Fast algorithms for Monte Carlo simulation of self-avoiding walks

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  - backbite moves for Hamiltonian paths
- Conclusion

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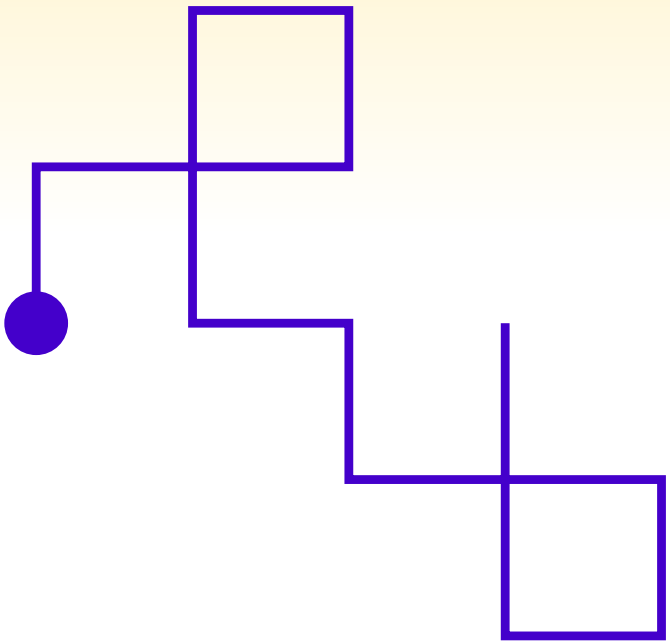

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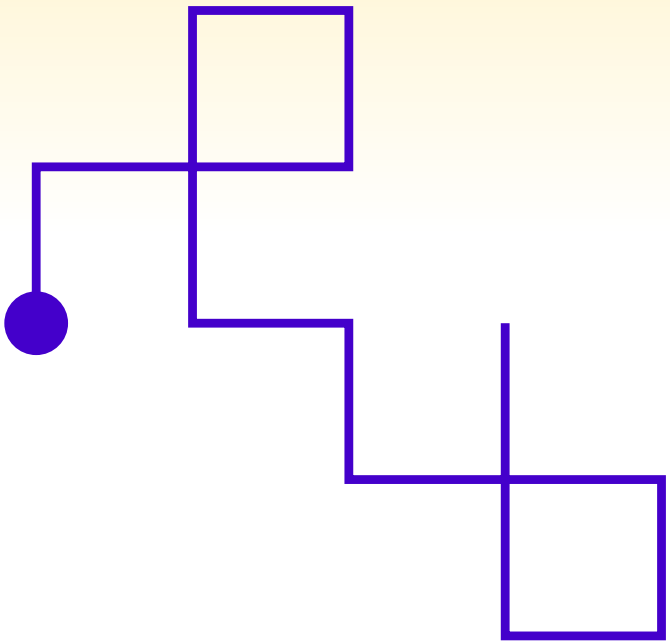

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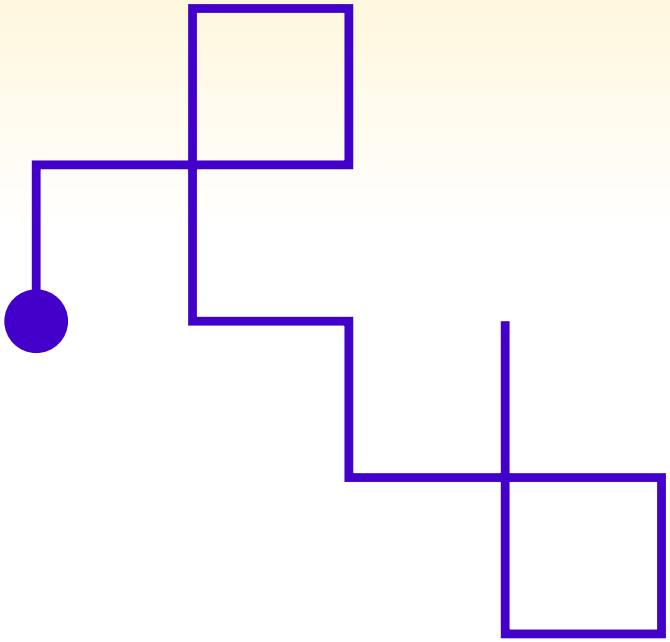

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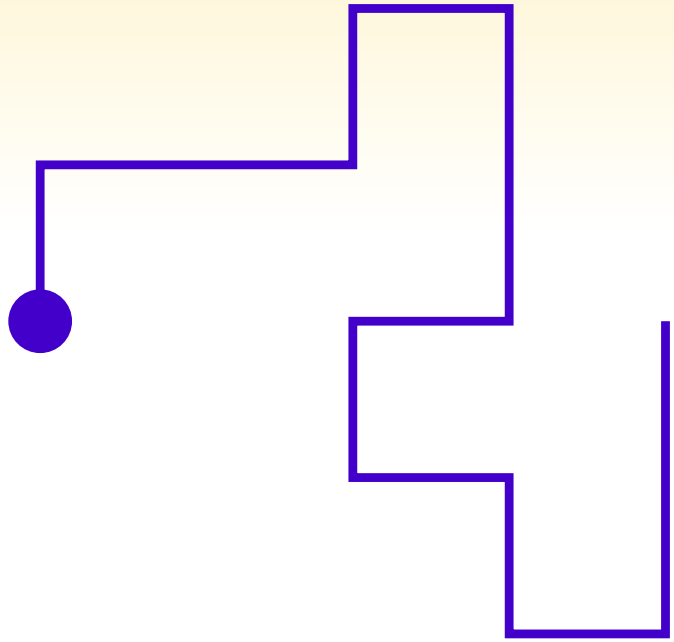
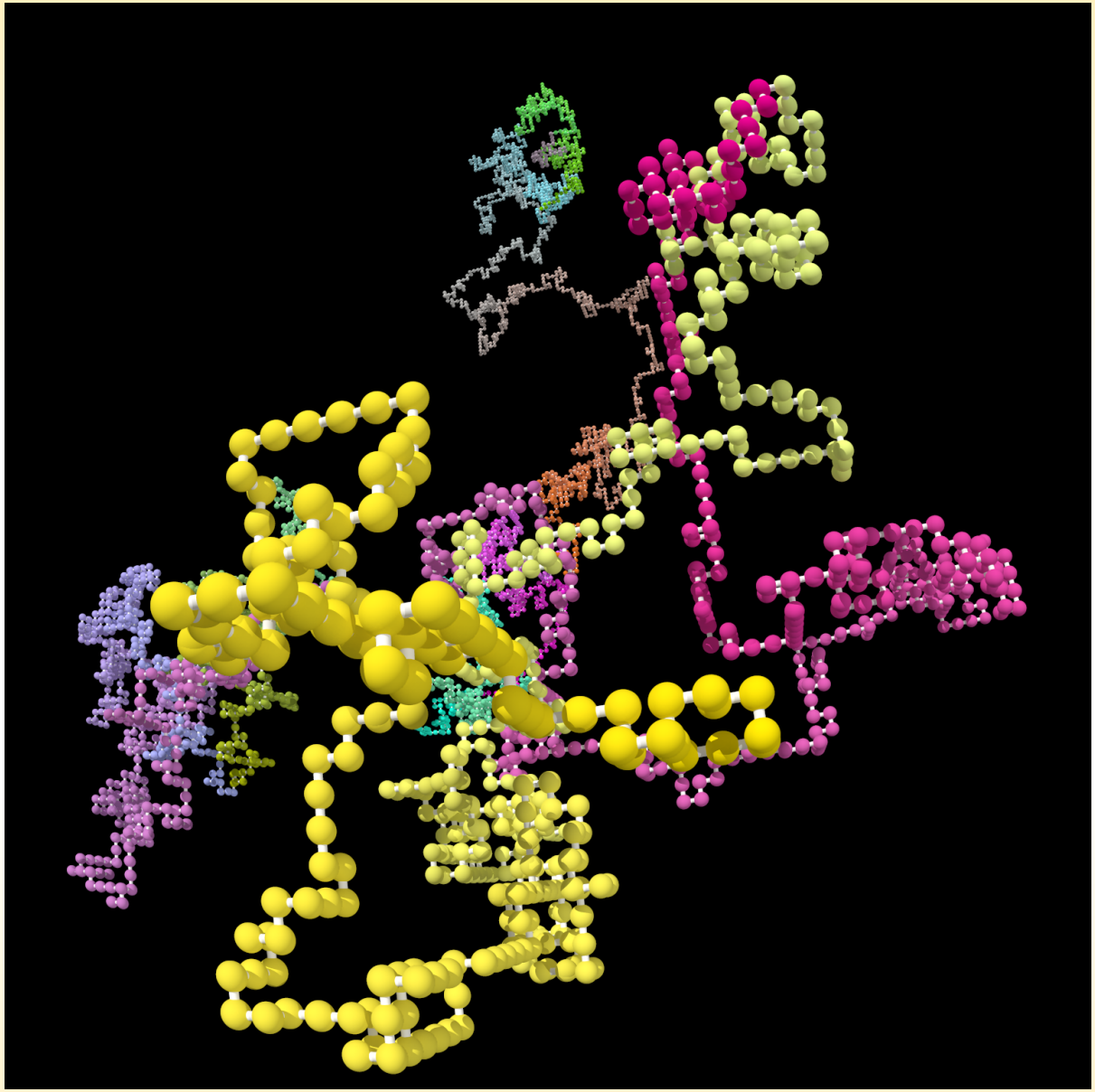


Self-avoiding walk

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



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- No exact solution for SAW.
- Markov chain Monte Carlo (MCMC) sampling very powerful for SAW, especially for $d = 3$.

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MCMC estimation of π

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- efficient implementation which implements global move for local cost.

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- Lal (1969) invented pivot algorithm, but key paper is by Madras and Sokal (1988).

