Advanced Monte Carlo algorithms

Bad Honnef Physics School

Computational Physics of Complex and Disordered Systemss

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23 September 2015

- Monte Carlo algorithms - basic notions.
- Hard disks: From detailed balance to global balance and to cluster algorithms.
- Integration and Sampling: From Gaussians to Maxwell and Boltzmann.
- Cluster algorithms for spin models: Ising, XY, Spin glasses.

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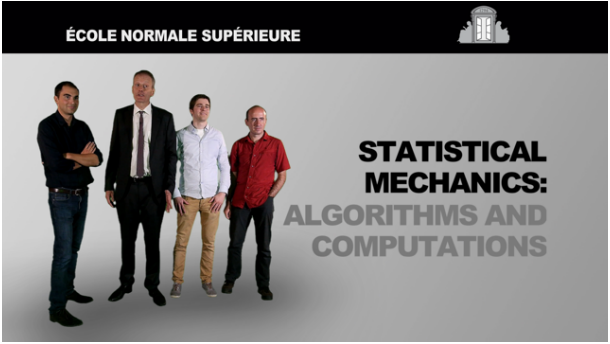
Breaking the rules

MOOC Statistical Mechanics: Algorithms and Computations



- Third edition starting in early 2016.
- 2014/15 edition reached 30,000 students.

3 × 3 pebble game

6	7	8
3	4	5
0	1	2

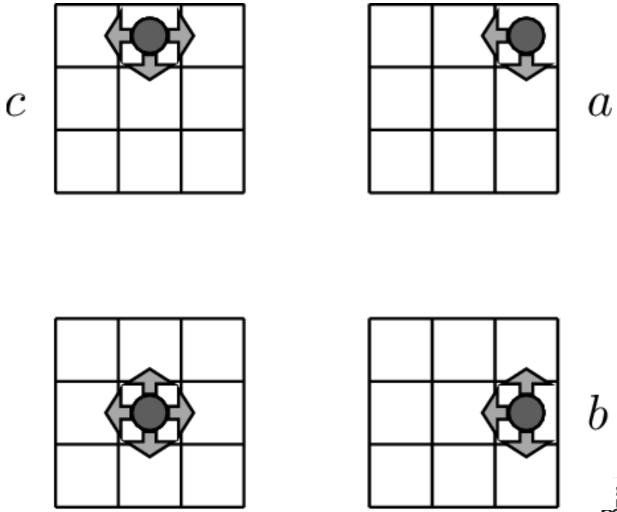
Visiting each site with equal probability:

$$\pi_k = \text{constant} \quad \forall k$$

Two sampling strategies

- Direct sampling (Buffon (1777))
- Markov-chain sampling (Metropolis et al (1953))

3×3 pebble game



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Detailed balance

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

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

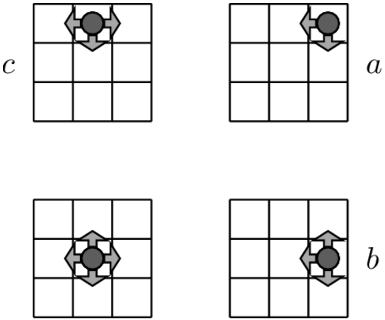
global balance condition

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

detailed balance condition

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

Detailed balance (3 × 3 pebble game)



$$p(a \to b) \stackrel{!}{=} p(b \to a)$$
$$p(a \to c) \stackrel{!}{=} p(c \to a)$$
$$p(b \to d) \stackrel{!}{=} p(d \to b)$$
$$\vdots \quad \stackrel{!}{=} \quad \vdots$$

- Only simple solution $p(\ldots \to \ldots) = \frac{1}{4}$
- implies rejections: $p(a \to a) = \frac{1}{2}$; $p(b \to b) = \frac{1}{4}$

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Pebble-basic.py

```
import random

neighbor =  [[1, 3, 0, 0], [2, 4, 0, 1], [2, 5, 1, 2],
             [4, 6, 3, 0], [5, 7, 3, 1], [5, 8, 4, 2],
             [7, 6, 6, 3], [8, 7, 6, 4], [8, 8, 7, 5]]
t_max = 4
site = 8
t = 0
print site
while t < t_max:
    t += 1
    site = neighbor[site][random.randint(0, 3)]
    print site
```

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Pebble-basic-multirun.py

```
import random

neighbor =  [[1, 3, 0, 0], [2, 4, 0, 1], [2, 5, 1, 2],
             [4, 6, 3, 0], [5, 7, 3, 1], [5, 8, 4, 2],
             [7, 6, 6, 3], [8, 7, 6, 4], [8, 8, 7, 5]]
t_max = 4
N_runs = 25600
for run in range(N_runs):
    site = 8
    t = 0
    while t < t_max:
        t += 1
        site = neighbor[site][random.randint(0, 3)]
    print site
```

