Advanced topics in Markov-chain Monte Carlo

Lecture 1:
Transition matrices - from the balance conditions to mixing
Part 1/2: Introduction

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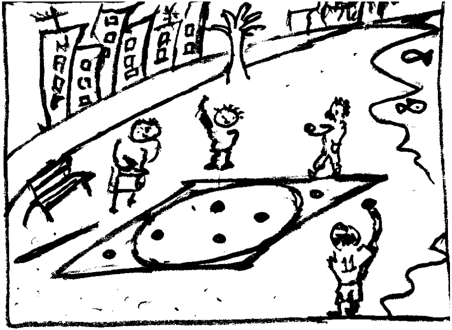
References

- W. Krauth "**Statistical Mechanics: Algorithms and Computations**" (Oxford University Press, 2006; second edition: "soon")

Monte Carlo



Direct sampling (algorithm)

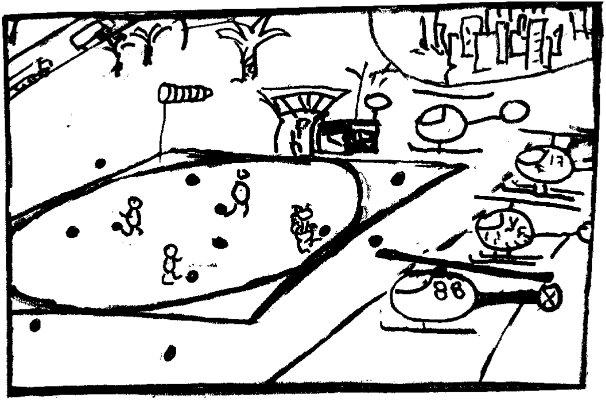
procedure `direct-pi`
$N_{\text{hits}} \leftarrow 0$ (initialize)
for $i = 1, \ldots, N$ **do**
$$\left\{ \begin{array}{l} x \leftarrow \texttt{ran}[-1,1] \\ y \leftarrow \texttt{ran}[-1,1] \\ \textbf{if } (x^2 + y^2 < 1)\ N_{\text{hits}} \leftarrow N_{\text{hits}} + 1 \end{array} \right.$$
output N_{hits}

Direct sampling (results)

Five trials with $N = 4000$

run	N_{hits}	estimation
1	3156	3.156
2	3129	3.129
3	3154	3.154
4	3134	3.134
5	3148	3.148

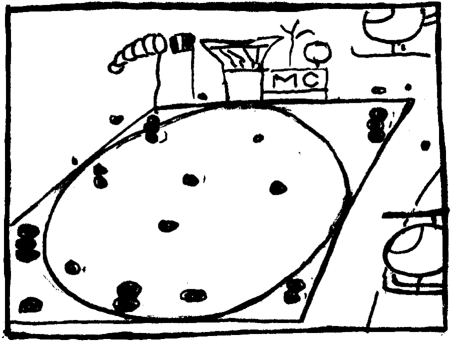
Markov-chain sampling (1/3)



Markov-chain sampling (2/3)

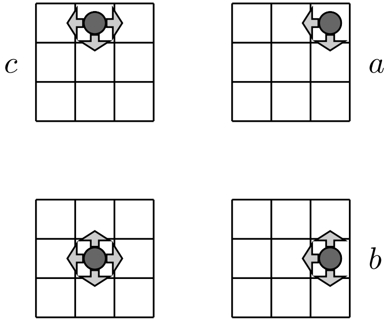
$$
\begin{array}{l}
\textbf{procedure } \texttt{markov-pi} \\
\text{hits} \leftarrow 0;\; x \leftarrow 1;\; y \leftarrow -1 \\
\textbf{for } i = 1, \ldots, N \textbf{ do} \\
\quad \left\{ \begin{array}{l}
\delta x \leftarrow \texttt{ran}[-\delta, \delta] \\
\delta y \leftarrow \texttt{ran}[-\delta, \delta] \\
\textbf{if } (|x + \delta x| < 1 \text{ and } |y + \delta y| < 1) \textbf{ then} \\
\quad \left\{ \begin{array}{l}
x \leftarrow x + \delta x \\
y \leftarrow y + \delta y
\end{array} \right. \\
\textbf{if } (x^2 + y^2 < 1)\; N_{\text{hits}} \leftarrow N_{\text{hits}} + 1
\end{array} \right. \\
\textbf{output } N_{\text{hits}}
\end{array}
$$

Markov-chain sampling (3/3)



- Metropolis et al. (1953).