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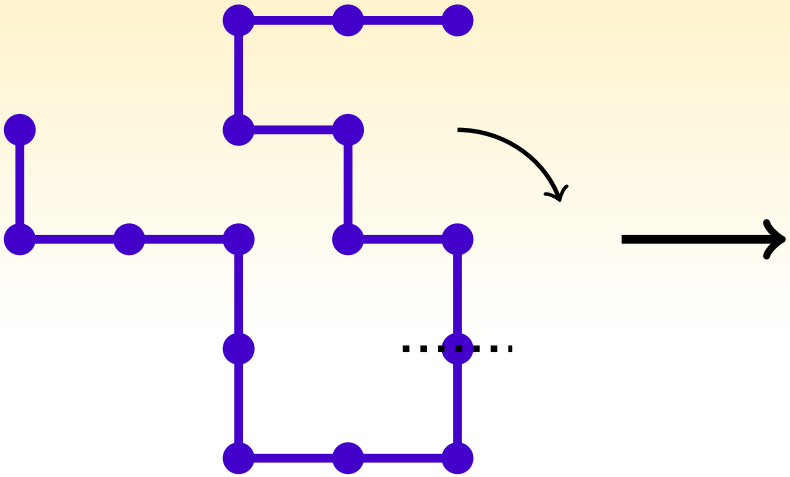
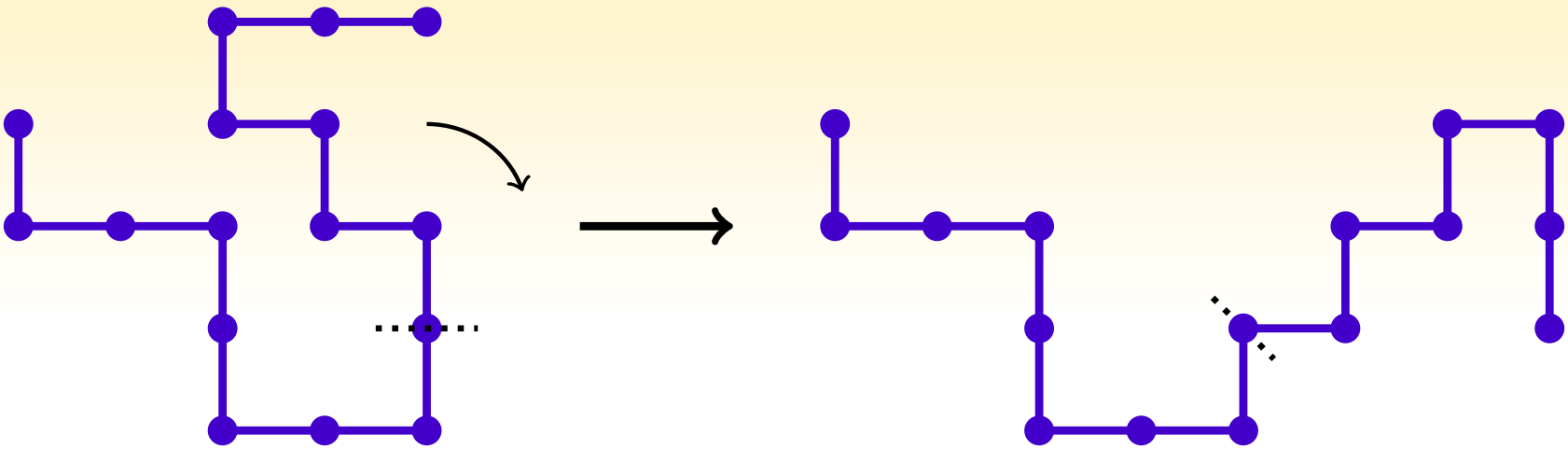
- Ergodic, samples SAWs uniformly at random.



Example pivot move



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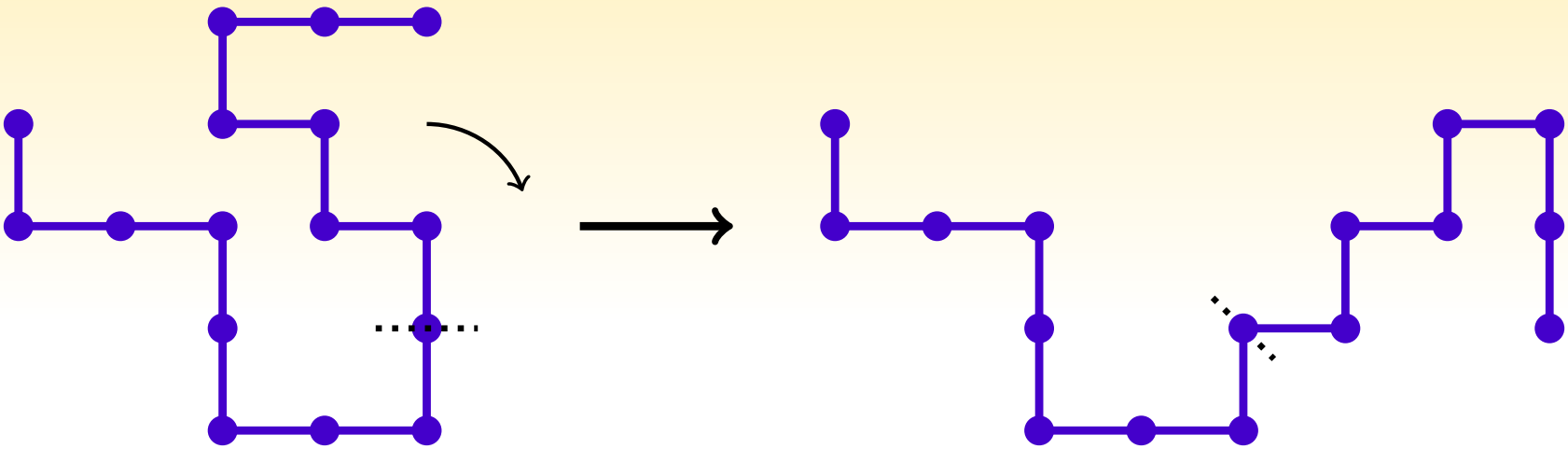

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- Bookkeeping can be handled efficiently in binary tree structure. $\Rightarrow O(\log N)$ (C., 2010)

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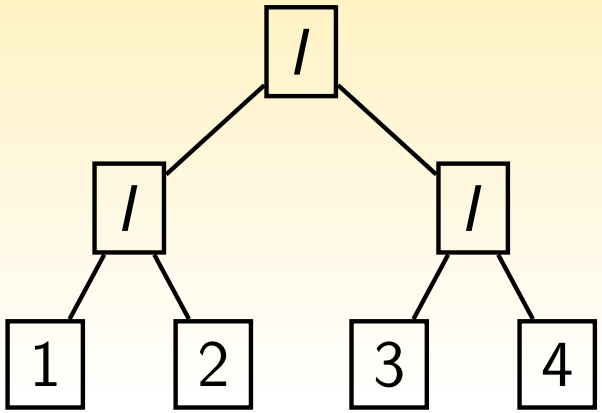
- Binary tree has typical height $O(\log N)$.

Example SAW-tree moves.



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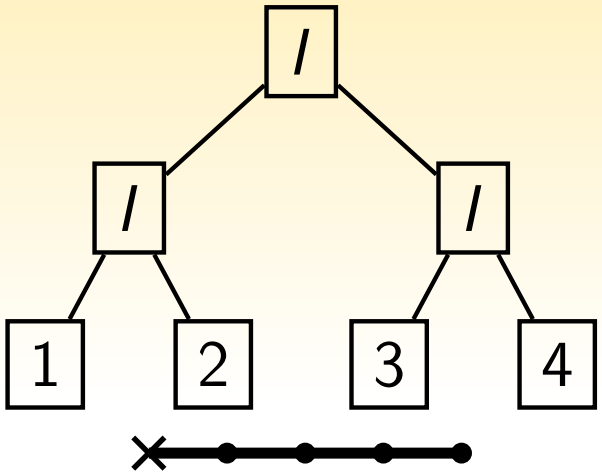

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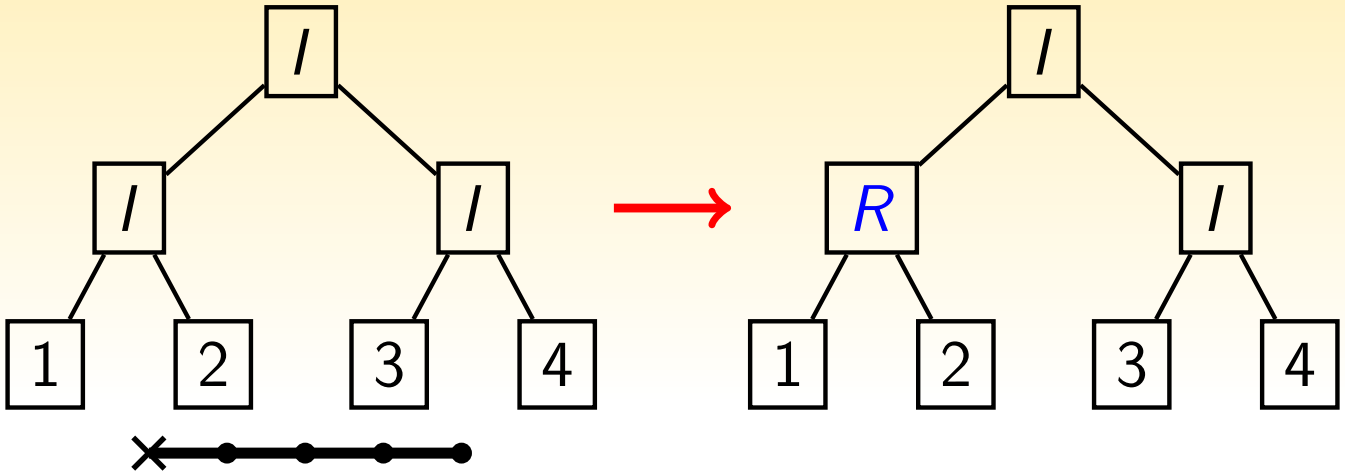

