REU PROJECT ON BRANCH POLYMERS

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1. Introduction

Fix a set of labeled disks $\{D_1, D_2, \ldots, D_n\}$ with radii $r_1, r_2, \ldots, r_n$ respectively. A *branched polymer of order* n in $\mathbb{R}^2$ is obtained by placing these disks in the plane in any configuration so that the disks form a connected subset of the plane, their interiors are disjoint, and D_1 is centered at the origin. Branched polymers have been studied in connection with molecular chemistry, statistical physics, random graphs, and geometry [1, 2, 3, 4, 5]. By a beautiful result of Brydges and Imbrie, the volume of the space of all possible branched polymers of order n in the plane is $(n-1)!(2\pi)^{n-1}$ [1]. Observe this result implies that the volume is independent of the specified radii. Kenyon and Winkler have recently provided a more elementary proof of this result [6]. In addition, Kenyon and Winkler give a recursive algorithm to grow branched polymers in the plane uniformly at random. In this REU, we implemented the Kenyon-Winkler algorithm and used it to examine some of the properties of branched polymers in the plane pertaining to abstract graph properties exhibited by the polymers. Several specific conjectures follow after we introduce the key concepts and notation following [6].

2. Background

Let X be a branched polymer of order n in the plane. We can associate to X a graph $G(X)$ with vertices $\{1, 2, \ldots, n\}$ and edges between two vertices if the associated disks are touching in the plane. $G(X)$ is connected since X is connected. Note that we sometimes informally refer to X as if it were the graph $G(X)$ and to the disks in X as they were the vertices of $G(X)$. Let T be any spanning tree for G. Consider T to be rooted at vertex 1. Then X can be encoded by the labeled tree T and an $(n-1)$-tuple of angles $\theta_i \in [0, 2\pi)$ for $2 \leq i \leq n$. First, D_1 is placed with its center at the origin. Then recursively stepping down the branches of T, if i is the parent of vertex j in T, then the angle θ_j determines the point on the boundary of D_i which is touching

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D_j as measured with respect to the positive horizontal ray through the center of D_i.

Given any labeled tree T of order n, let $BP_R(T)$ be the set of branched polymers with radii $R = (r_1, \ldots, r_n)$ such that the corresponding graph contains T as a subgraph. By the encoding above we see that $BP_R(T)$ is in bijective correspondence with a subset of $[0, 2\pi)^{n-1} = (S^1)^{n-1}$. In fact, $BP_R(T)$ corresponds with a manifold with boundary given by the subset of polymers whose graph strictly contains T [6]. The space of all branched polymers of order n with radii R, denoted $BP_R(n)$, is the union of the $BP_R(T)$ over all labeled trees of order n.

3. Kenyon-Winkler Simulation Algorithm

While it is easy to determine if a particular configuration of disks is a branched polymer, it is not obvious how to construct one uniformly at random. Given a particular tree T, not all angle vectors in $(S^1)^{n-1}$ will lead to valid branched polymers. The probability that a polymer chosen uniformly has a fixed tree T as a spanning subgraph of $G(X)$ changes with the radius vector R, in contrast to the invariance of volume for $BP_R(n)$. Below we describe the algorithm due to Kenyon and Winkler to "grow" a polymer $X \in BP_R(n)$ uniformly at random.

Before growing a polymer of order n, fix a radius vector $(r_1, \ldots, r_n)$ that will determine the final radius of each disk grown. Begin by placing D_1 with radius r_1 centered at the origin. For each $1 \leq i \leq n-1$, given a branched polymer of order i with radii $r_1, \ldots, r_i$, grow a polymer of order $i+1$ by means of the following steps:

(1) Choose an integer $j \in [1, i]$ uniformly and a real number $\theta \in [0, 2\pi)$ uniformly. Place a new disk D_{i+1} with radius 0 at the point on the boundary of D_j specified by the angle θ as measured from the positive x-axis through the center of D_j. Almost surely, D_{i+1} does not lie on the boundary of a disk other than D_j, since there are only a finite number of disks already adjacent to D_j.

(2) Increase the radius of D_{i+1} while holding constant $G(X)$, the accompanying angle vector $(\theta_2, \ldots, \theta_{i+1})$, and the position of D_1 until either the radius reaches r_{i+1}, in which case a new order $i+1$ polymer is generated as desired, or a collision occurs between two disks in the polymer at some positive radius $r < r_{i+1}$, introducing a cycle C into $G(X)$. (We refer to collisions between arbitrary disks in the polymer because, as the algorithm progresses, growing the radius of D_{i+1} may push two

other disks together.) If a collision occurs, proceed to the next step.

