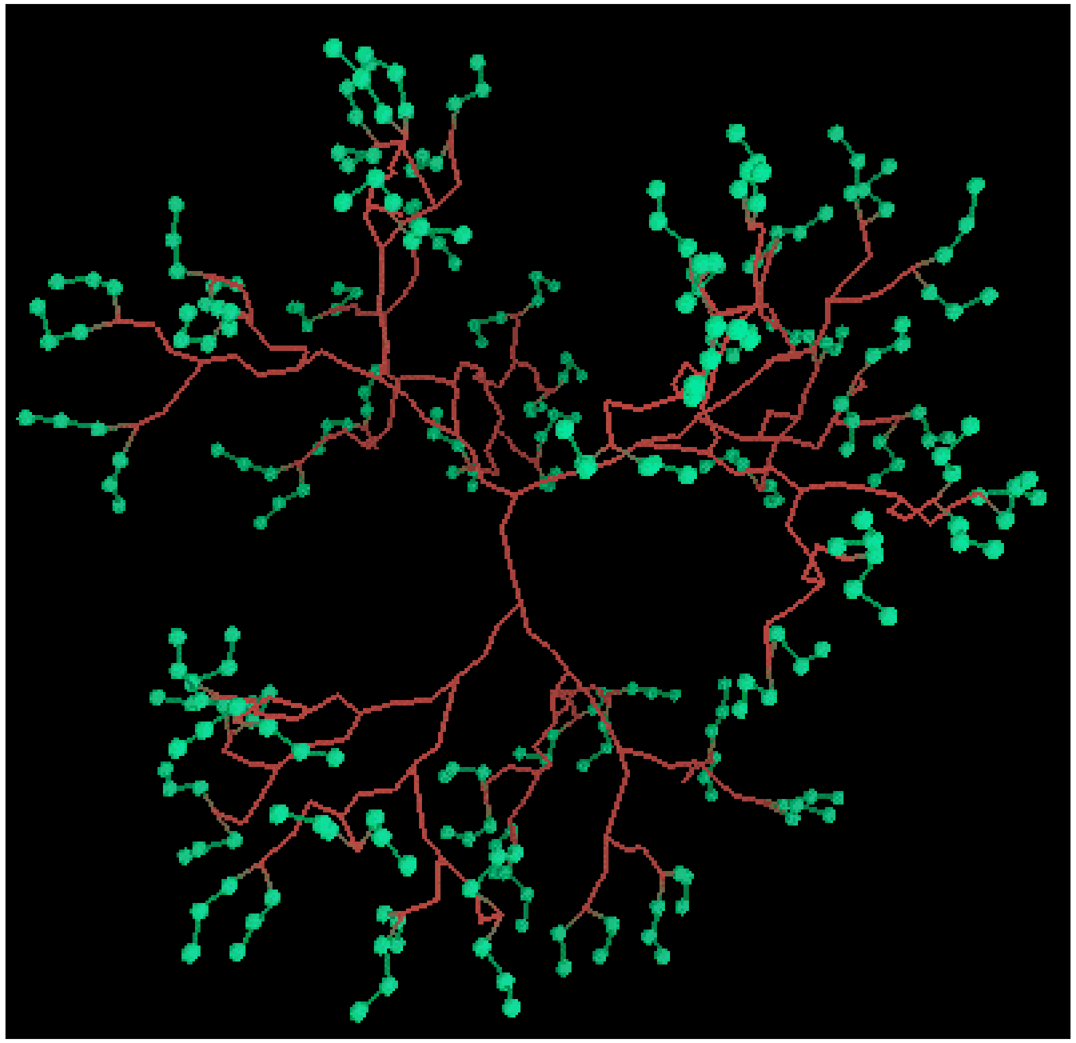
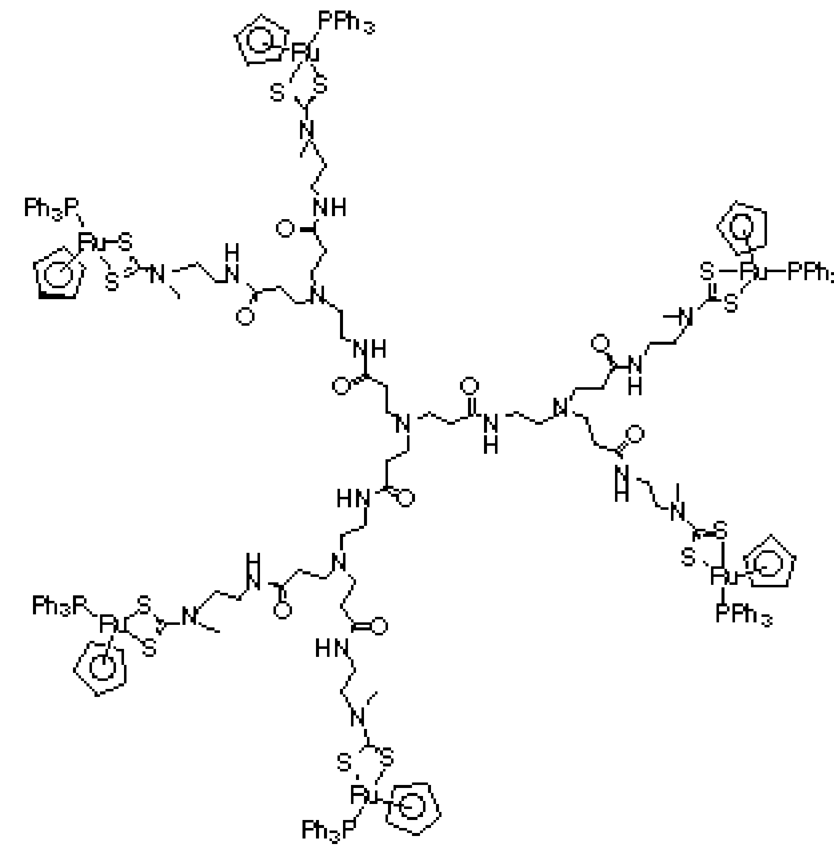
Branched Polymers

R. Kenyon, P. Winkler

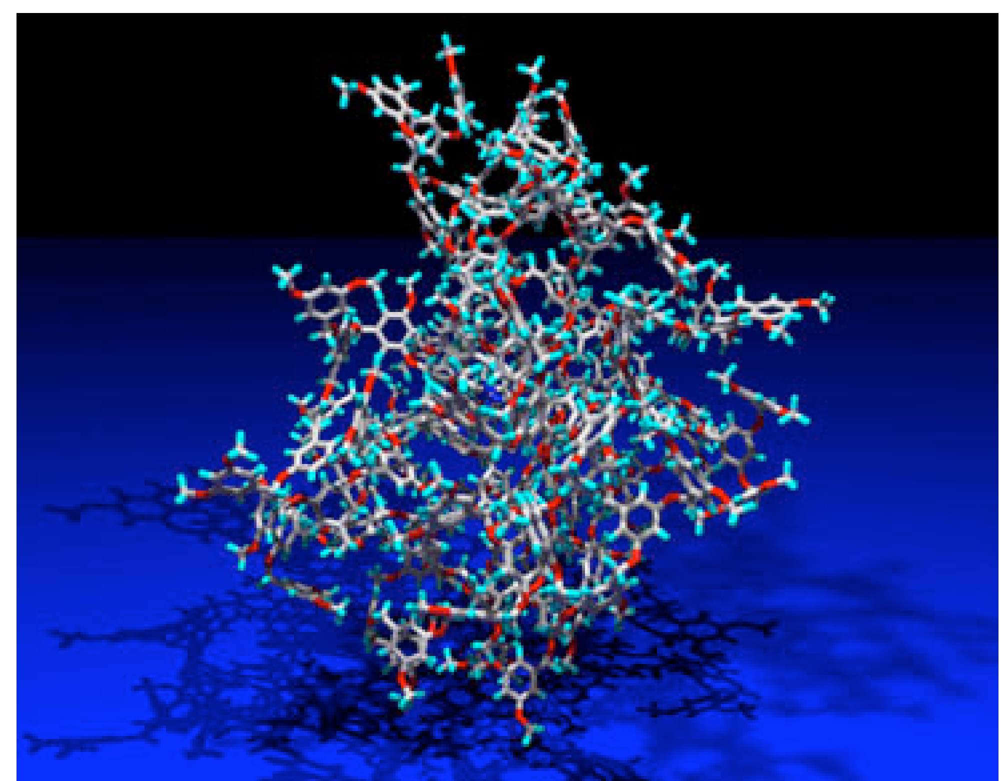
Branched polymers (dendrimers) in modern science