3×3 pebble game



- discretized version of heliport game

Global balance—detailed balance

$$\underbrace{p(a \to a)}_{\text{probability to go from } a \text{ to } a} + p(a \to b) + p(a \to c) = 1$$

global-balance condition

$$\underbrace{\pi(a)}_{\text{probability to be at } a} = \pi(a)p(a \to a) + \pi(b)p(b \to a) + \pi(c)p(c \to a)$$

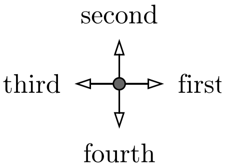
$$\pi(a)p(a \to c) + \pi(a)p(a \to b) = \pi(b)p(b \to a) + \pi(c)p(c \to a)$$

detailed-balance condition

$$\pi(a)p(a \to b) = \pi(b)p(b \to a) \quad \text{etc}$$

A priori probabilities, acceptance, implementation

7	8	9
4	5	6
1	2	3



site	Nbr(., k)			
k	1	2	3	4
1	2	4	0	0
2	3	5	1	0
3	0	6	2	0
4	5	7	0	1
5	6	8	4	2
6	0	9	5	3
7	8	0	0	4
8	9	0	7	5
9	0	0	8	6

Transition matrix

- P: matrix of conditional transition probabilities from i to j:

$$P = \begin{bmatrix}
\boxed{\frac{1}{2}} & \frac{1}{4} & \cdot & \frac{1}{4} & \cdot & \cdot & \cdot & \cdot & \cdot \\
\frac{1}{4} & \boxed{\frac{1}{4}} & \frac{1}{4} & \cdot & \frac{1}{4} & \cdot & \cdot & \cdot & \cdot \\
\cdot & \frac{1}{4} & \boxed{\frac{1}{2}} & \cdot & \cdot & \frac{1}{4} & \cdot & \cdot & \cdot \\
\frac{1}{4} & \cdot & \cdot & \boxed{\frac{1}{4}} & \frac{1}{4} & \cdot & \frac{1}{4} & \cdot & \cdot \\
\cdot & \frac{1}{4} & \cdot & \frac{1}{4} & \boxed{0} & \frac{1}{4} & \cdot & \frac{1}{4} & \cdot \\
\cdot & \cdot & \frac{1}{4} & \cdot & \frac{1}{4} & \boxed{\frac{1}{4}} & \cdot & \cdot & \frac{1}{4} \\
\cdot & \cdot & \cdot & \frac{1}{4} & \cdot & \cdot & \boxed{\frac{1}{2}} & \frac{1}{4} & \\
\cdot & \cdot & \cdot & \cdot & \frac{1}{4} & \cdot & \frac{1}{4} & \boxed{\frac{1}{4}} & \frac{1}{4} \\
\cdot & \cdot & \cdot & \cdot & \cdot & \frac{1}{4} & \cdot & \frac{1}{4} & \boxed{\frac{1}{2}}
\end{bmatrix}.$$

