A Stratification of the Space of Branched Polymers

Sara Billey
University of Washington

Combinatorics 2010:
Advances, Trends and Speculations
March 26, 2010

Outline

1. Background on Branched Polymers
2. Kenyon-Winkler Algorithm
3. Stratification of BP(n) / Rigidity Theory
4. Mészáros-Postnikov Theorem/Problem
5. Open Problems

New results and conjectures based on joint work with

- Dave Anderson (University of Washington)
- Tom Boothby, Morgan Eichwald, Chris Fox (REU 2009)

Branched Polymers

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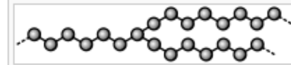
Branching (chemistry)

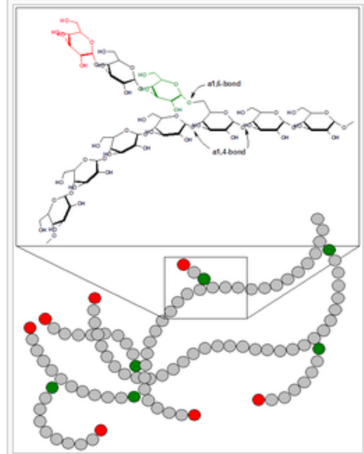
From Wikipedia, the free encyclopedia
(Redirected from Branched polymer)



Branch point in a polymer

In polymer chemistry, **branching** occurs by the replacement of a substituent, e.g., a hydrogen atom, on a monomer subunit, by another covalently bonded chain of that polymer; or, in the case of a graft copolymer, by a chain of another type. In crosslinking rubber by vulcanization, short sulfur branches link polyisoprene chains (or a synthetic variant) into a multiply-branched thermosetting elastomer. Rubber can also be so completely vulcanized that it becomes a rigid solid, so hard it can be used as the bit in a smoking pipe. Polycarbonate chains can be crosslinked to form the hardest, most impact-resistant thermosetting plastic, used in safety glasses.[1]

Branching may result from the formation of carbon-carbon or various other types of covalent bonds. Branching by ester and amide bonds is typically by a condensation reaction, producing one molecule of water (or HCl) for each bond formed.



Glycogen, a branched polysaccharide

Polymers which are branched but not crosslinked are generally thermoplastic. Branching sometimes occurs spontaneously during synthesis of polymers; e.g., by free-radical polymerization of ethylene to form polyethylene. In fact, preventing branching to produce linear polyethylene requires special methods. Because of the way polyamides are formed, nylon would seem to be limited to unbranched, straight chains. But "star" branched nylon can be produced by the condensation of dicarboxylic acids with polyamines having three or more amino groups. Branching also occurs naturally during enzymatically-catalyzed polymerization of glucose to form polysaccharides such as glycogen (animals), and amylopectin, a form of starch (plants). The unbranched form of starch is called amylose.

The ultimate in branching is a completely crosslinked network such as found in Bakelite, a phenol-formaldehyde thermoset resin.

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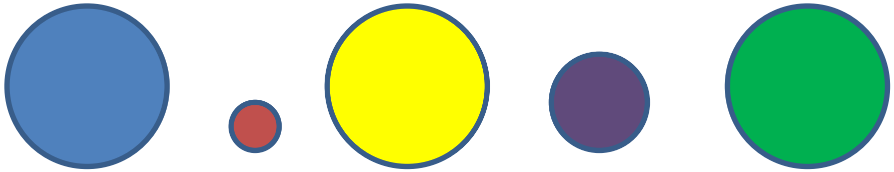
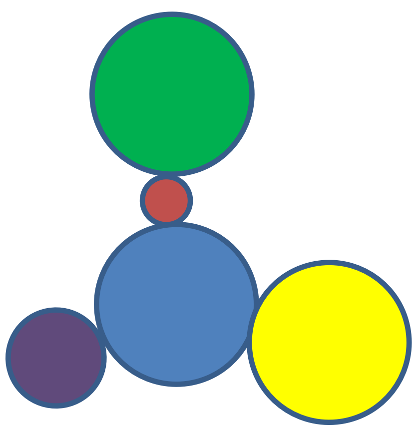
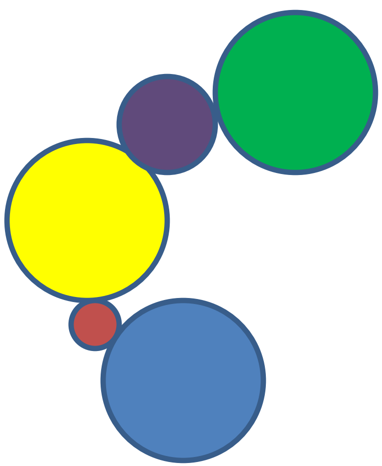
Modeling Branched Polymers

Given n labeled disks 

a branched polymer of order n is a placement of the disks in the plane such that

- Disk 1 has its center at (**0,0**)
- The union forms a connected subset of the plane
- No two disks overlap.

