Assorted Topics in the Monte Carlo Simulation of Polymers

Nathan Clisby
MASCOS / Department of Mathematics and Statistics
The University of Melbourne

SIAM Conference on Discrete Mathematics
Minneapolis
June 19, 2014

Outline

- Self-avoiding walks

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- Pivot algorithm

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- Conclusion

Self-avoiding walk model

- A walk on a lattice, step to neighbouring site provided it has not already been visited.

Simple random walk

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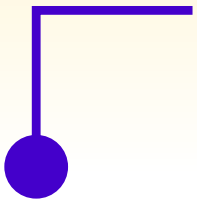

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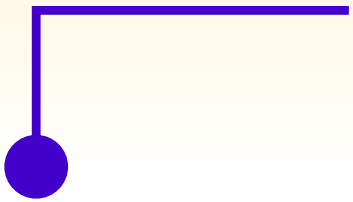

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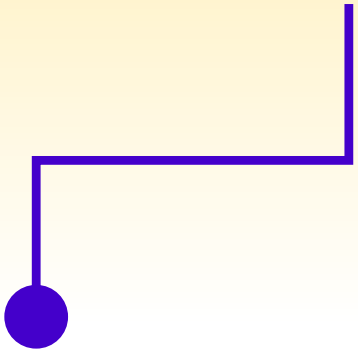

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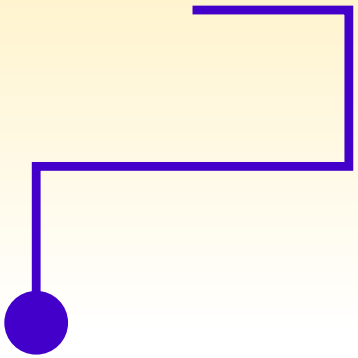

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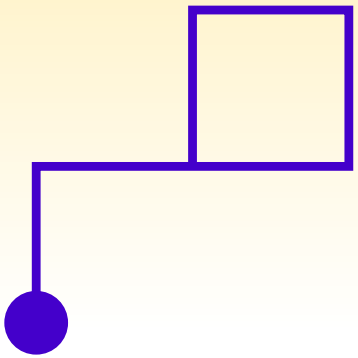

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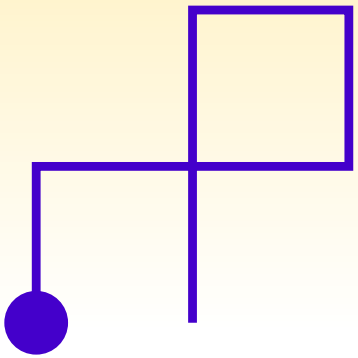

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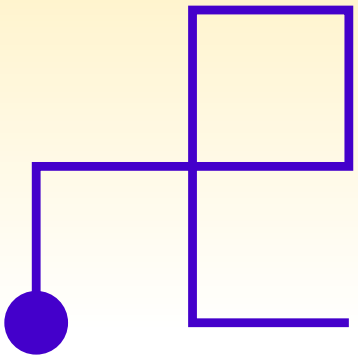

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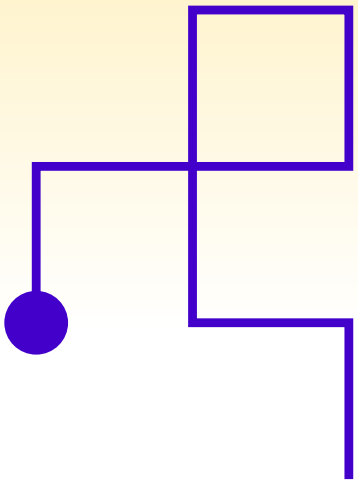

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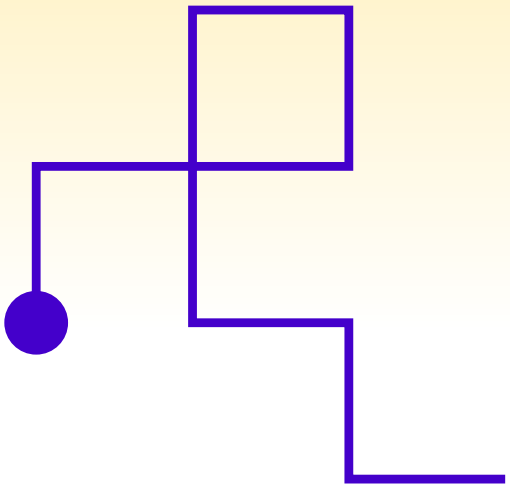

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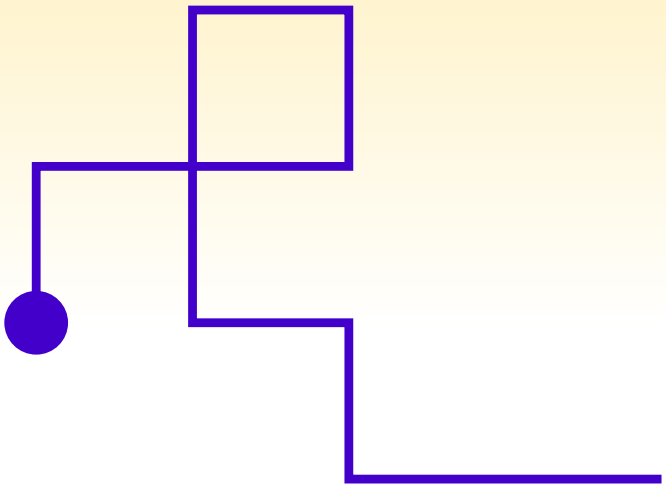

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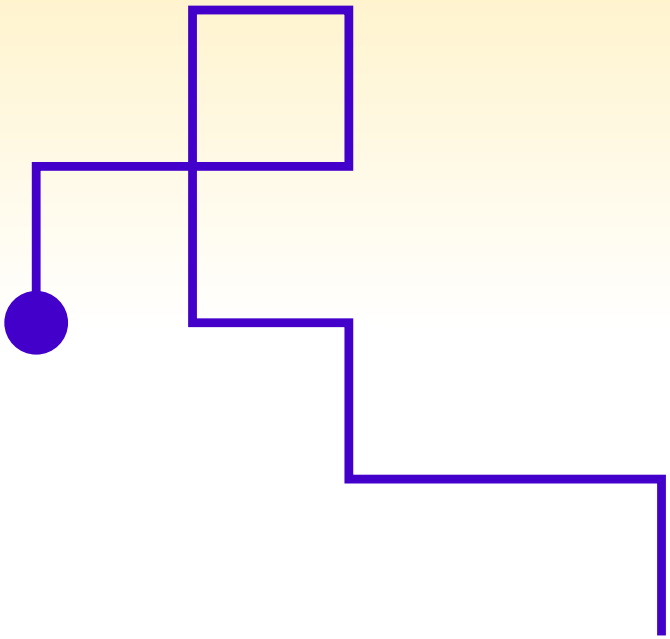

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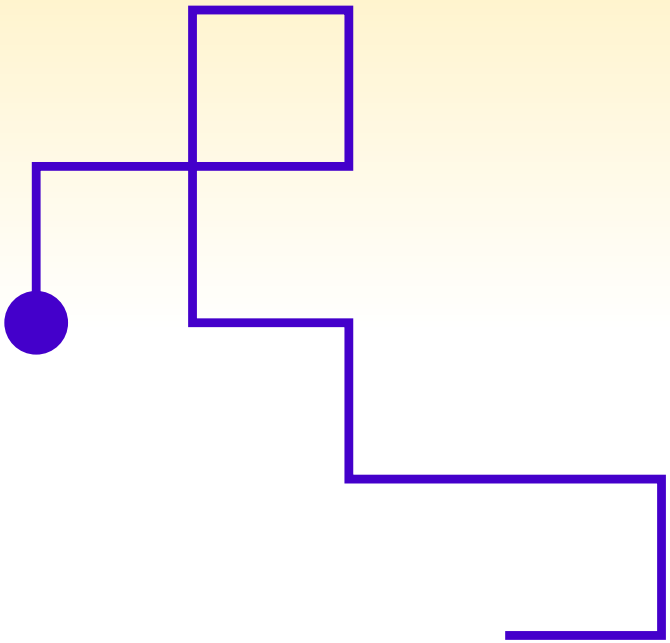

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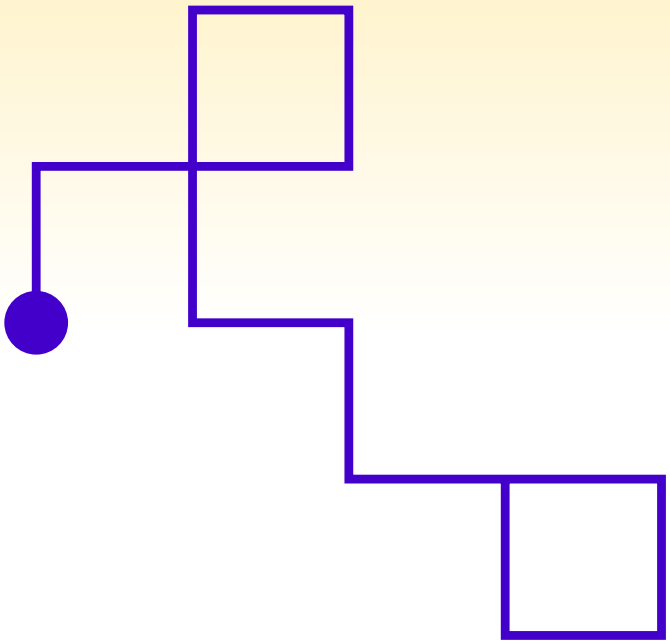

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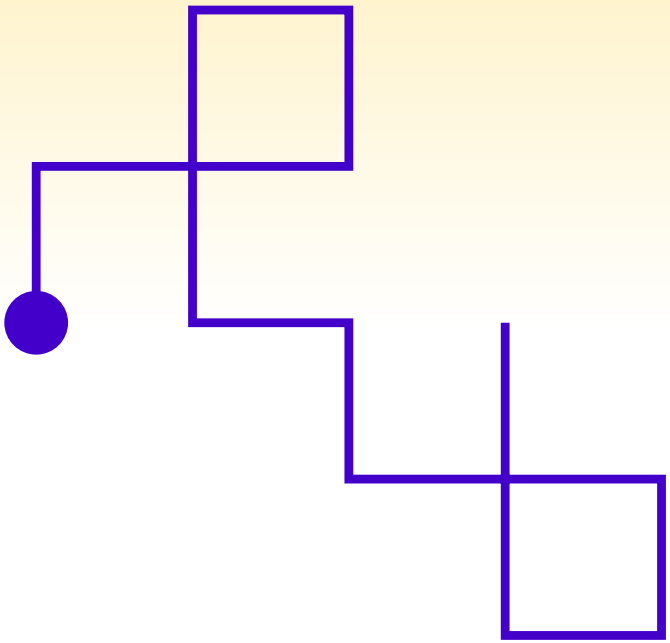

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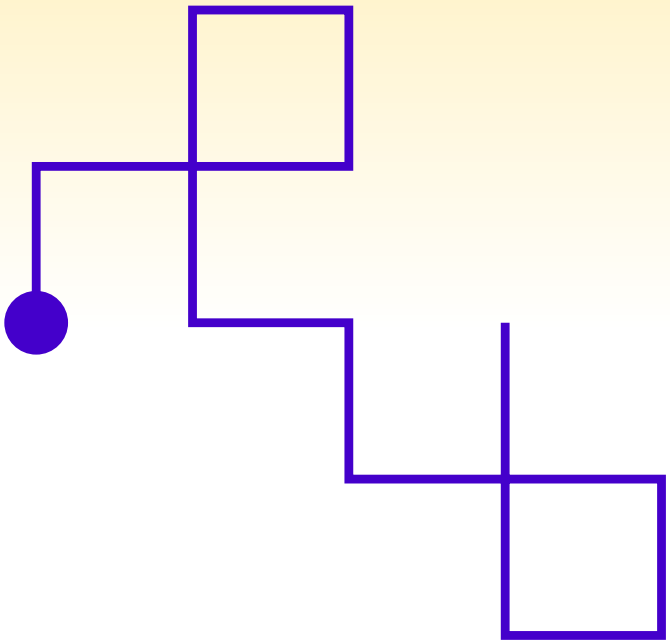

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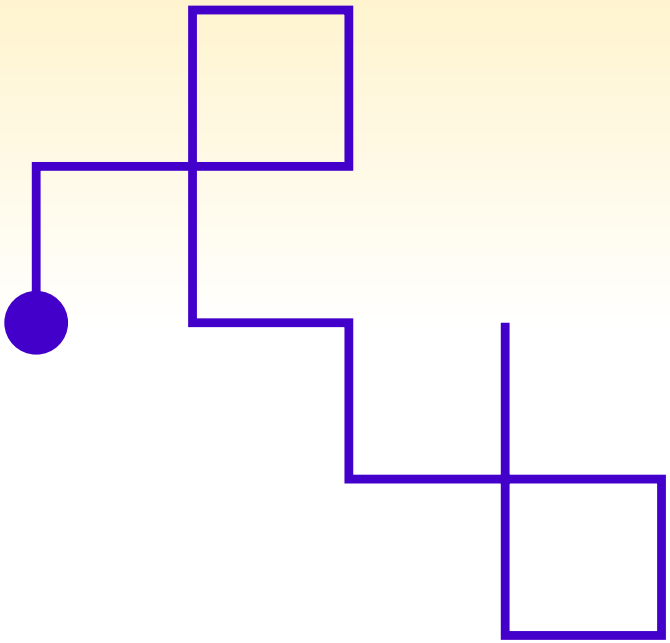

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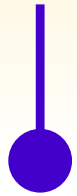

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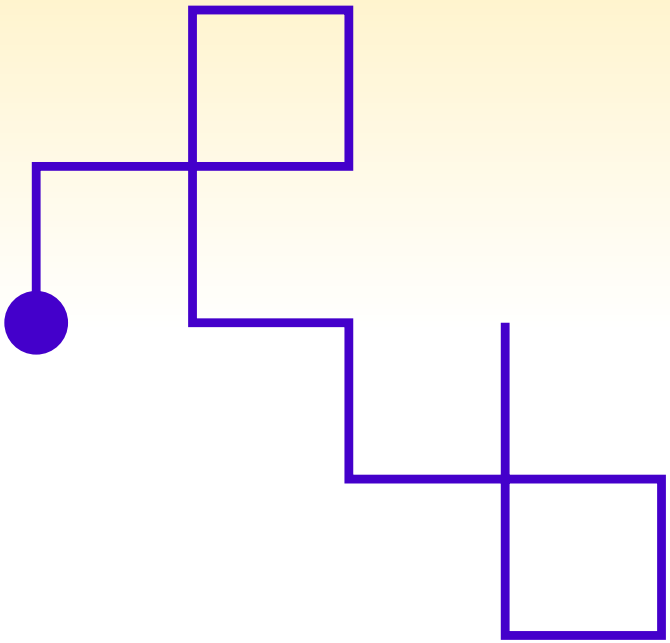

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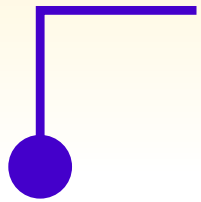

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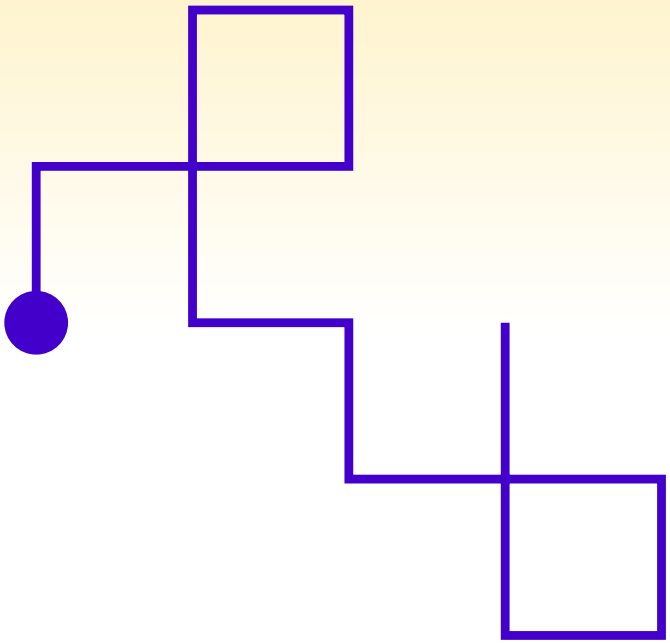

