

Advanced topics in Markov-chain Monte Carlo

Lecture 5:
Exact sampling for hard spheres
Part 1/2: Introduction / Recap

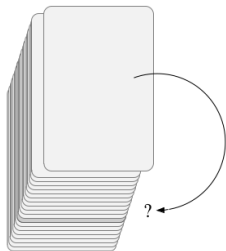
Werner Krauth

ICFP -Master Course Ecole Normale Supérieure, Paris, France

16 February 2022

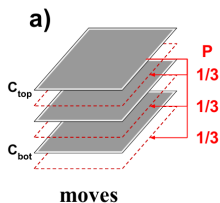
- J. G. Propp, D. B. Wilson **Exact sampling with coupled Markov chains and applications to statistical mechanics** <http://citeseerx.ist.psu.edu/viewdoc/summary?doi=10.1.1.27.1022>
- W. Krauth **“Statistical Mechanics: Algorithms and Computations”** (Oxford University Press, 2006)

Shuffling of cards 1/5



- $\Omega_N^{\text{shuffle}} = \{\text{Permutations of } \{1, \dots, N\}\}$
- For $N = 3$:
 $\Omega_3^{\text{shuffle}} = \{1 \equiv \{1, 2, 3\}, 2 \equiv \{1, 3, 2\}, 3 \equiv \{2, 1, 3\}, 4 \equiv \{2, 3, 1\}, 5 \equiv \{3, 1, 2\}, 6 \equiv \{3, 2, 1\}\}$.
- $\pi^{t=0} = \delta((1, \dots, N))$

Shuffling of cards 2/5

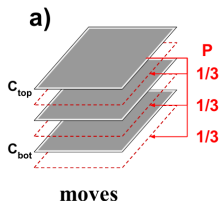


- $\Omega_3^{\text{shuffle}} = \{1 \equiv \{1, 2, 3\}, 2 \equiv \{1, 3, 2\}, 3 \equiv \{2, 1, 3\}, 4 \equiv \{2, 3, 1\}, 5 \equiv \{3, 1, 2\}, 6 \equiv \{3, 2, 1\}\}$.



$$P = \frac{1}{3} \begin{pmatrix} 1 & 0 & 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 1 \end{pmatrix}$$

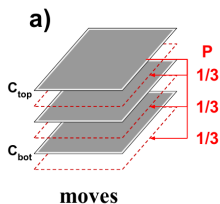
Shuffling of cards 3/5



```
procedure top-to-random
input  $\{c_1, \dots, c_n\}$ 
 $i \leftarrow \text{choice}(\{1, \dots, n\})$ 
 $\{\hat{c}_1, \dots, \hat{c}_n\} \leftarrow \{c_2, \dots, c_i, c_1, c_{i+1}, \dots, c_n\}$ 
output  $\{\hat{c}_1, \dots, \hat{c}_n\}$ 
```

- Insert upper card (c_1) after card i and before card $i + 1$
- NB: if $i = 1$, put it back on top.

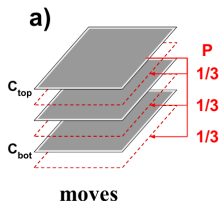
Shuffling of cards 4/5



```
procedure top2random-stop
input  $\{c_1, \dots, c_n\}$ 
 $c_{\text{first-}n} \leftarrow c_n$ 
for  $t = 1, 2, \dots$  do
     $\begin{cases} \tilde{c}_1 \leftarrow c_1 \\ \{c_1, \dots, c_n\} \leftarrow \text{top2random}(\{c_1, \dots, c_n\}) \\ \text{if } (\tilde{c}_1 = c_{\text{first-}n}) \text{ break} \end{cases}$ 
output  $\{c_1, \dots, c_n, t\}$ 
```

- Expected running time: $n \log n$.
- Closely related to $\mathcal{O}(n)$ algorithm for random permutations.

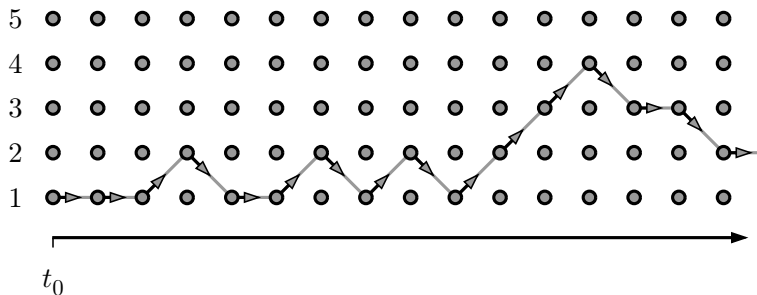
Shuffling of cards 5/5



```
procedure direct-shuffle
input  $\{c_1, \dots, c_n\}$ 
for  $t = 1, \dots, n$  do
     $i \leftarrow \text{choice}(\{n - t + 1, \dots, n\})$ 
     $\{c_1, \dots, c_n\} \leftarrow \{c_2, \dots, c_i, c_1, c_{i+1}, \dots, c_n\}$ 
output  $\{c_1, \dots, c_n\}$ 
```