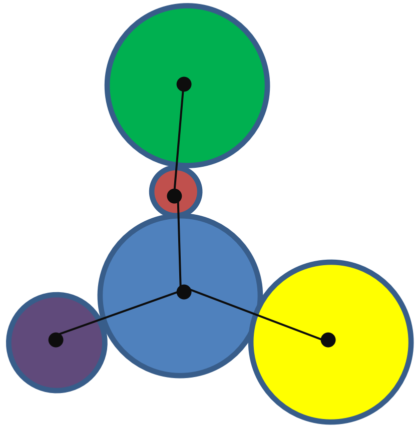




Embedding Branched Polymers

Notation:

- $R=(r_1,r_2,\ldots,r_n)$=list of radii for disks 1,2,…,n
- $BP_{\boldsymbol{R}}(n)$= branched polymers of order n.
- TG(P) = tangency graph of polymer P



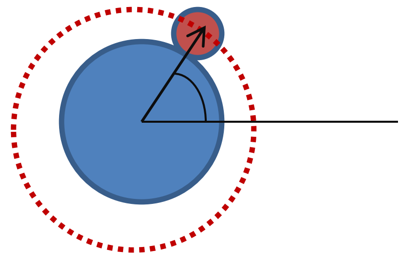
Two embeddings of $BP_{\boldsymbol{R}}$:

a) $BP_{\boldsymbol{R}}(n) \longrightarrow \mathbf{C}^n$ list centers of disks as complex numbers

b) $BP_{\boldsymbol{R}}(n) \longrightarrow \bigcup_T \mathbf{S}^{n-1}$ union over all labeled trees of order n

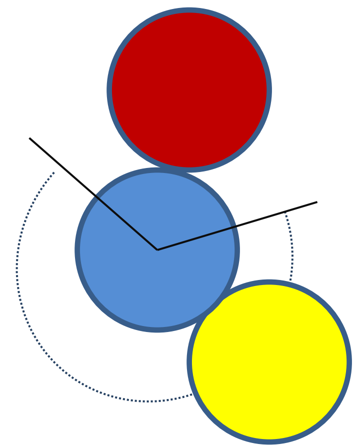
record angles of attachment from each disk to its parent.

Volume of $BP_R(n)$



Example: 2 disks

$\mathrm{vol}(BP_R(2)) = 2\pi$



Example: 3 disks, $R=(1,1,1)$

$\mathrm{vol}(BP_R(3)) = 3\ (4/3\ \pi)\ 2\pi$

$= 2\ (2\ \pi)^2$

Example: 3 disks, $R=(1,\varepsilon,\varepsilon)$

$\mathrm{vol}(BP_R(3)) = (2\pi)^2 + ½\ (2\ \pi)^2 + ½(2\pi)^2$

$= 2\ (2\ \pi)^2$

Volume of $BP_R(n)$

Theorem (Brydges-Imbrie) For any choice of radii, the space of branched polymers has volume

$$(n-1)!\,(2\pi)^{n-1}$$

Theorem (Brydges-Imbrie) The space of 3-dimensional branched polymers has volume

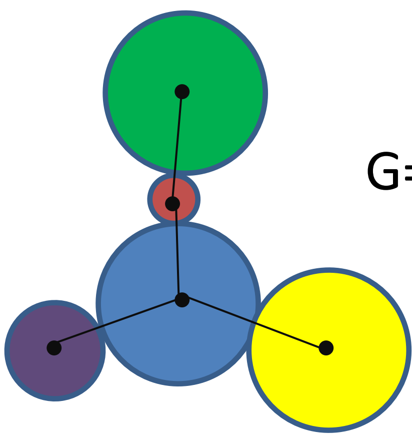
$$n^{n-1}(2\pi)^{n-1}$$

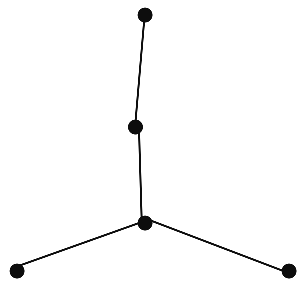
See also **"**Branched polymers" by Richard Kenyon and Peter Winkler, Amer. Math. Monthly **116** (2009).

