Randomised Algorithms

Lecture 4: Markov Chains and Mixing Times

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Lent 2022

UNIVERSITY OF CAMBRIDGE

Outline

Applications of Markov Chains in Computer Science

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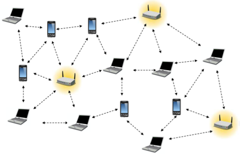
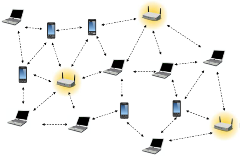


Broadcasting

Applications of Markov Chains in Computer Science



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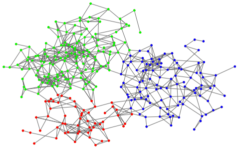
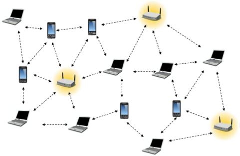


Clustering

Applications of Markov Chains in Computer Science



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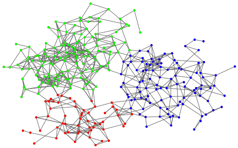

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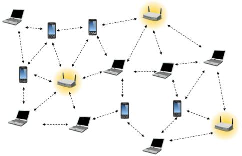

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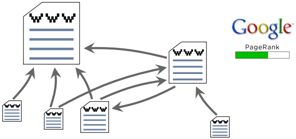

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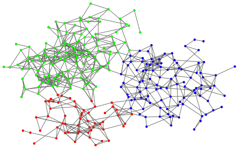

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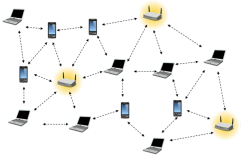

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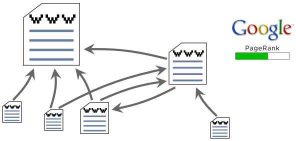

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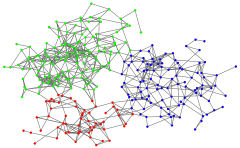

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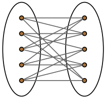
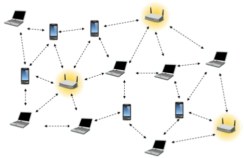


Sampling and Optimisation

Applications of Markov Chains in Computer Science



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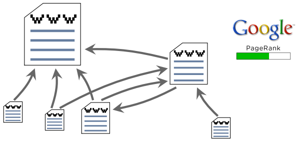

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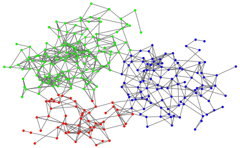

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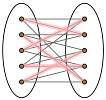

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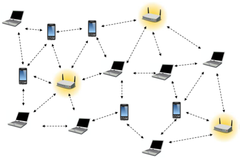

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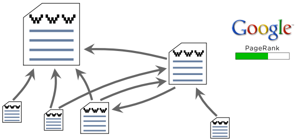

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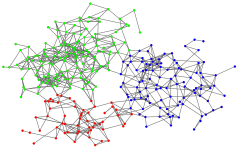

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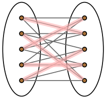

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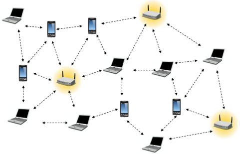

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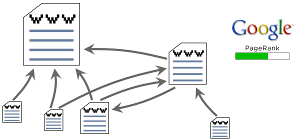

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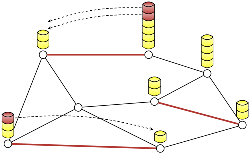
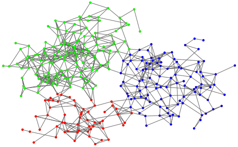


Load Balancing



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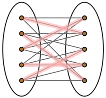

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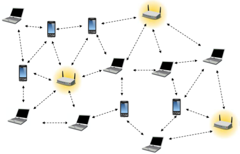

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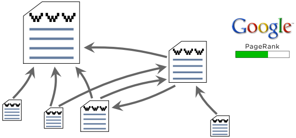

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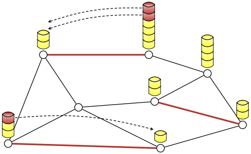

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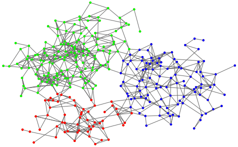

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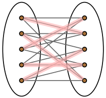

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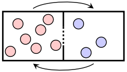

Particle Processes

Markov Chains

Markov Chain (Discrete Time and State, Time Homogeneous)

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From the definition one can deduce that (check!)

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

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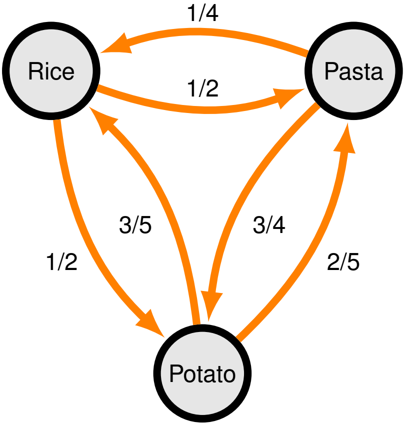
- For all $0 \leq t_1 < t_2, x \in \Omega$,

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

What does a Markov Chain Look Like?

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



This has transition matrix:

$$
\begin{array}{cc}
 & \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}
\end{array}
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$\Rightarrow$ can replace ρ by any (load) vector and view P as a balancing matrix!

Stopping and Hitting Times

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Example - College Carbs Stopping times:

✓ "We had rice yesterday"

Stopping and Hitting Times

A non-negative integer random variable τ is a stopping time for $(X_t)_{t \geq 0}$ if for every $s \geq 0$ the event $\{\tau = s\}$ depends only on $X_0, \ldots, X_s$.

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Some distinguish between $\tau_y^+ = \min\{t \geq 1 \colon X_t = y\}$ and $\tau_y = \min\{t \geq 0 \colon X_t = y\}$

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A Useful Identity

Hitting times are the solution to a set of linear equations:

$$h(x,y) \overset{\text{Markov Prop.}}{=} 1 + \sum_{z \in \Omega \setminus \{y\}} P(x,z) \cdot h(z,y) \qquad \forall x \neq y \in \Omega.$$

Outline

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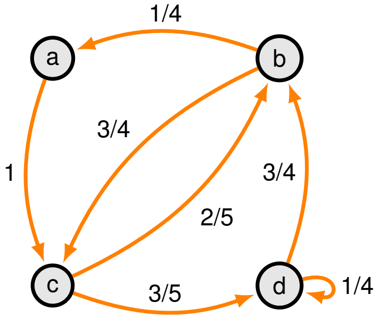

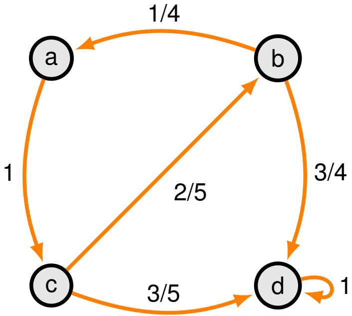

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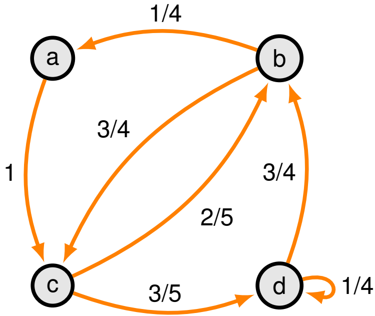

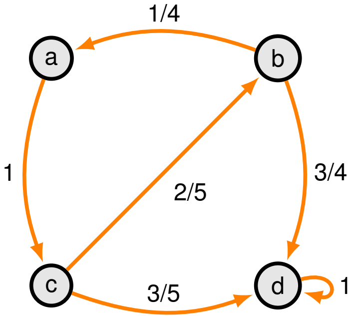

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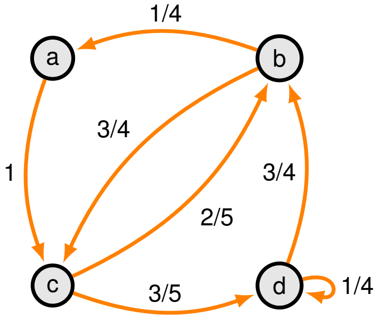

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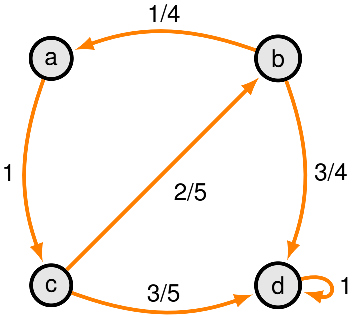

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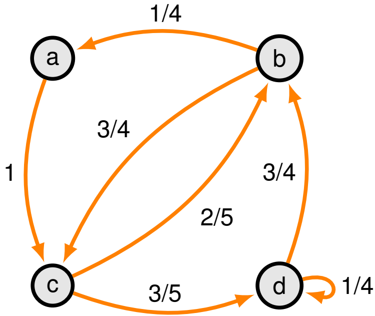

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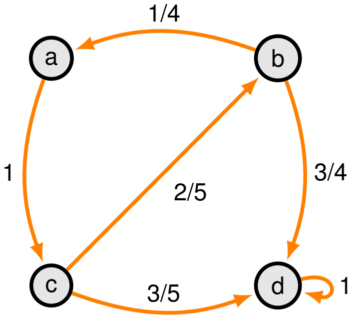

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Finite Hitting Time Theorem

For any states x and y of a finite irreducible Markov Chain $h(x, y) < \infty$.

Stationary Distribution

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

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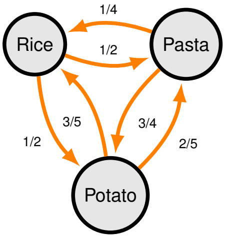

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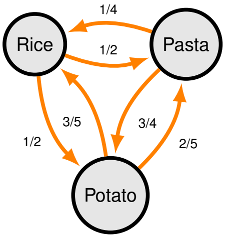

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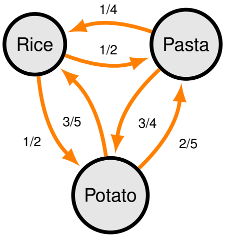

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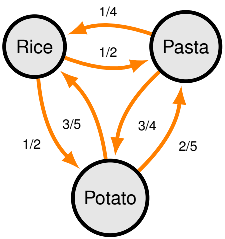

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Existence and Uniqueness of a Positive Stationary Distribution

Let P be finite, irreducible M.C., then there exists a unique probability distribution π on Ω such that $\pi = \pi P$ and $\pi(x) = 1/h(x,x) > 0$, $\forall x \in \Omega$.

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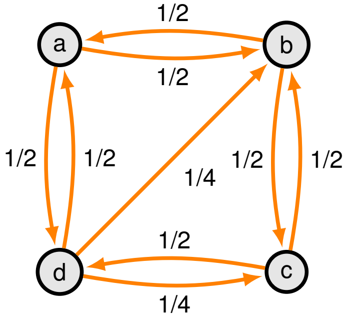

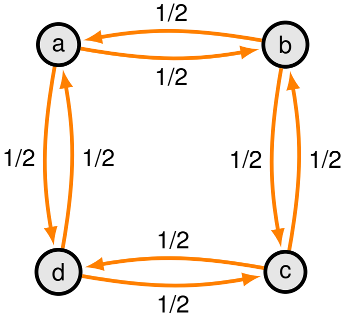

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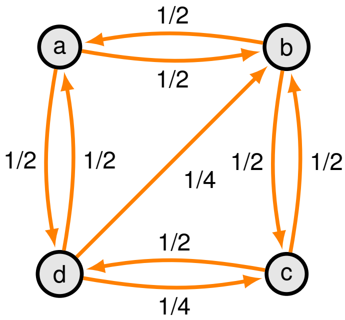

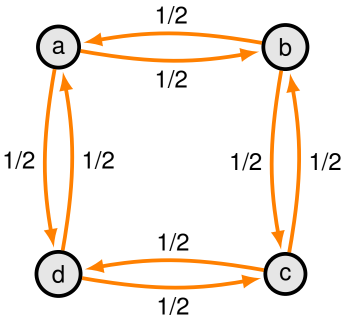

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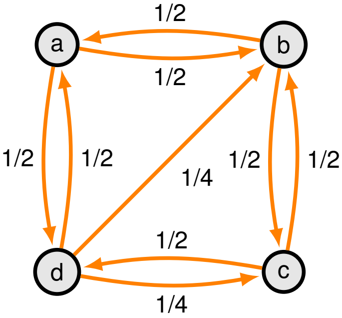

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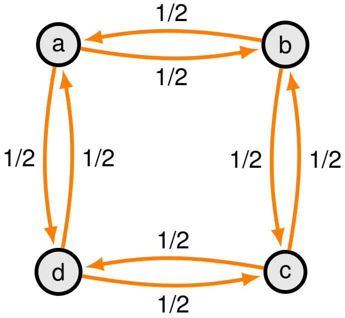

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- We will prove a simpler version of the Convergence Theorem after introducing Spectral Graph Theory.

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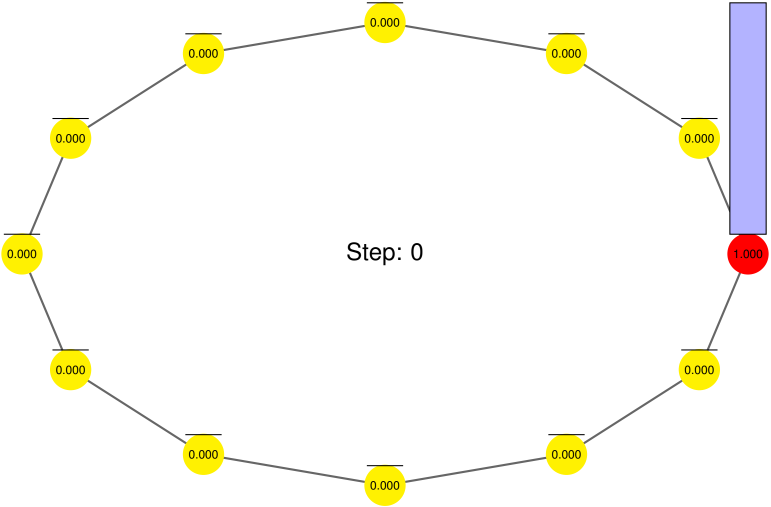

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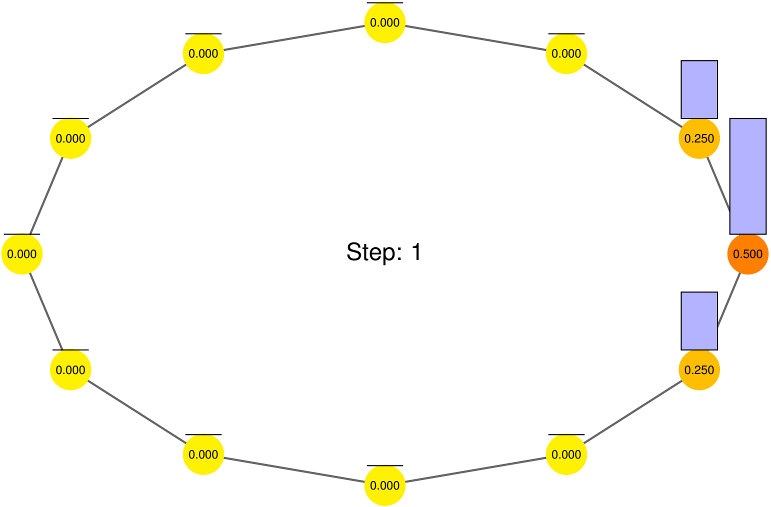

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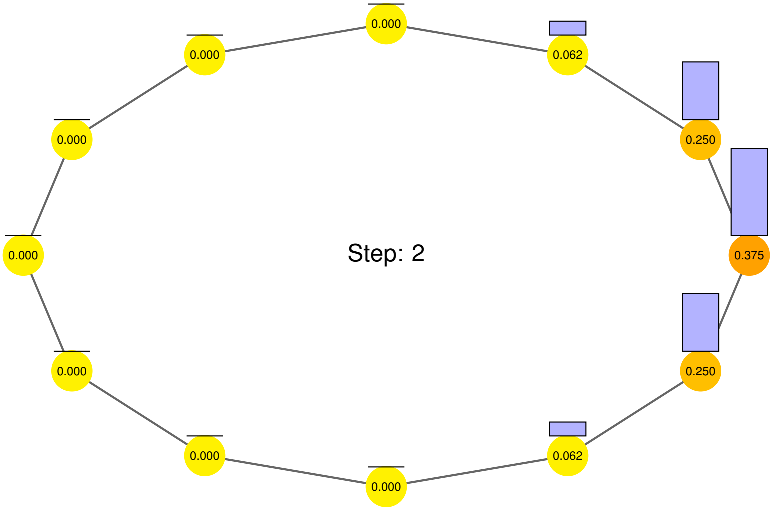