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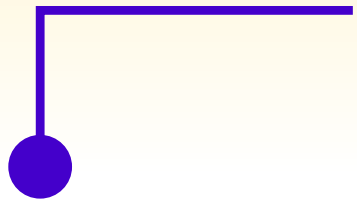

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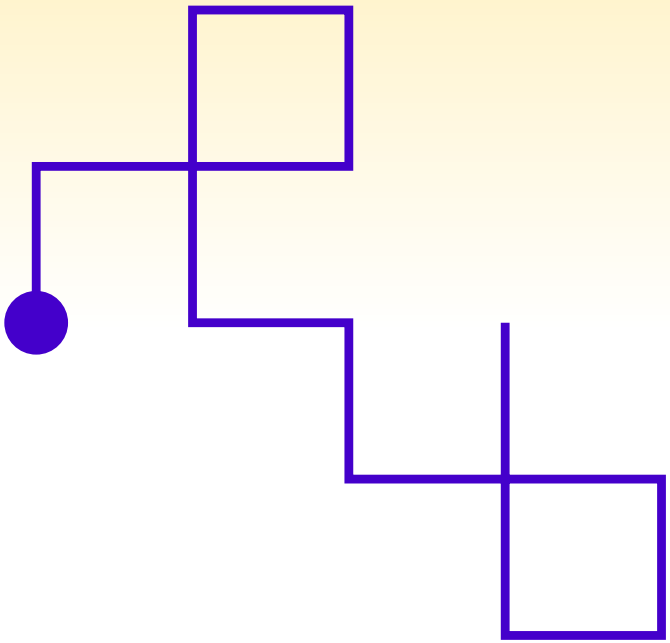

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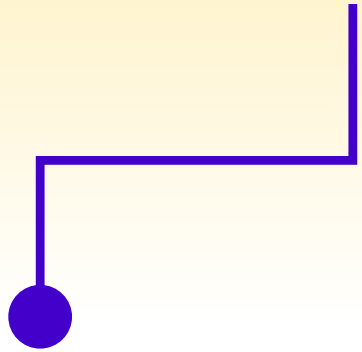

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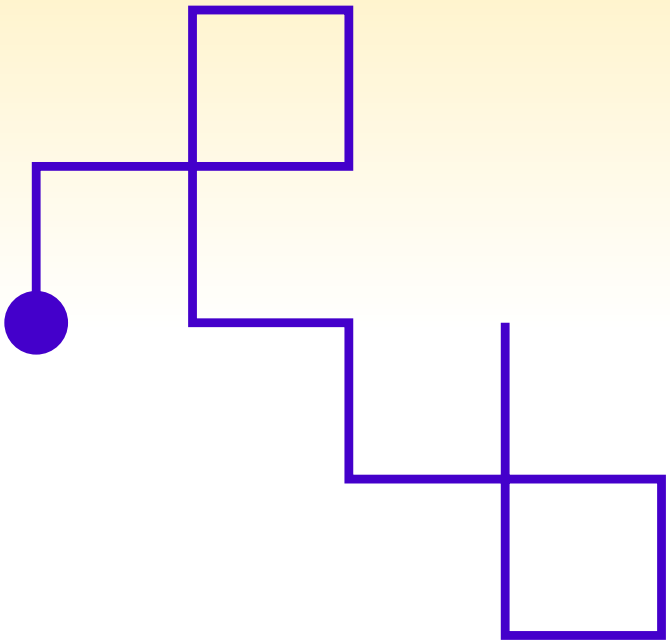

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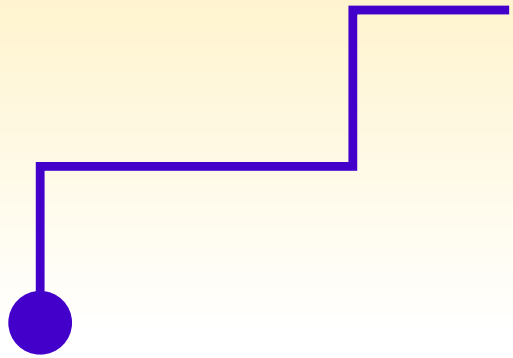

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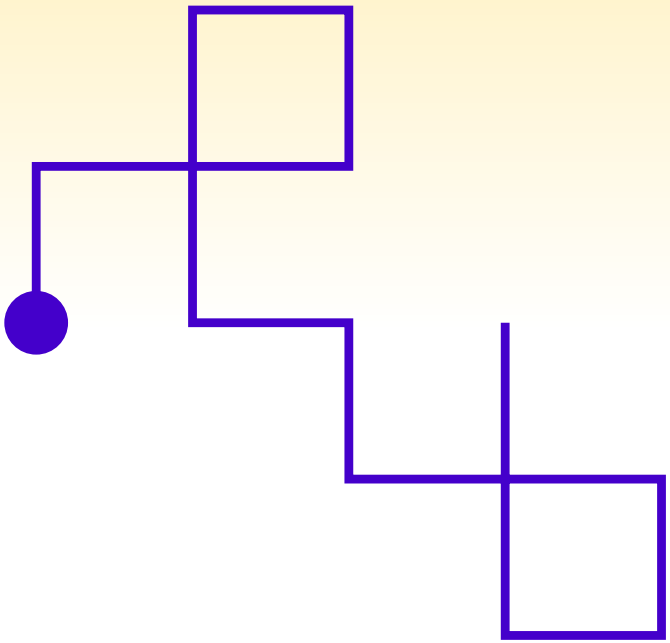

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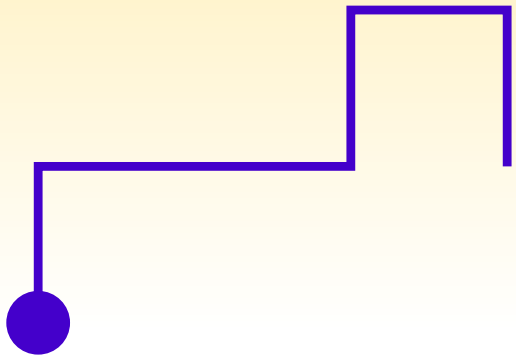

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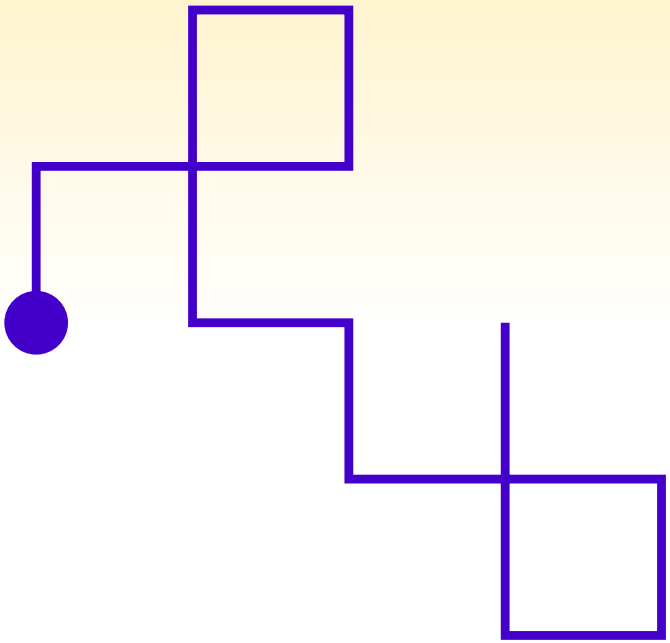

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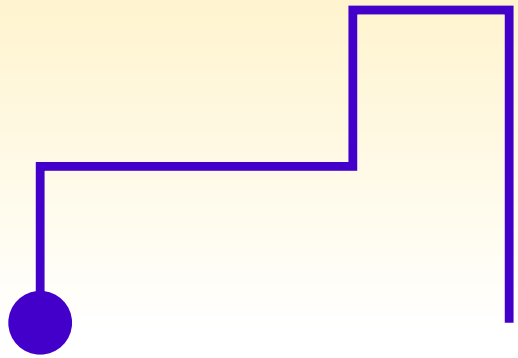

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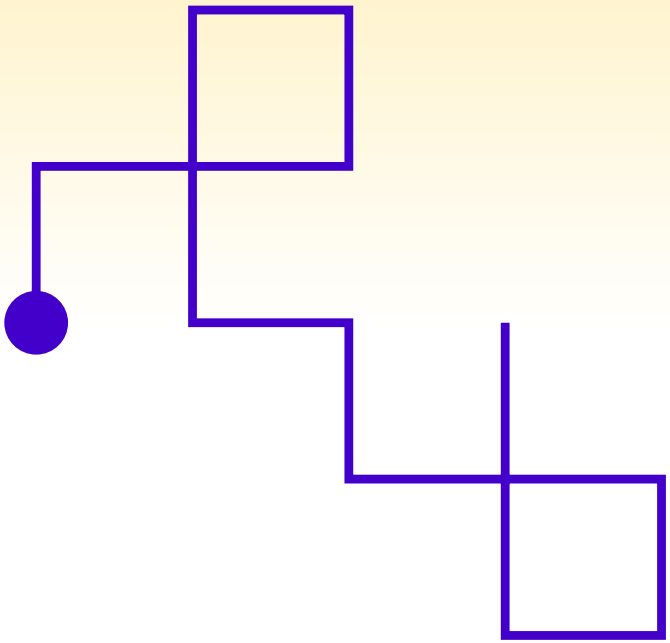

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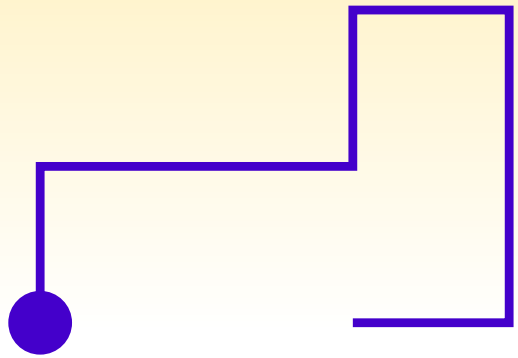

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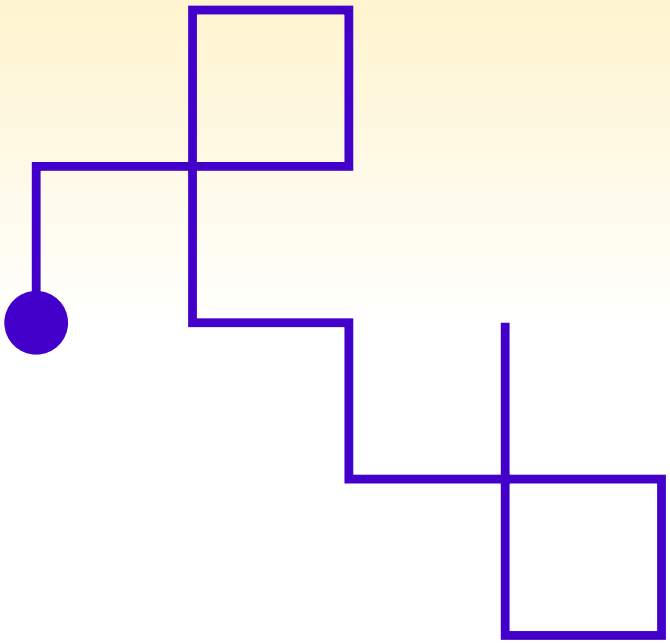

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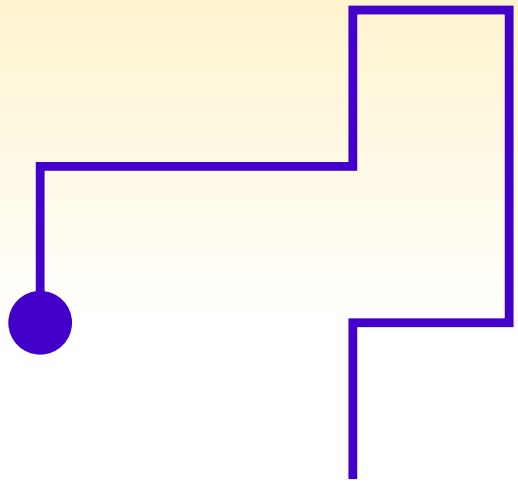

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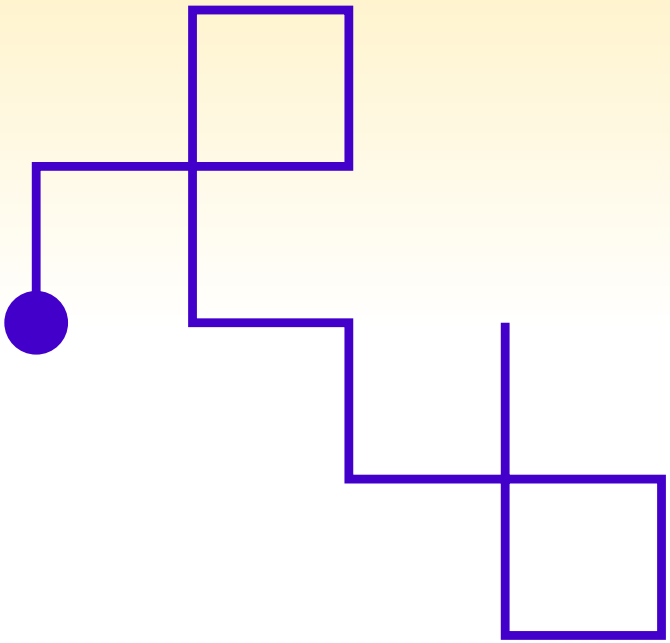

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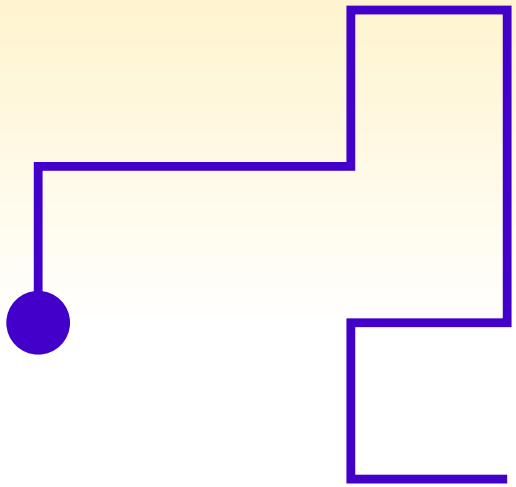

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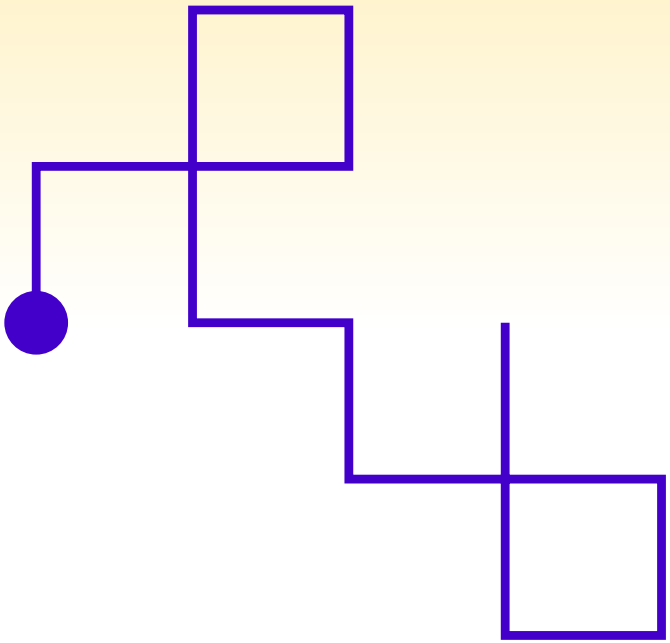

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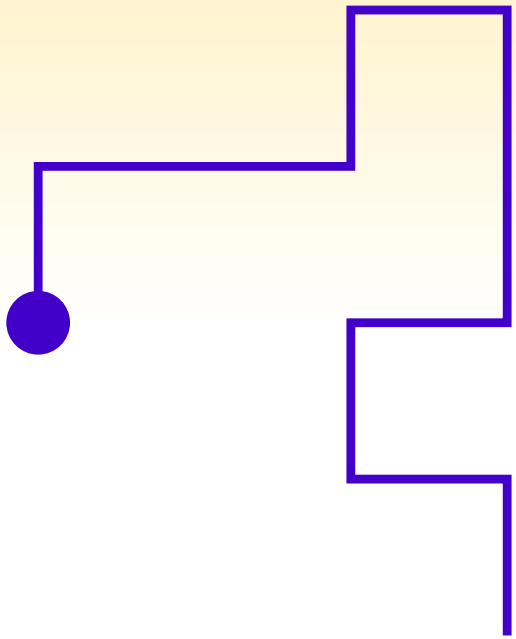