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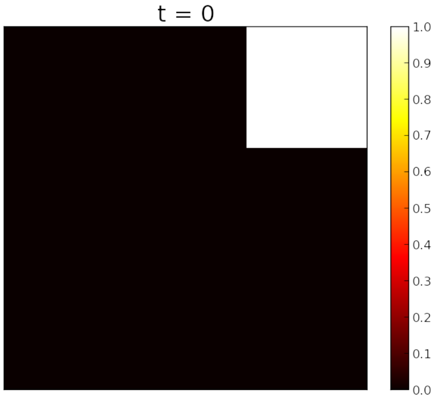
Monte Carlo simulation of the 3 × 3 pebble game



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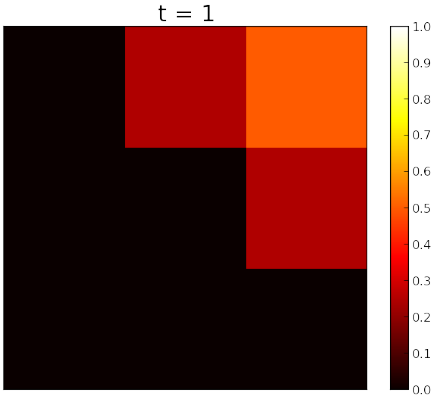
Monte Carlo simulation of the 3×3 pebble game



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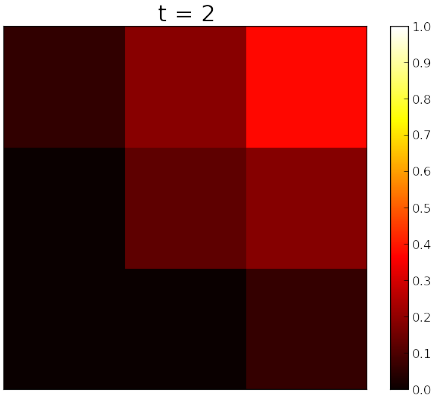
Monte Carlo simulation of the 3×3 pebble game



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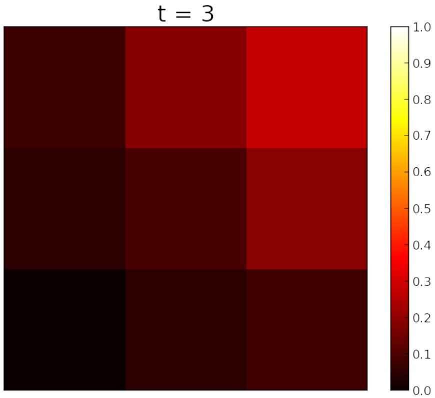
Monte Carlo simulation of the 3×3 pebble game



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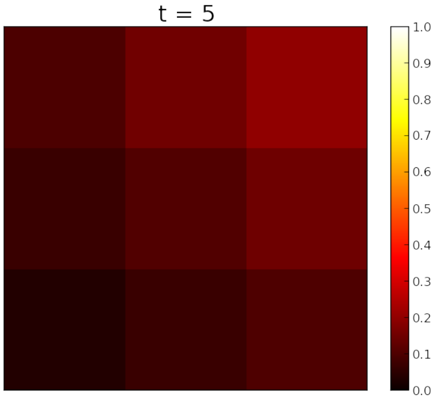
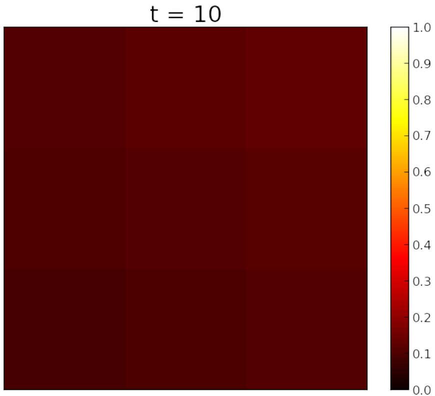
Monte Carlo simulation of the 3×3 pebble game



Monte Carlo simulation of the 3×3 pebble game



- Stationary distribution reached in the $t \to \infty$ limit

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Transfer matrix

- Algorithmic probabilities $p(a \to b)$...

