Preserving topology while sampling

Trials and tribulations

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Andrew Rechnitzer   Nick Beaton   Nathan Clisby

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How hard could it be?

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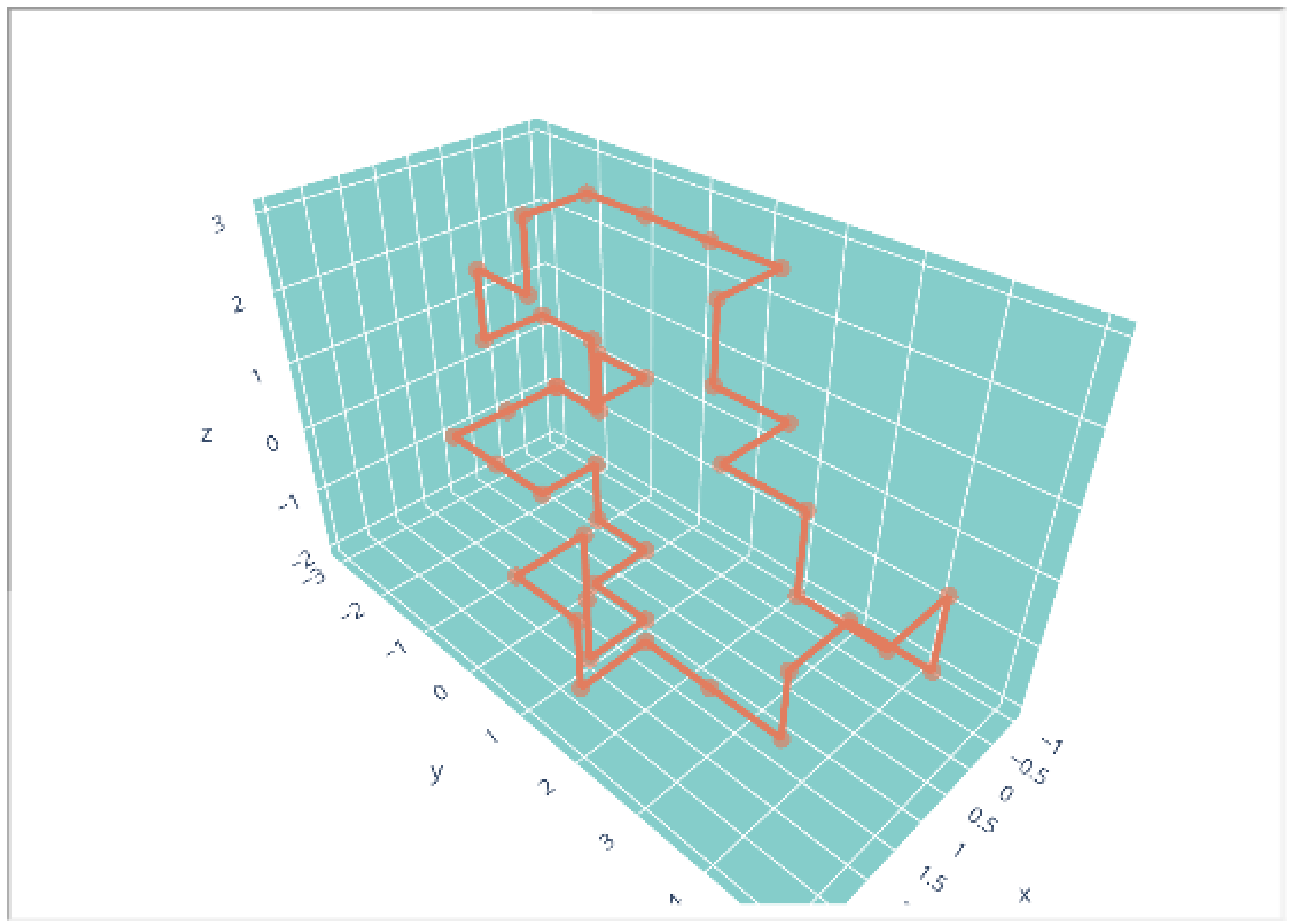
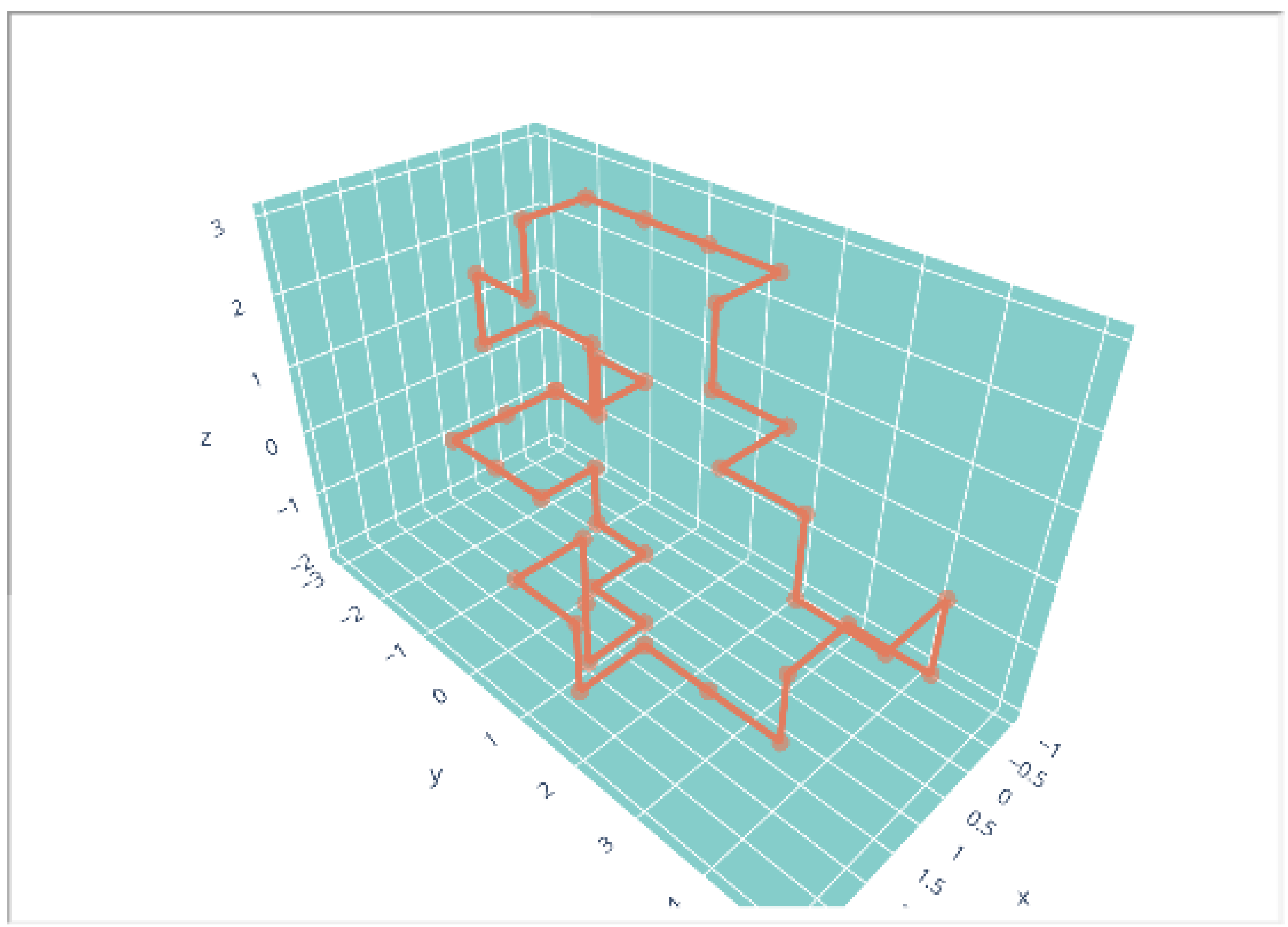
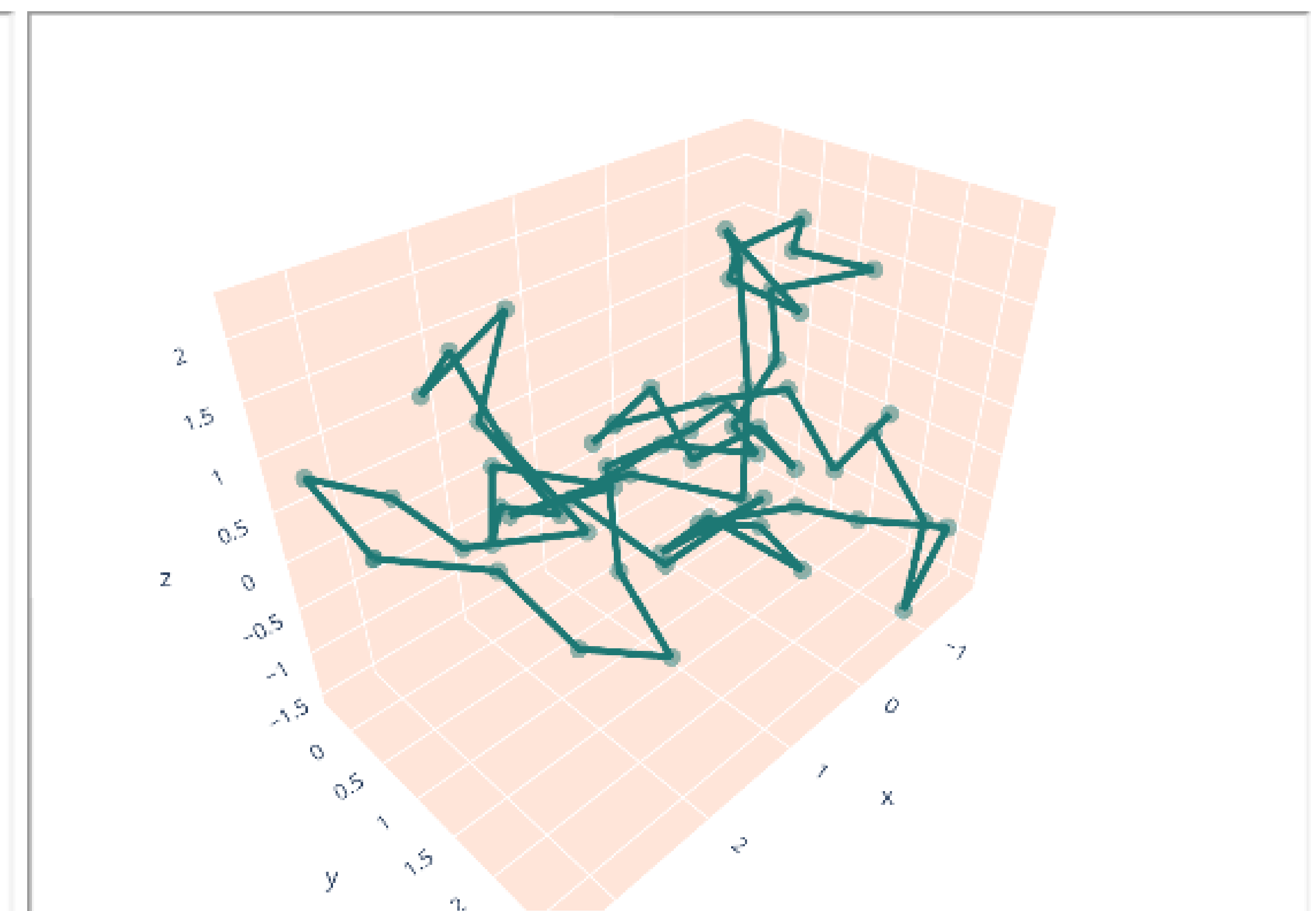
  - embedding of simple loop into lattice
  - each embedding of length n equally likely



My favourite two measures

- Self-avoiding polygons (SAP) in $\mathbb{Z}^3$
  - embedding of simple loop into lattice
  - each embedding of length n equally likely
- Equilateral random polygons (ERP) in $\mathbb{R}^3$
  - each edge has unit length
  - edge direction chosen uniformly on S^2, conditioned to close





Analytic results are very hard

- Work by Whittington, Sumners, Millett, Soteros, van Rensburg, Orlandini, Deguchi, Cantarella, Micheletti, Grosberg, …
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Resort to random sampling instead

- Sample a superset and then sieve out the ones you want, or
- Sample only curves of the given fixed topology

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- Exact random sampling of ERP — Cantarella et al (2015)
- Time $O(n^{5/2})$ to produce an completely independent ERP

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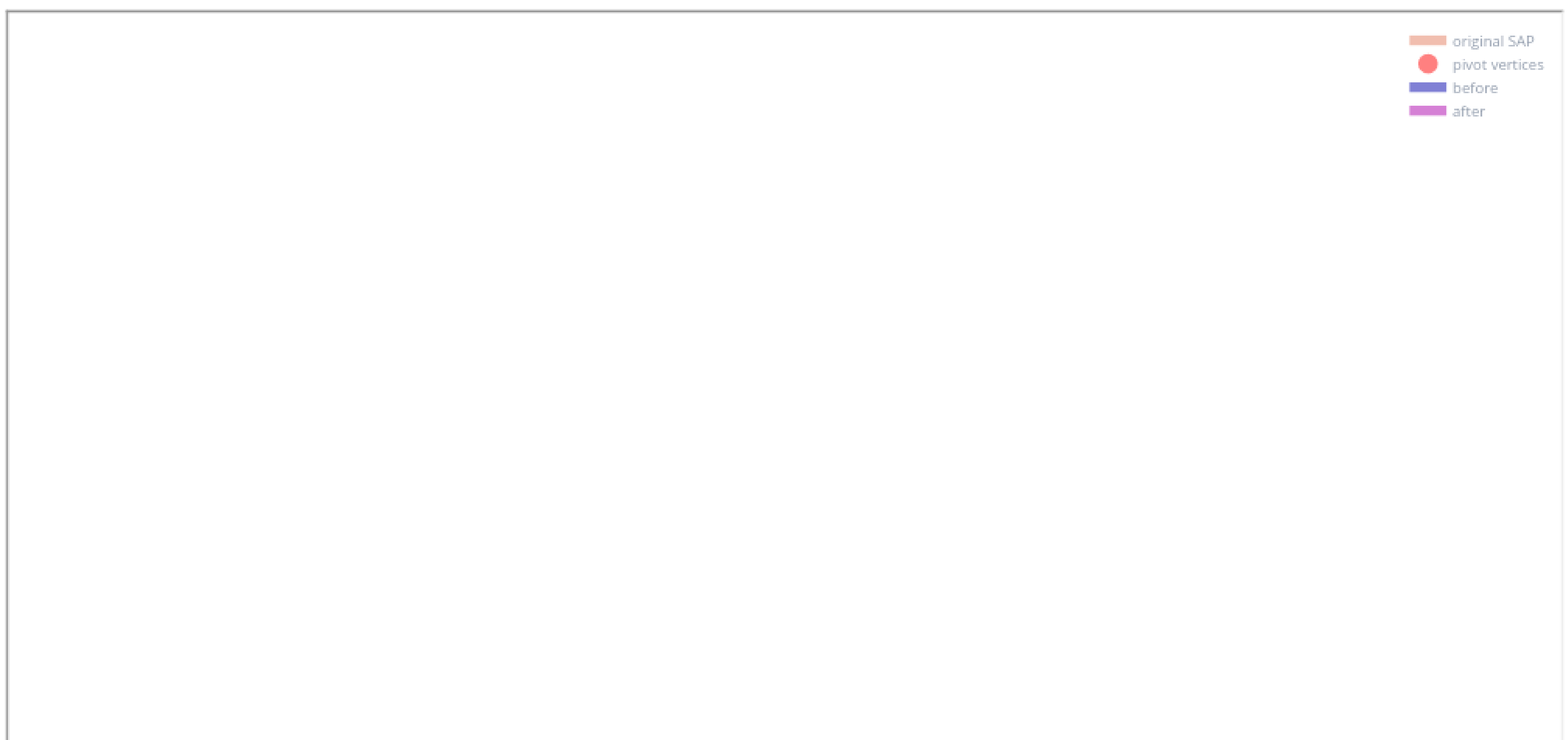
Sample superset then sieve #2

- Pivot algorithm on SAP of fixed length — Lai (1969), Madras & Sokal (1988), Madras et al (1990)
- Clisby (2010) implementation — $O(\log n)$ to sample statistically "*independent*" walk



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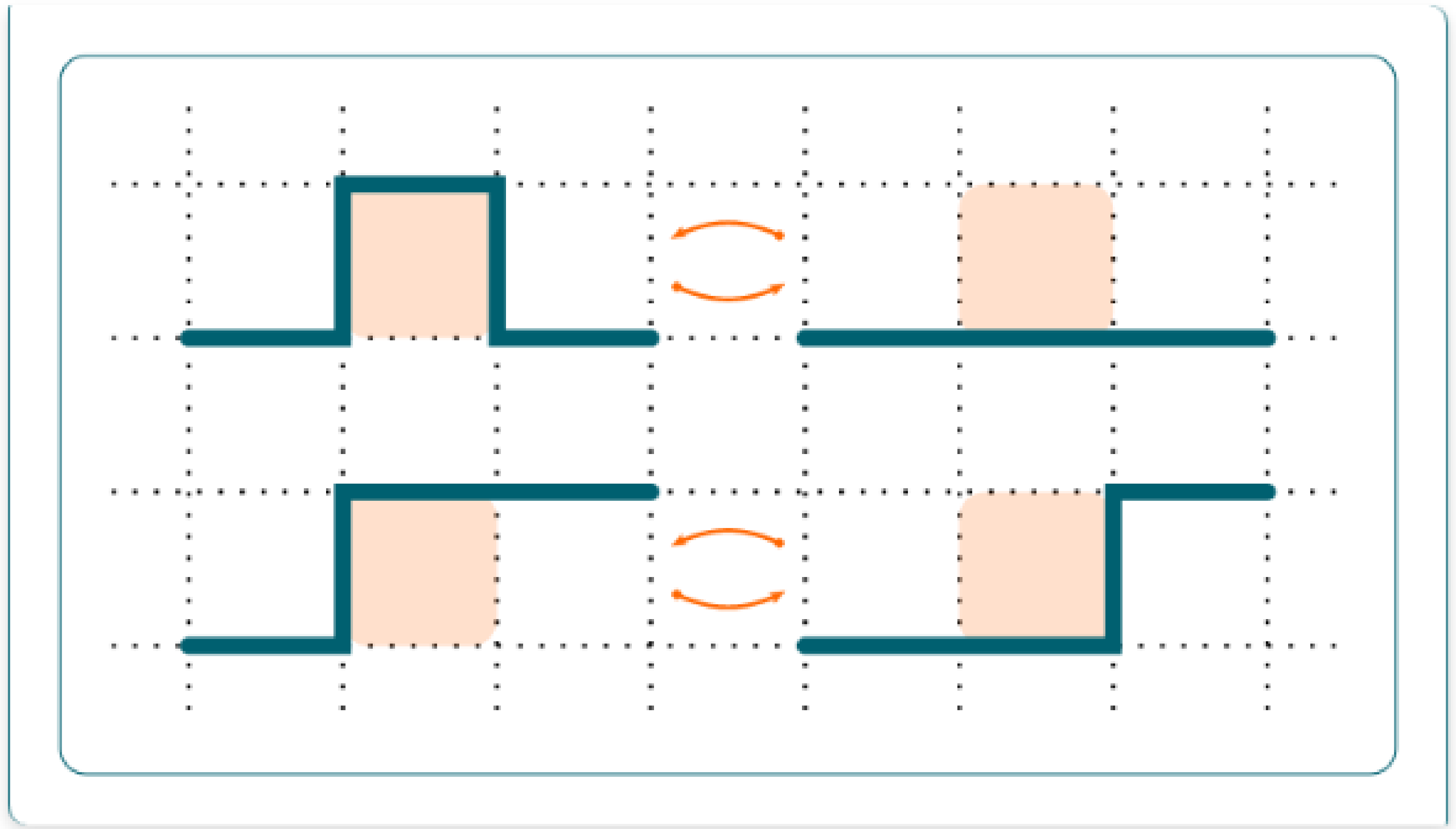
  - long polygon $\Longrightarrow$ many crossings $\Longrightarrow$ hard to ID
- Aside — how can we measure the trefoilness of a larger knot?