(3) The new disk cannot continue to grow as it did in the previous step without some pair of disks in the polymer overlapping. In order to allow D_{i+1} to continue growing, "remove" one of the edges in the cycle C, that is, choose a spanning tree of $G(X)$ to encode X and continue to grow D_{i+1} while holding constant the angles corresponding to the remaining edges and the position of D_1. Choosing which edge to remove is the key step in the algorithm in order to insure the final polymer comes from the uniform distribution. An edge will be deleted according to the probability distribution described in Section 3.1. After breaking the cycle, return to the previous step.

The algorithm is finished when each disk in turn has grown to its specified radius.

3.1. **Breaking Cycles.** Let X_r be the polymer obtained in the growth process where D_{i+1} has grown to radius $r < r_{i+1}$ and $G(X_r)$ contains a cycle. The cycle necessarily contains D_{i+1}. Let T be the graph $G(X_{r-\epsilon})$, just before the collision at radius r for some small $\epsilon > 0$. With probability 1, we can assume T is a tree and $G(X_r)$ is a graph with exactly one cycle. According to [6], the graphs with cycles only occur on the boundary of $BP_R(T)$ and graphs with multiple cycles only occur in codimension 2. The cycle C in $G(X_r)$ corresponds with a polygon P inscribed in the plane with vertices given by the centers of the disks in C.

Label the edges of the polygon P in counter clockwise order: say $E_1, E_2, \ldots, E_m$ so that D_{i+1} is centered at the vertex between edges E_1 and E_2. We think of the E_i's both as edges and as vectors in the plane so as vectors $E_1 + E_2 + \cdots + E_m = 0$.

Let T_i be the tree obtained from $G(X_r)$ by removing edge E_i. X_r now lies in the boundary of each submanifold $BP_{R'}(T_i)$ where $R' = (r_1, \ldots, r_i, r)$. For some of these trees, the corresponding local submanifold near X_r loses volume as r increases, whereas for others it gains volume.

From the proof of the Invariance Lemma [6, Sect. 5], we know that, given an infinitesimal increase in r, the local volume changes near X_r in each $BP_{R'}(T_i)$ sum to zero. One can observe that the local volume near X_r is necessarily decreasing for both $BP_{R'}(T_1)$ and $BP_{R'}(T_2)$ by our choice of labeling. Thus there must be at least one T_i for which the volume change is positive as r increases. In order to preserve uniform measure, we must choose among the trees with positive volume change according to a distribution that weights the trees according to the magnitude of their respective local volume changes.

Miraculously, there is a very simple way to determine the relative local volume changes near X_r. Let ϕ_i be the angle associated with E_i measured from the positive horizontal axis. Let U be the unit vector with angle $\frac{(\phi_1+\phi_2)}{2}$. Let $w_i = (U \cdot E_i)$, the dot product of U with E_i for $1 \leq i \leq m$.

Proposition 3.1. [6, Prop. 10] *Using the notation above, let v_i be the infinitesimal local volume change in $BP_{R'}(T_i)$ near X_r due to a small increase in r. Then v_1 is negative, and the vectors $V = (v_1, \ldots, v_m)$ and $W = (w_1, \ldots, w_m)$ only differ by a scalar multiple.*

From Proposition 3.1, we see that the positive infinitesimal volumes v_i are indexed by the positions of the positive values in the vector $X = (-w_1)W = (x_1, \ldots, x_m)$, a scaled multiple of W. Let $S = \sum_{x_i>0} x_i$. For $1 \leq i \leq m$, let

$$p_i = \begin{cases} \frac{x_i}{S} & \text{if } x_i > 0 \\ 0 & \text{if } x_i \leq 0. \end{cases}$$

Now we return to the algorithm for growing the radius of D_{i+1} in X_r. The p_i's determine a discrete probability distribution function on the edges $E_1, \ldots, E_m$ in the cycle of $G(X_r)$ containing D_{i+1}. Choose a number $1 \leq k \leq m$ according to the distribution $(p_1, \ldots, p_m)$. Delete edge k from $G(X_r)$. By construction, $X_r \in BP_{R'}(T_k)$ and increasing r slightly will move X_r into the interior of $BP_{R'}(T_k)$.

