Markov models

Source: Hastie et at. (2009), Daumé III. Thanks to D. Hsu.

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Sequence / time series modeling is an entire subfield in statistics, largely due to the plethora of sequence / time series data in applications:

- Economic / financial data over time
- Climate science
- Genomic sequences
- Speech and natural language
- ...

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If the X_t are discrete-valued, then the Markov property means that

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A sequence model for a Markov chain is called a **Markov model**.

Markov chain distributions

To specify a Markov chain (MC):

- Specify the distribution of the initial state X_1.
- Specify a **transition kernel**: $\Pr(X_{t+1} = x' \mid X_t = x)$ for all (x, x').

  (Nothing to do with *kernels* as in SVMs/kernel trick/RKHS.)

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- Initial state distribution given by a d-dimensional probability vector $\boldsymbol{\pi}$

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- Transition kernel can be written as a $d \times d$ matrix $\boldsymbol{A}$

$$A_{i,j} \;=\; \Pr(X_{t+1} = j \mid X_t = i)$$

  (rows of $\boldsymbol{A}$ are probability vectors).

  Also called a *transition matrix* or *(right) stochastic matrix*.

Example: a two-state Markov chain

State space: $\{1, 2\}$.
Parameters:

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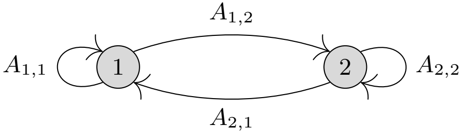

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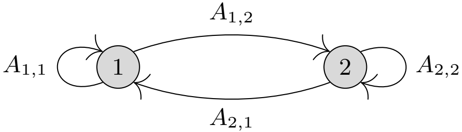

A random state sequence drawn from this MC:

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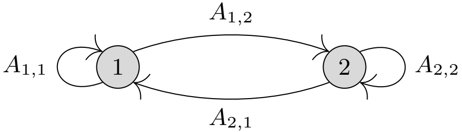

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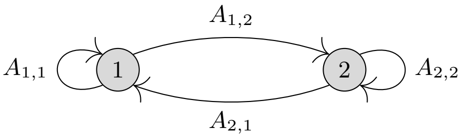

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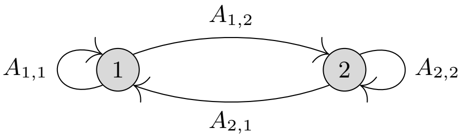

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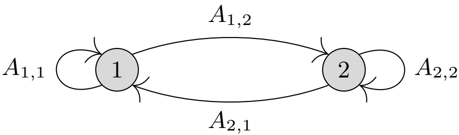

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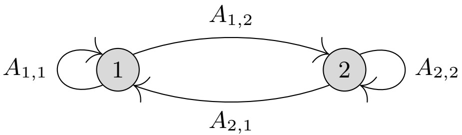

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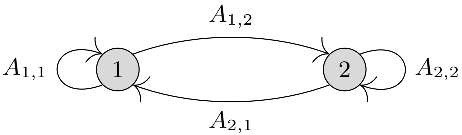

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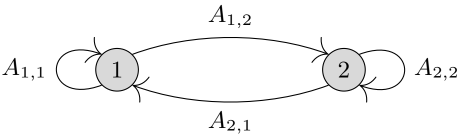

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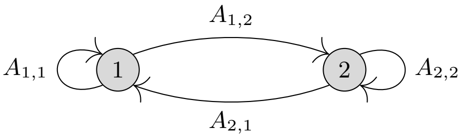

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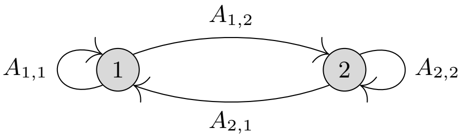

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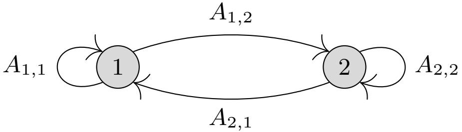

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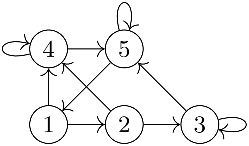
Example: random walk on a directed graph

Consider a directed graph $G = (V, E)$ over $|V| = d$ vertices (self-loops ok).