Sample only fixed topology #1

- Markov chain on SAPs of fixed topology — B.F. A.C.F. (1981, 1983)
- No topological testing needed — strand passage not possible
- Ergodic on knot type van Rensburg & Whittington (1991), van Rensburg & R (2011)



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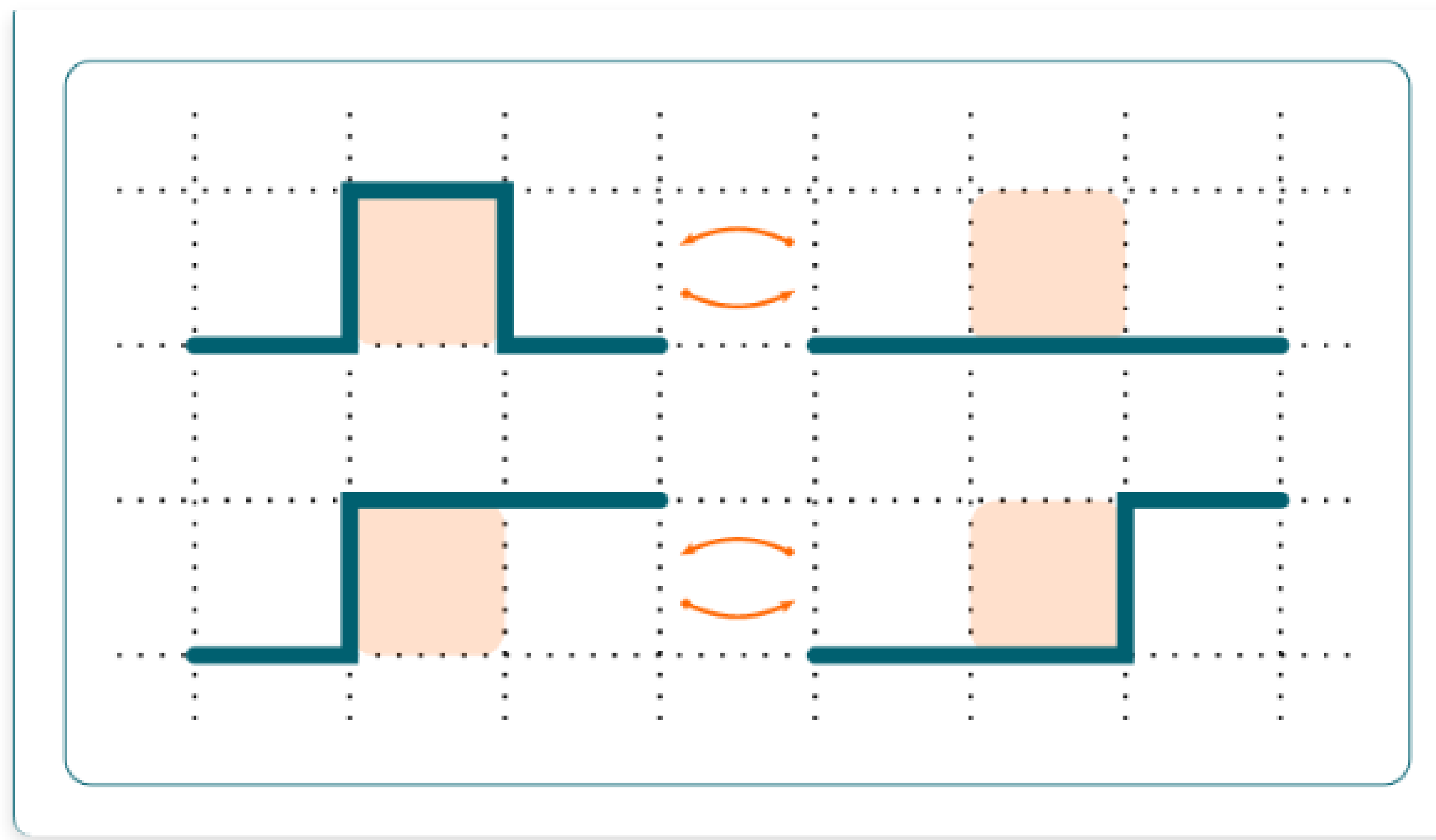

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- Tune so that grow/shrink moves equally likely to succeed

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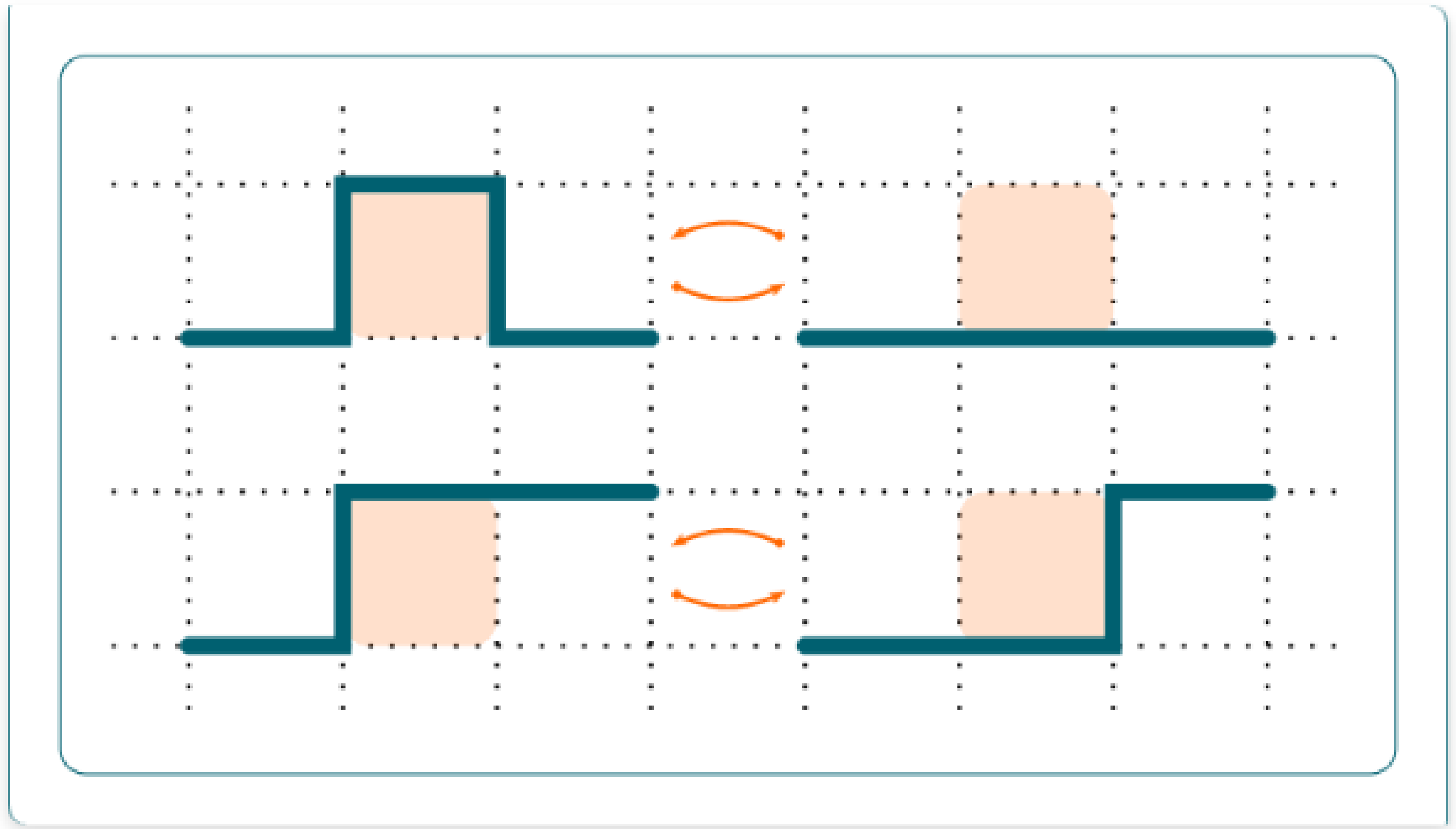
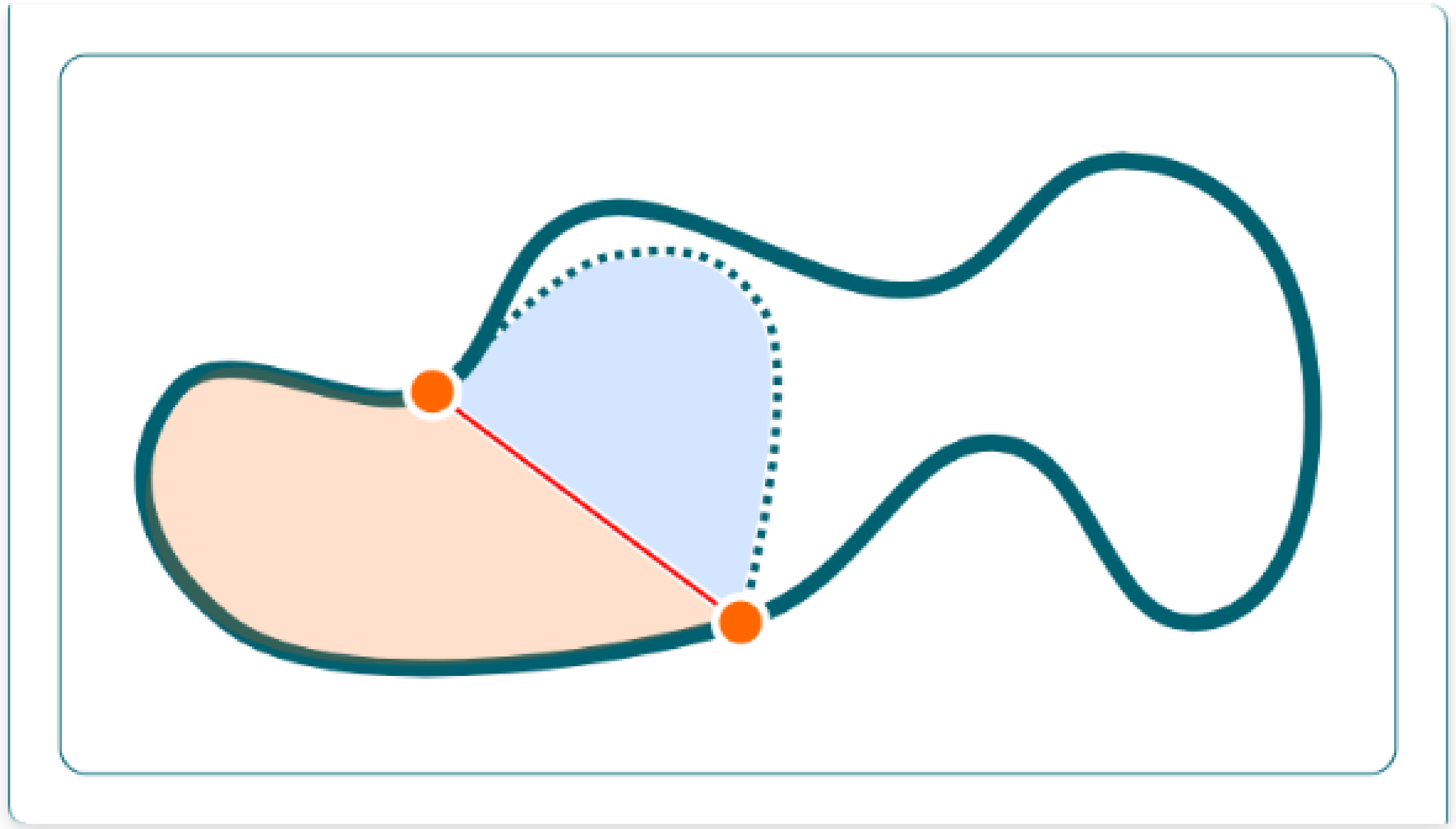


- Start with small conformation — deform with local moves
- Tune so that grow/shrink moves equally likely to succeed
- Random walk on polygon length — long time to sample *"independent"* long polygons

Fixed topology #2 — restricted pivots



- Pivot with excluded area algorithm Zhao & Ferrari (2012)
- Attempt pivot segment $\Phi \mapsto \Phi'$
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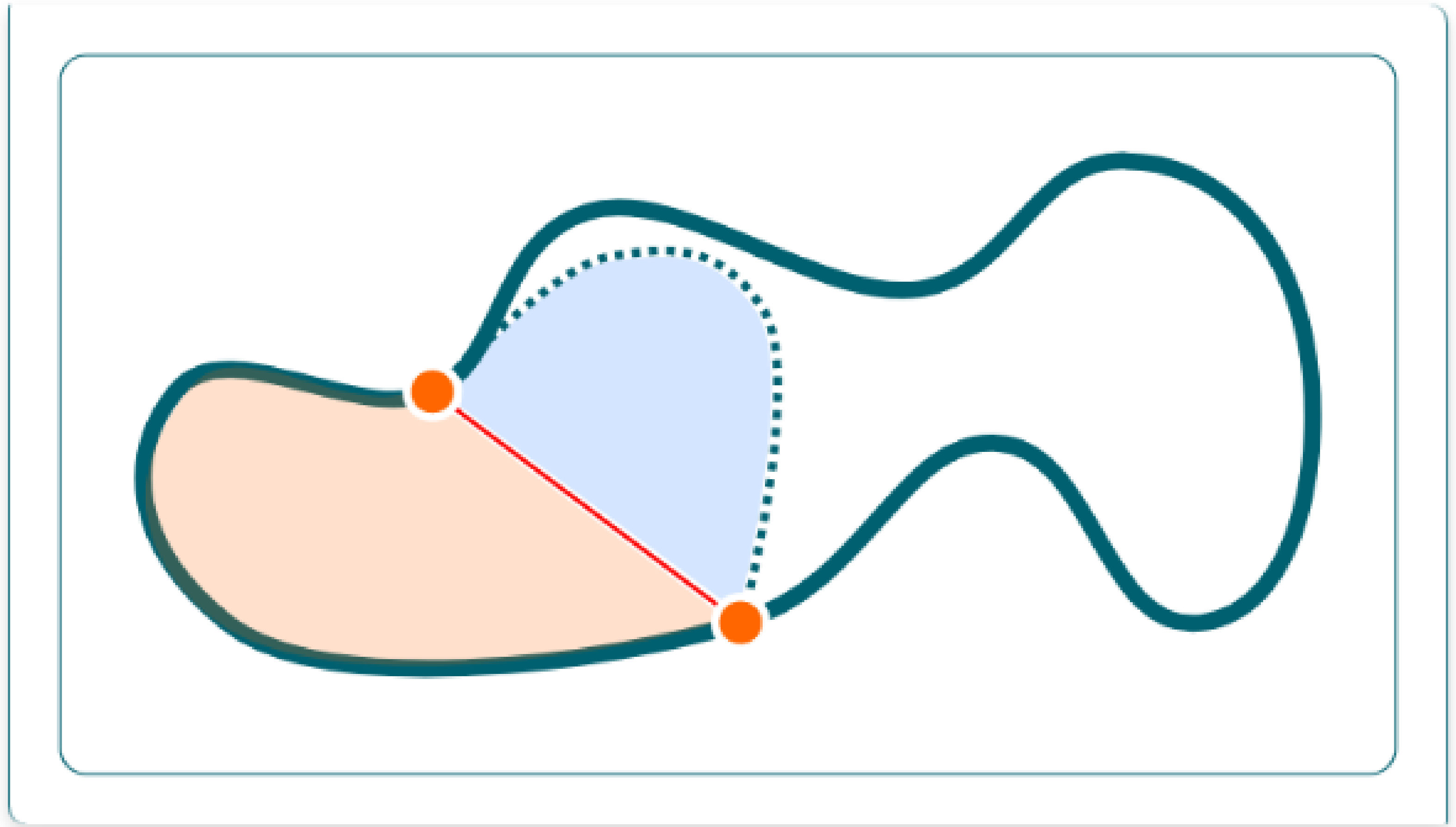

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- Computationally intensive — only allowed short segment $|\Phi| \leq 5$
- Probably *"okay"* for moderate size polygons — but not ergodic Madras & Sokal (1987)

So what can we do to speed things up?

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  - Store polygon and symmetries in binary tree
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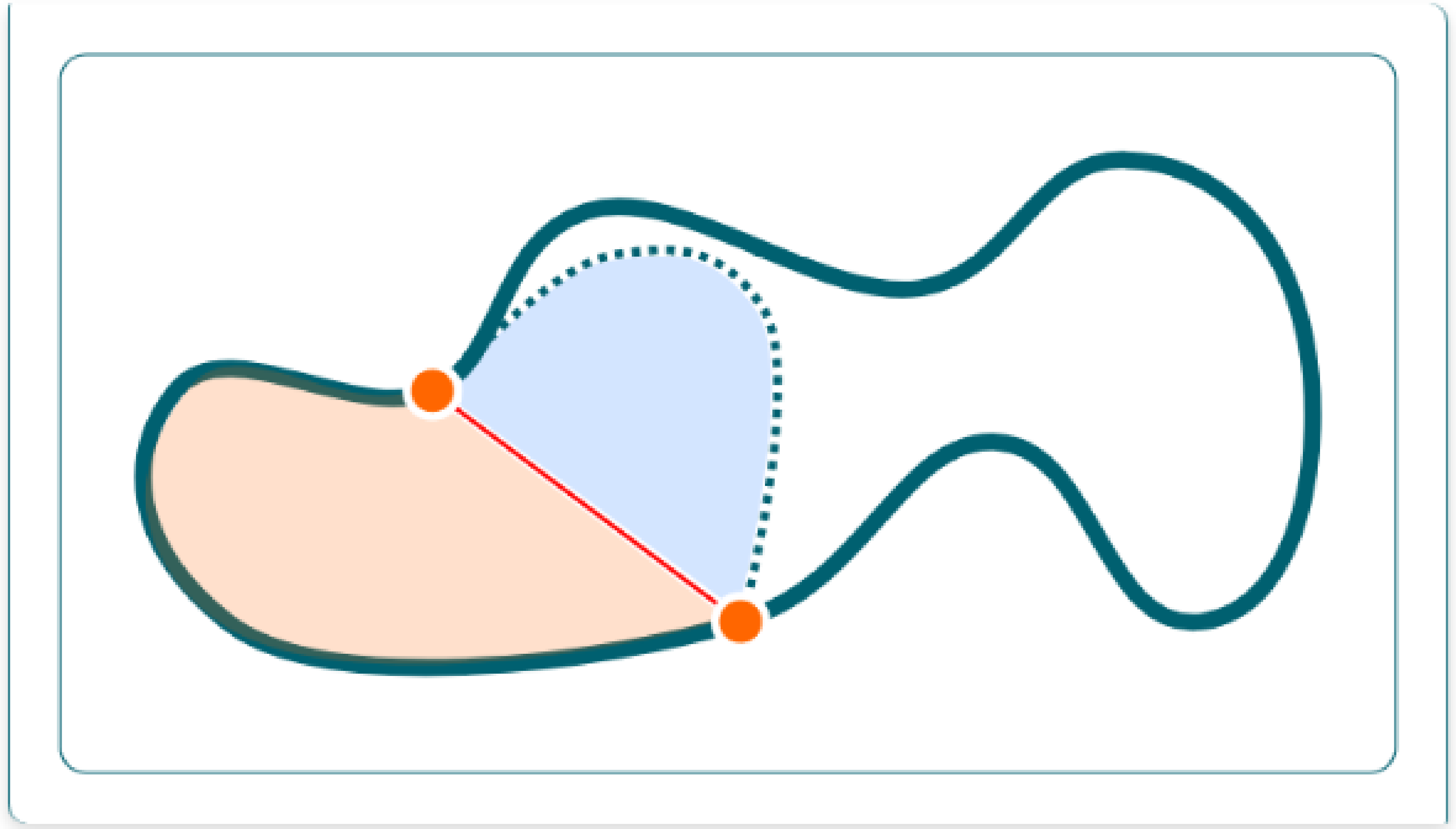
- Aside – this is actually not so far from Cantarellean encoding of polygons via triangulations

