Random Walks and Markov Chains

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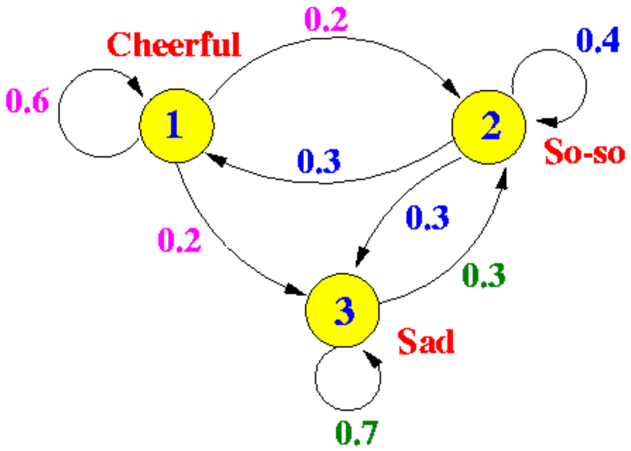
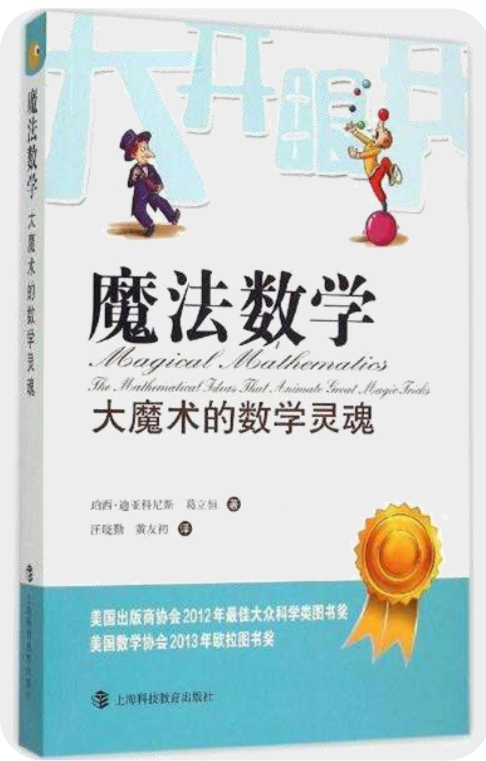




- 戴康尼斯（Persi Diaconis，1945年1月31日 - ）：美国数学家、统计学家。斯坦福大学的数学与统计学教授。

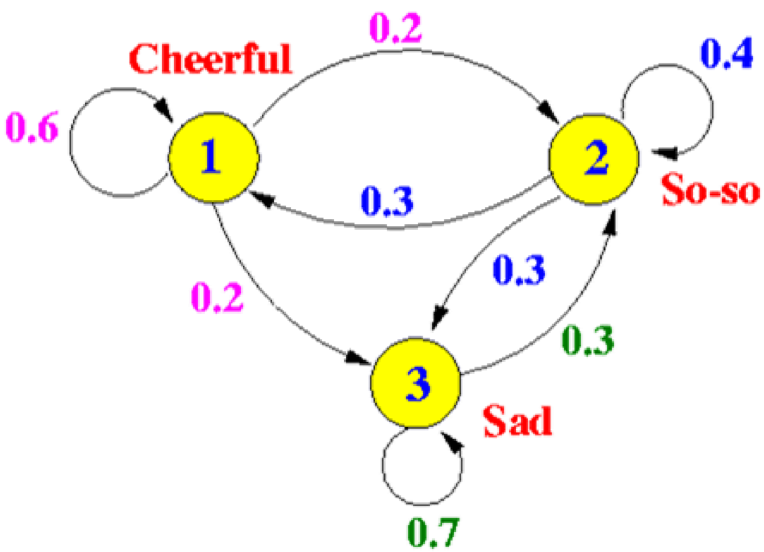
- 他解决了一些随机性的问题，包括掷币和洗牌。1992年，他和David Bayer证明完美的洗牌至少要洗七次。他又和说明从高处跌下的猫为何总能以脚着地的Richard Montgomery合作，证明了掷币哪面向上，物理因素比运气重要得多。

- 自14岁，他便跟随一个叫Dai Vernon的魔术师行走江湖。后来在赌场，他尝试研究防止他和其他魔术师被骗的方法。他18岁时买了一本An Introduction to Probability and Its Applications，但因为不懂微积分而看不明。24岁，他在City College of New York上数学课。其间他在《科学美国人》杂志投稿，介绍了他的两个纸牌戏法。马丁·葛登能认为那两个戏法十分精彩，注意到他的才华，为他写了一封推荐信。当时，哈佛大学的统计学家Fred Mosteller正在研究魔术，因此决定让Diaconis成为他的研究生。

——维基百科

Random walk

- **Random walk**. on a directed graph, a sequence of vertices generated from a start vertex by probabilistically selecting an incident edge, traveling the edge to a new vertex, and repeat the process.



Random walk

Probability distribution. $p = [p_1, p_2, \dots, p_n]$, where $\sum_{i=1}^{n} p_i$=1

Starting. $p = p(0) = [p_1(0), p_2(0), \dots, p_n(0)]$, $\sum_{i=1}^{n} p_i(0)$=1

and p_x is the probability of staring at x.

The probability of being at vertex x at time $t+1$:

$$p_x(t+1) = \sum_{(y,x)\in E} p_y(t) \cdot \Pr(y \to x)$$

Transition Matrix P: P_{ij} is the probability of the walk at vertex i selecting the edge to vertex j.

$$p(t) \cdot P = p(t+1)$$

Random walk

Fundamental property. in the limit, the long-term average property of being at a particular vertex is *independent of the start vertex*, or an initial probability distribution over vertices (provided the underlying graph is strongly connected) – the *stationary probabilities*.