$$
\{p(a \to b)\} = \begin{bmatrix}
\boxed{\frac{1}{2}} & \frac{1}{4} & \cdot & \frac{1}{4} & \cdot & \cdot & \cdot & \cdot & \cdot \\
\frac{1}{4} & \boxed{\frac{1}{4}} & \frac{1}{4} & \cdot & \frac{1}{4} & \cdot & \cdot & \cdot & \cdot \\
\cdot & \frac{1}{4} & \boxed{\frac{1}{2}} & \cdot & \cdot & \frac{1}{4} & \cdot & \cdot & \cdot \\
\frac{1}{4} & \cdot & \cdot & \boxed{\frac{1}{4}} & \frac{1}{4} & \cdot & \frac{1}{4} & \cdot & \cdot \\
\cdot & \frac{1}{4} & \cdot & \frac{1}{4} & \boxed{0} & \frac{1}{4} & \cdot & \frac{1}{4} & \cdot \\
\cdot & \cdot & \frac{1}{4} & \cdot & \frac{1}{4} & \boxed{\frac{1}{4}} & \cdot & \cdot & \frac{1}{4} \\
\cdot & \cdot & \cdot & \frac{1}{4} & \cdot & \cdot & \boxed{\frac{1}{2}} & \frac{1}{4} & \\
\cdot & \cdot & \cdot & \cdot & \frac{1}{4} & \cdot & \frac{1}{4} & \boxed{\frac{1}{4}} & \frac{1}{4} \\
\cdot & \cdot & \cdot & \cdot & \cdot & \frac{1}{4} & \cdot & \frac{1}{4} & \boxed{\frac{1}{2}}
\end{bmatrix}.
$$

Algorithmic probabilities II

- initial probability vector

$$\{\pi^0(1), \ldots, \pi^0(9)\} = \{0, \ldots, 0, 1\}.$$

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

$$\pi^{i+1}(a) = \sum_{b=1}^{9} p(b \to a)\pi^i(b)$$

- eigenvectors and eigenvalues

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

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Pebble-transfer.py

```
import numpy

neighbor =  [[1, 3, 0, 0], [2, 4, 0, 1], [2, 5, 1, 2],
             [4, 6, 3, 0], [5, 7, 3, 1], [5, 8, 4, 2],
             [7, 6, 6, 3], [8, 7, 6, 4], [8, 8, 7, 5]]
transfer = numpy.zeros((9, 9))
for k in range(9):
    for neigh in range(4): transfer[neighbor[k][neigh], k] += 0.25
position = numpy.zeros(9)
position[8] = 1.0
for t in range(100):
    print t,'  ',["%0.5f" % i for i in position]
    position = numpy.dot(transfer, position)
```

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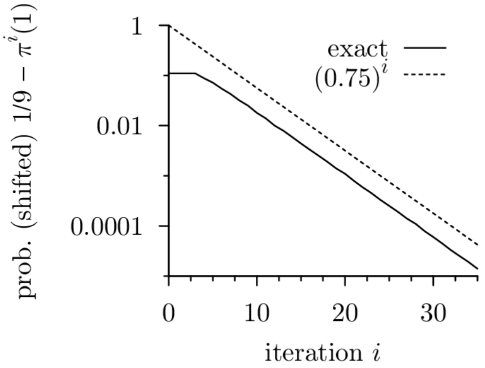
Exponential convergence in the 3×3 pebble game

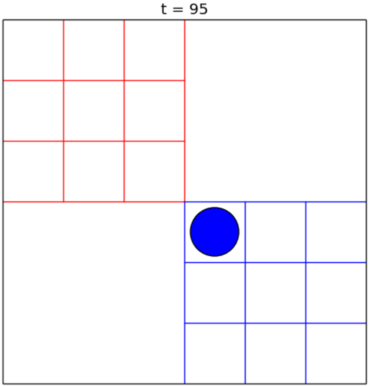
- Output of `pebble-transfer.py`:



- exponential convergence ≡ scale

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

Irreducibility 1/2 (red-blue pebble game)



This is a reducible Markov chain

- $t \to \infty$ behavior depends on initial configuration
- Multiple eigenvalues 1.

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Irreducibility 2/2 (red-blue pebble game)

$$\frac{1}{4}\begin{bmatrix}
2&1&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
1&1&1&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&1&2&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0\\
1&0&0&1&1&0&1&0&0&0&0&0&0&0&0&0&0&0\\
0&1&0&1&0&1&0&1&0&0&0&0&0&0&0&0&0&0\\
0&0&1&0&1&1&0&0&1&0&0&0&0&0&0&0&0&0\\
0&0&0&1&0&0&2&1&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&1&0&1&1&1&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&1&0&1&2&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&2&1&0&1&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&1&1&1&0&1&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&1&2&0&0&1&0&0&0\\
0&0&0&0&0&0&0&0&0&1&0&0&1&1&0&1&0&0\\
0&0&0&0&0&0&0&0&0&0&1&0&1&0&1&0&1&0\\
0&0&0&0&0&0&0&0&0&0&0&1&0&1&1&0&0&1\\
0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&2&1&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&1&1&1\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&1&2
\end{bmatrix}$$