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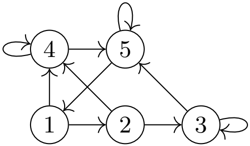

MC for random walk on G:

$$\pi_i \;=\; \mathbb{1}\{\text{start vertex is } i\}, \quad A_{i,j} \;=\; \frac{\mathbb{1}\{(i,j) \in E\}}{\text{out degree}(i)}.$$

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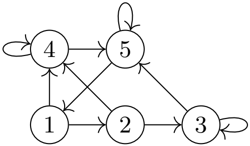

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 & * & & * & \\
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 & & * & & * \\
 & & & * & * \\
* & & & & *
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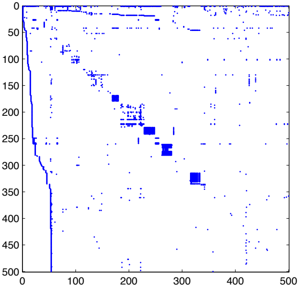
The non-zero pattern of $\boldsymbol{A}$ gives the adjacency structure of G (vertices = states).

Example: PageRank

Web graph $G = (V, E)$:
Vertices are webpages, directed edges are hyperlinks between webpages.



Adjacency matrix of the web graph for 500 web pages.

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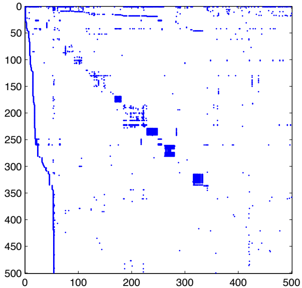

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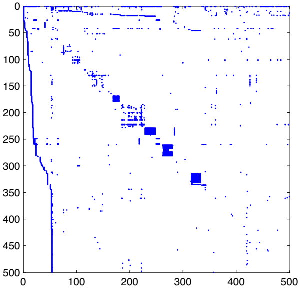

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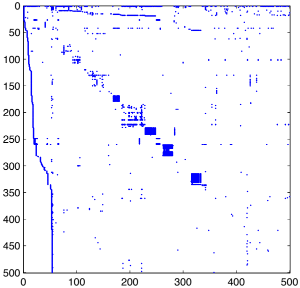

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$$\Pr(X_t = i) \quad \text{for large } t.$$

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What is the marginal distribution of X_2 in terms of $\boldsymbol{\pi}$ and $\boldsymbol{A}$?

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For each $j \in [d]$,

$$\Pr(X_2 = j)$$

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What is the marginal distribution of X_2 in terms of $\boldsymbol{\pi}$ and $\boldsymbol{A}$?

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\end{aligned}
$$

For any $t \in \mathbb{N}$, the marginal distribution of X_t in terms of $\boldsymbol{\pi}$ and $\boldsymbol{A}$ is

$$
\Pr(X_t = k) = k\text{-th entry of } \boldsymbol{\pi}^\top \underbrace{\boldsymbol{A}\boldsymbol{A}\cdots\boldsymbol{A}}_{t-1 \text{ times}}.
$$

Powers of the transition matrix

The (i,j)-th entry of $\boldsymbol{A}^p = \underbrace{\boldsymbol{A}\boldsymbol{A}\cdots\boldsymbol{A}}_{p \text{ times}}$ is the p-step transition matrix

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Convergence?

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\end{aligned}$$

Convergence? Doesn't even seem to matter what π is!

Limiting state distribution

Certain "nice" transition matrices $\boldsymbol{A} \in \mathbb{R}^{d \times d}$ have the property that

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A solution $\boldsymbol{q}$ to $(\star)$, is called a **stationary distribution**.

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Law of Large Numbers for MCs.

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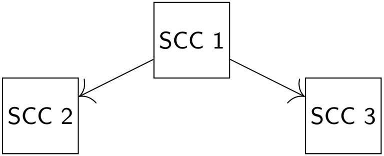
When does a MC even have a unique stationary distribution?

What can go wrong

1. **Directed graph underlying A has more than one strongly connected component "sinks"** $\longrightarrow$ stationary distribution may not be unique.



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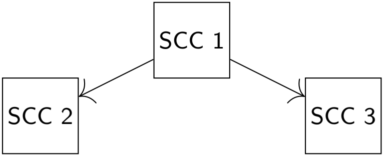

Markov chains with only one strongly connected component are called **irreducible**.

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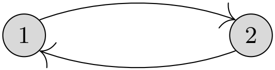
   Example:

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   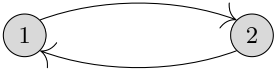

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   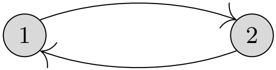

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   If every state $i \in [d]$ has $A_{i,i} > 0$, then aperiodicity is guaranteed.