Algorithmic probabilities II

- initial probability vector

$$\pi^{\{t=0\}} = \{0, \ldots, 0, 1\}.$$

- probability at iteration $i+1$ from iteration i

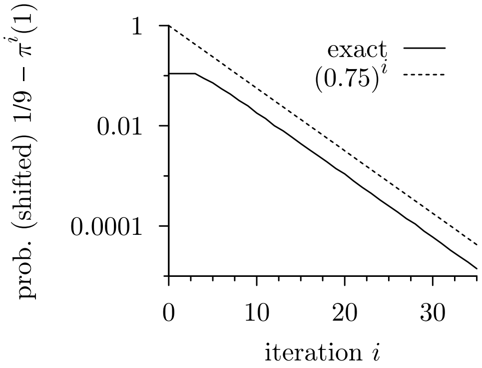
$$\pi_i^{\{t+1\}} = \sum_{j=1}^{9} \pi_j^{\{t\}} P_{j\to i}$$

- eigenvectors and eigenvalues

$$\{\pi_1^{\{t\}}, \ldots, \pi_9^{\{t\}}\} = \underbrace{\{\tfrac{1}{9}, \ldots, \tfrac{1}{9}\}}_{\substack{\text{first (left) eigenvector} \\ \text{eigenvalue } \lambda_1 = 1}} + \alpha_2 (0.75)^t \underbrace{\{-0.21, \ldots, 0.21\}}_{\substack{\text{second (left) eigenvector} \\ \text{eigenvalue } \lambda_2 = 0.75}} + \ldots$$

Transition matrices

- convergence of pebble game:

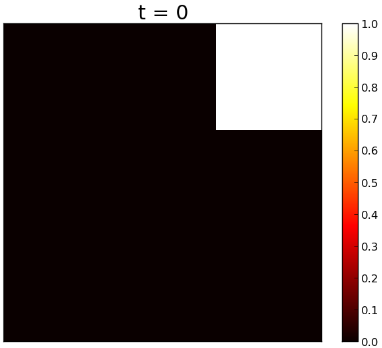


- exponential convergence ≡ scale

$$(0.75)^t = \exp\left[t \cdot \log\ 0.75\right] = \exp\left[-\frac{t}{3.476}\right].$$

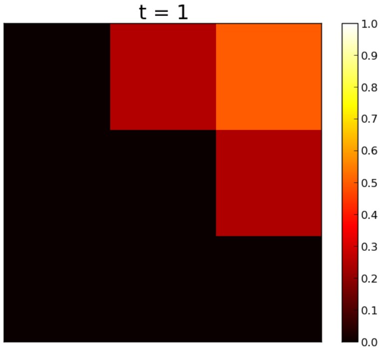
Mixing

- Distribution $\pi^{t=0}$ (starting from upper right)



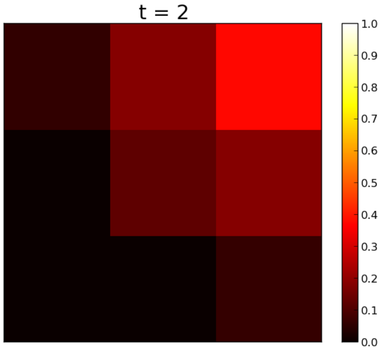
Mixing

- Distribution $\pi^{t=1}$ (starting from upper right)



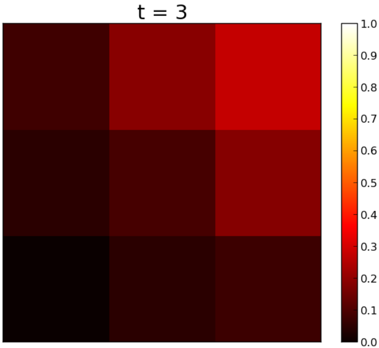
Mixing

- Distribution $\pi^{t=2}$ (starting from upper right)



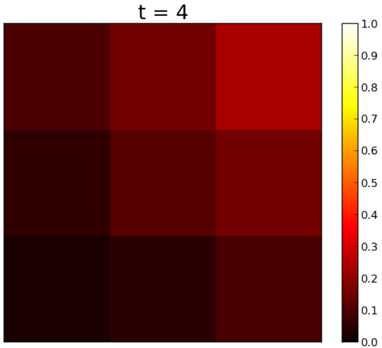
Mixing

- Distribution $\pi^{t=3}$ (starting from upper right)