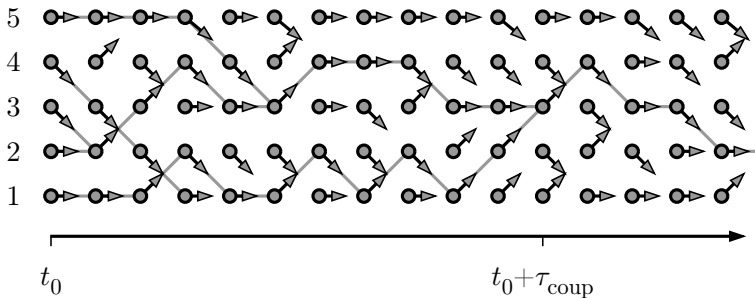
- Running time: n .
- Standard algorithm for generating random permutations.

Markov chain (traditional view)



- Configuration c_t , move δ_t .
- Set $t_0 = 0$.

Markov chain (random maps), coupling 1/4



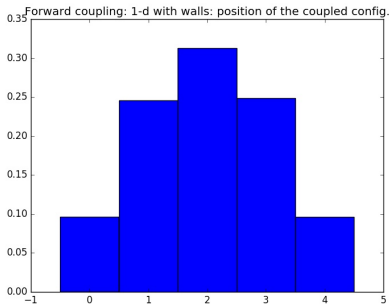
- Each configuration has its move at each time step.
- Coupling (Doebelin, 1930s).

Markov chain (random maps), coupling 2/4

```
pos=[]
for stat in range(10000):
    posit=set(range(N))
    for t in range(1000000):
        posit = set([min(max(b + random.randint(-1, 1), 0), N - 1) for b in posit])
        if len(posit) == 1: break
    pos.append(posit.pop())
```

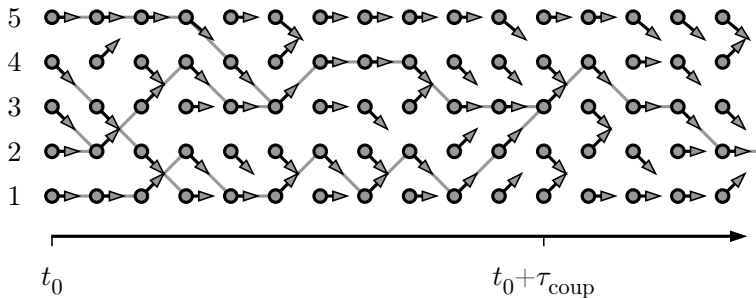
- Position of coupling not uniform.
- Coupling time larger than mixing time.

Markov chain (random maps), coupling 3/4



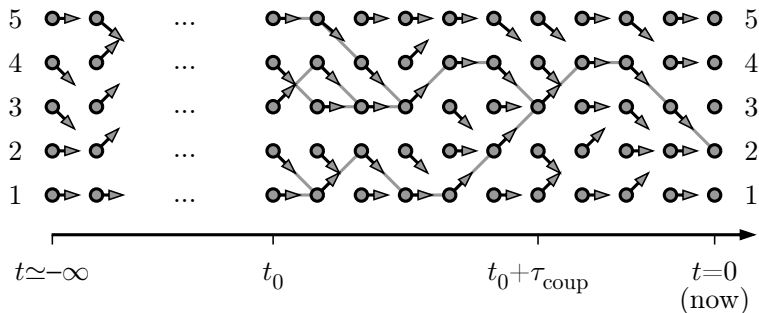
- Histogram of coupling position.

Markov chain (random maps), coupling 4/4



- Each configuration has its move at each time step.
- Coupling (Doebelin, 1930s).

