Randomised Algorithms

Lecture 4: Markov Chains and Mixing Times

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UNIVERSITY OF CAMBRIDGE

Outline

Recap of Markov Chain Basics

Irreducibility, Periodicity and Convergence

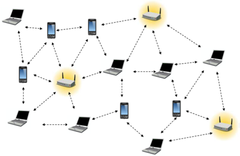
Total Variation Distance and Mixing Times

Application 1: Markov Chain Monte Carlo

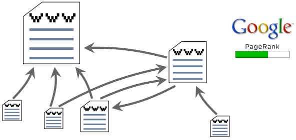
Application 2: Card Shuffling

Appendix: Remarks on Mixing Time (non-examin.)

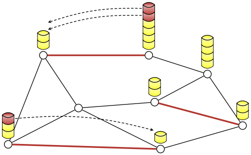
Applications of Markov Chains in Computer Science



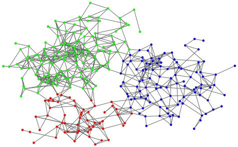
Broadcasting



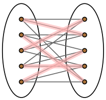
Ranking Websites



Load Balancing

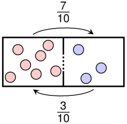


Clustering



$$A = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Sampling and Optimisation



Particle Processes

Markov Chains

Markov Chain (Discrete Time and State, Time Homogeneous)

The sequence $(X_t)_{t=0}^{\infty}$ is a Markov Chain on State Space Ω with Transition Matrix P if the Markov Property holds: for all $t \geq 0$, $x_0, \ldots, x_{t+1} \in \Omega$,

$$\mathbf{P}\left[X_{t+1} = x_{t+1} \,\middle|\, X_t = x_t, \ldots, X_0 = x_0 \right] = \mathbf{P}\left[X_{t+1} = x_{t+1} \,\middle|\, X_t = x_t \right]$$
$$:= P(x_t, x_{t+1}).$$

From the definition one can deduce that (check!)

- For all $t \geq 0, x_0, x_1, \ldots, x_t \in \Omega$,

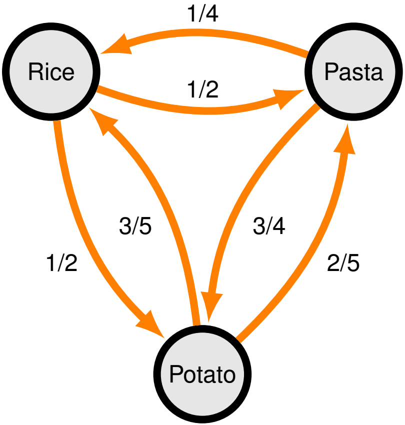
$$\mathbf{P}\left[X_t = x_t, X_{t-1} = x_{t-1}, \ldots, X_0 = x_0 \right] = P(x_0, x_1) \cdot \ldots \cdot P(x_{t-2}, x_{t-1}) \cdot P(x_{t-1}, x_t).$$

- For all $0 \leq t_1 < t_2, x \in \Omega$,

$$\mathbf{P}\left[X_{t_2} = x \right] = \sum_{y \in \Omega} \mathbf{P}\left[X_{t_2} = x \mid X_{t_1} = y \right] \cdot \mathbf{P}\left[X_{t_1} = y \right].$$

What does a Markov Chain Look Like?

Example: the carbohydrate served with lunch in the college cafeteria.



This has transition matrix:

$$P = \begin{array}{c} \\ \end{array} \begin{array}{ccc} \text{Rice} & \text{Pasta} & \text{Potato} \end{array}$$

$$P = \begin{bmatrix} 0 & 1/2 & 1/2 \\ 1/4 & 0 & 3/4 \\ 3/5 & 2/5 & 0 \end{bmatrix} \begin{array}{l} \text{Rice} \\ \text{Pasta} \\ \text{Potato} \end{array}$$