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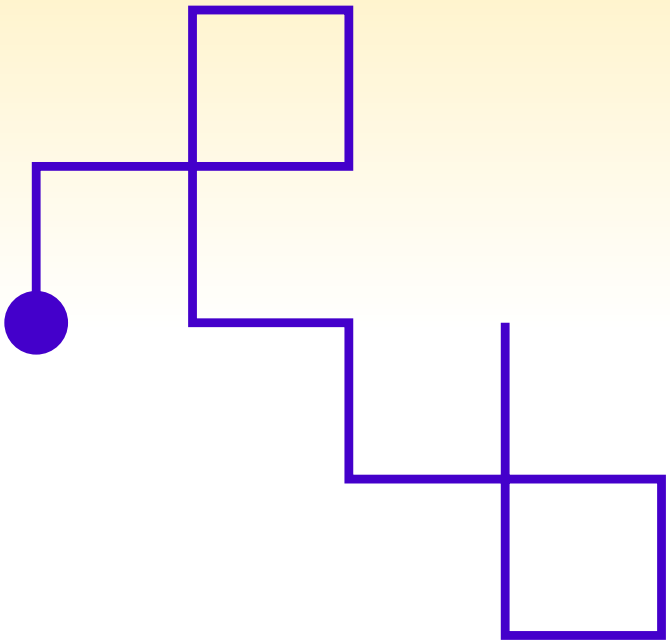

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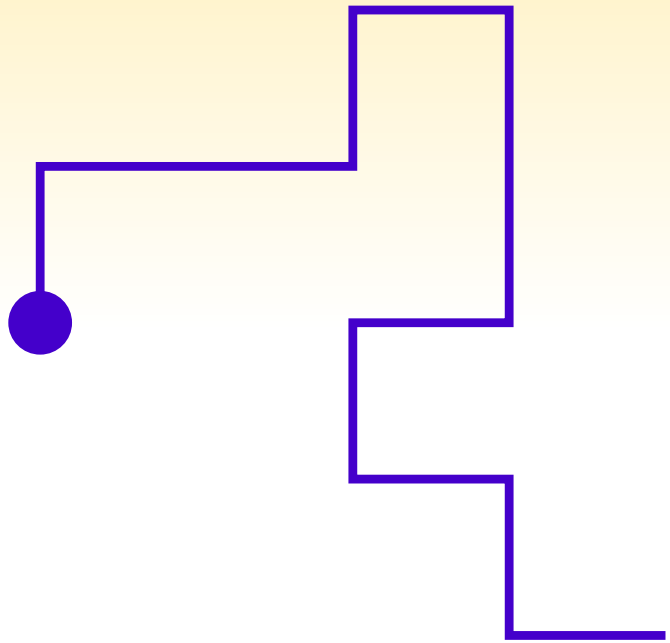

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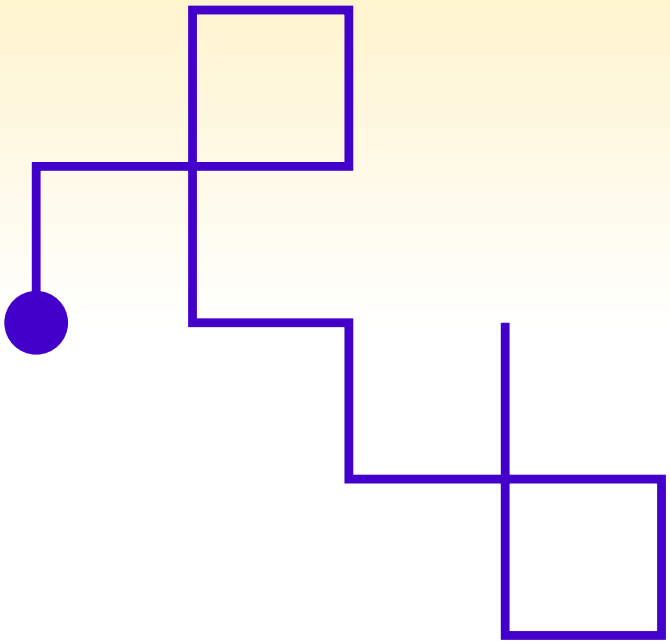

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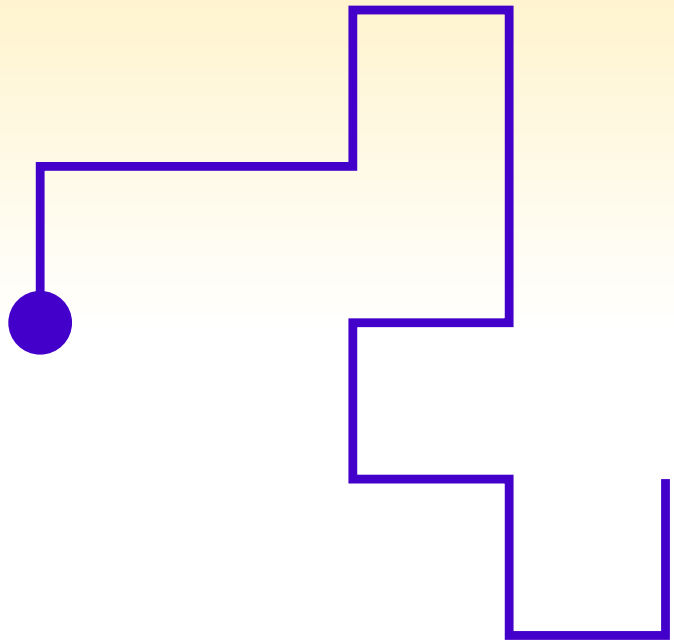

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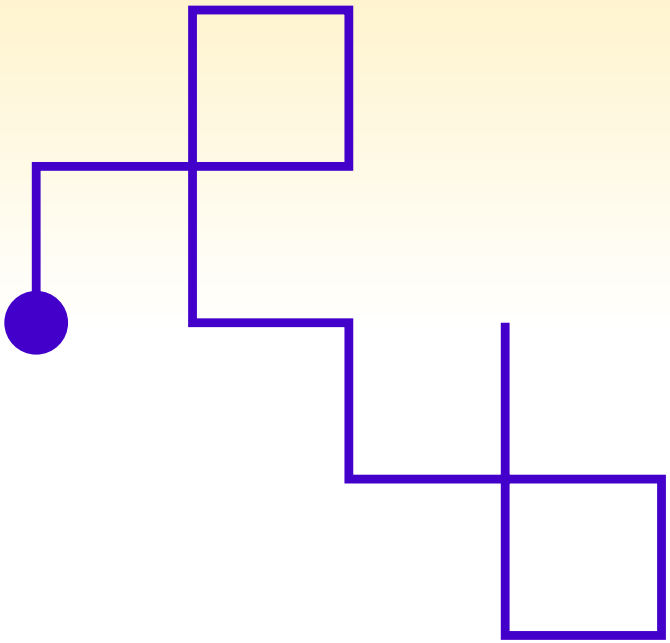

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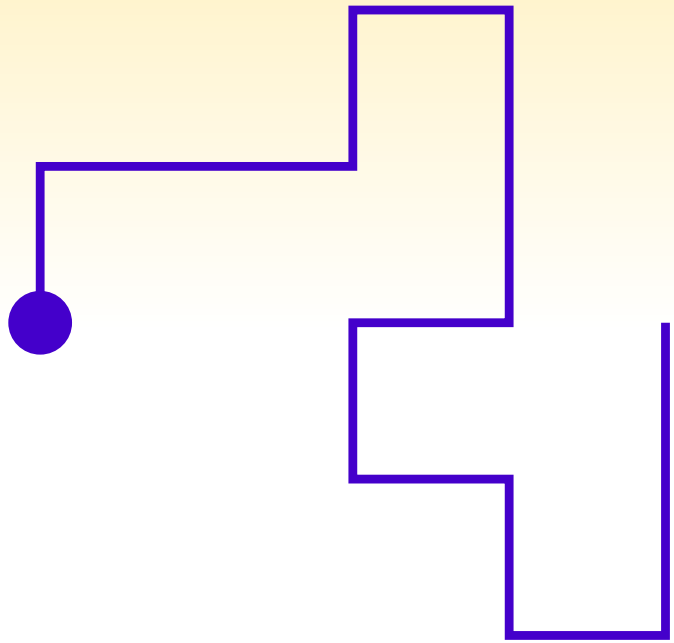
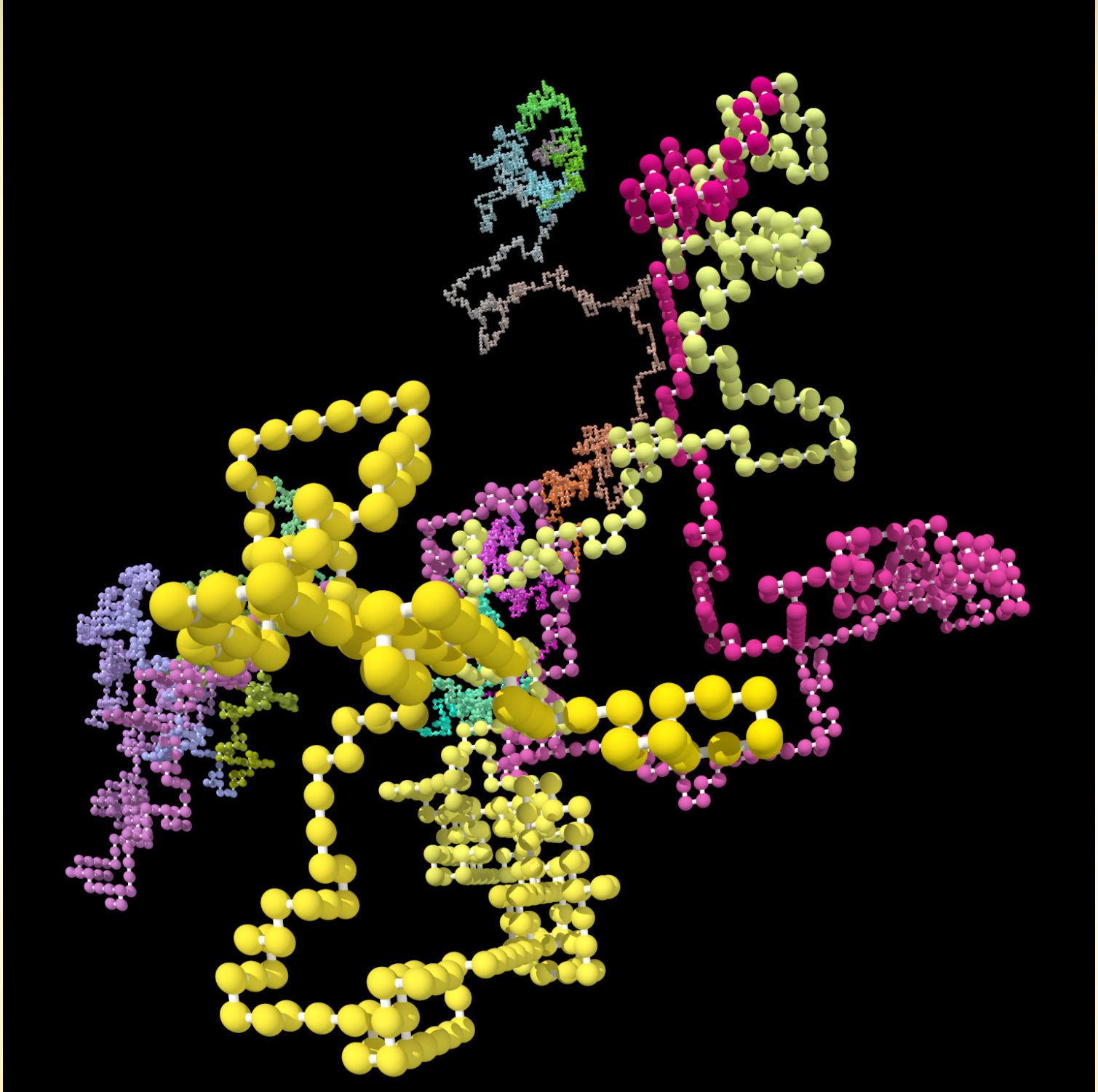


Self-avoiding walk

A typical SAW of 5000 steps on the simple cubic lattice:



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- D is model dependent, but the critical exponent ν is a universal quantity.

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- Markov chain Monte Carlo (MCMC) sampling very powerful for SAW, especially for $d = 3$.
- Estimate physical properties of system by sampling from all possible configurations (state space).
- Basic idea: generate new configurations by deforming current configuration via a "move".

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- Global moves can do much better.
- Pivot move: $O(1)$ successful moves for an essentially new configuration.
- Lal (1969) invented pivot algorithm, but key paper is by Madras and Sokal (1988).

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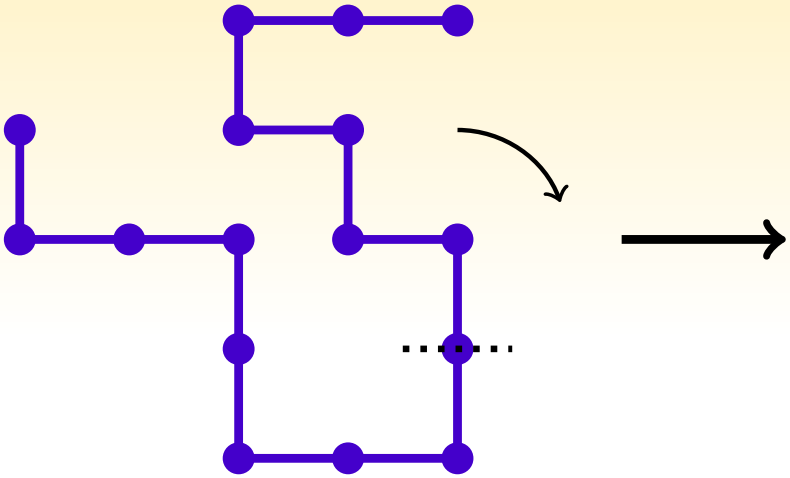
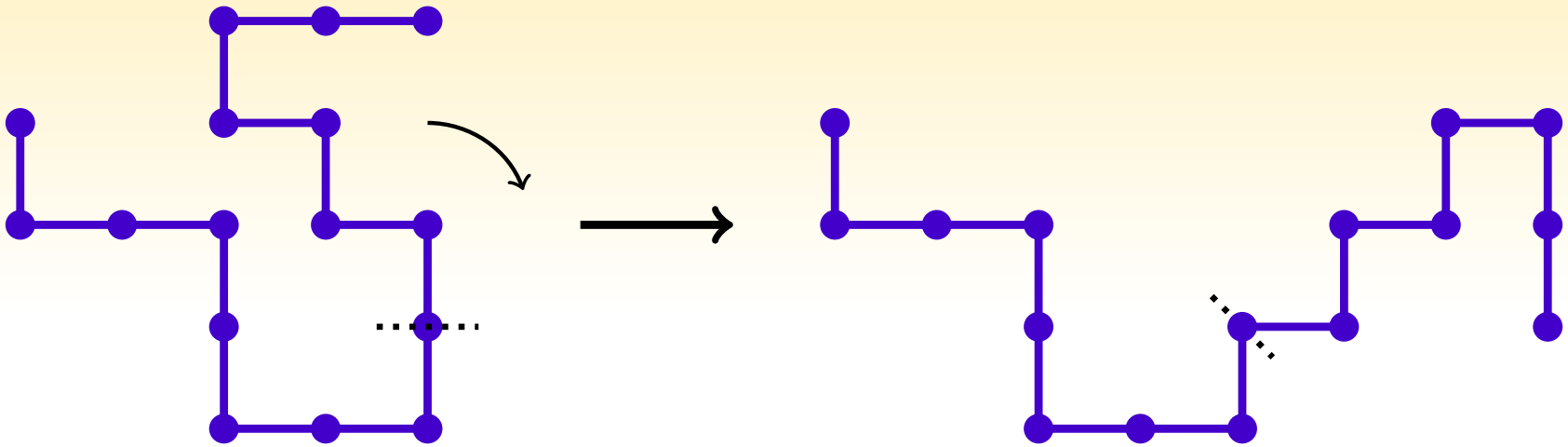
- "Global" because on average half of the monomers are moved.
- Ergodic, samples SAWs uniformly at random.