Stratifying $BP_R(n)$

Def: Given any graph G with n nodes, let

$$BP_R(G) := \{ P \in BP_R(n) : TG(P) = G \}$$

P = 

G= 

$\Rightarrow$ $P \in BP_R(G)$

Facts: $BP_R(n) = \bigcup BP_R(G)$ union over all labeled graphs G with n nodes. The boundary of $BP_R(n)$ consists of all $BP_R(G)$ where G has at least one cycle.

Volume of each strata

Open Problem: Given radii $R=(r_1,r_2,\ldots,r_n)$, what is $vol(BP_R(T))$ for any labeled tree T of order n?

Note: $vol(BP_R(G)) = 0$ if G contains a cycle.

Question: How can we approximate the volumes for the $vol(BP_R(T))$'s ?

Kenyon-Winkler Algorithm

Input: $R = (r_1, r_2, \ldots, r_n)$

Output: uniformly chosen branched polymer of order n

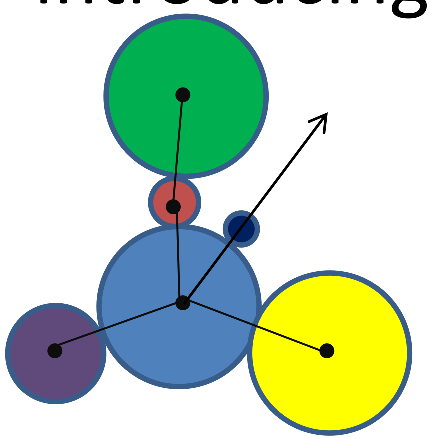
Start: Place disk 1 centered at origin.

Loop: For each j>1,

- Choose an integer $i \in [1,j)$ uniformly and a real number Φ in $[0, 2\pi)$ uniformly.
- Place a new disk labeled j with radius 0 at the point on the boundary of disk i specified at the angle Φ.
- Begin to grow the radius of disk j.

Growing disk j

- Increase the radius of disk j while holding constant the tangency graph, the angle vector, and the center of disk 1 until either
  a) The radius reaches r_j
  b) Or collision occurs between two disks in the polymer introducing a cycle into TG(P).



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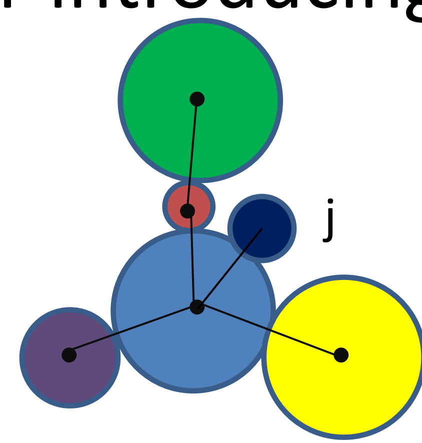

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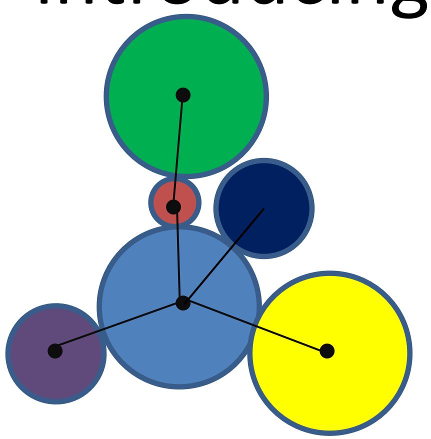