3.2. **Detecting Collisions.** There are two types of collisions possible: collisions between D_{i+1} and another disk, and collisions in which neither disk is D_{i+1}. In each case, we can easily solve for the smallest positive value of the radius of D_{i+1} such that a collision occurs. The analysis is simplified by holding the center of D_{i+1} fixed at the origin rather than holding the center of D_1 fixed and determining the location of all other disks by taking $i+1$ to be the root of tree T.

Detection of D_{i+1}-branch collisions. Let $N(D_{i+1})$ be the set of disks that are adjacent to D_{i+1}. If a disk $D_k \in N(D_{i+1})$, define $\mathrm{B}(k \setminus i+1)$ to be the maximal connected subgraph of X containing D_k but not D_{i+1}. Suppose ϕ is the angle of the vector from the center of D_{i+1} to the center of D_k measured counterclockwise from the x-axis. Let r be the change in radius and r_0 be the initial radius of D_{i+1}. As r increases, $\mathrm{B}(k \setminus i+1)$ will move in the direction of the vector $\vec{v} = \langle \cos\phi, \sin\phi \rangle$. For a given $D_l \in \mathrm{B}(k \setminus i+1)$ with initial center (a_0, b_0), the center as a function of r is

$$(a, b) = (a_0 + r\cos\phi, b_0 + r\sin\phi)$$

Suppose D_l has radius r_l. When the distance between the center of D_l and the center of D_{i+1} is $r + r_0 + r_l$, D_l and D_{i+1} are tangent, i.e. a collision occurs. Thus we can solve for the value of r such that a collision occurs using the distance formula. We collect terms in the equation

$$(a_0 + r\cos\phi - 0)^2 + (b_0 + r\sin\phi - 0)^2 = (r + r_0 + r_l)^2$$

and find that the quadratic terms cancel, leaving us with a linear equation in r,

$$a_0^2 + b_0 - r_l^2 = 2r(r_l - (a_0\cos\phi + b_0\sin\phi))$$

which we solve to obtain

$$r = \frac{a_0^2 + b_0^2 - r_l^2}{2(r_l - (a_0\cos\phi + b_0\sin\phi))}.$$

In our implementation, we apply this formula to each disk in X and record the smallest positive value of r thus obtained as well as which disk collided with D_{i+1}.

Detection of branch-branch collisions. We will now consider the collision of two disks that are in different branches of D_{i+1}. Let $D_j, D_k \in N(D_{i+1})$, D_j and D_k distinct, and let ϕ_j and ϕ_k be the angles at which D_j and D_k attach to D_{i+1}, respectively. Suppose $D_l \in \mathrm{B}(j \setminus i+1)$ and $D_m \in \mathrm{B}(k \setminus i+1)$, and suppose that their initial centers are (a_0, b_0) and (c_0, d_0), respectively. Then the centers of D_l and D_m as functions of r are:

$$(a, b) = (a_0 + r\cos\phi_j, b_0 + r\sin\phi_j) \tag{3.1}$$

$$(c, d) = (c_0 + r\cos\phi_k, d_0 + r\sin\phi_k) \tag{3.2}$$

Let r_l be the radius of D_l and r_m be the radius of D_m. A collision occurs if the distance between D_l and D_m is $r_l + r_m$. Again, we use the distance formula to solve for r. Substitute (3.1) and (3.2) into

$$(a - c)^2 + (b - d)^2 = (r_l + r_m)^2$$

to obtain

$$\begin{aligned}
\left[(\cos\phi_j - \cos\phi_k)^2 + (\sin\phi_j - \sin\phi_k)^2\right] r^2 +& \\
[2(a_0 - c_0)(\cos\phi_j - \cos\phi_k) + 2(b_0 - d_0)(\sin\phi_j - \sin\phi_k)]\, r +& \\
\left[(a_0 - c_0)^2 + (b_0 - d_0)^2 - (r_l + r_m)^2\right] &= 0,
\end{aligned}$$

and solve for r with the quadratic formula. Of the solutions obtained, we keep the smallest positive solution if one exists or nothing otherwise.

