

# Markov-chain Monte Carlo: A modern primer

Lecture 1: Fundamentals

Part 2/2: Single particle on the path graph

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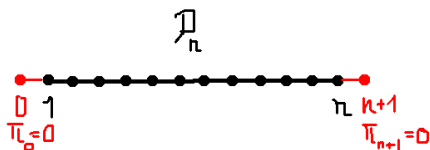
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28 February 2022

# References

- F. Chen, L. Lovasz, I. Pak, **Lifting Markov Chains to Speed up Mixing**. Proceedings of the 17th Annual ACM Symposium on Theory of Computing, 275 (1999) <http://www.math.ucla.edu/~pak/papers/stoc2.pdf>
- P. Diaconis, S. Holmes, R. M. Neal, **Analysis of a nonreversible Markov chain sampler** Ann. Appl. Probab. 10, 726–752 (2000) [https://projecteuclid.org/download/pdf\\_1/euclid.aoap/1019487508](https://projecteuclid.org/download/pdf_1/euclid.aoap/1019487508)
- M. Hildebrand, **Rates of convergence of the Diaconis-Holmes-Neal Markov chain sampler with a V-shaped stationary probability**, Markov Proc. Rel. Fields 10, 687–704 (2004)
- W. Krauth, **Event-Chain Monte Carlo: Foundations, Applications, and Prospects**, Front. Phys. 9:663457. <https://www.frontiersin.org/article/10.3389/fphy.2021.663457>

# Metropolis algorithm on path graph (1/5)

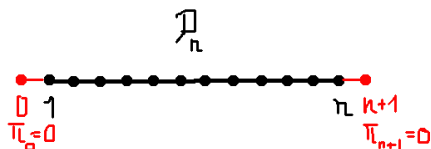


- Path graph  $\mathcal{P}_n$  so that  $\Omega_n = \{1, \dots, n\}$ .
- **Phantom vertices and edges.**

Metropolis algorithm (NB:  $P_{ij} = \mathcal{A}_{ij}P_{ij}$  for  $i \neq j$ ):

- 1 Move set  $\mathcal{L} = \{+, -\}$ .
- 2  $\mathcal{A}$  flat  $\rightarrow \sigma = \text{choice}(\mathcal{L})$ .
- 3 Metropolis filter: Accept with probability  $\min(1, \pi_j/\pi_i)$ .

# Metropolis algorithm on path graph (2/5)



- Detailed balance:

$$\underbrace{\pi_i P_{ij}}_{\mathcal{F}_{ij}} = \underbrace{\pi_j P_{ji}}_{\mathcal{F}_{ji}}$$

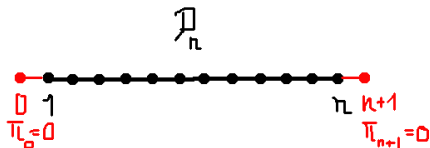
- Metropolis **algorithm**:

$$\mathcal{F}_{ij} = \frac{1}{2} \min(\pi_i, \pi_j) \Leftrightarrow P_{ij} = \frac{1}{2} \min(1, \pi_j/\pi_i)$$

- Metropolis **filter** (NB:  $P_{ij} = \mathcal{A}_{ij} P_{ij}$ ):

$$\mathcal{P}_{ij} = \min(1, \pi_j/\pi_i)$$

# Metropolis algorithm on path graph (3/5)



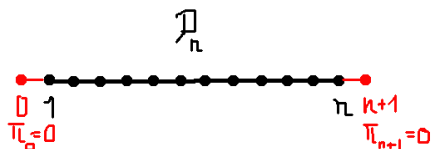
- Global balance ( $\pi_i = \sum_j \pi_j P_{ji} = \sum_j \mathcal{F}_{ji}$ ):

$$\underbrace{\pi_i - \frac{1}{2} \min(\pi_i, \pi_{i-1}) - \frac{1}{2} \min(\pi_i, \pi_{i+1})}_{\text{curved arrow}}$$

$$\boxed{i-1} \begin{array}{c} \xrightarrow{\frac{1}{2} \min(\pi_{i-1}, \pi_i)} \\ \xleftarrow{\frac{1}{2} \min(\pi_i, \pi_{i-1})} \end{array} \boxed{i} \begin{array}{c} \xrightarrow{\frac{1}{2} \min(\pi_i, \pi_{i+1})} \\ \xleftarrow{\frac{1}{2} \min(\pi_{i+1}, \pi_i)} \end{array} \boxed{i+1}$$