artificial blood



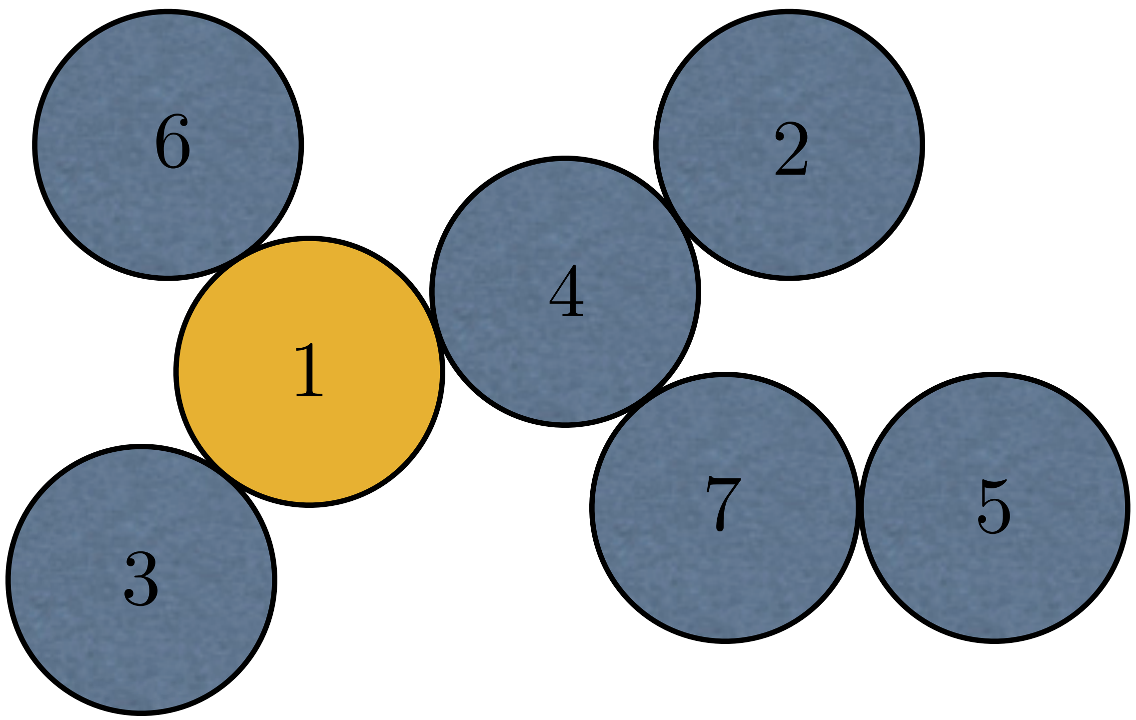
catalyst recovery



artificial photosynthesis

A branched polymer is a connected collection of unit disks with non-overlapping interiors

(generically, a tree of disks)



X_n = space of branched polymers with n labelled disks.

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?

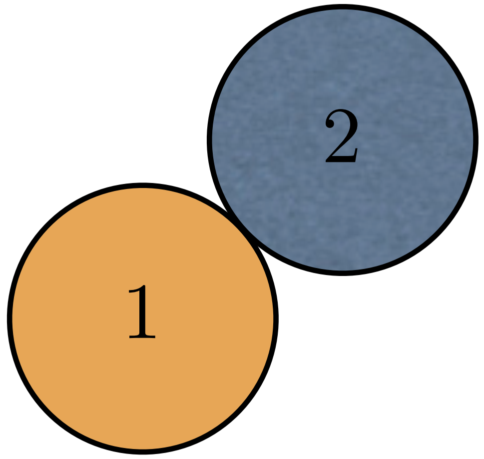
Theorem [Brydges/Imbrie 2002]

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

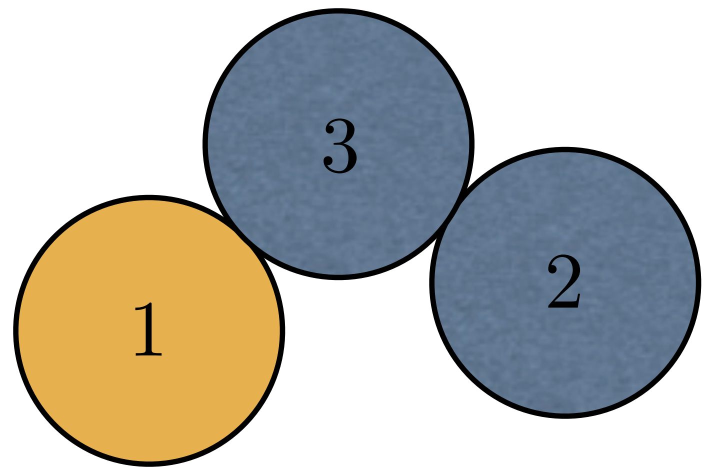
$3D$: The volume of X_n, measured in terms of angles, is $(2\pi)^{n-1}n^{n-1}$.

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

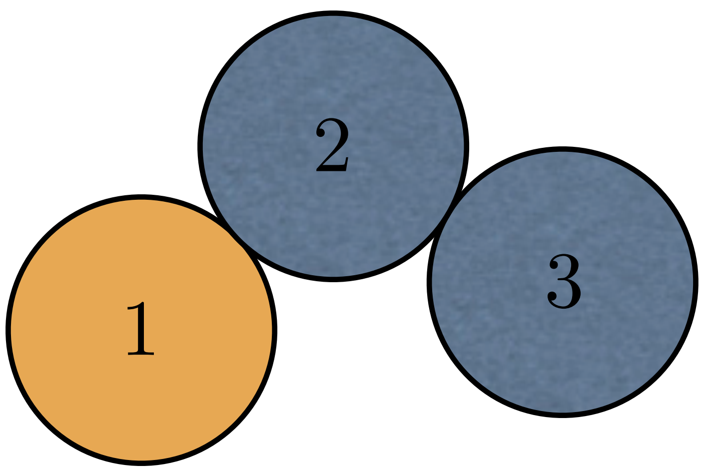
$2D$ examples:



$\text{Volume}(X_2) = 2\pi$

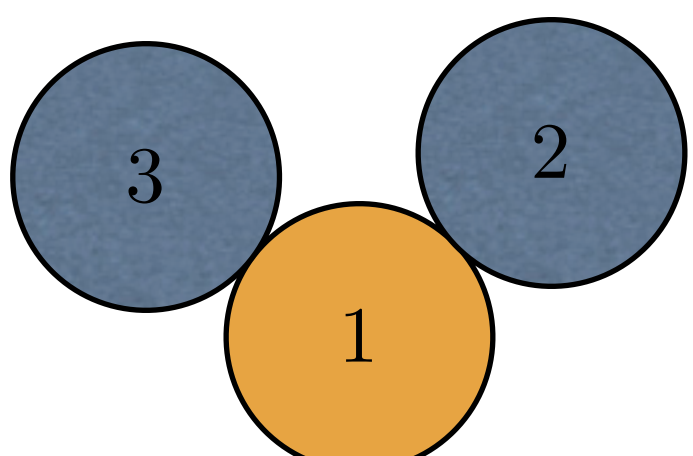


$2\pi \cdot \frac{4\pi}{3}$



$2\pi \cdot \frac{4\pi}{3}$

$\text{Volume}(X_3) = 2(2\pi)^2$

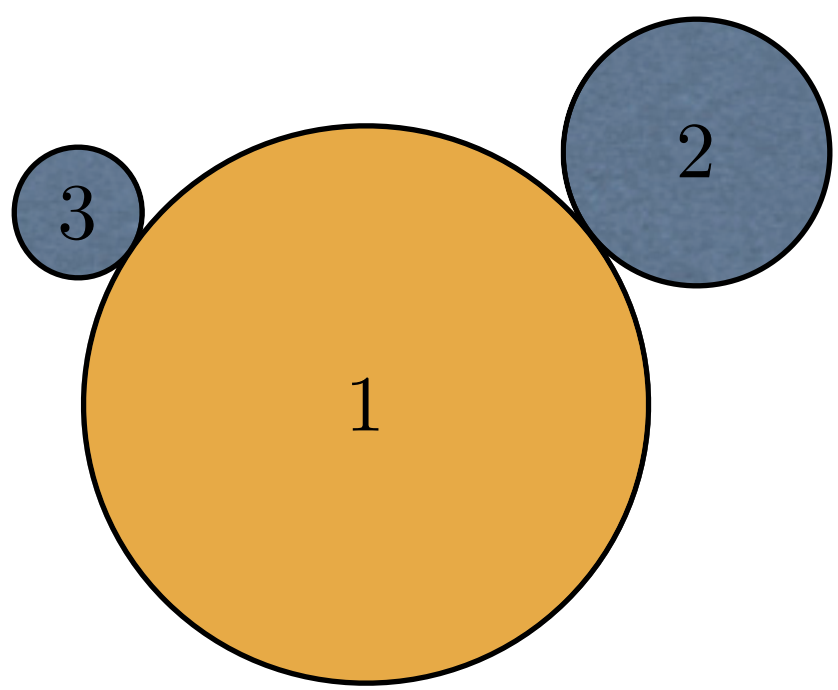


$2\pi \cdot \frac{4\pi}{3}$

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)