Transition Matrices and Distributions

The Transition Matrix P of a Markov chain on $\Omega = \{1, \ldots n\}$ is given by

$$P = \begin{pmatrix} P(1,1) & \ldots & P(1,n) \\ \vdots & \ddots & \vdots \\ P(n,1) & \ldots & P(n,n) \end{pmatrix}.$$

- $\rho^t = (\rho^t(1), \rho^t(2), \ldots, \rho^t(n))$: state vector at time t (row vector).
- Multiplying ρ^t by P corresponds to advancing the chain one step:

$$\rho^t(y) = \sum_{x \in \Omega} \rho^{t-1}(x) \cdot P(x,y) \qquad \text{and thus} \qquad \rho^t = \rho^{t-1} \cdot P.$$

- The Markov Property and line above imply that for any $t \geq 0$

$$\rho^t = \rho \cdot P^{t-1} \qquad \text{and thus} \qquad P^t(x,y) = \mathbf{P}\left[\, X_t = y \mid X_0 = x \,\right].$$

- Everything boils down to deterministic vector/matrix computations

$\Rightarrow$ can replace ρ by any (load) vector and view P as a balancing matrix!

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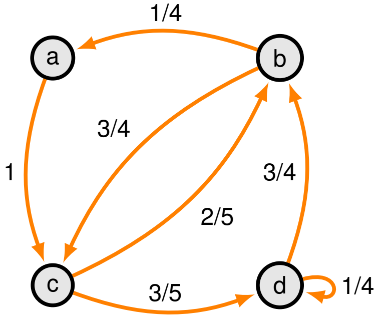
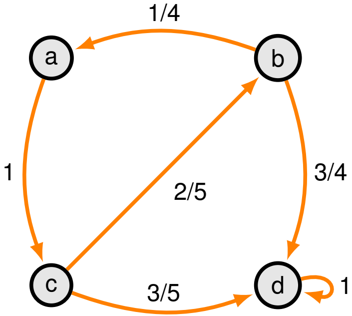
Irreducible Markov Chains

A Markov Chain is irreducible if for every pair of states $x, y \in \Omega$ there is an integer $k \geq 0$ such that $P^k(x, y) > 0$.



✓ irreducible



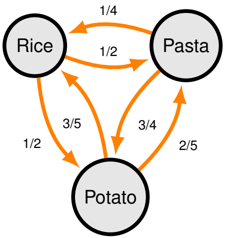
× not irreducible (thus reducible)

Stationary Distribution

A probability distribution $\pi = (\pi(1), \dots, \pi(n))$ is the stationary distribution of a Markov Chain if $\pi P = \pi$ (π is a left eigenvector with eigenvalue 1)

College carbs example:

$$\underbrace{\left(\frac{4}{13}, \frac{4}{13}, \frac{5}{13}\right)}_{\pi} \cdot \underbrace{\begin{pmatrix} 0 & 1/2 & 1/2 \\ 1/4 & 0 & 3/4 \\ 3/5 & 2/5 & 0 \end{pmatrix}}_{P} = \underbrace{\left(\frac{4}{13}, \frac{4}{13}, \frac{5}{13}\right)}_{\pi}$$



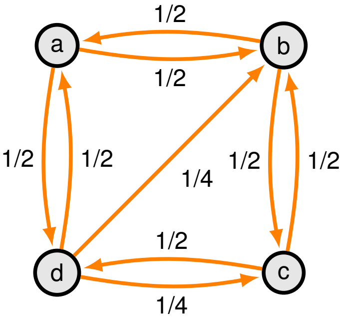
- A Markov Chain reaches stationary distribution if $\rho^t = \pi$ for some t.
- If reached, then it persists: If $\rho^t = \pi$ then $\rho^{t+k} = \pi$ for all $k \geq 0$.