Example pivot move



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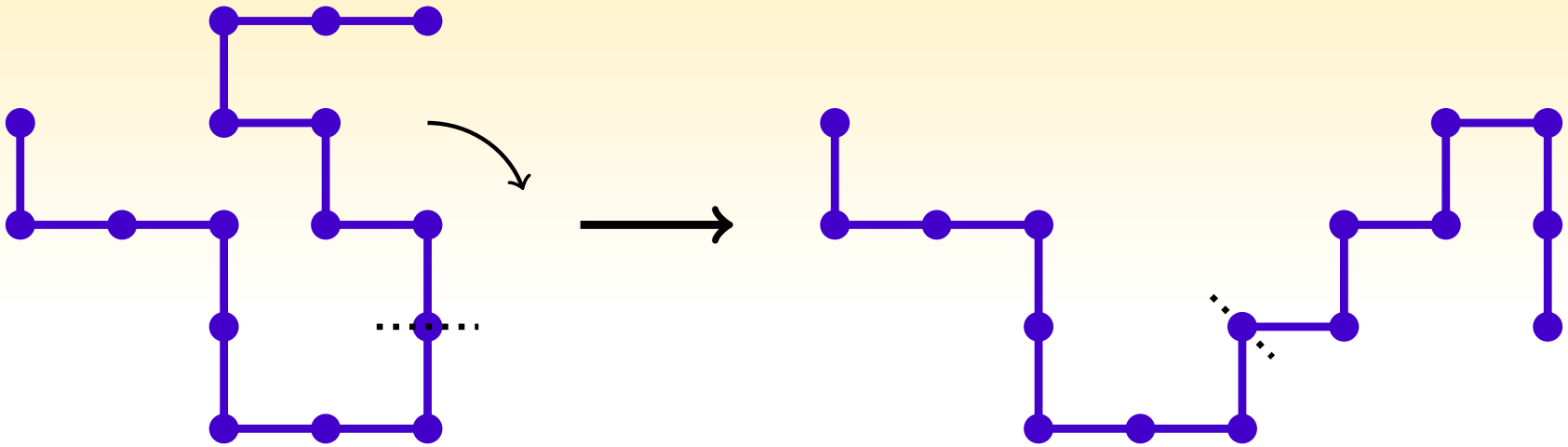

Example pivot move

Run simulation

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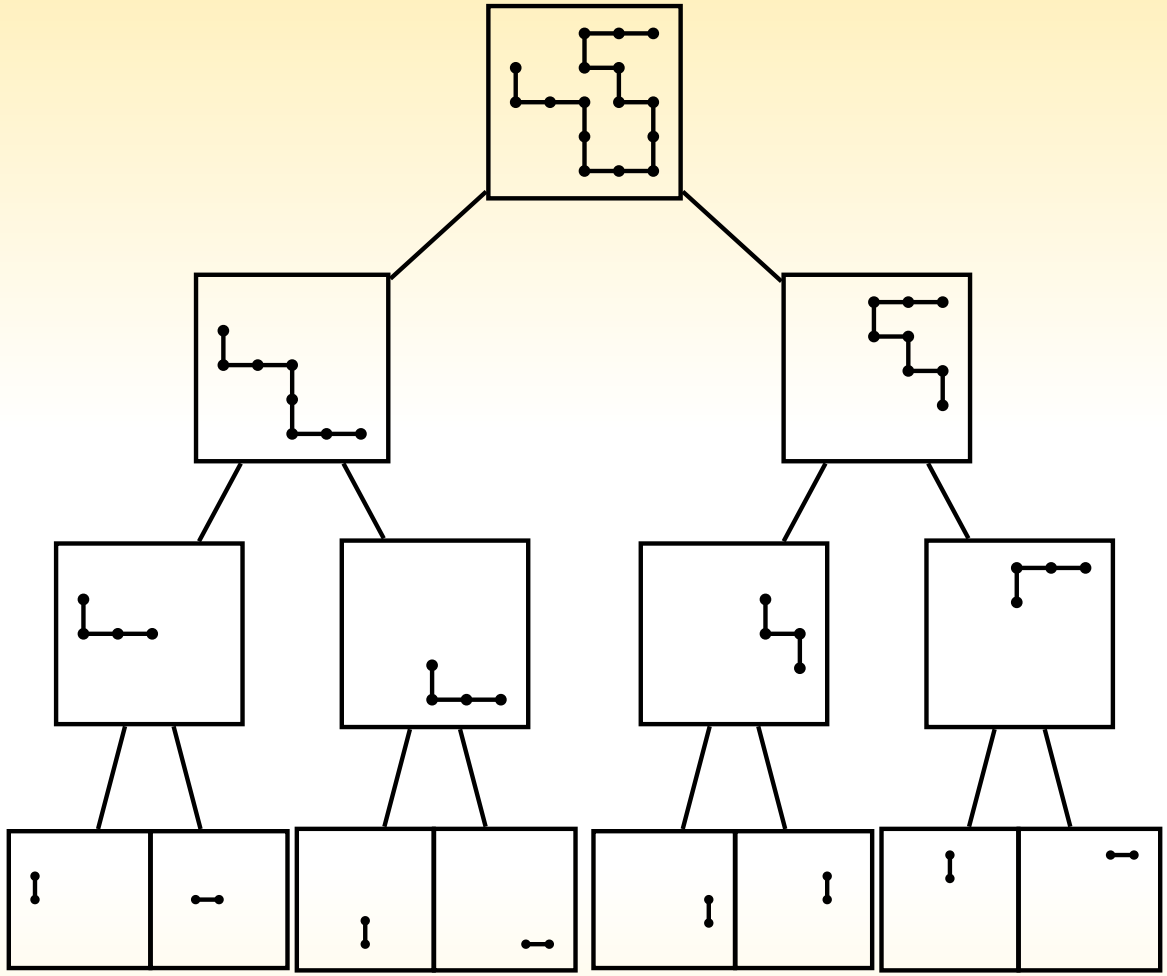
- Bookkeeping can be handled efficiently in binary tree structure. $\Rightarrow O(\log N)$ (C., 2010)



SAW-tree representation of a walk.

Key properties of the SAW-tree data structure.

- Each node contains:

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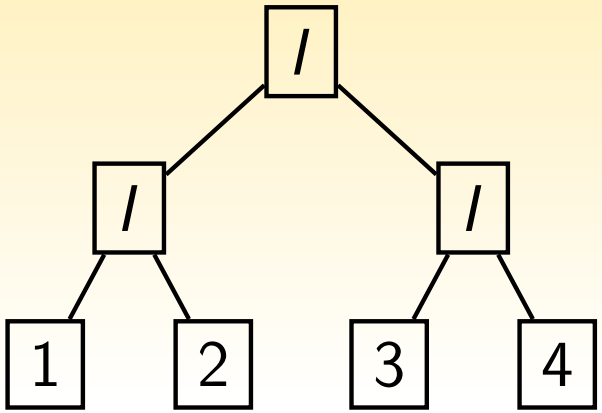

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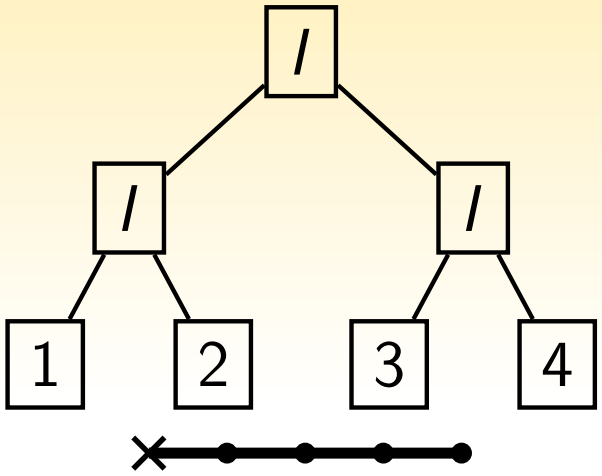

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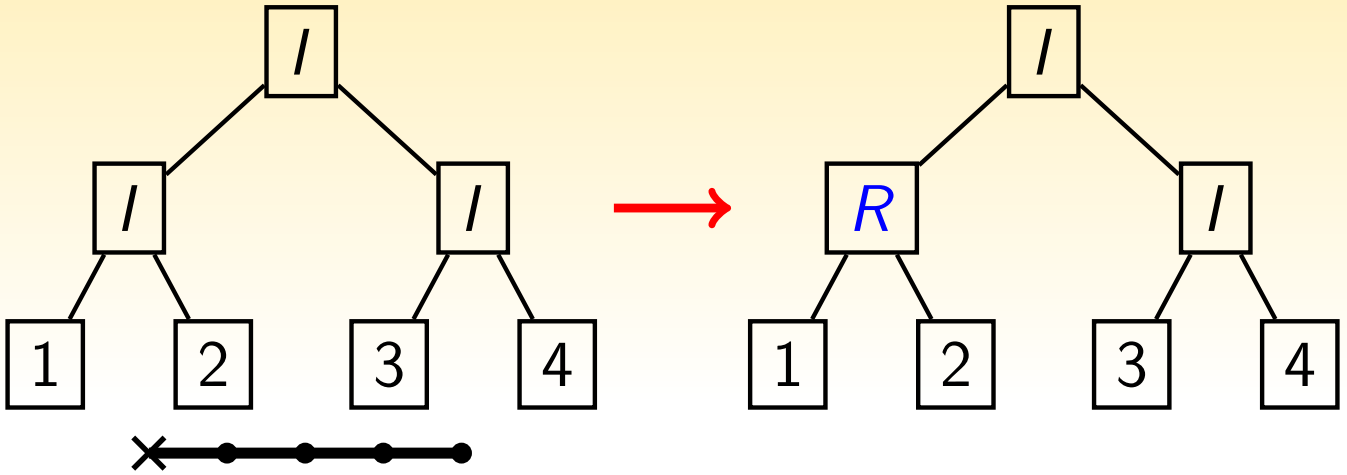

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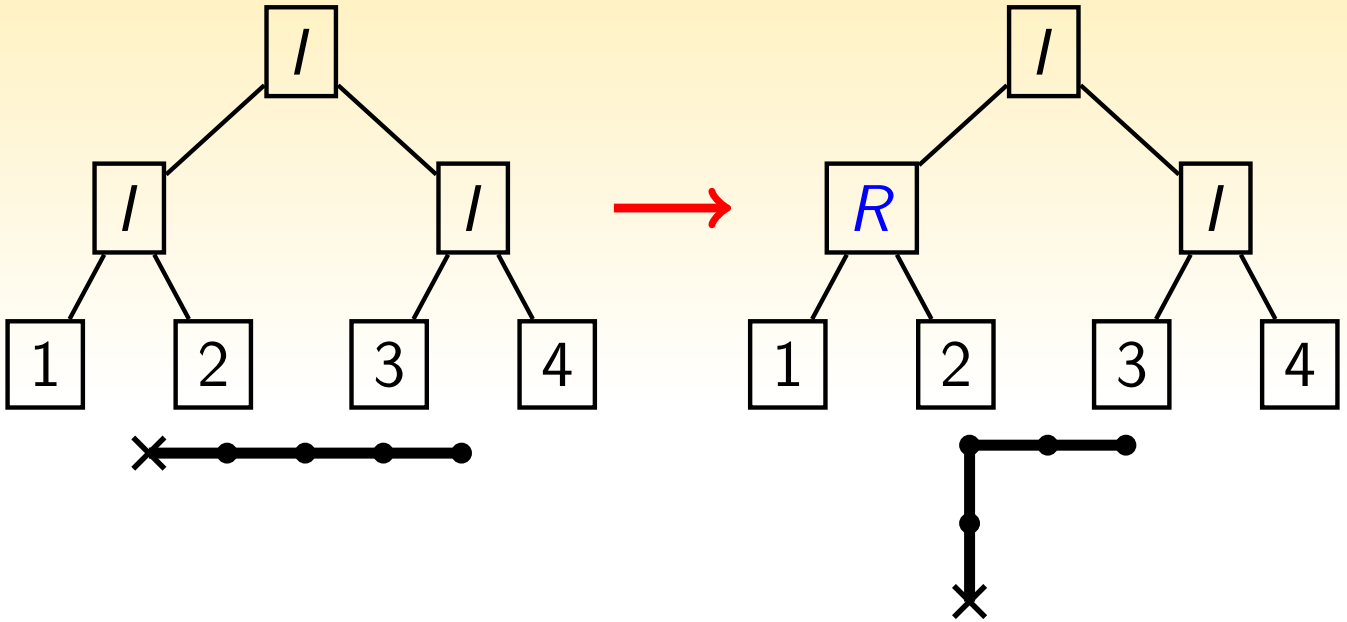

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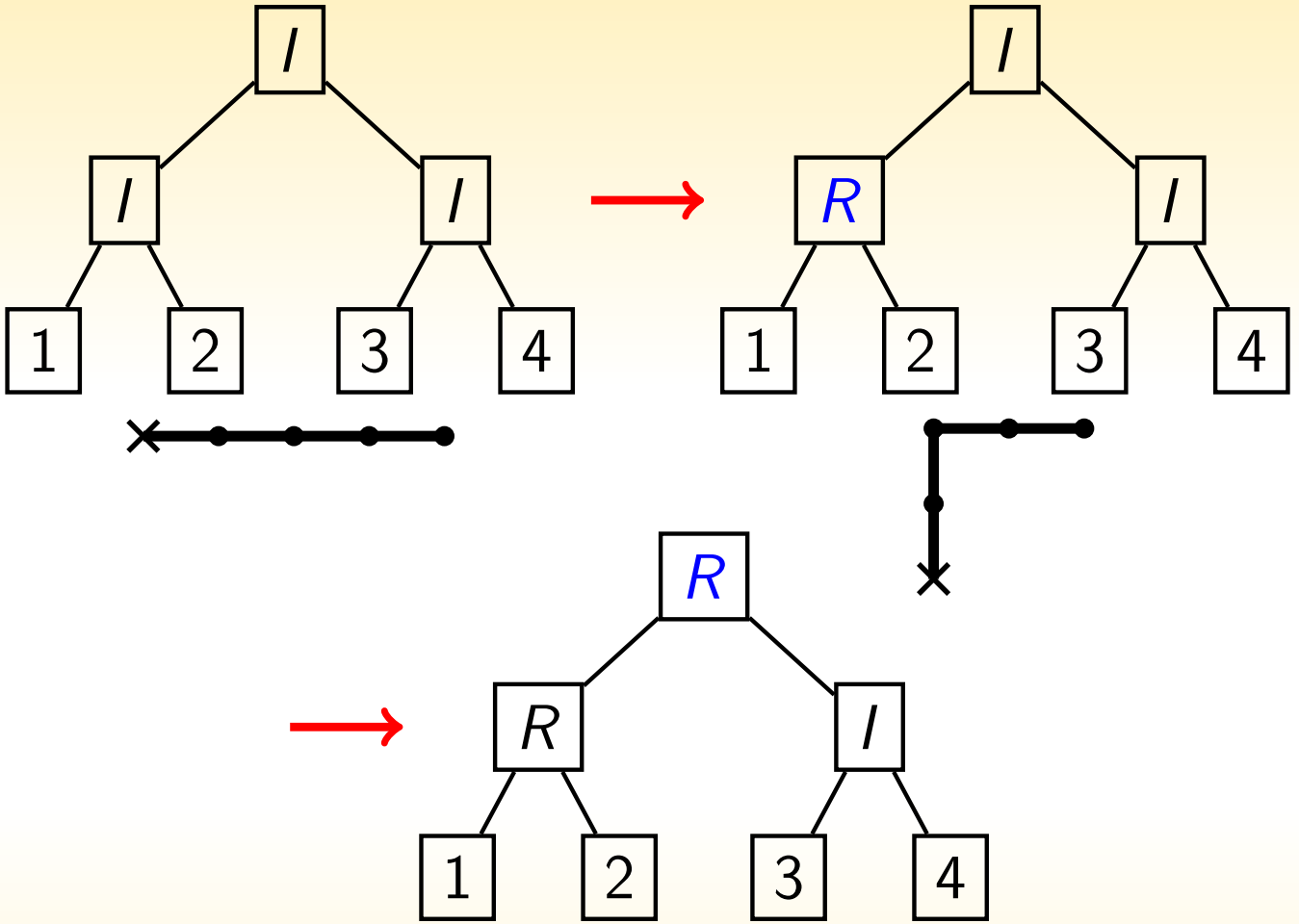