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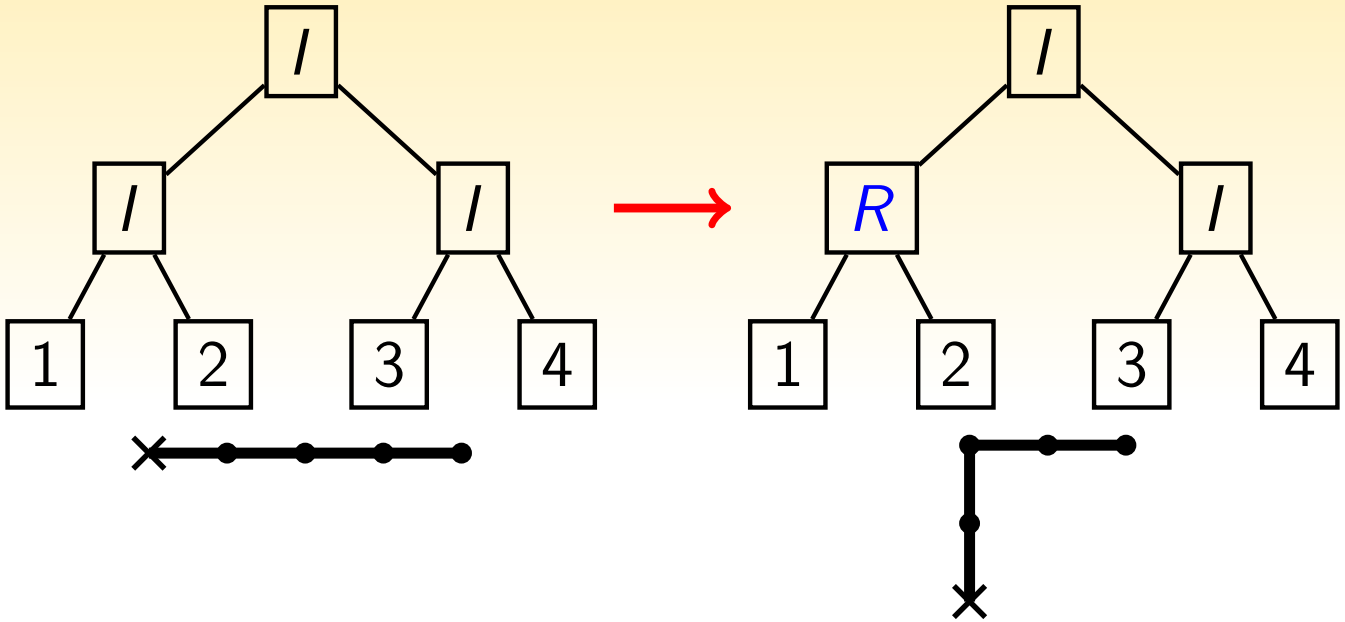

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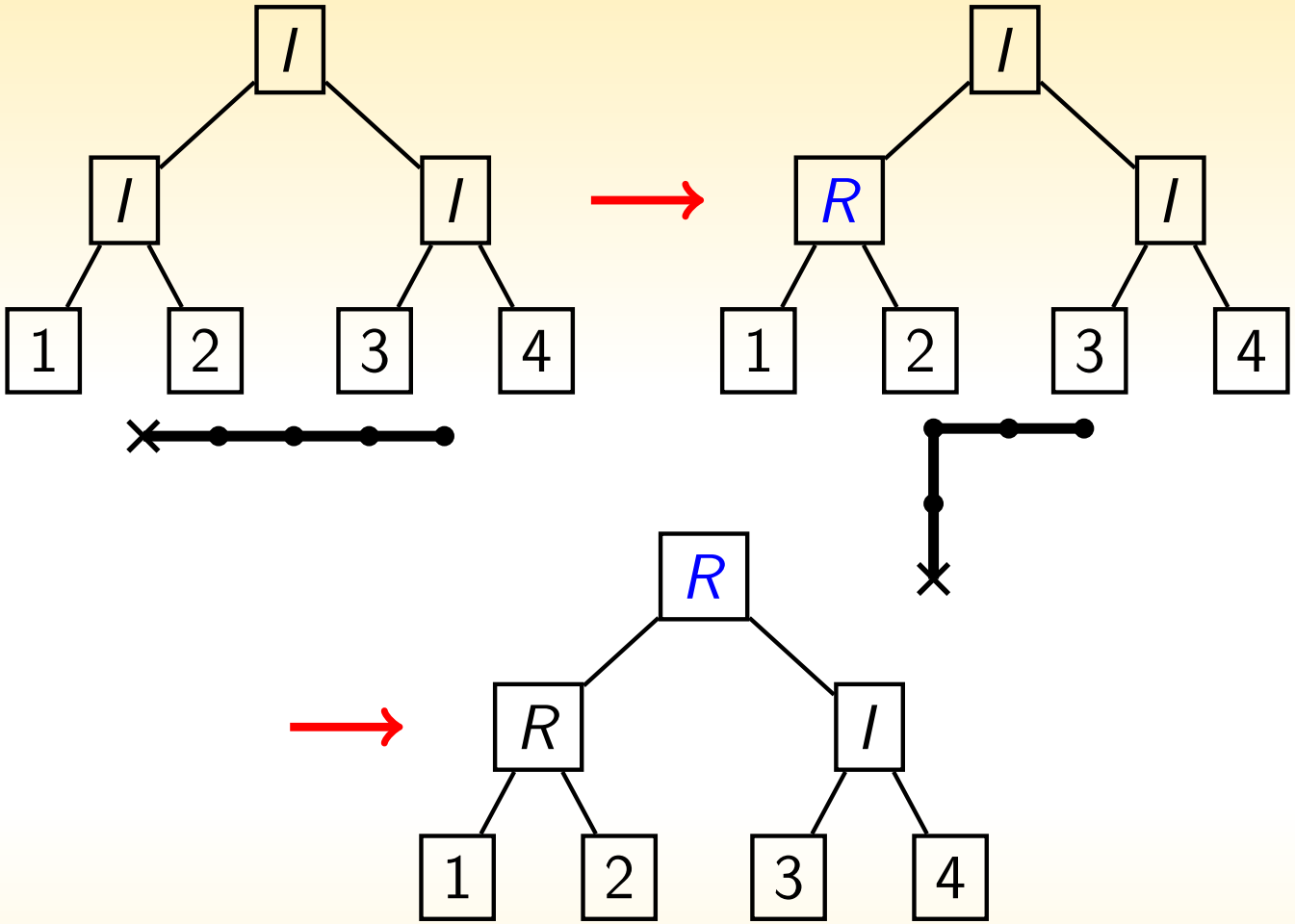

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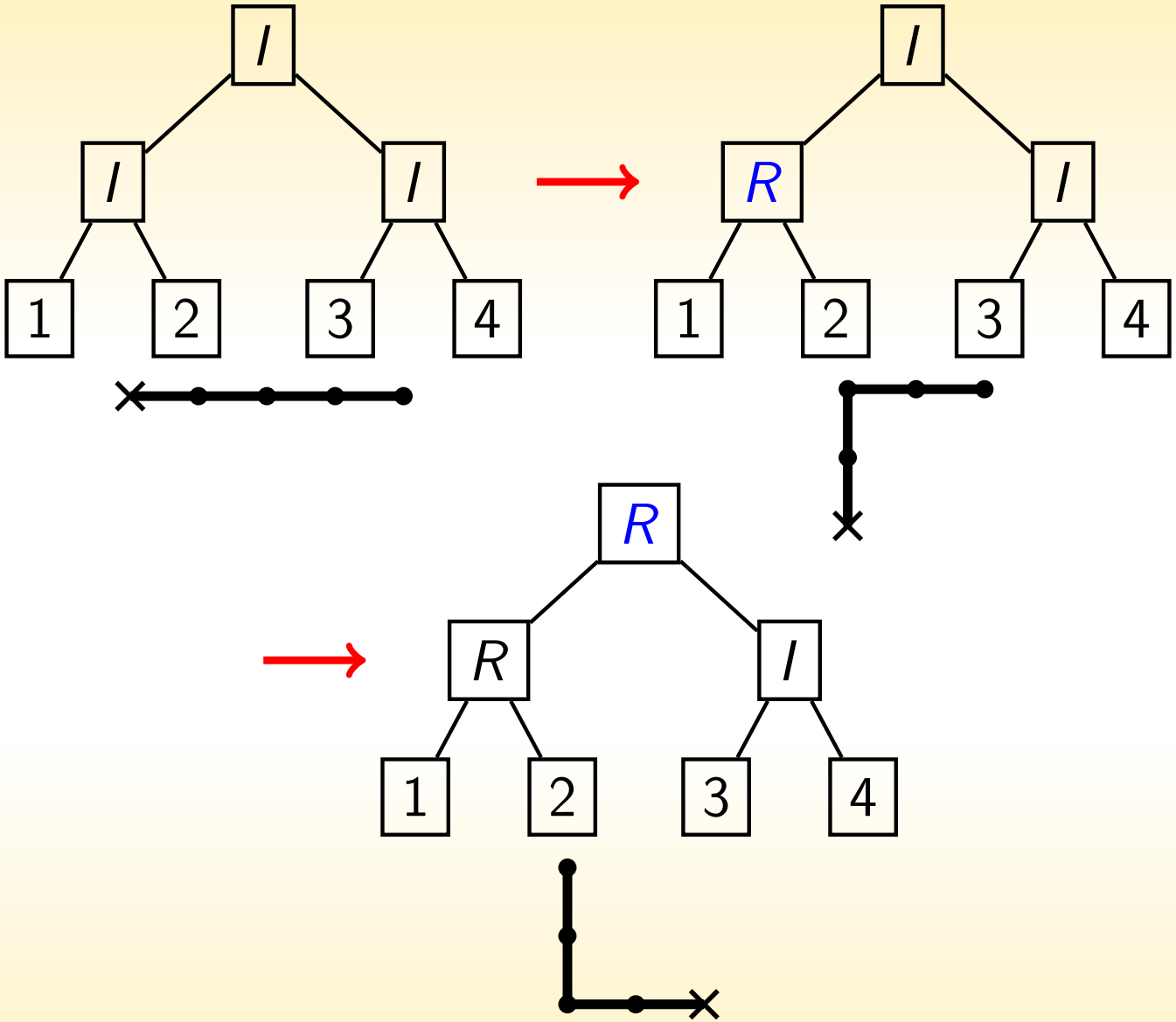

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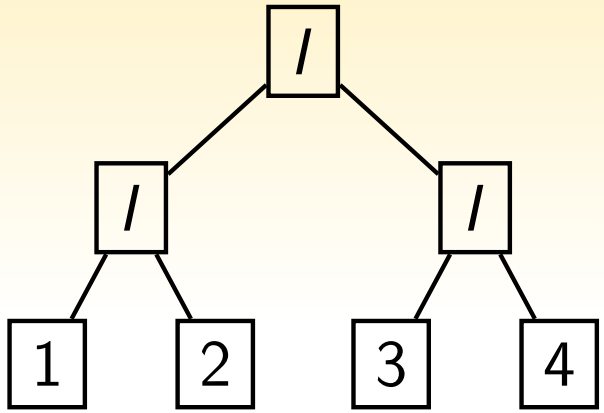