Existence and Uniqueness of a Positive Stationary Distribution

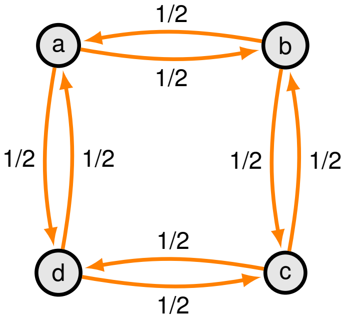
Let P be finite, irreducible MC, then there exists a unique probability distribution π on Ω such that $\pi = \pi P$ and $\pi(x) = 1/h(x,x) > 0, \forall x \in \Omega$; $h(x,x)$ is the expected time for the MC starting in x to return to x.

Periodicity

- A Markov Chain is aperiodic if for all $x \in \Omega$, $\gcd\{t \geq 1 : P^t(x,x) > 0\} = 1$.
- Otherwise we say it is periodic.



✓ Aperiodic



× Periodic

???

Question: Which of the two chains (if any) are aperiodic?

Convergence Theorem

Ergodic = Irreducible + Aperiodic

Convergence Theorem

Let P be any finite, irreducible, aperiodic Markov Chain with stationary distribution π. Then for any $x, y \in \Omega$,

$$\lim_{t\to\infty} P^t(x,y) = \pi(y).$$

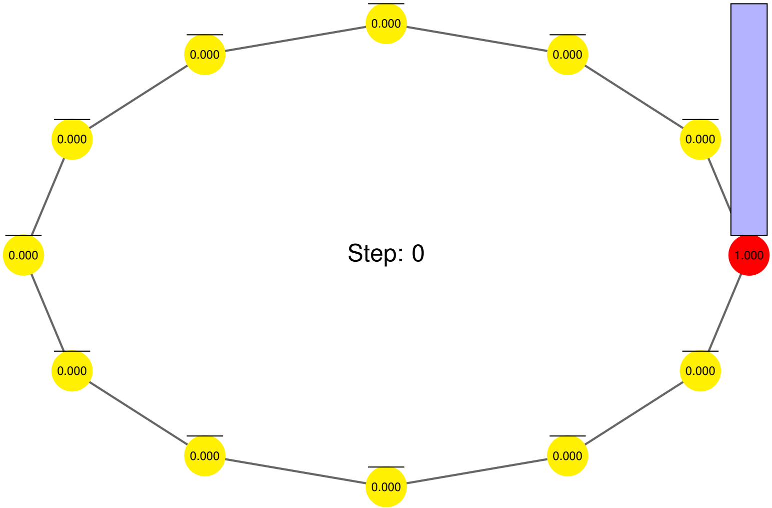
- mentioned before: For finite irreducible MC's π exists, is unique and

$$\pi(y) = \frac{1}{h(y,y)} > 0.$$

- We will prove a quantitative version of the Convergence Theorem after introducing Spectral Graph Theory.

Convergence to Stationarity (Example)

- Markov Chain: stays put with $1/2$ and moves left (or right) w.p. $1/4$
- At step t the value at vertex $x \in \{1, 2, \ldots, 12\}$ is $P^t(1, x)$.



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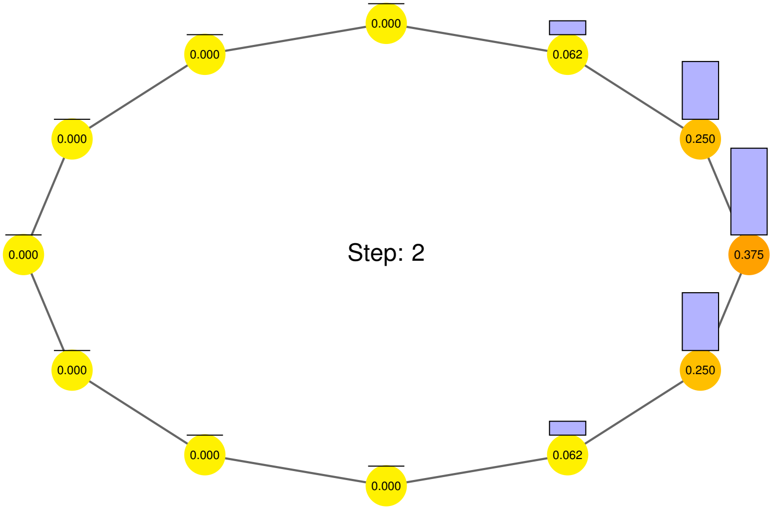

