Assorted Topics in the Monte Carlo Simulation of Polymers

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Outline

- Self-avoiding walks
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- Pivot algorithm
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- SAW-tree, a data structure for fast pivot moves
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  - $\mu$ - neither local nor global
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  - Dense polymers - new symmetries
  - $R_h$ - estimate observables
  - $\mu$ - neither local nor global
- 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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Self-avoiding walk
A typical SAW of 5000 steps on the simple cubic lattice:
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• E.g. typical size of a SAW / polymer grows with the number of monomers, \( N \), as:

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R = D N^\nu
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E.g. typical size of a SAW / polymer grows with the number of monomers, \( N \), as:

\[ R = D N^\nu \]

\( D \) is model dependent, but the critical exponent \( \nu \) is a universal quantity.
Pivot algorithm

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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”.
Pivot algorithm

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Pivot algorithm

- Procedure:
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1. Choose a pivot site at random

"Global" because on average half of the monomers are moved.

Ergodic, samples SAWs uniformly at random.
Pivot algorithm

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Example pivot move
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Run simulation
Time $O(N)$ to write down an $N$-step walk, so this must be best possible for pivot move?
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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:
  - Symmetry information (for rotations / reflections);
  - "Bounding box" information (for intersection testing);
  - Information about moments of positions, allowing for exact calculation of $R_e^2$ and $R_g^2$. 

Tree structure can be altered via "tree rotations", so that symmetry operations can be applied to any section of the walk.

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

Assorted Monte Carlo
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Example SAW-tree moves.
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How do we apply symmetry to steps 2, 3, 4? Restructure the binary tree via a “tree rotation”.

```
                /
               /   
              /     
             /       
            /         
           /           
          1  2  3  4  
```
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```
    / \
   /   \
  /     \
1 2 3 4
```

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![Diagram of binary tree rotation](image_url)
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\[
\begin{array}{c}
\begin{array}{c}
/ \\
/ \\
/ \\
1 2 3 4
\end{array}
\end{array}
\rightarrow
\begin{array}{c}
\begin{array}{c}
/ \\
/ \\
/ \\
1 2 / \\
\end{array}
\end{array}
\rightarrow
\begin{array}{c}
\begin{array}{c}
/ \\
/ \\
/ \\
1 R/
\end{array}
\end{array}
\rightarrow
\begin{array}{c}
\begin{array}{c}
/ \\
/ \\
/ \\
2 3 4
\end{array}
\end{array}
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```
1 2 3 4
```

```
1
```

```
R
```

```
2
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```
3 4
```

```
1
```

```
2
```

```
3 4
```
• With a binary tree implementation, pivot move has *global effect for local cost*.
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- $O(\log N)$ for:
  - Rotating part of the walk.
  - Checking for self-intersections between two pieces.
  - Calculating global observables such as $R_2^e$ and $R_2^g$. 

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

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

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- Examples on $20 \times 20$ and $200 \times 200$ lattice (from generator at:
  http://lattice.complex.unimelb.edu.au/hamiltonian_path)
Hamiltonian paths

Some effective MCMC moves for sampling dense polymers are based on changing the topology of configurations.
Hamiltonian paths

- Some effective MCMC moves for sampling dense polymers are based on changing the topology of configurations.
- 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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```
\begin{align*}
\text{Backbite moves for sampling Hamiltonian paths.}
\end{align*}
```
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- This suggests time $O(N)$ to perform a backbite move.
- However, can use binary tree data structure with *time reversal* as our symmetry operation.
- Only trick required is bookkeeping for determining neighbours.
This time binary tree has time reversal symmetry elements in the nodes.

![Binary Tree Diagram]
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1 2 3 4
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2 1 3 4
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\[
\begin{array}{cccc}
+ & + & - & + \\
1 & 2 & 3 & 4 \\
1234 & & & 2134 \\
\end{array}
\]
How do we reverse sequences of steps which don’t align with the tree?
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1 2 3 4

\[ \text{1234} \]
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1 2 3 4

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1 4 3 2

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Results

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- \( L = 8192, \ N = 67\,108\,864: \ 360\,000 \text{ steps, versus 6.77 tree rotations.} \)
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- $\mathbb{Z}^2$:
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- $\mathbb{Z}^3$:
Results

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  - Moves have mean size $O(N^{\approx 0.75})$.
  - $L = 8192$, $N = 67108864$: 360 000 steps, versus 6.77 tree rotations.

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  - Moves have mean size $O(N)$.
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$\mathbb{Z}^3$:
- Moves have mean size $O(N)$.
- $L = 512, \; N = 134\,217\,728$: 46 million steps, versus 20.6 tree rotations.
Hydrodynamic radius

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- Why not $R_h$?

\[
R_h^{-1} = \frac{1}{N^2} \sum_{i \neq j} \frac{1}{r_{ij}}
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\[
\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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- Relevant to experiments.
- Strong corrections to scaling, large $N$ should make a big difference.
Hydrodynamic radius

- Can’t rapidly calculate $R_h$, as it depends non-linearly on all $O(N^2)$ interparticle distances, c.f. $O(\log N)$ to perform a pivot.
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- Our estimator is a weighted version of $1/r_{ij}$, monomers $i$ and $j$ chosen at random.
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- Key insight: for an unbiased estimator $E(O)$, Time average($E(O)$) = Ensemble average($O$).
- Our estimator is a weighted version of $1/r_{ij}$, monomers $i$ and $j$ chosen at random.
- $1.591 \pm 0.007$, (Dünweg et al., 2002), vs $1.58040 \pm 0.00002$. 
Counting SAW

Number of SAW of length $N$, $c_N$, tells us about how many conformations are available to SAW of a particular length:

$$c_N \sim A N^{\gamma-1} \mu^N [1 + \text{corrections}]$$
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- Can estimate $c_N/(c_{N/2})^2$ via pivot algorithm - probability that when two SAW are concatenated the result is self-avoiding.
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- Then use

\[ c_N = \frac{c_N}{c_{N/2}^2} \left( \frac{c_{N/2}}{c_{N/4}^2} \right)^2 \cdots c_{N/k}^{N/k}. \]
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- Sites of the walk which are close to the concatenation point have a much greater influence on the probability, than sites which are far away.
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- Pivot sites chosen uniformly: $\tilde{\tau}_{\text{int}} = \Omega(N)$ (due to trapped configurations).
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- Instead, choose distance from joint uniformly from all distance scales.
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- \( \Rightarrow \mu = 4.684\,039\,931(27) \) (C., 2013)
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- Instead, choose distance from joint uniformly from all distance scales.
- $\Rightarrow \mu = 4.684\,039\,931(27)$ (C., 2013)
- This idea can be applied to other systems with additional length scales: confined polymers, bridges, star polymers, perhaps $\theta$-polymers.
Conclusion

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- Pivot algorithm only part of the story.