Markov chain

- A finite set S of states
- Transition probability: For $x, y \in S$, p_{xy} is the probability going from state x to y.
- $\sum_y p_{xy} = 1$

Markov chain ➔ Random graph

① A vertex ➔ a state

② p_{xy} ➔ weighted edge from x to y.

Markov chain

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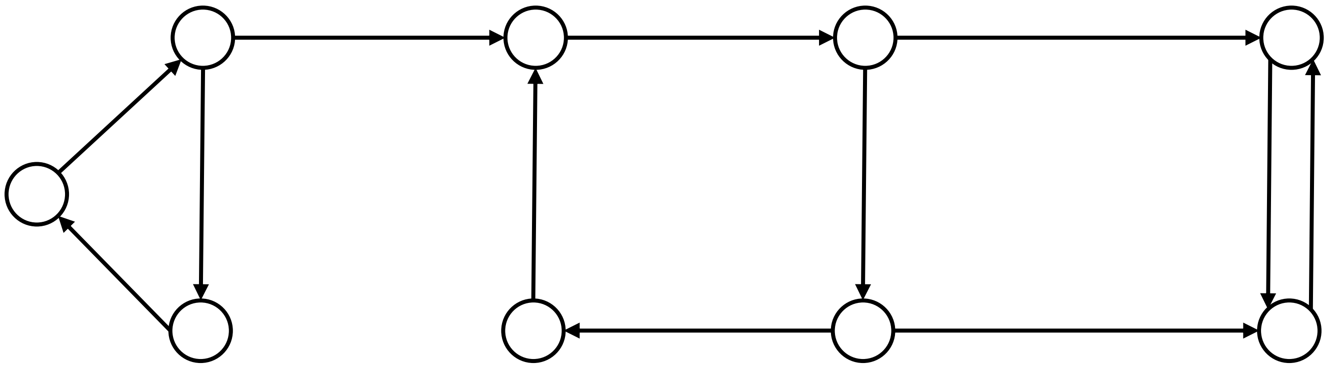
② p_{xy}➔weighted edge from x to y.

Connected Markov chain: if the underlying directed graph is strongly connected.

Transition probability matrix P: P_{xy} is the probability of changing from state x to y.

Markov chain

Persistent state. If the state ever be reached, the random process will return to it with probability 1.



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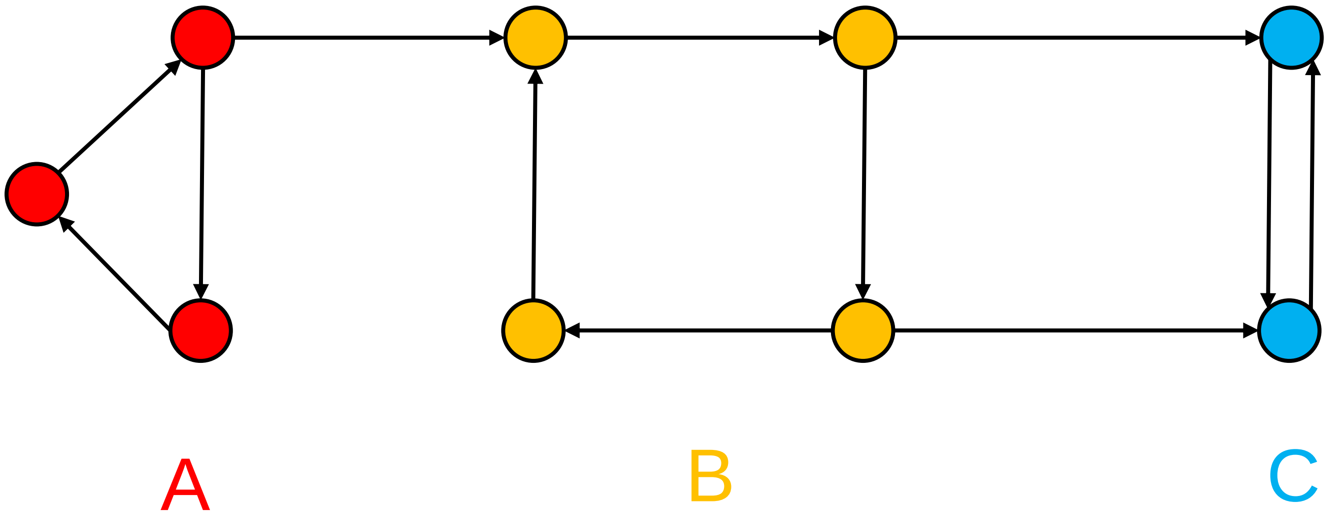

Markov chain

Aperiodic. If the greatest common divisor of the lengths of directed cycles in one.

Random walk	**Markov Chain**
Graph	Stochastic process
Vertex	State
Strongly connected	Persistent/Connected
Aperiodic	Aperiodic
Strongly connected +Aperiodic	Ergodic
Undirected graph	Time reversible

We will assume strongly connectness by default.

Stationary distribution

$p(t)$: the probability distribution after t steps of a random walk.

Long-term average probability distribution:

$$\boldsymbol{a}(\boldsymbol{t}) = \frac{1}{t}\big(p(0) + p(1) + \cdots + p(t-1)\big)$$

Fundatmental theorem of Markov chains:
For a connected MC, $\boldsymbol{a}(\boldsymbol{t})$ converges to a limit probability x which satisfies $x \cdot P = x$.