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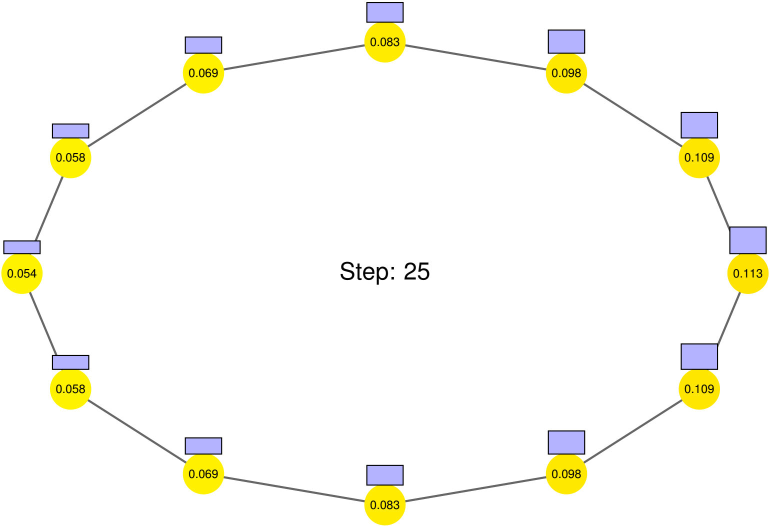

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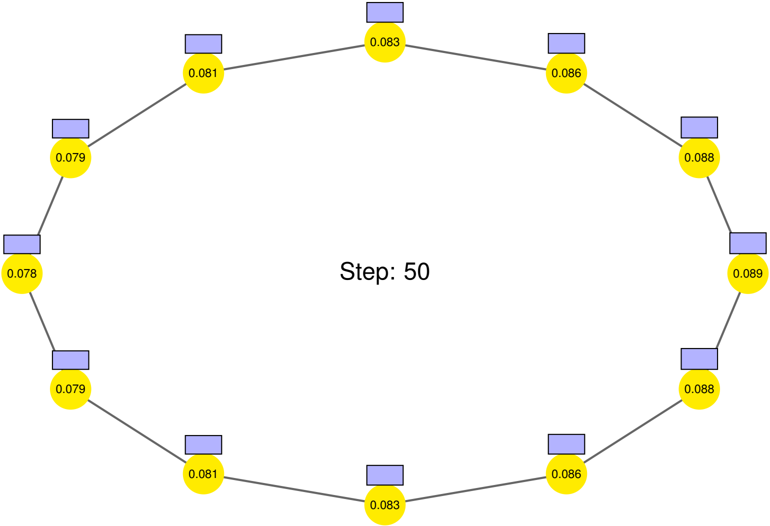


Outline

How Similar are Two Probability Measures?

Loaded Dice

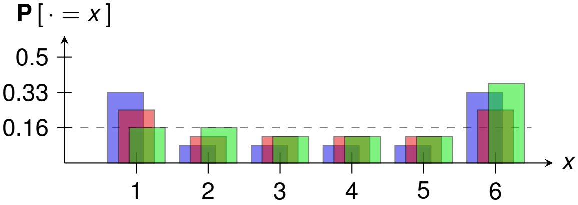
- You are presented three loaded (unfair) dice A, B, C:

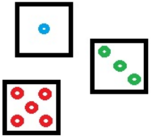
x	1	2	3	4	5	6
$\mathbf{P}[A = x]$	1/3	1/12	1/12	1/12	1/12	1/3
$\mathbf{P}[B = x]$	1/4	1/8	1/8	1/8	1/8	1/4
$\mathbf{P}[C = x]$	1/6	1/6	1/8	1/8	1/8	9/24

Question 1: Which dice is the least fair? Most choose A. Why?