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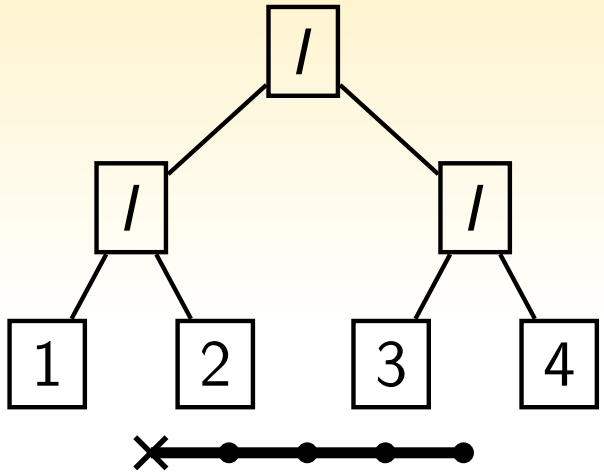

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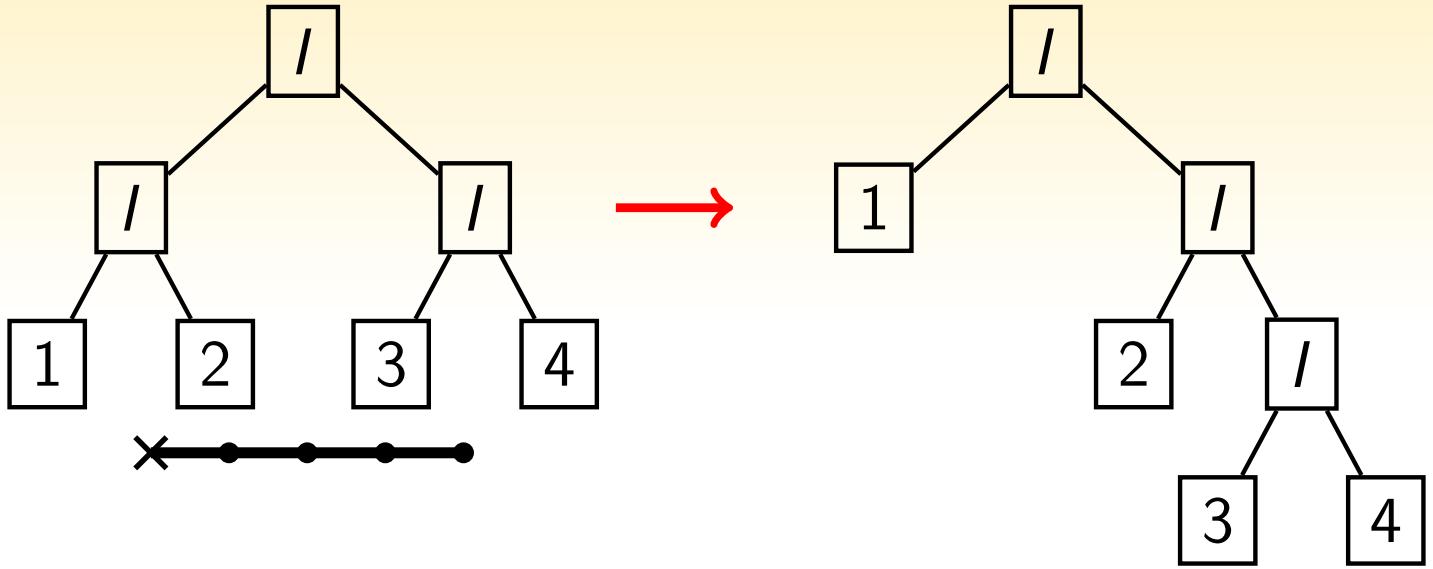

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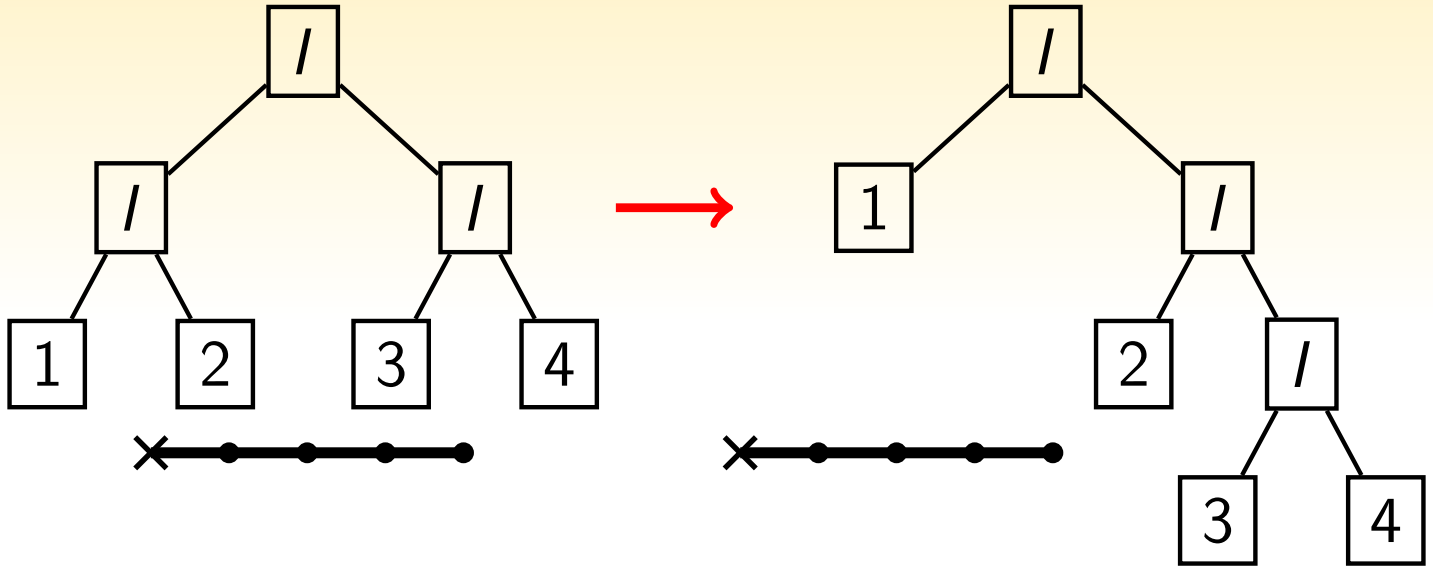

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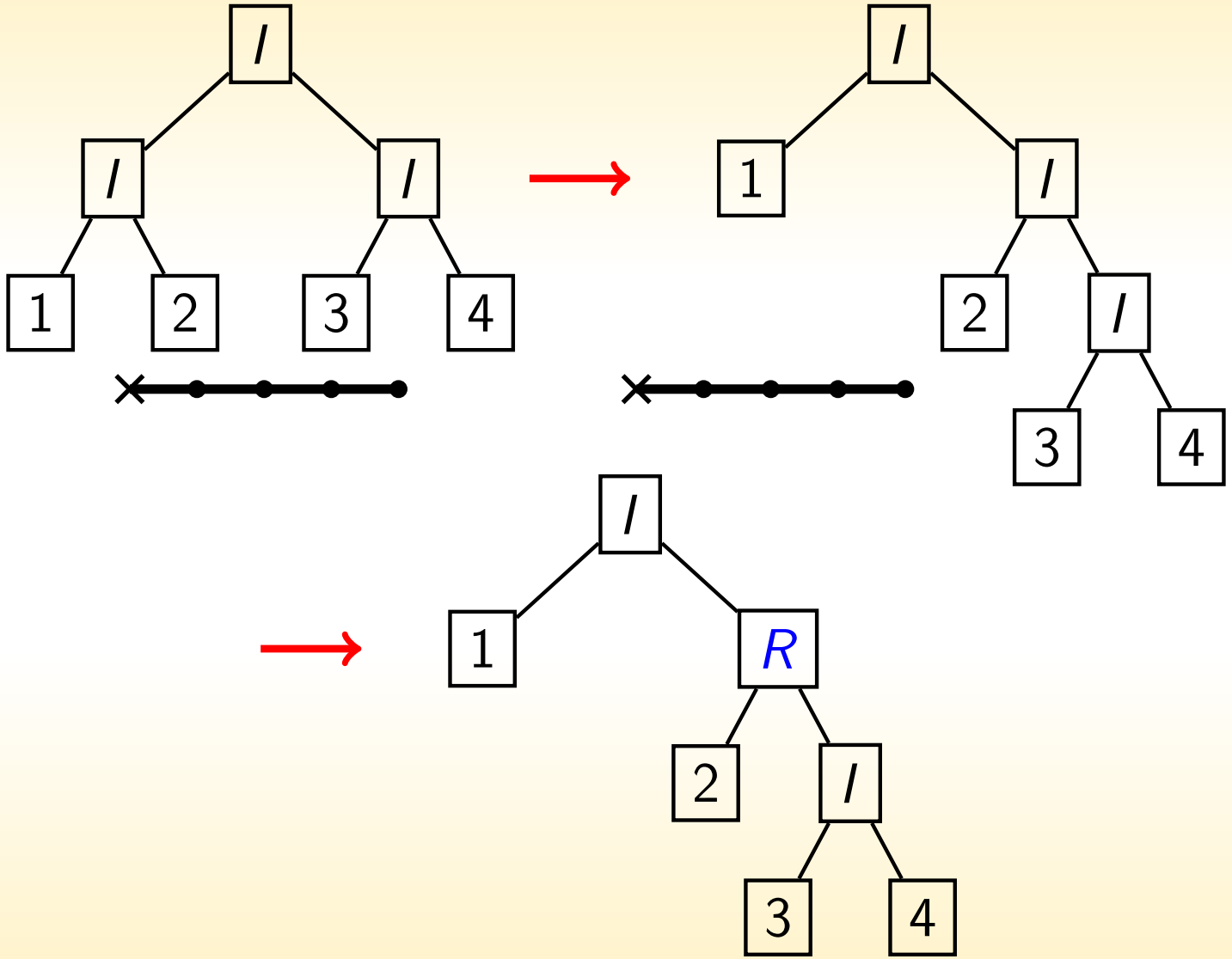