Fundamental Theorem

Lemma: Let P be the transition probability matrix for a connected Markov chain. The $n \times (n+1)$ matrix $A = [P - \boldsymbol{I}, \boldsymbol{1}]$ obtained by augmenting the matrix $P - \boldsymbol{I}$ with an additional column of ones has rank n.

Fundamental Theorem of Markov Chains: For a connected Markov chain there is a unique vector $\boldsymbol{\pi}$ satisfying $\boldsymbol{\pi} \cdot P = \boldsymbol{\pi}$. Moreover, for any starting distribution, $\lim_{t \to \infty} \boldsymbol{a}(\boldsymbol{t})$ exists and equals $\boldsymbol{\pi}$.

Lemma: For a random walk on a strongly connected graph with probabilities on the edge, if the vector $\boldsymbol{\pi}$ satisfies $\boldsymbol{\pi}_x p_{xy} = \pi_y p_{yx}$ for all x and y and $\sum_x \pi_x = 1$, then $\boldsymbol{\pi}$ is the stationary distribution of the walk.

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Markov Chain Monte Carlo

MCMC. A technique for sampling a multivariate probability distribution $p(\boldsymbol{x})$, where $\boldsymbol{x} = (x_1, x_2, \ldots, x_d)$.

Application. to estimate the expected value of a function $f(x)$

$$E(f) = \sum_{\boldsymbol{x}} f(\boldsymbol{x}) \cdot p(\boldsymbol{x})$$

Markov Chain Monte Carlo

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Realization:

① Draw a set of samples. Each sample $\boldsymbol{x}$ is selected with probability $p(\boldsymbol{x})$.

② Averaging f over these samples.

Markov Chain Monte Carlo

Sample according to $p(\boldsymbol{x})$. Design a MC whose states correspond to the value space of $\boldsymbol{x}$ and whose stationary probability distribution is $p(\boldsymbol{x})$.

Recall:

- ✓ $p(\boldsymbol{t})$ is the row vector of probabilities of the random walk being at each state at time t.
- ✓ $\boldsymbol{a}(\boldsymbol{t}) = \frac{1}{t}(p(0) + p(1) + \cdots + p(t-1))$

$$E(r) = \sum_i f_i(\frac{1}{t}\sum_{j=1}^{t} \Pr(walk\ is\ in\ state\ i\ at\ time\ j)) = \sum_i f_i a_i(t)$$

Markov Chain Monte Carlo

Sample according to $p(\boldsymbol{x})$. Design a MC whose states correspond to the value space of $\boldsymbol{x}$ and whose *stationary probability distribution* is $p(\boldsymbol{x})$.

$$E(r) = \sum_i f_i \left(\frac{1}{t}\sum_{j=1}^{t} \Pr(walk\ is\ in\ state\ i\ at\ time\ j)\right) = \sum_i f_i a_i(t)$$

$$\left|\sum_i f_i p_i - E(r)\right| \le f_{max} \cdot \sum_i |p_i - a_i(t)|$$
$$= f_{max} \cdot \boxed{\|p - a(t)\|_1}$$

Markov Chain Monte Carlo

Sample according to $p(\boldsymbol{x})$. Design a MC whose states correspond to the value space of $\boldsymbol{x}$ and whose stationary probability distribution is $p(\boldsymbol{x})$.

Two general approach:

- The Metropolis-Hastings algorithm
- The Gibbs sampling

Metropolis-Hastings Algorithm

MHA. A general method to design a Markov chain whose stationary distribution is a given target distribution $\boldsymbol{p}$.

Given random graph G, with $\Delta(G) = r$. The transitions of the MC are defined as

$$\begin{cases} p_{ij} = \frac{1}{r}\min\left(1, \frac{p_j}{p_i}\right) \\ p_{ii} = 1 - \sum_{i \neq j} p_{ij} \end{cases}$$

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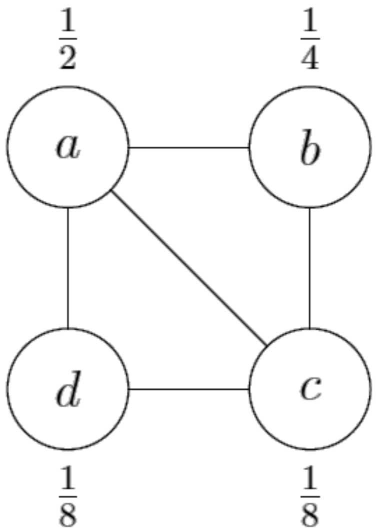
$p(a) = \frac{1}{2}$
$p(b) = \frac{1}{4}$
$p(c) = \frac{1}{8}$
$p(d) = \frac{1}{8}$



$a \to b \quad \frac{1}{3}\,\frac{1}{4}\,\frac{2}{1} = \frac{1}{6}$
$a \to c \quad \frac{1}{3}\,\frac{1}{8}\,\frac{2}{1} = \frac{1}{12}$
$a \to d \quad \frac{1}{3}\,\frac{1}{8}\,\frac{2}{1} = \frac{1}{12}$
$a \to a \quad 1 - \frac{1}{6} - \frac{1}{12} - \frac{1}{12} = \frac{2}{3}$

$b \to a \quad \frac{1}{3}$
$b \to c \quad \frac{1}{3}\,\frac{1}{8}\,\frac{4}{1} = \frac{1}{6}$
$b \to b \quad 1 - \frac{1}{3} - \frac{1}{6} = \frac{1}{2}$

$c \to a \quad \frac{1}{3}$
$c \to b \quad \frac{1}{3}$
$c \to d \quad \frac{1}{3}$
$c \to c \quad 1 - \frac{1}{3} - \frac{1}{3} - \frac{1}{3} = 0$

