-valued function. Let* X *be a random variable with distribution* π*. Then, with probability* 1,

$$\lim_{n\to\infty} \frac{g(X_1) + \cdots + g(X_n)}{n} = E(g(X)) = \sum_j \pi_j g(j).$$

Basic Idea of Metropolis–Hastings Algorithm

- Proposed by Nicholas Metropolis in 1953 & further developed by Wilfred Keith Hastings in 1970.
- Start with any irreducible Markov chain on the state space of interest
- Then modify it into a new Markov chain with desired stationary distribution
- Modification: moves are proposed according to the original chain, but the proposal may or may not be accepted.
- Art: choice of the probability of accepting the proposal

Algorithm 1 Metropolis-Hastings

Require:

Stationary distribution $\pi = (\pi_1, ..., \pi_M)$;

Original transition matrix $P = (p_{i,j})$;

State X_0 (chosen randomly or deterministically);

Ensure:

Modified transition matrix $P' = (p'_{i,j})$;

repeat

If $X_n = i$, propose a new state j using the transition probabilities in the ith row of the original transition matrix P;

Compute the acceptance probability $a_{i,j} = \min\left(\frac{\pi_j p_{j,i}}{\pi_i p_{i,j}}, 1\right)$;

Flip a coin that lands Heads with probability $a_{i,j}$;

If the coin lands Heads, accept the proposal (i.e., go to j), setting $X_{n+1} = j$. Otherwise, reject the proposal (i.e., stay at i), setting $X_{n+1} = i$;

until Convergence;

return P';

Basic Idea of Gibbs Sampling

- At each stage, one variable is updated (keeping all the other variables fixed) by drawing from the conditional distribution of that variable given all the other variables.
- Two major kinds of Gibbs sampler:
  - systematic scan: the updates sweep through the components in a deterministic order.
  - random scan: a randomly chosen component is updated at each stage.

Algorithm: Systematic Scan Gibbs Sampler

Let X and Y be discrete r.v.s with joint PMF $p_{X,Y}(x,y) = P(X = x, Y = y)$. We wish to construct a two-dimensional Markov chain (X_n, Y_n) whose stationary distribution is $p_{X,Y}$. The systematic scan Gibbs sampler proceeds by updating the X-component and the Y-component in alternation. If the current state is $(X_n, Y_n) = (x_n, y_n)$, then we update the X-component while holding the Y-component fixed, and then update the Y-component while holding the X-component fixed.

Algorithm 2 Systematic Scan Gibbs Sampler

Require:
Joint PMF $p_{X,Y}$;
Initial state (X_0, Y_0);

Ensure:
Two-dimensional Markov chain (X_n, Y_n);

repeat
    Draw a value x_{n+1} from the conditional distribution of X given $Y = y_n$, i.e. $P(X|Y = y_n)$, and set $X_{n+1} = x_{n+1}$;
    Draw a value y_{n+1} from the conditional distribution of Y given $X = x_{n+1}$, i.e. $P(Y|X = x_{n+1})$, and set $Y_{n+1} = y_{n+1}$;
    return (X_{n+1}, Y_{n+1});
until $n \geq N$;

Algorithm: Random Scan Gibbs Sampler

As above, let X and Y be discrete r.v.s with joint PMF $p_{X,Y}(x, y)$. We wish to construct a two-dimensional Markov chain (X_n, Y_n) whose stationary distribution is $p_{X,Y}$. Each move of the random scan Gibbs sampler picks a uniformly random component and updates it, according to the conditional distribution given the other component.

Algorithm 3 Random scan Gibbs sampler

Require:

Joint PMF $p_{X,Y}$;

Initial state (X_0, Y_0);

Ensure:

Two-dimensional Markov chain (X_n, Y_n);

```
repeat
    Choose which component to update, with equal probabilities;
    If the X-component was chosen, draw a value x_{n+1} from the conditional distribution of X given Y = y_n, and set X_{n+1} = x_{n+1}, Y_{n+1} = y_n. Similarly, if the Y-component was chosen, draw a value y_{n+1} from the conditional distribution of Y given X = x_n, and set X_{n+1} = x_n, Y_{n+1} = y_{n+1};
    return (X_{n+1}, Y_{n+1});
until n ≥ N;
```

References

- Chapter 11 of **BH**
- Chapter 7 of **BT**
- Reading: Chapter 12 of **BH**