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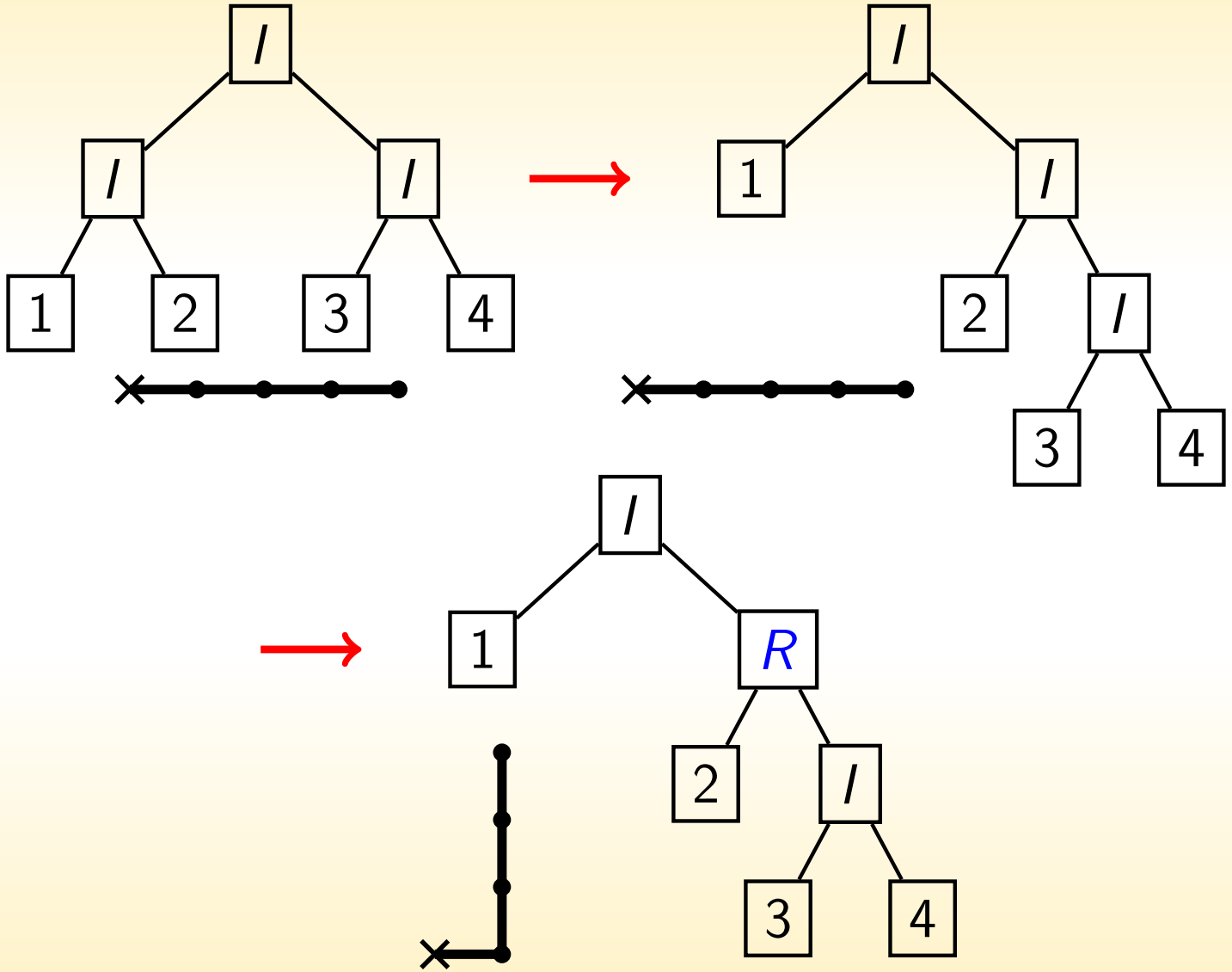

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- How can we extend this key idea - fast global moves - to other models?

Hamiltonian paths

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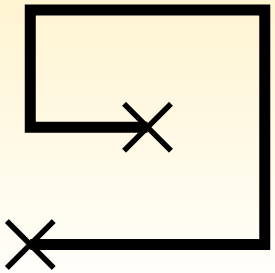
- Hamiltonian path generator, see
  `http://lattice.complex.unimelb.edu.au/hamiltonian_path`

Backbite moves for sampling Hamiltonian paths.



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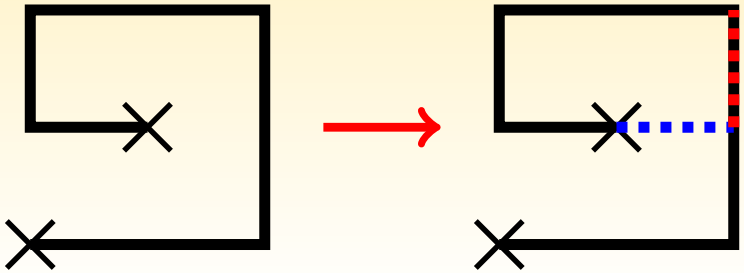

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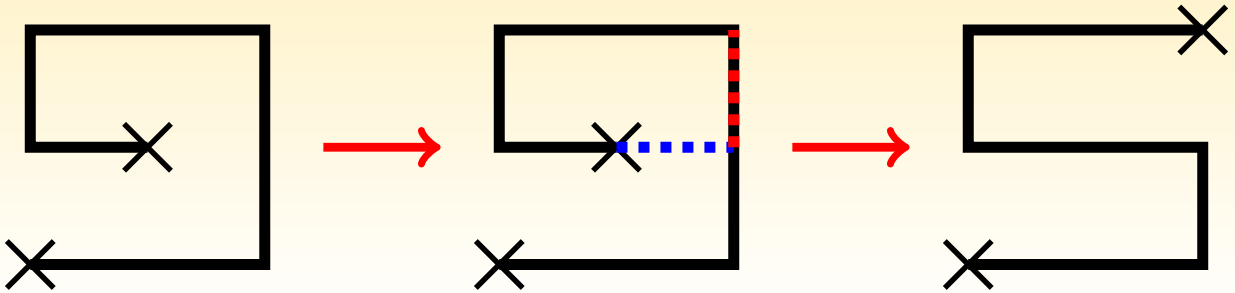

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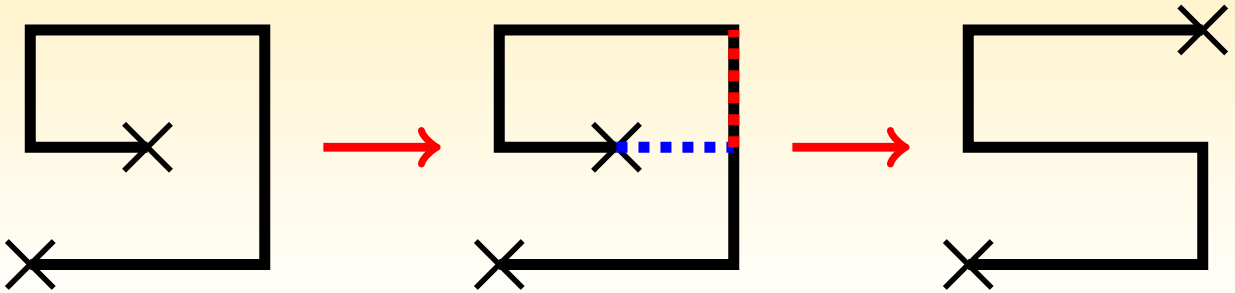

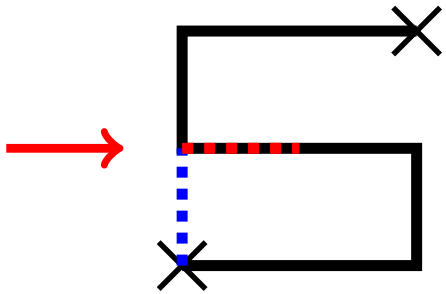

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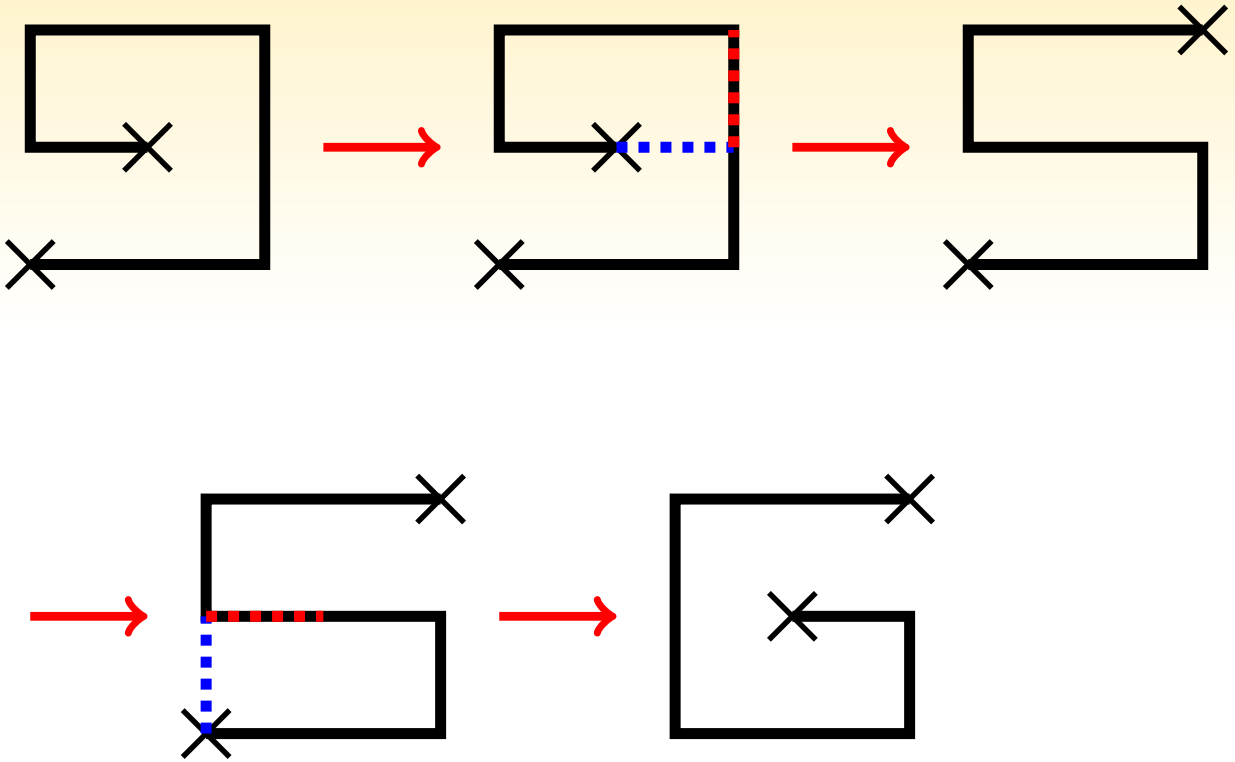