$d \to a \quad \frac{1}{3}$
$d \to c \quad \frac{1}{3}$
$d \to d \quad 1 - \frac{1}{3} - \frac{1}{3} = \frac{1}{3}$

$$\begin{aligned} p(a) &= p(a)p(a \to a) + p(b)p(b \to a) + p(c)p(c \to a) + p(d)p(d \to a) \\ &= \frac{1}{2}\,\frac{2}{3} + \frac{1}{4}\,\frac{1}{3} + \frac{1}{8}\,\frac{1}{3} + \frac{1}{8}\,\frac{1}{3} = \frac{1}{2} \end{aligned}$$

$$\begin{aligned} p(b) &= p(a)p(a \to b) + p(b)p(b \to b) + p(c)p(c \to b) \\ &= \frac{1}{2}\,\frac{1}{6} + \frac{1}{4}\,\frac{1}{2} + \frac{1}{8}\,\frac{1}{3} = \frac{1}{4} \end{aligned}$$

$$\begin{aligned} p(c) &= p(a)p(a \to c) + p(b)p(b \to c) + p(c)p(c \to c) + p(d)p(d \to c) \\ &= \frac{1}{2}\,\frac{1}{12} + \frac{1}{4}\,\frac{1}{6} + \frac{1}{8}\,0 + \frac{1}{8}\,\frac{1}{3} = \frac{1}{8} \end{aligned}$$

$$\begin{aligned} p(d) &= p(a)p(a \to d) + p(c)p(c \to d) + p(d)p(d \to d) \\ &= \frac{1}{2}\,\frac{1}{12} + \frac{1}{8}\,\frac{1}{3} + \frac{1}{8}\,\frac{1}{3} = \frac{1}{8} \end{aligned}$$

Metropolis-Hastings Algorithm

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Correctness.

To prove the stationary distribution is indeed the target distribution $\boldsymbol{p}$.

$$p_i p_{ij} = \frac{p_i}{r}\min\left(1, \frac{p_j}{p_i}\right) = \frac{1}{r}\min(p_i, p_j) = \frac{p_j}{r}\min\left(1, \frac{p_i}{p_j}\right) = p_j p_{ji}$$

Gibbs Sampling

Let $p(\boldsymbol{x})$ be the target distribution where $\boldsymbol{x} = (x_1, \dots, x_d)$.
Now the undirected random graph is a hyper cube: there is an edge between $\boldsymbol{x}$ and $\boldsymbol{y}$ if $\boldsymbol{x}$ and $\boldsymbol{y}$ differ in only 1 coordinate.

Sampling process: for $\boldsymbol{x} = (x_1, \dots, x_d)$

① Choose one of the x_i to update;

② ${x_i}'$ is chosen based on the marginal probability of x_i

$$p_{xy} = \frac{1}{d} \cdot p(y_i \,|\, x_1 \cdots x_{i-1} x_{i+1} \cdots x_d)$$

where $x_i \neq y_i$ and $x_j = y_j$ for all $i \neq j$,

(i.e., $x_{i \neq j}$ does not change).

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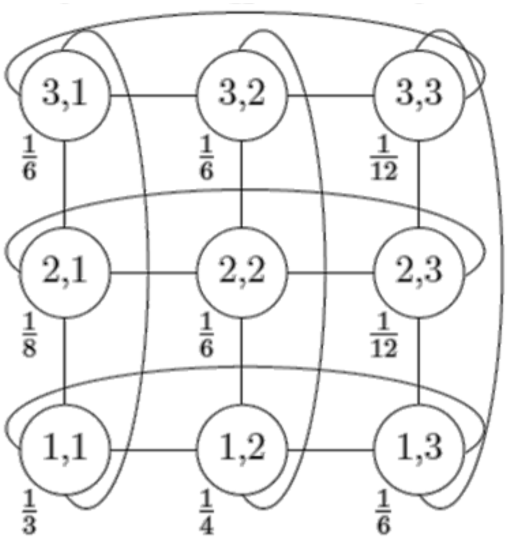

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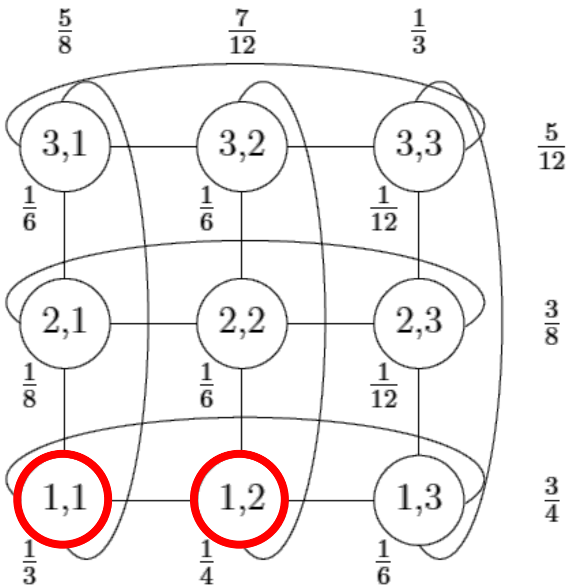