Conditions for unique stationary distribution

Theorem: If MC with transition matrix $\boldsymbol{A}$ is *irreducible* and *aperiodic*, then

- There is a unique stationary distribution $\boldsymbol{q}$ (which satisfies $\boldsymbol{q}^\top \boldsymbol{A} = \boldsymbol{q}^\top$).
- $$\lim_{p \to \infty} \boldsymbol{A}^p = \begin{pmatrix} \text{——} & \boldsymbol{q}^\top & \text{——} \\ \text{——} & \boldsymbol{q}^\top & \text{——} \\ & \vdots & \\ \text{——} & \boldsymbol{q}^\top & \text{——} \end{pmatrix}.$$

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Power method:

initialize $\boldsymbol{q}$ arbitrarily.
repeat
  $\boldsymbol{q}^\top := \boldsymbol{q}^\top \boldsymbol{A}$.
until bored.
return $\boldsymbol{q}$.

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PageRank scores = stationary distribution of this new MC.

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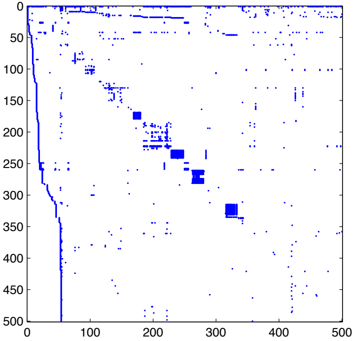
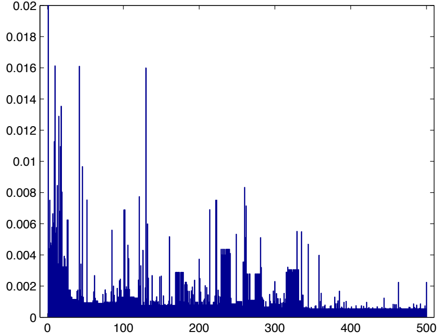


Adjacency matrix of the web graph for 500 web pages.



PageRank distribution.

(From K. Murphy, "Machine Learning", MIT Press 2012.)

Example: semi-supervised learning

Have some **labeled data** $(x_1, y_1), (x_2, y_2), \ldots, (x_m, y_m)$ from $\mathcal{X} \times \{\pm 1\}$, and also many **unlabeled data** $x_{m+1}, x_{m+1}, \ldots, x_{m+n}$ from $\mathcal{X}$.

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- Start weighted random walk starting from **unlabeled point** x_{m+i}.

  If **first labeled point reached** has label $y \in \{\pm 1\}$, then use $\hat{y}_{m+i} := y$ as the label for x_{m+i}.

  (Can actually compute, in closed form, the probabilities of $\hat{y}_{m+i} = y$ for each y.)

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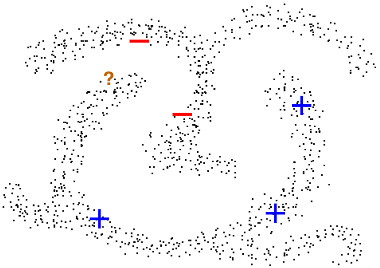

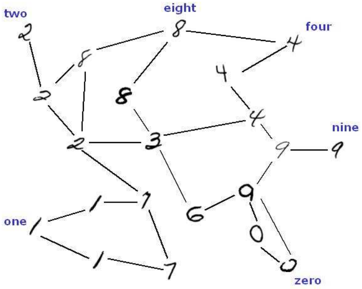

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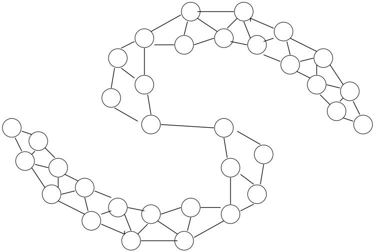

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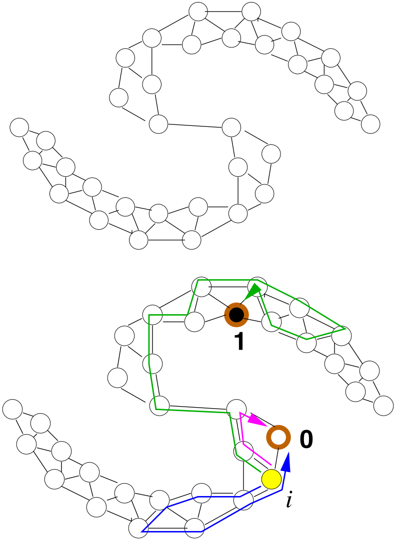

Recap

- Markov property: past and future are conditionally independent given the present.
- Transition matrix: the conditional next-state distributions for each state.
- Random walk on graphs: extremely important process, very well-studied, many applications (including in ML, statistics, etc).
- **Irreducible and aperiodic Markov chains have limiting behavior**: doesn't matter where you start, eventually marginal state distribution is the stationary distribution.

  Some qualities similar to iid processes, some rather different.

  Related to eigenvectors/eigenvalues, computation via power method.
- Forms the basis of PageRank.