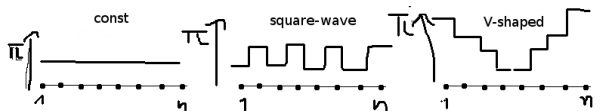
- Irreducibility **OK** if no holes in  $\pi$ .
- Aperiodicity **OK**, thanks to boundaries

# Metropolis algorithm on path graph (4/5)



```
procedure metro-path
input  $x$ 
 $\sigma \leftarrow \text{choice}(\mathcal{L})$  ( $\mathcal{L} = \{-1, +1\}$ )
if ( $\text{ran}(0, 1) < \pi_{x+\sigma} / \pi_x$ ) then
  {  $x_i \leftarrow x_i + \sigma$ 
output  $x$ 
```

# Metropolis algorithm on path graph (5/5)



Model	Definition	Conductance	$t_{\text{mix}}$
Flat	$\pi_i = \frac{1}{n}$	$\mathcal{O}(1/n)$	$\mathcal{O}(n^2)$
Square	$\pi_{2k-1} = \frac{2}{3n}, \pi_{2k} = \frac{4}{3n}$	$\sim 2/(3n)$	$\mathcal{O}(n^2)$
V-shape	$\pi_i = \frac{4}{n^2} \left  \frac{n+1}{2} - i \right $	$\sim 2/n^2$	$\mathcal{O}(n^2 \log n)$

NB: Graph diameter  $n$ .

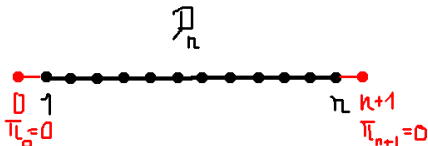
NNB:  $\pi$  normalized.

NNNB: Bottleneck between  $i = \frac{n}{2}$  and  $j = \frac{n}{2} + 1$ .

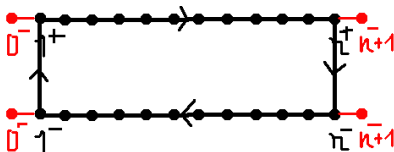
# Lifting on the path graph (1/7)

Probability distribution  $\pi = (1/n, \dots, 1/n)$  (Diaconis et al. 2000)

- “Collapsed” Markov chain:



- “Lifted” Markov chain  $\hat{\Omega} = \Omega \times \{-, +\}$ :



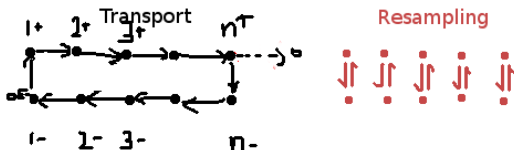
- Irreducible, but not aperiodic.  $\hat{\pi}_{i,\sigma} = \frac{1}{2}\pi_i = 1/(2n)$



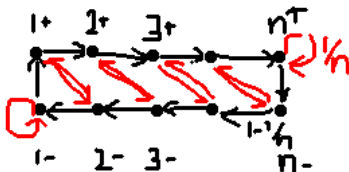
# Lifting on the path graph (2/7)

Probability distribution  $\pi = (1/n, \dots, 1/n)$  (Diaconis et al. 2000)

- Transport + **resampling**



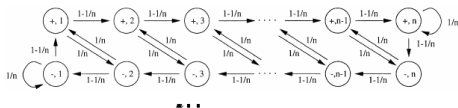
- “Lifted” Markov chain  $\hat{\Omega} = \Omega \times \{-, +\}$ :



# Lifting on the path graph (3/7)

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P. DIACONIS, S. HOLMES AND R. M. NEAL



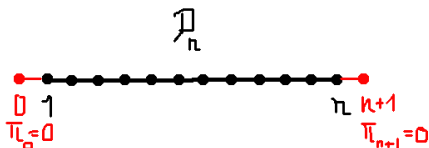
The transition matrix is doubly stochastic, and thus the stationary distribution is uniform.