Inner pivot



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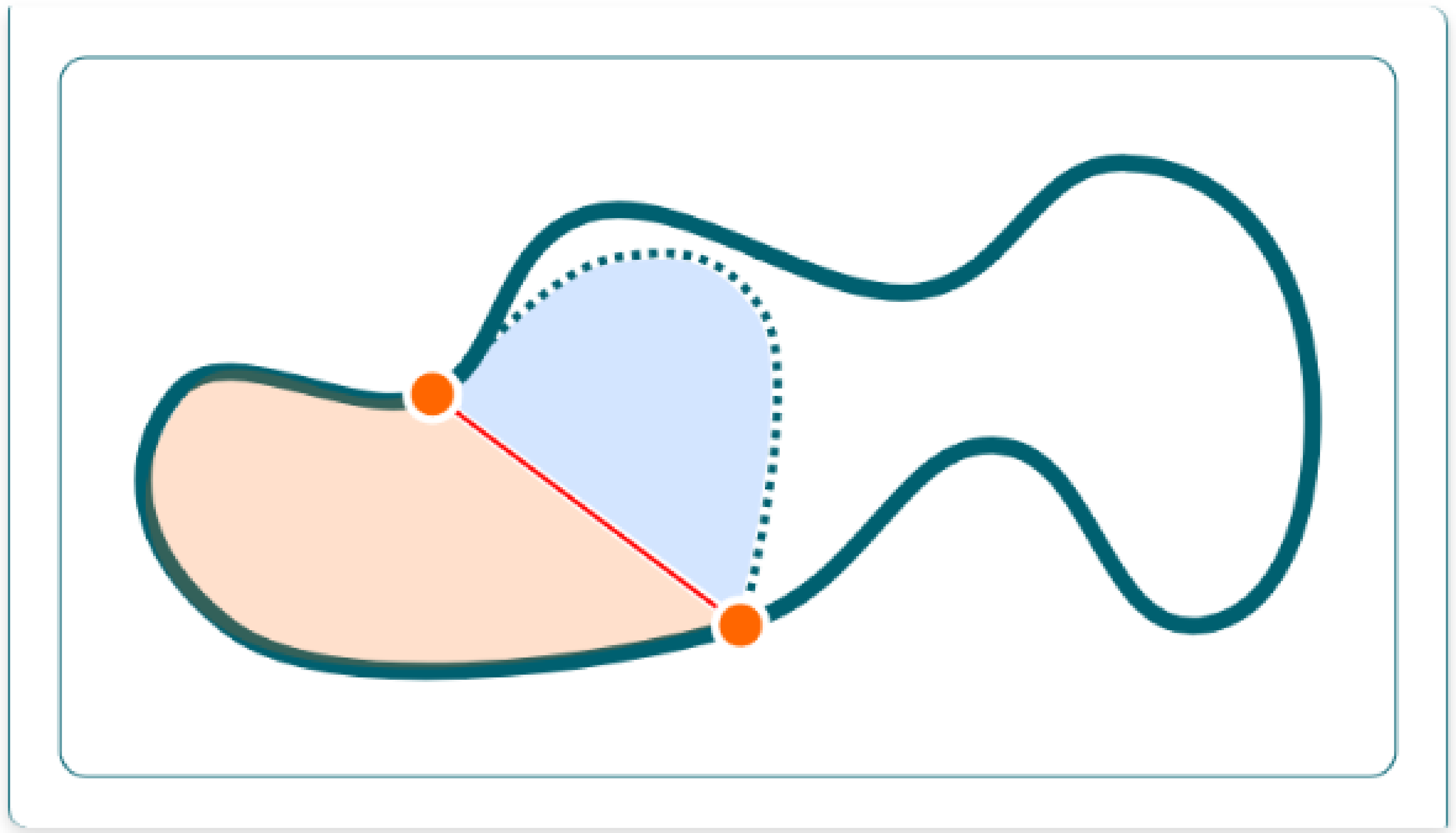
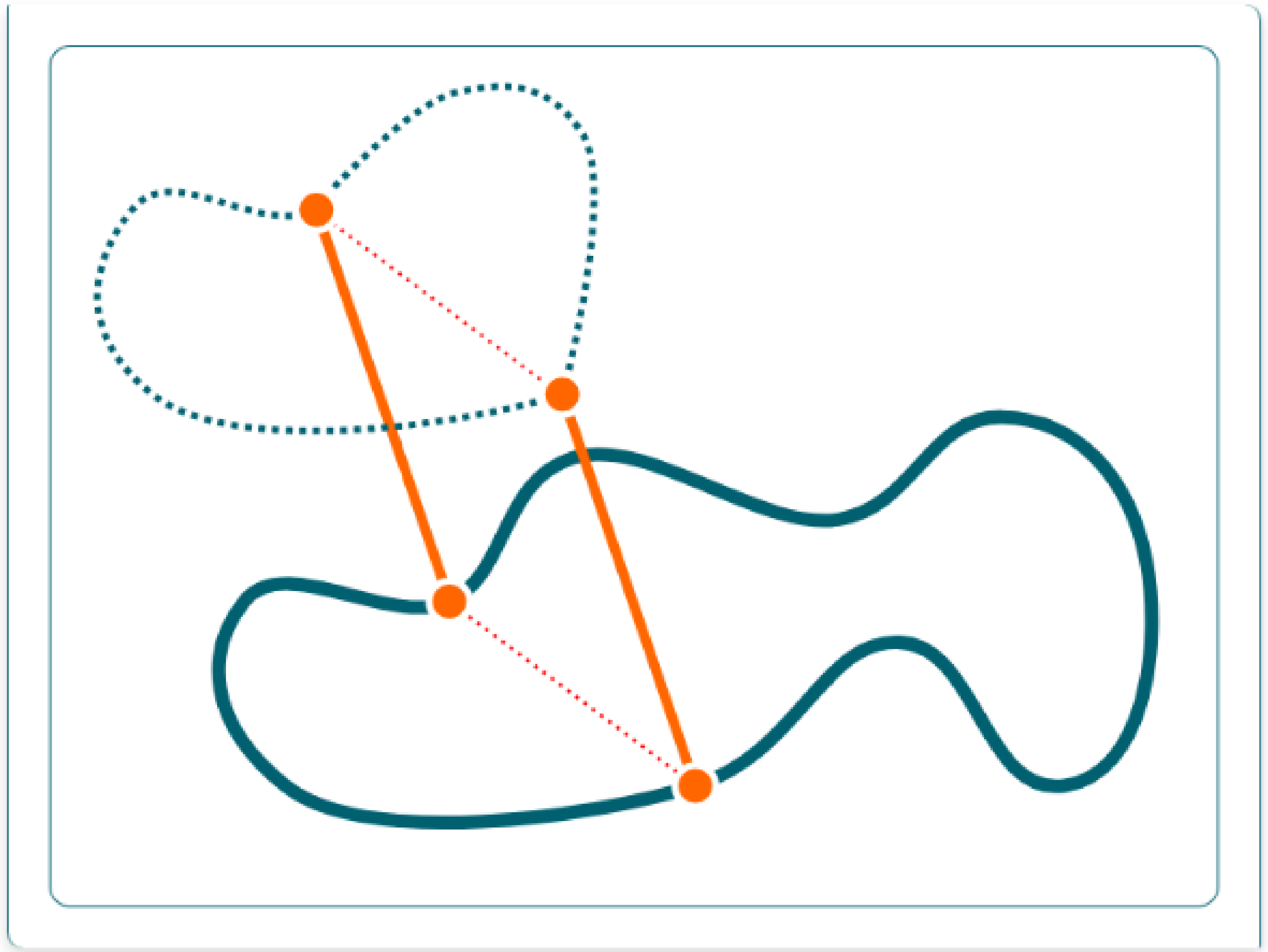


- Pick pivot segment and rotation angle
- Topology checking
  - Each pivot edge maps out a twisted quadrilateral
  - Check intersection of fixed edges with triangulation of those quadrilaterals
  - Use ray-tracing methods — eg Möller-Trumbore (1997)

Outer pivot



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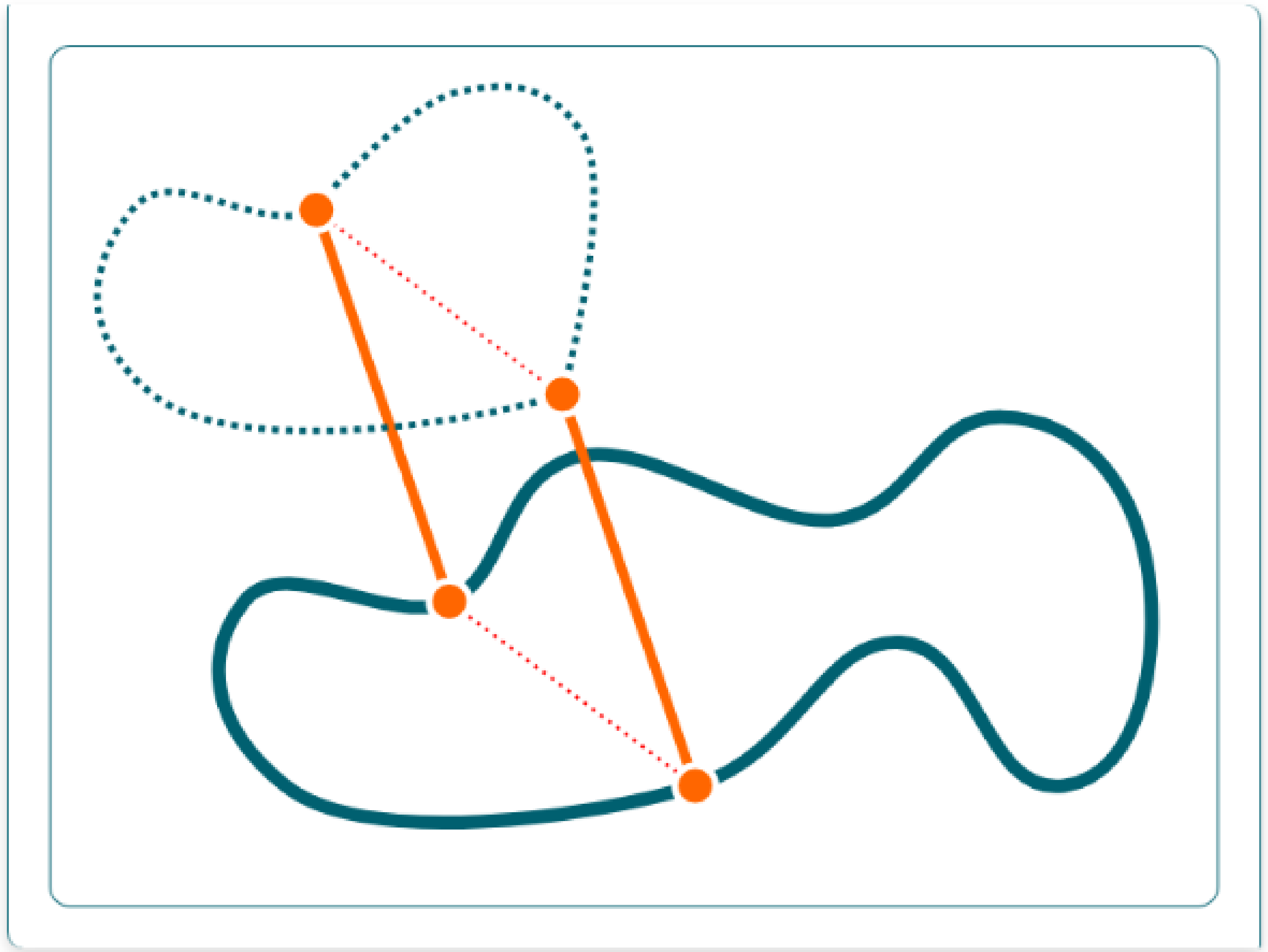

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  - drag the segment to infinity
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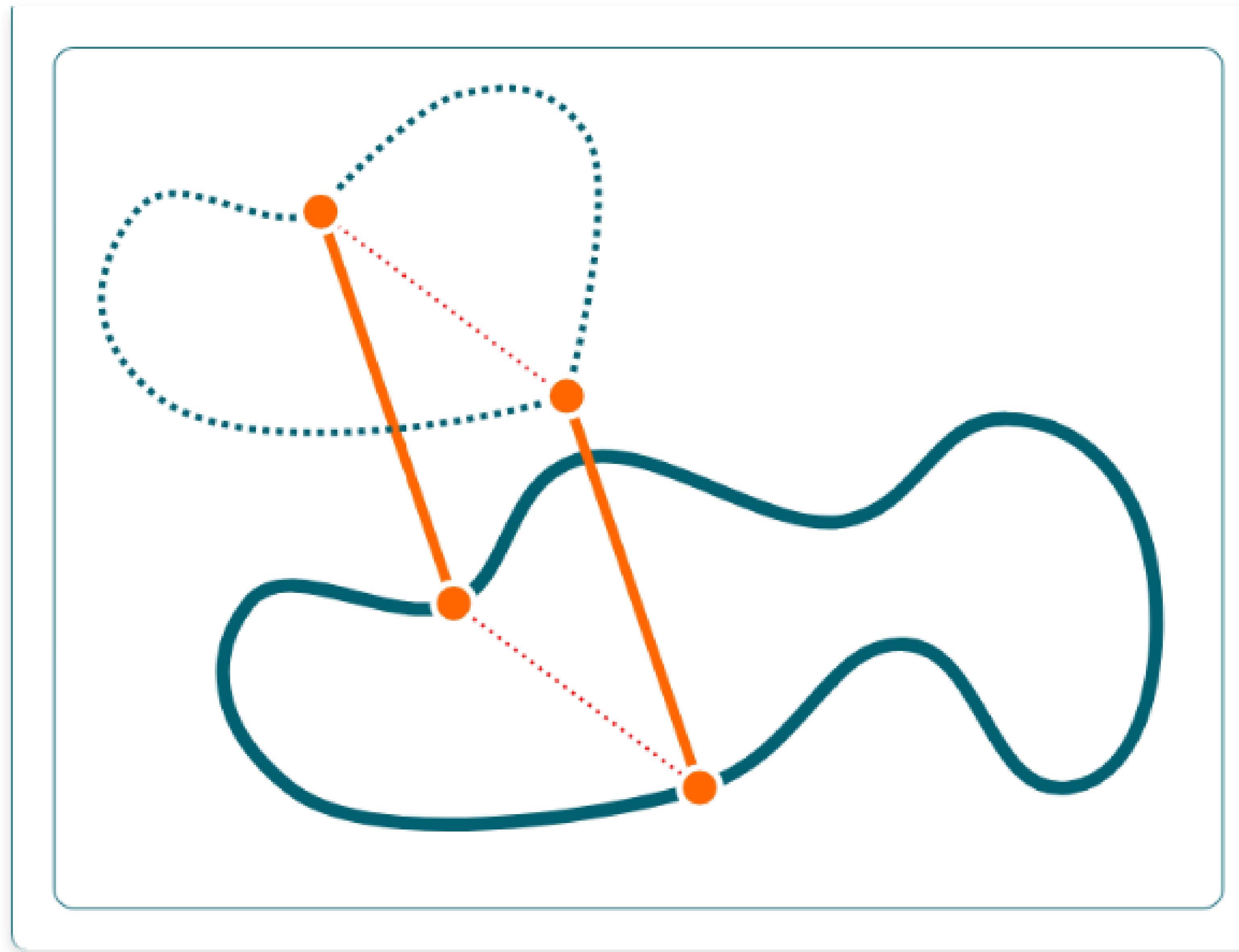

- Pick the pivot segment and an orthogonal drag direction
  - drag the segment to infinity
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  - drag the segment back from infinity
- Topology checking
  - drag to/from infinity $\mapsto$ segment overlap in projection
  - pivot at infinity $\mapsto$ check intersection with drag lines

Simple implementation of inner and outer pivots

- Computation time is $O(n^2)$ or $O(n \log n)$:
  - pick pivot vertices: $O(1)$ on $\mathbb{R}^3$
  - inner pivot: naive $O(n^2)$, but maybe as fast as $O(n \log n)$?
  - drag to infinity: naive $O(n^2)$, or Shamos-Hoey (1976) $O(n \log n)$
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- Autocorrelation time?

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- Consider the product $q = x^a y^b z^c$
  - Numbers $x, y, z \in \mathbb{R}$ changed rarely
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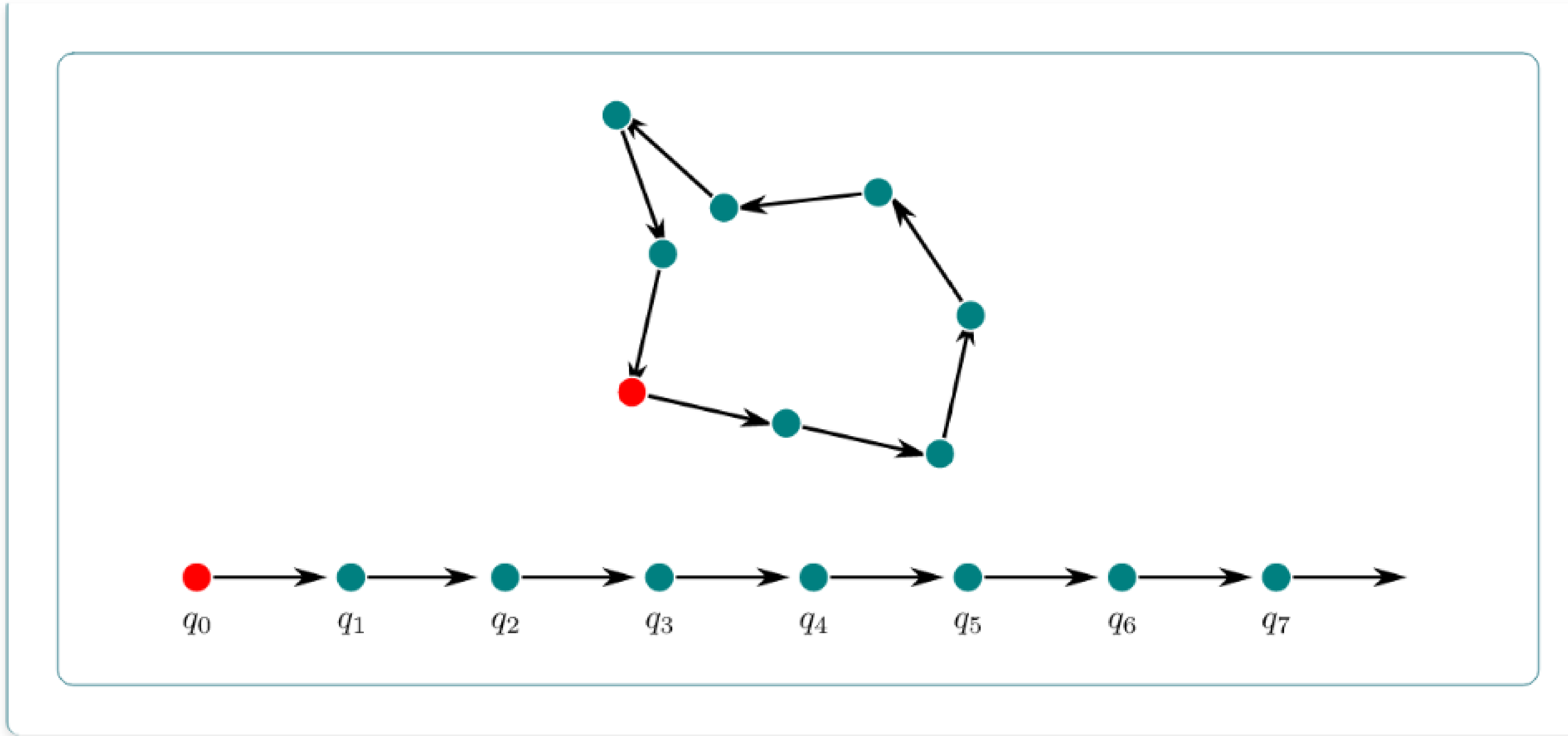
- Careful precomputation and lazy evaluation

Clisbification

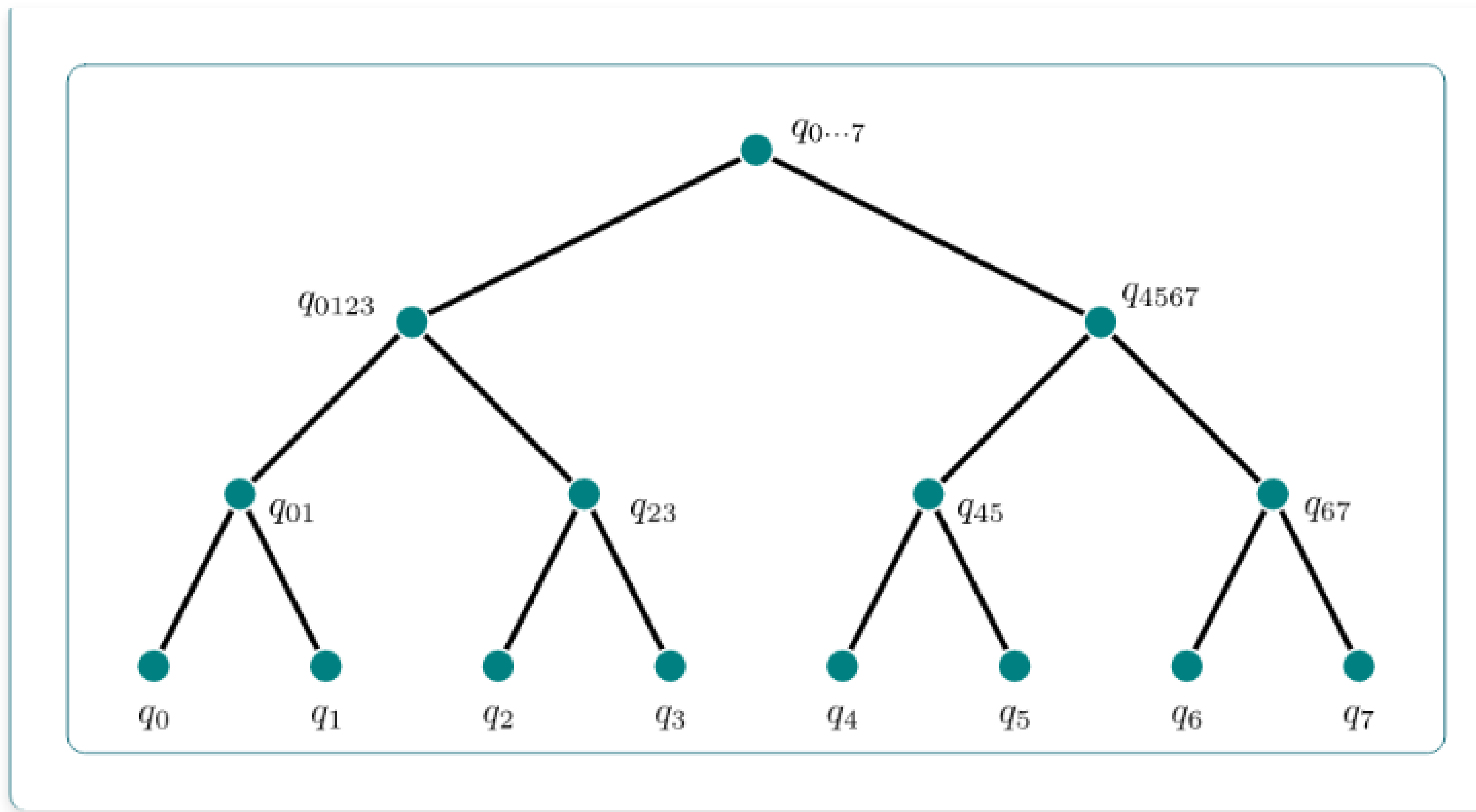
- Successful pivot in $O(\log n)$ time



- Write polygon as symmetries acting on $\vec{e} = (1, 0, 0)$
- Position of vertex n is

$$\vec{X}_n = \sum_{k=0}^{n-1} (q_0 q_1 \cdots q_k)\, \vec{e}$$

Store polygon in a tree



- Leaf k stores symmetry q_k and a position $\vec{P}_k = q_k\vec{e}$
- Internal nodes stores $q_n = q_\ell q_r$ and a position $\vec{P}_n = \vec{P}_\ell + q_\ell\vec{P}_r$