Transfer matrix of the red-blue pebble game

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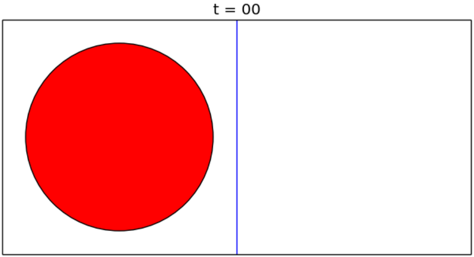
Aperiodicity 1/2



Aperiodicity 2/2

$$T = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$\lambda_1 = 1 \qquad v_1 = \begin{pmatrix} 1/2 \\ 1/2 \end{pmatrix}$$

$$\lambda_2 = -1 \qquad v_2 = \begin{pmatrix} +1/2 \\ -1/2 \end{pmatrix}$$

Convergence conditions of Markov chains

Three conditions:

- Global balance
- Irreducibility
- Aperiodicity

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Properties of Markov chains

- Independence of initial condition in $t \to \infty$ limit.
- Exponential convergence $\Rightarrow$ time scale.
- Convergence time scale related to gap of transfer matrix.
- Convergence concerns π.
- reflects in correlation functions of “slow” variables.

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Metropolis algorithm (1953)

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

is solved by the Metropolis Algorithm (1953):

$$p(a \to b) = \min\left(1, \frac{\pi(b)}{\pi(a)}\right)$$

Proof of Metropolis algorithm:

case	$\pi(a) > \pi(b)$	$\pi(b) > \pi(a)$	
$p(a \to b)$			1
$\pi(a)p(a \to b)$			2
$p(b \to a)$			3
$\pi(b)p(b \to a)$			4

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Metropolis-Hastings algorithms (a priori probabilities)

The probability to go from a to b is composite:

$$\mathcal{P}(a \to b) = \underbrace{\mathcal{A}(a \to b)}_{\text{consider } a \to b} \times \underbrace{p(a \to b)}_{\text{accept } a \to b}$$

Generalized Metropolis algorithm

$$\frac{p(a \to b)}{p(b \to a)} = \frac{\pi(b)}{\mathcal{A}(a \to b)} \frac{\mathcal{A}(b \to a)}{\pi(a)}$$

$$p(a \to b) = \min\left[1, \frac{\pi(b)}{\mathcal{A}(a \to b)} \frac{\mathcal{A}(b \to a)}{\pi(a)}\right]$$

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Breaking the Metropolis algorithm

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

is solved by the Metropolis Algorithm (1953):

$$p^{\text{MET}}(a \to b) = \min\left(1, \frac{\pi(b)}{\pi(a)}\right)$$

If $\pi(a) = \pi_0(a)\pi_1(a)\dots\pi_{n-1}(k)$, we may use:
Factorized Metropolis Algorithm (Michel et al, 2014):

$$p^{\text{FACT}}(a \to b) = \prod_k \min\left(1, \frac{\pi_k(b)}{\pi_k(a)}\right)$$

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Breaking detailed balance

Global balance

$$\underbrace{\pi(a)p(a \to c))}_{\text{Flow } P(a \to c)} + \pi(a)p(a \to b) = \pi(b)p(b \to a) + \pi(c)p(c \to a)$$

- Flow out of a = Flow into a.

Detailed balance

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

- Flow from a to b = Flow from b to a

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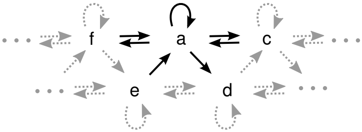
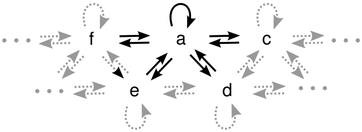
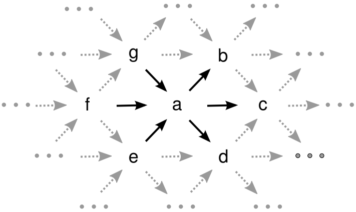
Detailed balance and global balance



global balance



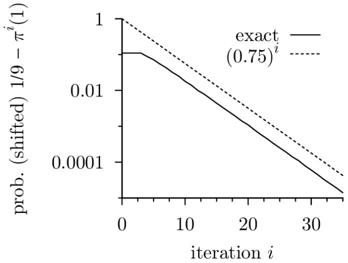
detailed balance



maximal global balance

Understanding exponential convergence

- Output of `pebble-transfer.py`:



- exponential convergence not incompatible with perfect sampling (Propp, Wilson 1996)
- Each individual realization of the Markov chain can reach total independence from initial conditions (Propp, Wilson 1996)

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Conclusions

Concepts considered:

- Sampling (direct, Markov-chain)
- Detailed balance, global balance
- Transfer matrix
- Exponential convergence
- Irreducibility
- Aperiodicity

Algorithms considered:

- pebble-basic.py
- pebble-basic-multirun.py
- pebble-transfer.py