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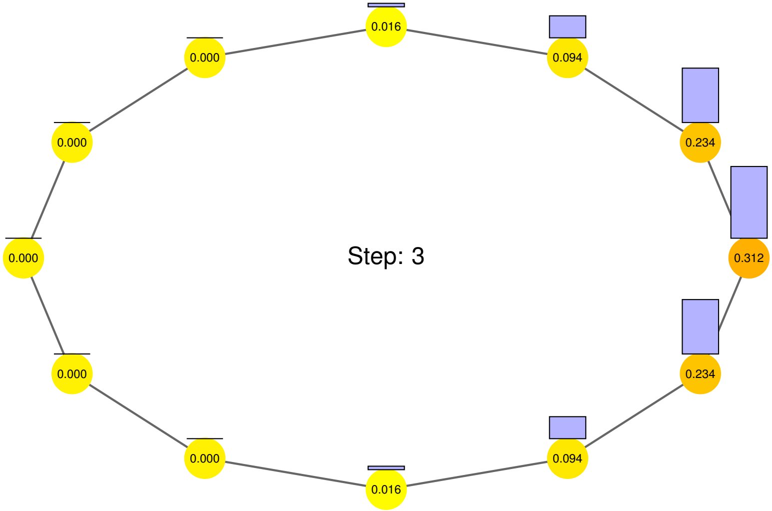

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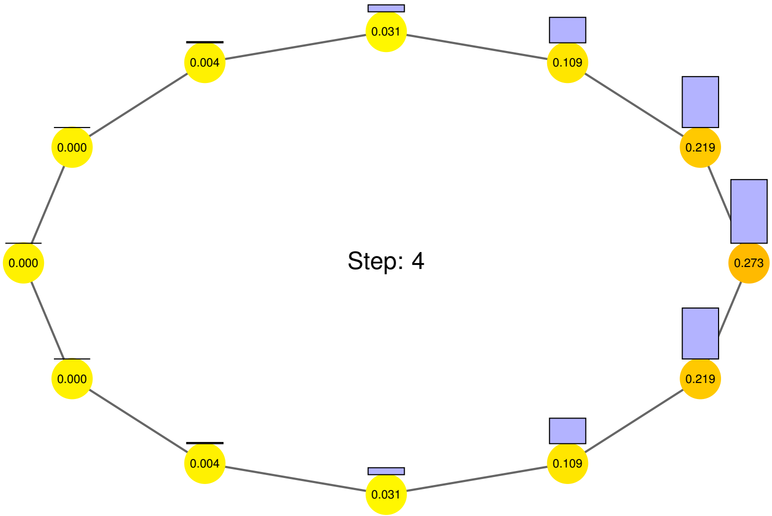

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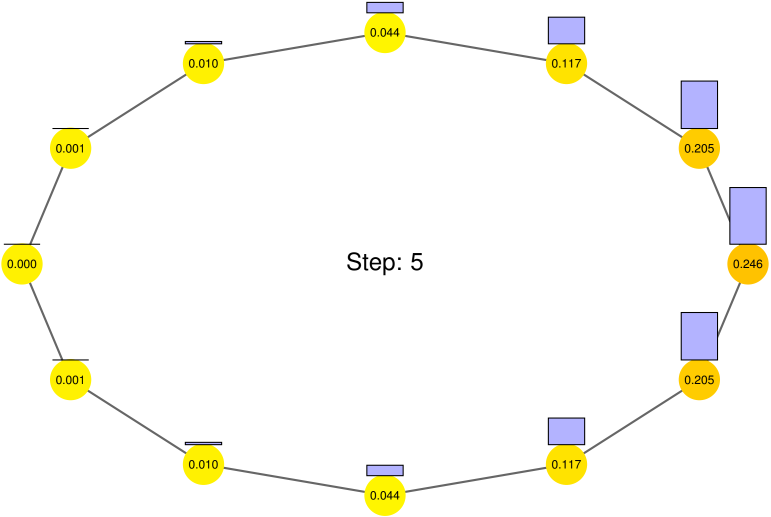

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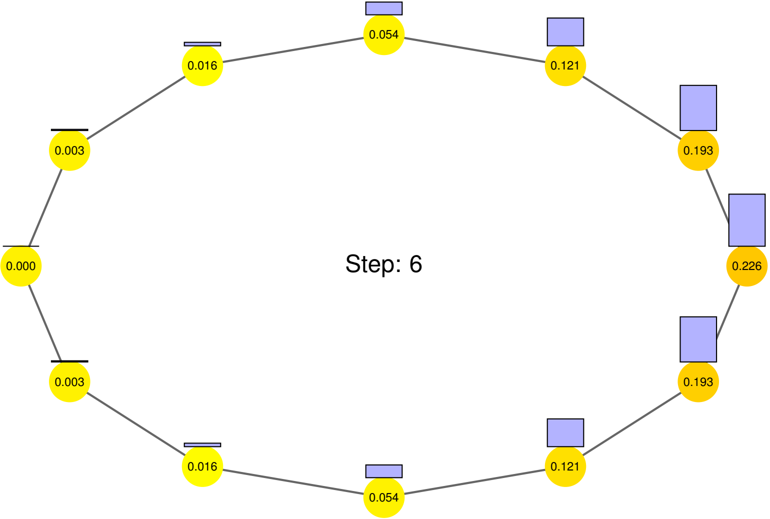

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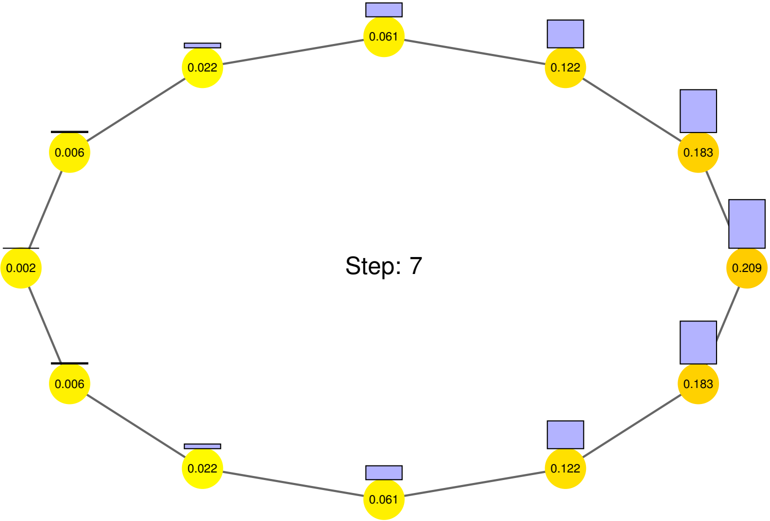

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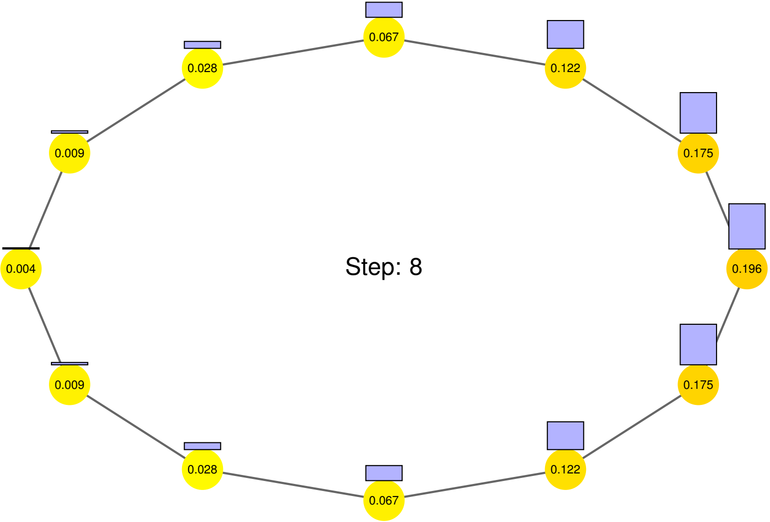

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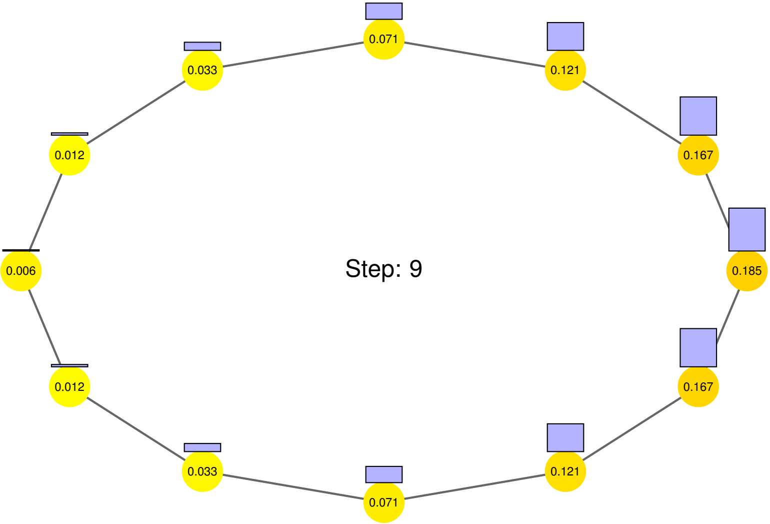

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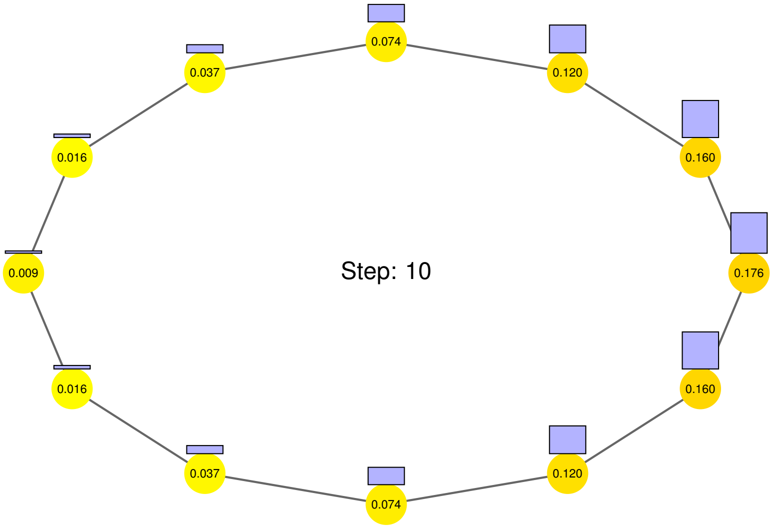

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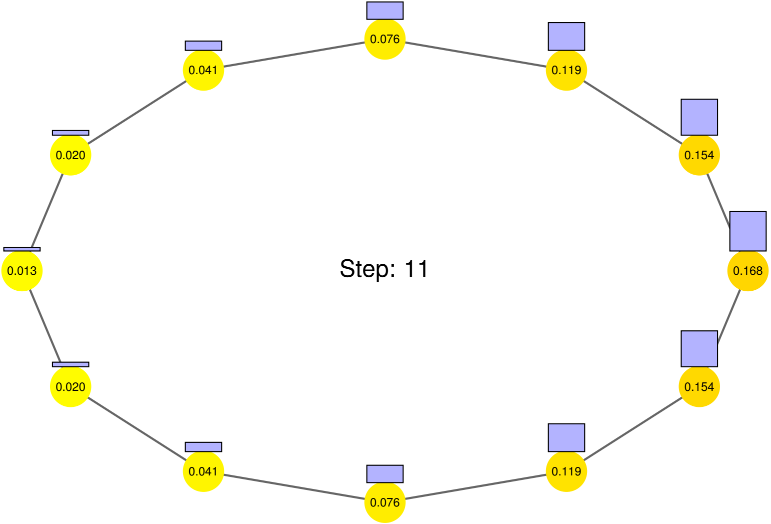

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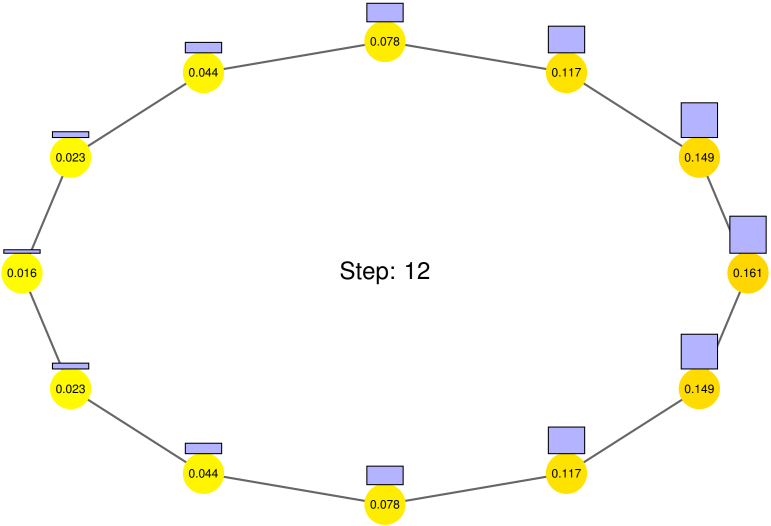

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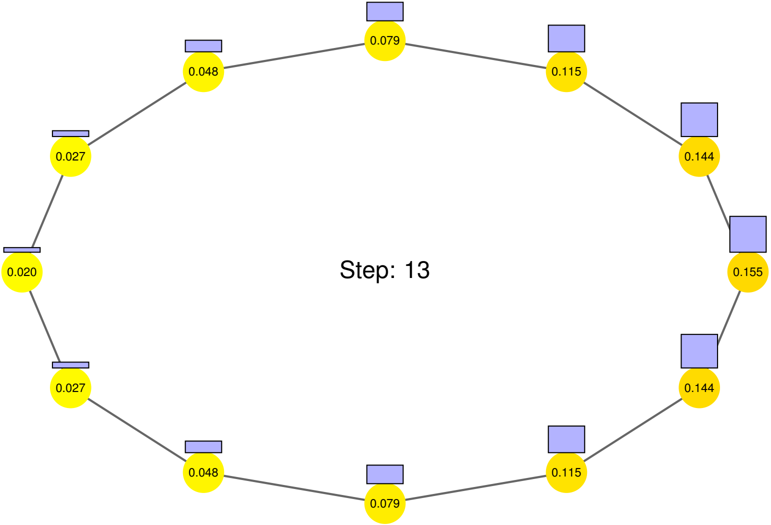

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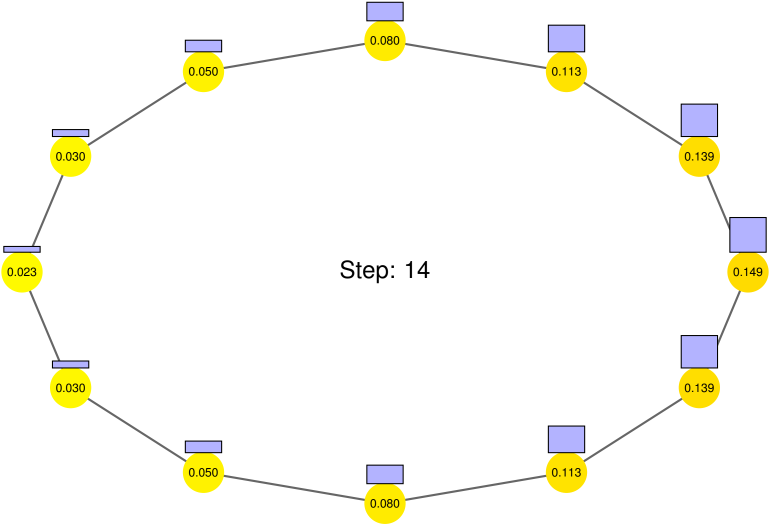

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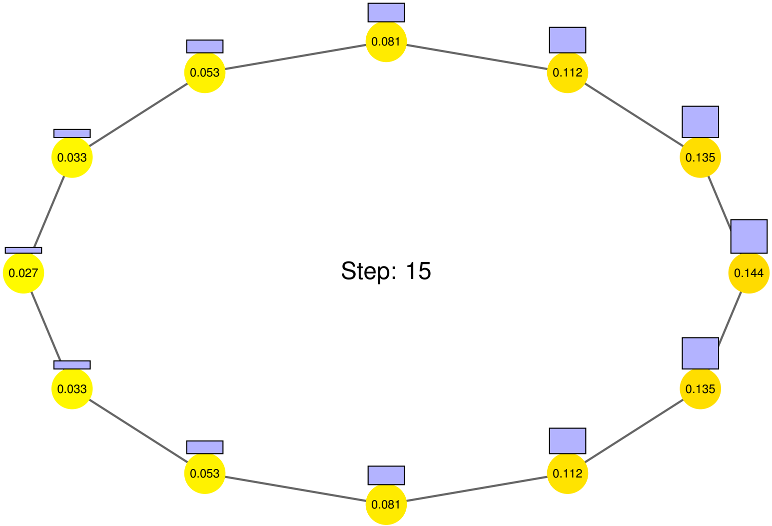