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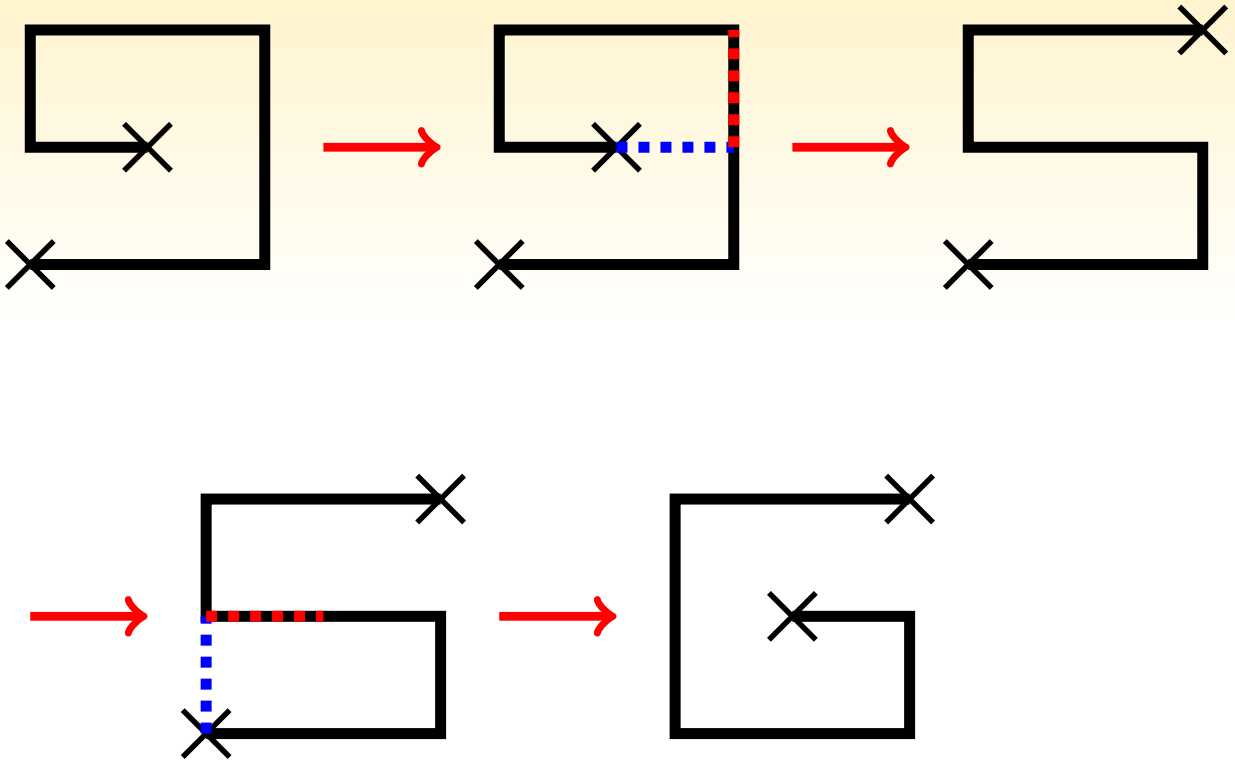

Each time we make a backbite move we create a loop, delete the edge which completes the loop, and *reverse* the orientation of the remaining edges of the loop.

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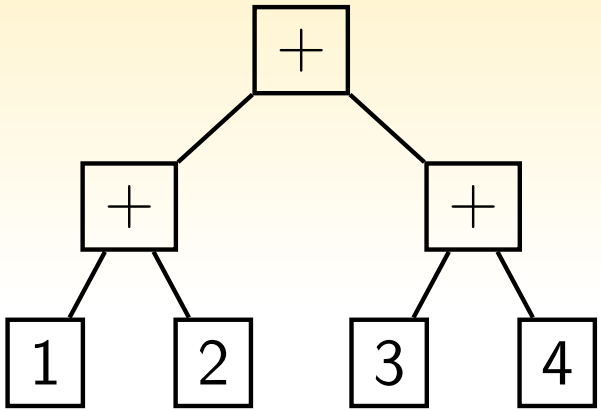
- Use binary tree data structure with *time reversal* as our symmetry operation, with bookkeeping for determining neighbours.

This time binary tree has time reversal symmetry elements in the nodes.



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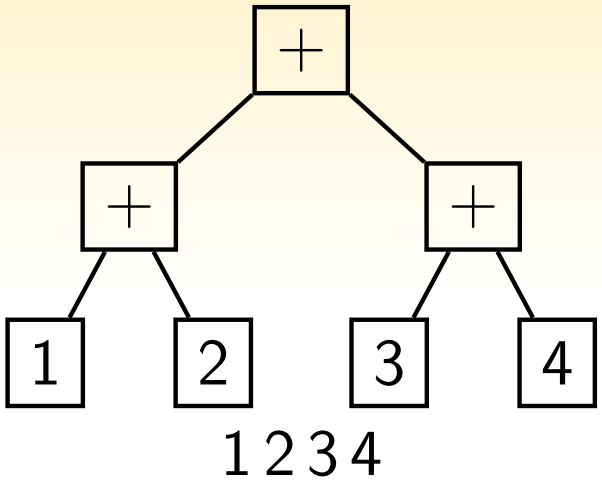

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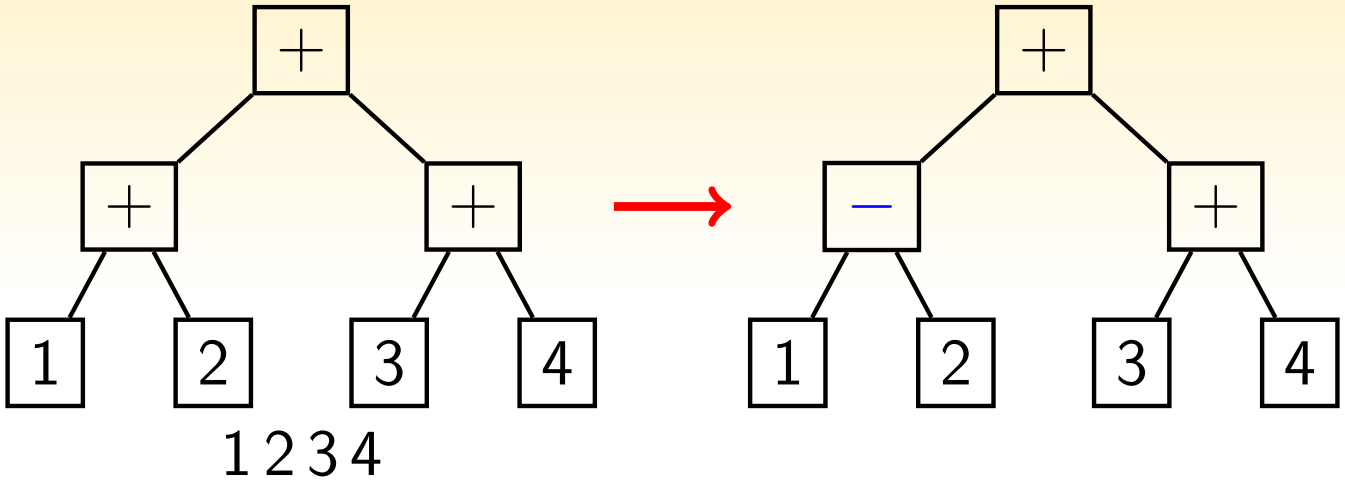

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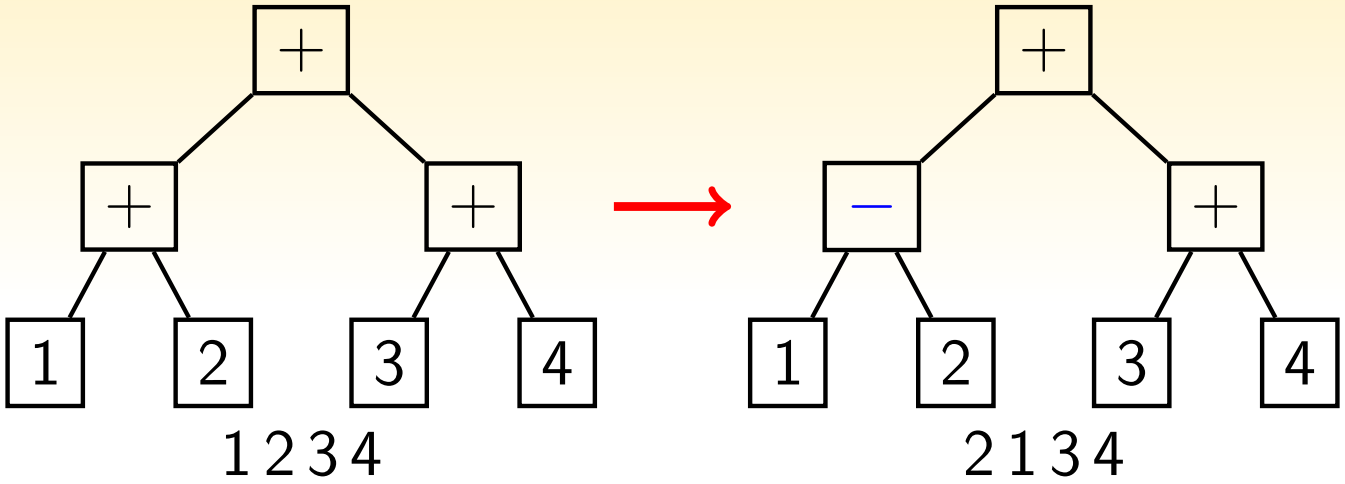