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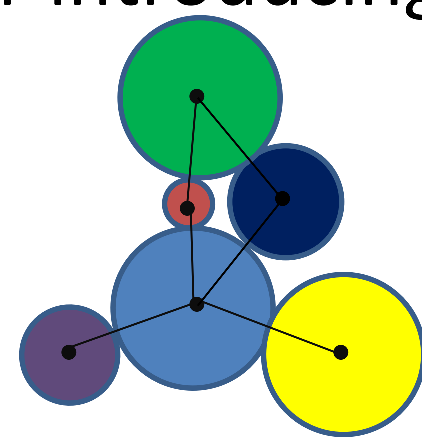
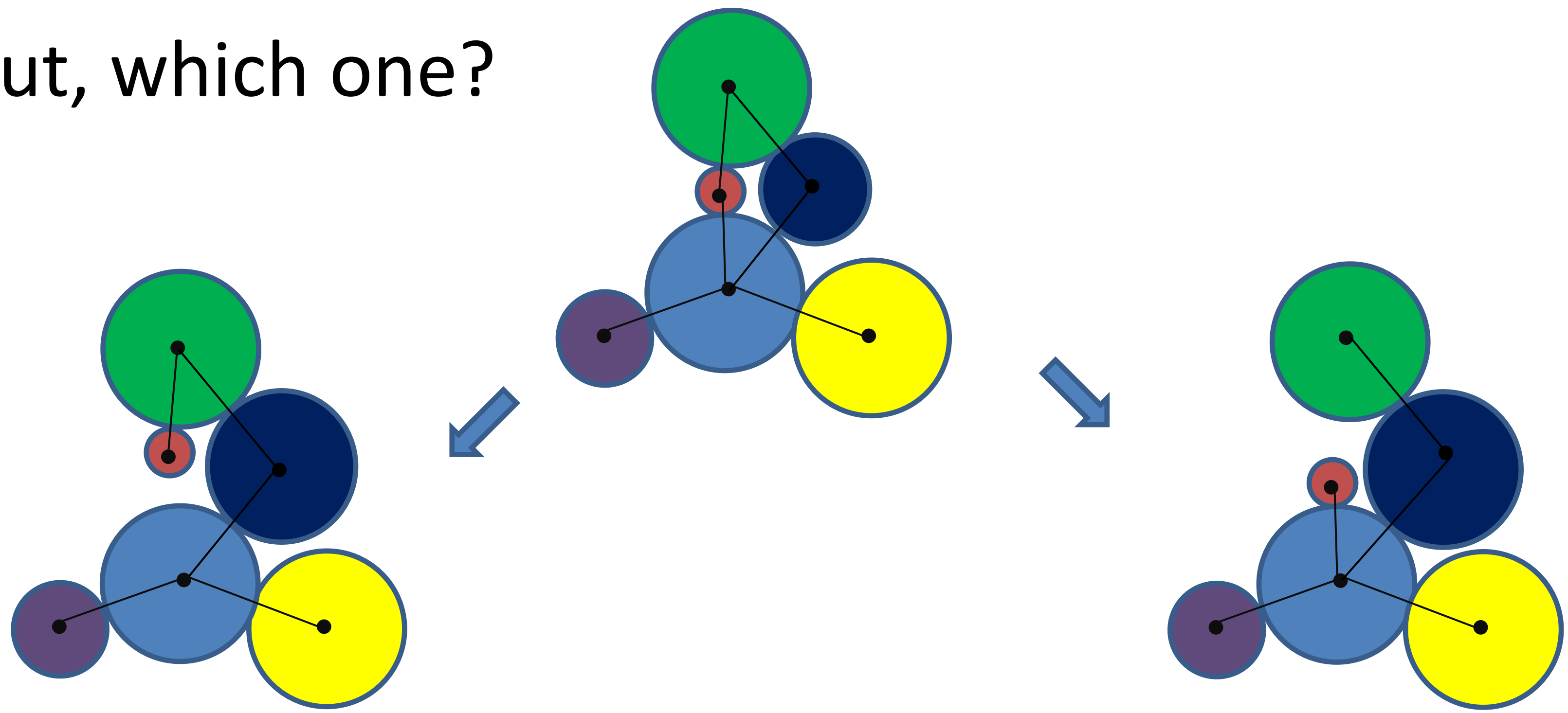


Choosing a spanning tree

If a cycle occurs while growing disk j, we must delete an edge from the tangency graph to continue growing without overlap.

But, which one?



Choosing a spanning tree

- Label the edges around the cycle $E_1,\ldots, E_k$ in counter clockwise order so that E_1 and E_2 meet at the center of disk j.
- T_i =tree obtained from TG(P) by removing E_i.
- Among all T_i such that locally vol(BP(T_i)) is increasing near P, choose with probability proportional to these positive volume forms.

Choosing a spanning tree

Miraculously, there is a very simple way to determine the relative local volume changes near P.

- Φ_i = angle of E_i measured from the positive horizontal axis.
- U=unit vector with angle $(\Phi_1 + \Phi_2)/2$.
- $w_i = (U \cdot E_i)$

v_1 is negative

Theorem (Kenyon-Winkler) Let v_i be the infinitesimal local volume change in $BP(T_i)$ near P due to a small increase in radius. Then