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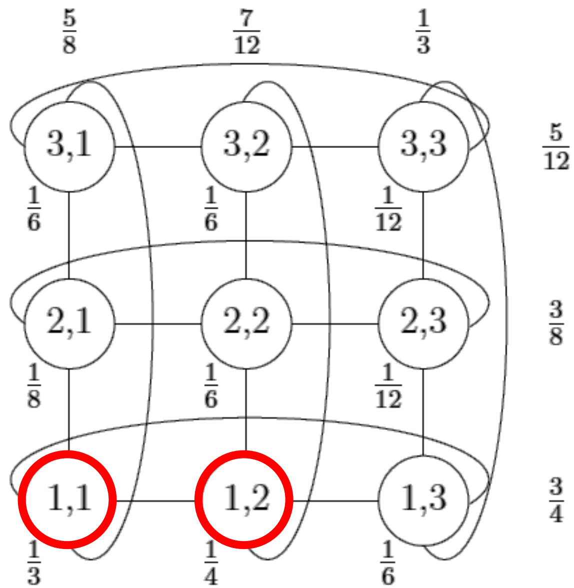

$$p_{(11)(12)} = \frac{1}{d} p_{12} / (p_{11} + p_{12} + p_{13}) = \frac{1}{2}\ (\frac{1}{4}) / (\frac{1}{3}\ \frac{1}{4}\ \frac{1}{6}) = \frac{1}{8} / \frac{9}{12} = \frac{1}{8}\ \frac{4}{3} = \frac{1}{6}$$

$$p_{(11)(12)} = \frac{1}{2}\ \frac{1}{4}\ \frac{4}{3} = \frac{1}{6} \quad p_{(12)(11)} = \frac{1}{2}\ \frac{1}{3}\ \frac{4}{3} = \frac{2}{9} \quad p_{(13)(11)} = \frac{1}{2}\ \frac{1}{3}\ \frac{4}{3} = \frac{2}{9} \quad p_{(21)(22)} = \frac{1}{2} \frac{1}{6} \frac{8}{3} = \frac{2}{9}$$

$$p_{(11)(13)} = \frac{1}{2}\ \frac{1}{6}\ \frac{4}{3} = \frac{1}{9} \quad p_{(12)(13)} = \frac{1}{2}\ \frac{1}{6}\ \frac{4}{3} = \frac{1}{9} \quad p_{(13)(12)} = \frac{1}{2}\ \frac{1}{4}\ \frac{4}{3} = \frac{1}{6} \quad p_{(21)(23)} = \frac{1}{2} \frac{1}{12} \frac{8}{3} = \frac{1}{9}$$

$$p_{(11)(21)} = \frac{1}{2}\ \frac{1}{8}\ \frac{8}{5} = \frac{1}{10} \quad p_{(12)(22)} = \frac{1}{2}\ \frac{1}{6}\ \frac{12}{7} = \frac{1}{7} \quad p_{(13)(23)} = \frac{1}{2}\ \frac{1}{12}\ \frac{3}{1} = \frac{1}{8} \quad p_{(21)(11)} = \frac{1}{2} \frac{1}{3} \frac{8}{5} = \frac{4}{15}$$

$$p_{(11)(31)} = \frac{1}{2}\ \frac{1}{6}\ \frac{8}{5} = \frac{2}{15} \quad p_{(12)(32)} = \frac{1}{2}\ \frac{1}{6}\ \frac{12}{7} = \frac{1}{7} \quad p_{(13)(33)} = \frac{1}{2}\ \frac{1}{12}\ \frac{3}{1} = \frac{1}{8} \quad p_{(21)(31)} = \frac{1}{2} \frac{1}{6} \frac{8}{5} = \frac{2}{15}$$

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Correctness. To prove the stationary distribution is indeed the target distribution $\boldsymbol{p}$.

$$p_{\boldsymbol{x}\boldsymbol{y}} = \frac{1}{d} \frac{p(y_i |\, x_1 \cdots x_{i-1} x_{i+1} \cdots x_d) p(x_1 \cdots x_{i-1} x_{i+1} \cdots x_d)}{p(x_1 \cdots x_{i-1} x_{i+1} \cdots x_d)}$$

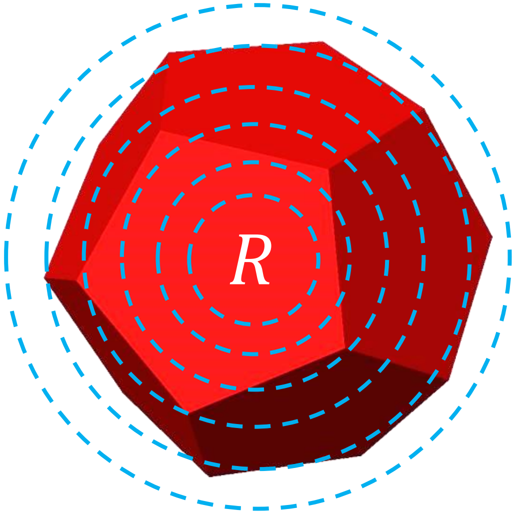
$$= \frac{1}{d} \frac{p(x_1 \cdots x_{i-1} y_i x_{i+1} \cdots x_d)}{p(x_1 \cdots x_{i-1} x_{i+1} \cdots x_d)} = \frac{1}{d} \frac{p(\boldsymbol{y})}{p(x_1 \cdots x_{i-1} x_{i+1} \cdots x_d)}$$

Similarly $p_{\boldsymbol{y}\boldsymbol{x}} = \frac{1}{d} \frac{p(\boldsymbol{x})}{p(x_1 \cdots x_{i-1} x_{i+1} \cdots x_d)}$

It follows that $p(\boldsymbol{x}) p_{\boldsymbol{x}\boldsymbol{y}} = p(\boldsymbol{y}) p_{\boldsymbol{y}\boldsymbol{x}}$.

Areas and Volumes

For general convex sets in d space, there are no close form formulae for volume.

