THE CONFIGURATION SPACE OF BRANCHED POLYMERS

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Branched polymers (dendrimers) in modern science

- artificial blood
- catalyst recovery
- artificial photosynthesis
A branched polymer is a connected collection of unit disks with non-overlapping interiors
(generically, a tree of disks)

\[ X_n = \text{space of branched polymers with } n \text{ labelled disks.} \]
$2D$ examples:

Volume($X_2$) = $2\pi$

Volume($X_3$) = $2(2\pi)^2$
\[ 1 \cdot (2\pi)^3 \quad 5 \cdot (2\pi)^3 \]
\[ \frac{5}{27} \cdot (2\pi)^4 \quad \frac{230}{27} \cdot (2\pi)^4 \quad \frac{413}{27} \cdot (2\pi)^4 \]
Questions

1. What does a random BP looks like?
   (diameter? number of leaves? scaling limit?)

2. Does the space $X_n$ have a nice geometric structure?

Theorem [Brydges/Imbrie 2002]

2D: The volume of $X_n$, measured in terms of angles, is $(2\pi)^{n-1}(n-1)!$.

3D: The volume of $X_n$, measured in terms of angles, is $(2\pi)^{n-1}n^{n-1}$.

Generally, they related BPs in $\mathbb{R}^{D+2}$ with the “hard sphere” model in $\mathbb{R}^D$. 
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Key observation:

**Invariance Lemma in 2D:** The volume of $X_n$ doesn’t change when you change the radii.

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$$\text{Vol} = 2\pi(2\pi - 2\theta_1)$$
Key observation:

**Invariance Lemma in 2D**: The volume of $X_n$ doesn’t change when you change the radii.

([BI] proved this using localization/ equivariant cohomology)
Assuming this Lemma, we can compute $\text{Vol}(X_n)$ as follows:

Take disks of radii $1, \epsilon, \epsilon^2, \ldots, \epsilon^{n-1}$.

In this case, we can ignore BPs like:

since they have small volume ($\to 0$ as $\epsilon \to 0$).

So we need consider only configurations where balls are attached in order of decreasing radius.
Attach $i$ to one of $1, 2, \ldots, i - 1$. 

$2\pi \cdot (i - 1) + O(\epsilon)$ choices

Total volume $\prod_{i=2}^{n} 2\pi (i - 1) = (2\pi)^{n-1}(n - 1)!$

in limit $\epsilon \to 0$. □
Proof of Invariance Lemma

The proof is based on the following (trivial) fact:

**Lemma:** If $v_1, \ldots, v_n \in \mathbb{R}^{n-1}$ and the $n \times n$ matrix

$$A = \begin{pmatrix} 1 & 1 & \ldots & 1 \\ v_1 & v_2 & \ldots & v_n \end{pmatrix}$$

is singular, then

$$\sum_{j=1}^{n} (-1)^j v_1 \wedge \cdots \wedge \hat{v}_j \wedge \cdots \wedge v_n = 0.$$

Now, change the radii of the disks continuously.

The volumes of the components of $X_n$ (one for each tree) change because their boundaries in the space of angles move.
Codimension-1 boundaries are where the BP has a cycle:

![Diagram showing codimension-1 boundaries]

A BP with a $k$-cycle is in the boundary of $k$ components (break one of the $k$ edges of the cycle).

Show using Lemma that the net volume lost to each component sums to zero:
Codimension-1 boundaries are where the BP has a cycle:

Let $\theta_i$ be the angle of edge $i$ of $P$. 

When increasing $R$, this component loses volume near $P$. 
When increasing $R$, this component gains volume near $P$. 
Computing volume changes:

Let \( \frac{\partial}{\partial t_1}, \ldots, \frac{\partial}{\partial t_{k-2}} \) be coordinates for perturbations of a \( k \)-gon \( P \) preserving edge lengths.