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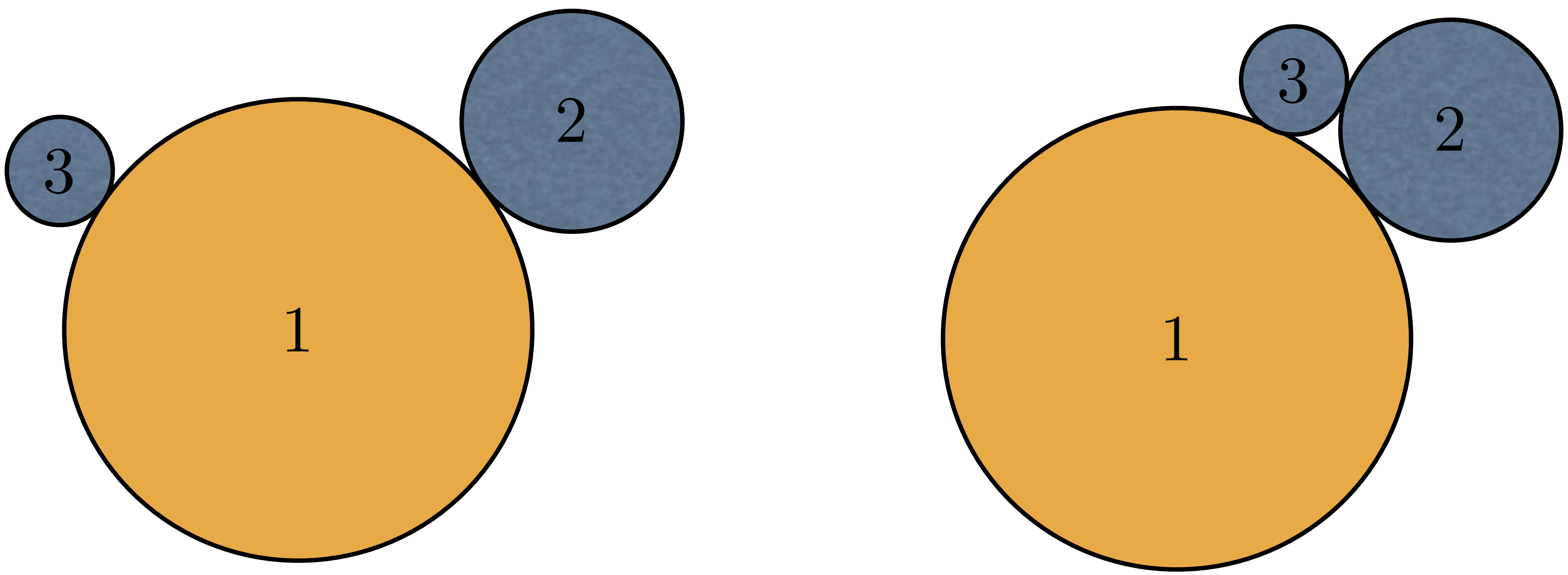

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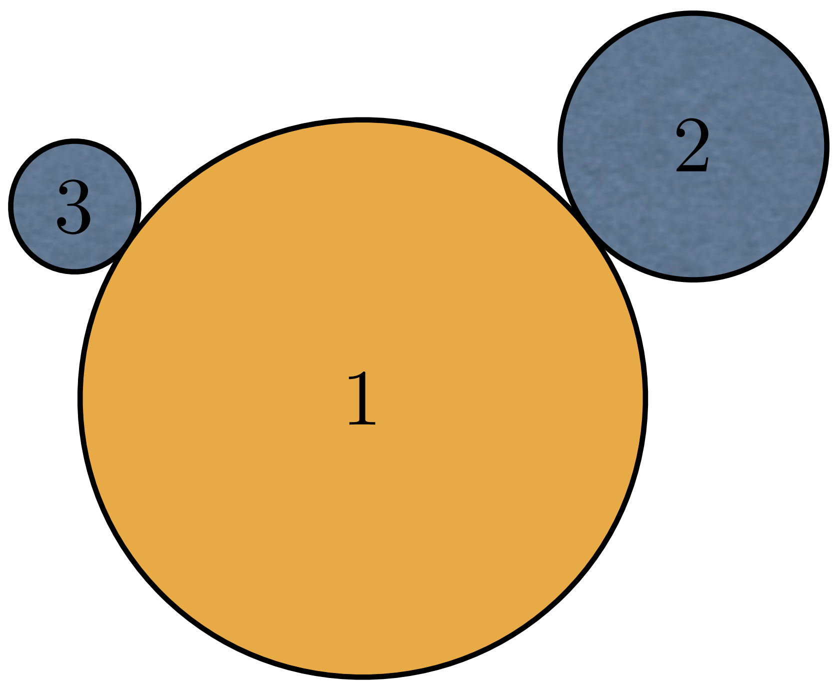
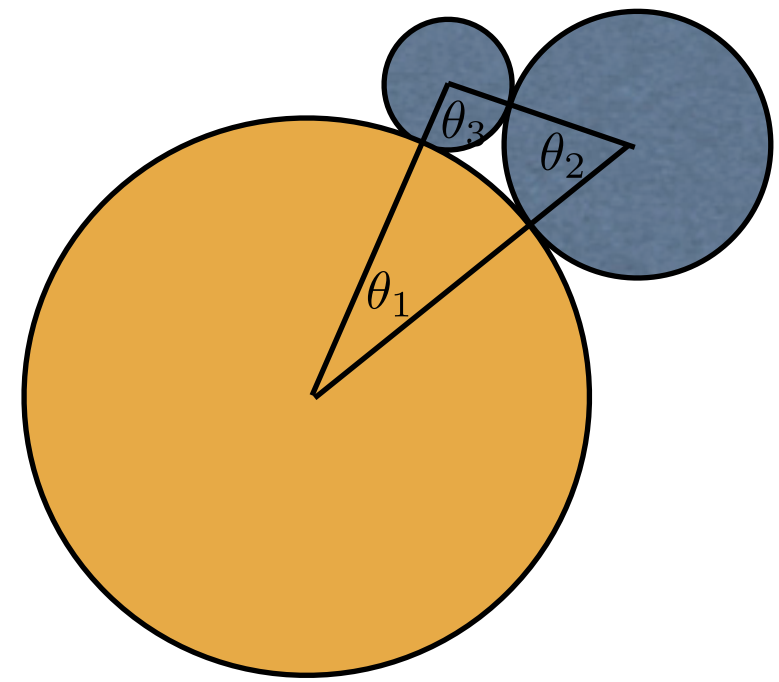


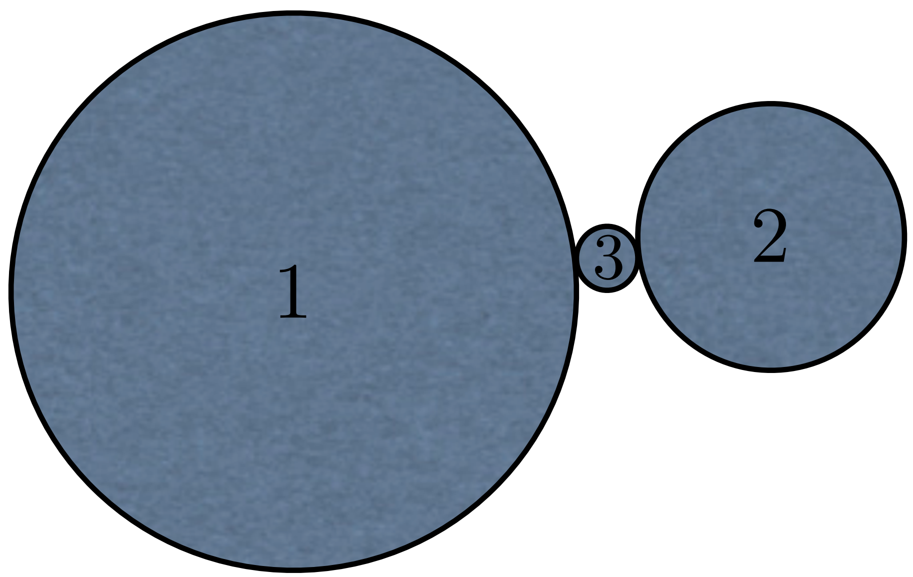


Vol$= 2\pi(2\pi - 2\theta_1)$

Assuming this Lemma, we can compute $\mathrm{Vol}(X_n)$ as follows:

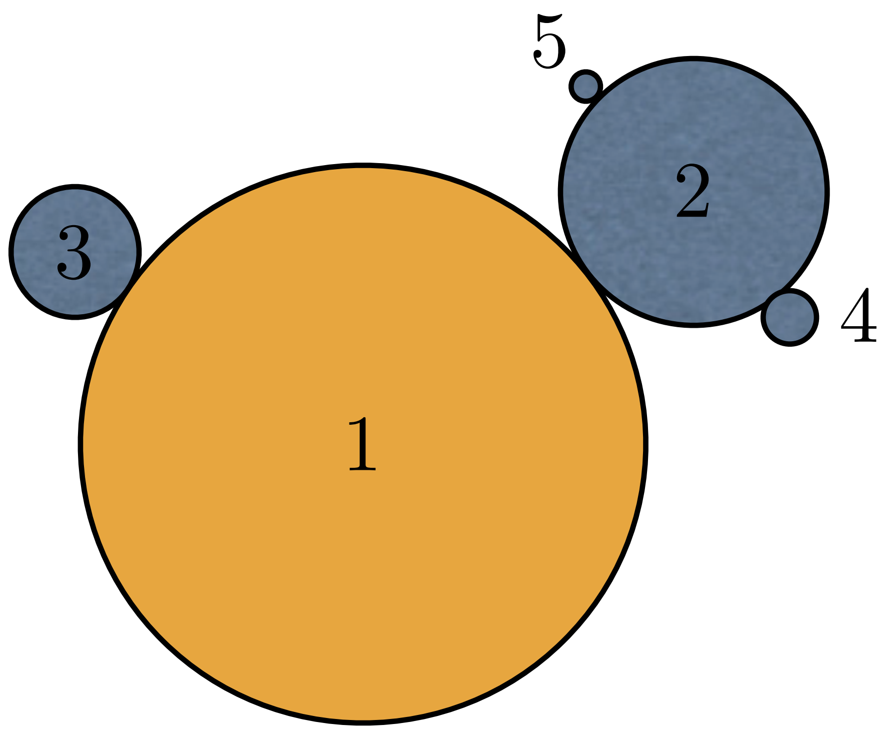
Take disks of radii $1, \epsilon, \epsilon^2, \ldots, \epsilon^{n-1}$.

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 $1, 2, \ldots, i-1$ $\qquad$ $2\pi \cdot (i-1) + O(\epsilon)$ 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 fact.

Lemma: If $\theta_1 + \cdots + \theta_k = constant$, then

$$\sum_{i=1}^{k} d\theta_1 \wedge \cdots \wedge \widehat{d\theta_i} \wedge \widehat{d\theta_{i+1}} \wedge \cdots \wedge d\theta_k = 0.$$

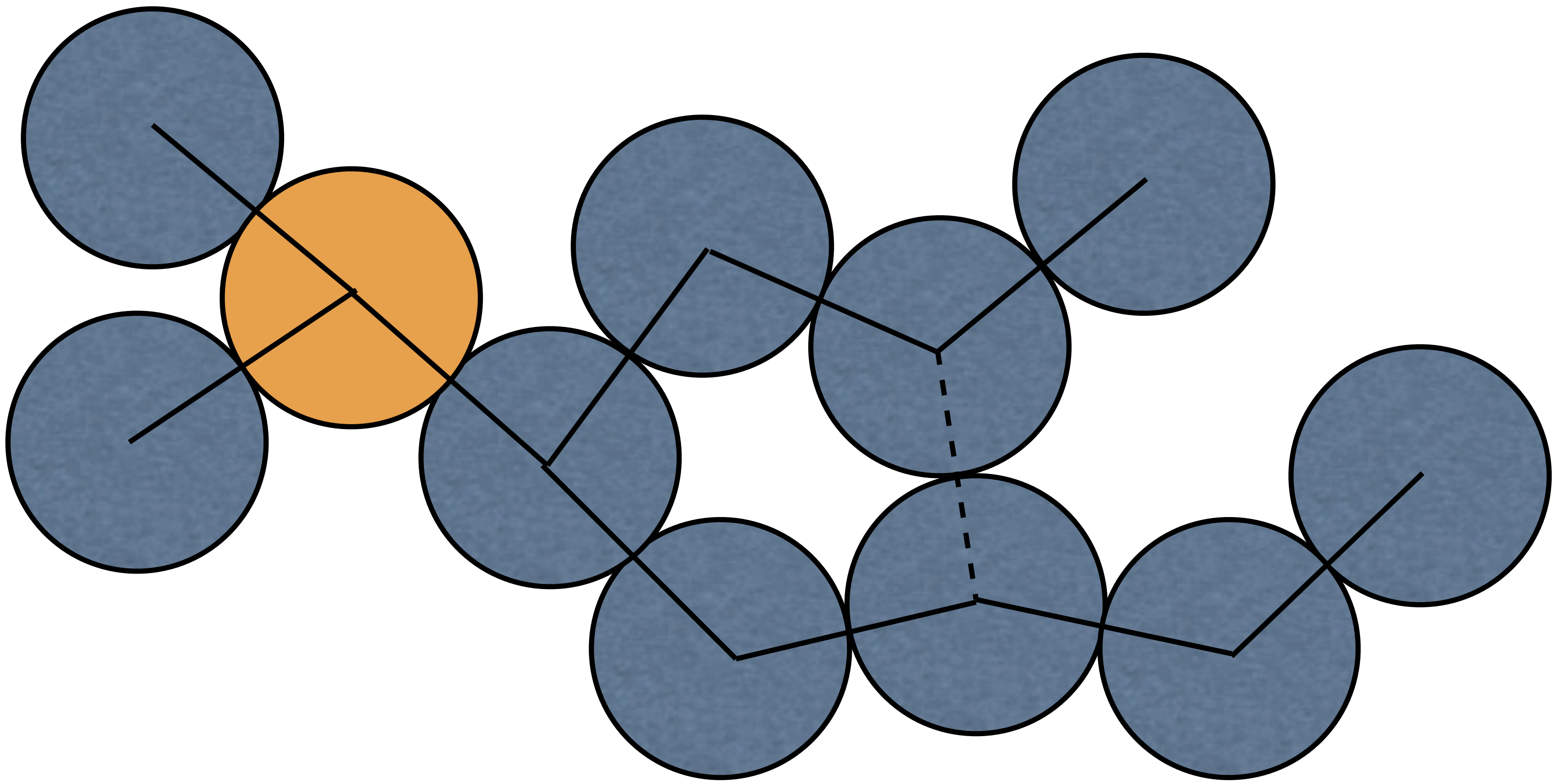
e.g. $d\theta_3 \wedge d\theta_4 + d\theta_1 \wedge d\theta_4 + d\theta 1 \wedge d\theta_2 - d\theta_2 \wedge d\theta_3$

$$= d\theta_3 \wedge (-d\theta_1 - d\theta_2 - d\theta_3) + d\theta_1 \wedge (-d\theta_1 - d\theta_2 - d\theta_3) + d\theta_1 \wedge d\theta_2 - d\theta_2 \wedge d\theta_3 = 0.$$

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:



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. $\square$

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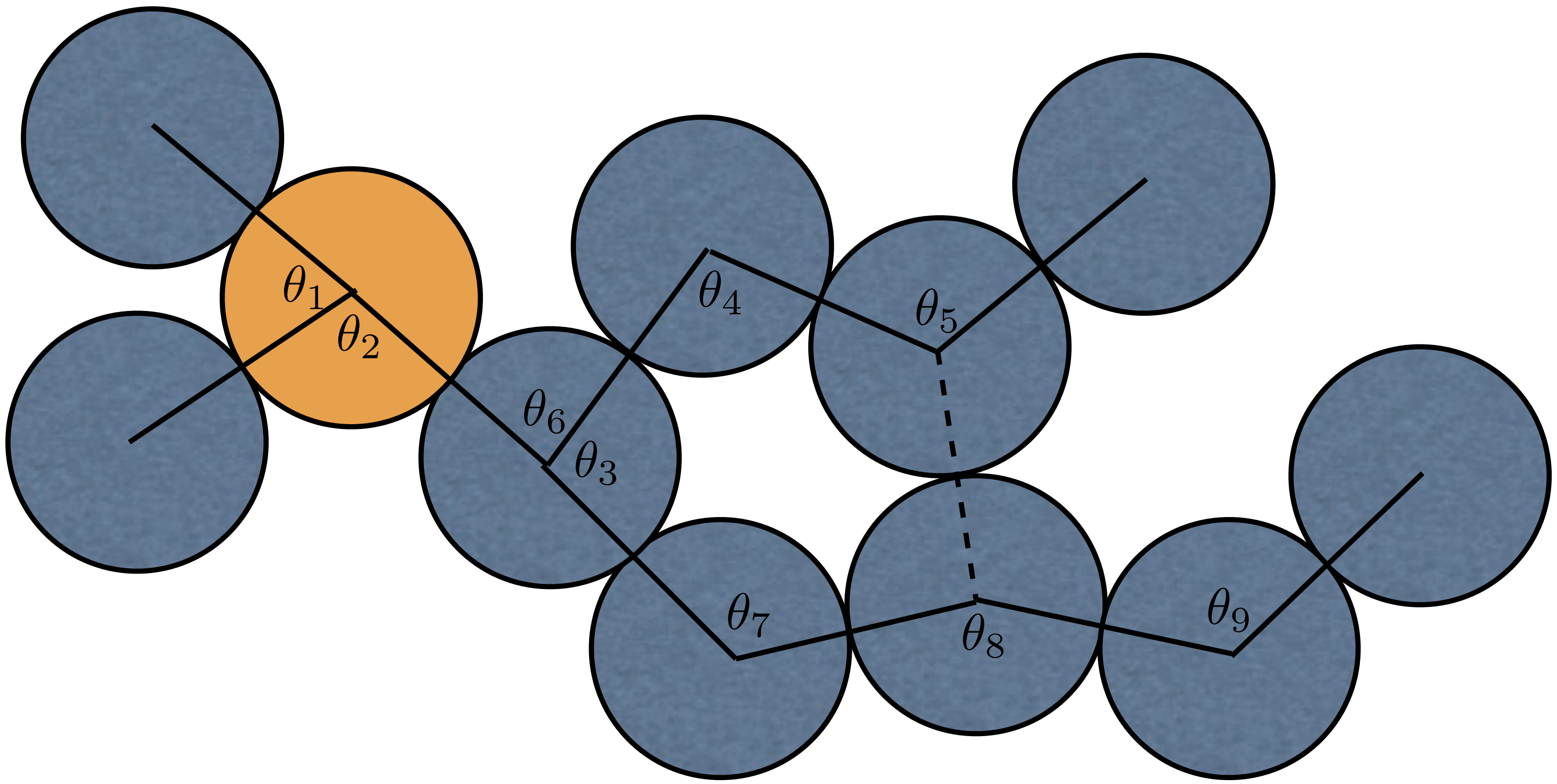