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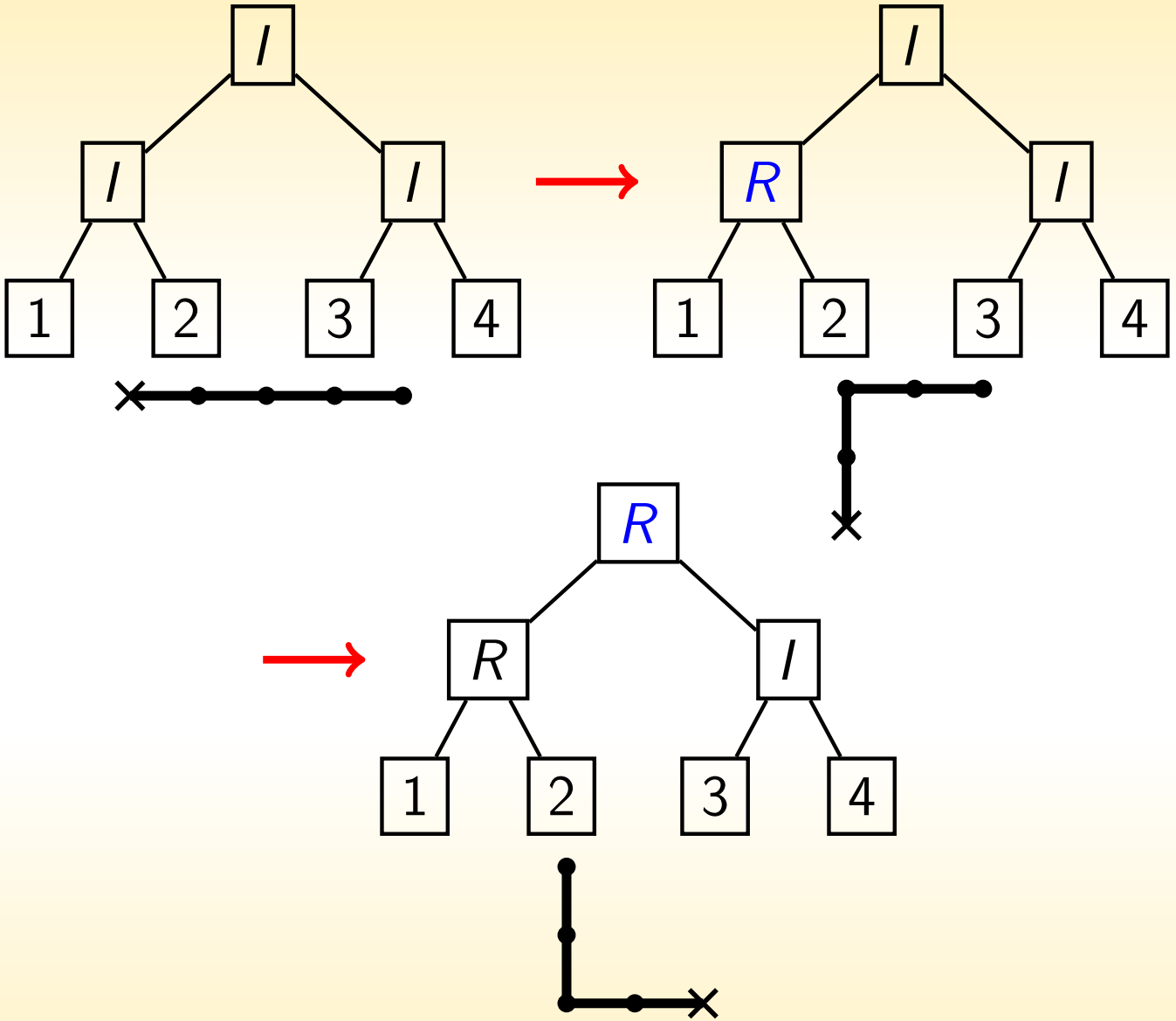

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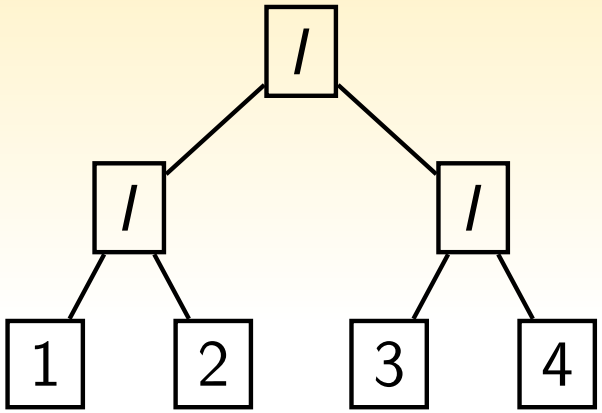

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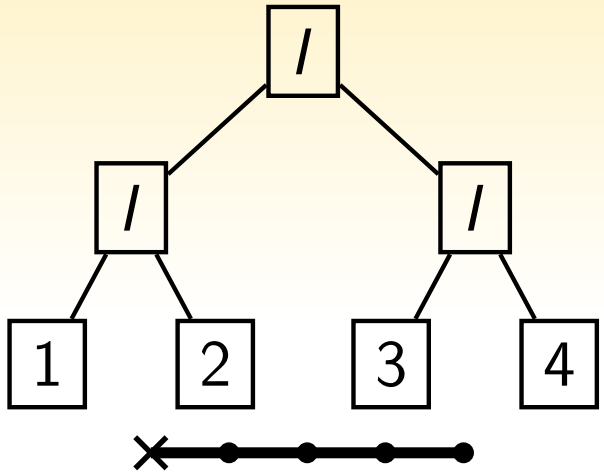

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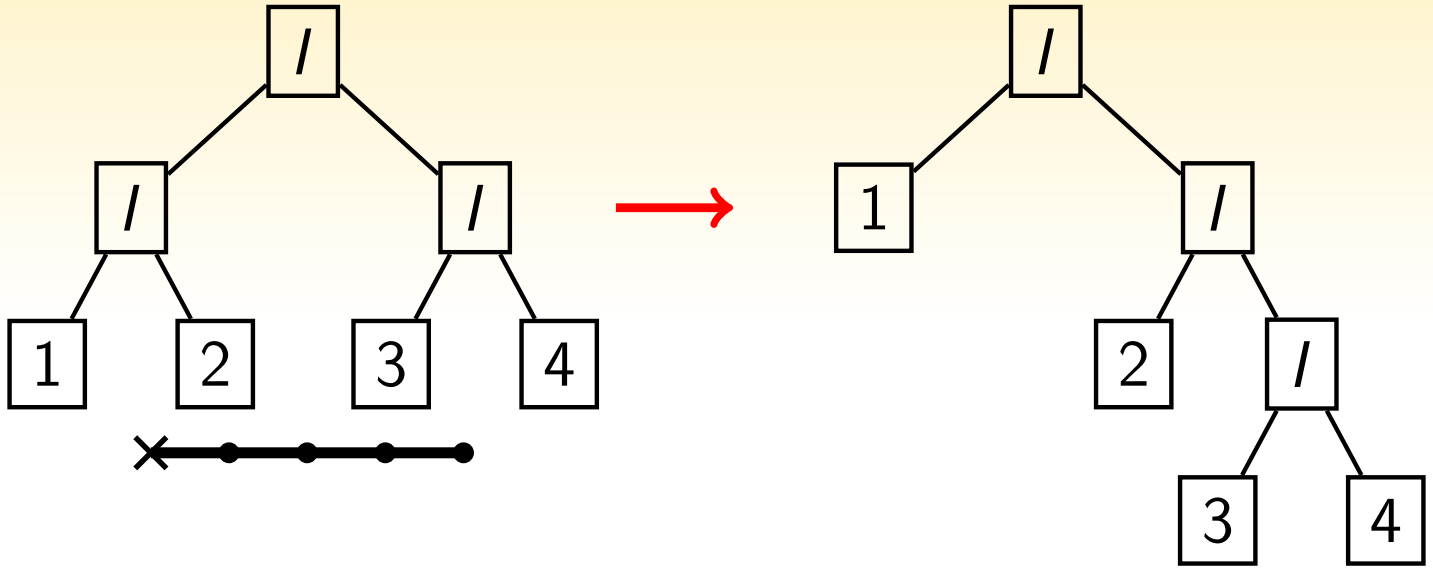

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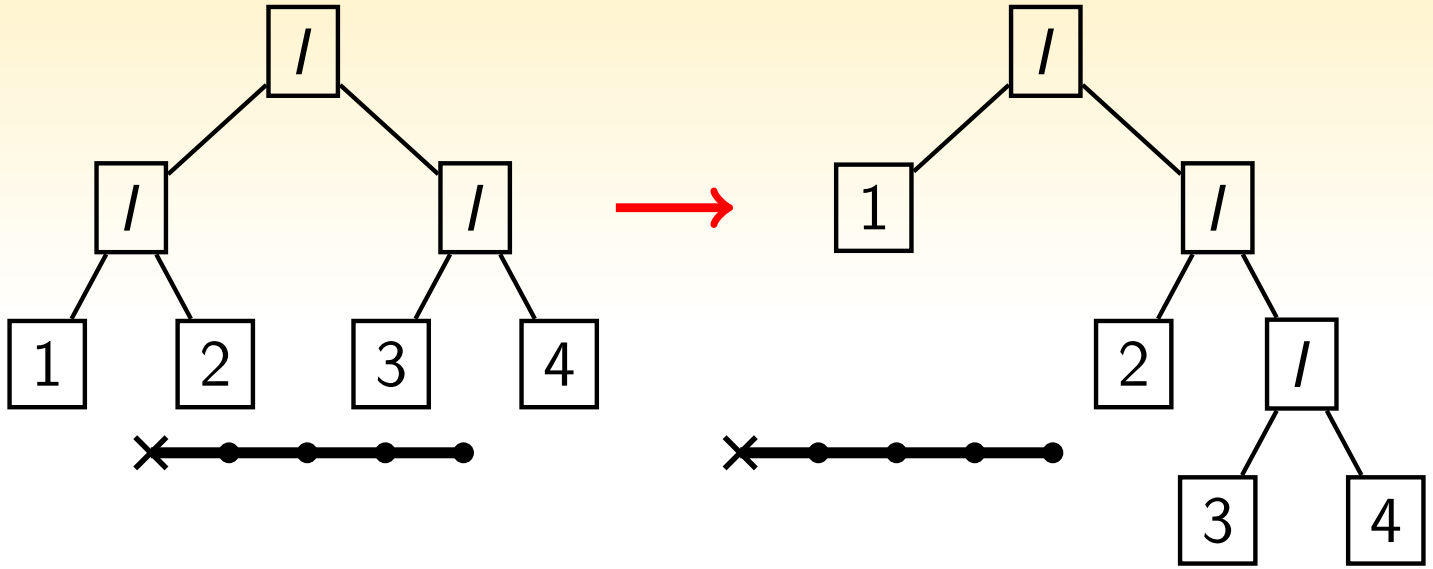

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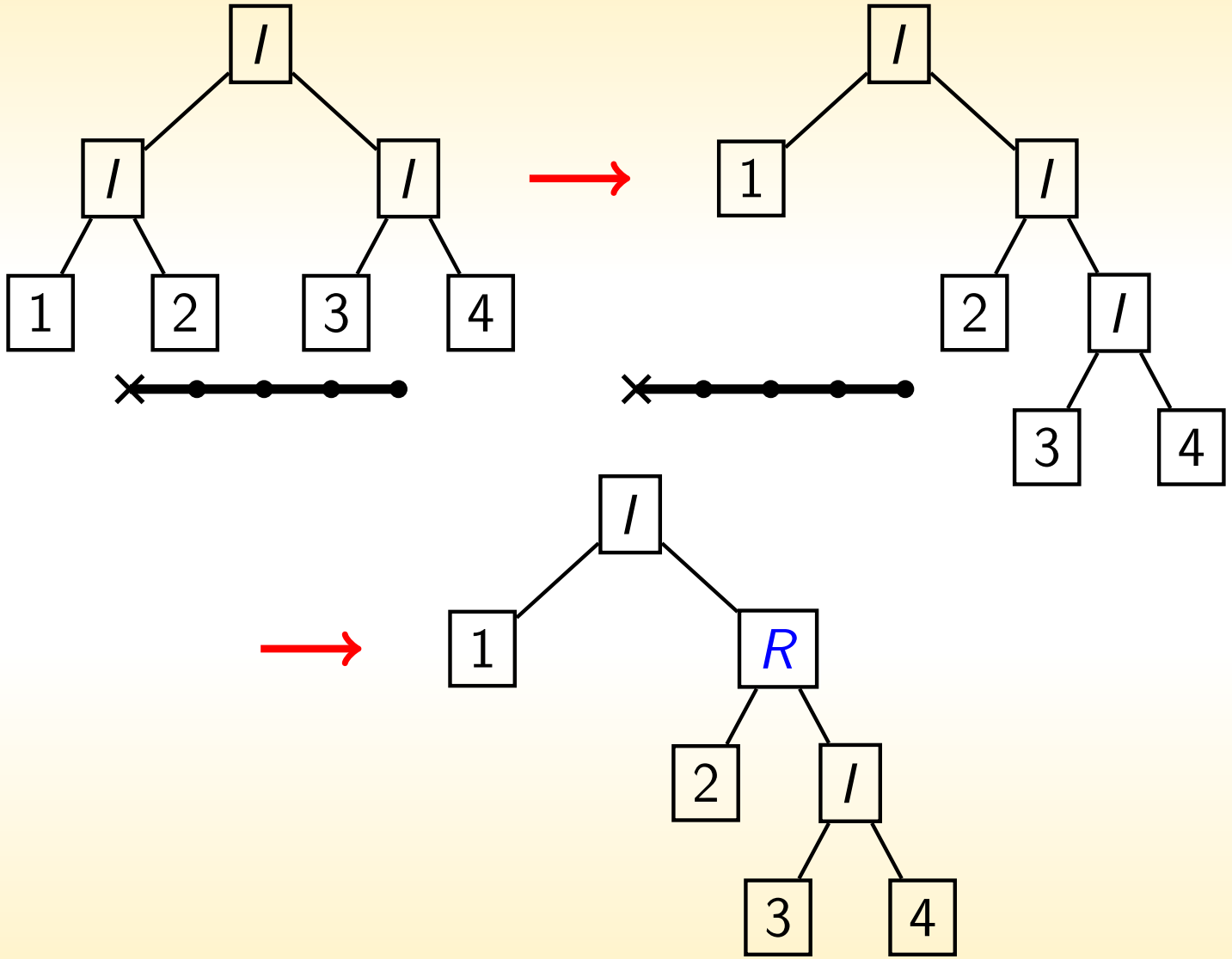

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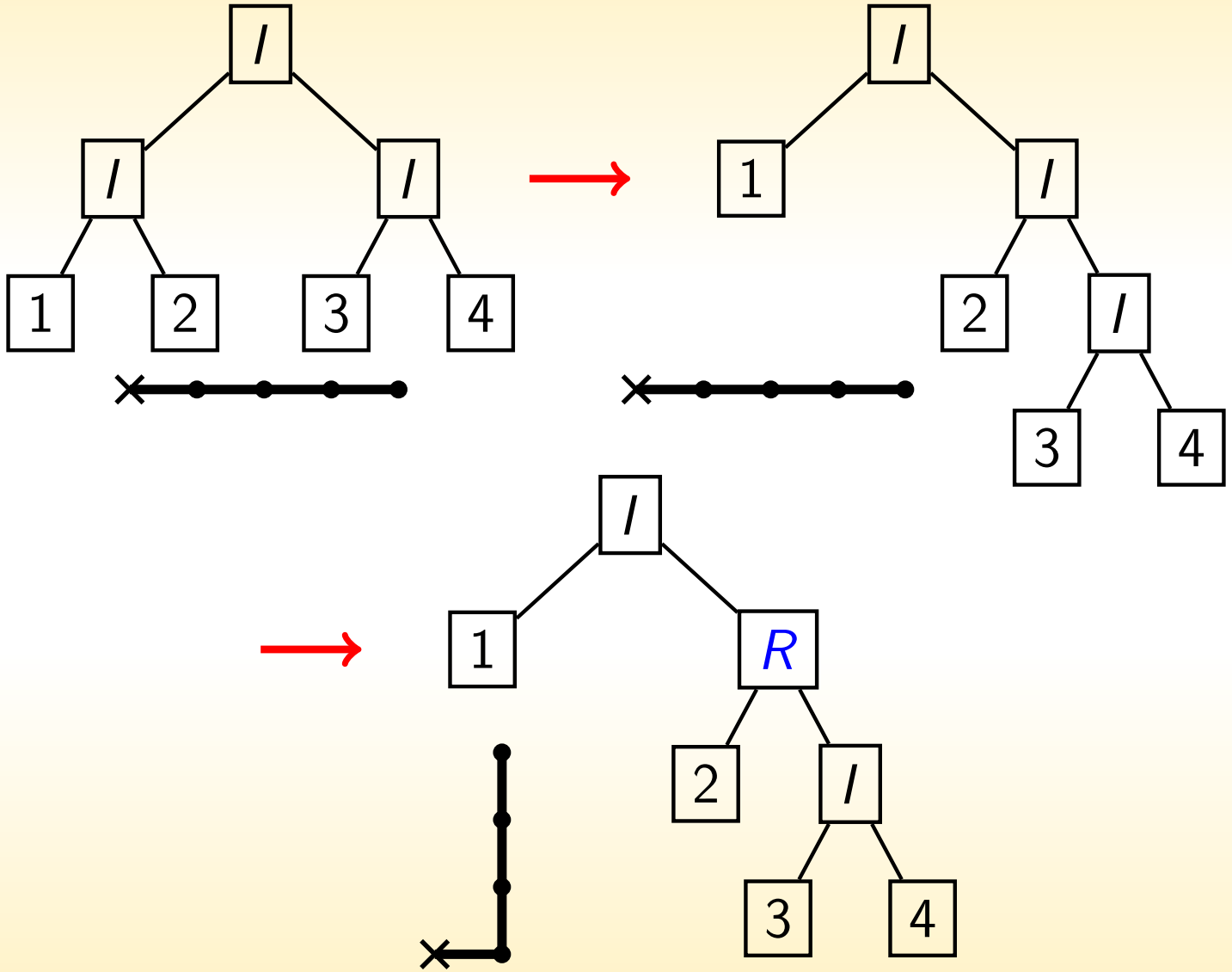

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- How can we extend this key idea - fast global moves - to other models?