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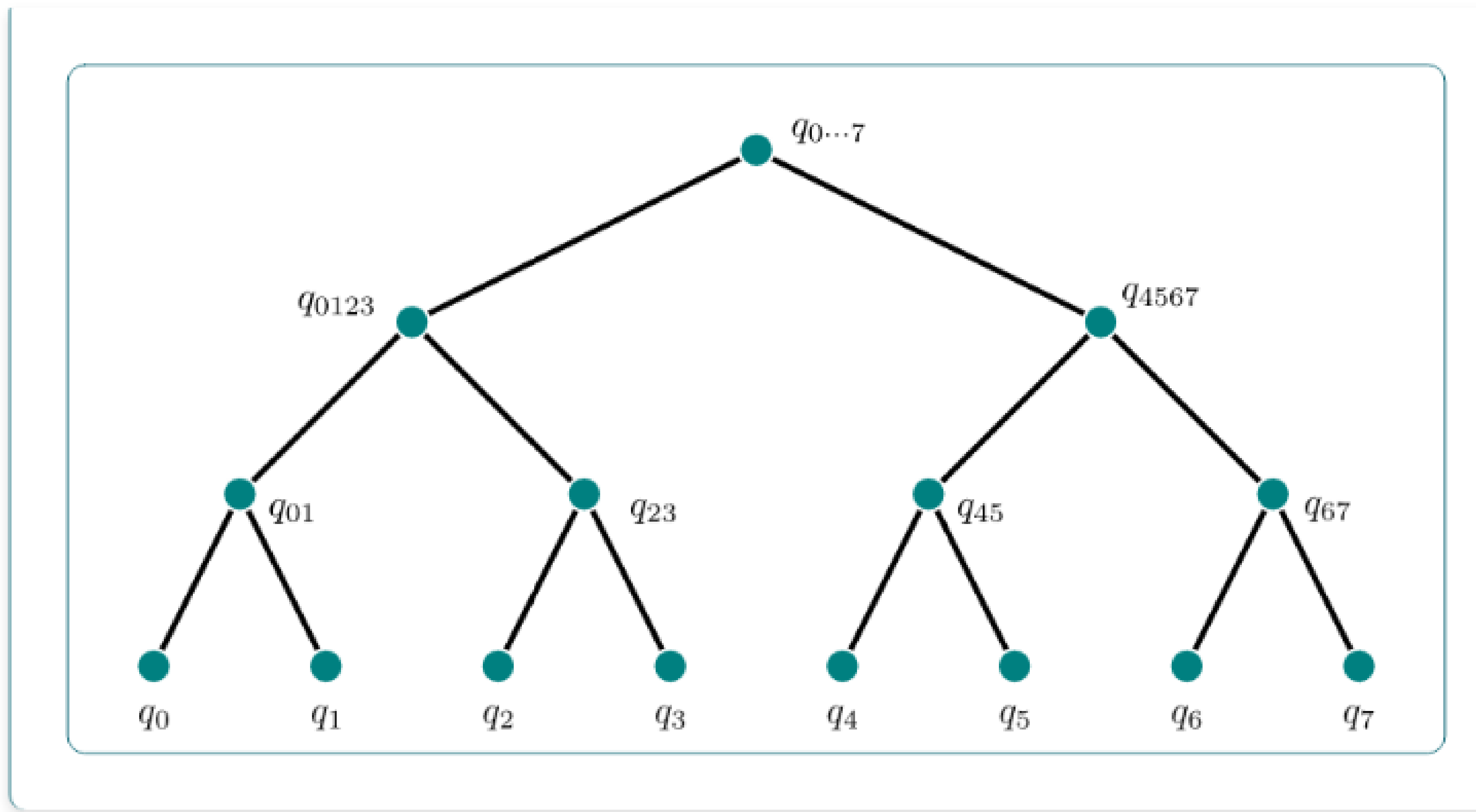

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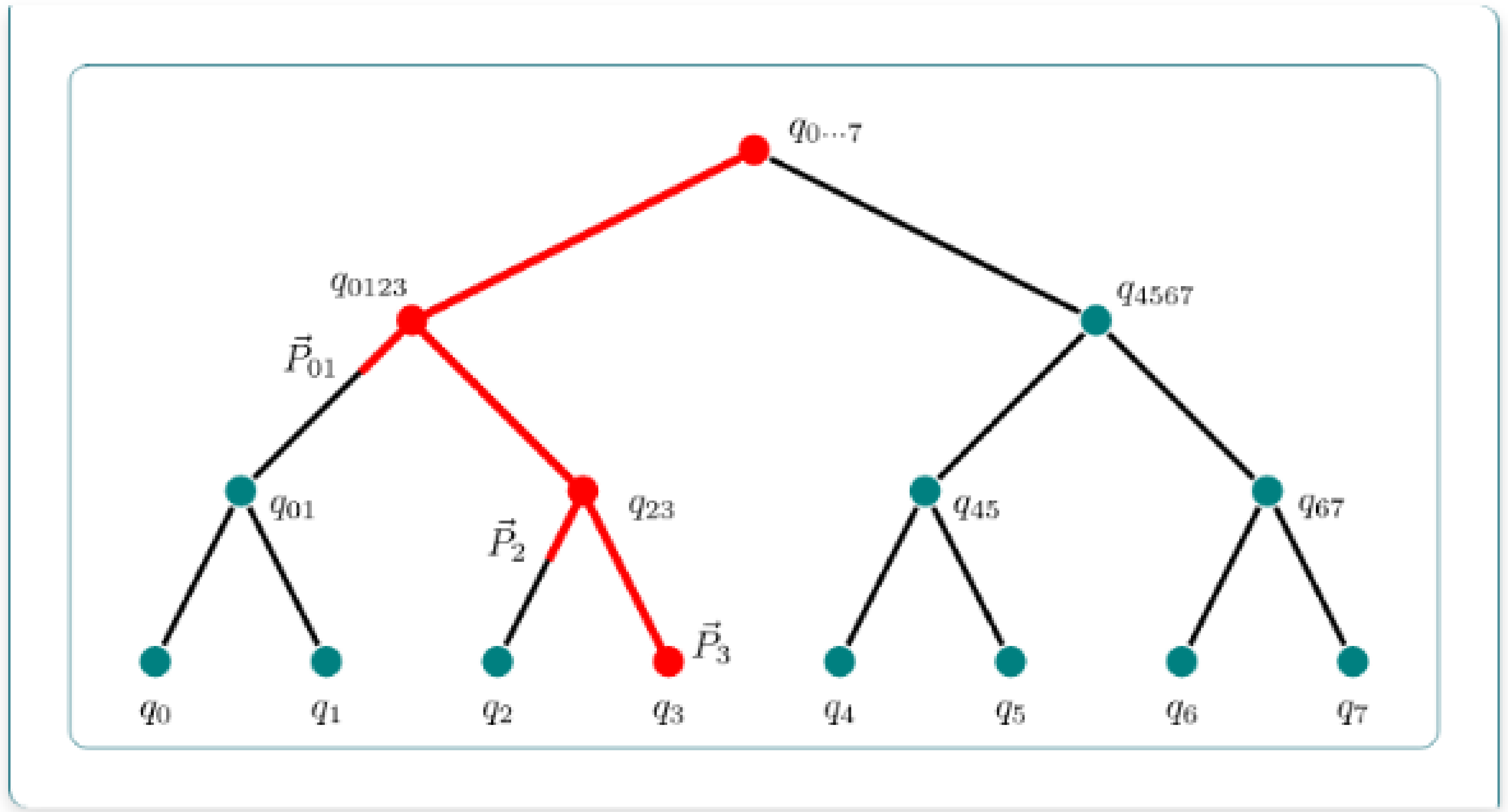
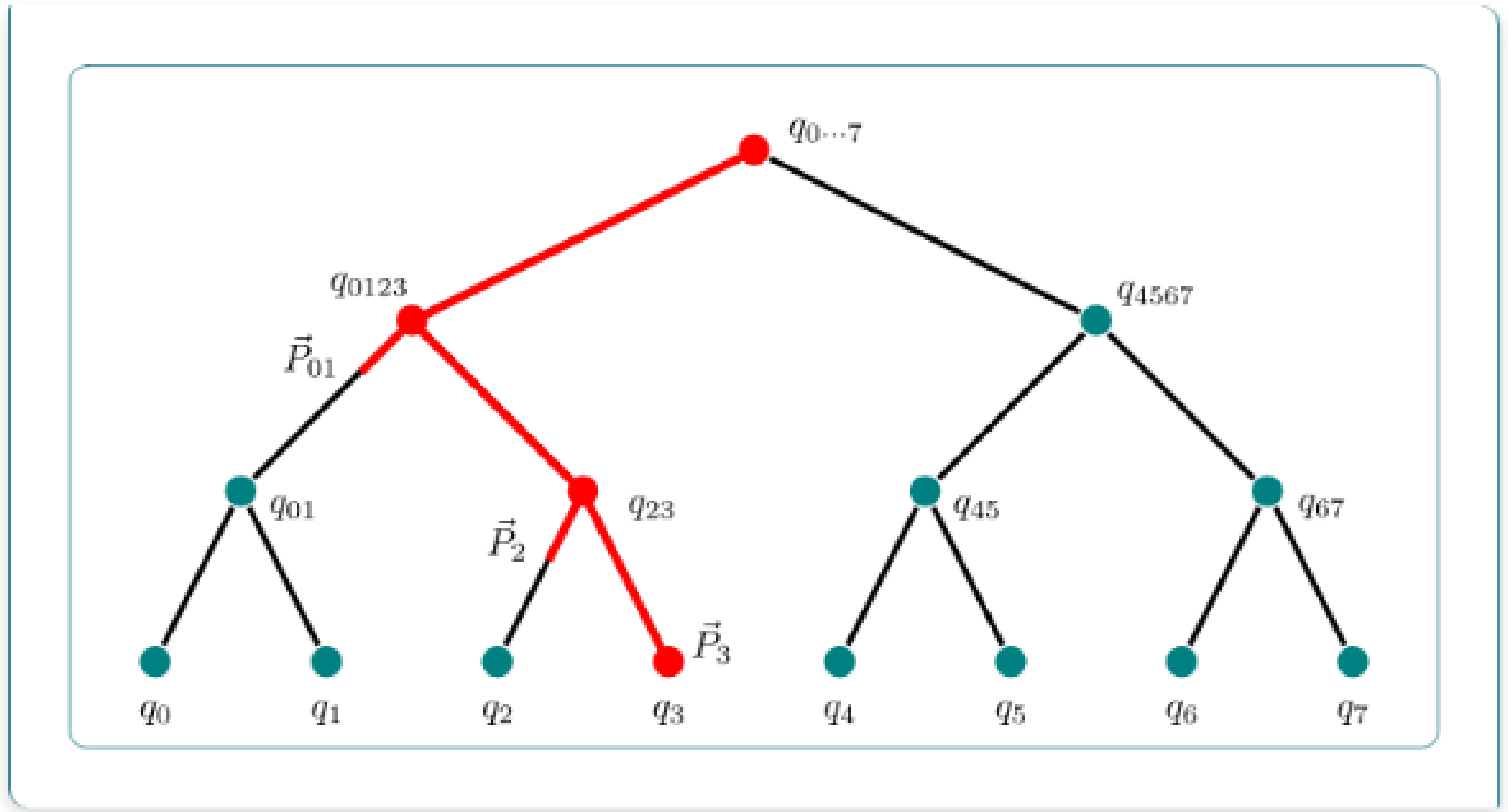
- Internal nodes stores $q_n = q_\ell q_r$ and a position $\vec{P}_n = \vec{P}_\ell + q_\ell \vec{P}_r$
- Compute polygon vertex positions using $q_n, \vec{P}_n$

Compute a position



- Position of vertex 4 $\equiv$ end of 3rd polygon edge

Compute a position



- Position of vertex 4 $\equiv$ end of 3rd polygon edge
  - $\vec{X}_4 = (q_0 + q_{01} + q_{012} + q_{0123})\,\vec{e}$

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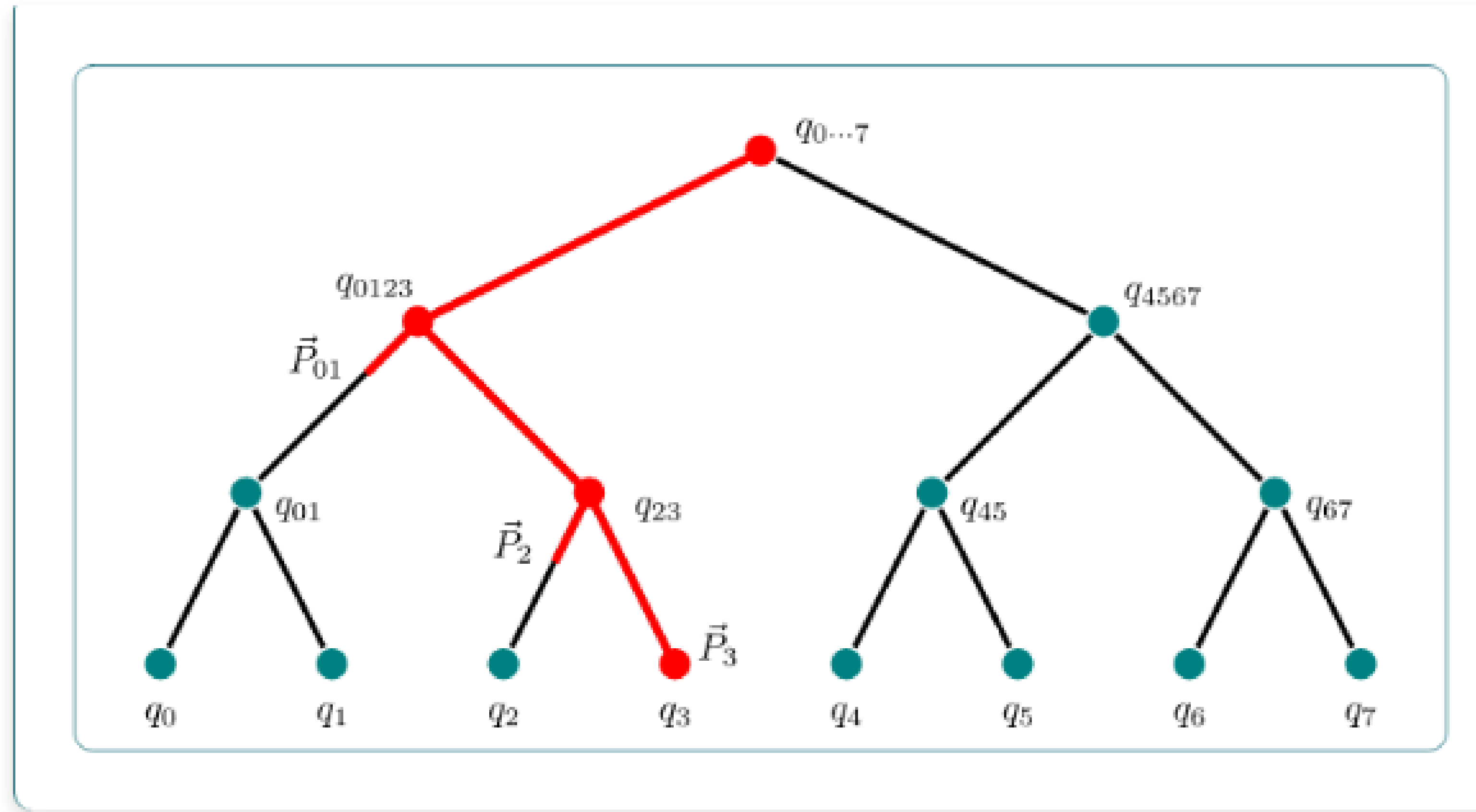

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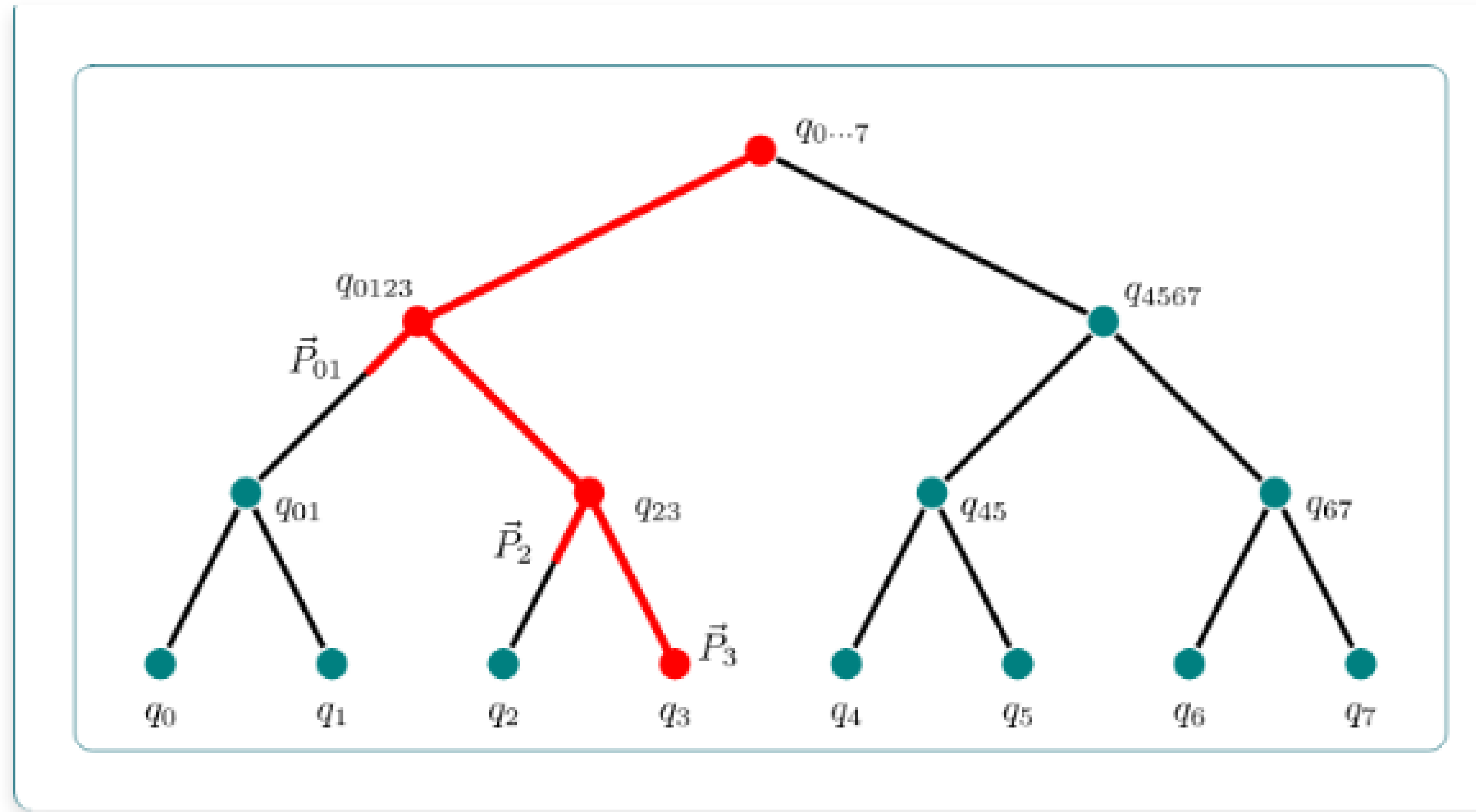

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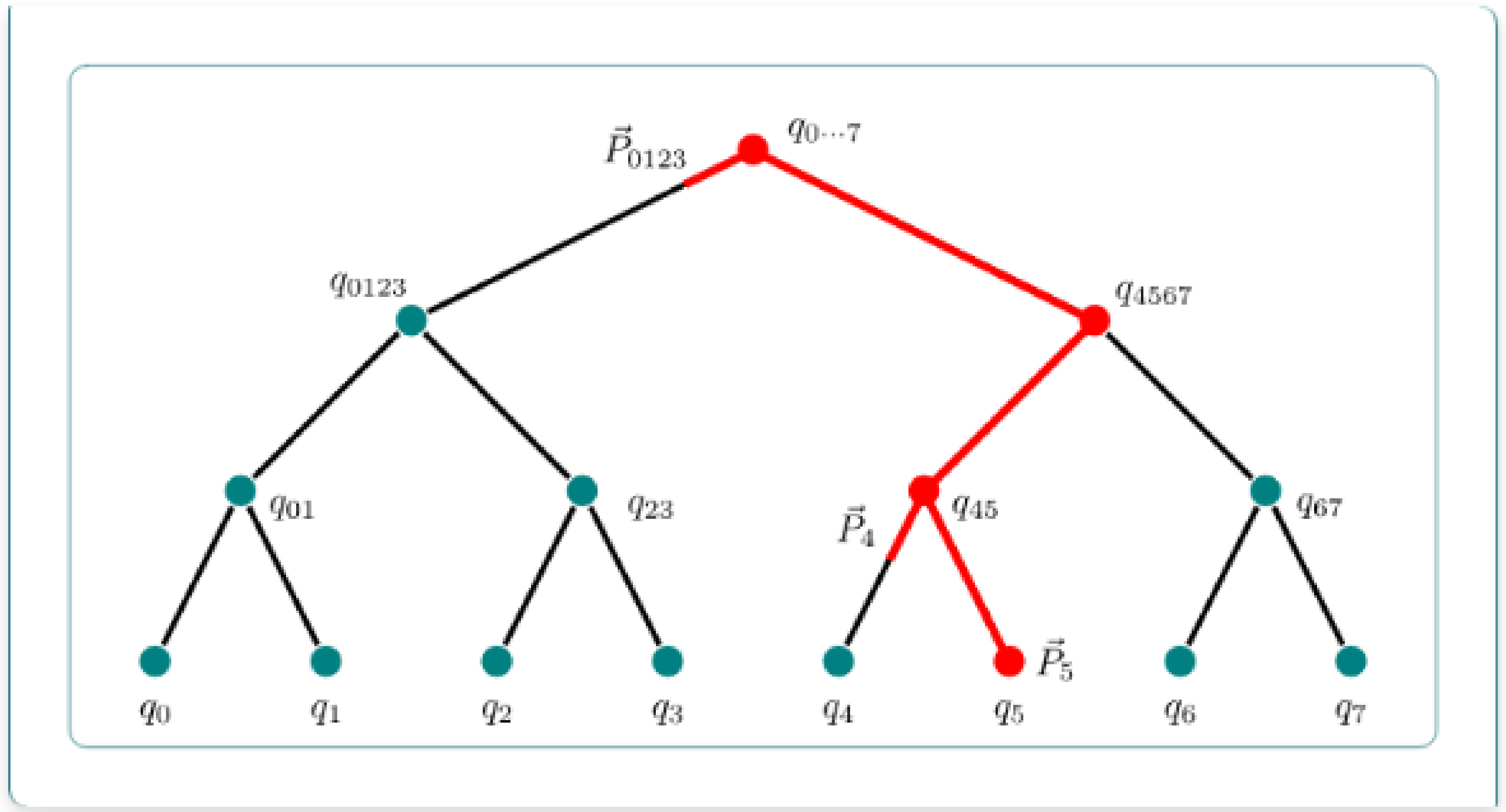
  - $\vec{X}_4 = \vec{P}_{01} + q_{01}\left(\vec{P}_2 + (q_2\vec{P}_3)\right)$
- Already computed q_{01} and P_{01}, P_2, P_3.
- Requires $O(\text{tree-depth}) = O(\log n)$ operations