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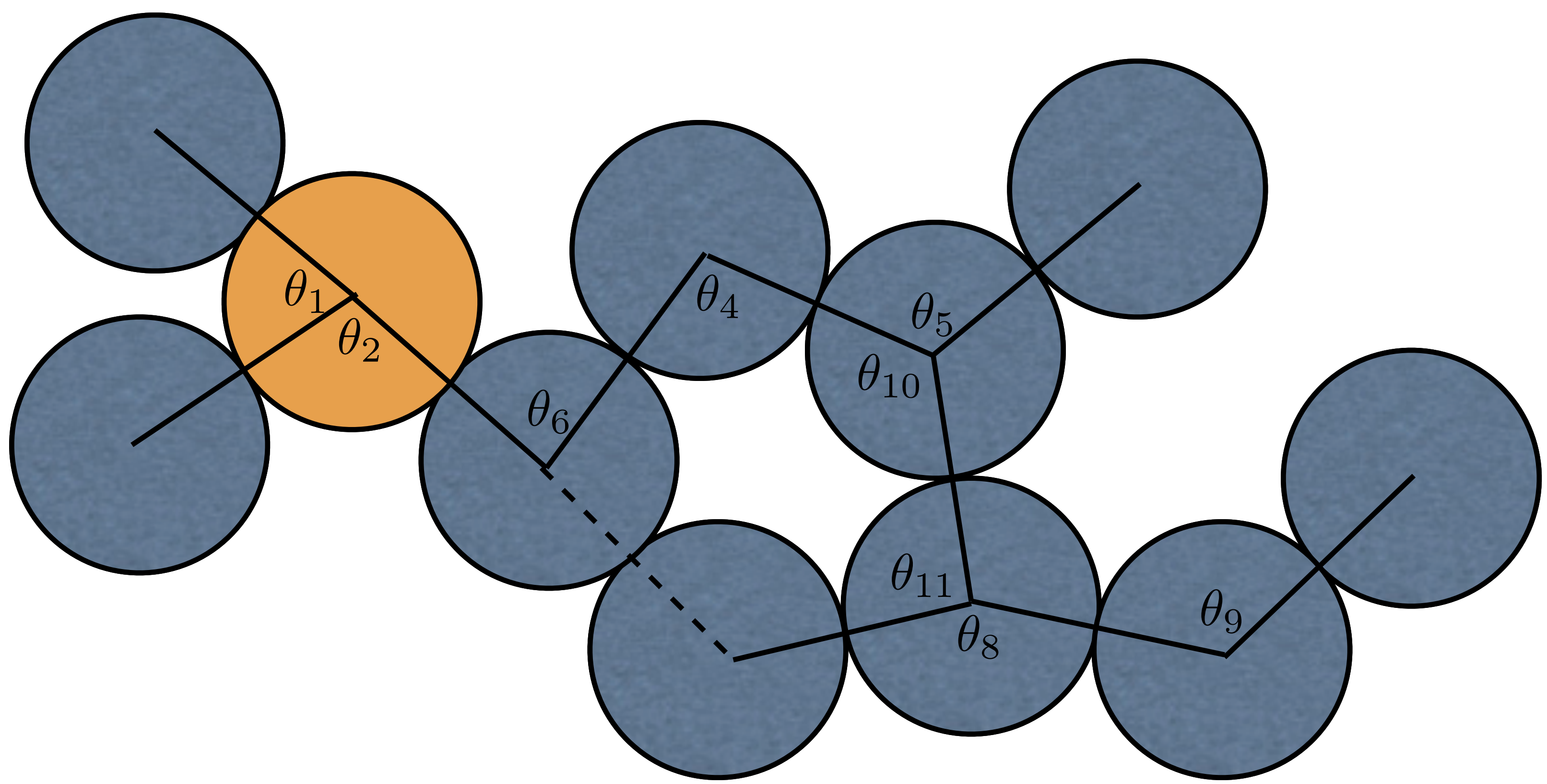

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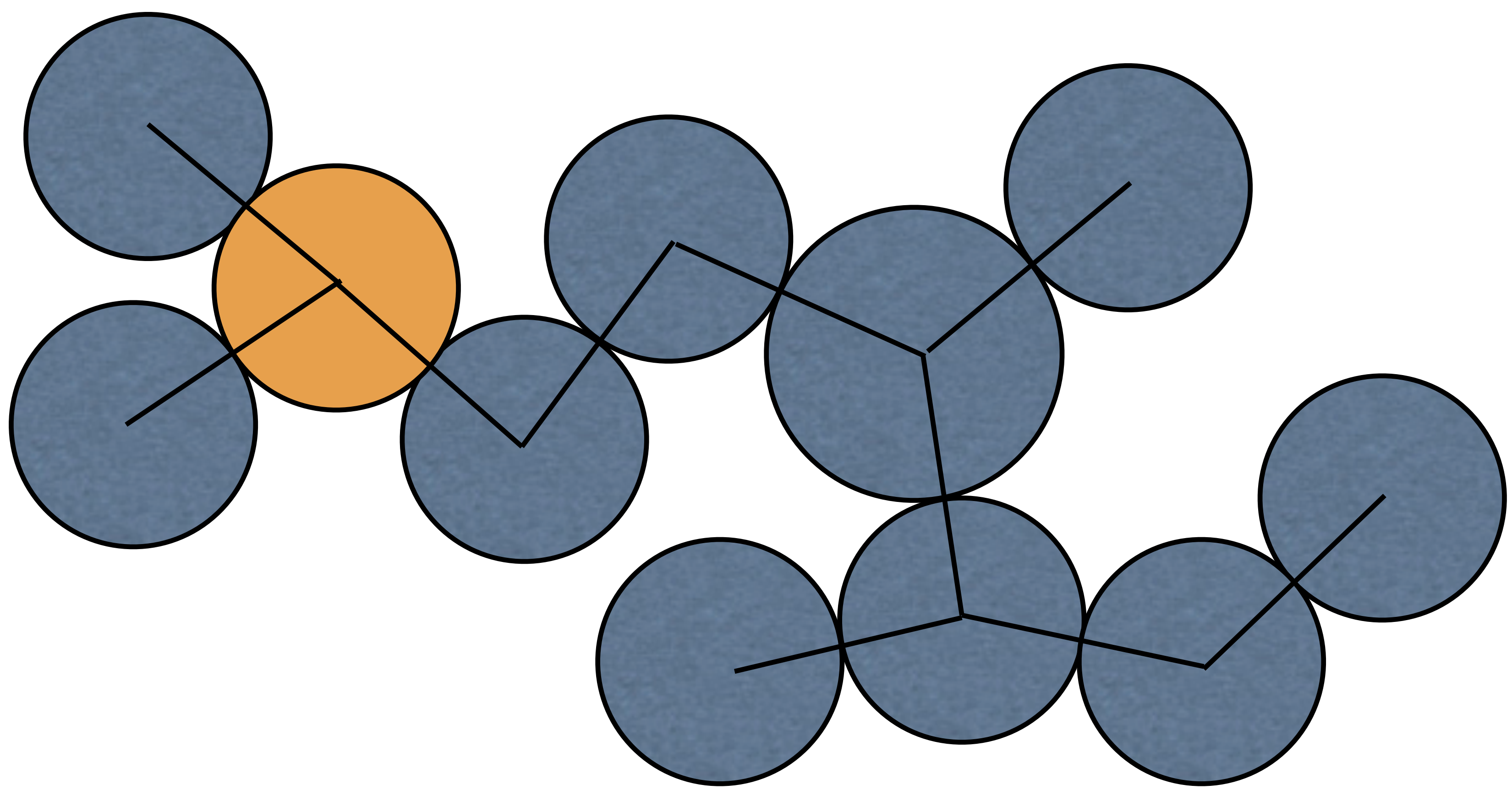