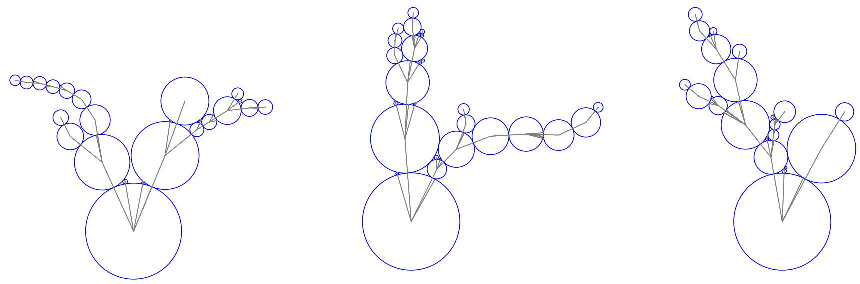

Figure 1. A few "organic"-looking trees

We apply this formula to each pair of disks (D_l, D_m) fulfilling the above preconditions, recording the value of r and the corresponding pair of disks whenever a positive solution is found. To determine when a collision first occurs as r increases, then, we compare the minimum positive value of r found for each type of collision.

4. Applications

The simulation algorithm for branch polymers can be adapted to model physical forms in nature. Different possible models include organic tree growth, the chemical reactions in polyethanol and polyesters, and the growth of cancerous tumors. The images in Figure 4 below were created with slight modifications to our implementation of the Kenyon-Winkler algorithm to create models of two-dimensional organic trees.

These trees were created by restricting the attachment angle and allowing for collisions instead of the edge breaking process. As before, D_1 is fixed at the origin with unit radius. D_2 is attached to D_1 at an angle $theta_2$ such that $theta_2 \in [\frac{\pi}{2} - \frac{\pi}{6}, \frac{\pi}{2} + \frac{\pi}{56}]$. Suppose $DiskX \in BP_R(T)$ and $DiskX \neq Disk1$.

Say D_i is attached to its parent at an angle of θ_i relative to the x-axis. A new disk D_j can be grown off of D_i only at an angle in the range $[\theta_i - \frac{\pi}{6}, \theta_i + \frac{\pi}{6}]$. As D_j expands its radius from zero to one, if there is a collision, D_j ceases to expand further and the cycle remains intact. At this point a new disk then begins to grow from a randomly chosen disk. This construction is guaranteed to produce a branched polymer, but we don't know in advance what the radius vector will be.

5. Open Problems

There are many open problems on branched polymers. Kenyon and Winkler posed several interesting problems in [6]. After implementing the algorithm to generate planar branched polymers, we have made a few observations which lead to more questions. We summarize this list below. Unless otherwise noted, all of these problems refer to branched polymers with disks of unit radius, denoted $BP_{\mathbf{1}}(n)$.

(1) Compute $BP_{\mathbf{1}}(T)$ for each T [6]. See data in appendix for trees up to order 10.

(2) We conjecture that the expected percentage of disks with a given vertex degree in the graph stabilizes rather quickly also to approximately the distribution $[0.23, 0.56, 0.19, 0.011, 10^{-5}, 0]$ so about 23% have degree 1, 56% have degree 2 etc.

(3) Based on our data, we conjecture that the following quantities all follow the same asymptotic growth for $BP_{\mathbf{1}}(n)$:
   (a) Combinatorial diameter: maximal path length between pairs of disks in the polymer, where path length is measured between disk centers.
   (b) Geometric diameter: maximal distance between pairs of points in the polymer, where distance is measured in the Euclidean metric.
   (c) Geometric radius: maximal distance from points in the polymer to the center of mass.
   (d) Distance from the center of mass to the origin.

   Moreover, the ratios between these quantities seem to stabilize rather quickly. What are their exact values? Also, while the values above appear to grow linearly in n, we have no proof of this, and no conjecture for a better formula – for small n, any linear function is wildly inaccurate.

(4) Given a vertex $v \in T$ of degree k, are the gaps between the neighbors around D_v equidistributed? Equivalently, is the volume of polymers with fixed neighbors $D_2, \ldots, D_k$ around D_1 invariant under small changes in angle among $\theta_2, \ldots, \theta_k$.

(5) Given an algorithm to uniformly produce a random polymer of order n; if one selects any order$k$ subpolymer, in a uniformly random manner, is the result a random order k polymer? This defines a weak notion of self-similarity. Is there a stronger one?

(6) Given a minimal bounding circle for a polymer, what is the expected density; the ratio between the area of that circle and the total area of the polymer?

