Introduction to MCMC and PageRank

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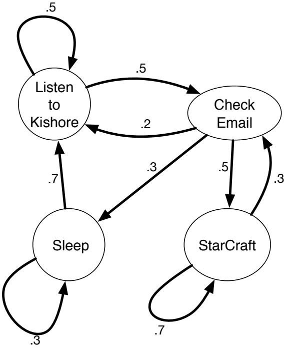
Lecture for CS 6505

What is a Markov chain?

Example: Life in CS 6210, discrete time $t = 0, 1, 2, \ldots$:



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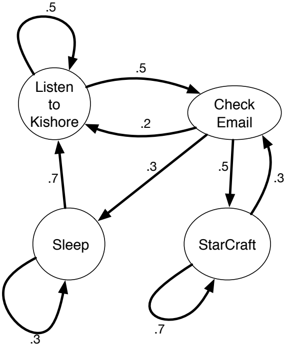


Each vertex is a state of the Markov chain.

Directed graph, possibly with self-loops.

Edge weights represent probability of a transition, so:
non-negative and sum of weights of outgoing edges $= 1$.

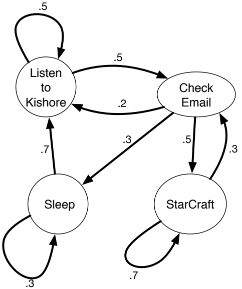
Transition matrix

In general: N states $\Omega = \{1, 2, \ldots, N\}$.

$N \times N$ transition matrix P where:

$\mathrm{P}(i, j) =$ weight of edge $i \to j = \mathbf{Pr}$ (going from i to j)

For earlier example:



$$\mathrm{P} = \begin{bmatrix} .5 & .5 & 0 & 0 \\ .2 & 0 & .5 & .3 \\ 0 & .3 & .7 & 0 \\ .7 & 0 & 0 & .3 \end{bmatrix}$$

P is a stochastic matrix = rows sum to 1.

One-step transitions

Time: $t = 0, 1, 2, \ldots$.
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in state k_0 at time 0, in k_1 at time 1, ..., in k_{t-1} at time $t-1$, what's the probability of being in state j at time t?

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$$\begin{aligned}\mathbf{Pr}\left(X_t = j \mid X_0 = k_0, X_1 = k_1, \ldots, X_{t-1} = k_{t-1}\right) \\ &= \mathbf{Pr}\left(X_t = j \mid X_{t-1} = k_{t-1}\right) \\ &= \mathrm{P}(k_{t-1}, j).\end{aligned}$$

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Process is **memoryless** –

only current state matters, previous states do not matter.

Known as **Markov property**, hence the term Markov chain.

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What's probability *Listen* at time 2 given *Email* at time 0?
Try all possibilities for state at time 1.

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Try all possibilities for state at time 1.

$$\begin{aligned}
&\mathbf{Pr}\left(X_2 = Listen \mid X_0 = Email\right) \\
&\quad = \quad \mathbf{Pr}\left(X_2 = Listen \mid X_1 = Listen\right) \times \mathbf{Pr}\left(X_1 = Listen \mid X_0 = Email\right) \\
&\qquad\quad + \mathbf{Pr}\left(X_2 = Listen \mid X_1 = Email\right) \times \mathbf{Pr}\left(X_1 = Email \mid X_0 = Email\right) \\
&\qquad\quad + \mathbf{Pr}\left(X_2 = Listen \mid X_1 = StarCraft\right) \times \mathbf{Pr}\left(X_1 = StarCraft \mid X_0 = Email\right) \\
&\qquad\quad + \mathbf{Pr}\left(X_2 = Listen \mid X_1 = Sleep\right) \times \mathbf{Pr}\left(X_1 = Sleep \mid X_0 = Email\right)
\end{aligned}$$

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&\quad + \mathbf{Pr}(X_2 = Listen \mid X_1 = Email) \times \mathbf{Pr}(X_1 = Email \mid X_0 = Email) \\
&\quad + \mathbf{Pr}(X_2 = Listen \mid X_1 = StarCraft) \times \mathbf{Pr}(X_1 = StarCraft \mid X_0 = Email) \\
&\quad + \mathbf{Pr}(X_2 = Listen \mid X_1 = Sleep) \times \mathbf{Pr}(X_1 = Sleep \mid X_0 = Email) \\
&= (.5)(.2) + 0 + 0 + (.7)(.3) = .31
\end{aligned}
$$

$$
\mathrm{P} = \begin{bmatrix} .5 & .5 & 0 & 0 \\ .2 & 0 & .5 & .3 \\ 0 & .3 & .7 & 0 \\ .7 & 0 & 0 & .3 \end{bmatrix} \qquad \mathrm{P}^2 = \begin{bmatrix} .35 & .25 & .25 & .15 \\ .31 & .25 & .35 & .09 \\ .06 & .21 & .64 & .09 \\ .56 & .35 & 0 & .09 \end{bmatrix}
$$