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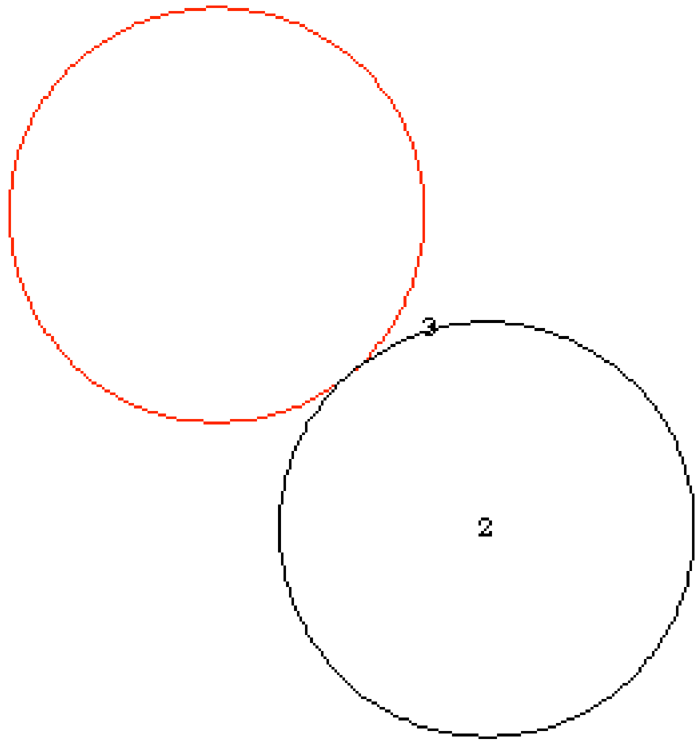
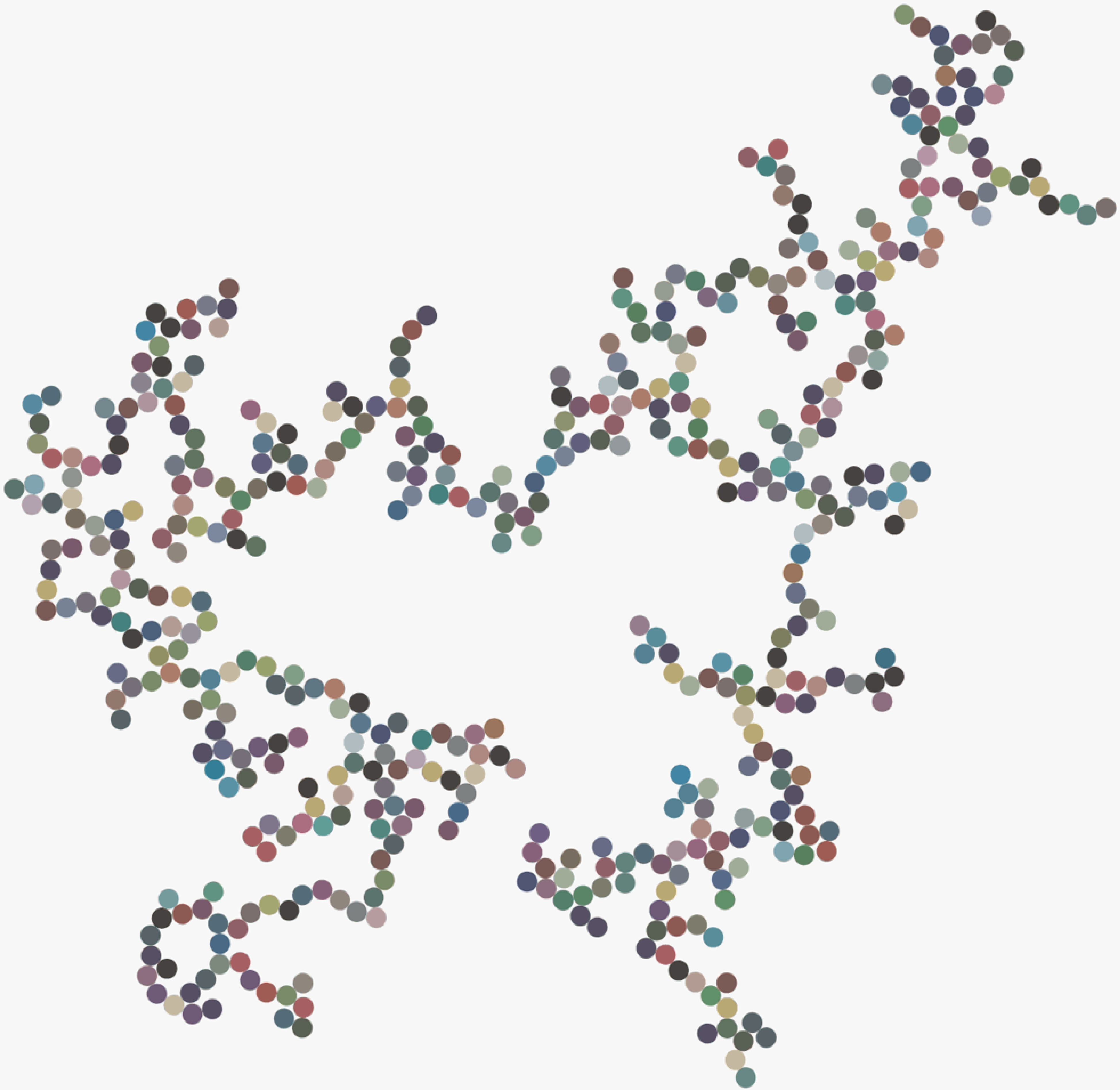
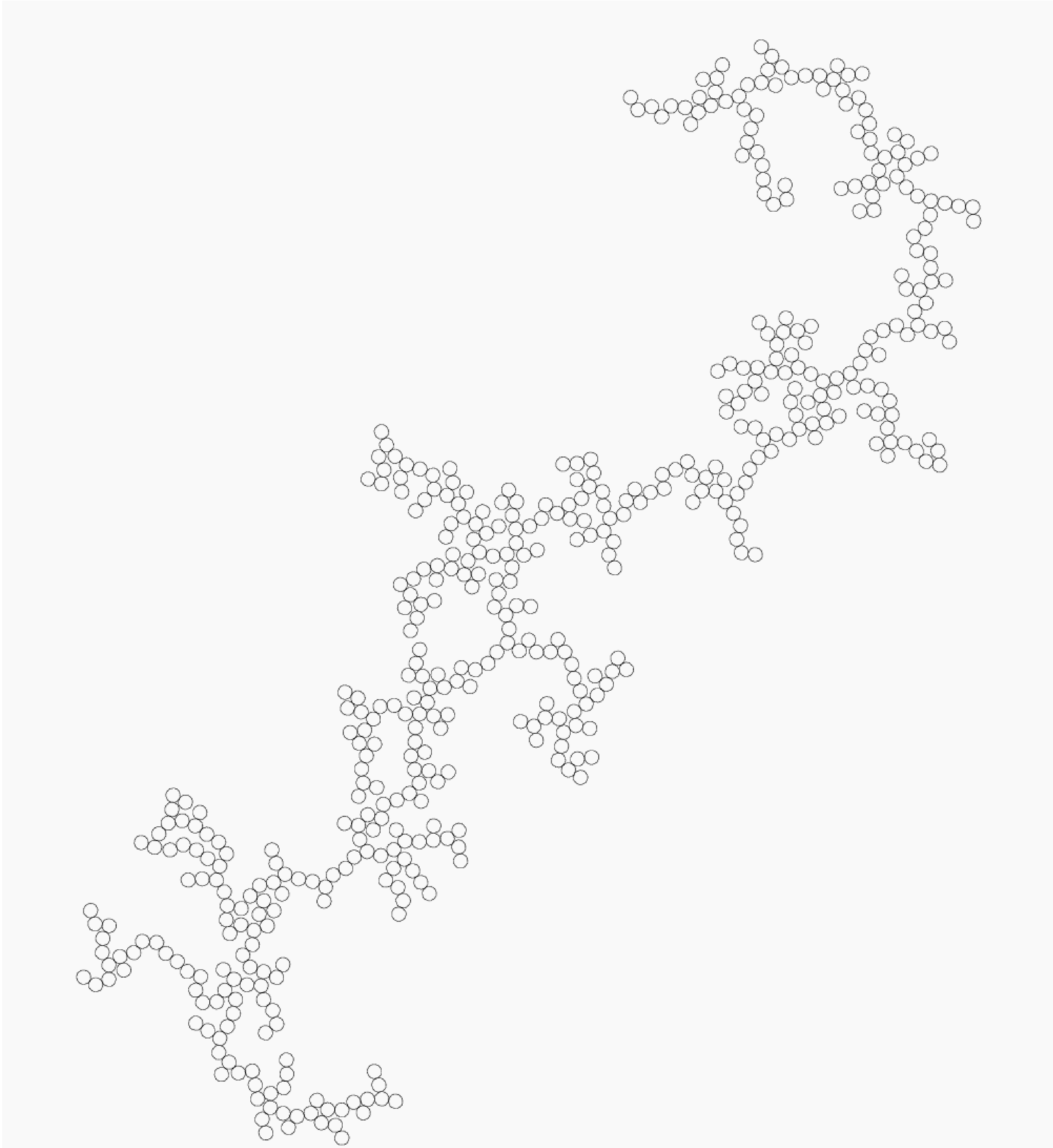
Perfect simulation of a $2D$ branched polymer.