Hamiltonian paths

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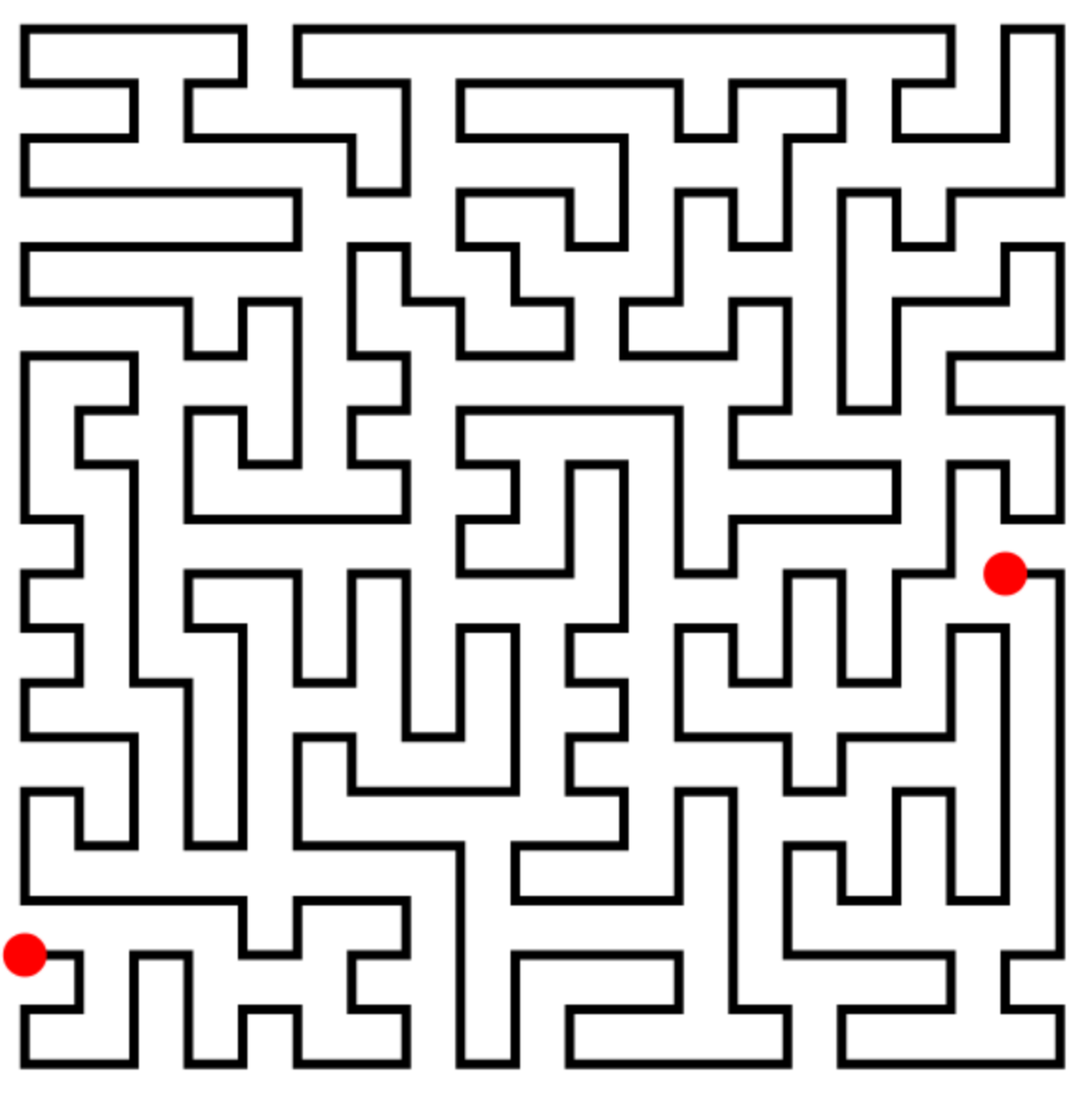
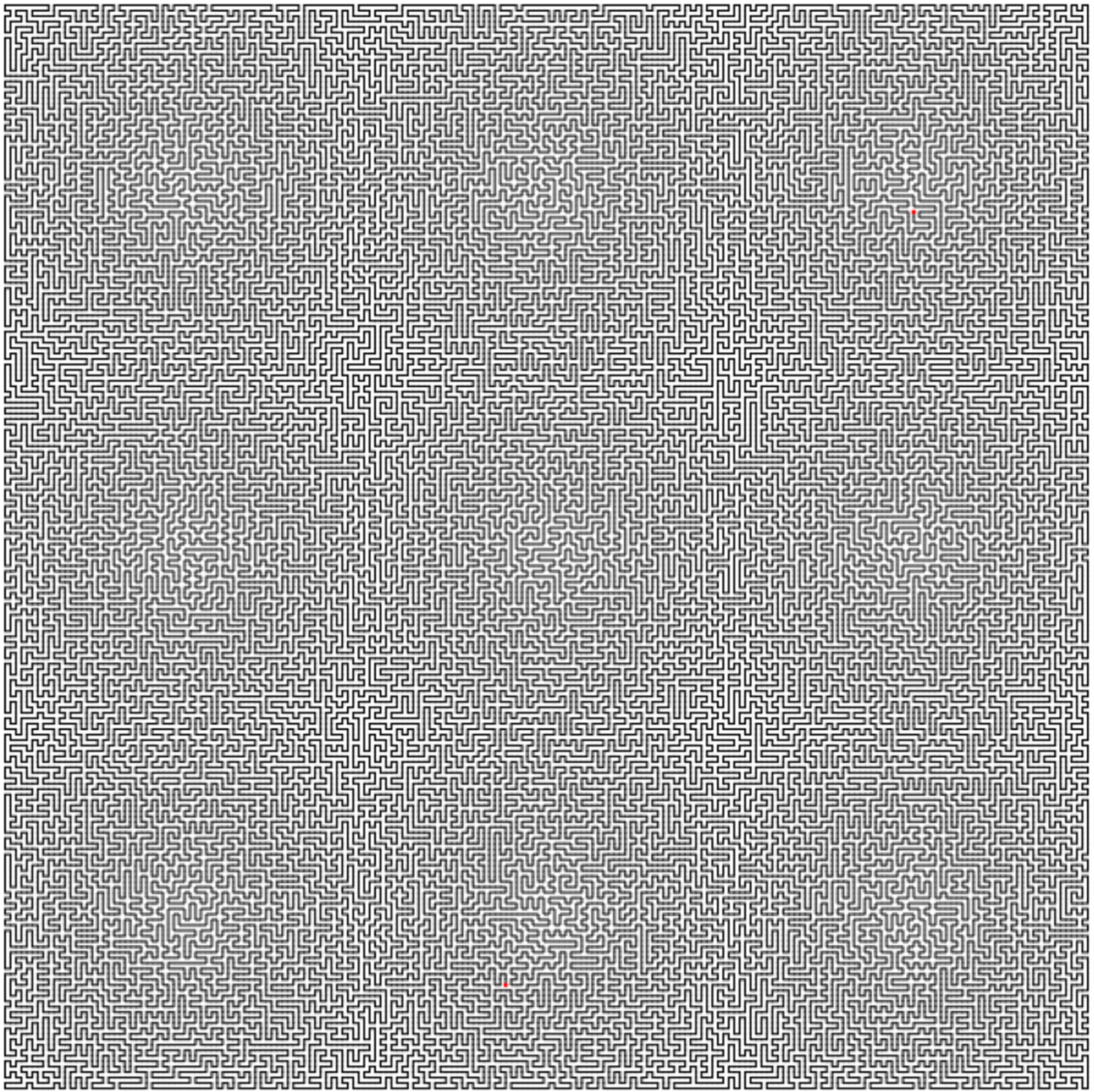
  `http://lattice.complex.unimelb.edu.au/hamiltonian_path`)





Hamiltonian paths

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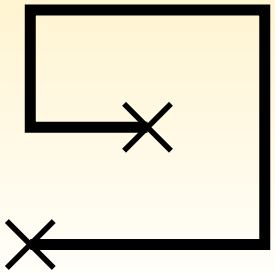
- One example: backbite move, which is likely to be ergodic for the simple cubic lattice.

Backbite moves for sampling Hamiltonian paths.



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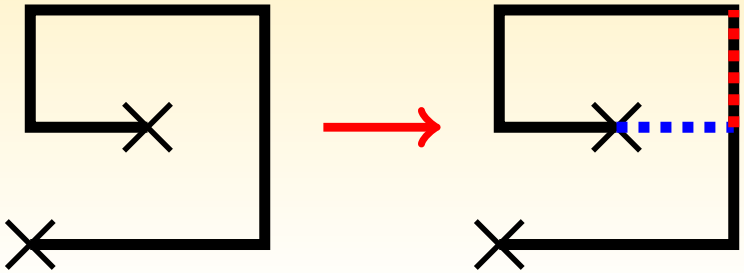

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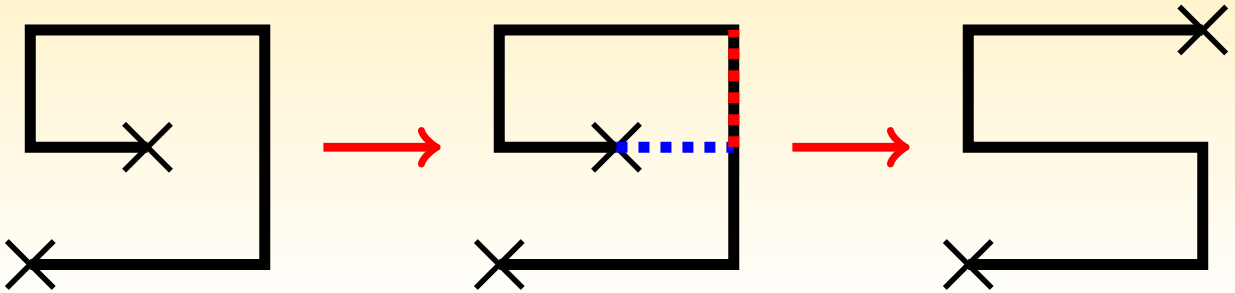

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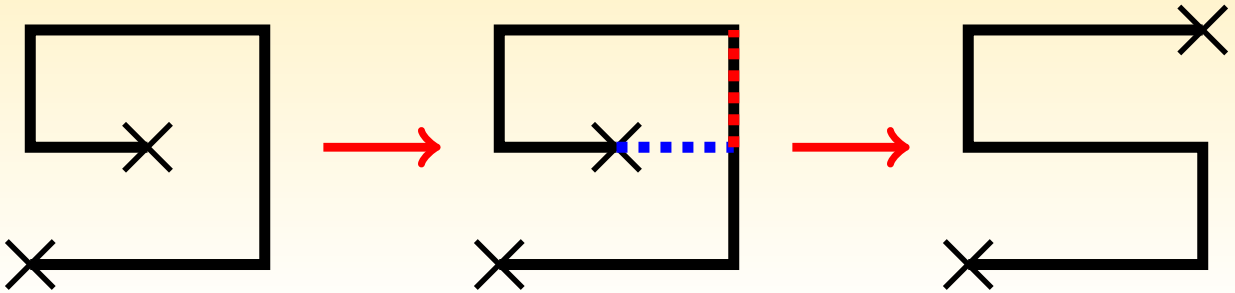

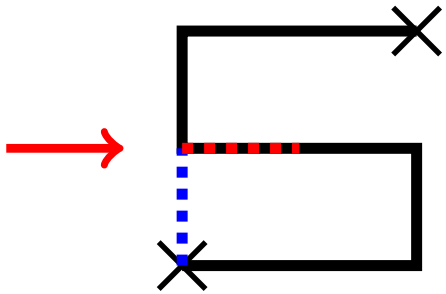

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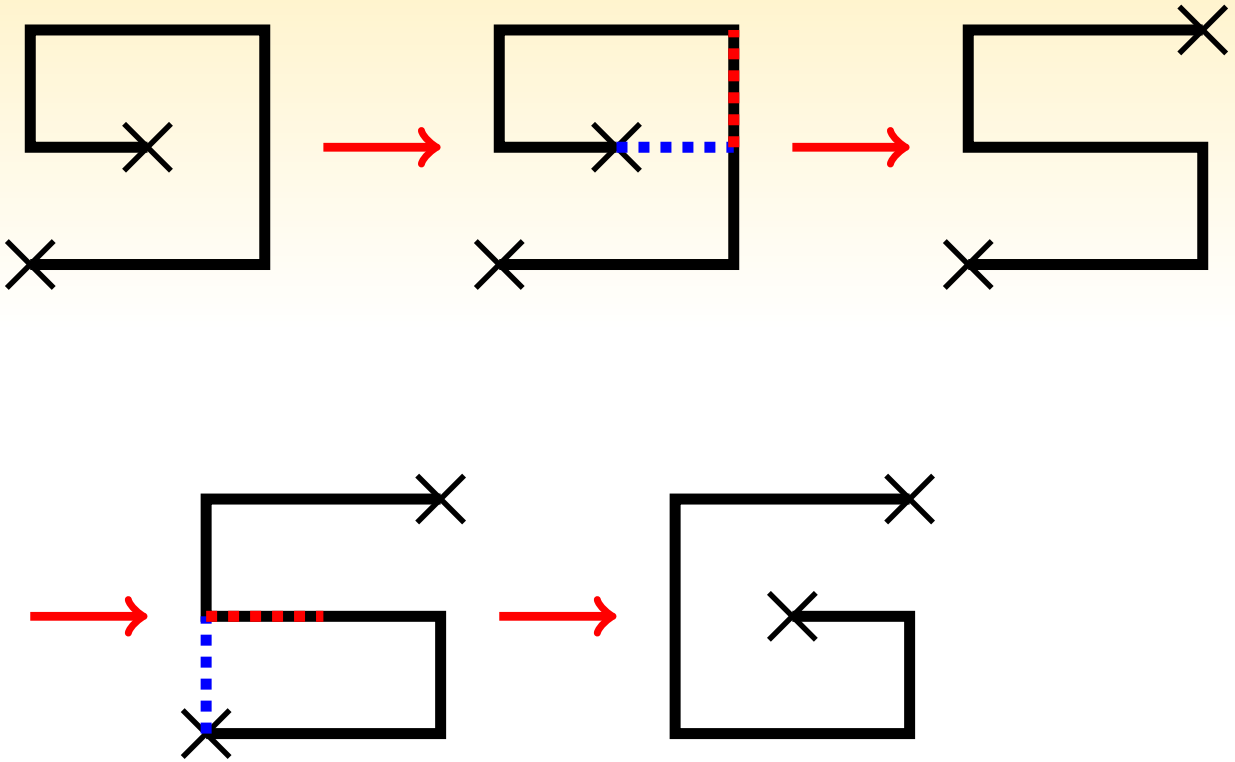

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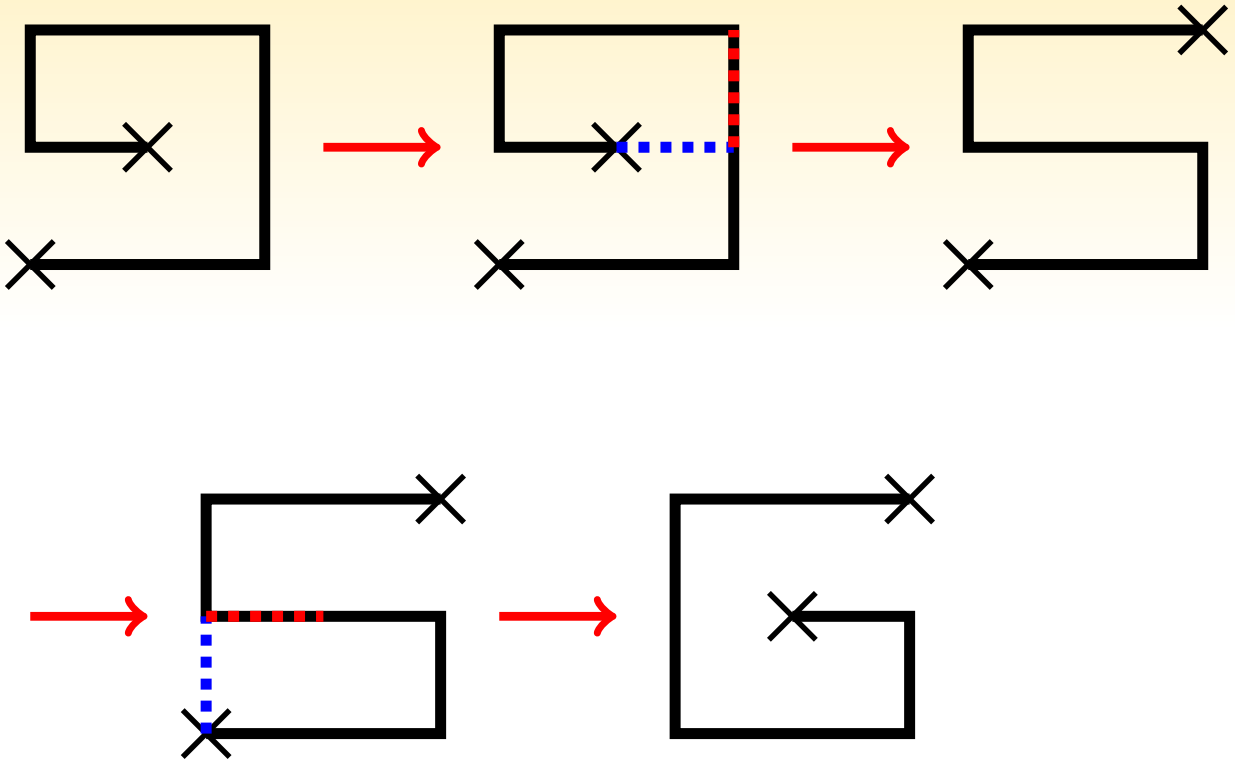

Each time we make a backbite move we create a loop, delete the edge which completes the loop, and *reverse* the orientation of the remaining edges of the loop.