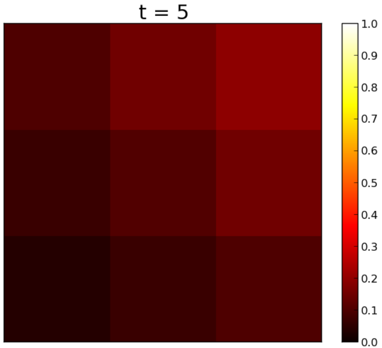
Mixing

- Distribution $\pi^{t=4}$ (starting from upper right)



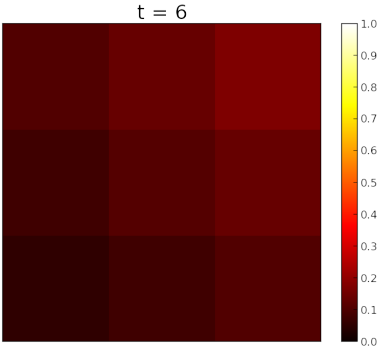
Mixing

- Distribution $\pi^{t=5}$ (starting from upper right)



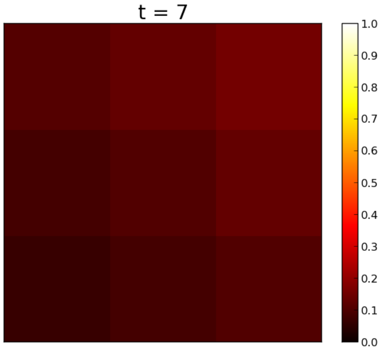
Mixing

- Distribution $\pi^{t=6}$ (starting from upper right)



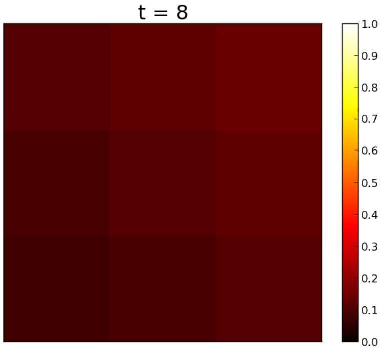
Mixing

- Distribution $\pi^{t=7}$ (starting from upper right)



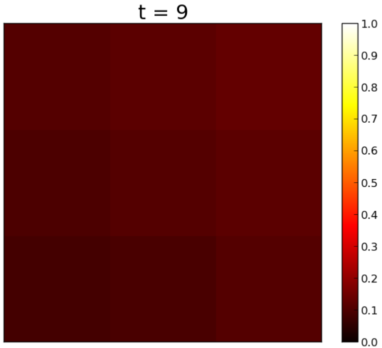
Mixing

- Distribution $\pi^{t=8}$ (starting from upper right)



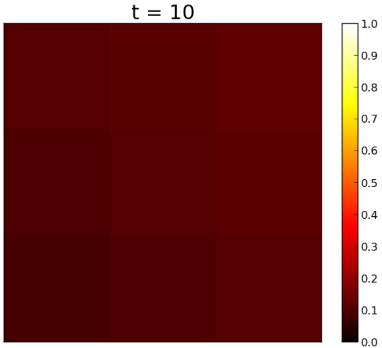
Mixing

- Distribution $\pi^{t=9}$ (starting from upper right)



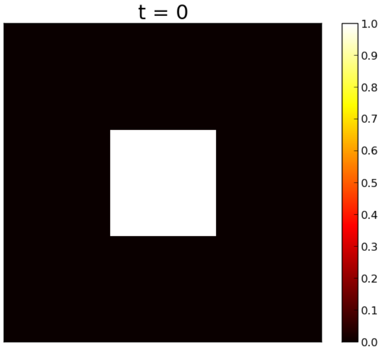
Mixing

- Distribution $\pi^{t=10}$ (starting from upper right)



Mixing

- Distribution $\pi^{t=0}$ (starting from center)



Mixing

- Distribution $\pi^{t=1}$ (starting from center)