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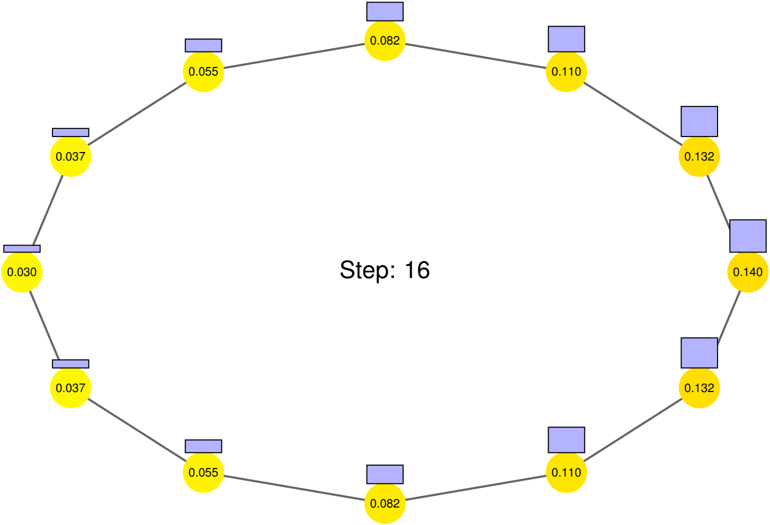

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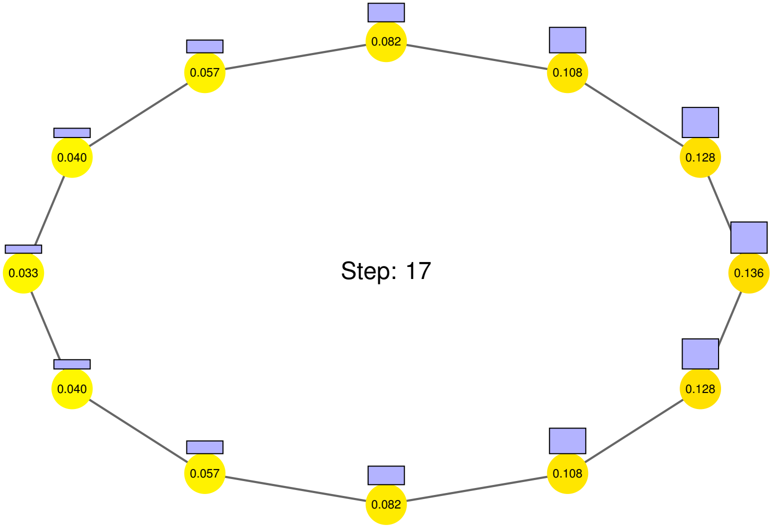

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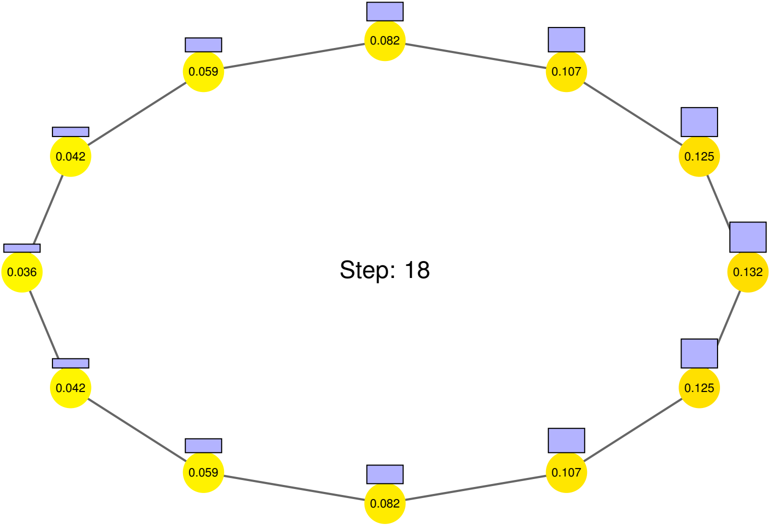

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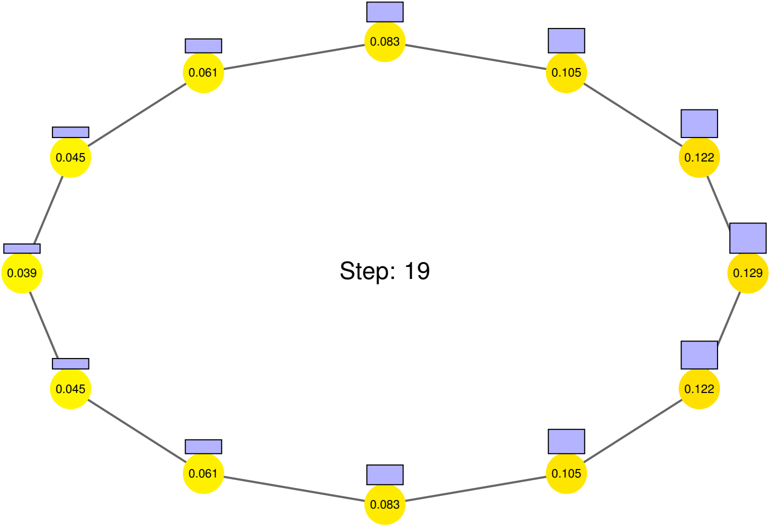

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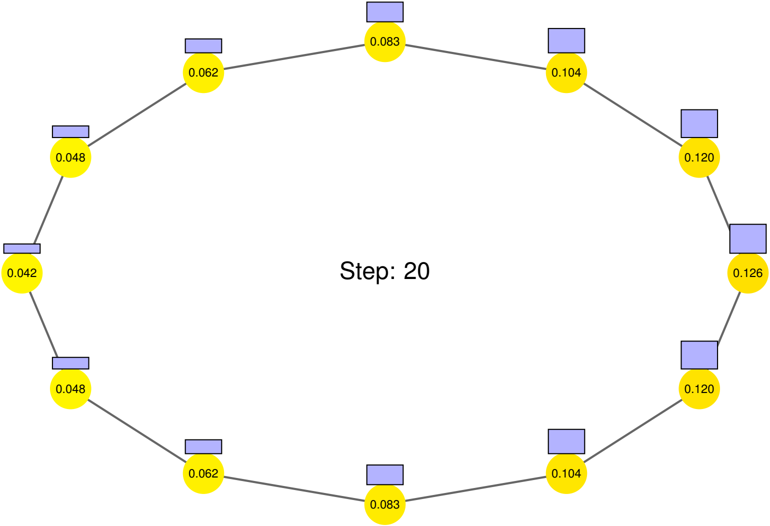

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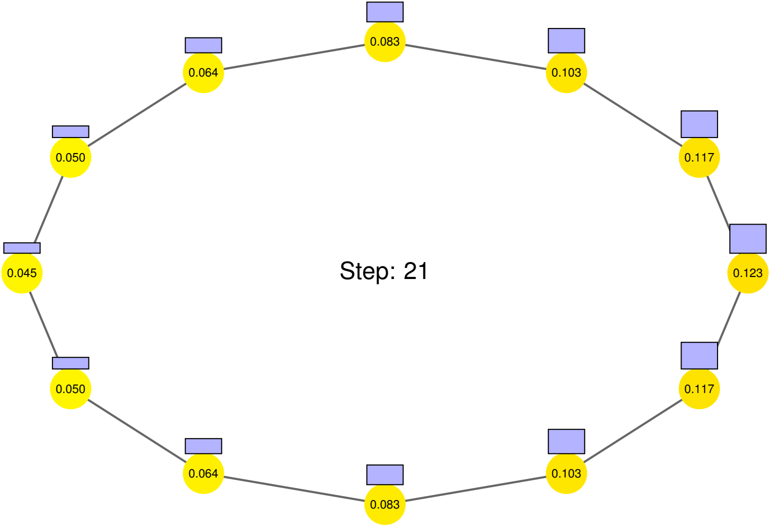

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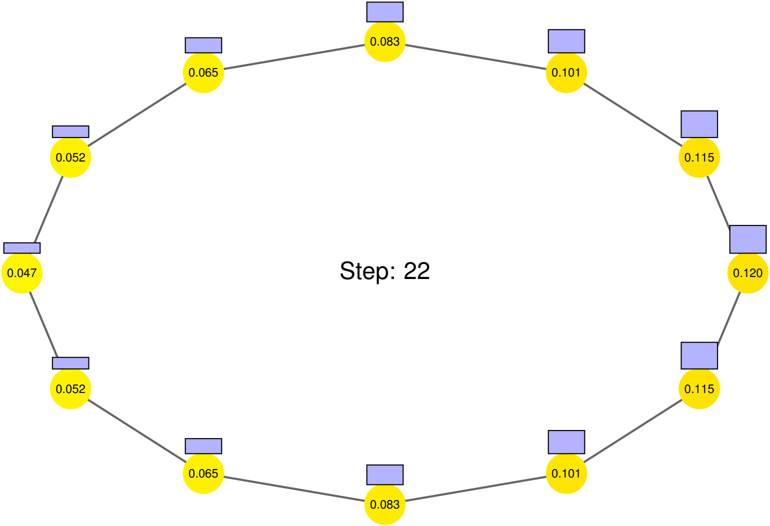

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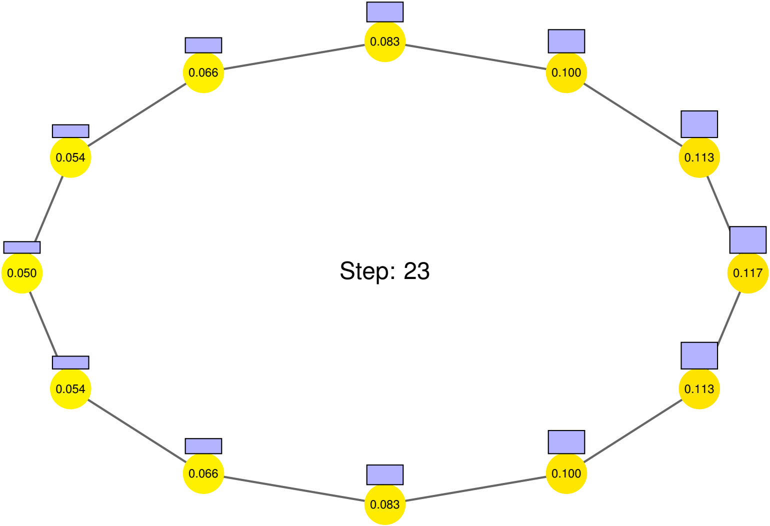

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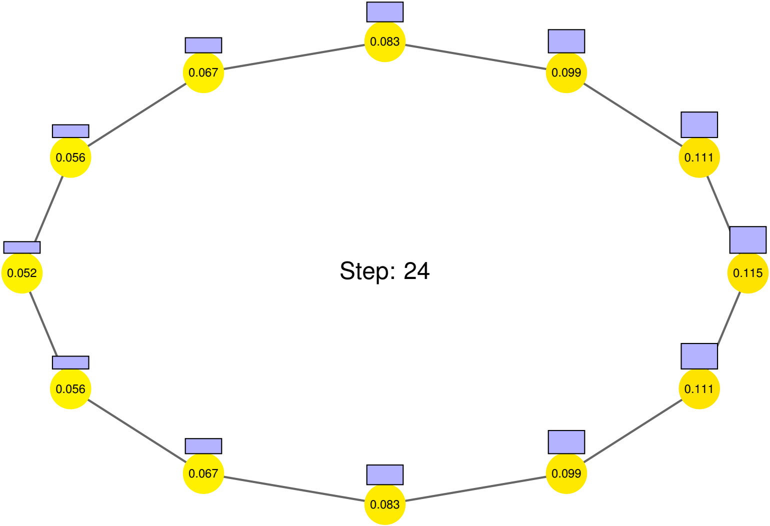

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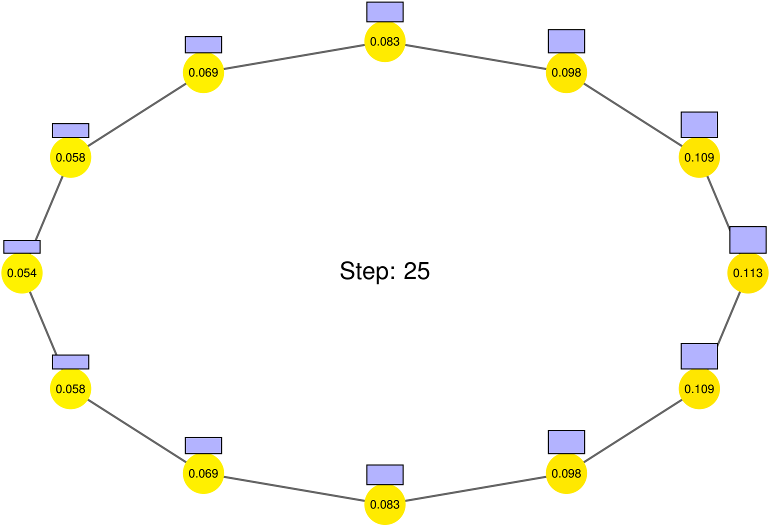

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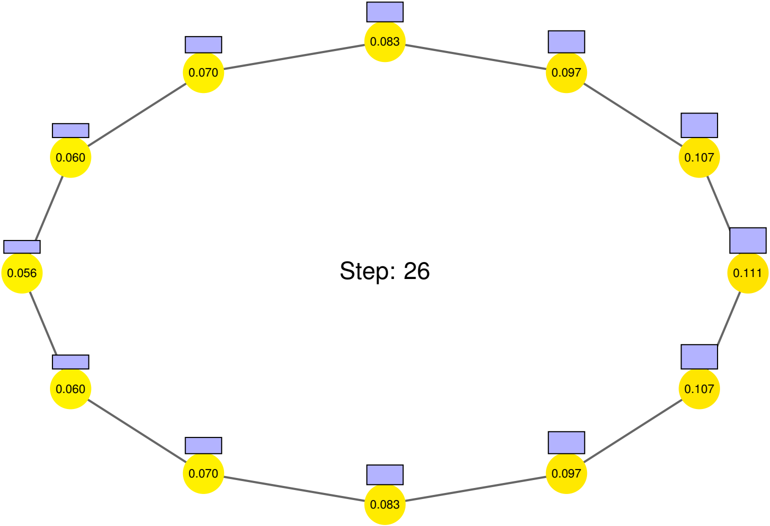

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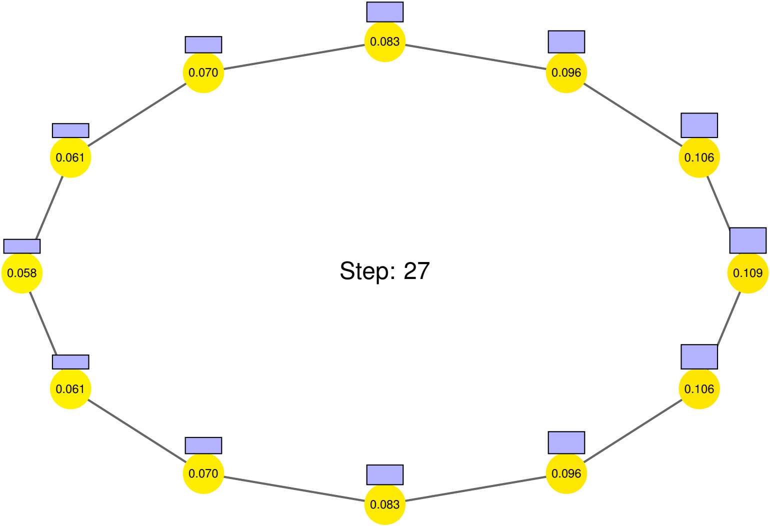

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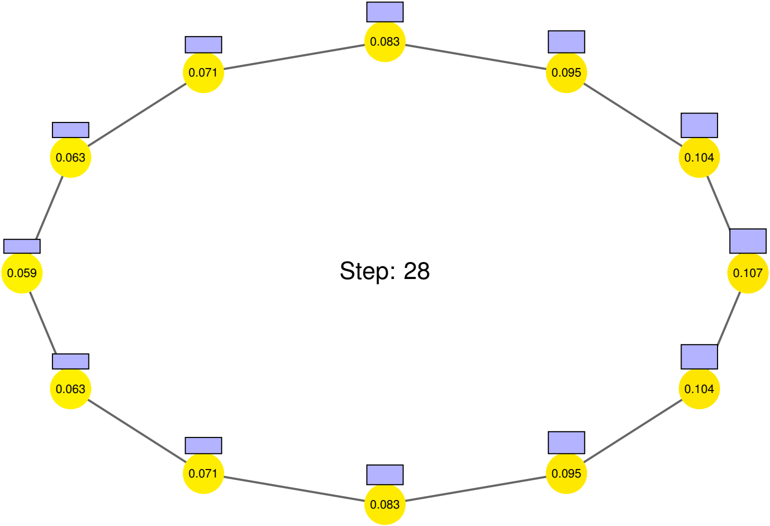