$$V=(v_1,\ldots,v_k) \text{ and } W = (w_1,\ldots,w_k)$$

only differ by a scalar multiple and v_1 is negative

Kenyon-Winkler Algorithm

Input: R= $(r_1,r_2,\ldots,r_n)$

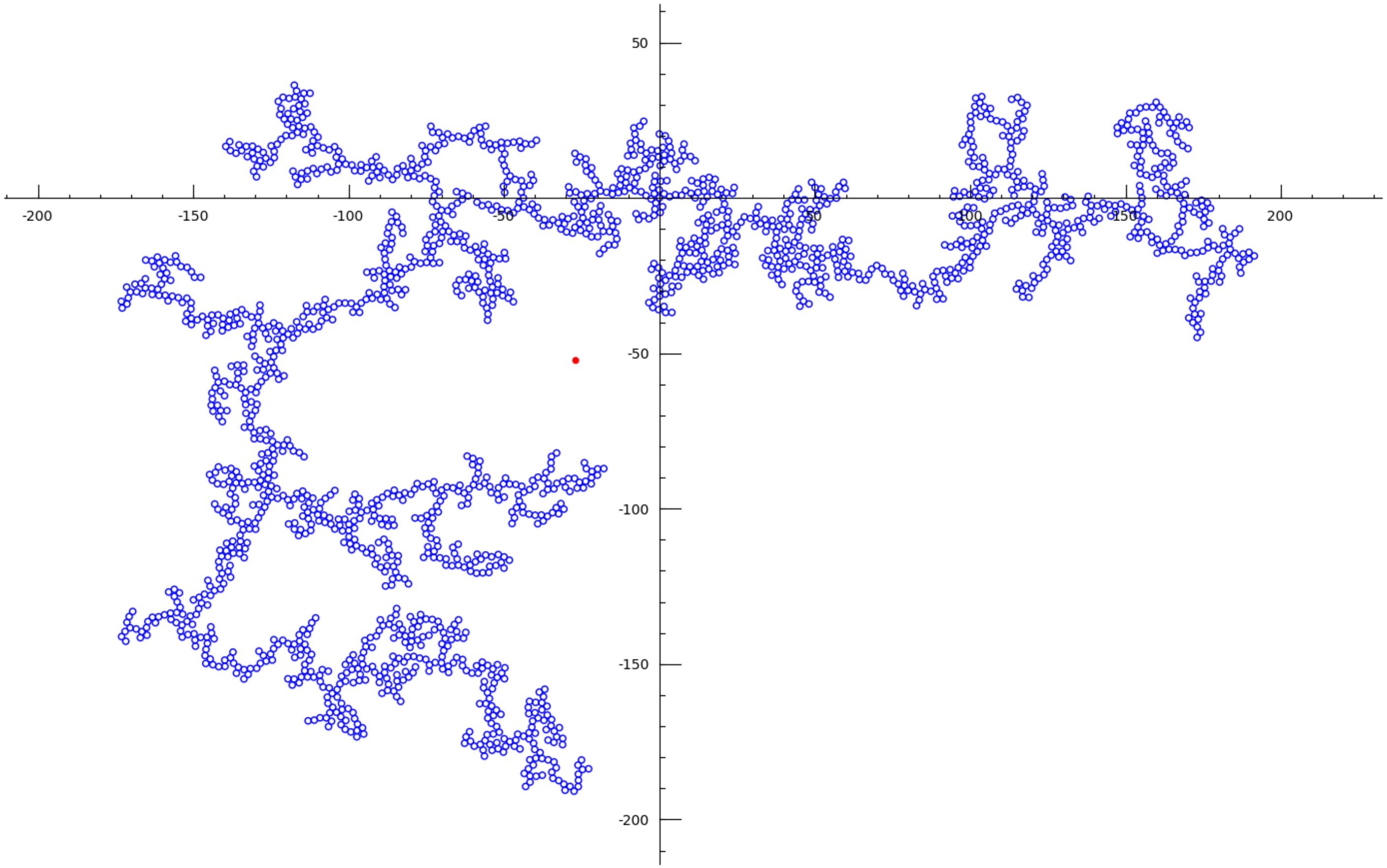
Output: uniformly chosen branched polymer of order n

Start: Place disk 1 centered at origin.

Loop: For each j>1,

- Choose an integer i $\in[1,j)$ uniformly and a real number Φ in $[0,2\pi)$ uniformly.
- Place a new disk labeled j with radius 0 at the point on the boundary of disk i specified at the angle Φ.
- Begin to grow the radius of disk j up to r_j. When a collision occurs, a cycle forms in the graph. Choose a spanning tree in proportion to the local changes in volume with respect to each tree.