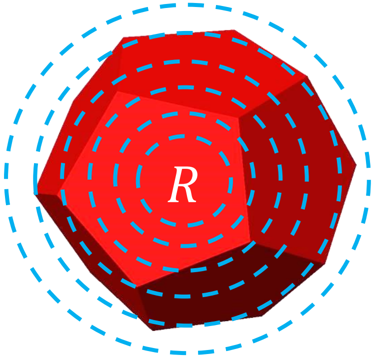


Sequence of concentric spheres:

$$R \supset S_1 \subseteq S_2 \subseteq \cdots \subseteq S_k \supset R$$

$$\begin{aligned} Vol(R) &= Vol(S_k \cap R) \\ &= \frac{Vol(S_k \cap R)}{Vol(S_{k-1} \cap R)} \cdot \frac{Vol(S_{k-1} \cap R)}{Vol(S_{k-2} \cap R)} \cdots \frac{Vol(S_2 \cap R)}{Vol(S_1 \cap R)} \cdot Vol(S_1) \end{aligned}$$

Areas and Volumes



$$Vol(R) = \frac{Vol(S_k \cap R)}{Vol(S_{k-1} \cap R)} \cdot \frac{Vol(S_{k-1} \cap R)}{Vol(S_{k-2} \cap R)} \cdots \frac{Vol(S_2 \cap R)}{Vol(S_1 \cap R)} \cdot Vol(S_1)$$

$$Radius(S_i) = \left(1 + \frac{1}{d}\right) \cdot Radius(S_{i-1})$$

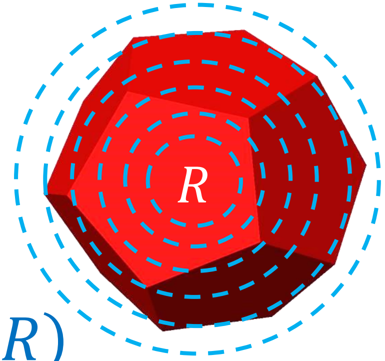
Thus $1 \leq \frac{Vol(S_i \cap R)}{Vol(S_{i-1} \cap R)} = \left(1 + \frac{1}{d}\right)^d \leq e$

Let $r = \left(1 + \frac{1}{d}\right)^k$ then the number of spheres k is at most

$$O\left(\log_{1+\frac{1}{d}} r\right) = O(d\ln(r))$$

To estimate the overall volume to error $1 \pm \epsilon$:
Estimate each volume ratio to a factor of $1 \pm \frac{\epsilon}{ed\ln(r)}$.

Areas and Volumes



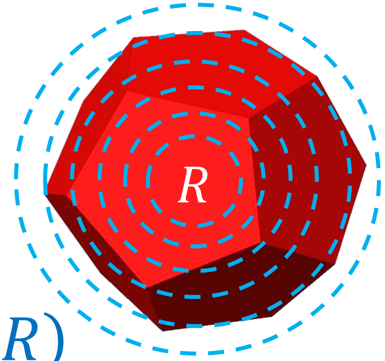
$$Radius(S_i) = \left(1 + \frac{1}{d}\right) \cdot Radius(S_{i+1}),\ 1 \leq \frac{Vol(S_i \cap R)}{Vol(S_{i-1} \cap R)} \leq e$$

Estimate the ratio $\frac{Vol(S_i \cap R)}{Vol(S_{i-1} \cap R)}$:

① Selecting points in $S_i \cap R$ uniformly at random;

② Computing the fraction in $S_{i-1} \cap R$.

Areas and Volumes



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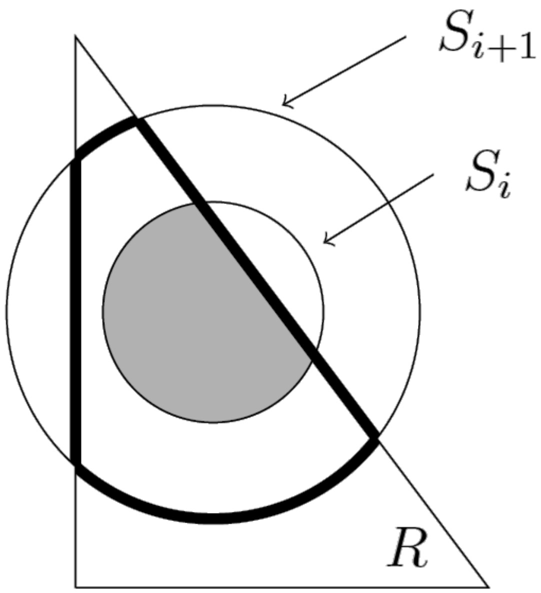
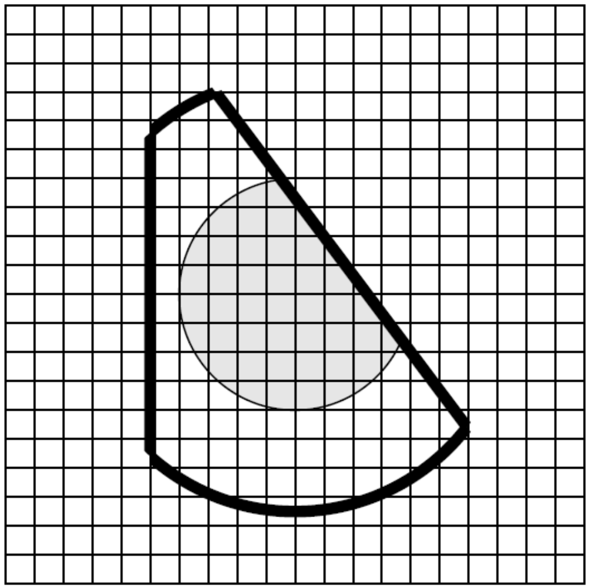