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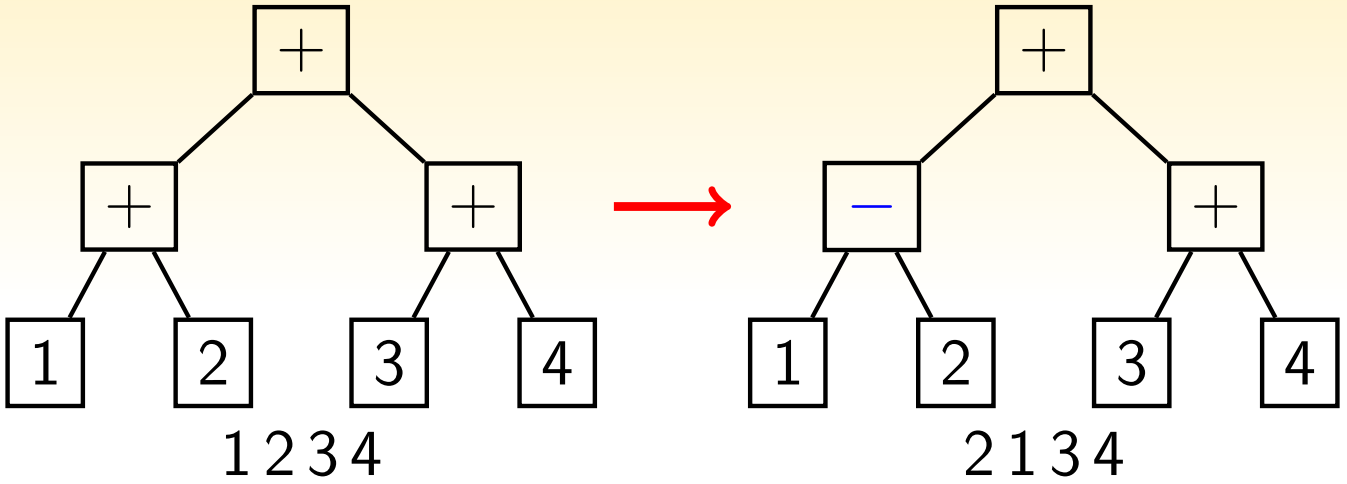

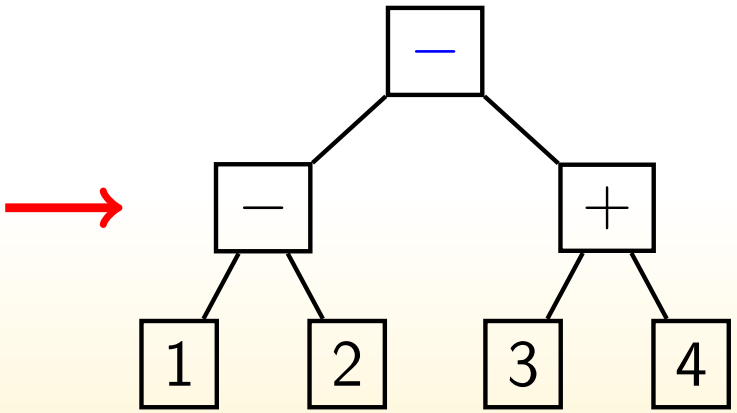

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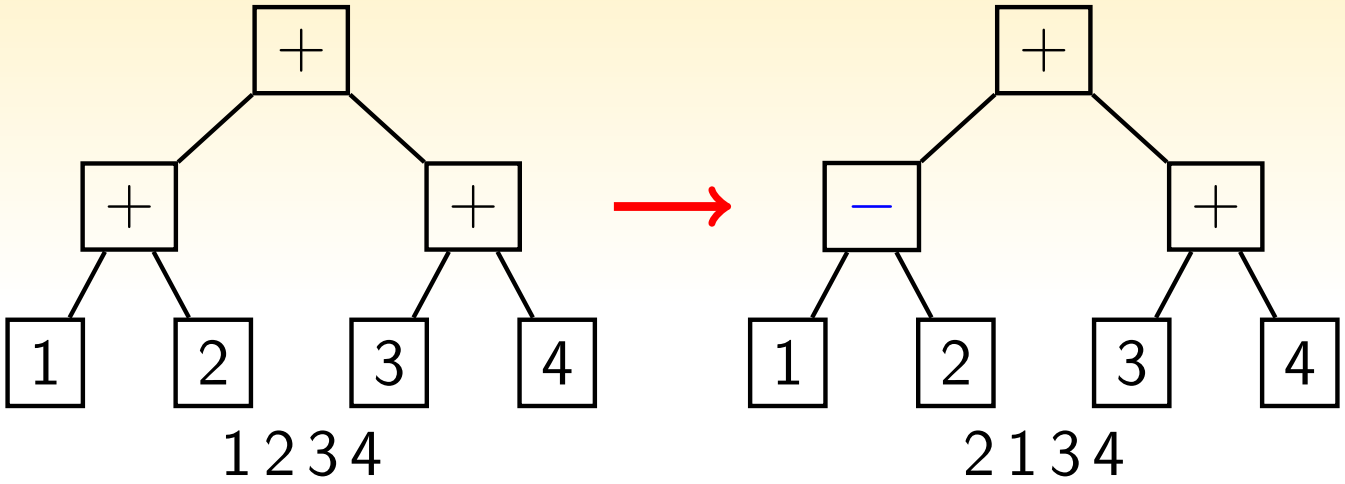

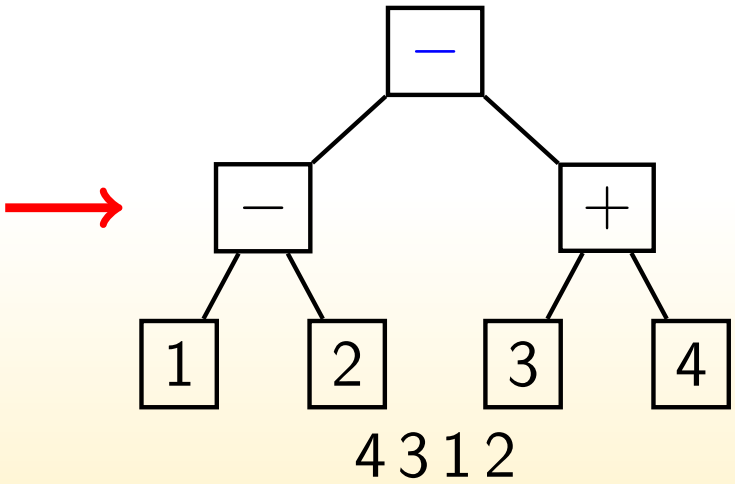

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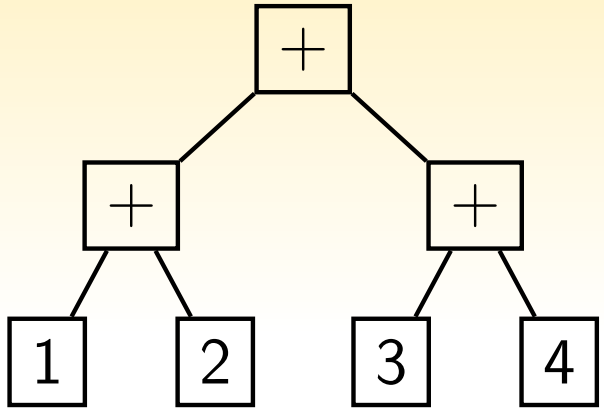

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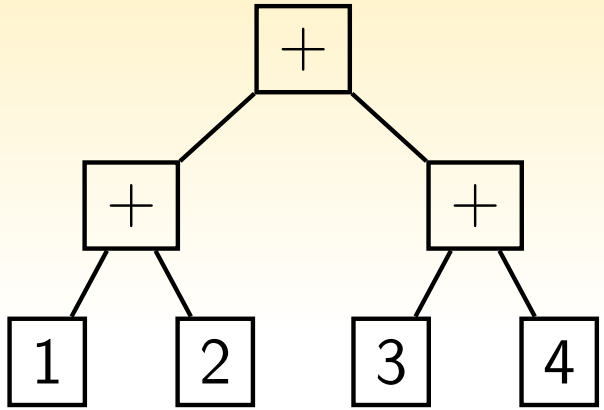

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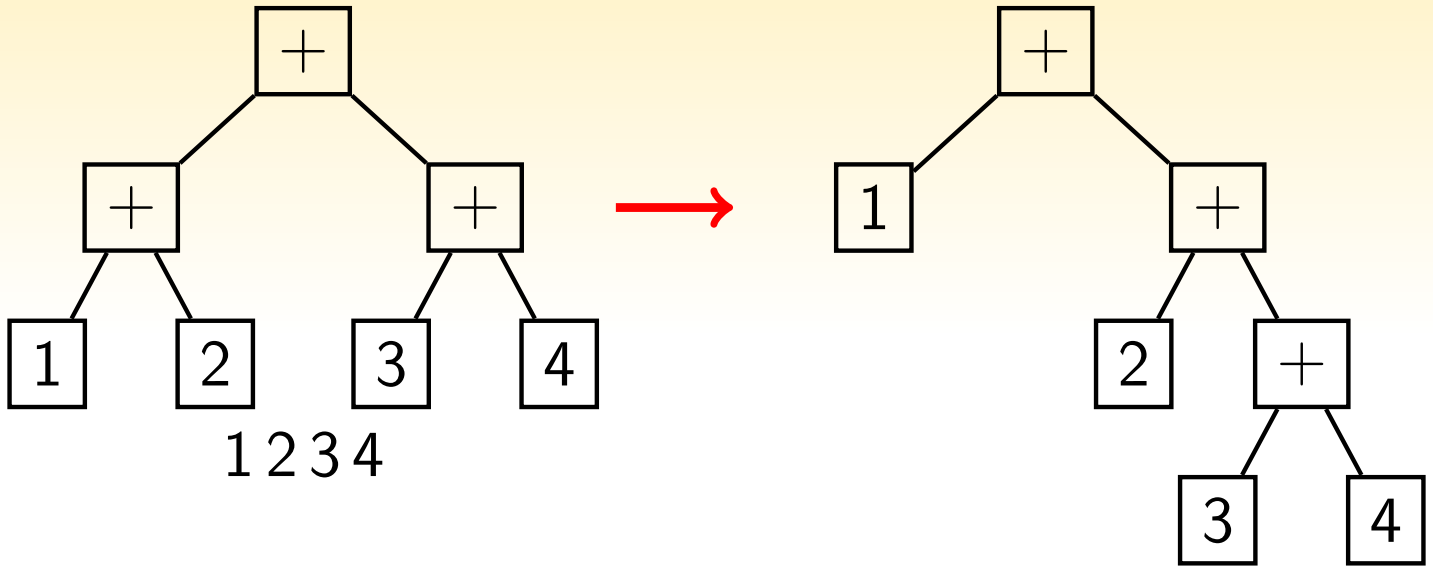