Question 2: Which dice is the most fair? Dice B and C seem "fairer" than A but which is fairest?

We need a formal "fairness measure" to compare probability distributions!





Total Variation Distance

The Total Variation Distance between two probability distributions μ and η on a countable state space Ω is given by

$$\|\mu - \eta\|_{tv} = \frac{1}{2} \sum_{\omega \in \Omega} |\mu(\omega) - \eta(\omega)|.$$

Loaded Dice: let $D = Unif\{1,2,3,4,5,6\}$ be the law of a fair dice:

$$\|D - A\|_{tv} = \frac{1}{2}\left(2\left|\frac{1}{6} - \frac{1}{3}\right| + 4\left|\frac{1}{6} - \frac{1}{12}\right|\right) = \frac{1}{3}$$

$$\|D - B\|_{tv} = \frac{1}{2}\left(2\left|\frac{1}{6} - \frac{1}{4}\right| + 4\left|\frac{1}{6} - \frac{1}{8}\right|\right) = \frac{1}{6}$$

$$\|D - C\|_{tv} = \frac{1}{2}\left(3\left|\frac{1}{6} - \frac{1}{8}\right| + \left|\frac{1}{6} - \frac{9}{24}\right|\right) = \frac{1}{6}.$$

Thus

$$\|D - B\|_{tv} = \|D - C\|_{tv} \quad \text{and} \quad \|D - B\|_{tv}, \|D - C\|_{tv} < \|D - A\|_{tv}.$$

So A is the least "fair", however B and C are equally "fair" (in TV distance).

TV Distances and Markov Chains

Let P be a finite Markov Chain with stationary distribution π.

- Let μ be the initial distribution on Ω (might be just one vertex) and $t \geq 0$. Then
$$P_{\mu}^{t} := \mathbf{P}\left[X_t = \cdot \mid X_0 \sim \mu \right],$$
is a probability measure on Ω.
- *[Exercise 4/5.5]* For any μ,
$$\left\| P_{\mu}^{t} - \pi \right\|_{tv} \leq \max_{x \in \Omega} \left\| P_{x}^{t} - \pi \right\|_{tv}.$$

We will see a similar result later after introducing spectral techniques (Lecture 12)!

Convergence Theorem (Implication for TV Distance)

For any finite, irreducible, aperiodic Markov Chain,
$$\lim_{t \to \infty} \max_{x \in \Omega} \left\| P_{x}^{t} - \pi \right\|_{tv} = 0.$$

We have seen that $\lim_{t \to \infty} P^t(x, y) = \pi(y)$ (Slide 10)

Mixing Time of a Markov Chain

Convergence Theorem: "Nice" Markov Chains converge to stationarity.

Question: How fast do they converge?

Mixing Time

The mixing time $\tau_x(\epsilon)$ of a finite Markov Chain P with stationary distribution π is defined as

$$\tau_x(\epsilon) = \min \left\{ t \geq 0 \colon \left\| P_x^t - \pi \right\|_{tv} \leq \epsilon \right\},$$

and,

$$\tau(\epsilon) = \max_x \tau_x(\epsilon).$$

- This is how long we need to wait until we are "ϵ-close" to stationarity
- We often take $\epsilon = 1/4$, indeed let $t_{mix} := \tau(1/4)$

See final slides for some comments on why we choose $1/4$.

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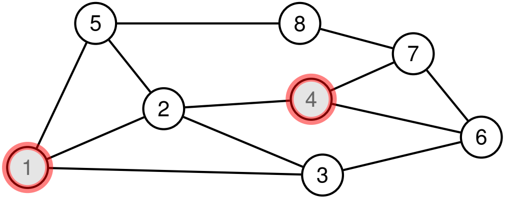
Appendix: Remarks on Mixing Time (non-examin.)

The Independent Set Problem



$S = \{1, 4\}$ is an independent set ✓

Independent Set

Given an undirected graph $G = (V, E)$, an independent set (IS) is a subset $S \subseteq V$ such that there are no two $u, v \in S$ with $\{u, v\} \in E(G)$.