Branched polymers in $3D$

Invariance Lemma in $3D$

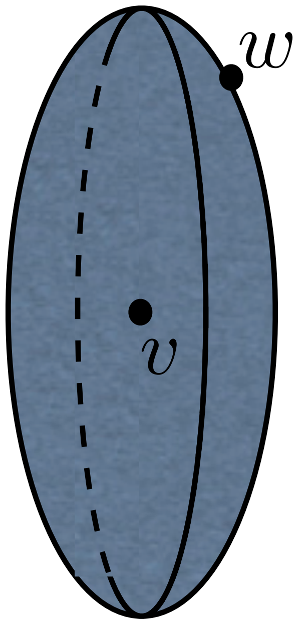
The volume of X_n doesn't change when you change the interactions as indicated below.

Instead of $\|v - w\| \geq 2$

we have

$$(v_x - w_x)^2 + \beta(v_y - w_y)^2 + \beta(v_z - w_z)^2 \geq 2$$

(w lies outside a certain ellipsoid centered at v.)



we can have a different β for each pair of points.

We can take $\beta_i = \epsilon^{-i}$. cigar-shaped hard-core repulsion
(Then as $\epsilon \to 0$, no interaction.)

Another key observation: the spherical measure on S^2 (or surface area measure on one of these ellipsoids) projects to uniform Lebesgue measure on a segment in the x-direction. (Archimedes)

Now project the ball centers to the x-axis:

$$x_1 < x_2 < x_3 < \cdots < x_n.$$

Lemma: The volume of the set of $3DBP$s 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: Use the invariance principle. □

e.g. if $|x_n - x_1| < 1$, $n_i = i - 1$ and volume is $(2\pi)^{n-1}(n-1)!$
(This is a $2DBP$ in disguise!)

e.g. maximally spread case: $x_{i+2} - x_i > 1$ for all i.
$n_i = 1$ and volume is $(2\pi)^{n-1}$.

Question: when we project the points of a $3DBP$,
what is their distribution?

Answer:

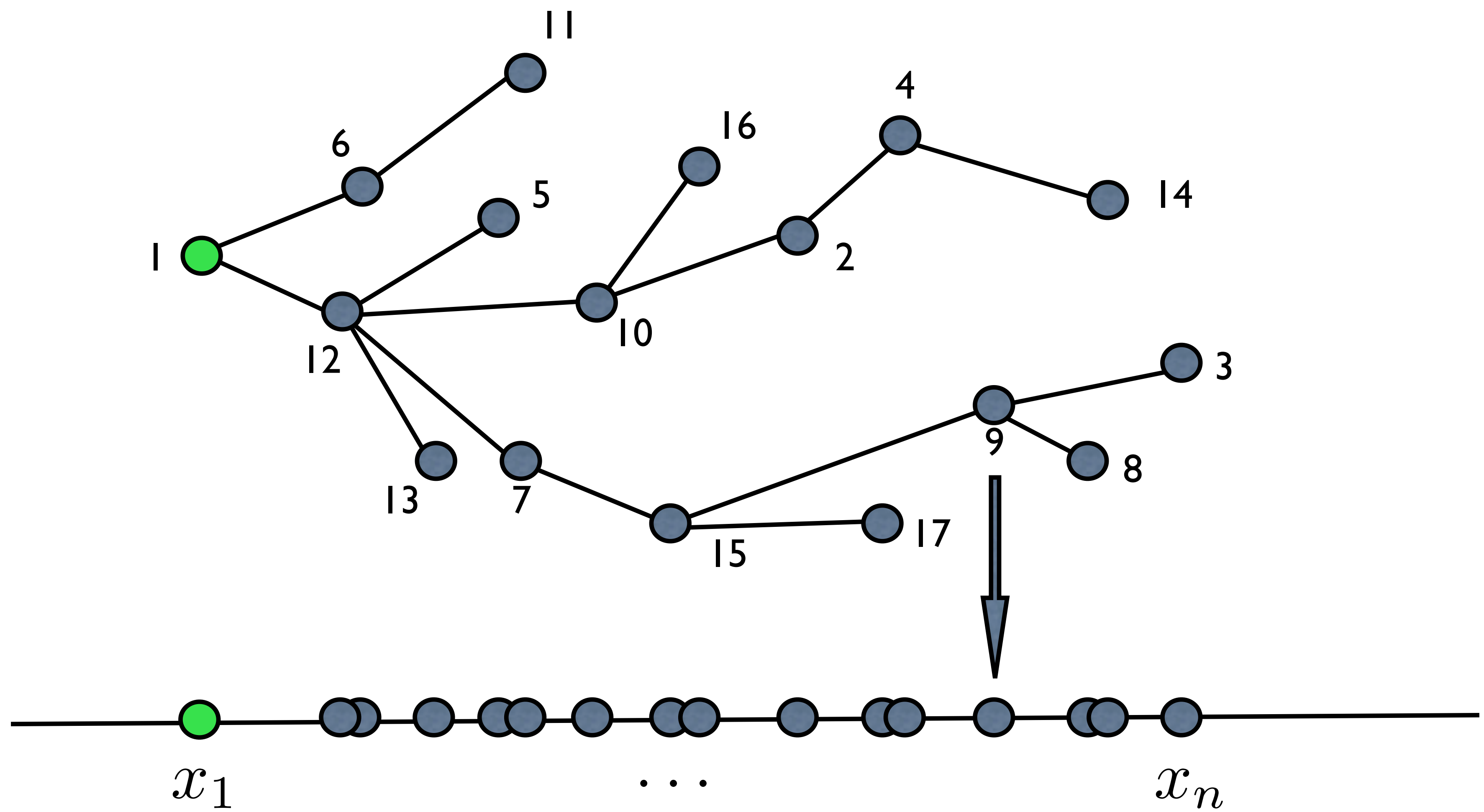
(1) Construct a random labelled tree on n vertices.

(2) Assign a uniform [0,1] length to each edge, independently.