Coupling from the past 1/8



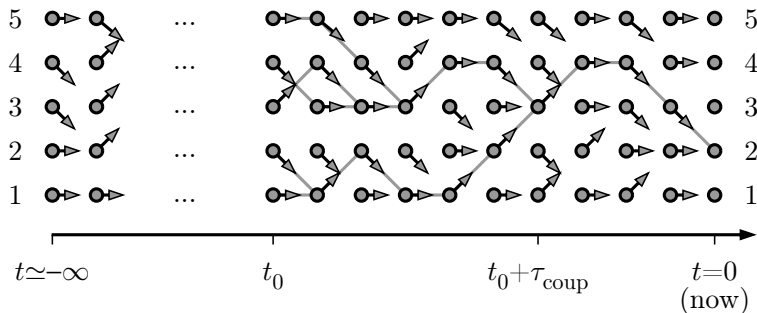
- Starting an MCMC simulation at $t = -\infty$
- Propp & Wilson (1997)

Coupling from the past 2/8

```
pos = []
for statistic in range(100000):
    all_arrows = {}
    time_tot = 0
    while True:
        time_tot -= 1
        arrows = [random.randint(-1, 1) for i in range(N)]
        if arrows[0] == -1: arrows[0] = 0
        if arrows[N - 1] == 1: arrows[N - 1] = 0
        all_arrows[time_tot]=arrows
        positions=set(range(0, N))
        for t in range(time_tot, 0):
            positions = set([b + all_arrows[t][b] for b in positions])
            if len(positions) == 1: break
        if len(positions) == 1: break
```

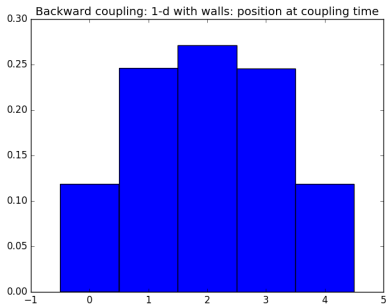
- Starting an MCMC simulation at $t = -\infty$
- Propp & Wilson (1997)

Coupling from the past 3/8



- Starting an MCMC simulation at $t = -\infty$
- Propp & Wilson (1997)

Coupling from the past 4/8



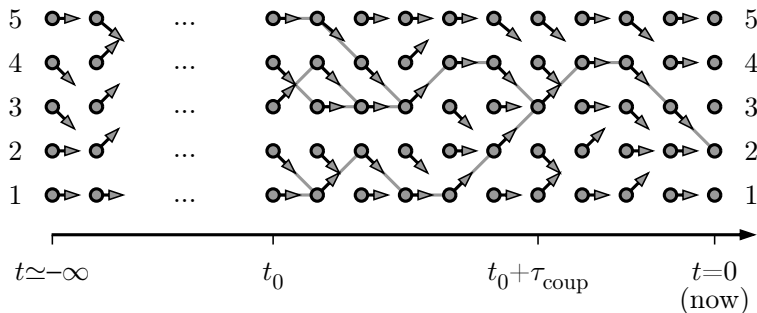
- Coupling position (in the past) non-uniform)

Coupling from the past 5/8

```
for statistic in range(10000):
    all_arrows = {}
    time_tot = 0
    while True:
        time_tot -= 1
        old_pos = set(range(0, N))
        arrows = [random.randint(-1, 1) for i in range(N)]
        if arrows[0] == -1: arrows[0] = 0
        if arrows[N - 1] == 1: arrows[N - 1] = 0
        all_arrows[time_tot] = arrows
        positions = set(range(N))
        for t in range(time_tot, 0):
            positions = set([b + all_arrows[t][b] for b in positions])
        if len(positions) == 1: break
    a=positions.pop()
    pos.append(a)
```

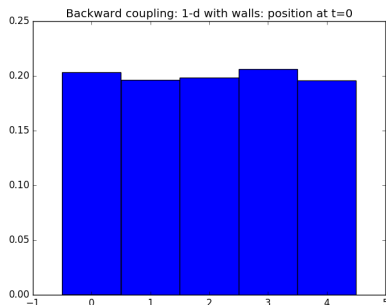
- Dictionary of random maps going back in time.

Coupling from the past 6/8



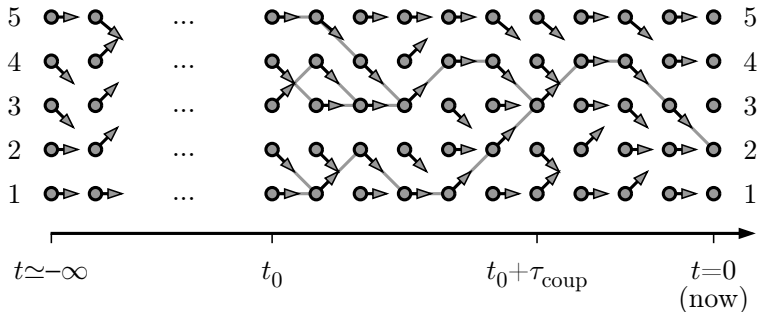
- Starting an MCMC simulation at $t = -\infty$
- Propp & Wilson (1997)

Coupling from the past 7/8



- Perfect sample at $t = 0$, starting from $t = -\infty$
- Propp & Wilson (1997)

Coupling from the past 8/8



- Try it yourself!