# 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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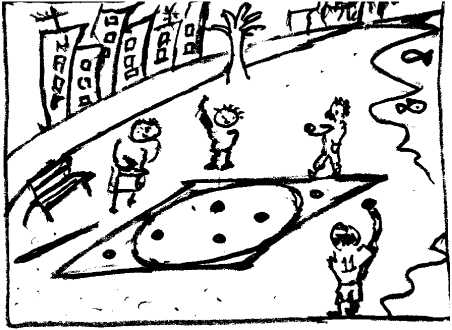
# References

- 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**

$$\left\{ \begin{array}{l} x \leftarrow \texttt{ran}[-1,1] \\ y \leftarrow \texttt{ran}[-1,1] \\ \textbf{if } (x^2 + y^2 < 1) \; N_{\text{hits}} \leftarrow N_{\text{hits}} + 1 \end{array} \right.$$

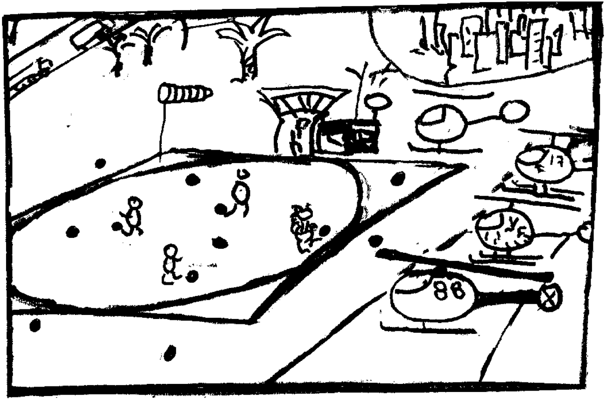
**output** $N_{\text{hits}}$

# Direct sampling (results)

Five trials with $N = 4000$

| run | $N_{\text{hits}}$ | 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)

**procedure** `markov-pi`

hits $\leftarrow 0$; $x \leftarrow 1$; $y \leftarrow -1$

**for** $i = 1, \ldots, N$ **do**

$$\left\{ \begin{array}{l} \delta x \leftarrow \texttt{ran}[-\delta, \delta] \\ \delta y \leftarrow \texttt{ran}[-\delta, \delta] \\ \textbf{if } (|x + \delta x| < 1 \text{ and } |y + \delta y| < 1) \textbf{ then} \\ \quad \left\{ \begin{array}{l} x \leftarrow x + \delta x \\ y \leftarrow y + \delta y \end{array} \right. \\ \textbf{if } (x^2 + y^2 < 1)\ N_{\text{hits}} \leftarrow N_{\text{hits}} + 1 \end{array} \right.$$

**output** $N_{\text{hits}}$

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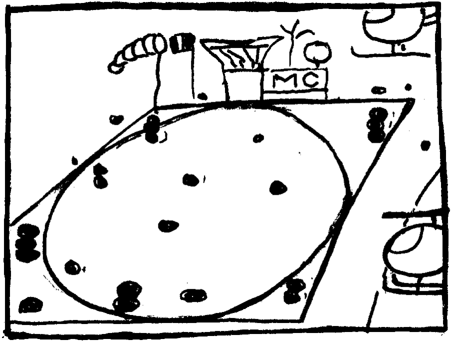
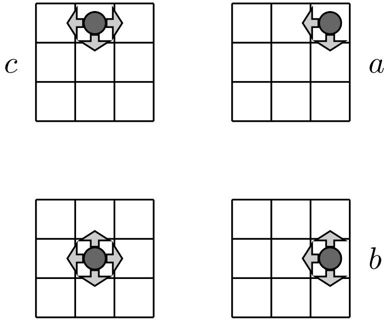
# Markov-chain sampling (3/3)




- Metropolis et al. (1953).

# 3 × 3 pebble game




- discretized version of heliport game

# Detailed balance

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

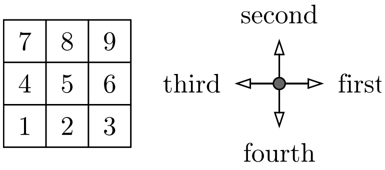
$$\underbrace{\pi(a)}_{\text{probability to be at } a} = \pi(a)p(a \to a) + \pi(b)p(b \to a) + \pi(c)p(c \to a)$$

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

## detailed balance condition

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

# A priori probabilities, acceptance, implementation




| 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 $i$

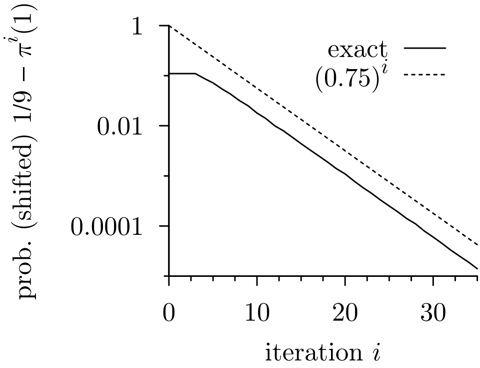
$$\pi_i^{\{t+1\}} = \sum_{j=1}^{9} \pi_j^{\{t\}} P_{j \to i}$$

- eigenvectors and eigenvalues

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

# Transition matrices

- convergence of pebble game:

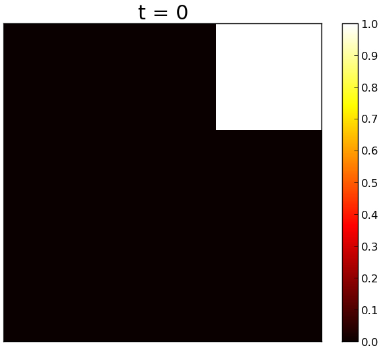



- exponential convergence $\equiv$ scale

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

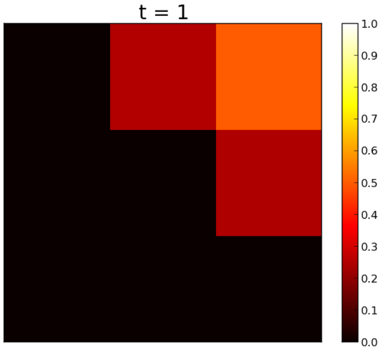
# Mixing

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



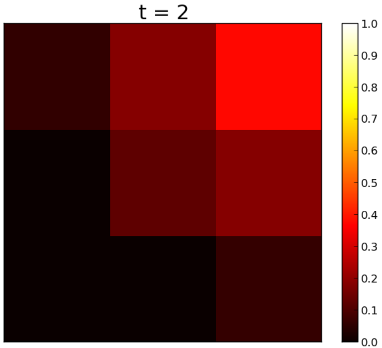
# Mixing

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



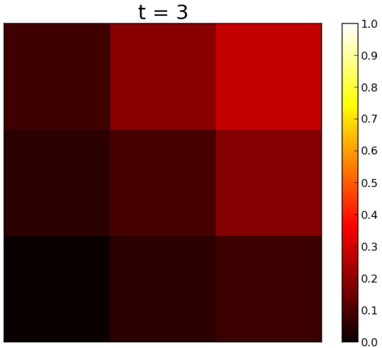
# Mixing

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



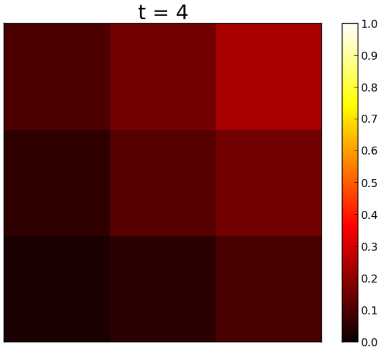
# Mixing

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



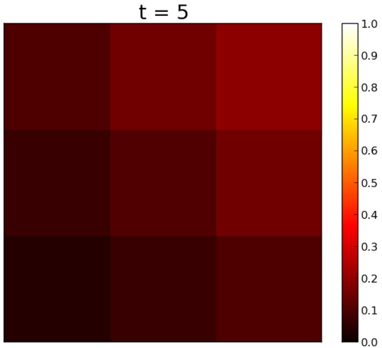
# Mixing

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



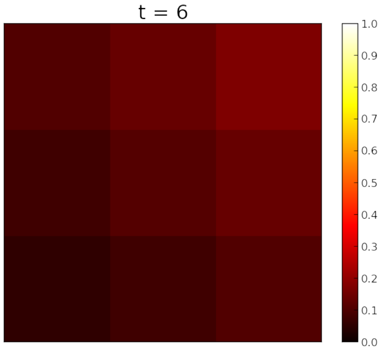
# Mixing

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



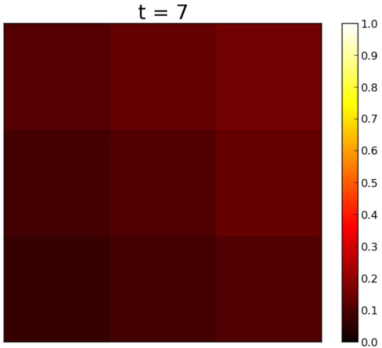
# Mixing

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



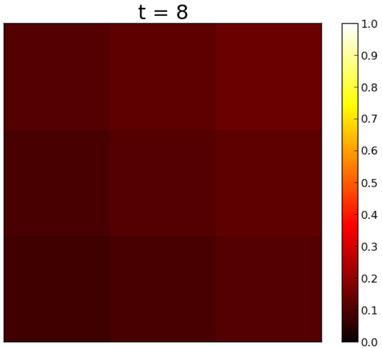
# Mixing

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



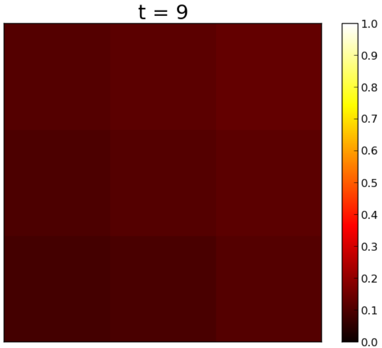
# Mixing

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



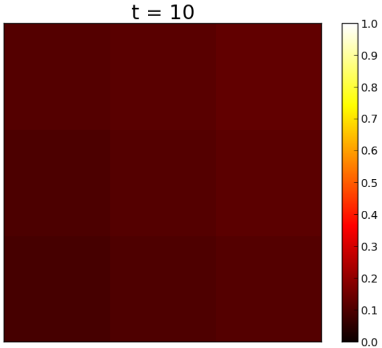
# Mixing

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



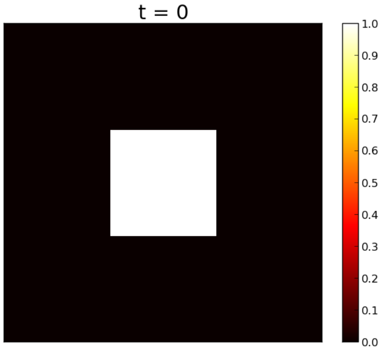
# Mixing

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



# Mixing

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



# Mixing

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