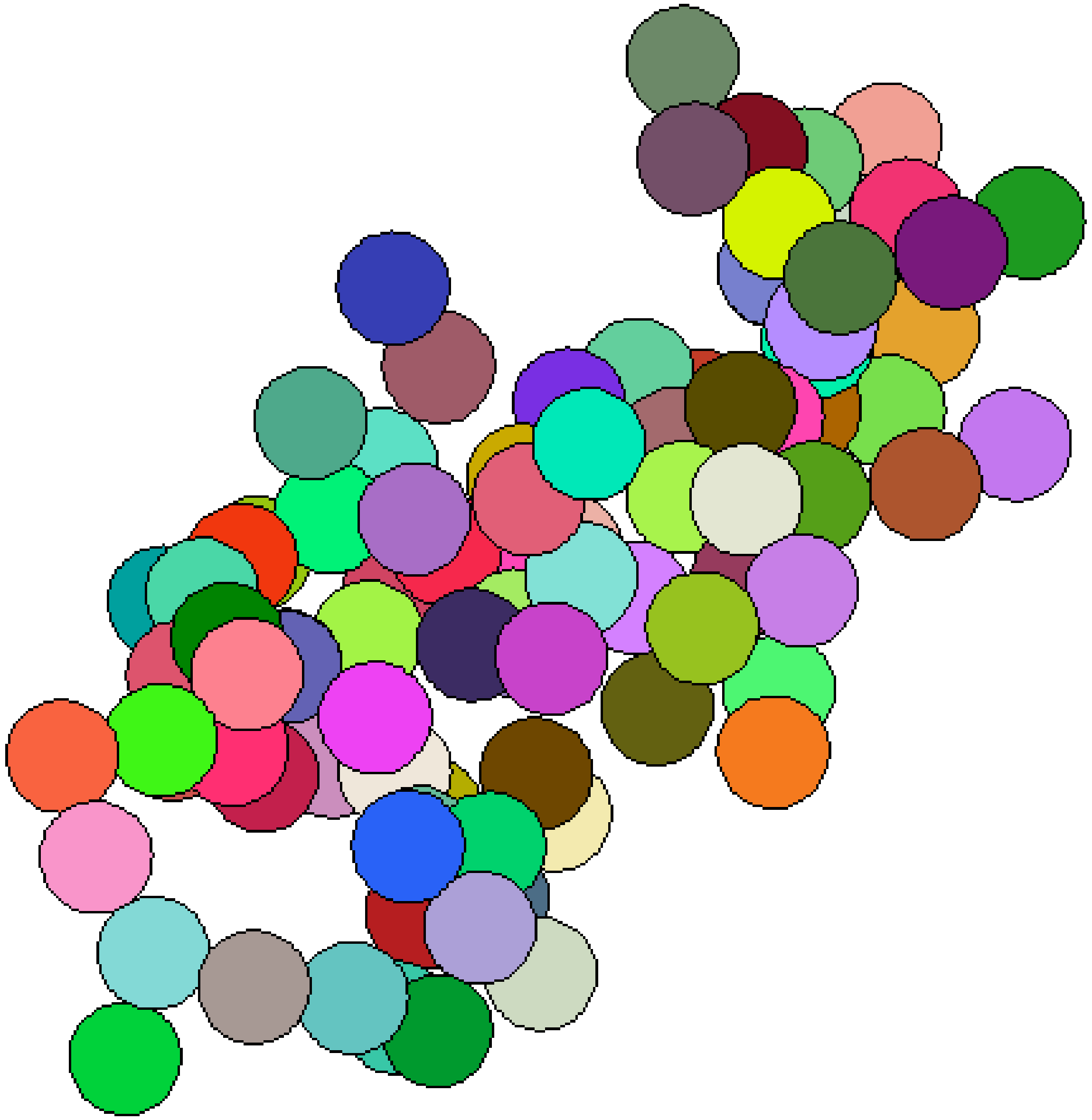
(3) Dangle the tree from the root.

(4) Let x_i be the distance of the ith 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 $\sqrt{n}$.

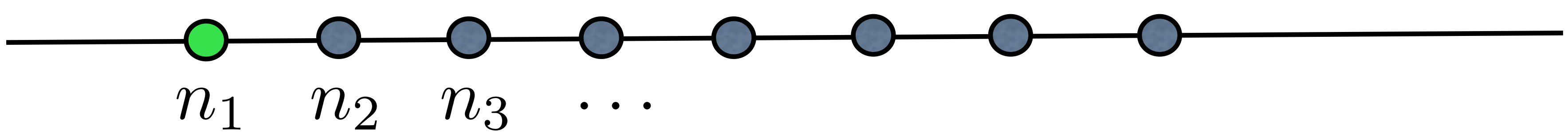


Theorem proof idea.

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

Consider a simpler case: projected points lie in $\frac{1}{2}\mathbb{Z}$.

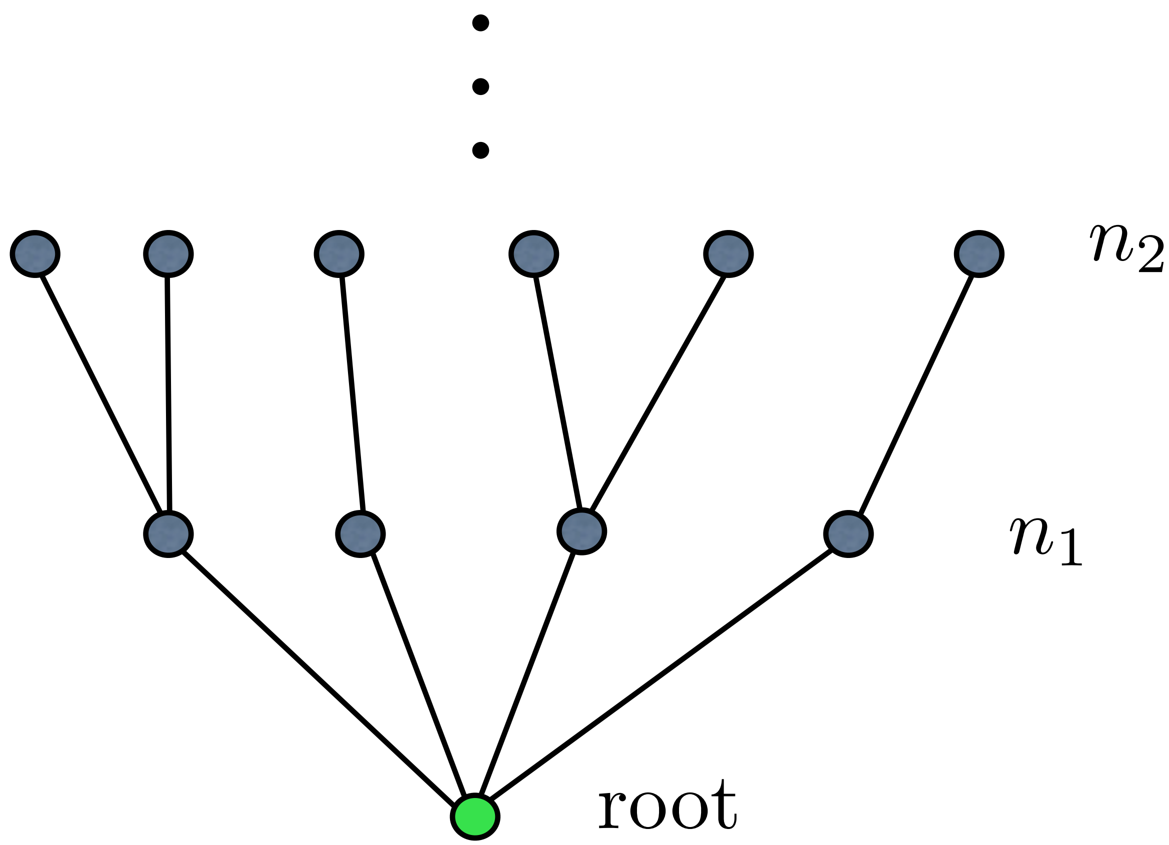
n_1 points project to 0,
n_2 points project to $\frac{1}{2}$, etc.



$$\# \text{ preimages} = \frac{(n_1+n_2-1)!}{(n_2-1)!} \frac{(n_2+n_3-1)!}{(n_3-1)!} \cdots \frac{(n_{k-1}+n_k-1)!}{(n_k-1)!} \frac{(n_k-1)!}{1}$$

$$(\# \text{ preimage}) \times (\text{volume}) = \binom{n_1+n_2-1}{n_2-1} \binom{n_2+n_3-1}{n_3-1} \cdots \binom{n_{k-1}+n_k-1}{n_k-1} \frac{1}{n_k}$$

This quantity also counts rooted planar trees with n_i vertices at level i.


n_2
n_1
root

Open questions

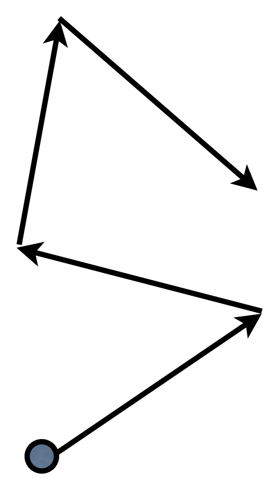
1. Dynamics on polymers

2. $4D$ polymers ($\approx$ 2D hard disk model).

3. Diameter of a 2DBP

A puzzle:

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



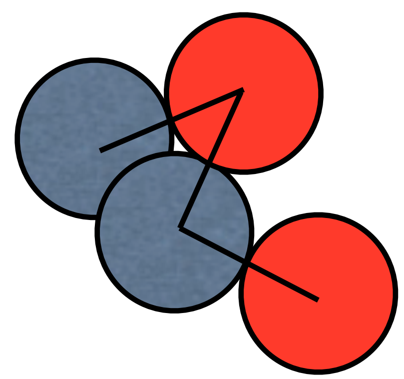
Show: probability that you are back within 1 of the origin is $\frac{1}{n+1}$.

What if you weaken the hard core interaction?

... Allow certain pairs of disks to overlap each other.

Define an "interaction" graph G: $v \sim v'$ if v and v' cannot overlap.

E.g. Two species of balls: blues & reds "Bipartite polymers"
(G is complete bipartite graph)



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.