- Finding a maximal independent set in G is NP-complete
- Counting the number of independent sets in G is "even harder", it is #P-complete
- Goal: find a randomised approximation algorithm for counting the number of independent sets

Counting the Number of Independent Sets

Approach 1 (Naive Monte Carlo):

- Pick a random subset $S \subseteq V$ with each vertex included w.p. $1/2$

$\Rightarrow$ works well if the number of IS is $\Omega(2^n)$ (or $\Omega(2^n/\operatorname{poly}(n))$)

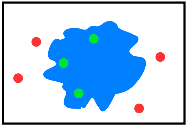
- But: number of IS may be $\ll 2^n$!

Approach 2 (Sampling IS):

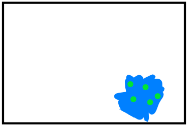
- Set up a Markov Chain with state space being all IS of G
- If we can generate a random IS, then we can also approximately count the number of IS in G

not obvious, see Chapter 10 in Mitzenmacher & Upfal

$\Omega = 2^V$



$\Omega = 2^V$

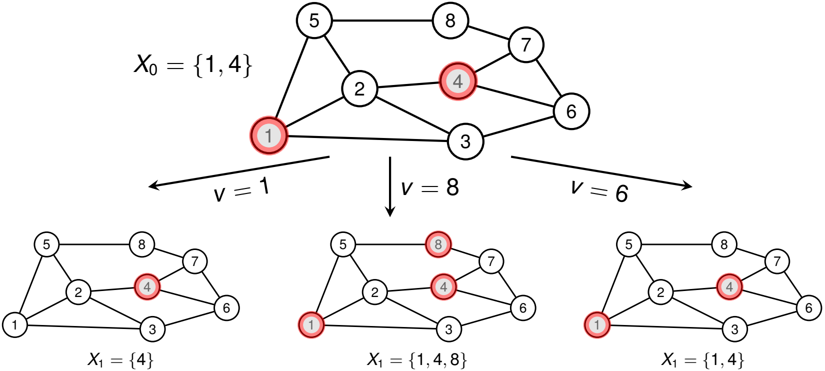


How can we set up a Markov Chain to sample from the set of all IS?

Markov Chain for Sampling Independent Sets

INDEPENDENTSETSAMPLER

```
Let X_0 be an arbitrary independent set in G
For t = 0, 1, 2, ...:
    Pick a vertex v ∈ V(G) uniformly at random
    If v ∈ X_t then X_{t+1} ← X_t \ {v}
    elif v ∉ X_t and X_t ∪ {v} is an independent set then X_{t+1} ← X_t ∪ {v}
    else X_{t+1} ← X_t
```



Markov Chain for Sampling Independent Sets

INDEPENDENTSETSAMPLER

Let X_0 be an arbitrary independent set in G
For $t = 0, 1, 2, \ldots$:
    Pick a vertex $v \in V(G)$ uniformly at random
    If $v \in X_t$ **then** $X_{t+1} \leftarrow X_t \setminus \{v\}$
    elif $v \notin X_t$ **and** $X_t \cup \{v\}$ is an independent set **then** $X_{t+1} \leftarrow X_t \cup \{v\}$
    else $X_{t+1} \leftarrow X_t$

Properties of the Markov Chain

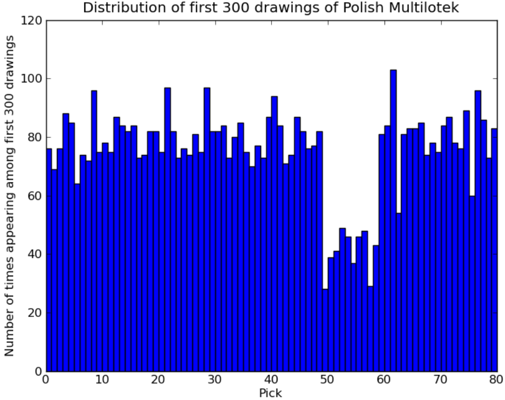
- This is a local definition (no explicit definition of P!)
- This chain is irreducible (every independent set is reachable)
- This chain is aperiodic (Check!)
- The stationary distribution is uniform, since $P_{u,v} = P_{v,u}$

Key Question: What is the mixing time of this Markov Chain?