States: 1=*Listen*, 2=*Email*, 3=*StarCraft*, 4=*Sleep*.

k-step transitions

2-step transition probabilities: use P^2.
In general, for states i and j:

$$
\begin{aligned}
&\mathbf{Pr}\left(X_{t+2} = j \mid X_t = i\right) \\
&= \sum_{k=1}^{N} \mathbf{Pr}\left(X_{t+2} = j \mid X_{t+1} = k\right) \times \mathbf{Pr}\left(X_{t+1} = k \mid X_t = i\right) \\
&= \sum_{k} \mathrm{P}(k,j)\mathrm{P}(i,k) = \sum_{k} \mathrm{P}(i,k)\mathrm{P}(k,j) = \mathrm{P}^2(i,j)
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ℓ-step transition probabilities: use P^ℓ.
For states i and j and integer $\ell \geq 1$,

$$\mathbf{Pr}\left(X_{t+\ell}=j \mid X_t=i\right) = \mathrm{P}^\ell(i,j),$$

Random Initial State

Suppose the state at time 0 is not fixed
but is chosen from a probability distribution μ_0.

Notation: $X_0 \sim \mu_0$.

What is the distribution for X_1?

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So $X_1 \sim \mu_1$ where $\mu_1 = \mu_0\mathrm{P}$.

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And $X_t \sim \mu_t$ where $\mu_t = \mu_0\mathrm{P}^t$.

Back to CS 6210 example: big t?

Let's look again at our CS 6210 example:

$$P = \begin{bmatrix} .5 & .5 & 0 & 0 \\ .2 & 0 & .5 & .3 \\ 0 & .3 & .7 & 0 \\ .7 & 0 & 0 & .3 \end{bmatrix}$$

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Columns are converging to

$$\pi = [\ .244186, \ \ .244186, \ \ .406977, \ \ .104651].$$

Limiting Distribution

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Let $\pi = [\ .244186,\ \ .244186,\ \ .406977,\ \ .104651]$.
In other words, for big t, $X_t \sim \pi$.

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in other words, $\pi \mathrm{P} = \pi$.

Any distribution π where $\pi \mathrm{P} = \pi$ is called a stationary distribution of the Markov chain.

Stationary Distributions

Key questions:

- When is there a stationary distribution?
- If there is at least one, is it unique or more than one?
- Assuming there's a unique stationary distribution:
  - Do we always reach it?
  - What is it?
  - *Mixing time* = Time to reach unique stationary distribution

Algorithmic Goal:

- If we have a distribution π that we want to sample from, can we design a Markov chain that has:
  - Unique stationary distribution π,
  - From every X_0 we always reach π,
  - Fast mixing time.

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Want a unique stationary distribution π and that
get to it from every starting state X_0.

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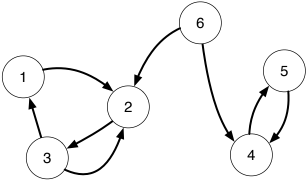

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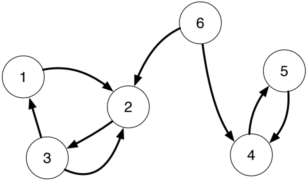


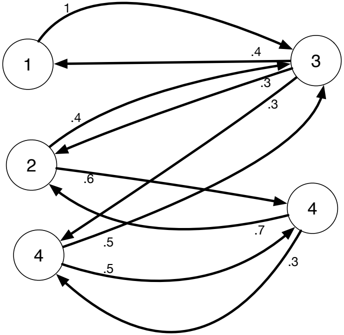
Starting at 1 gets to different distribution than starting at 5.

State i communicates with state j if starting at i can reach j:

$$\text{there exists } t, \ \mathrm{P}^t(i,j) > 0.$$

Markov chain is irreducible if all pairs of states communicate..

Example of bipartite Markov chain:



Starting at 1 gets to different distribution than starting at 3.