Let \( \frac{\partial}{\partial R} \) be a perturbation of \( P \) increasing two adjacent edge lengths at the same rate.

\[
B = \begin{pmatrix}
\frac{\partial \theta_1}{\partial t_1} & \cdots & \frac{\partial \theta_k}{\partial t_1} \\
\vdots & \ddots & \vdots \\
\frac{\partial \theta_1}{\partial t_{k-2}} & \cdots & \frac{\partial \theta_k}{\partial t_{k-2}} \\
\frac{\partial \theta_1}{\partial R} & \cdots & \frac{\partial \theta_k}{\partial R}
\end{pmatrix}
\]

Note that \((1,1,\ldots,1)\) is in the span of the \( \frac{\partial}{\partial t_i} \) (rotate \( P \)).

So by the lemma, \( \sum_{j=1}^{k} (-1)^j d\theta_1 \land \cdots \land \widehat{d\theta_j} \land \cdots \land d\theta_k = 0 \).
The volume changes are proportional to the projection lengths along the angle bisector. (Calculation omitted.)
Perfect simulation of a 2D branched polymer.
\[ \approx 1000 \text{ balls} \]

\[ \approx 2000 \text{ balls} \]
What if you weaken the hard core interaction?

that is, allow certain pairs of disks to overlap each other.

Define an “interaction” graph $G$:

$v \sim v'$ if $v$ and $v'$ are not allowed to overlap.

E.g. Two species of balls: blues & reds “Bipartite polymers”

(G is complete bipartite graph)

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**Theorem**

The volume of the configuration space is $(2\pi)^{n-1}T_G(1, 0)$.

$$T_G(1, 0) = \sum_{\text{spanning subgraphs}} (-1)^{\text{edges}}$$

$T_G(x, y)$ is the Tutte polynomial of $G$. 
Branched polymers in 3D

Project the ball centers to the $x$-axis:

Let $G$ be the graph with vertices $x_i$ and edges when $|x_i - x_j| < 1$. 
**Lemma:** The $n$-dimensional volume of the set of 3DBPs whose centers project to $x_1 < x_2 < \cdots < x_n$ is $(2\pi)^{n-1} \prod_{i=1}^{n-2} n_i$ where $n_i$ is the number of $x_j$ with $j > i$, with $|x_j - x_i| < 1$.

**Proof:** Compute $T_G(1,0)$. Use Archimedes’ theorem. □

**Theorem:** [Archimedes] The Lebesgue measure on $S^2$ projects to uniform Lebesgue measure on a segment in the $x$-direction.
Question: when we project the points of a 3DBP, what is their distribution?

Answer:
(1) Construct a random labelled tree on $n$ vertices.
(2) Assign a uniform $[0,1]$ length to each edge, independently.
(3) Dangle the tree from the root.
(4) Let $x_i$ be the distance of the $i$th vertex from the root. (and $x_1 = 0$)

Theorem: These points are equidistributed with the projected points of a BP.
Corollary. The 3DBP with $n$ balls has diameter of order $\sqrt{n}$. 
Proof of Theorem

Let \(x_1, \ldots, x_n \in \mathbb{R}\) be the projections of the centers.

Build a tree by gluing each \(x_k\) to some \(x_j\) to its left with \(|x_k - x_j| < 1\)

The number of ways to do this is \(\prod_{i=1}^{n-1} n_i\)

Integrate over positions of the \(x_i\):

Each tree contributes \(\int_{[0,1]^{n-1}} dx\)

So get \(n^{n-1}\) (total number of rooted trees). \(\square\)
Open questions

1. Dynamics on polymers

2. 4D polymers \((\approx 2D \text{ hard disk model})\).

3. Diameter of a 2DBP

4. \(X_n \times [0, 1]^M \approx \mathbb{T}^{n-1} \times [0, 1]^M\)
A puzzle: [Spitzer]

Starting at origin in \( \mathbb{R}^2 \), take a random walk, each step being a uniformly chosen unit vector.

Show: the probability that you are within 1 of the origin after \( n \) steps is \( \frac{1}{n+1} \).

Hint: Use \( G=\text{n-cycle} \).
Computing $Z_{4D}$.

Take points $x_1, \ldots, x_n \in \mathbb{R}^2$, with $x_1 = 0$.
Define a graph $G$ by: $x_i \sim x_j$ if $|x_i - x_j| < 1$.

$$Z_{4D} = \int T_G(1, 0) dx_2 \ldots dx_n.$$