Example 2000 disks



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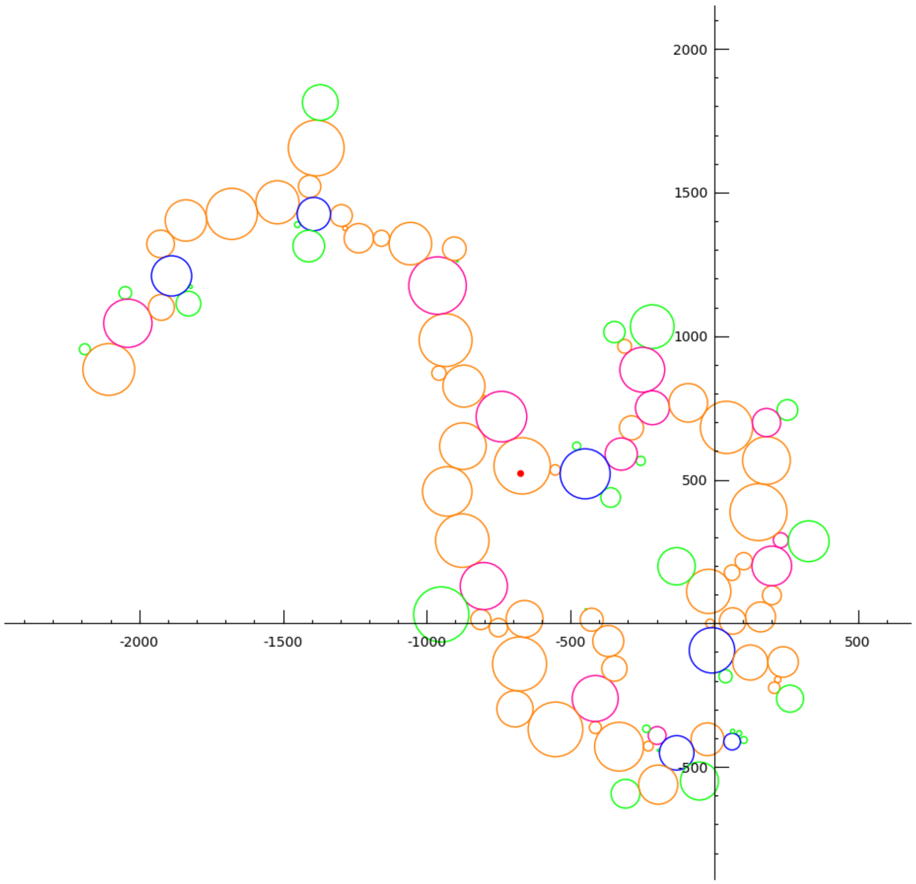
Example 100 disks



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Data Inspired Conjectures

Fix R=(1,1,…,1)

- Collected data approximating the frequency each tree up to order 10 occurs among uniformly chosen random branched polymers.
- Conjectured distribution on vertex degrees:

  [0.23, 0.56, 0.19, 0.011, 10^-5, 0]

- Conjectured relationship between diameter of T and expected diameter of P in BP(T).

Stratifying $BP_R(n)$

- $BP_R(G) := \{ P \in BP_R(n) : TG(P) = G \}$
- $BP_R(n) = \bigcup BP_R(G)$ (manifold with boundary)

Questions:

Could $BP_R(n)$ have a cell decomposition?

What does each $BP_R(G)$ look like?

What are the "points" in this stratification?

Rigid Graphs

What are the “points” in this stratification?

$$BP_R(G) = \overline{BP_R(G)} \quad \text{iff } \dim(BP_R(G))=1 \quad \text{iff}$$

The only continuous motions of the embedding of G which preserve edge lengths are rotations and translations.

$$\Updownarrow$$

Def: G is infinitesimally rigid.

Laman's Theorem

Theorem: G is minimally infinitesimally rigid for generic embeddings iff

$$\#E_G = 2\ \#V_G - 3$$

and for all subgraphs H of G, $\#E_H \leq 2\ \#V_H - 3$.

Note: Non-generic embeddings of a graph can exist which satisfy Laman's condition but aren't infinitesimally rigid!

Rigid Graphs

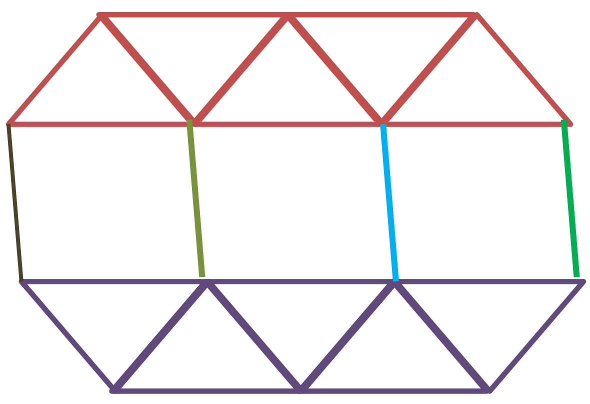
Application: We can use Laman's criterion to identify "points" in $BP_R(n)$.