Periodicity

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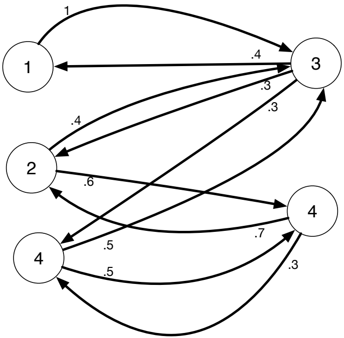
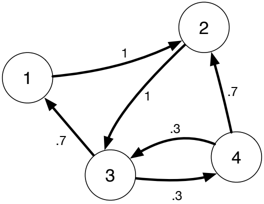


Starting at 1 gets to different distribution than starting at 3.

Need that no periodicity.

Aperiodic

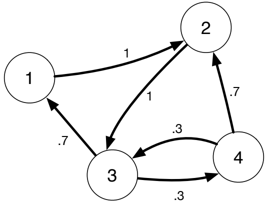


Return times for state i are times $R_i = \{t : P^t(i, i) > 0\}$.

Above example: $R_1 = \{3, 5, 6, 8, 9, \ldots\}$.

Let $r = \gcd(R_i)$ be the period for state i.

Aperiodic



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If P is irreducible then all states have the same period.
If $r = 2$ then the Markov chain is bipartite.
A Markov chain is aperiodic if $r = 1$.

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Ergodic Markov chain has a unique stationary distribution π.
And for all initial $X_0 \sim \mu_0$ then:

$$\lim_{t \to \infty} \mu_t = \pi.$$

In other words, for big enough t, all rows of P^t are π.

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How big does t need to be?

What is π?

Determining π: Symmetric Markov Chain

Symmetric if for all pairs i, j: $\mathrm{P}(i,j) = \mathrm{P}(j,i)$.
Then π is uniformly distributed over all of the states $\{1, \ldots, N\}$:

$$\pi(j) = \frac{1}{N} \text{ for all states } j.$$

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(\pi\mathrm{P})(j) &= \sum_{i=1}^{N} \pi(i)\mathrm{P}(i,j) \\
&= \frac{1}{N}\sum_{i=1}^{N} \mathrm{P}(i,j) \\
&= \frac{1}{N}\sum_{i=1}^{N} \mathrm{P}(j,i) \quad \text{since P is symmetric}
\end{aligned}$$

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&= \frac{1}{N} \quad \text{since rows of P always sum to 1}
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&= \frac{1}{N} \quad \text{since rows of P always sum to 1} \\
&= \pi(j) \qquad \square
\end{aligned}$$

Determining π: Reversible Markov Chain

Reversible with respect to π if for all pairs i, j:

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If can find such a π then it is the stationary distribution.

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Proof: Similar to the symmetric case.
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$$\pi(i)\mathrm{P}(i,j) = \pi(j)\mathrm{P}(j,i).$$

If can find such a π then it is the stationary distribution.

Proof: Similar to the symmetric case.
Need to check that for all states j: $(\pi\mathrm{P})(j) = \pi(j)$.

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&= \pi(j) \qquad \square
\end{aligned}$$

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What is π?

Some Examples

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Symmetric: for edge (i,j), $\mathrm{P}(i,j) = \mathrm{P}(j,i) = 1/d$.

So π is uniform: $\pi(i) = 1/n$.

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Random walk on a general connected undirected graph G:

- What is π?
  - Consider $\pi(i) = d(i)/Z$ where
    - $d(i) =$ degree of vertex i and
    - $Z = \sum_{j \in V} d(j)$. (Note, $Z = 2m = 2|E|$.)
  - Check it's reversible: $\pi(i)\mathrm{P}(i,j) = \frac{d(i)}{Z}\frac{1}{d(i)} = \frac{1}{Z} = \pi(j)\mathrm{P}(j,i)$.

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What if G is a directed graph?

Then it may not be reversible, and if it's not reversible:

then usually we can't figure out the stationary distribution since typically N is HUGE.

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Notation:
For page $x \in V$, let:

$$\begin{aligned} \mathrm{Out}(x) &= \{y : x \to y \in E\} = \text{outgoing edges from } x \\ \mathrm{In}(x) &= \{w : w \to x \in E\} = \text{incoming edges to } x \end{aligned}$$

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First Ranking Idea

First idea for ranking pages: like academic papers

use citation counts

Here, citation = link to a page.

So set $\pi(x) = |\mathrm{In}(x)| =$ number of links to x.

Refining the Ranking Idea

What if:

a webpage has 500 links and one is to Eric's page.

another webpage has only 5 links and one is to Santosh's page.