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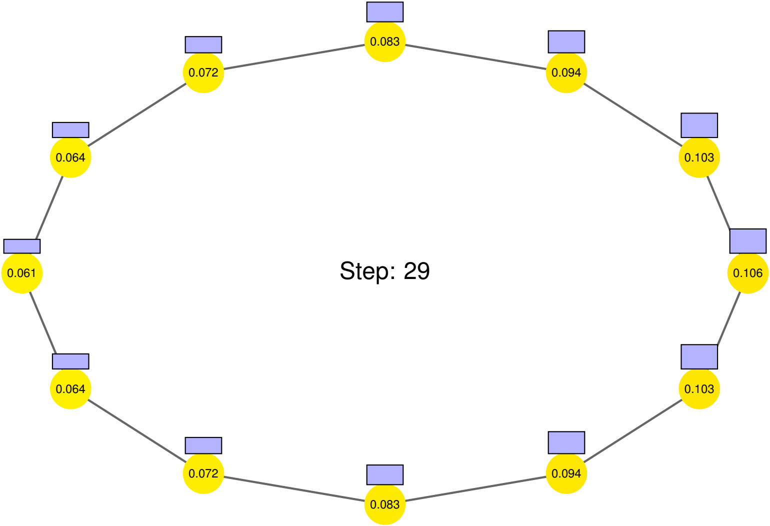

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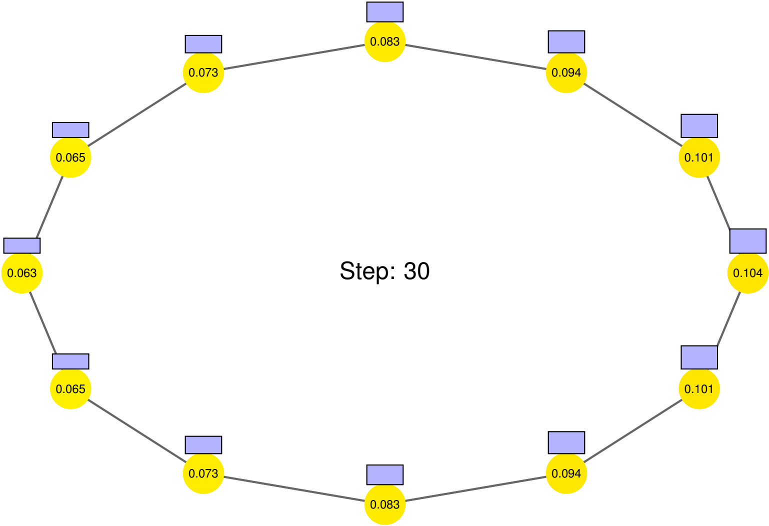

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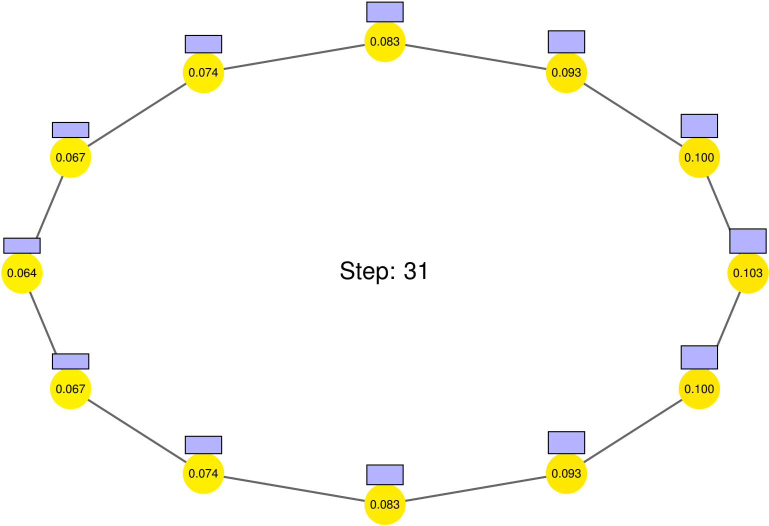

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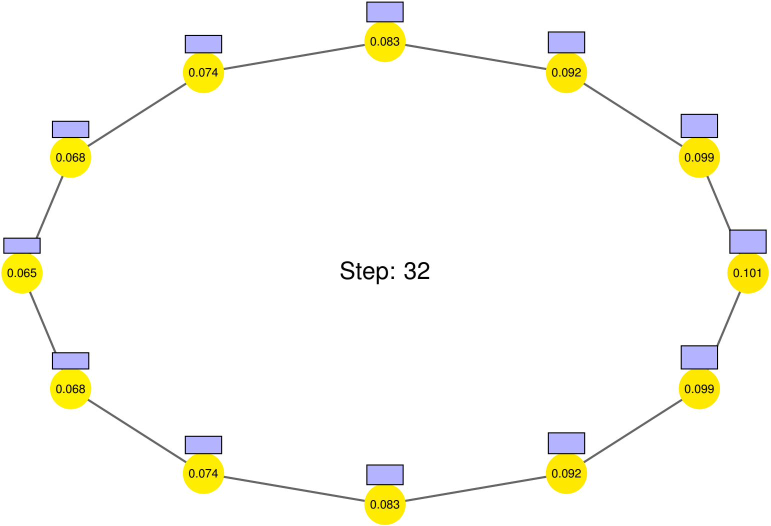

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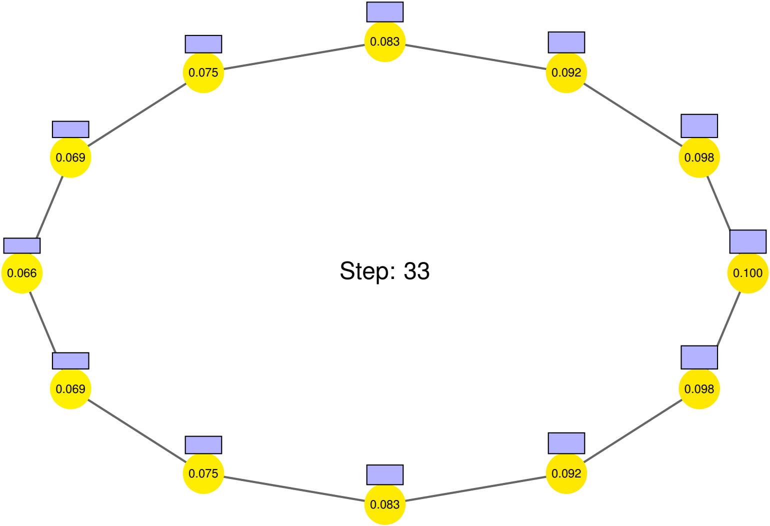

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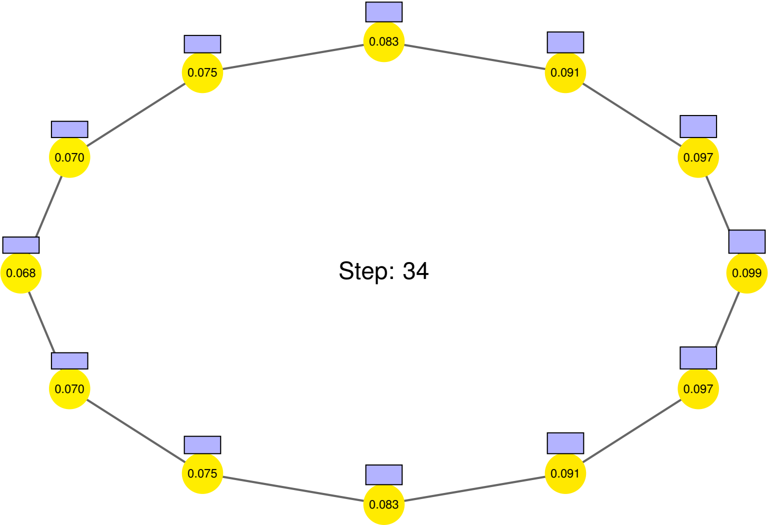

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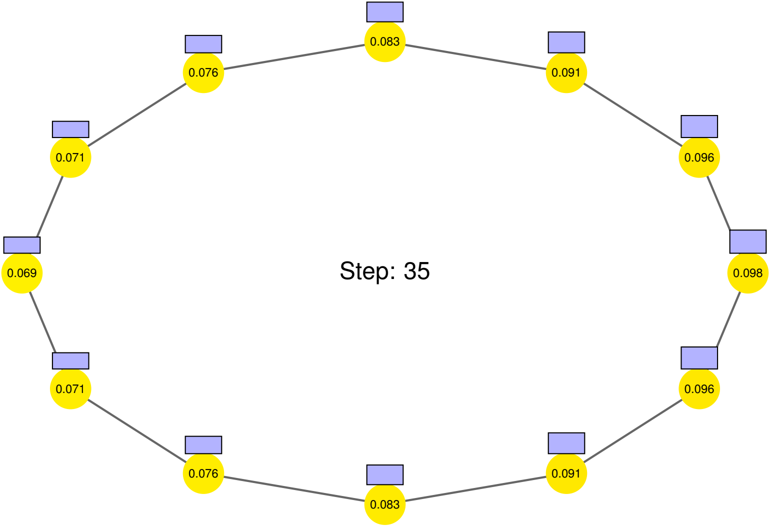

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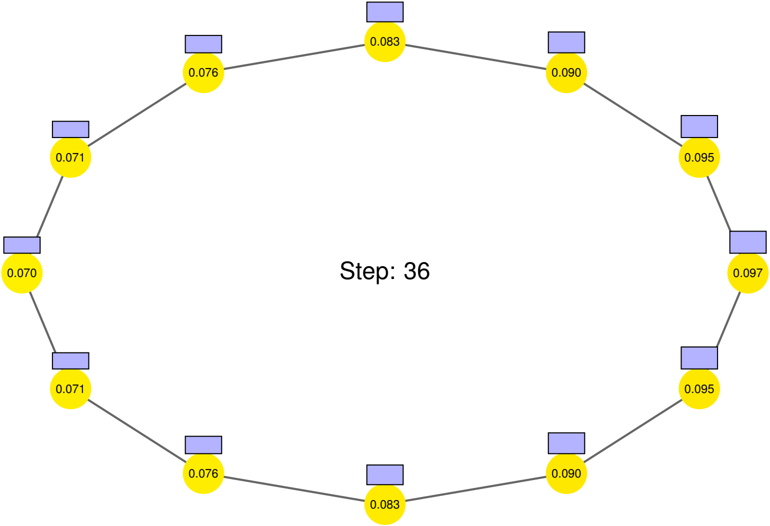

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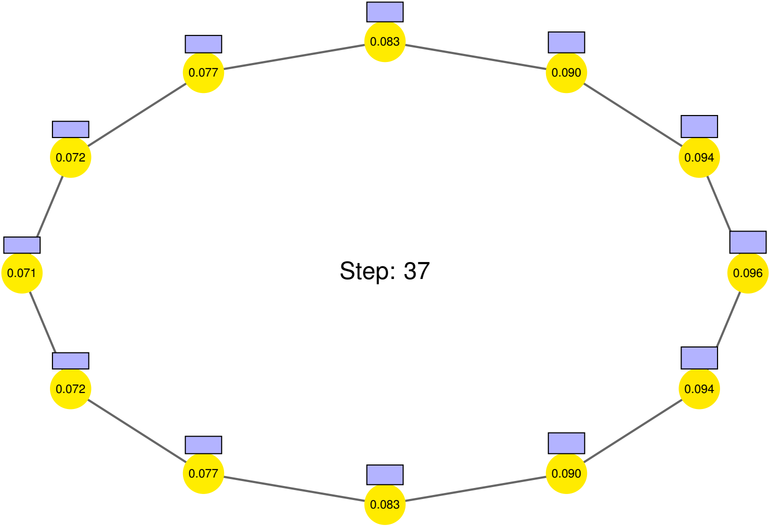

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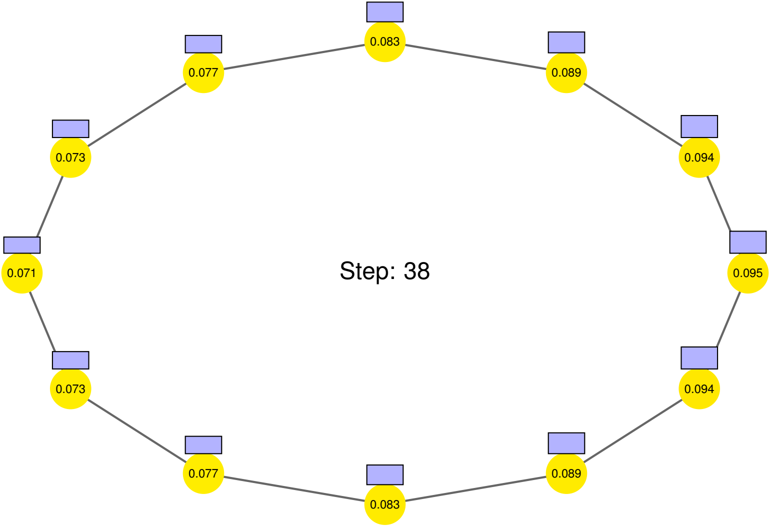

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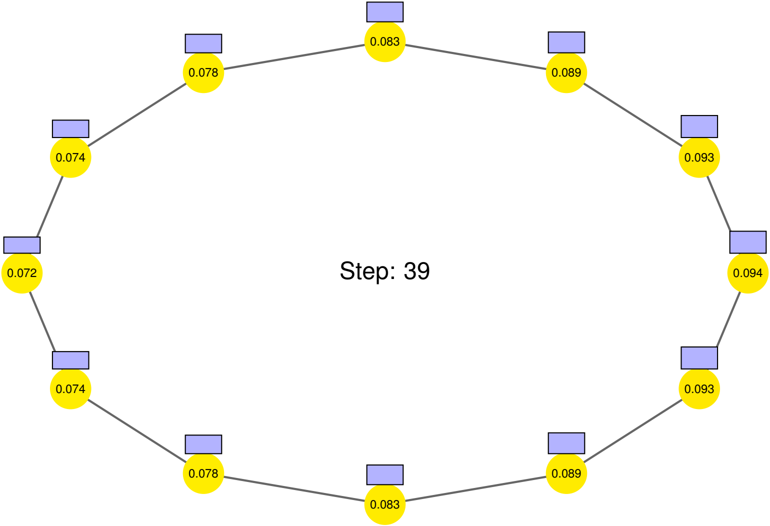

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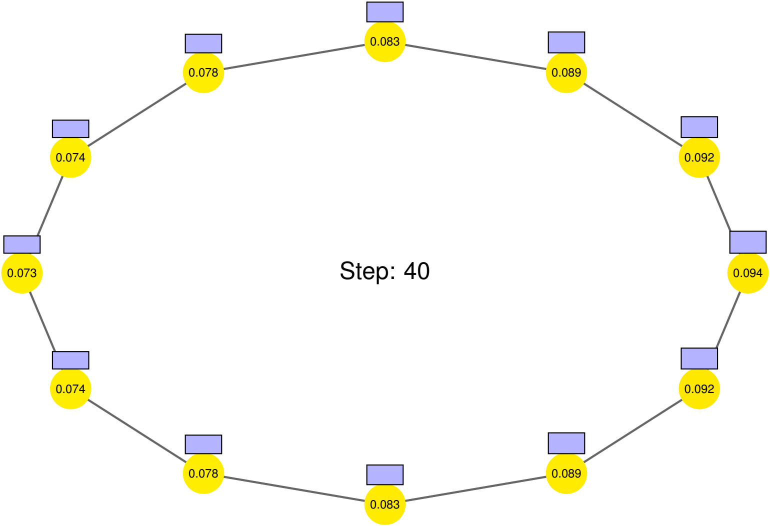

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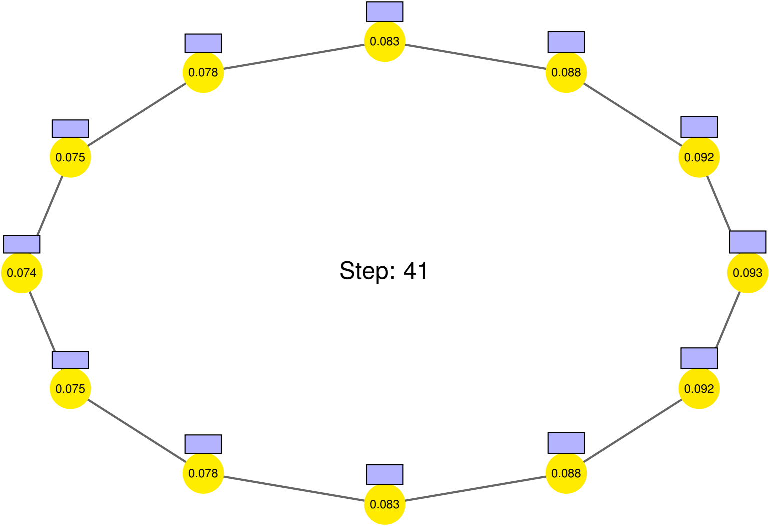