Corollary: For generic radii, $\dim(BP_R(G)) = 1$ iff G contains a spanning subgraph satisfying Laman's condition.

Rigid Components

Question: What is $\dim(BP_R(G))$ in general?

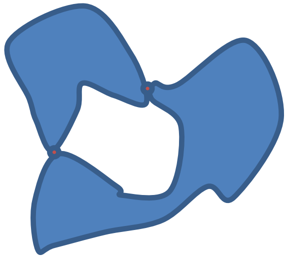
Def: H is a rigid component of G if H is infinitesimally rigid and no other rigid subgraph of G properly contains H.



Attachment Graph

Assume G has rigid components $C_1,\ldots,C_k$.

Note: Two rigid components share at most one vertex.



Def: A(G) = attachment graph

Init: $V = \{1,2,\ldots,k\}$ $E = \{ij: C_i, C_j \text{ overlap}\}$

Replace all cliques by spanning trees.

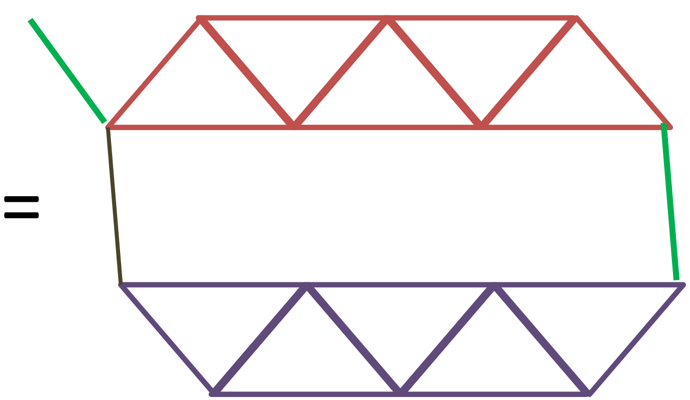
Example

Def: A(G) = attachment graph

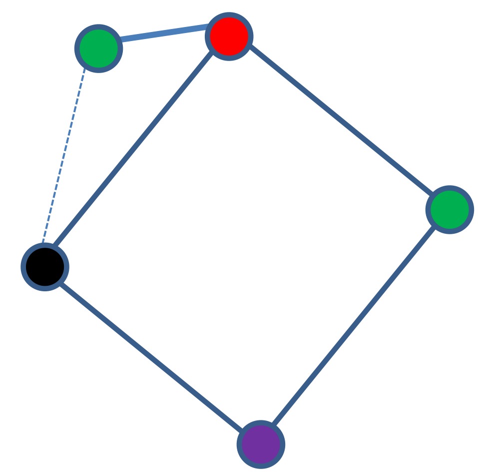
Init: $V = \{1,2,\ldots,k\}$ $E = \{ij: C_i, C_j \text{ overlap}\}$

Replace all cliques by spanning trees.

G=



A(G) =



Generic Dimension Formula

Theorem (Anderson-Billey): For generic radii, each connected component of $BP_R(G)$ is a manifold of dimension

$$\dim(BP_R(G)) = 3\,\#V_{A(G)} - 2\#E_{A(G)} - 2$$

$$= \#V_{A(G)} - 2\,\#\,(\text{bd faces } A(G)),$$

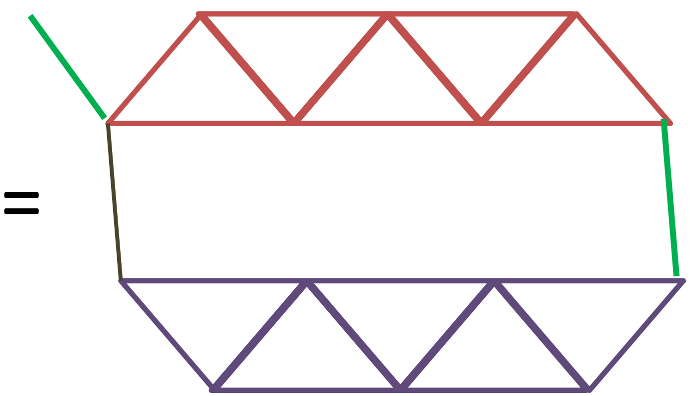
assuming the analogus dimension formula holds for each proper connected subgraph of A(G).