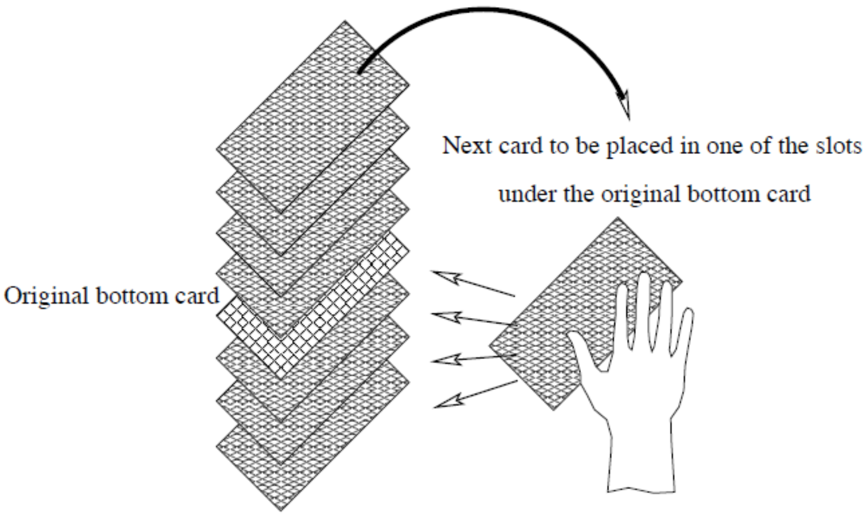


Some conceptions

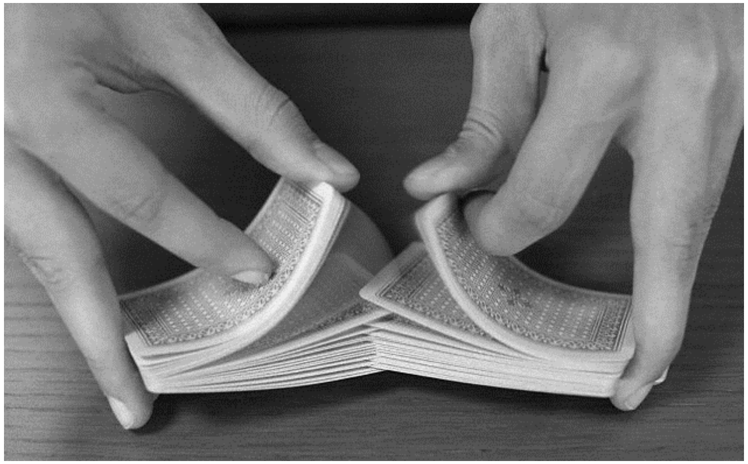
Mixing time. Fix $\epsilon > 0$. The ϵ −mixing time of a MC is the minimum integer t such that for any starting distribution p_0, the 1-norm distance between the t −step running average probability distribution and the stationary distribution is at most ϵ.

Hitting time h_{xy}. The expected time of a random walk starting at vertex x (or a starting probability distribution) to reach vertex y.

Cover time. The expected time of a random walk starting at vertex x in the graph G to reach each vertex at least once.



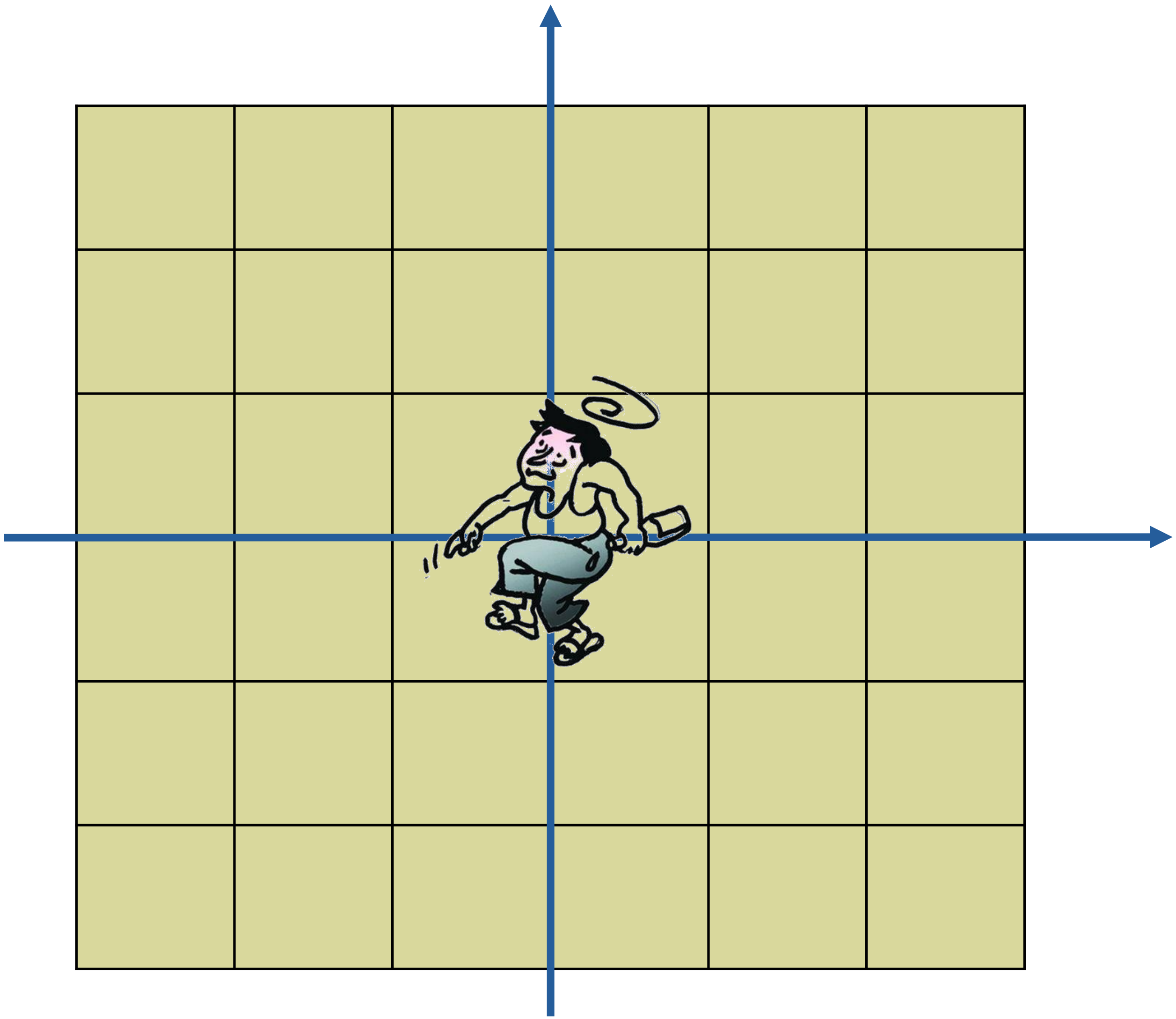
Next card to be placed in one of the slots
under the original bottom card
Original bottom card