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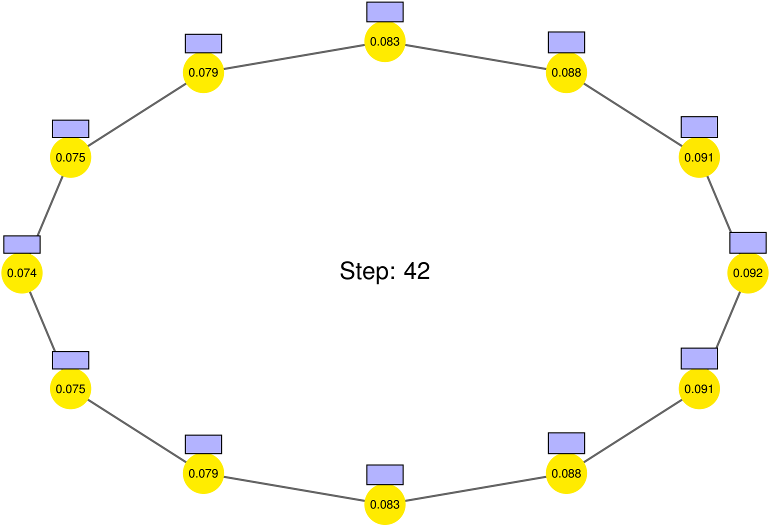

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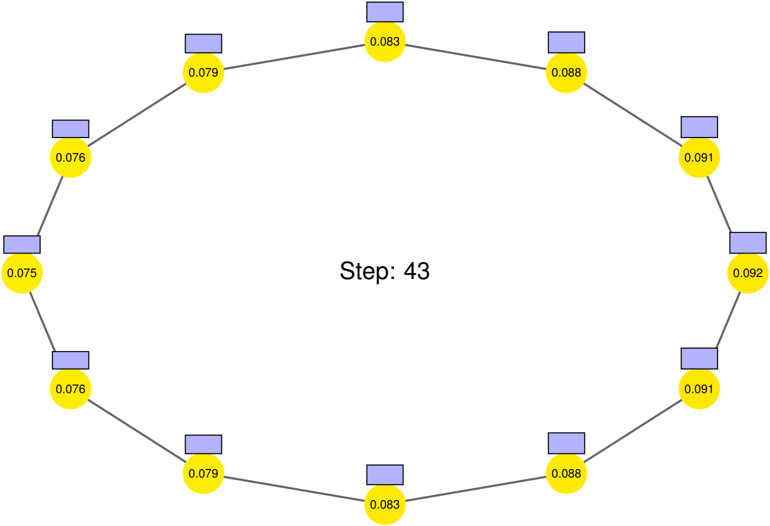

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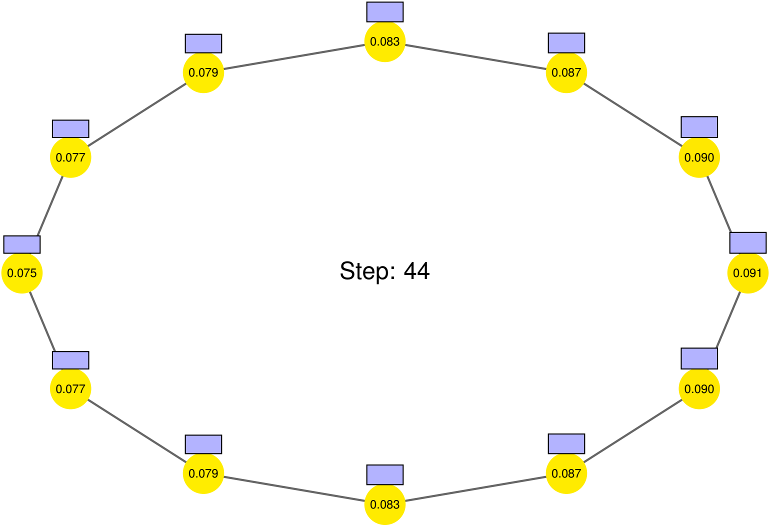

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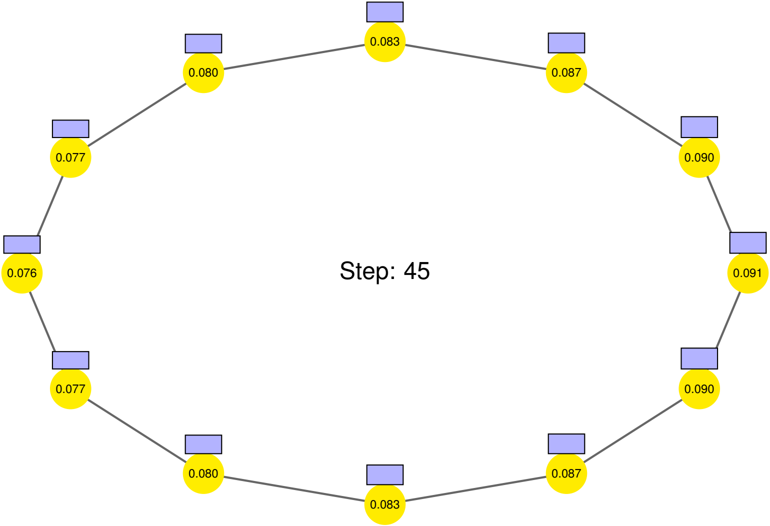

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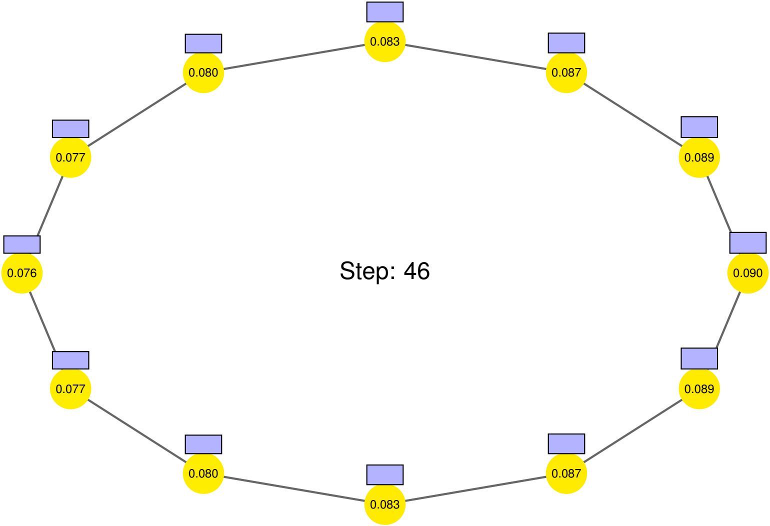

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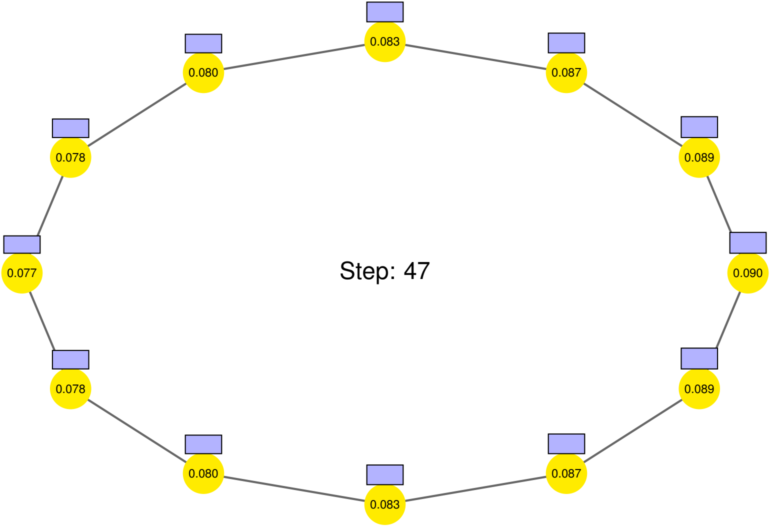

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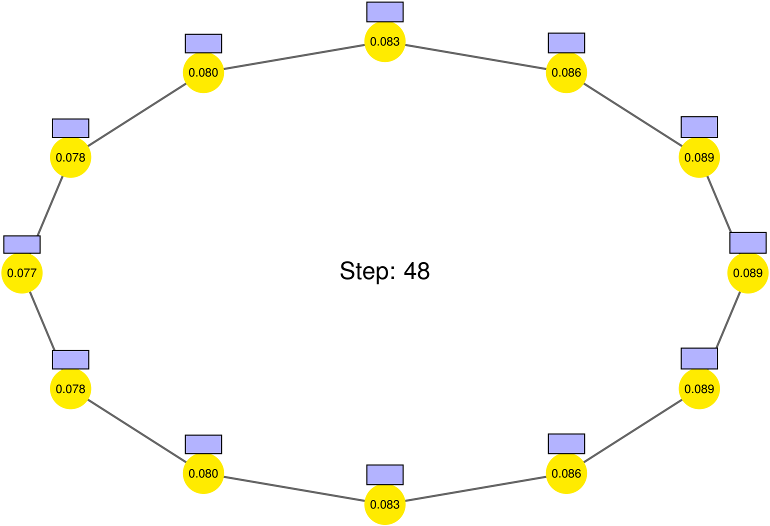

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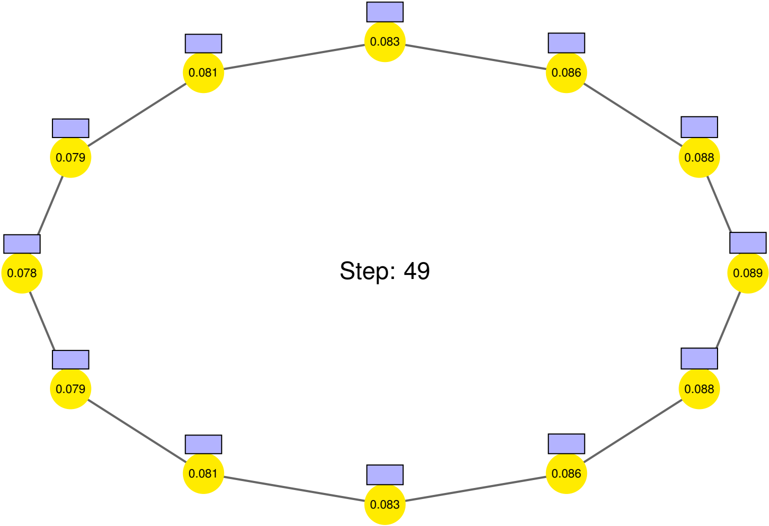

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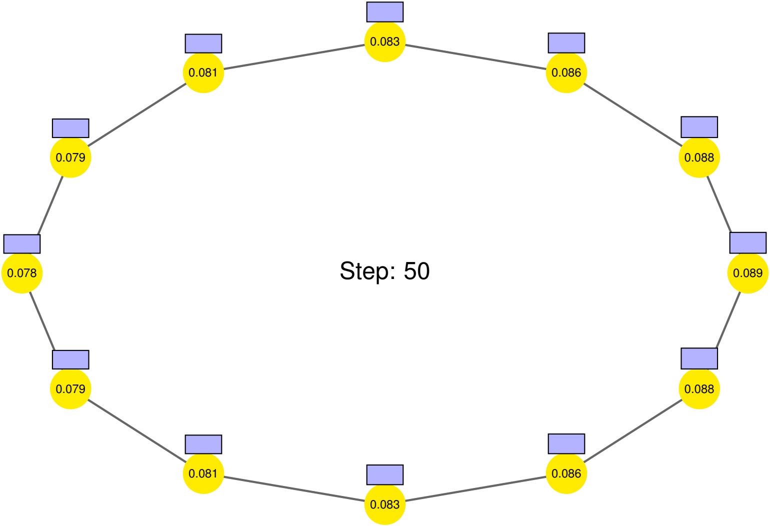

Outline

Recap of Markov Chain Basics

Irreducibility, Periodicity and Convergence

Total Variation Distance and Mixing Times

Application 1: Card Shuffling

Application 2: Ehrenfest Chain and Hypercubes

Application 3: Markov Chain Monte Carlo

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
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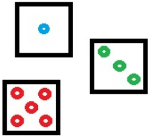

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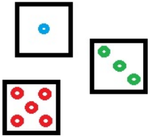

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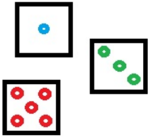

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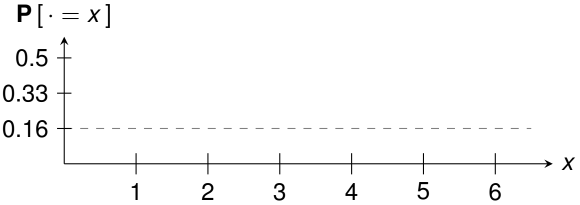

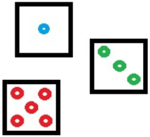

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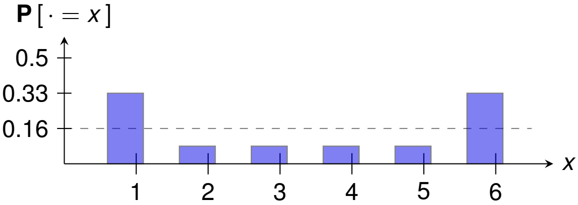

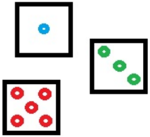

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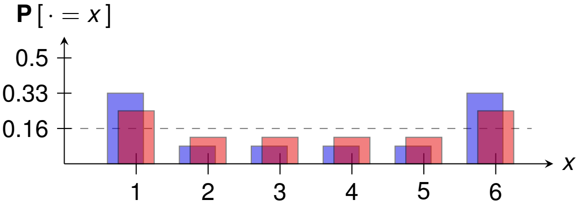

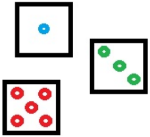

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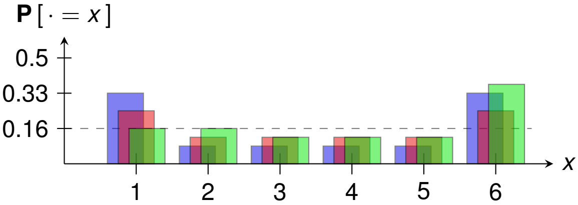

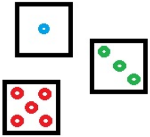

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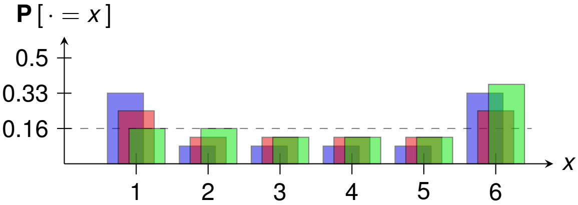

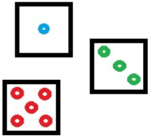

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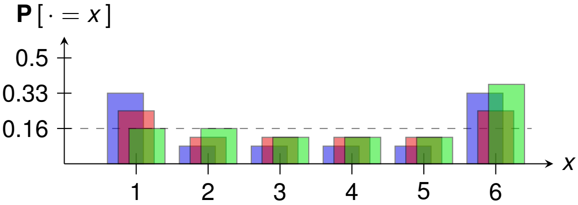

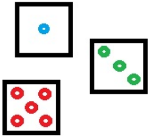

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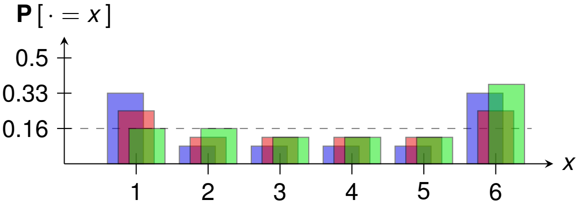

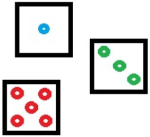

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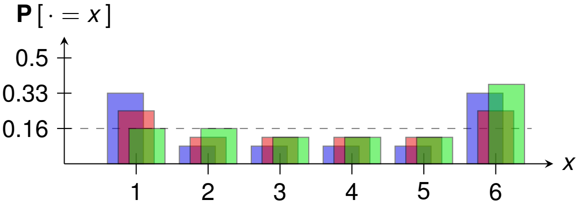
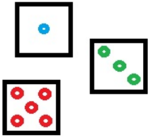
We need a formal "fairness measure" to compare probability distributions!





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Thus

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

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

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We will prove a similar result later after introducing spectral techniques!