- Diaconis, Holmes, Neal (2000).
- $\Omega$  (samples) +  $\mathcal{L}$  (moves)  $\rightarrow \hat{\Omega} = \Omega \times \mathcal{L}$  (lifted samples)
- Resampling with rate  $1/n$ .
- **Phantoms** illustrate the “rejection  $\rightarrow$  lifting” mystery.
- Let’s generalize.

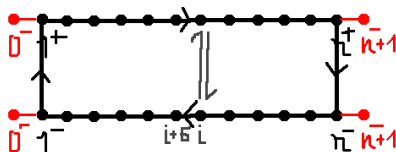
# Lifting on the path graph (4/7)

General probability distribution  $\pi = (\pi_1, \dots, \pi_n)$

- “Collapsed” Markov chain:



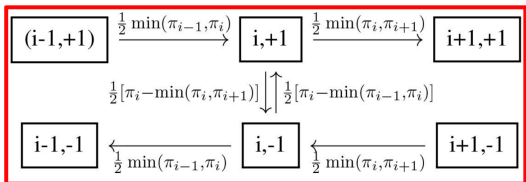
- “Lifted” Markov chain  $\hat{\Omega} = \Omega \times \{-, +\}$ :



- Replace all rejections by lifting moves.

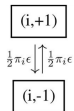
# Lifting on the path graph (5/7)

- “Lifted Markov chain: **Transport**”



NB: The  $\frac{1}{2} \Leftrightarrow \hat{\pi}_{i,\sigma} = \frac{1}{2} \pi_i$

- “Lifted Markov chain: **Resampling**”



- Resampling can often be dropped

# Lifting on the path graph (6/7)

- **Transport**

```
procedure transport-path
input {x,  $\sigma$ } (configuration  $\in \widehat{\Omega} = \Omega \times \{+, -\}$ )
if (ran(0, 1) <  $\pi_{x+\sigma}/\pi_x$ ) then
  {  $x_i \leftarrow x_i + \sigma$  }
else
  {  $\sigma \leftarrow -\sigma$  }
output {x,  $\sigma$ }
```

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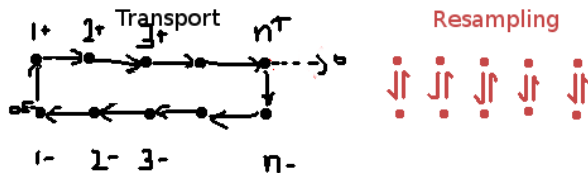
- **Resampling**

```
procedure resample-path
input {x,  $\sigma$ } (configuration  $\in \widehat{\Omega} = \Omega \times \{+, -\}$ )
if (ran(0, 1) < p) then (p: resampling rate)
  {  $\sigma \leftarrow -\sigma$  }
output {x,  $\sigma$ }
```

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- **Mix freely!**

# Lifting on the path graph (7/7)



Model	Conductance	$t_{\text{mix}}$ (collapsed)	$t_{\text{mix}}$ (lifted)
Flat	$\mathcal{O}(1/n)$	$\mathcal{O}(n^2)$	$\mathcal{O}(n)$
Square	$\mathcal{O}(1/n)$	$\mathcal{O}(n^2)$	$\mathcal{O}(n^2)$
V-shape	$\mathcal{O}(1/n^2)$	$\mathcal{O}(n^2 \log n)$	$\mathcal{O}(n^2)$