This is a very deep question and goes beyond the scope of this course. Many positive and negative results are known here, and they often depend on the density of the graph G.

Outline

Experiment Gone Wrong...



Thanks to Krzysztof Onak (pointer) and Eric Price (graph)

Source: Slides by Ronitt Rubinfeld

What is Card Shuffling?

Source: wikipedia

Here we will focus on one shuffling scheme which is easy to analyse.

How long does it take to shuffle a deck of 52 cards?

How quickly do we converge to the uniform distribution over all $n!$ permutations?

One of the leading experts in the field who has related card shuffling to many other mathematical problems.

Persi Diaconis (Professor of Statistics and former Magician)

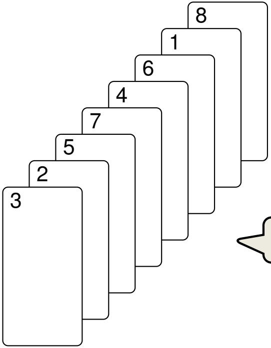
Source: `www.soundcloud.com`

The Card Shuffling Markov Chain

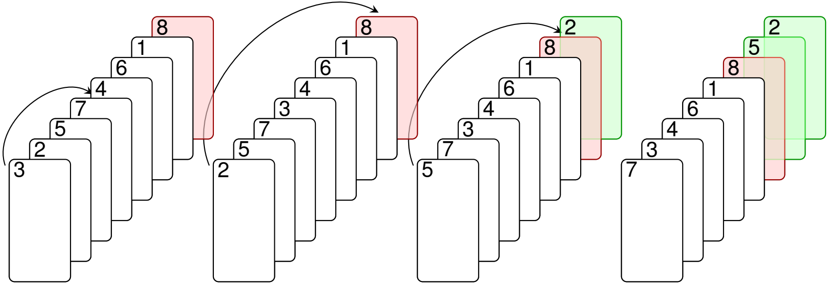
TOPTORANDOMSHUFFLE (Input: A pile of n cards)

For $t = 1, 2, \ldots$
    Pick $i \in \{1, 2, \ldots, n\}$ uniformly at random
    Take the top card and insert it behind the i-th card

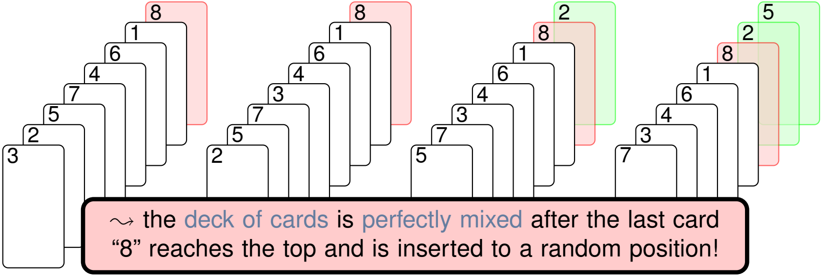
This is a slightly informal definition, so let us look at a small example...



We will focus on this "small" set of cards ($n = 8$)

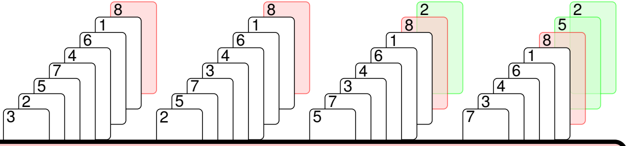


Even if we know which set of cards come after 8, every permutation is equally likely!



$\rightsquigarrow$ the deck of cards is perfectly mixed after the last card "8" reaches the top and is inserted to a random position!

Analysing the Mixing Time (Intuition)



$\rightsquigarrow$ deck of cards is perfectly mixed after the last card "8" reaches the top and is inserted to a random position!