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- We often take $\varepsilon = 1/4$, indeed let $t_{mix} := \tau(1/4)$

Outline

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Source: wikipedia

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The Card Shuffling Markov Chain

TopToRandomShuffle (Input: A pile of n cards)

1: **For** $t = 1, 2, \ldots$

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

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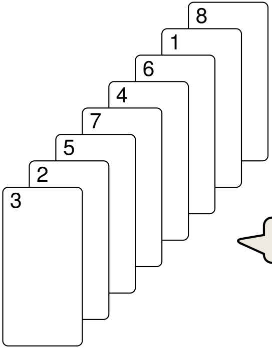
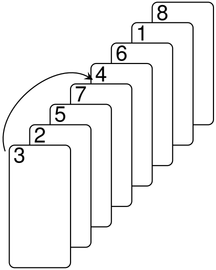


We will focus on this "small" set of cards ($n = 8$)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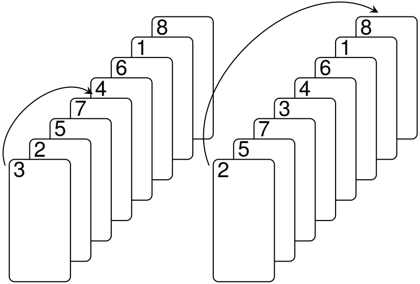
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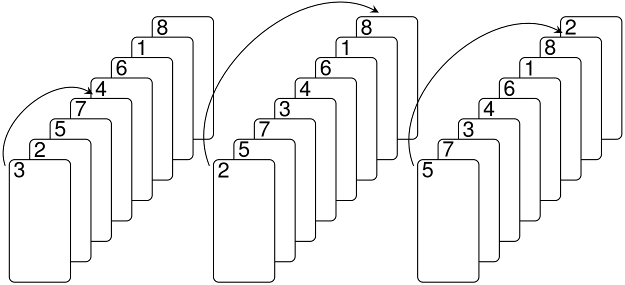
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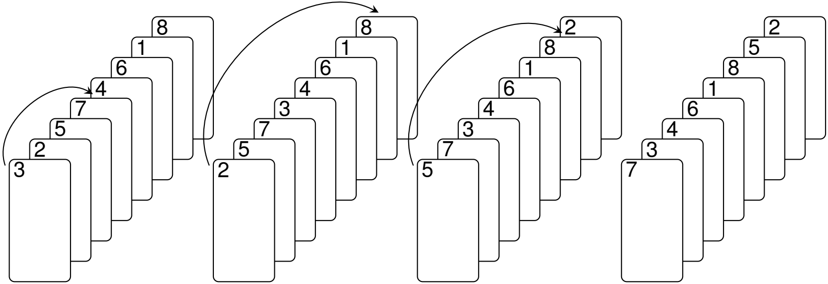
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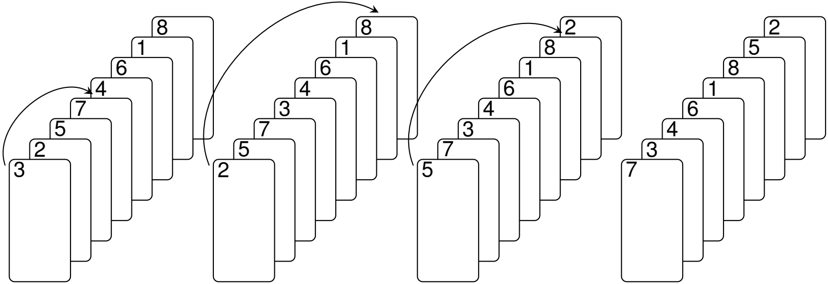

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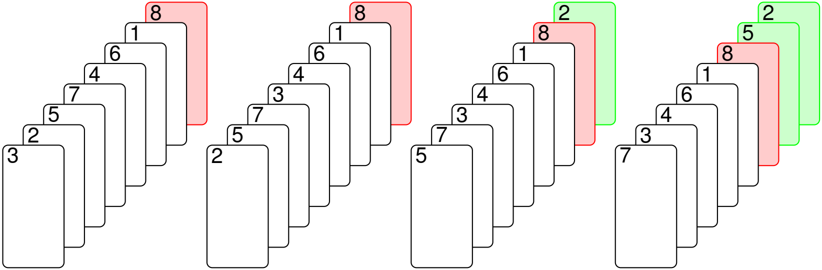

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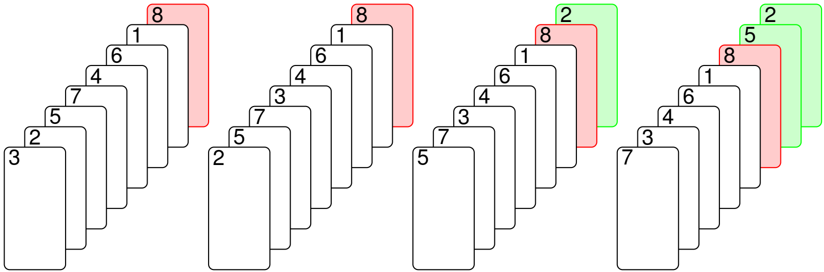

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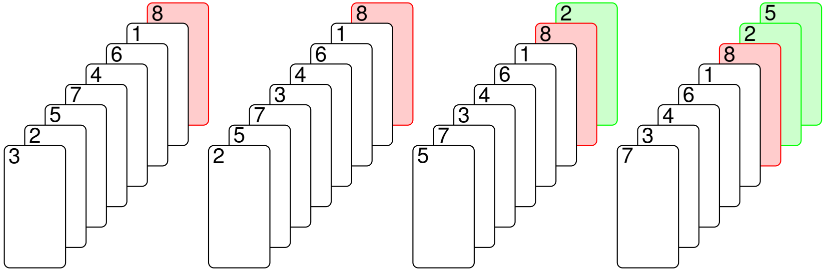

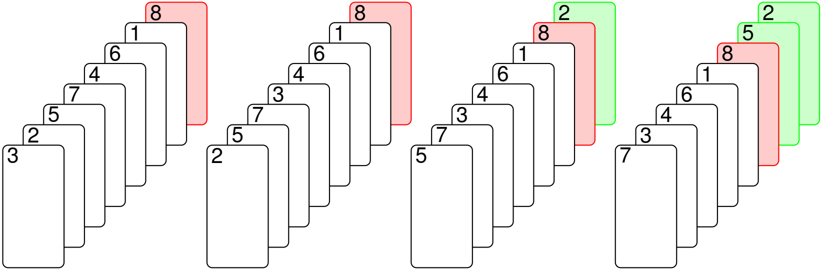

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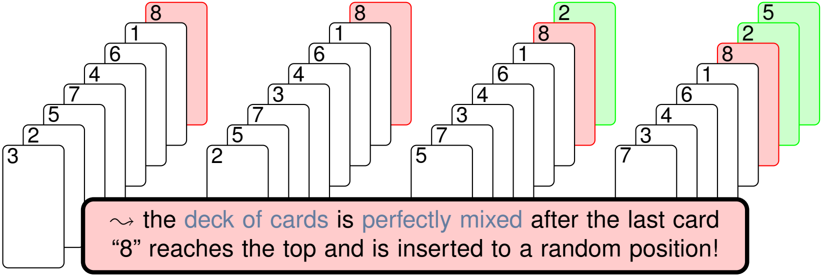
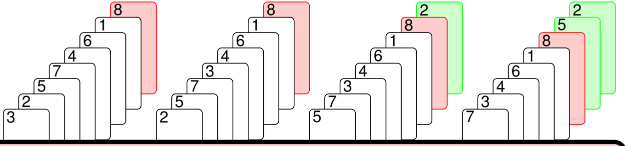


$\rightsquigarrow$ the deck of cards is perfectly mixed after the last card "8" reaches the top and is inserted to a random position!

Analysing the Mixing Time (Intuition)



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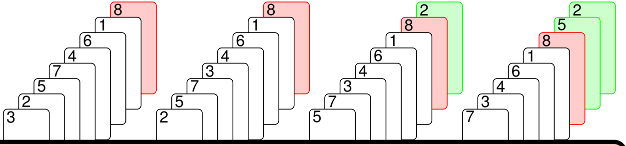

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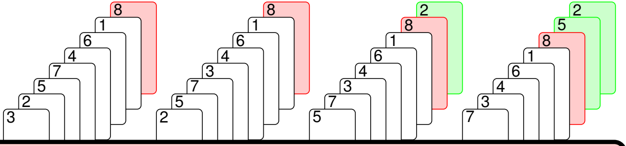

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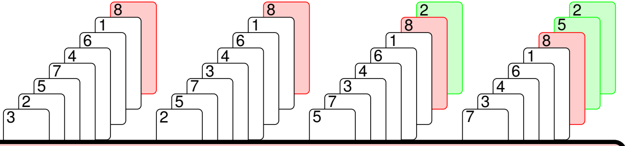

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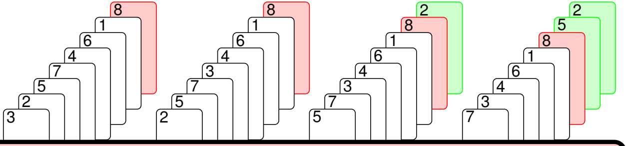

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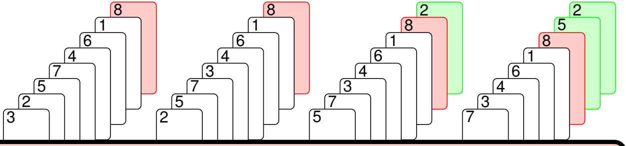

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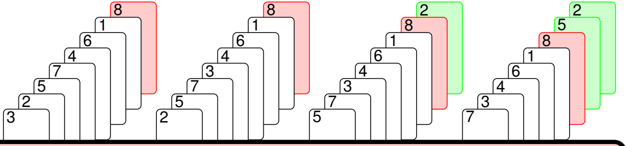

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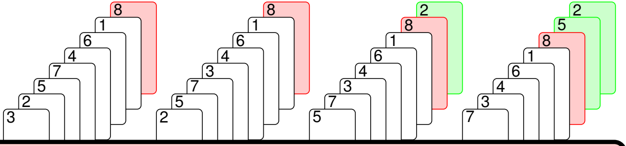

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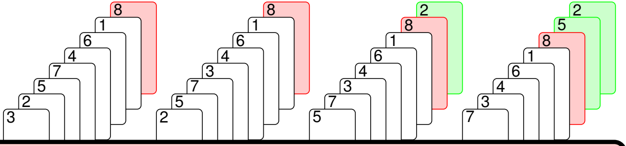

$\rightsquigarrow$ deck of cards is perfectly mixed after the last card "8" reaches the top and is inserted to a random position!

- 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
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- 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.

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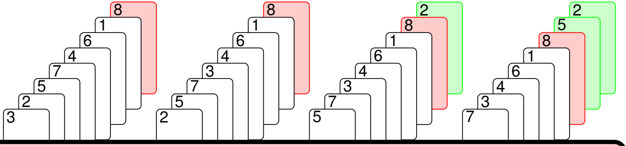

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Using the so-called coupling method, one could prove $t_{mix} \leq n \log n$.

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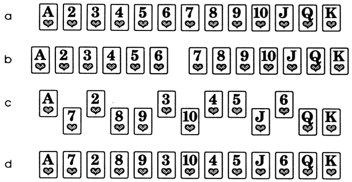

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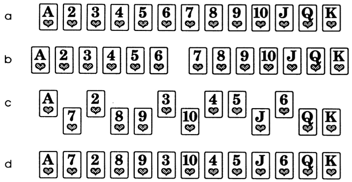

t	1	2	3	4	5	6	7	8	9	10
$\|P^t - \pi\|_{tv}$	1.000	1.000	1.000	1.000	0.924	0.614	0.334	0.167	0.085	0.043

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

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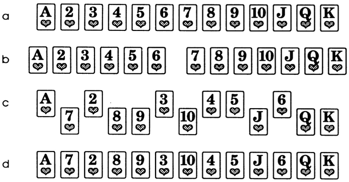

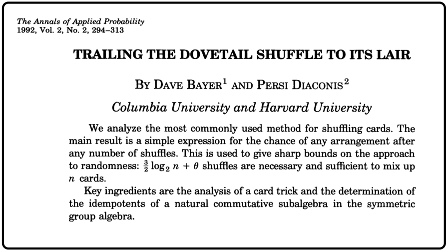

The Annals of Applied Probability
1992, Vol. 2, No. 2, 294–313

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
$\|P^t - \pi\|_{tv}$	1.000	1.000	1.000	1.000	0.924	0.614	0.334	0.167	0.085	0.043

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Outline

The Ehrenfest Markov Chain

Ehrenfest Model

- A simple model for the exchange of molecules between two boxes

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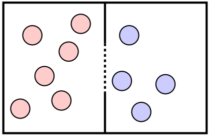

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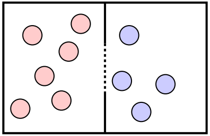

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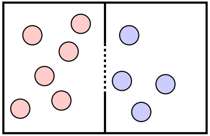

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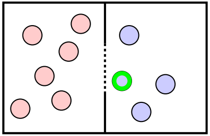

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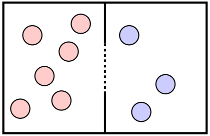

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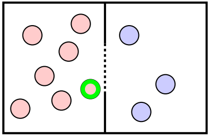

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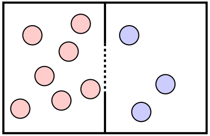
$$P_{x,x-1} = \frac{x}{d} \qquad \text{and} \qquad P_{x,x+1} = \frac{d-x}{d}.$$



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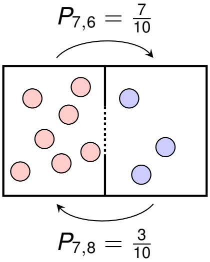

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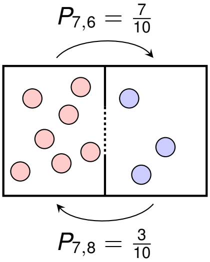

Let us now enlarge the state space by looking at each particle individually!

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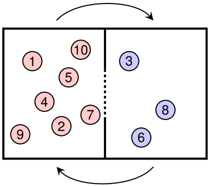
$P_{7,6} = \frac{7}{10}$



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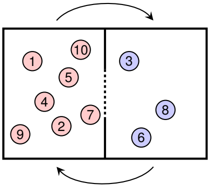

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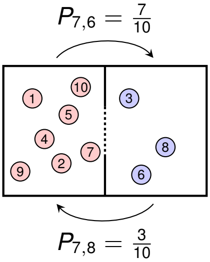

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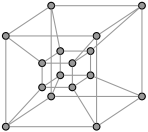

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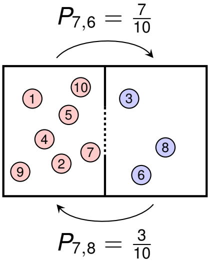

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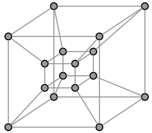

Analysis of the Mixing Time

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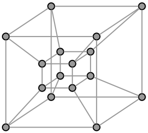

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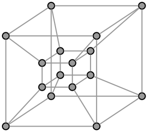

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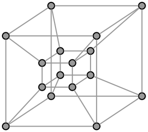

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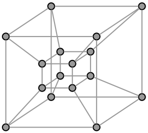

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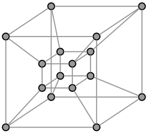

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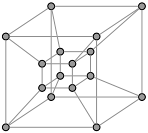

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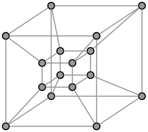

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- At each step $t = 0, 1, 2 \ldots$
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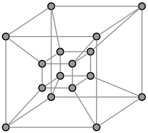

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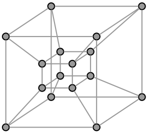

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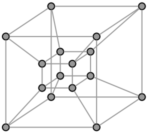

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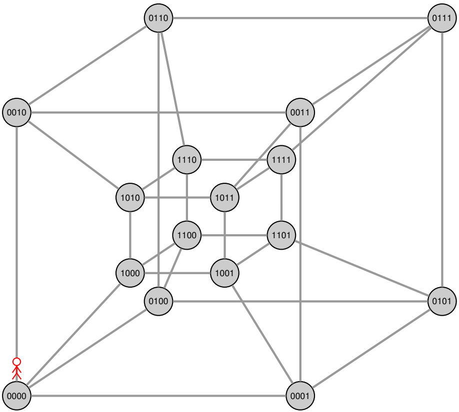
These two chains are equivalent!