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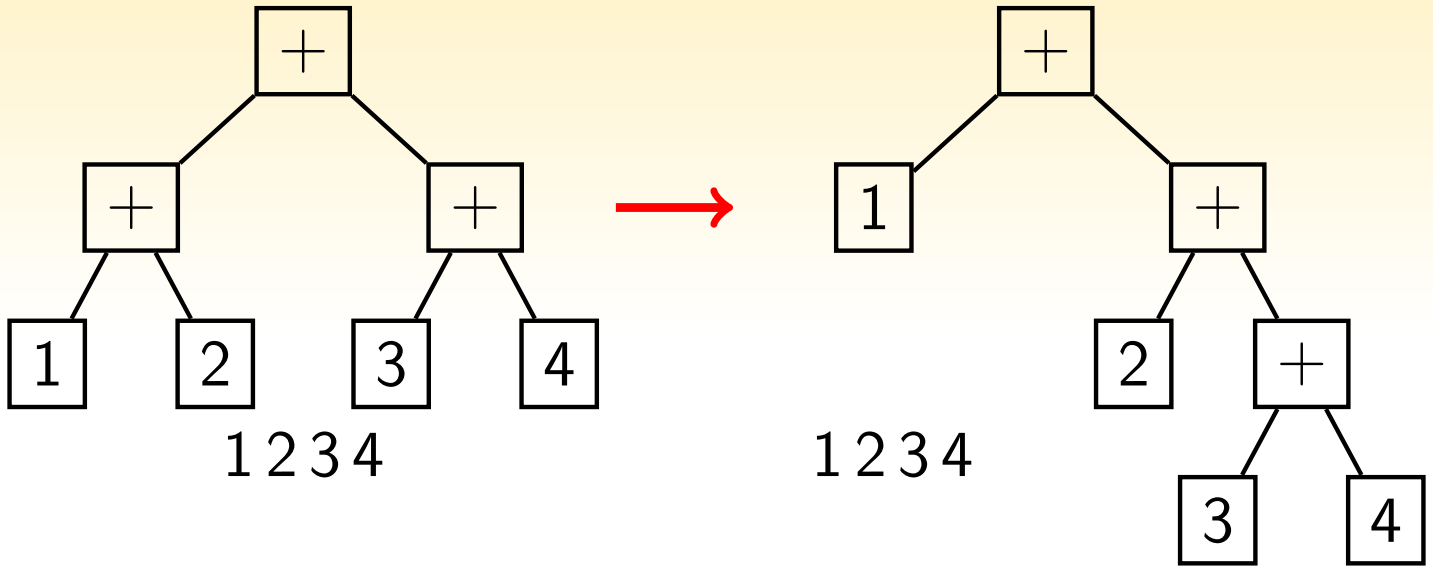

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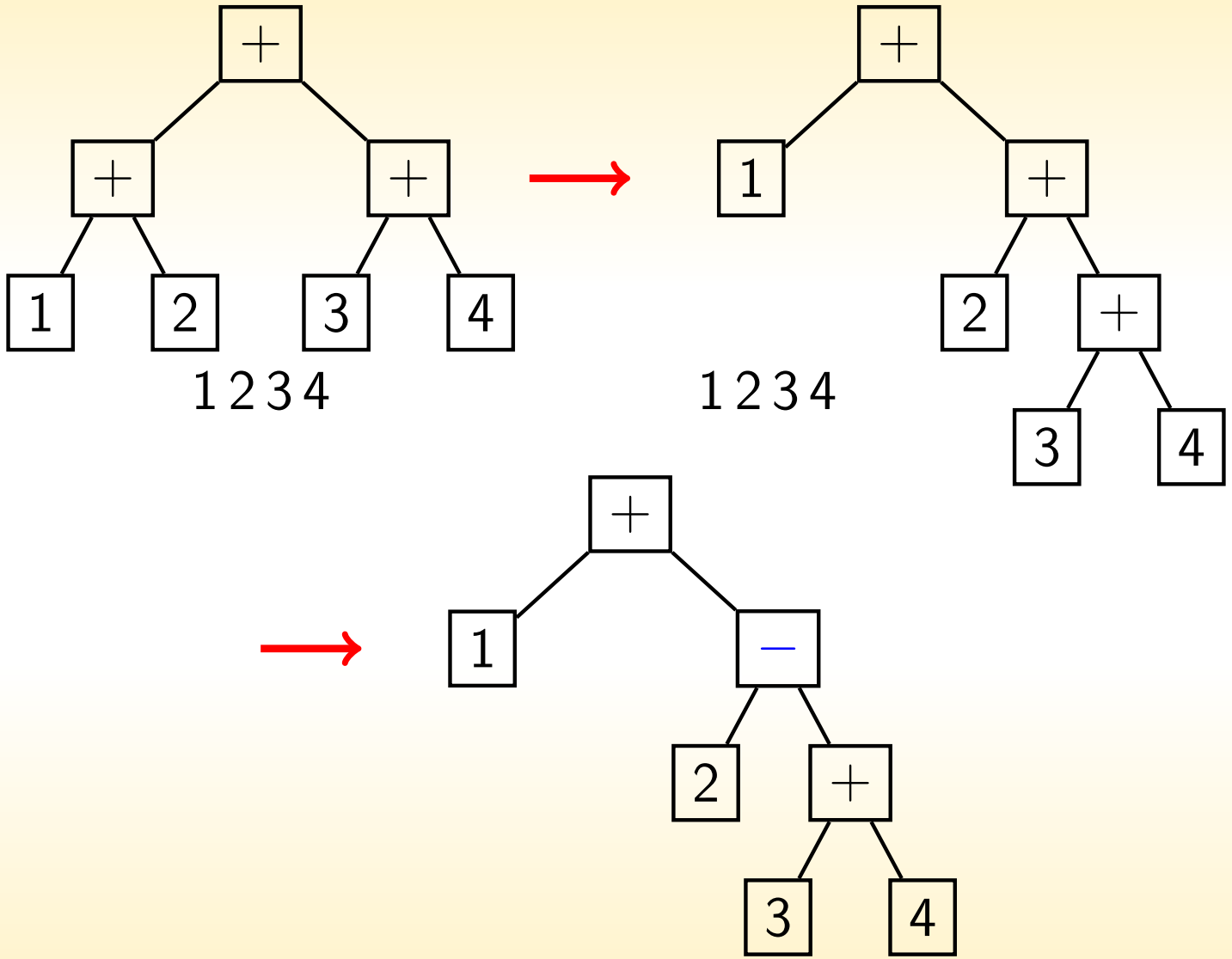

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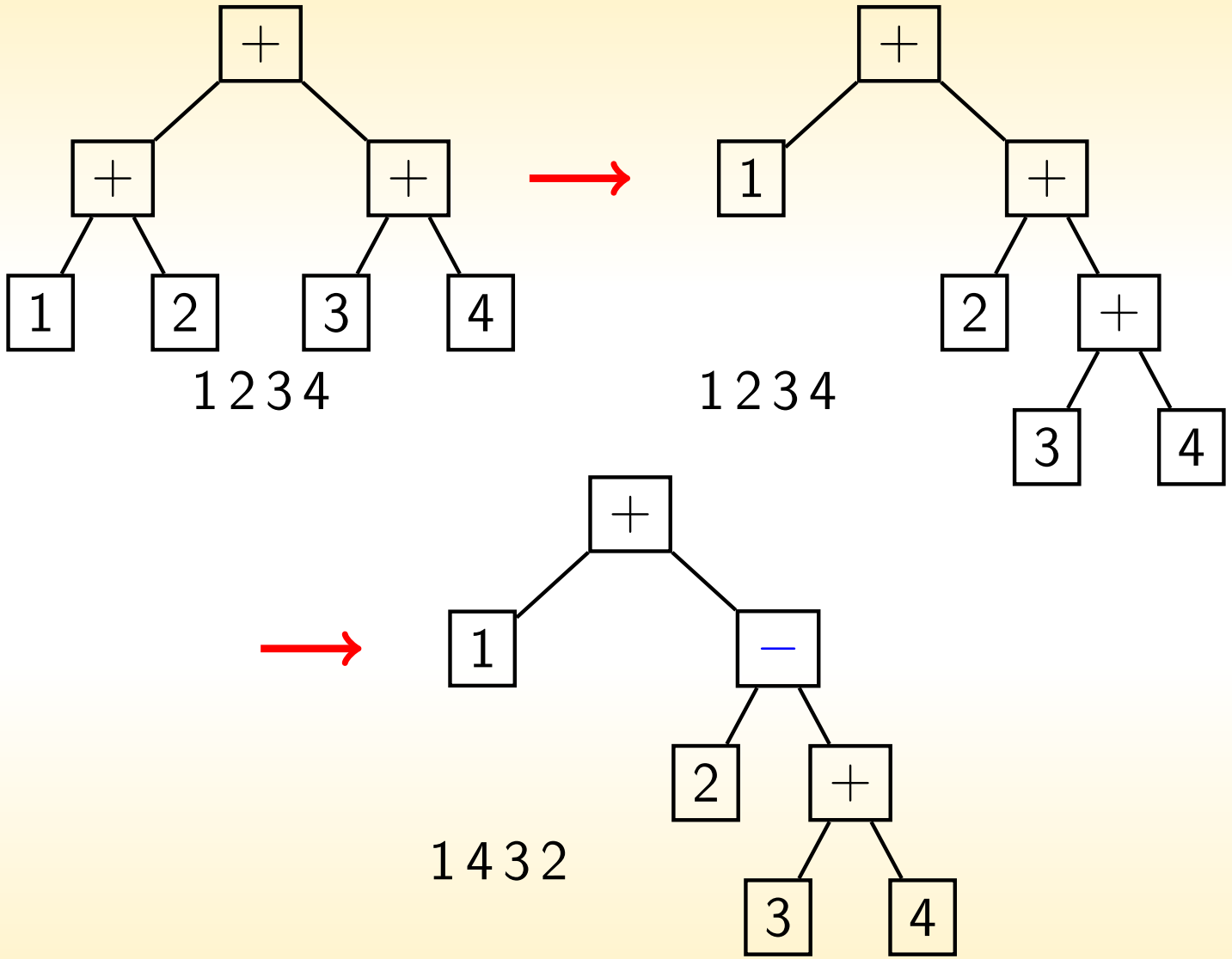

Results

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- $\mathbb{Z}^3$: $L = 512$, $N = 134\,217\,728$: 46 million steps, versus 20.6 tree rotations.

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- Apply global move without explicitly evaluating all of the effects of the move - just need to be able to test some properties of the object efficiently.
- Linear order of walks makes things easy; can we apply these principles elsewhere?