Compute another position



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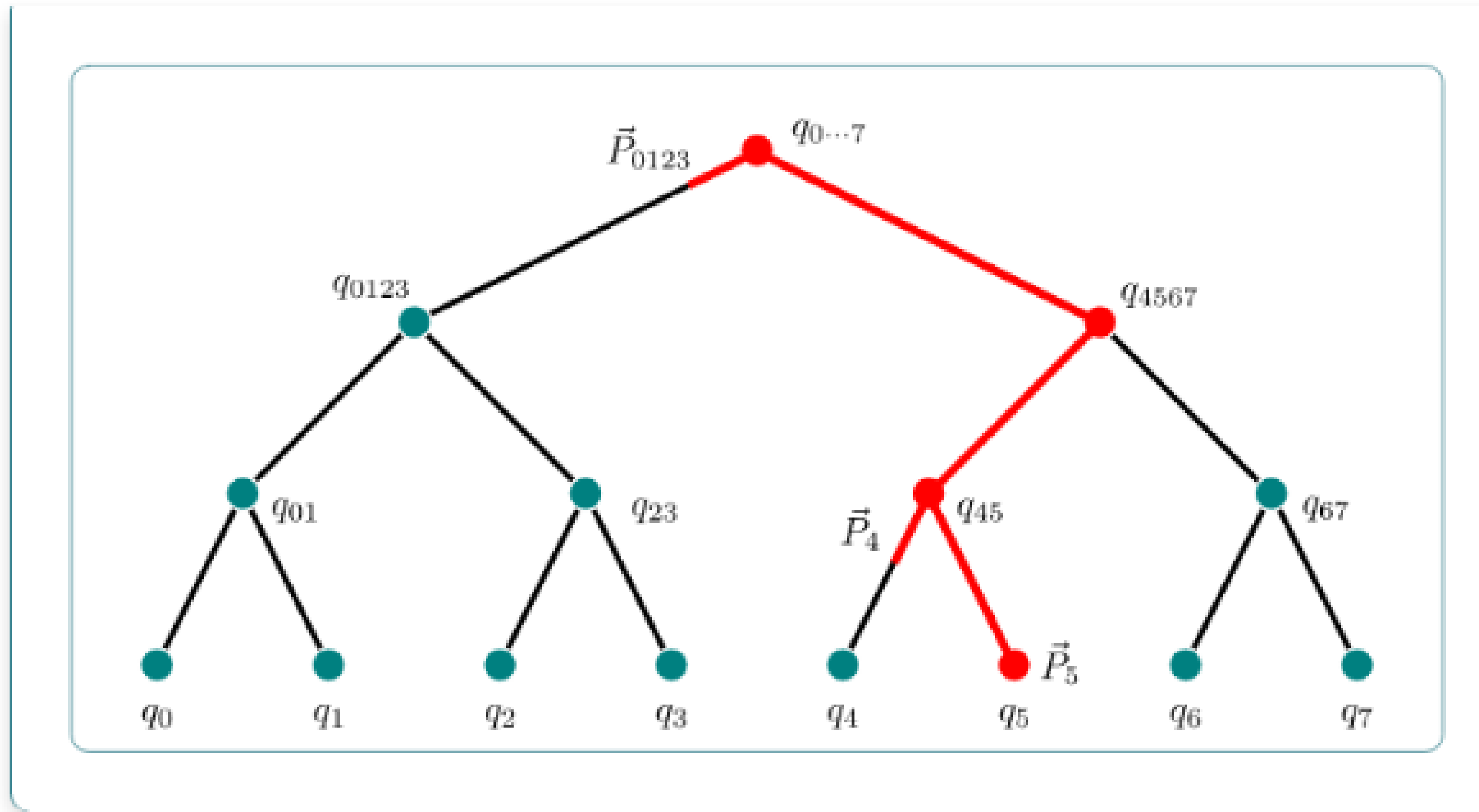

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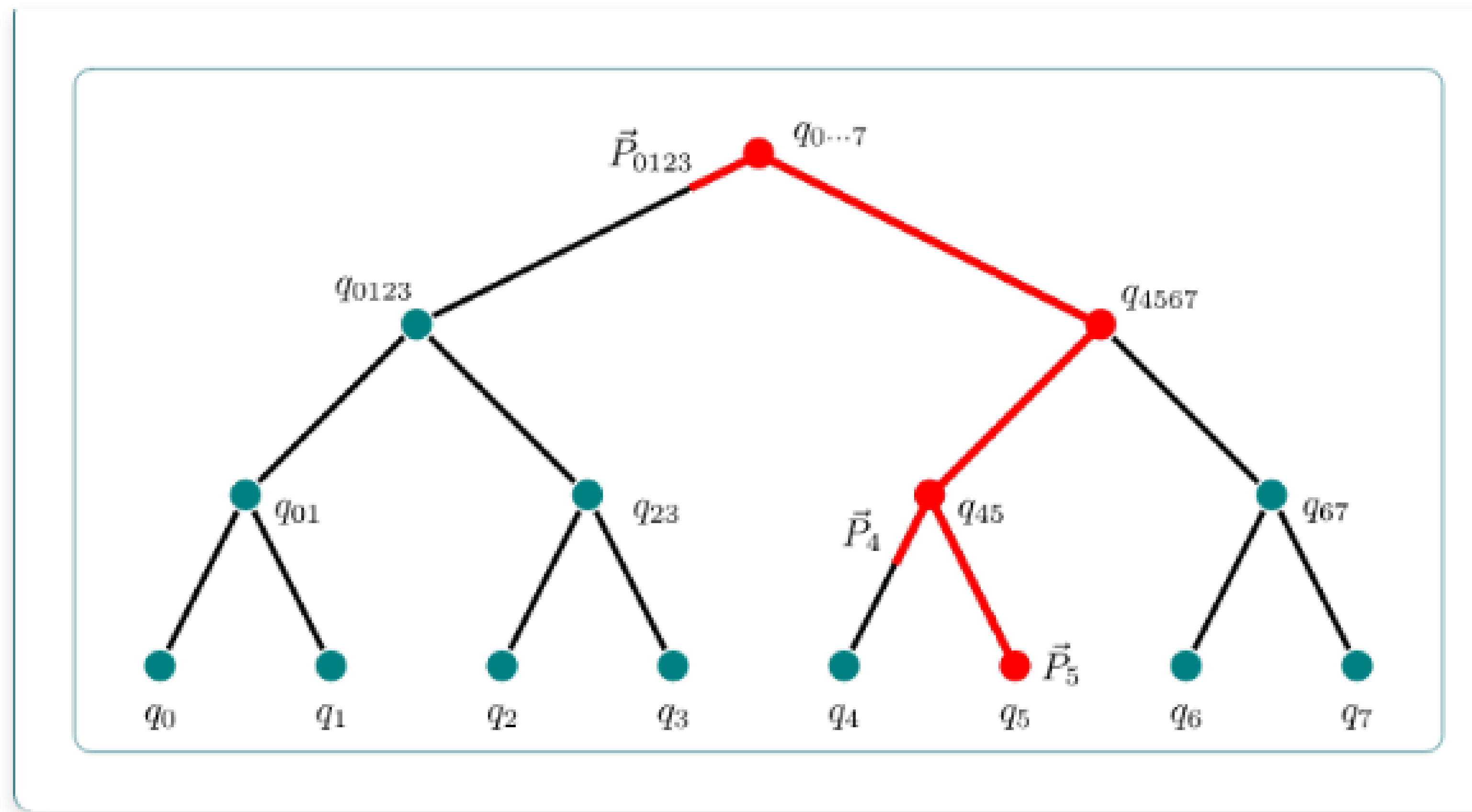

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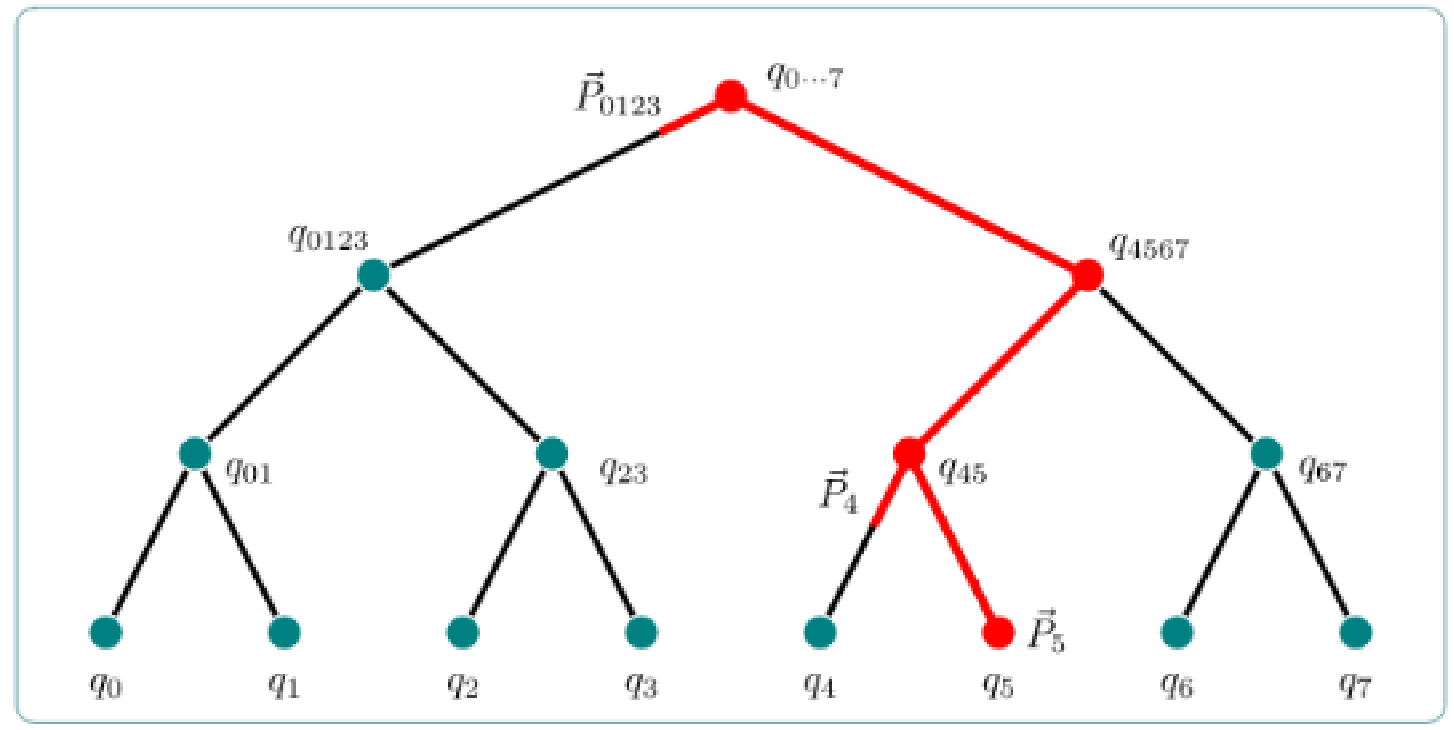

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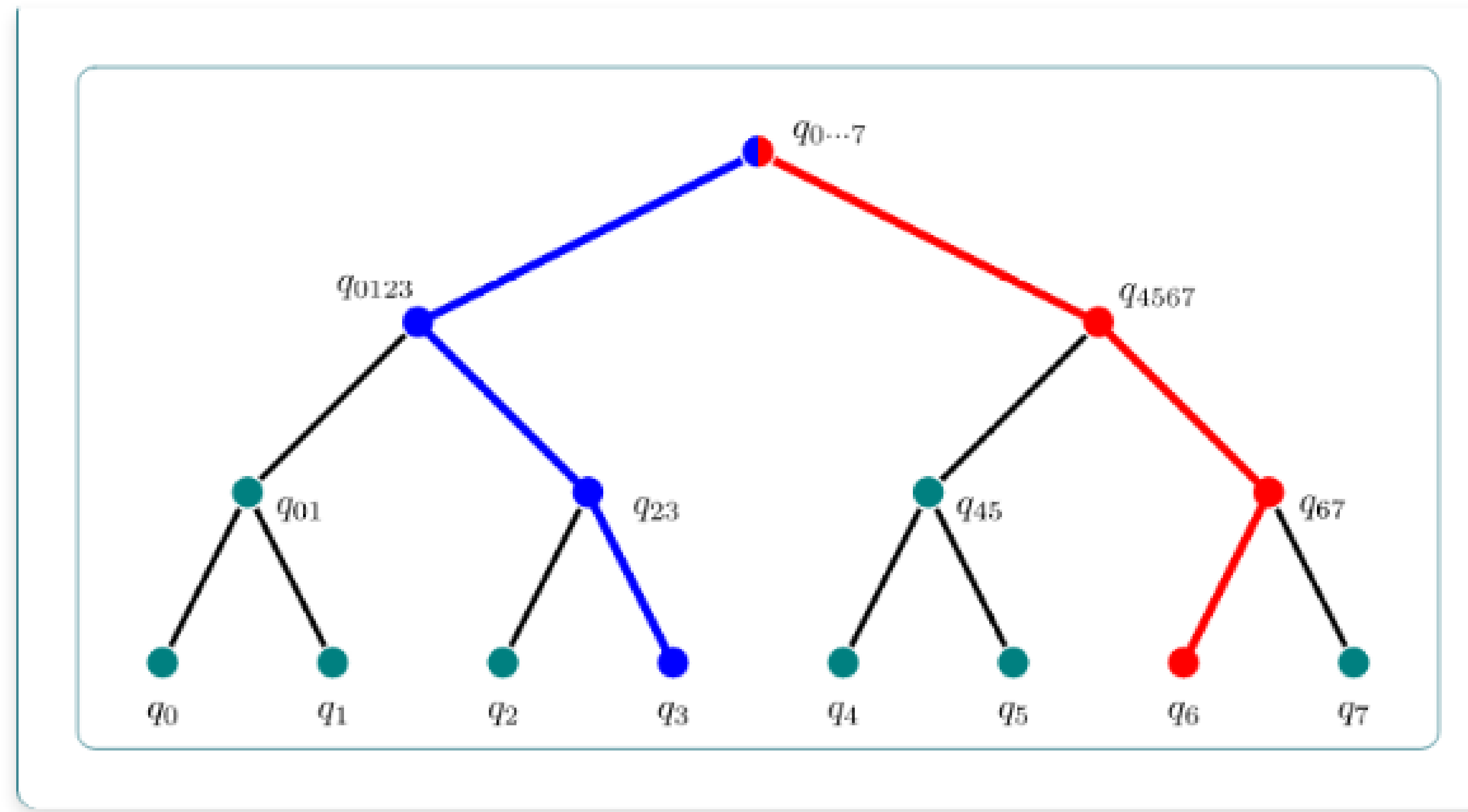
Update after pivot at vertices 3 and 6



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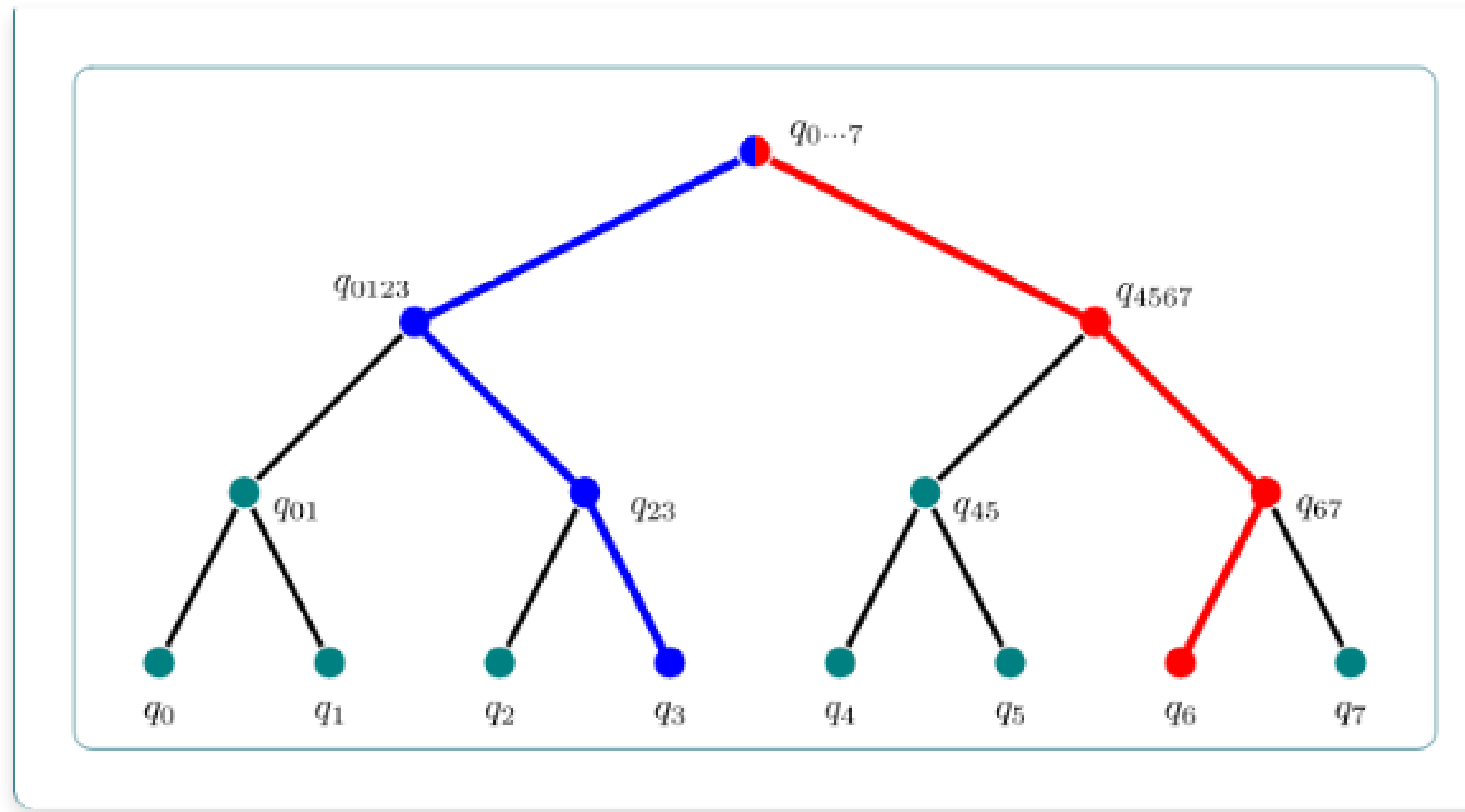

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  - ERP sampling in sublinear time
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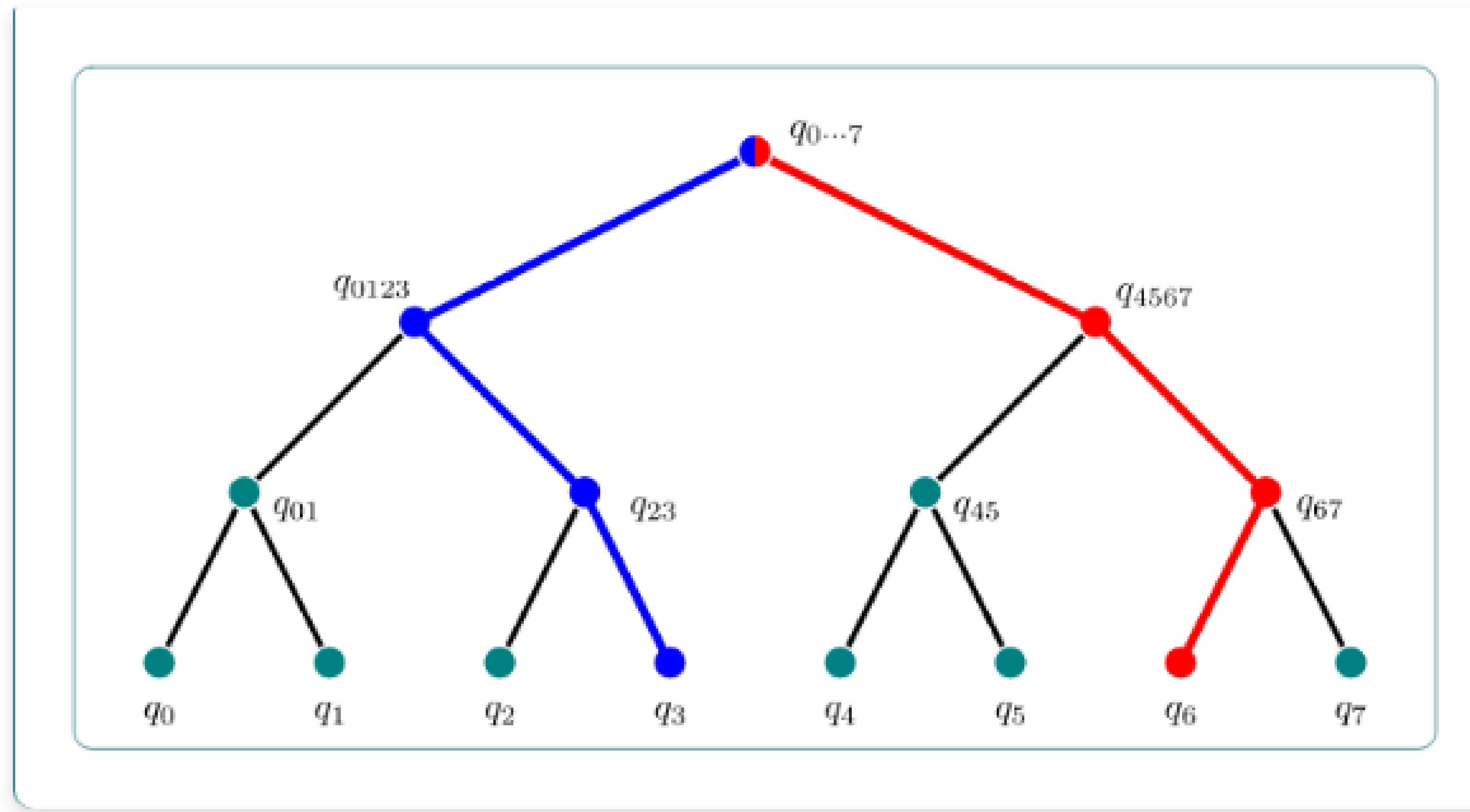