- How long does it take for the last card "n" to become top card?
- At the last position, card "n" moves up with probability $\frac{1}{n}$ at each step
- At the second last position, card "n" moves up with probability $\frac{2}{n}$

$\vdots$

- At the second position, card "n" moves up with probability $\frac{n-1}{n}$
- One final step to randomise card "n" (with probability 1)

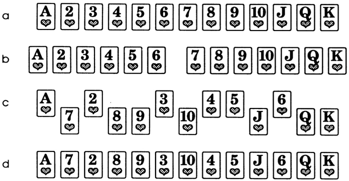
This is a **"reversed" coupon collector** process with n cards, which takes $n \log n$ in expectation.

Using the so-called coupling method, one could prove $t_{mix} \leq n \log n$.

Riffle Shuffle (non-examinable)

Riffle Shuffle

1. Split a deck of n cards into two piles (thus the size of each portion will be Binomial)
2. Riffle the cards together so that the card drops from the left (or right) pile with probability proportional to the number of remaining cards



The Annals of Applied Probability
1992, Vol. 2, No. 2, 294–313

TRAILING THE DOVETAIL SHUFFLE TO ITS LAIR

By Dave Bayer[1] and Persi Diaconis[2]

Columbia University and Harvard University

We analyze the most commonly used method for shuffling cards. The main result is a simple expression for the chance of any arrangement after any number of shuffles. This is used to give sharp bounds on the approach to randomness: $\frac{3}{2}\log_2 n + \theta$ shuffles are necessary and sufficient to mix up n cards.

Key ingredients are the analysis of a card trick and the determination of the idempotents of a natural commutative subalgebra in the symmetric group algebra.

t	1	2	3	4	5	6	7	8	9	10
$\lVert P^t - \pi \rVert_{tv}$	1.000	1.000	1.000	1.000	0.924	0.614	0.334	0.167	0.085	0.043

Figure: Total Variation Distance for t riffle shuffles of 52 cards.

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Further Remarks on the Mixing Time (non-examin.)

- One can prove $\max_x \left\|P_x^t - \pi\right\|_{tv}$ is non-increasing in t (this means if the chain is "ϵ-mixed" at step t, then this also holds in future steps) *[Mitzenmacher, Upfal, 12.3]*
- We chose $t_{mix} := \tau(1/4)$, but other choices of ϵ are perfectly fine too (e.g, $t_{mix} := \tau(1/e)$ is often used); in fact, any constant $\epsilon \in (0, 1/2)$ is possible.

Remark: This freedom on how to pick ϵ relies on the sub-multiplicative property of a (version) of the variation distance. First, let

$$d(t) := \max_x \left\|P_x^t - \pi\right\|_{tv}$$

be the variation distance after t steps when starting from the worst state. Further, define

$$\overline{d}(t) := \max_{\mu,\nu} \left\|P_\mu^t - P_\nu^t\right\|_{tv}.$$

These quantities are related by the following double inequality

$$d(t) \leq \overline{d}(t) \leq 2d(t).$$

This 2 is the reason why we ultimately need $\epsilon < 1/2$ in this derivation. On the other hand, see *[Exercise (4/5).8]* why $\epsilon < 1/2$ is also necessary.

Further, $\overline{d}(t)$ is sub-multiplicative, that is for any $s, t \geq 1$,

$$\overline{d}(s+t) \leq \overline{d}(s) \cdot \overline{d}(t).$$

Hence for any fixed $0 < \epsilon < \delta < 1/2$ it follows from the above that

$$\tau(\epsilon) \leq \left\lceil \frac{\ln \epsilon}{\ln(2\delta)} \right\rceil \tau(\delta).$$

In particular, for any $\epsilon < 1/4$

$$\tau(\epsilon) \leq \left\lceil \log_2 \epsilon^{-1} \right\rceil \tau(1/4).$$

Hence smaller constants $\epsilon < 1/4$ only increase the mixing time by some constant factor.