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- Only trick required is bookkeeping for determining neighbours.

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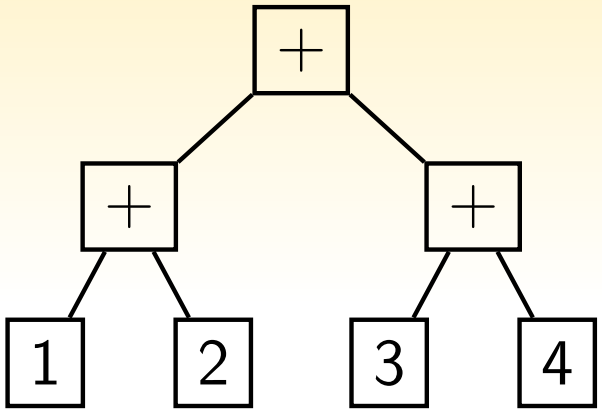

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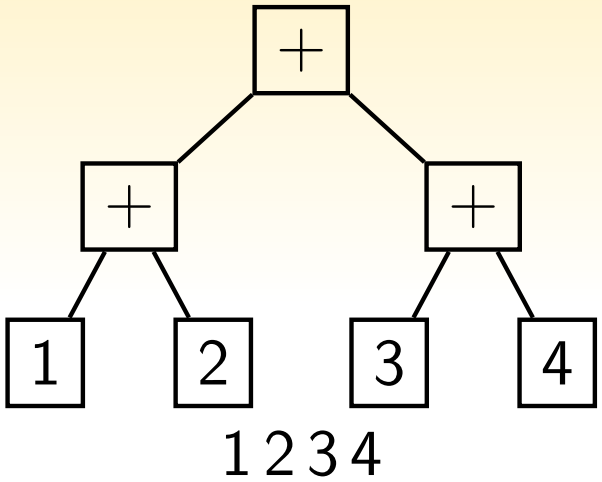

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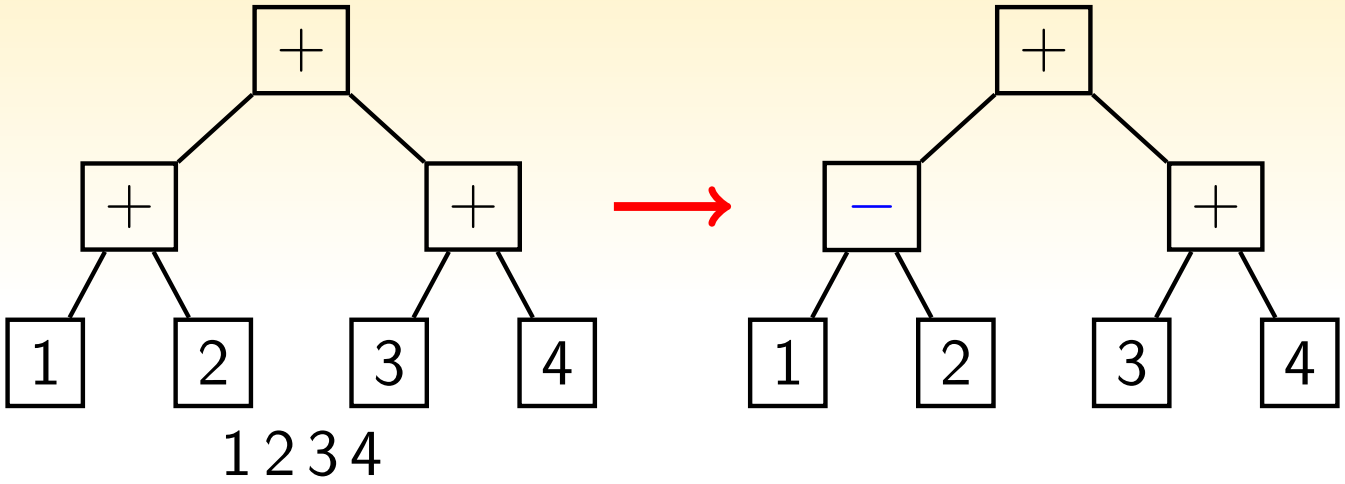

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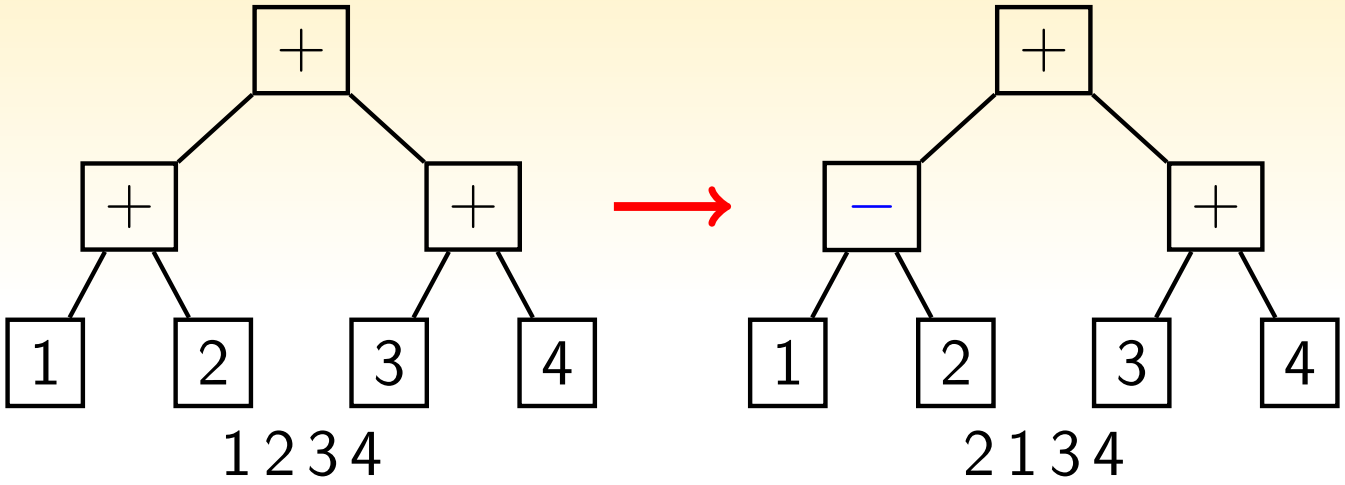

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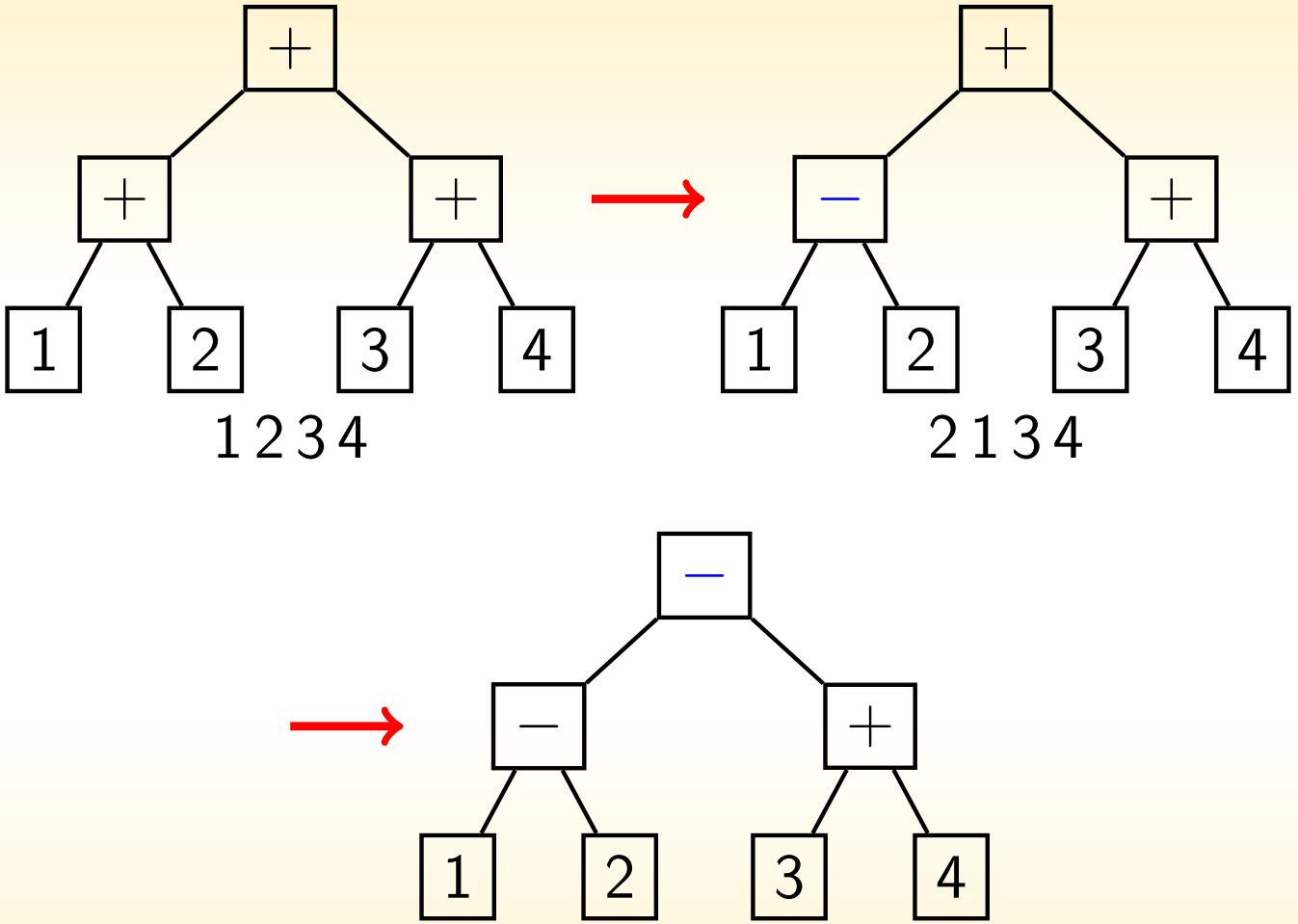

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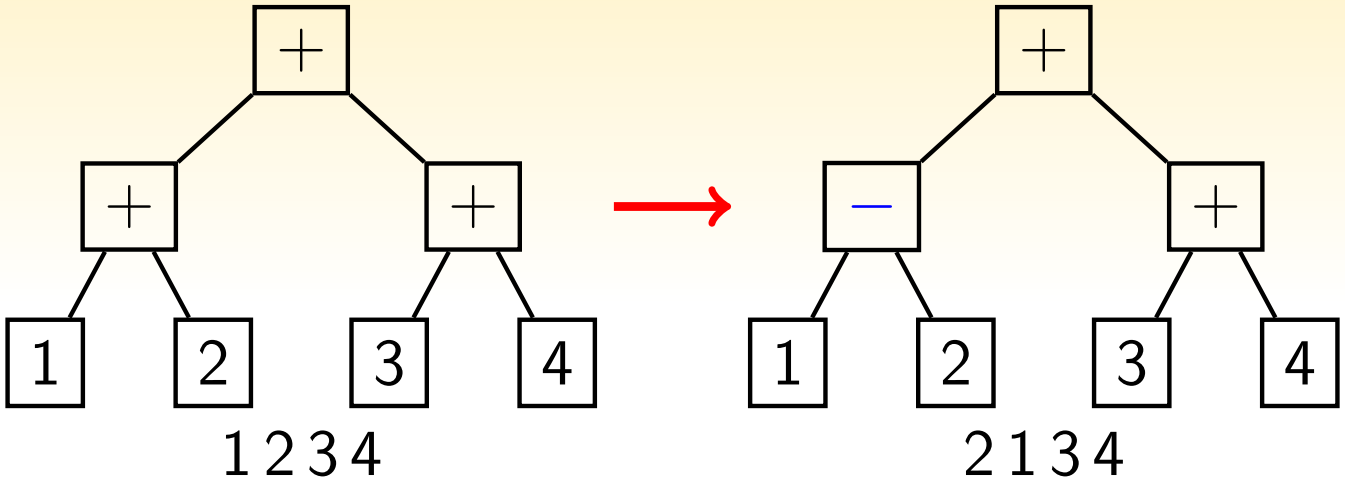

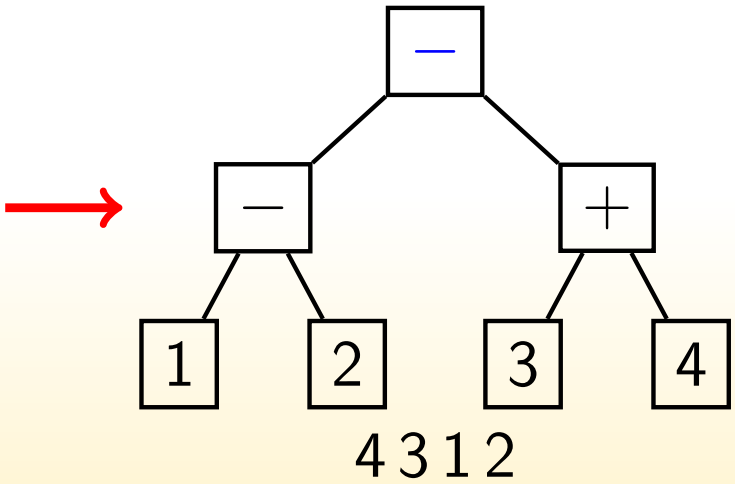

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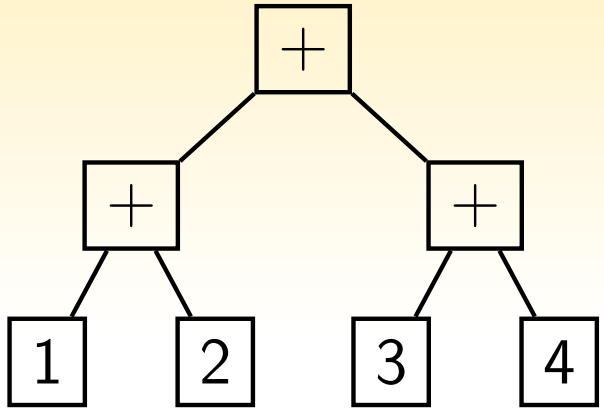