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- Harder on lattice — must pick pairs carefully to stay on lattice

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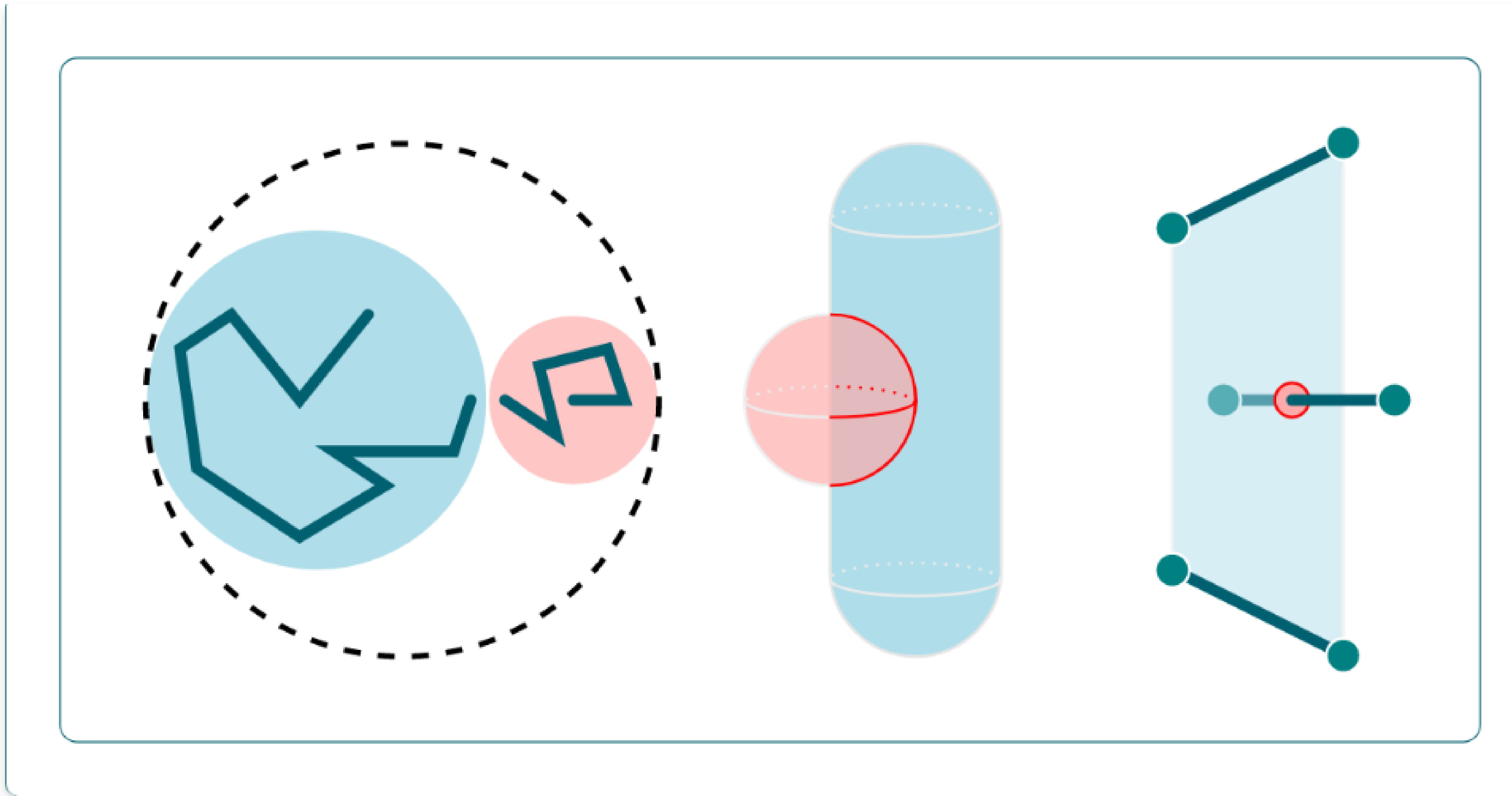

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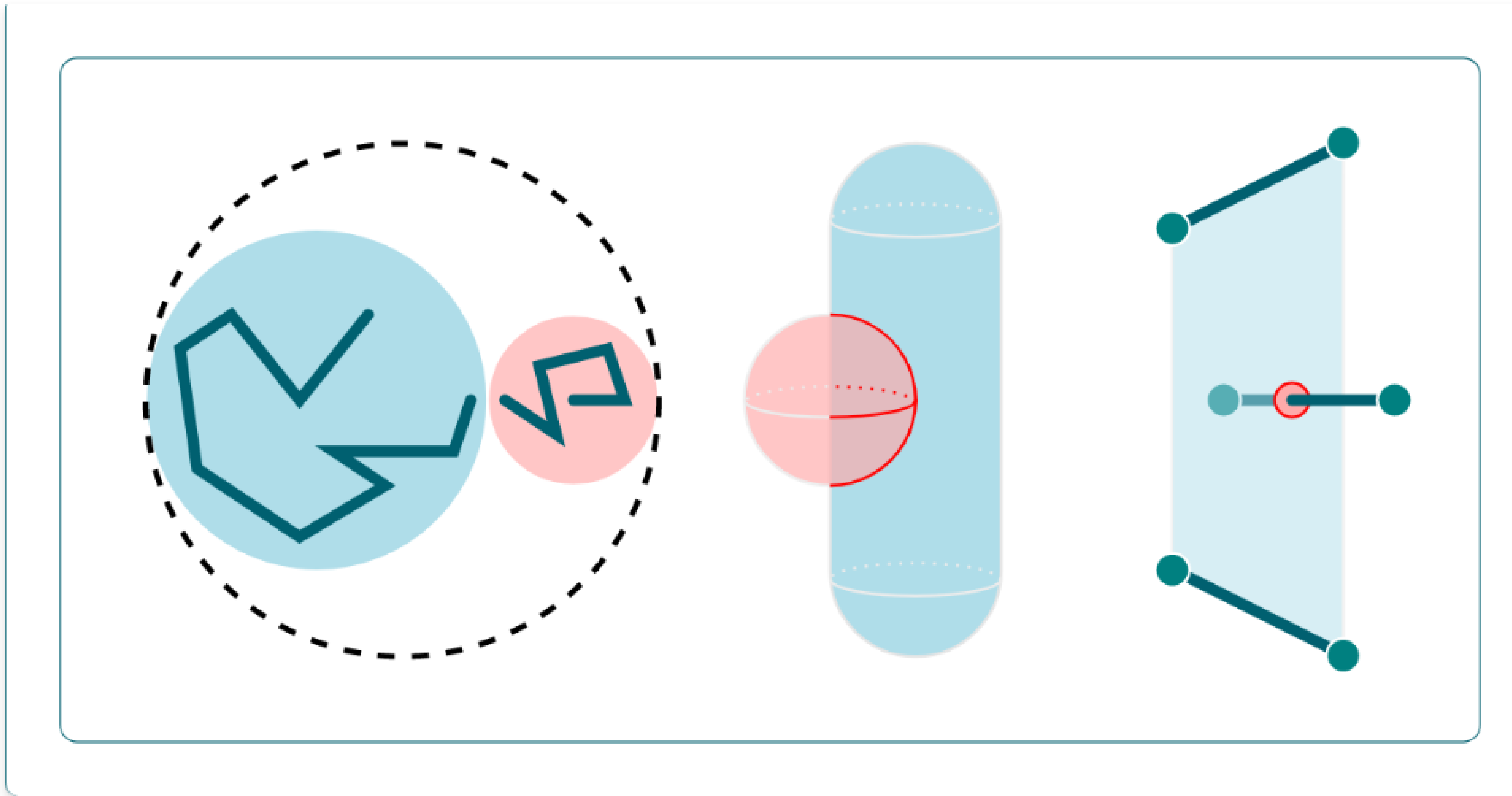

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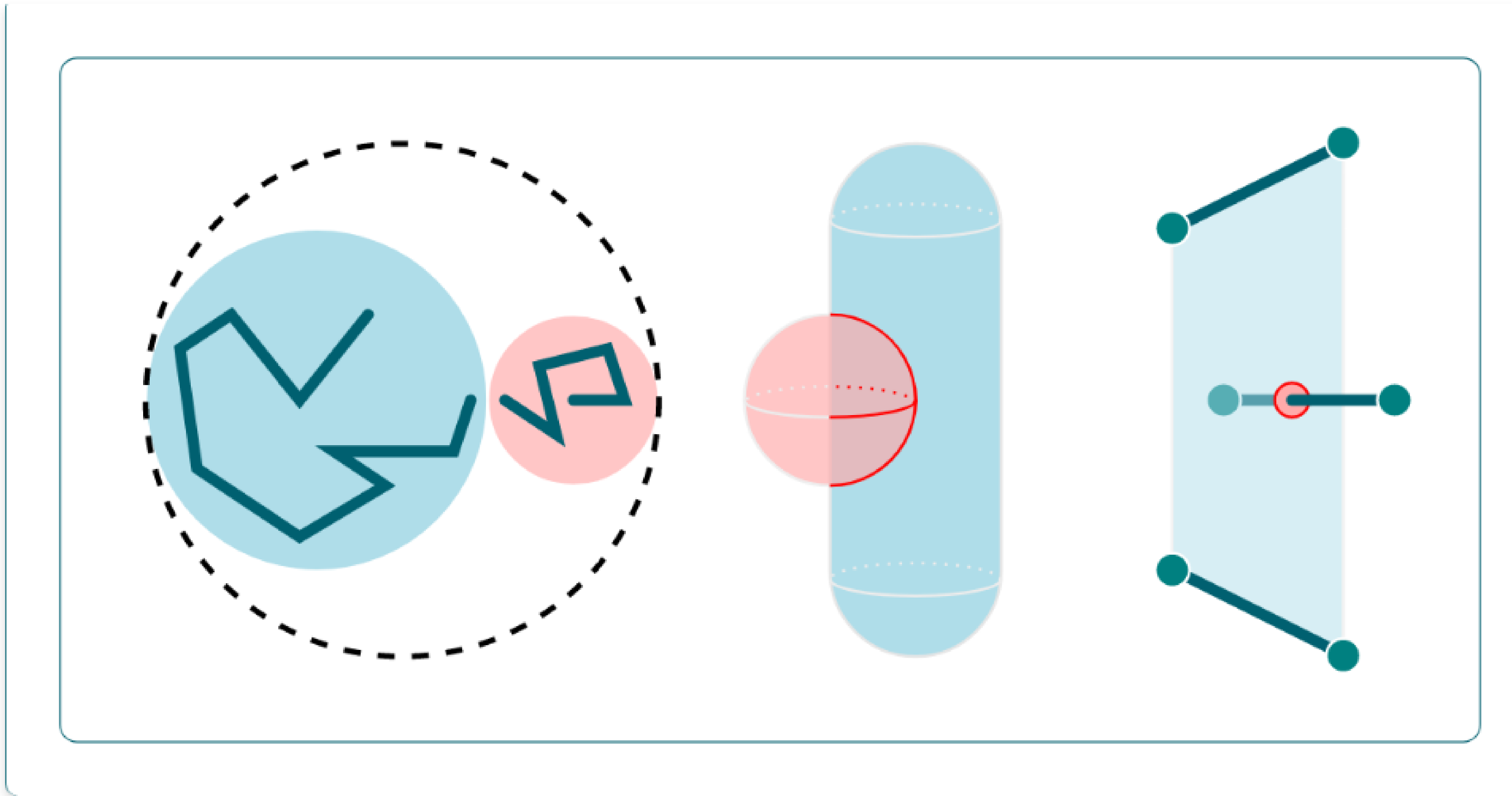

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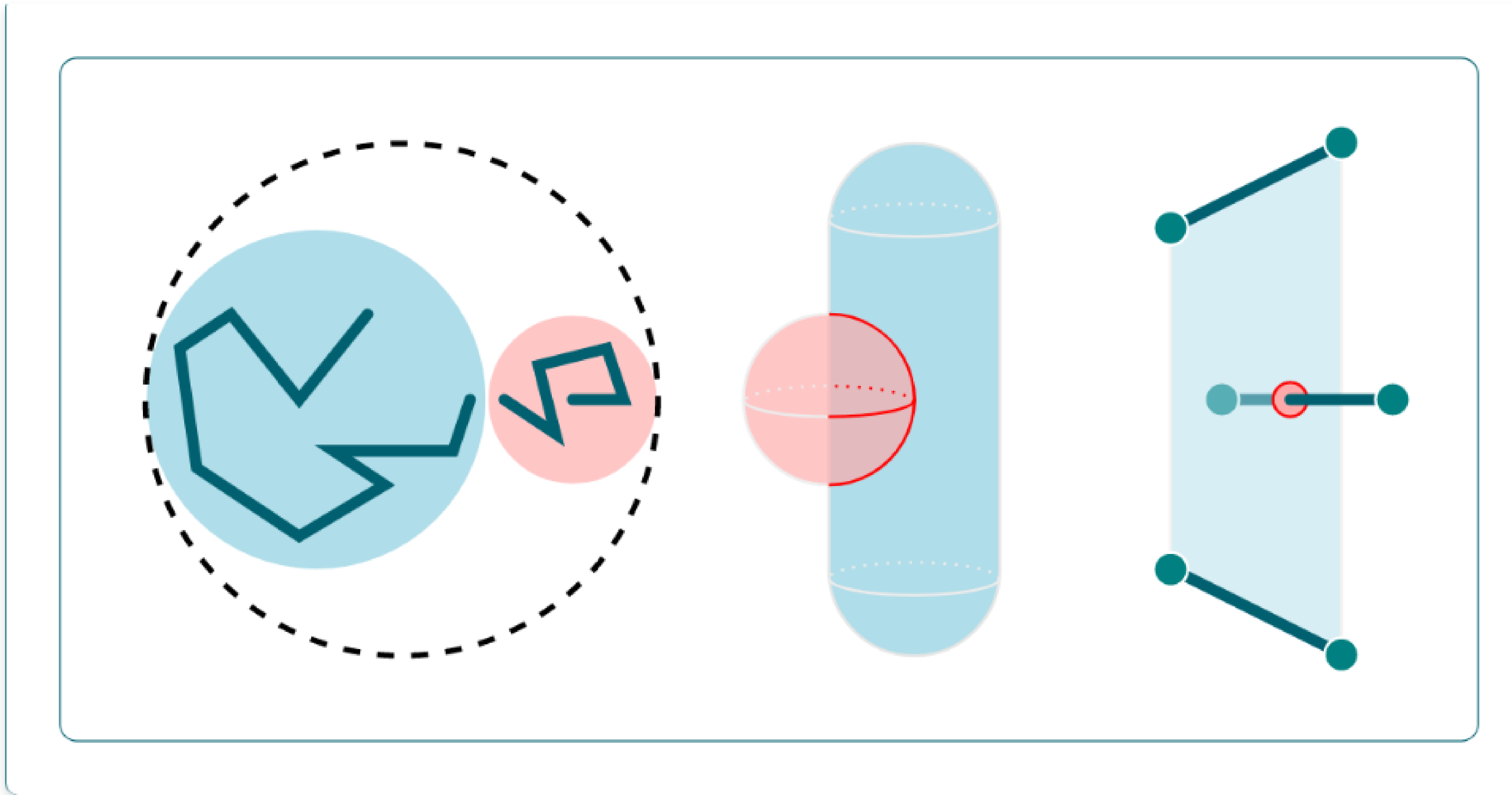

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- Bounding sphere construction
- Sphere intersects sphere-capped-cylinder test
- Segment intersects quadrilateral test $\equiv$ Möller-Trumbore

Fast intersection checks via bounding sphere refinements

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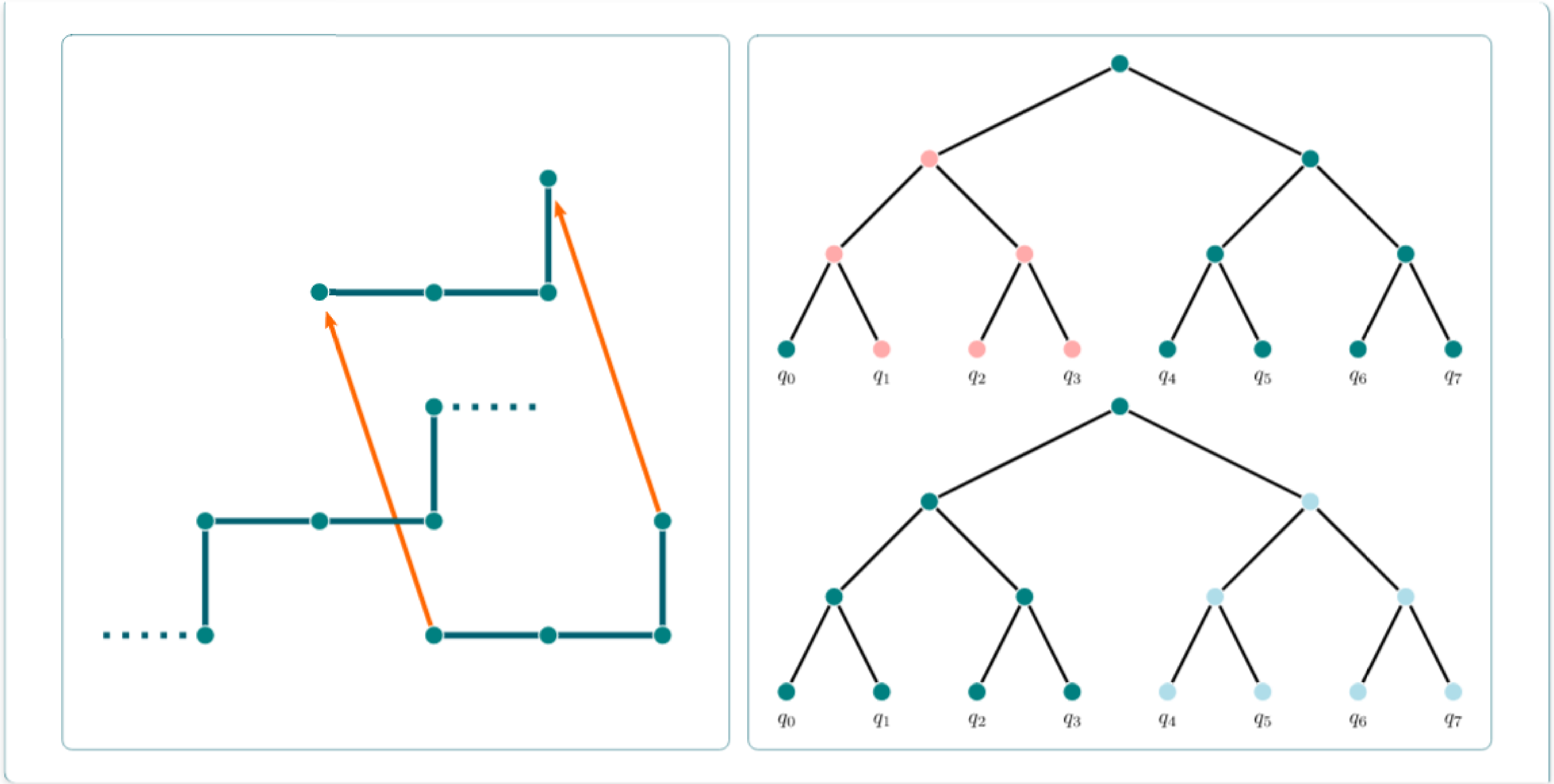