Example of a Random Walk on a 4-Dimensional Hypercube



t	Coord.	X_t
0		0 0 0 0

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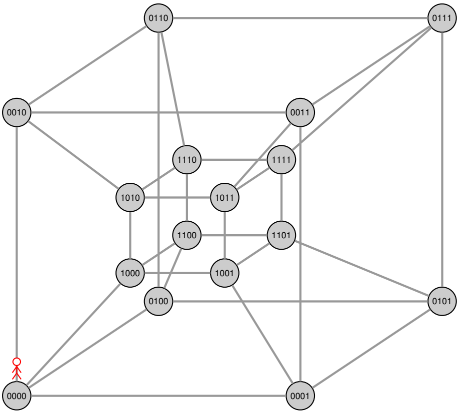

t	Coord.	X_t			
0	2	0	0	0	0
1		0	?	0	0

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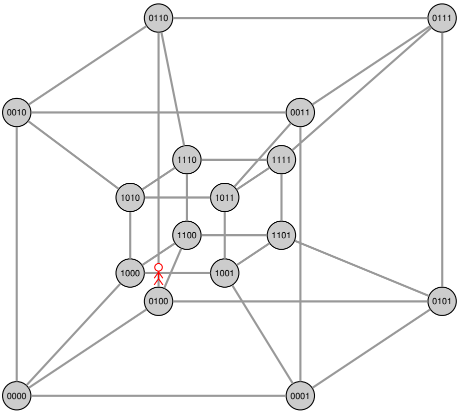

t	Coord.	X_t			
0	2	0	0	0	0
1		0	1	0	0

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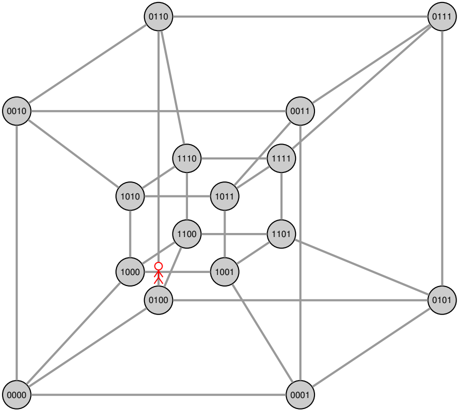

t	Coord.	X_t			
0	2	0	0	0	0
1	3	0	1	0	0
2		0	1	?	0

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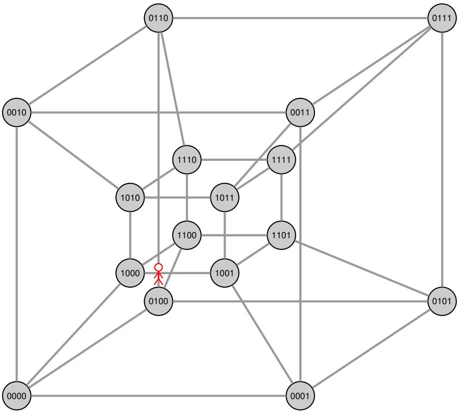

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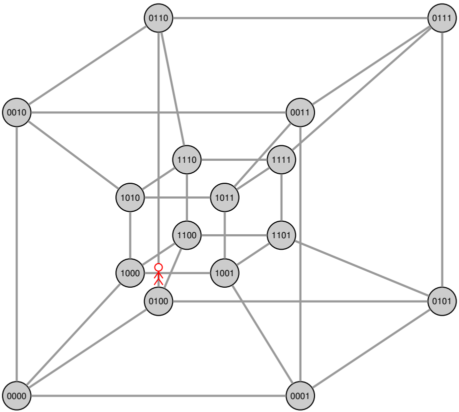

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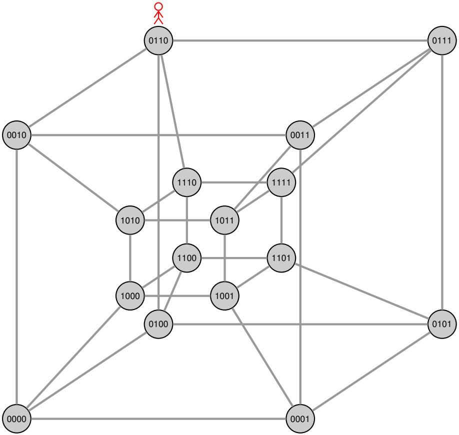
1	3	0	1	0	0
2	3	0	1	0	0
3		0	1	?	0

Example of a Random Walk on a 4-Dimensional Hypercube



t	Coord.	X_t			
0	2	0	0	0	0
1	3	0	1	0	0
2	3	0	1	0	0
3		0	1	1	0

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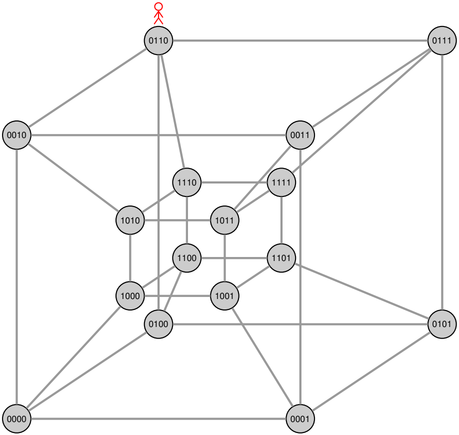
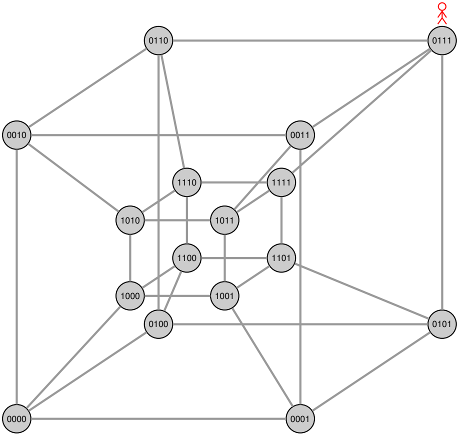


t	Coord.	X_t			
0	2	0	0	0	0
1	3	0	1	0	0
2	3	0	1	0	0
3	4	0	1	1	0
4		0	1	1	?

Example of a Random Walk on a 4-Dimensional Hypercube



t	Coord.	X_t			
0	2	0	0	0	0
1	3	0	1	0	0
2	3	0	1	0	0
3	4	0	1	1	0
4		0	1	1	1

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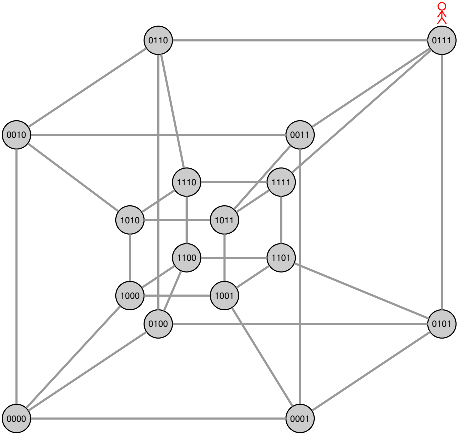

t	Coord.	X_t			
0	2	0	0	0	0
1	3	0	1	0	0
2	3	0	1	0	0
3	4	0	1	1	0
4	2	0	1	1	1
5		0	?	1	1

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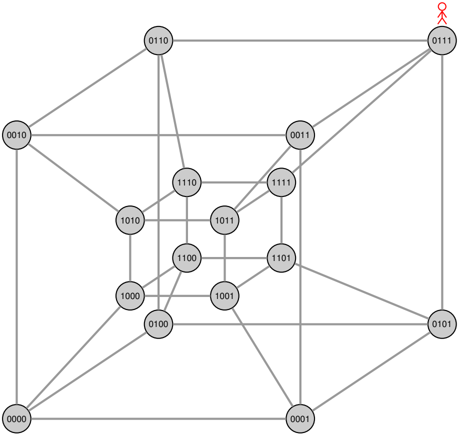

t	Coord.	X_t			
0	2	0	0	0	0
1	3	0	1	0	0
2	3	0	1	0	0
3	4	0	1	1	0
4	2	0	1	1	1
5		0	1	1	1

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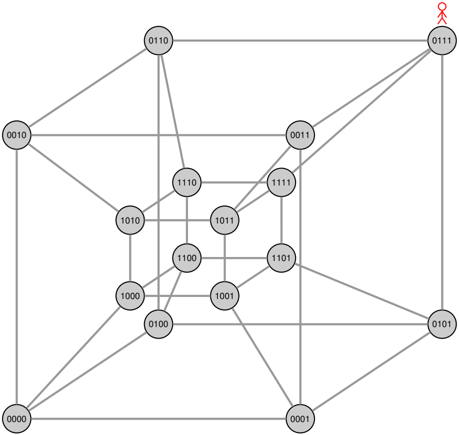
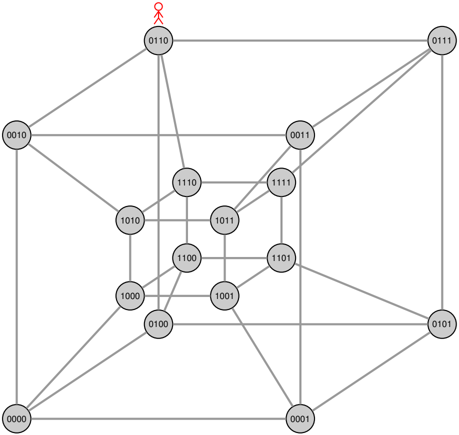


t	Coord.	X_t			
0	2	0	0	0	0
1	3	0	1	0	0
2	3	0	1	0	0
3	4	0	1	1	0
4	2	0	1	1	1
5	4	0	1	1	1
6		0	1	1	?

Example of a Random Walk on a 4-Dimensional Hypercube



t	Coord.	X_t			
0	2	0	0	0	0
1	3	0	1	0	0
2	3	0	1	0	0
3	4	0	1	1	0
4	2	0	1	1	1
5	4	0	1	1	1
6		0	1	1	0

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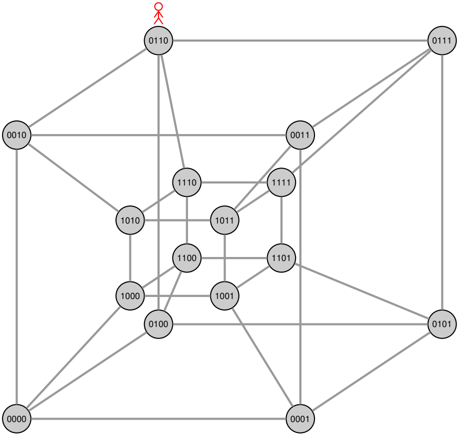
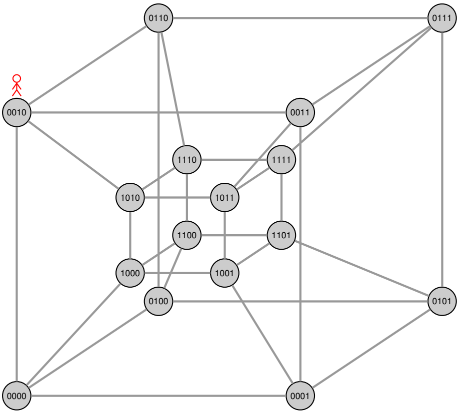


t	Coord.	X_t			
0	2	0	0	0	0
1	3	0	1	0	0
2	3	0	1	0	0
3	4	0	1	1	0
4	2	0	1	1	1
5	4	0	1	1	1
6	2	0	1	1	0
7		0	?	1	0

Example of a Random Walk on a 4-Dimensional Hypercube



t	Coord.	X_t			
0	2	0	0	0	0
1	3	0	1	0	0
2	3	0	1	0	0
3	4	0	1	1	0
4	2	0	1	1	1
5	4	0	1	1	1
6	2	0	1	1	0
7		0	0	1	0

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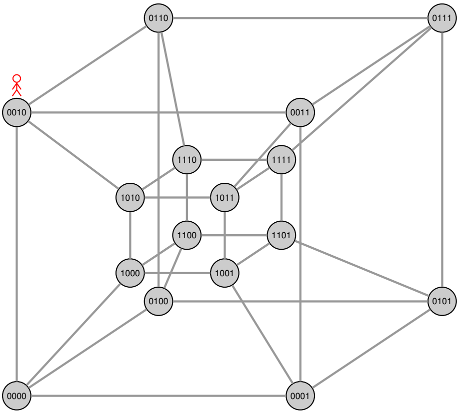

t	Coord.	X_t			
0	2	0	0	0	0
1	3	0	1	0	0
2	3	0	1	0	0
3	4	0	1	1	0
4	2	0	1	1	1
5	4	0	1	1	1
6	2	0	1	1	0
7	4	0	0	1	0
8		0	0	1	?

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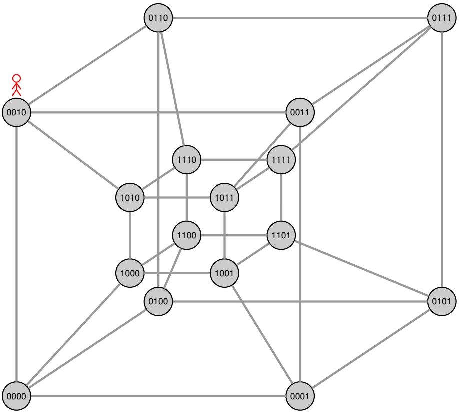

t	Coord.	X_t			
0	2	0	0	0	0
1	3	0	1	0	0
2	3	0	1	0	0
3	4	0	1	1	0
4	2	0	1	1	1
5	4	0	1	1	1
6	2	0	1	1	0
7	4	0	0	1	0
8		0	0	1	0

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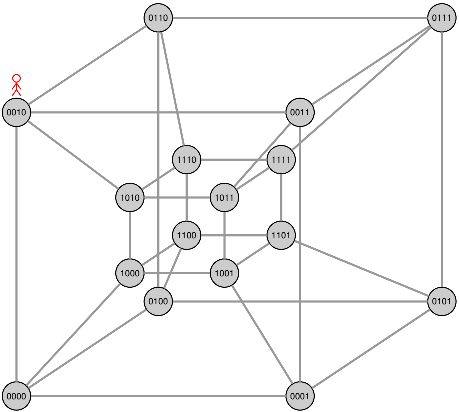
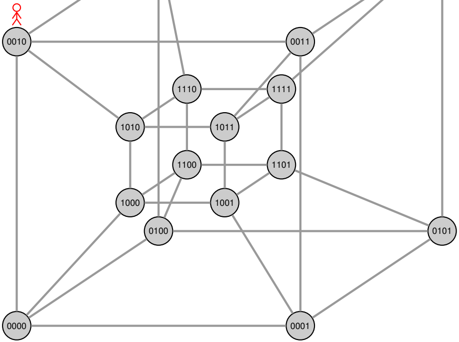


t	Coord.	X_t			
0	2	0	0	0	0
1	3	0	1	0	0
2	3	0	1	0	0
3	4	0	1	1	0
4	2	0	1	1	1
5	4	0	1	1	1
6	2	0	1	1	0
7	4	0	0	1	0
8	3	0	0	1	0
9		0	0	?	0

Example of a Random Walk on a 4-Dimensional Hypercube



t	Coord.	X_t			
0	2	0	0	0	0
1	3	0	1	0	0
2	3	0	1	0	0
3	4	0	1	1	0
4	2	0	1	1	1
5	4	0	1	1	1
6	2	0	1	1	0
7	4	0	0	1	0
8	3	0	0	1	0
9		0	0	1	0

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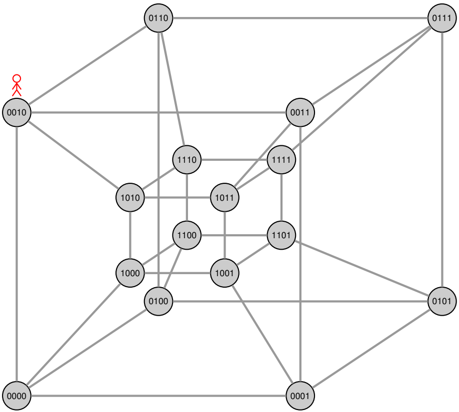
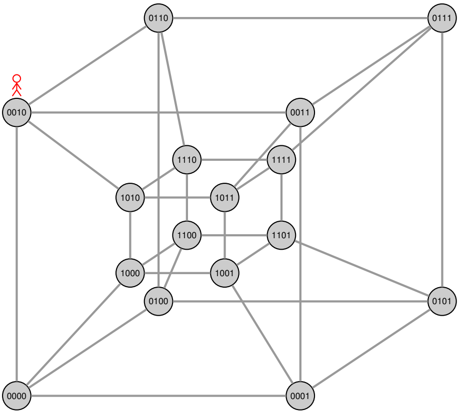


t	Coord.	X_t			
0	2	0	0	0	0
1	3	0	1	0	0
2	3	0	1	0	0
3	4	0	1	1	0
4	2	0	1	1	1
5	4	0	1	1	1
6	2	0	1	1	0
7	4	0	0	1	0
8	3	0	0	1	0
9	1	0	0	1	0
10	done!	?	0	1	0

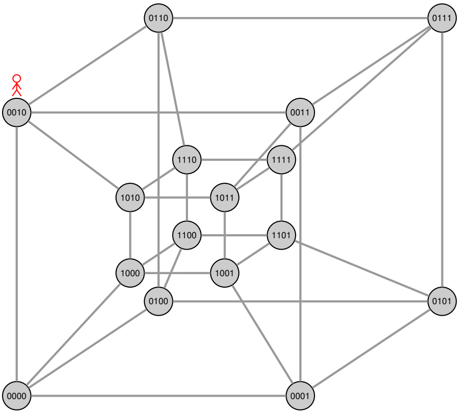
Example of a Random Walk on a 4-Dimensional Hypercube



Once all coordinates have been picked at least once, the state is uniformly at random in $\{0,1\}^d$.

t	Coord.	X_t			
0	2	0	0	0	0
1	3	0	1	0	0
2	3	0	1	0	0
3	4	0	1	1	0
4	2	0	1	1	1
5	4	0	1	1	1
6	2	0	1	1	0
7	4	0	0	1	0
8	3	0	0	1	0
9	1	0	0	1	0
10	done!	0	0	1	0

Example of a Random Walk on a 4-Dimensional Hypercube

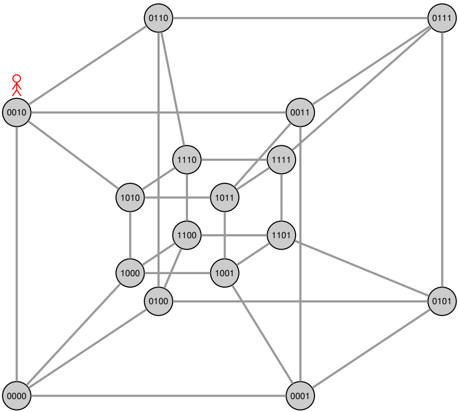


t	Coord.	X_t			
0	2	0	0	0	0
1	3	0	1	0	0
2	3	0	1	0	0
3	4	0	1	1	0
4	2	0	1	1	1
5	4	0	1	1	1
6	2	0	1	1	0
7	4	0	0	1	0
8	3	0	0	1	0
9	1	0	0	1	0
10	done!	0	0	1	0

Once all coordinates have been picked at least once, the state is uniformly at random in $\{0,1\}^d$.

