Monte Carlo calculation of the hydrodynamic radius for self-avoiding walks

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Statistical mechanics of soft matter, (SM)$^2$
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Self-avoiding walk model

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- Models polymers in good solvent limit.
- Exactly captures universal properties such as critical exponents.
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Hydrodynamic radius for SAW
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Self-avoiding walk
A typical SAW of 5000 steps on the simple cubic lattice:
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- SAW *exactly* captures universal properties of polymers.
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• This is the key property of polymers in a good solvent.
• SAW exactly captures universal properties of polymers.
• E.g. growth in size of a polymer grows as number of monomers increases.
Typical size of a SAW / polymer grows with the number of monomers, $N$, as:

$$R = DN^\nu$$
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Size can be defined in various ways:

- $\langle R^2 \rangle$: mean square end-to-end distance
- $\langle R_g^2 \rangle$: mean square radius of gyration
- $\langle R_h \rangle$: mean hydrodynamic radius

$D$ is non-universal, different for every kind of polymer molecule, or every choice of grid for SAW. Flory exponent $\nu$ is universal!
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- 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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- Local moves make a small deformation, e.g. adding or removing a monomer, $O(N^2)$ moves to get an “essentially new” configuration.
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- Pivot move: $O(1)$ successful moves for an essentially new configuration.
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- Ergodic, samples SAWs uniformly at random.
Example pivot move
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Run simulation
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Bookkeeping can be handled efficiently in binary tree structure.
SAW-tree representation of a walk.
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    (Relies on the fact that monomers which are close on the chain are also close in space.)
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- Calculating global observables such as *R_e*^2^ and *R_g*^2^.

Very fast, can rapidly simulate SAW with many millions of steps.

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$$R_h^{-1} = \frac{1}{N^2} \sum_{i \neq j} \frac{1}{r_{ij}}$$

$$\langle R_h \rangle \sim D_h N^\nu \left(1 + \frac{a}{N^{1-\nu}} + \frac{b}{N^{0.53}} + \cdots \right)$$
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- Strong corrections to scaling, large $N$ should make a big difference.
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- Our estimator is a weighted version of $1/r_{ij}$, monomers $i$ and $j$ chosen at random.
Results

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