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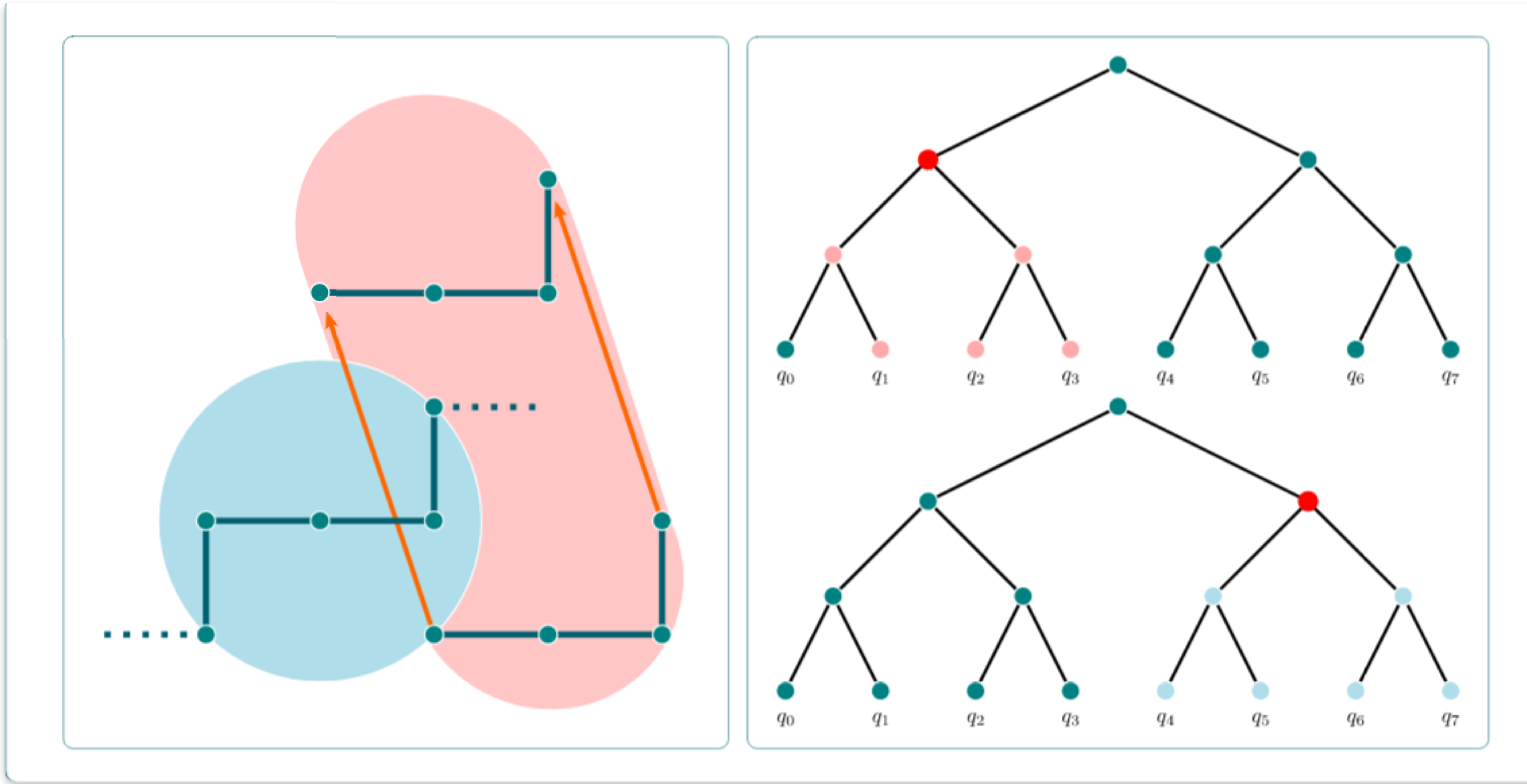

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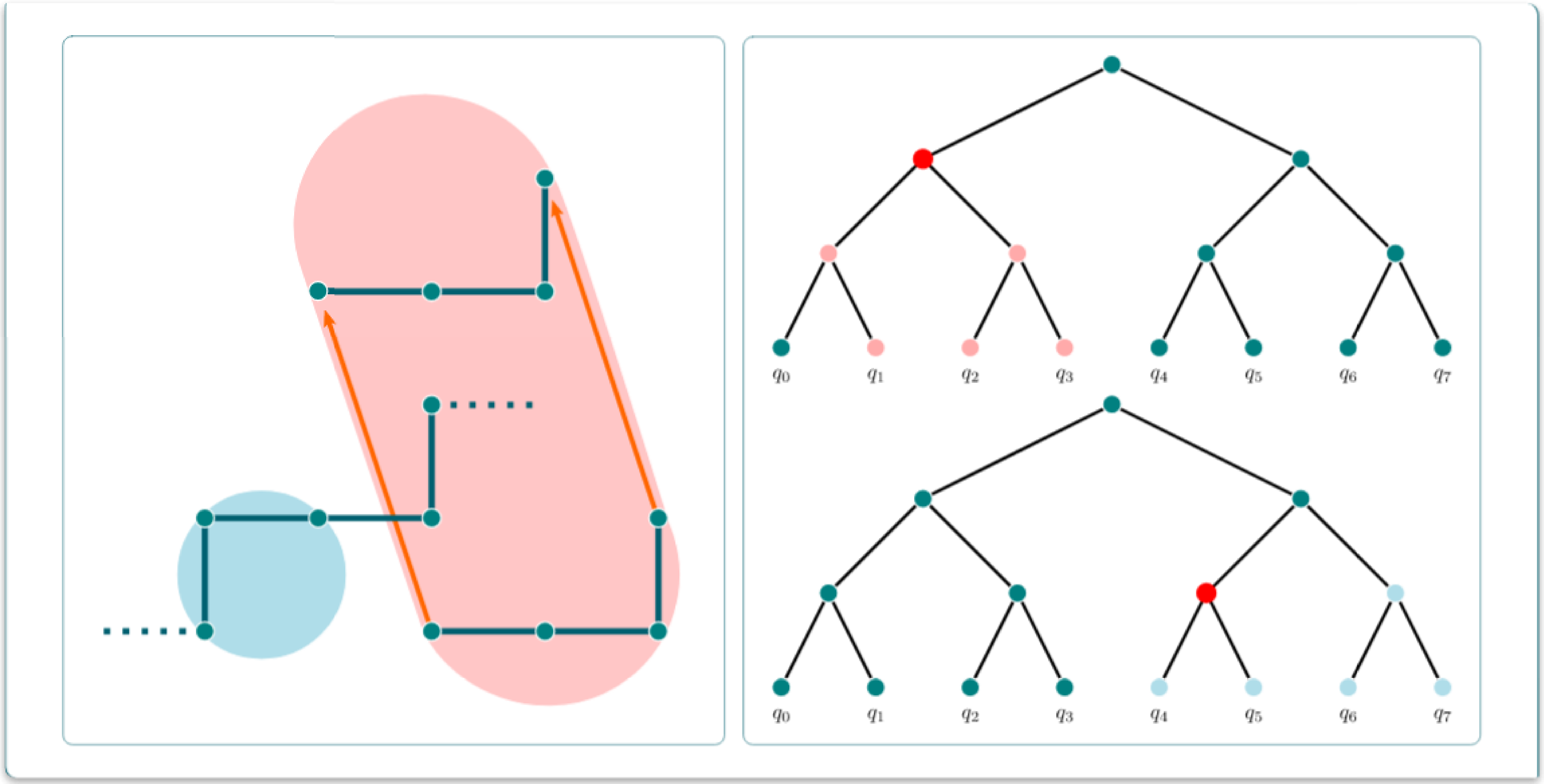

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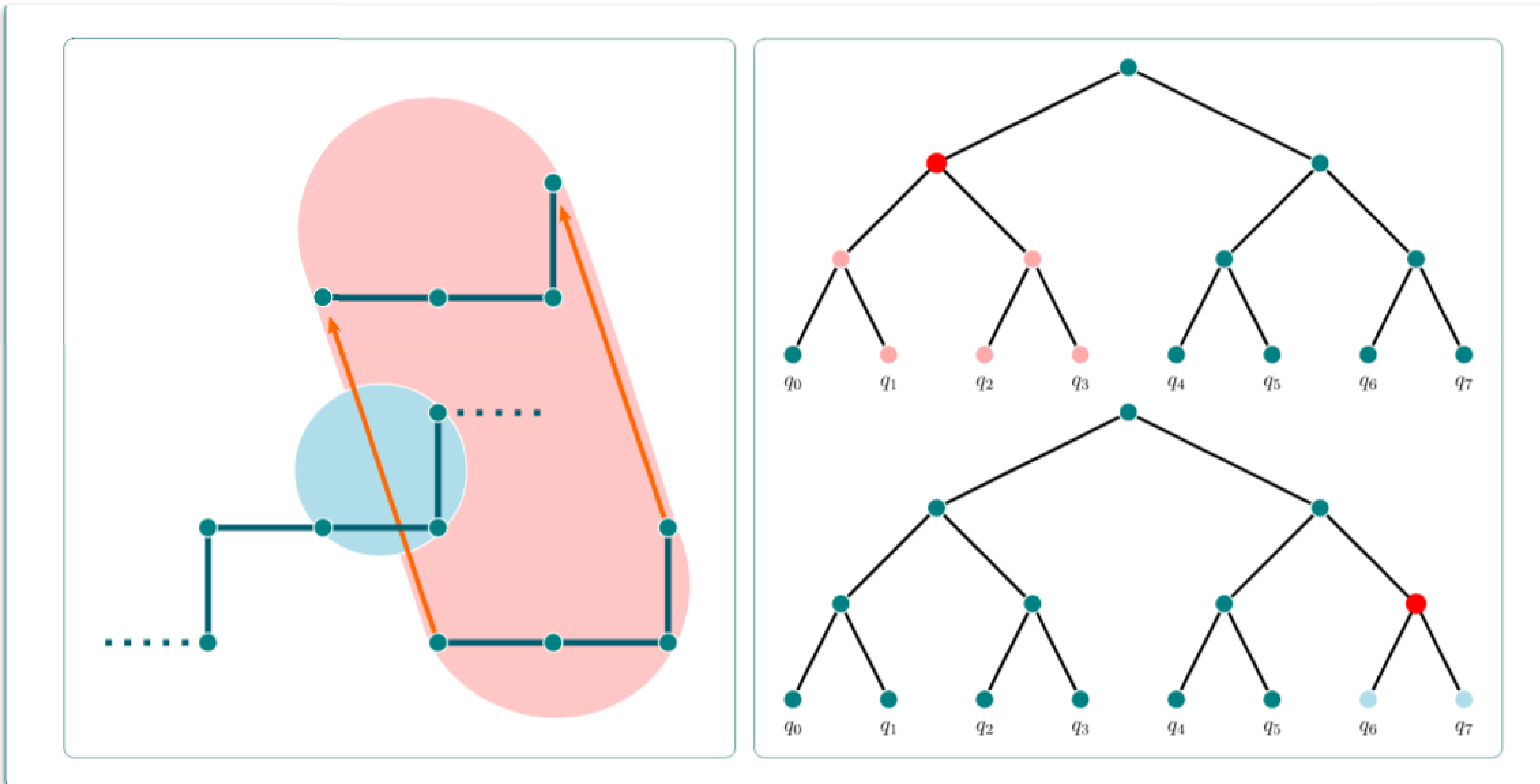

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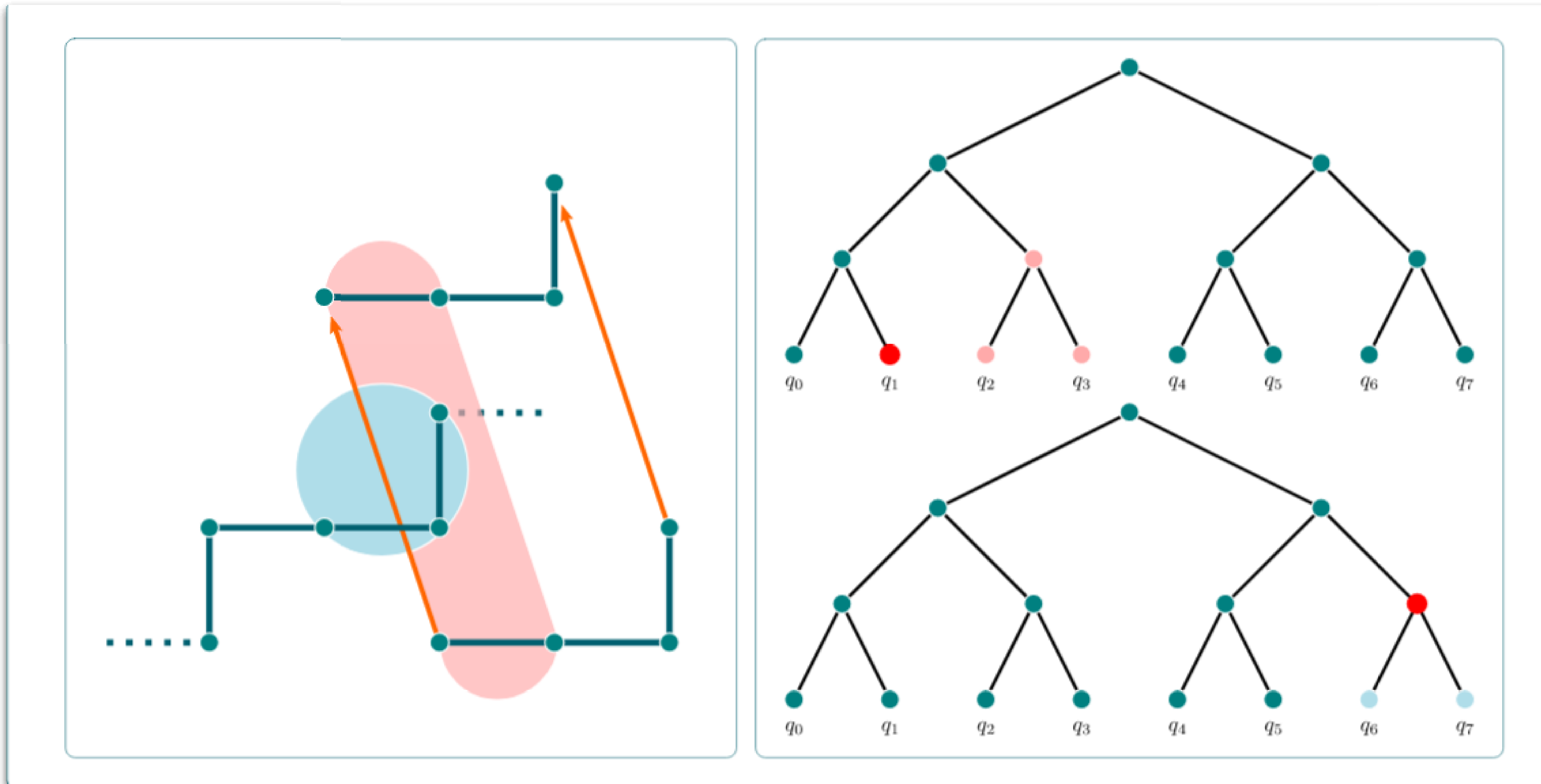

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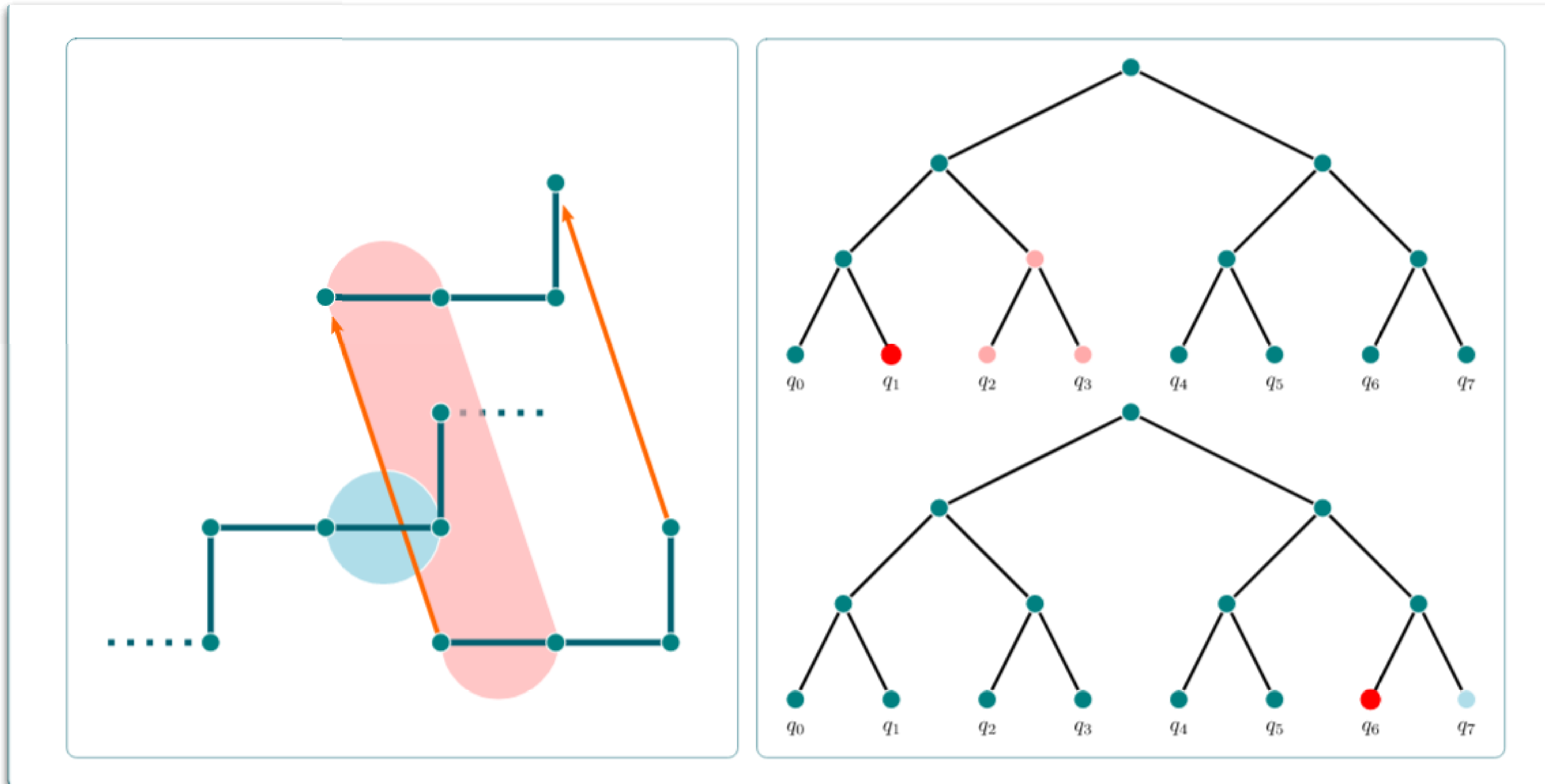
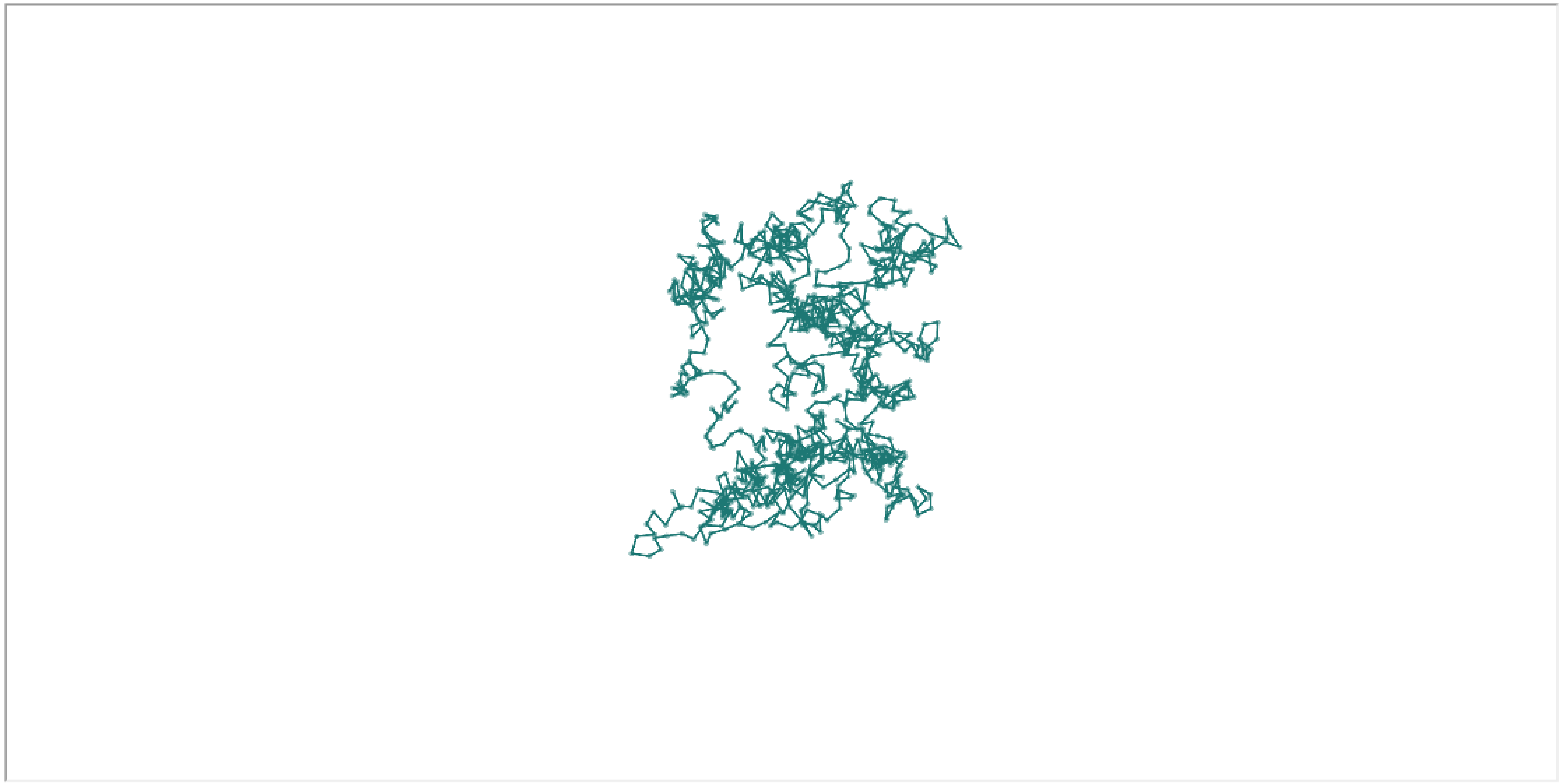


- Check segment-quadrilateral intersection via Möller-Trumbore

Does it work? Is topology conserved?