Coupon Collector $\rightsquigarrow$ mixing time should be $O(n \log n)$

Example of a Random Walk on a 4-Dimensional Hypercube



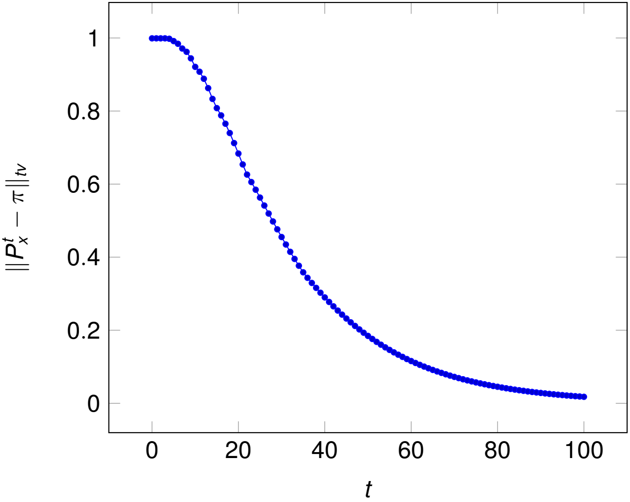
t	Coord.	X_t			
0	2	0	0	0	0
1	3	0	1	0	0
2	3	0	1	0	0
3	4	0	1	1	0
4	2	0	1	1	1
5	4	0	1	1	1
6	2	0	1	1	0
7	4	0	0	1	0
8	3	0	0	1	0
9	1	0	0	1	0
10	done!	0	0	1	0

Once all coordinates have been picked at least once, the state is uniformly at random in $\{0,1\}^d$.

Coupon Collector $\rightsquigarrow$ mixing time should be $O(n \log n)$

We will not formalise this argument here (see exercise question)

Total Variation Distance of Random Walk on Hypercube $(d = 22)$



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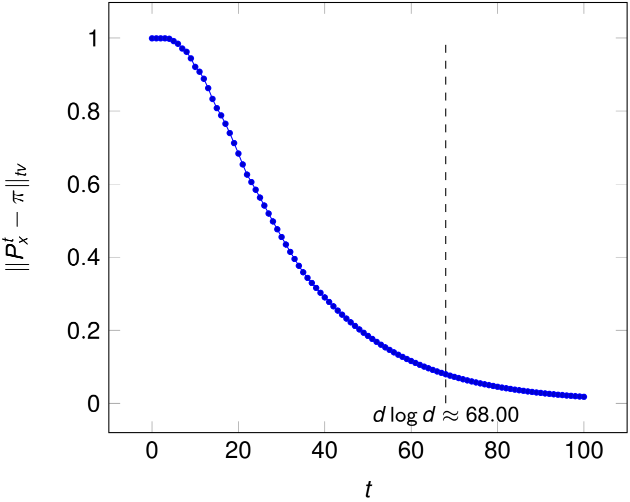

Theoretical Results (by Diaconis, Graham and Morrison)

RANDOM WALK ON A HYPERCUBE 53

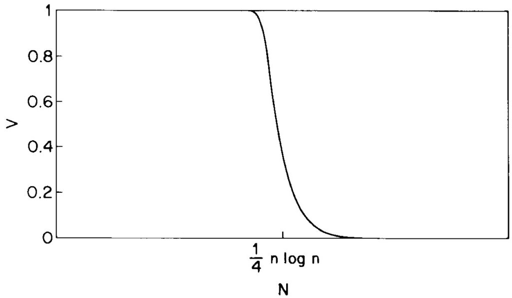

Fig. 1. The variation distance V as a function of N, for $n = 10^{12}$.

Source: "Asymptotic analysis of a random walk on a hypercube with many dimensions", P. Diaconis, R.L. Graham, J.A. Morrison; Random Structures & Algorithms, 1990.

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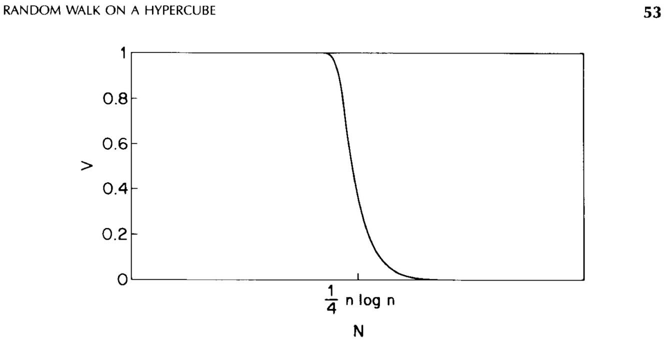

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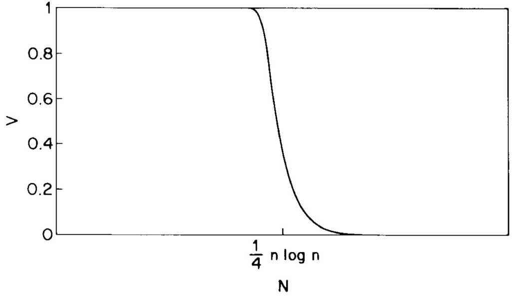
- This is a numerical plot of a theoretical bound, where $d = 10^{12}$
  (Minor Remark: This random walk is with a loop probability of $1/(d+1)$)
- The variation distance exhibits a so-called cut-off phenomena:

Theoretical Results (by Diaconis, Graham and Morrison)

RANDOM WALK ON A HYPERCUBE 53



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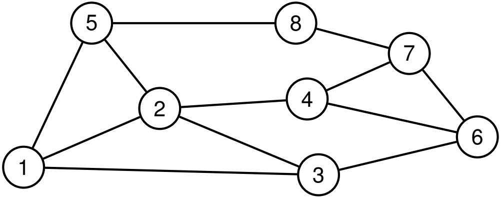
- This is a numerical plot of a theoretical bound, where $d = 10^{12}$
  (Minor Remark: This random walk is with a loop probability of $1/(d+1)$)
- The variation distance exhibits a so-called cut-off phenomena:
  - Distance remains close to its maximum value 1 until step $\frac{1}{4} n \log n - \Theta(n)$
  - Then distance moves close to 0 before step $\frac{1}{4} n \log n + \Theta(n)$

Outline

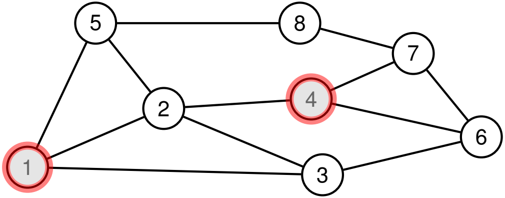
A Markov Chain for Sampling Independent Sets (1/2)



Independent Set

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

A Markov Chain for Sampling Independent Sets (1/2)



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

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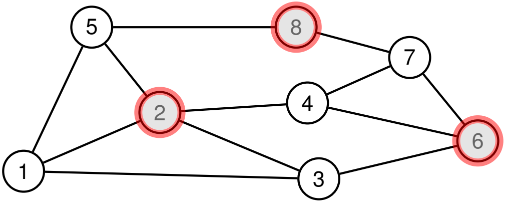
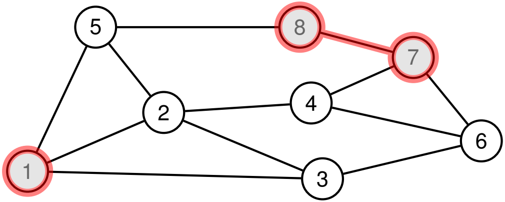


$S = \{2, 6, 8\}$ is an independent set ✓

Independent Set

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

A Markov Chain for Sampling Independent Sets (1/2)



$S = \{1, 7, 8\}$ is **not** an independent set ×

Independent Set

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

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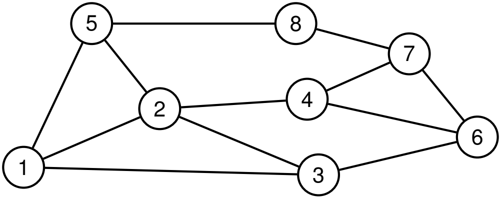

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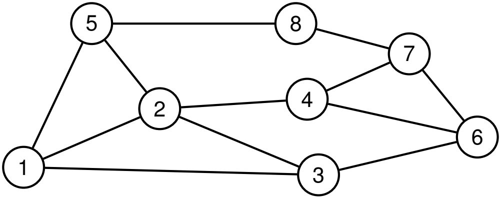

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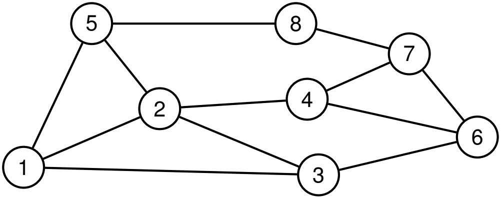
Given an undirected graph $G = (V, E)$, an independent set is a subset $S \subseteq V$ such that there are no two vertices $u, v \in S$ with $\{u, v\} \in E(G)$.

How can we take a sample from the space of all independent sets?

A Markov Chain for Sampling Independent Sets (1/2)



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Naive brute-force would take an insane amount of time (and space)!

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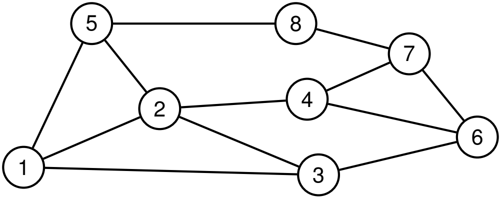

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We can use a generic Markov Chain Monte Carlo approach to tackle this problem!

A Markov Chain for Sampling Independent Sets (2/2)

INDEPENDENTSETSAMPLER

Let X_0 be an arbitrary independent set in G
For $t = 1, 2, \ldots$:
    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 $X_{t+1} \leftarrow X_t$

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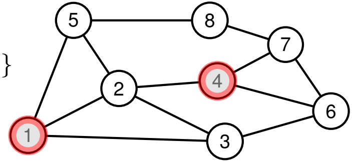
$X_0 = \{1, 4\}$



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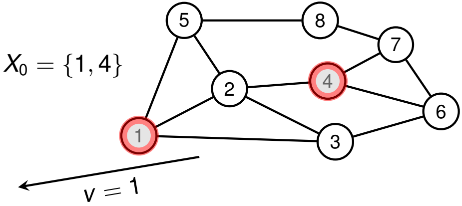

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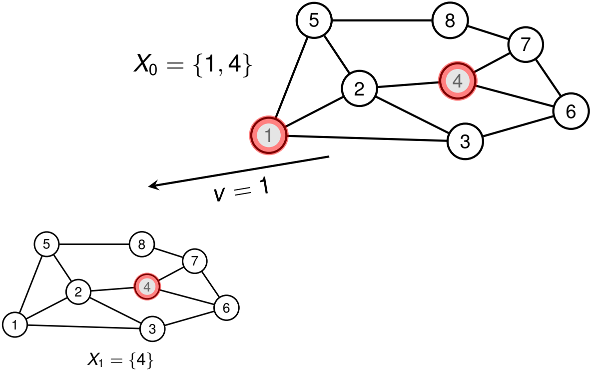

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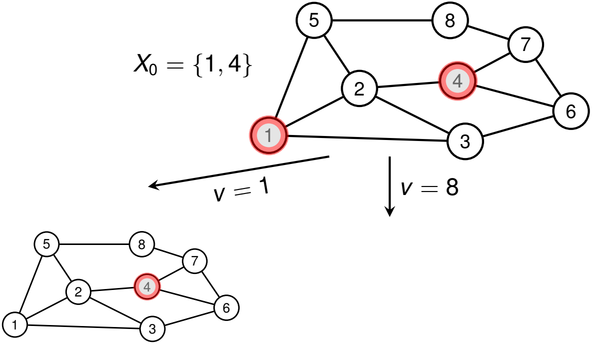

$X_1 = \{4\}$

A Markov Chain for Sampling Independent Sets (2/2)

INDEPENDENTSETSAMPLER

Let X_0 be an arbitrary independent set in G
For $t = 1, 2, \ldots$:
    Pick a vertex $v \in V(G)$ uniformly at random
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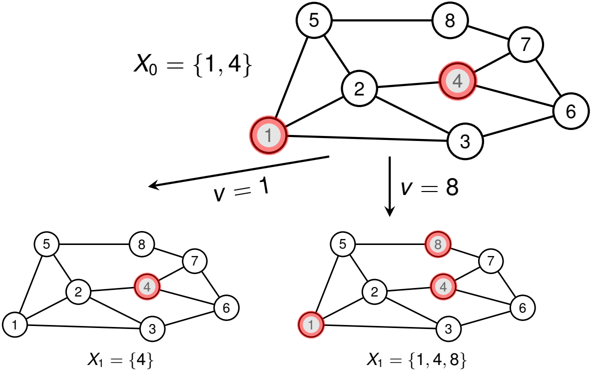

A Markov Chain for Sampling Independent Sets (2/2)

INDEPENDENTSETSAMPLER

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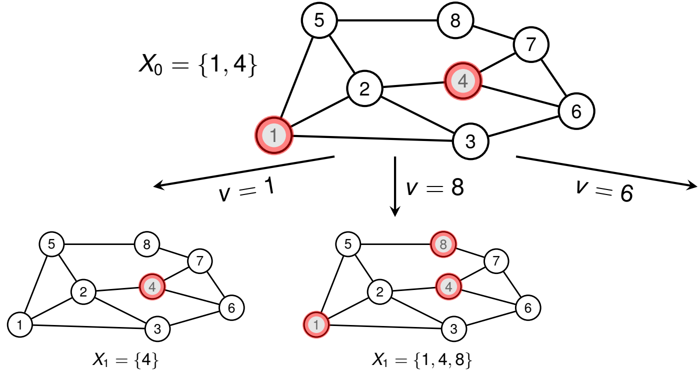

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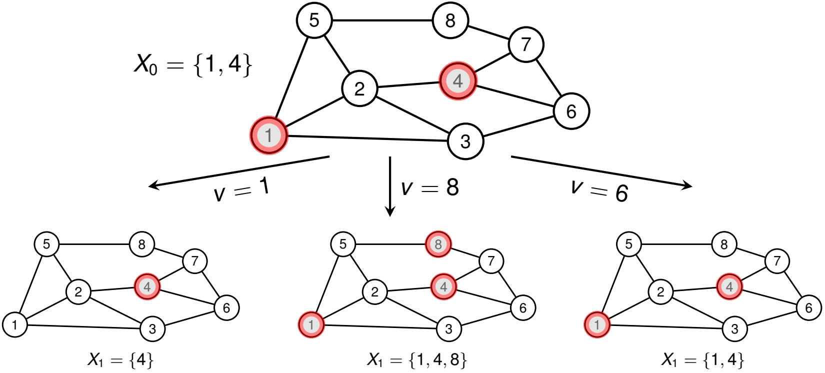

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Remark

A Markov Chain for Sampling Independent Sets (2/2)

INDEPENDENTSETSAMPLER

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Remark

- This is a local definition (no explicit definition of P!)

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- This chain is irreducible (every independent set is reachable)

A Markov Chain for Sampling Independent Sets (2/2)

INDEPENDENTSETSAMPLER

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

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not covered here, see the textbook of Mitzenmacher & Upfal