Which link is more valuable?

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Academic papers: If a paper cites 50 other papers, then each reference gets $1/50$ of a citation.

Webpages: If a page y has $|\mathrm{Out}(y)|$ outgoing links, then:

each linked page gets $1/|\mathrm{Out}(y)|$.

New solution:

$$\pi(x) = \sum_{y \in \mathrm{In}(x)} \frac{1}{|\mathrm{Out}(y)|}.$$

Further Refining the Ranking Idea

Previous:

$$\pi(x) = \sum_{y \in \text{In}(x)} \frac{1}{|\text{Out}(y)|}.$$

But if *Eric's children's webpage* has a link to a Eric's page and *CNN* has a link to Santosh's page, which is more important?

Further Refining the Ranking Idea

Previous:

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But if *Eric's children's webpage* has a link to a Eric's page and *CNN* has a link to Santosh's page, which is more important?

Solution: define $\pi(x)$ recursively.
Page y has importance $\pi(y)$.
A link from y gets $\pi(y)/|\mathrm{Out}(y)|$ of a citation.

$$\pi(x) = \sum_{y \in \mathrm{In}(x)} \frac{\pi(y)}{|\mathrm{Out}(y)|}.$$

Random Walk

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Recursive definition of π, how do we find it?

Look at the random walk on the webgraph $G = (V, E)$.
From a page $y \in V$, choose a random link and follow it.
This is a Markov chain.
For $y \to x \in E$ then:

$$\mathrm{P}(y, x) = \frac{1}{|\mathrm{Out}(y)|}$$

What is the stationary distribution of this Markov chain?

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Need to find π where $\pi = \pi \mathrm{P}$.
Thus,

$$\pi(x) = \sum_{y \in V} \pi(y) \mathrm{P}(y, x) = \sum_{y \in \mathrm{In}(x)} \frac{\pi(y)}{|\mathrm{Out}(y)|}.$$

This is identical to the definition of the importance vector π.

Summary: the stationary distribution of the random walk on the webgraph gives the importance $\pi(x)$ of a page x.

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Random Walk on the Webgraph

Random walk on the webgraph $G = (V, E)$.

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Solution to make it ergodic:
Introduce "damping factor" α where $0 < \alpha \leq 1$.
(in practice apparently use $\alpha \approx .85$)

From page y,
with prob. α follow a random outgoing link from page y.
with prob. $1 - \alpha$ go to a completely random page
(uniformly chosen from all pages V).

Let $N = |V|$ denote number of webpages.
Transition matrix of new Random Surfer chain:

$$\mathrm{P}(y,x) = \begin{cases} \frac{1-\alpha}{N} & \text{if } y \to x \notin E \\ \frac{1-\alpha}{N} + \frac{\alpha}{|\mathrm{Out}(y)|} & \text{if } y \to x \in E \end{cases}$$

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How to find π?

Take last week's π, and compute πP^t for big t.

What's a big enough t?

Mixing Time

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Example: $\Omega = \{1, 2, 3, 4\}$.
μ is uniform: $\mu(1) = \mu(2) = \mu(3) = \mu(4) = .25$.
And ν has: $\nu(1) = .5, \nu(2) = .1, \nu(3) = .15, \nu(4) = .25$.

$$d_{TV}(\mu, \nu) = \frac{1}{2}(.25 + .15 + .1 + 0) = .25$$

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Consider ergodic MC with states Ω, transition matrix P, and unique stationary distribution π.
For state $x \in \Omega$, time to mix from x:

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> mixing time is time to get within distance $\leq 1/4$ of π from the worst initial state X_0.

Choice of constant $1/4$ is somewhat arbitrary.
Can get within distance $\leq \epsilon$ in time $O(\mathrm{T_{mix}} \log(1/\epsilon))$.

Mixing Time of Random Surfer

Coupling proof:
Consider 2 copies of the Random Surfer chain (X_t) and (Y_t).

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If $X_{t-1} = Y_{t-1}$ then they choose the same transition at time t.
If $X_{t-1} \neq Y_{t-1}$ then with prob. $1 - \alpha$ choose the same random page z for both chains.

Therefore,

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Setting: $t \geq -2/\log(\alpha)$ we have $\mathbf{Pr}\left(X_t \neq Y_t\right) \leq 1/4$.
Therefore, mixing time:

$$\mathrm{T}_{\mathrm{mix}} \leq \frac{-2}{\log \alpha} \approx 8.5 \text{ for } \alpha = .85.$$