- 1024 edge square after $\approx$ 250k pivots
- Still an unknot

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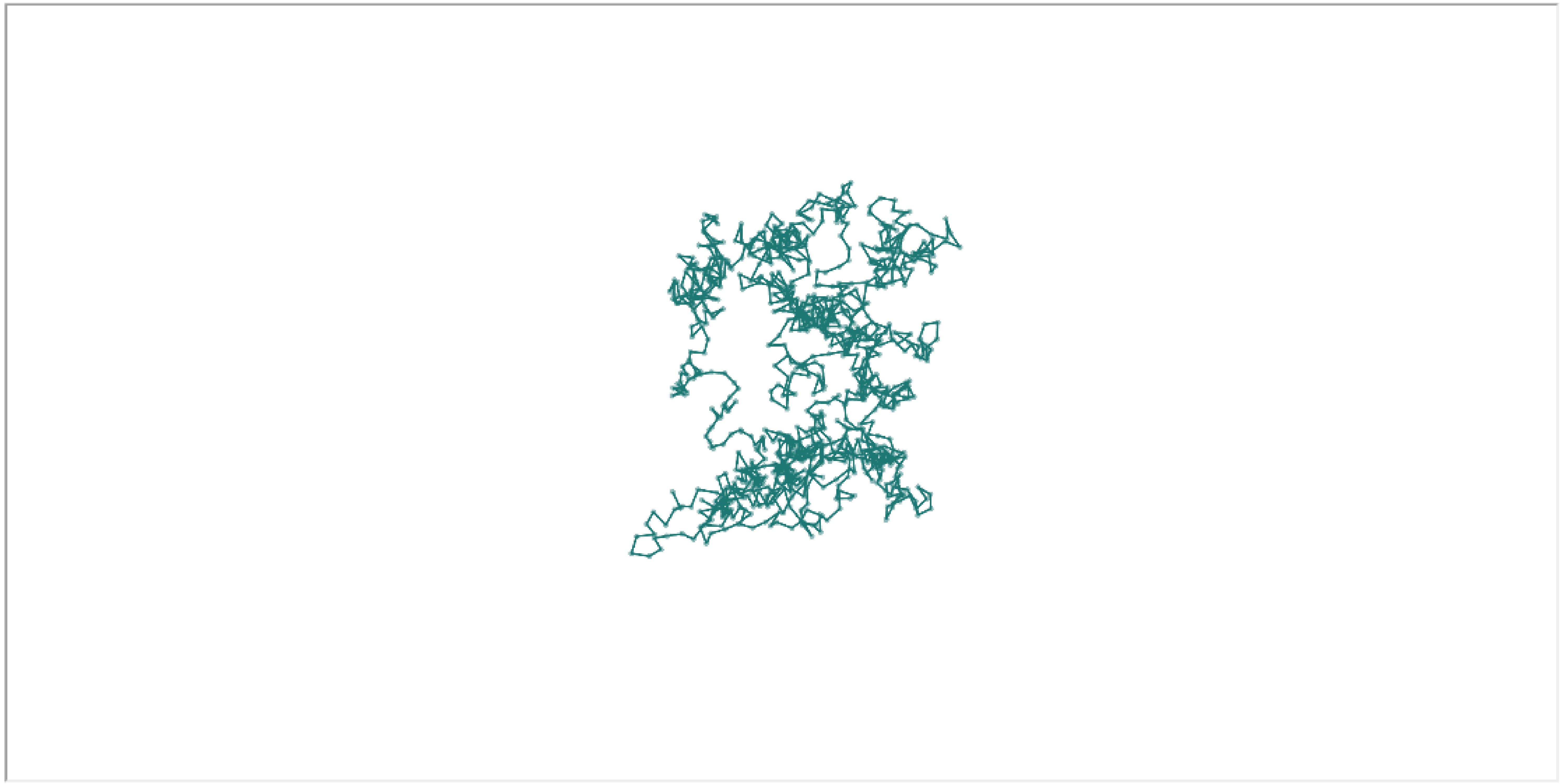
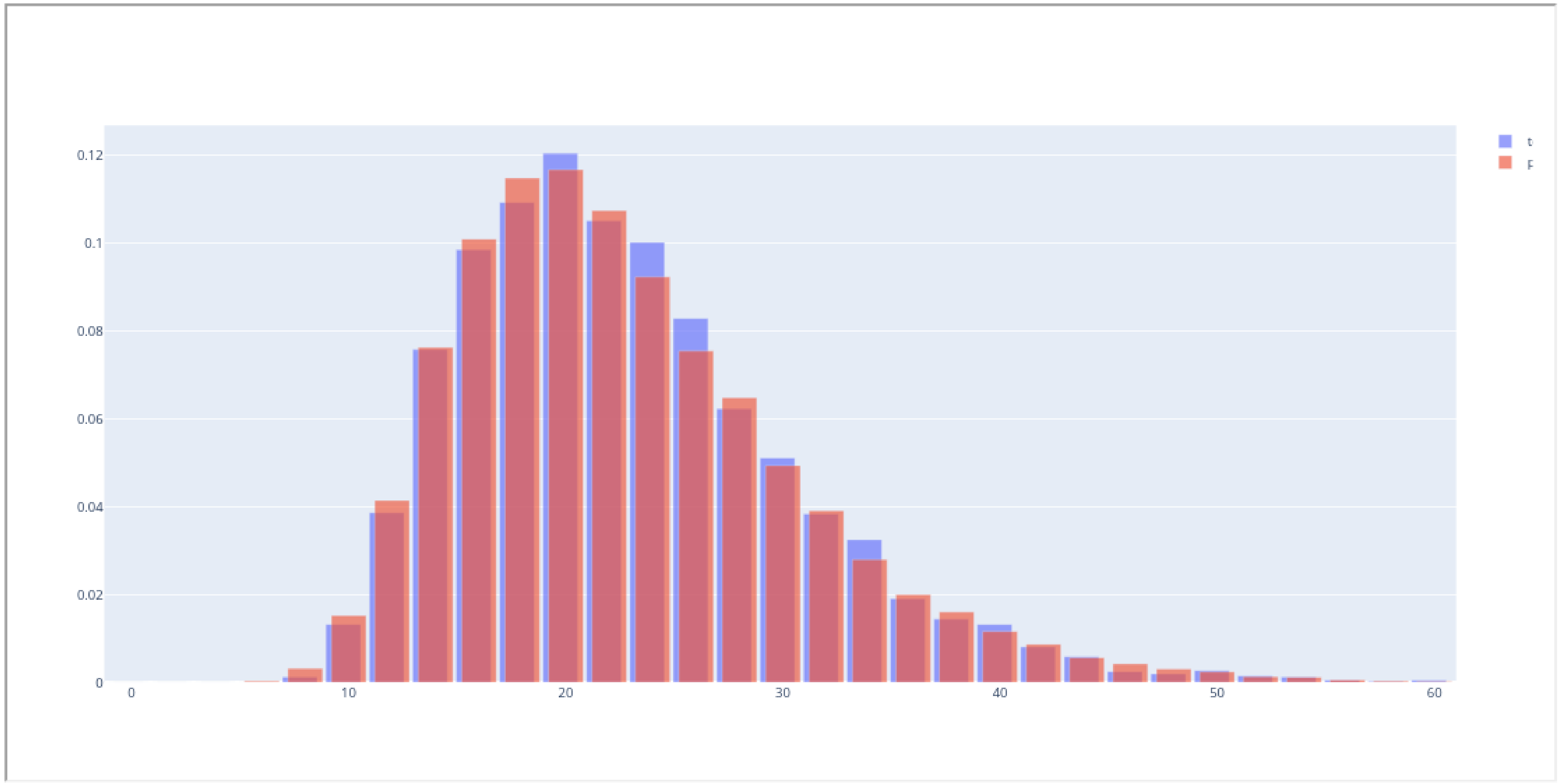


- 1024 edge square after $\approx$ 250k pivots
- Still an unknot
- Important aside — the topoly library is extremely helpful!

Does it work? Compare R_g histograms



- Generate 2^{12} length 256 unknots with the topoly library
- Generate 2^{14} length 256 unknots by pivots
- Close agreement

Does it work? Is it fast? Autocorrelation is everything

Warning: research still in progress

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- Had great difficulty computing reliable autocorrelation time estimates
  - Windowing method via EMCEE python module
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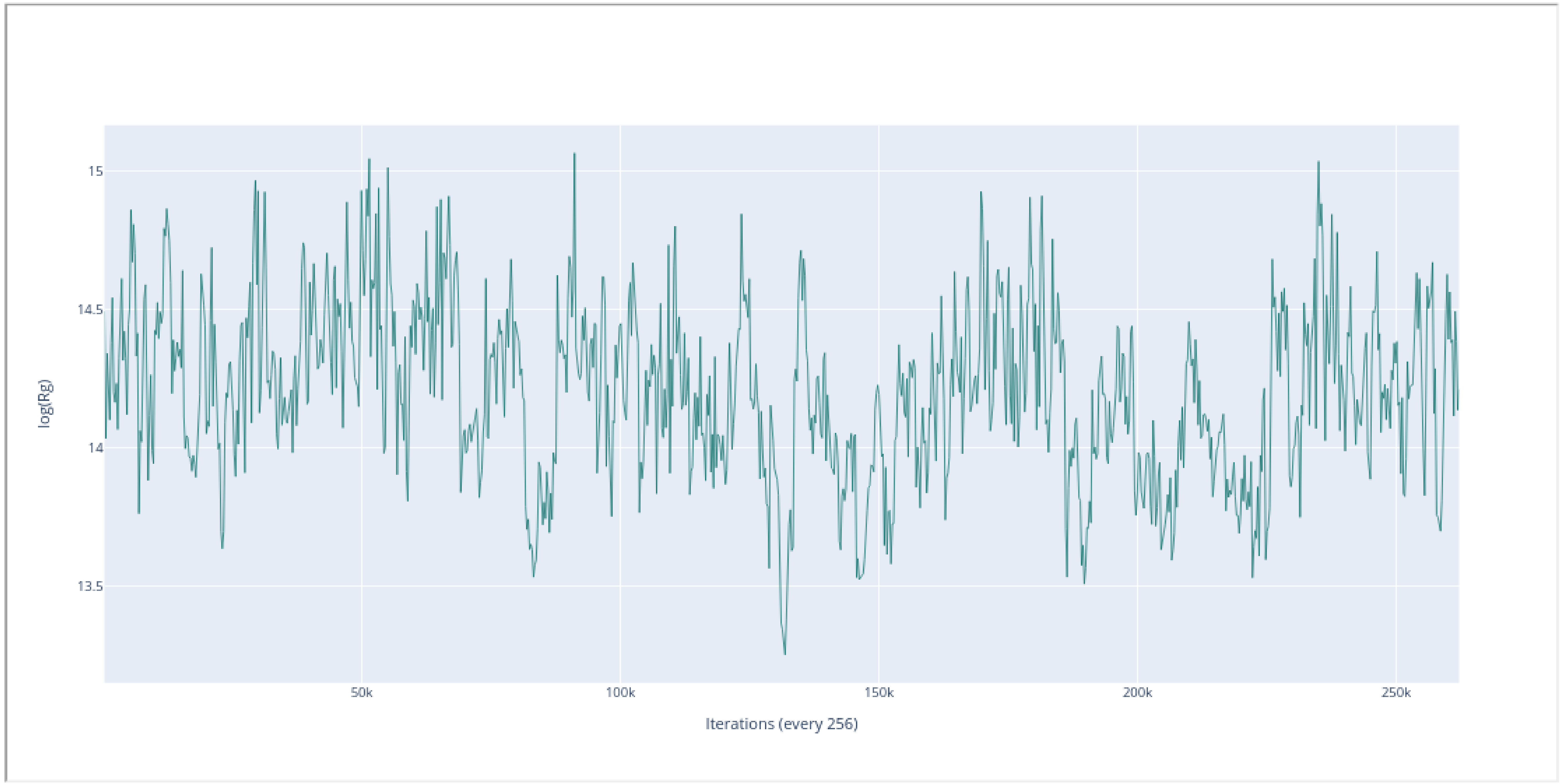
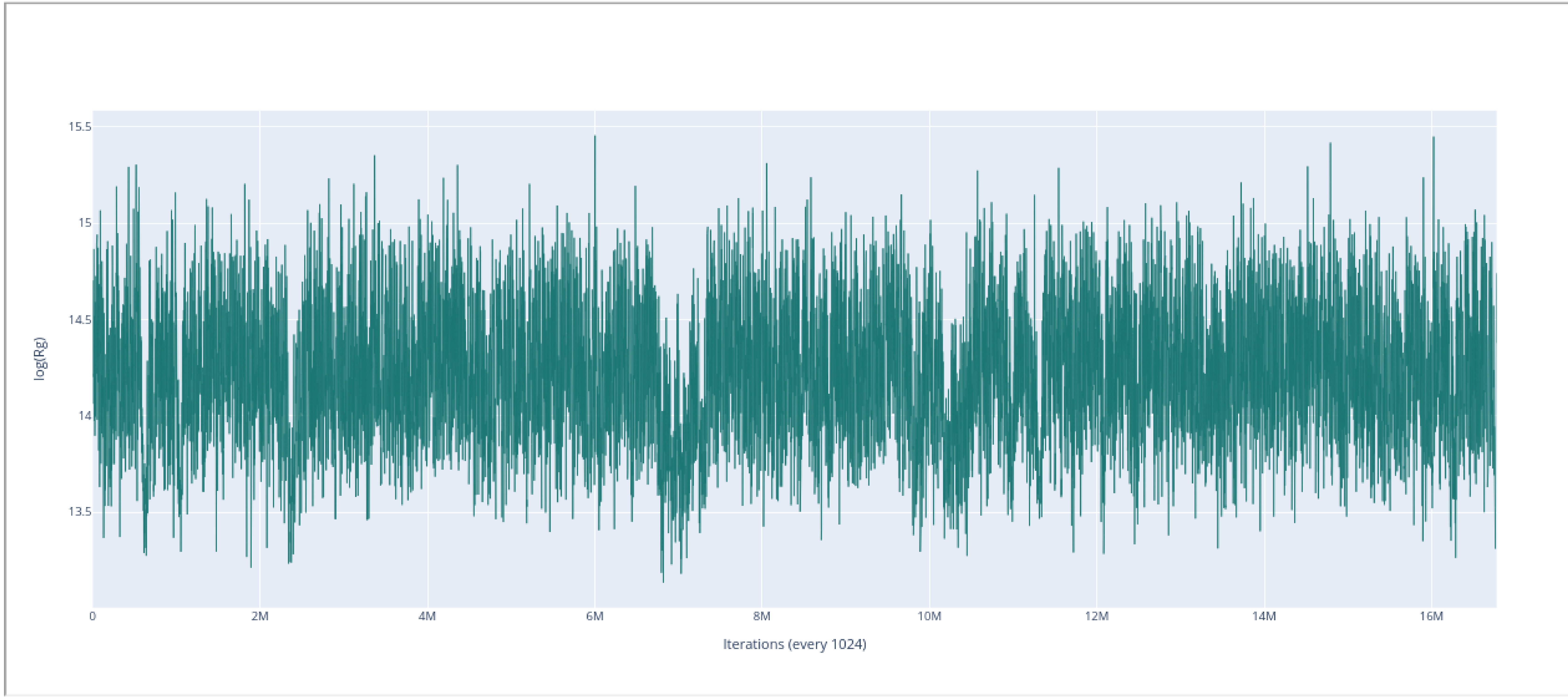
- Huh? What is going on

Plot evolution of R_g with iterations



- Unknot length 256, every 256th iteration shown
- Looks okay, but those *"canyons"* are worrying

Plot evolution of R_g with iterations



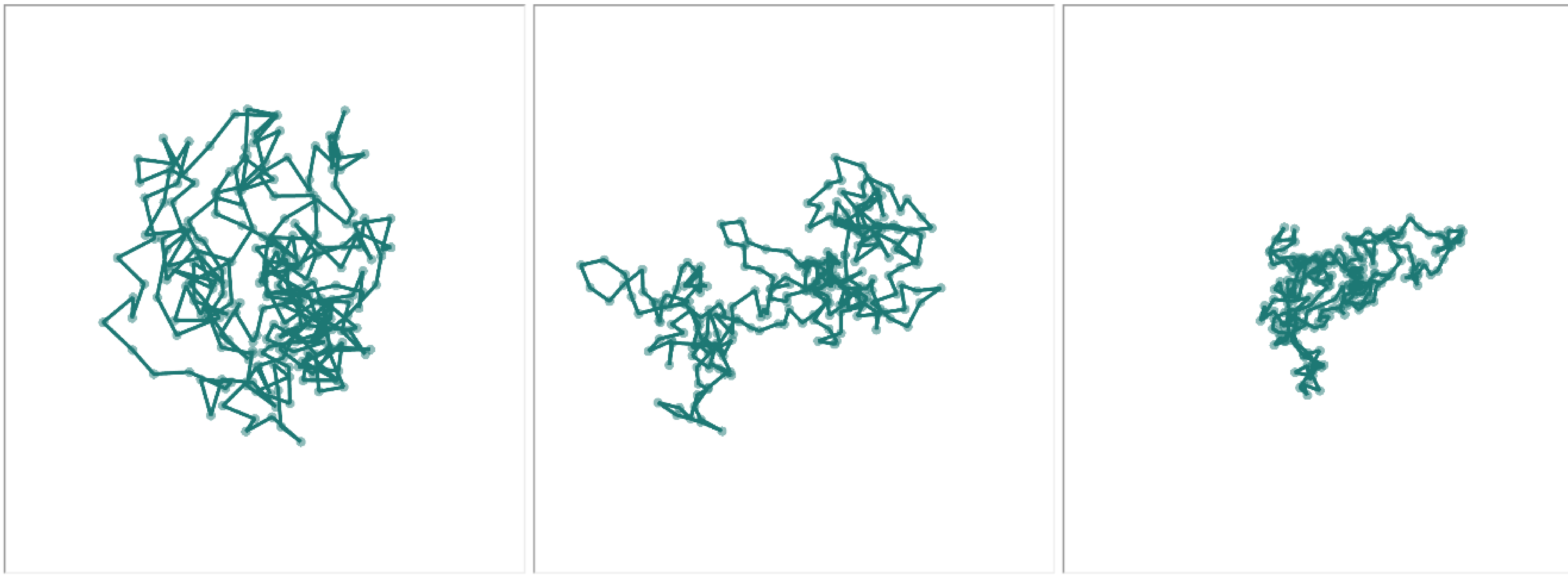
- Unknot length 256, every 1024th iteration shown
- Now *"canyons"* are very worrying

Possibility 1

bugs in my code

Possibility 2

Compact conformations are not so rare



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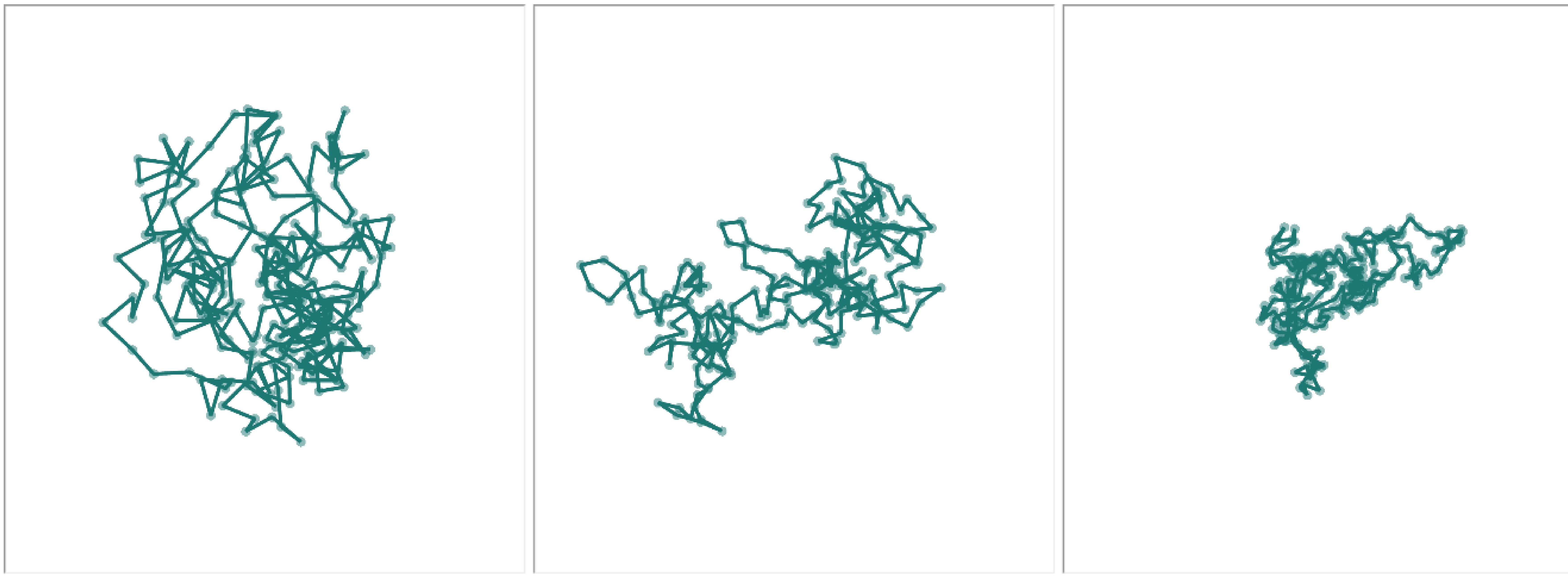

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Does not exclude Possibility 1

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Many thanks to the organisers for today

Richard

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YXE after cancelled flight June 2015

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- He made a big impact on my mathematics; how I do it, how I present it, and how I teach it