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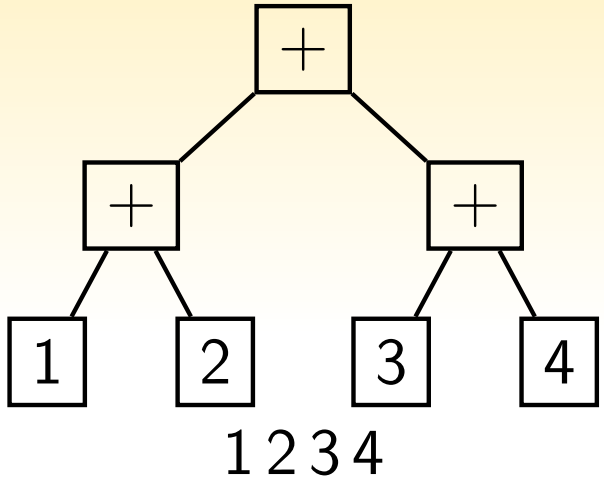

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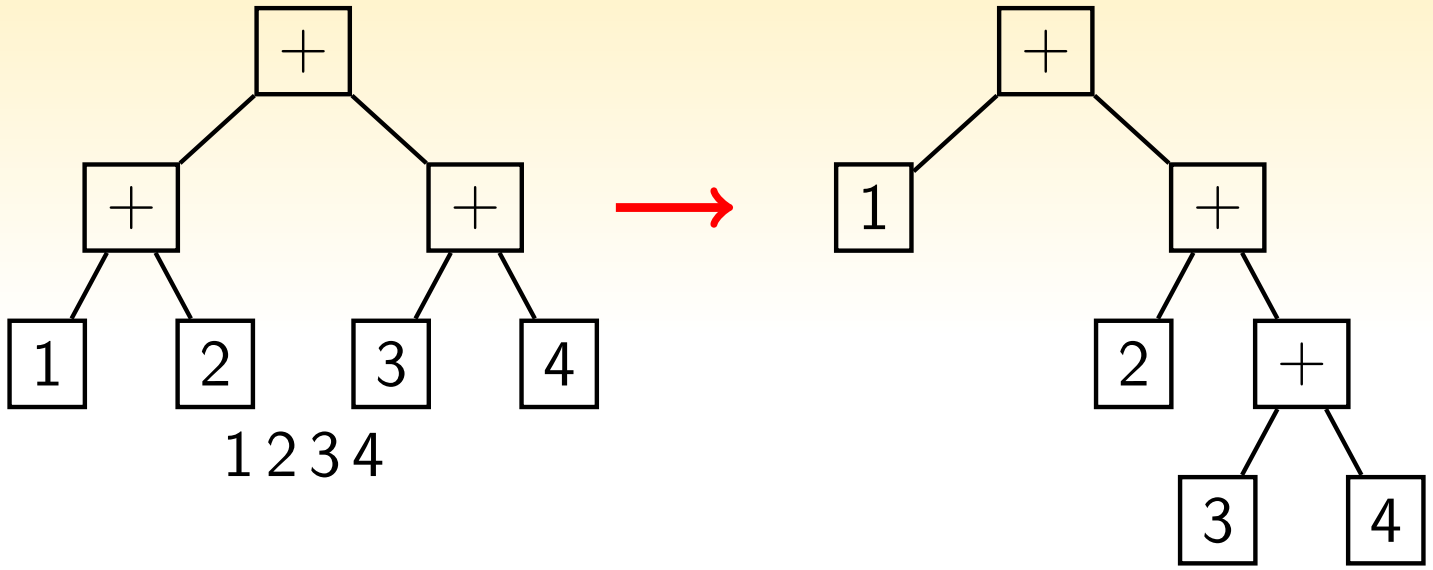

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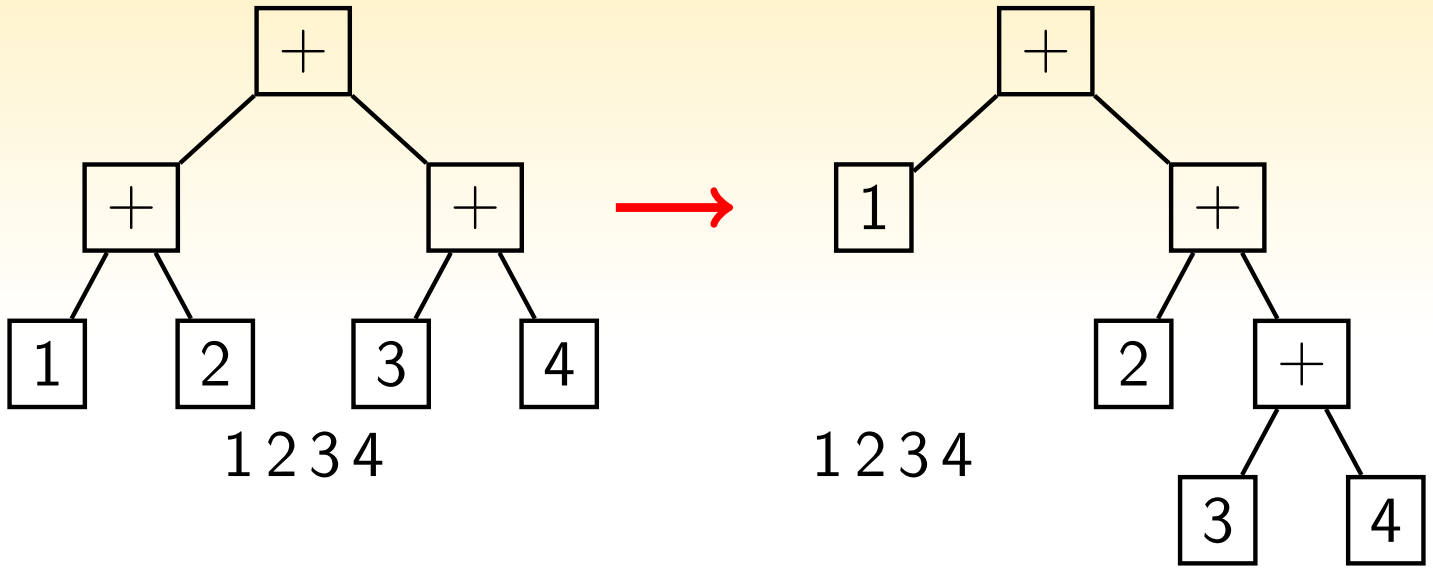

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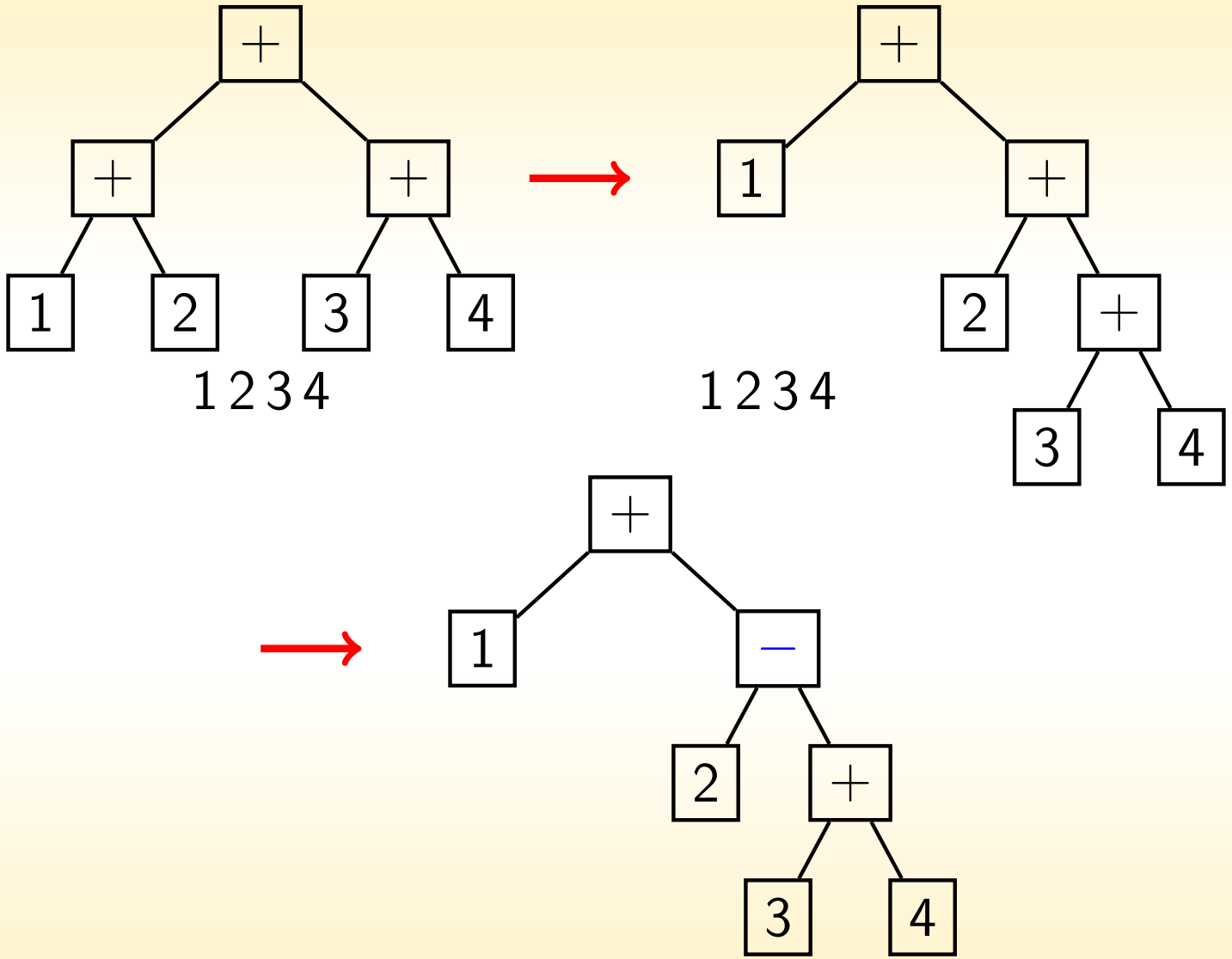

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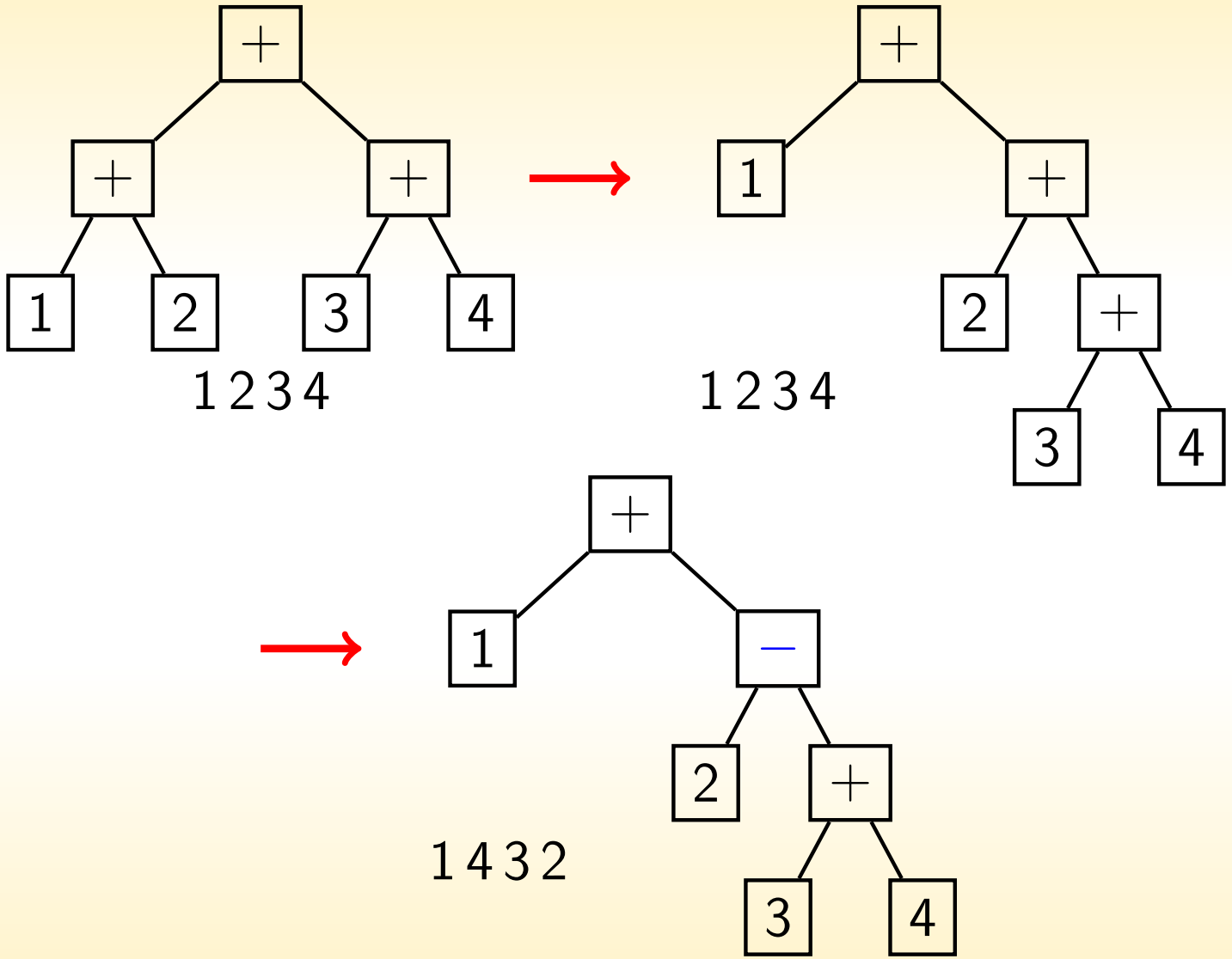

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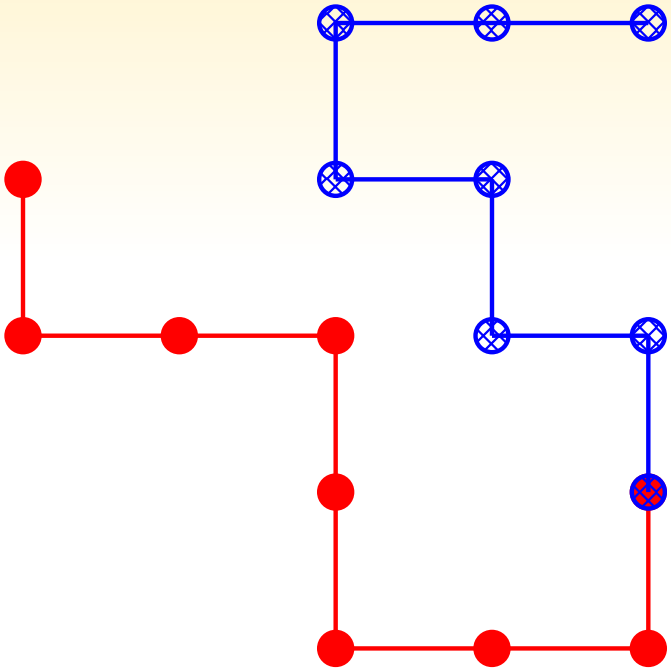
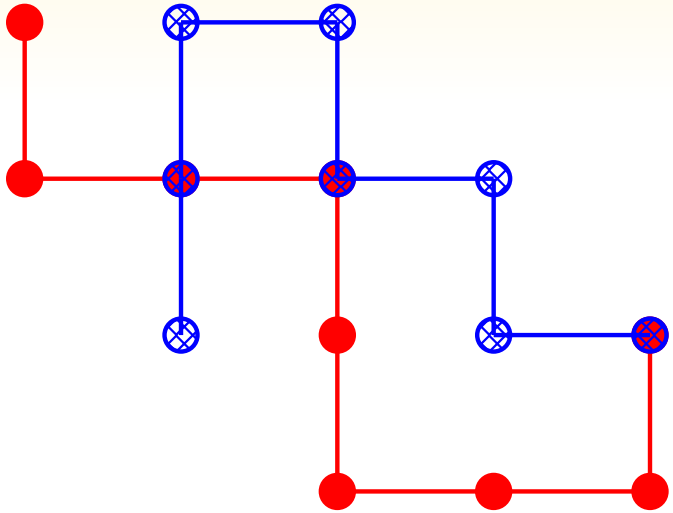
- Then use

$$c_N = \frac{c_N}{c_{N/2}^2}\left(\frac{c_{N/2}}{c_{N/4}^2}\right)^2 \cdots c_k^{N/k}.$$





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- This idea can be applied to other systems with additional length scales: confined polymers, bridges, star polymers, perhaps θ-polymers.

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- Pivot algorithm only part of the story.