$O(n \ln n)$

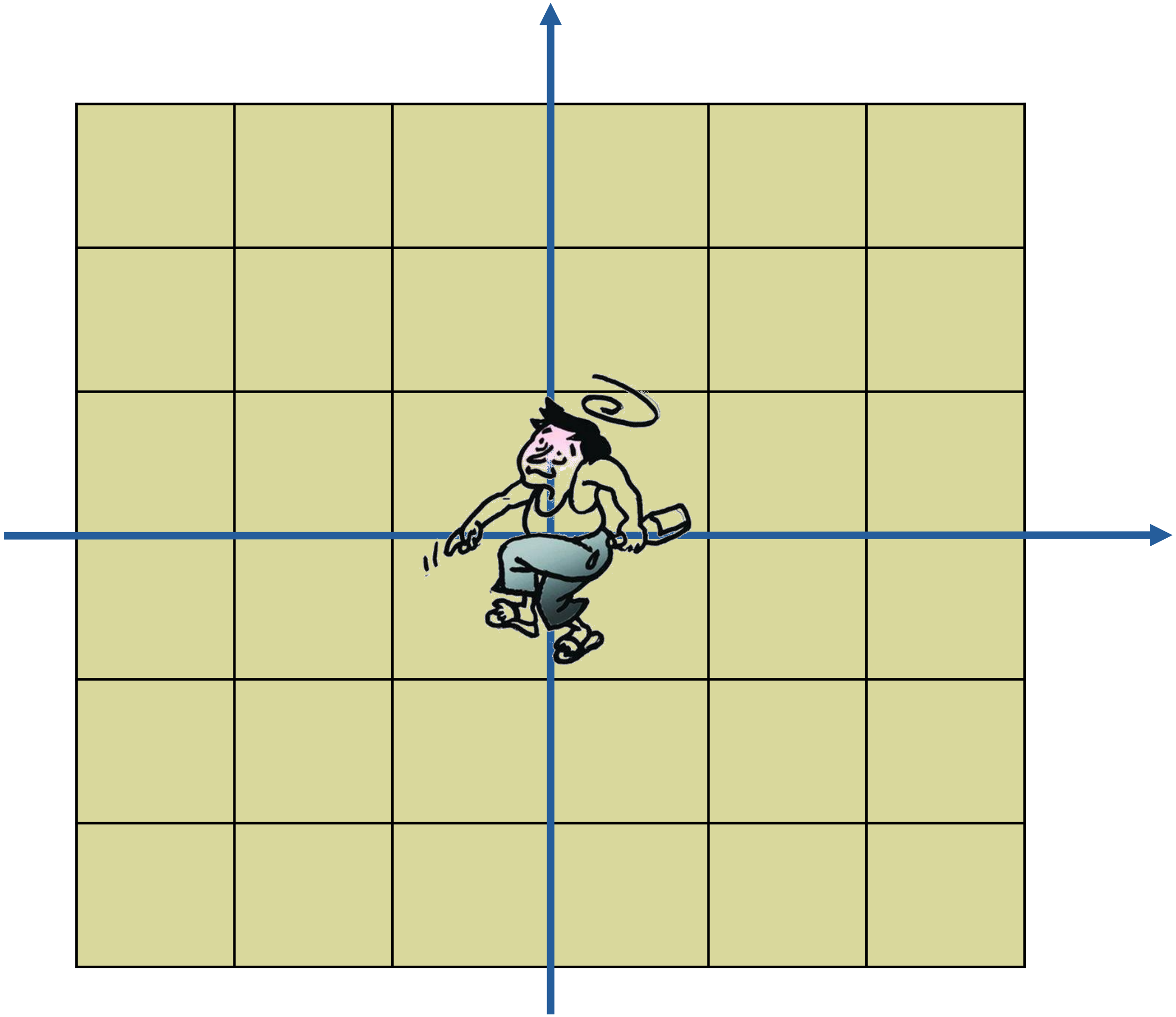
$O(\ln n)$

Random walks in Euclidean Space



George Pólya,1921

Random walks in Euclidean Space



Random walks in Euclidean Space

Random walks in Euclidean Space

- “A drunk person will always find their way home, while a drunk bird may get lost forever.”