Example

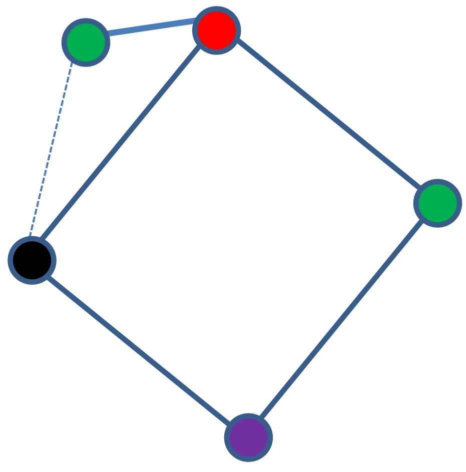
Here: dim(BP(G))= $\#V_{A(G)} - 2 \#$ (bd faces A(G))

$= 5 - 2*1 = 3.$

G=



A(G) =



Proof Outline

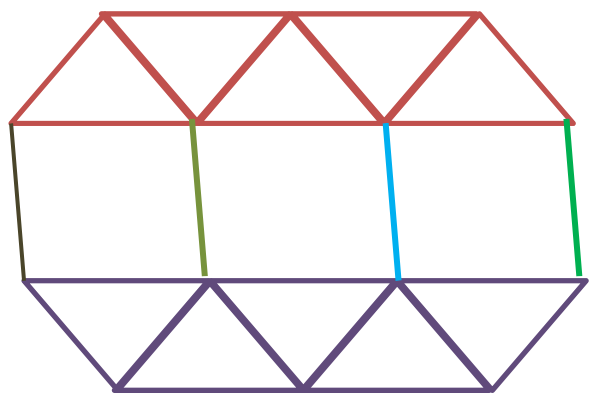
- Write equations for BP(G) in terms of translation and rotation of rigid components (3k variables).
- Each edge of A(G) defines 2 equations.
- Compute the Jacobian and apply Submersion Theorem.

General Dimension Formula

Theorem (Anderson-Billey): For all radii, $BP_R(G)$ is a variety of dimension

$$\dim(BP_R(G)) = 3\,\#V_{A(G)} - 2\#E_{A(G)} - 2 - \mathrm{corank}(\mathrm{Crit}J)$$

Example: take $R=(1,1,\ldots,1)$ and the tangency graph



Review

Stratifying $BP_R(n)$

- $BP_R(G) := \{ P \in BP_R(n) : TG(P) = G \}$
- $BP_R(n) = \bigcup BP_R(G)$

Questions:

What does each $BP_R(G)$ look like?

Answer: finite number of manifolds with given dimension determined by G (generically).

What are the “points” in this stratification?

Answer: BP(G)’s of dimension -- rigid graphs.

Mészáros-Postnikov Theorem

Mészáros-Postnikov (2009) give generalization of BP(n) using the theory of hyperplane arrangements.

Recall: Given n labeled disks with radii $r_1, \ldots, r_n$, a branched polymer is a placement of the disks in the plane such that

- ~~Disk 1 has its center at (**0,0**)~~
- ~~The union forms a connected subset of the plane~~
- No two disks overlap.

Braid arrangement to BP(n)

Braid arrangement: hyperplanes in V given by

$$h_{ij} = x_i - x_j = 0 \ \ \forall \ 1 \leq i < j \leq n$$

$$V = \mathbb{C}^n/(1,1 \dots ,1)$$

Branched polymers:

$$BP_n = \{x \in V\colon \ \left|h_{ij}(x)\right| \geq r_i + r_j\}$$

Generalized Polymers

Definition: For any central hyperplane arrangement A defined by linear forms h_i(x)=0 and real numbers r_i, define

$$BP_A = \{x \in \mathbb{C}^m : |h_i(x)| \geq r_i\}$$

Generalized Polymers

Theorem (Mészáros-Postnikov):
The q-volume of BP_A is $(-2\pi)^{rank\,A}\chi_A(-q)$
and the usual volume is obtained by setting q=0.

Theorem (M-P): BP_A & $C_A = \mathbb{C}^r \setminus \cup \{x\colon\ h_{i(x)} = 0\}$
have the same cohomology ring given by the Orlik-Solomon algebra.

Open (M-P): What is $H^*(BP_R(n))$?

Open Problems

1. What is $vol(BP_R(T))$? Open for $R=(1,1,\ldots,1)$.
2. Conjectured distribution on vertex degrees: $[0.23, 0.56, 0.19, 0.011, 10^{-5}, 0]$.
3. What is expected diameter of P in $BP_R(T)$?
4. Is $BP_R(G)$ contractible?
5. What is $H^*(BP_R(n))$?

   -- See (Mészáros-Postnikov hyperplane arr.)