(7) One can define eccentricity in a number of ways. If we consider the smallest (in surface area, perhaps) ellipse that a polymer fits into, what is the eccentricity of that ellipse? Similarly, we can bound the polymer in a rectangle, and look at the ratio between its side lengths. This is intended to measure the tendency of branched polymers to be "stringy" and oblong – is this even the right notion?

(8) From a combinatorial perspective, it is interesting to consider the possible trees that may be realized. How many trees on n vertices can be embedded in the plane, if the edges have length 1 and the vertices are placed at hexagonal lattice points? It isn't difficult to count the number of such trees for up to 8 vertices, and already, the sequence does not appear in Sloane's encyclopedia.

Appendix A. Frequencies of Degree Sequences and Trees

The following data was collected by running the Kenyon-Winkler algorithm to grow 1 million unit polymers of each order 5, 6, $\cdots$ 10.

From the polymers generated, we observed that the degree sequences of the underlying trees had the following frequencies, in percentage. Degree sequences which provably have zero volume have been denoted by 0, whereas those with zero observed frequency have been denoted 0.0.

The frequencies of individual trees are given in Figures A - A, and are given in proportion, not percentage. Several trees (for example, a central vertex with 9 neighbors) cannot be realized as trees of unit polymers,

Order 5		Order 6	
(1 1 1 1 4)	0.7718	(1 1 1 1 1 5)	0.0038
(1 1 1 2 3)	35.4813	(1 1 1 1 2 4)	1.8194
(1 1 2 2 2)	63.7469	(1 1 1 1 3 3)	3.1142
		(1 1 2 2 2 2)	46.2374
		(1 1 1 2 2 3)	48.8252

FIGURE 2. Order 5 Tree Frequencies

Order 7

(1 1 1 1 1 1 6)	0
(1 1 1 1 1 2 5)	0.0088
(1 1 1 1 1 3 4)	0.2313
(1 1 1 1 2 2 4)	2.6841
(1 1 1 1 2 3 3)	9.9973
(1 1 2 2 2 2 2)	32.5268
(1 1 1 2 2 2 3)	54.5517

Order 8

(1 1 1 1 1 1 2 6)	0
(1 1 1 1 1 1 3 5)	0.0005
(1 1 1 1 1 1 4 4)	0.0027
(1 1 1 1 1 2 2 5)	0.0146
(1 1 1 1 1 3 3 3)	0.5554
(1 1 1 1 1 2 3 4)	0.8296
(1 1 1 1 2 2 2 4)	3.2738
(1 1 1 1 2 2 3 3)	19.0304
(1 1 2 2 2 2 2 2)	22.2310
(1 1 1 2 2 2 2 3)	54.0620

Order 9

(1 1 1 1 1 1 1 3 6)	0
(1 1 1 1 1 1 2 2 6)	0
(1 1 1 1 1 1 1 4 5)	0.0
(1 1 1 1 1 1 2 3 5)	0.0033
(1 1 1 1 1 1 2 4 4)	0.0102
(1 1 1 1 1 2 2 2 5)	0.0173
(1 1 1 1 1 1 3 3 4)	0.0529
(1 1 1 1 1 2 2 3 4)	1.7496
(1 1 1 1 1 2 3 3 3)	2.4499
(1 1 1 1 2 2 2 2 4)	3.4818
(1 1 2 2 2 2 2 2 2)	14.8640
(1 1 1 1 2 2 2 3 3)	28.2088
(1 1 1 2 2 2 2 2 3)	49.1622

Order 10

(1 1 1 1 1 1 1 1 4 6)	0
(1 1 1 1 1 1 1 1 5 5)	0
(1 1 1 1 1 1 1 2 3 6)	0
(1 1 1 1 1 1 2 2 2 6)	0
(1 1 1 1 1 1 1 2 4 5)	0.0
(1 1 1 1 1 1 1 3 3 5)	0.0
(1 1 1 1 1 1 1 3 4 4)	0.0010
(1 1 1 1 1 1 2 2 3 5)	0.0058
(1 1 1 1 1 2 2 2 2 5)	0.0191
(1 1 1 1 1 1 2 2 4 4)	0.0268
(1 1 1 1 1 1 3 3 3 3)	0.1021
(1 1 1 1 1 1 2 3 3 4)	0.2539
(1 1 1 1 1 2 2 2 3 4)	2.7840
(1 1 1 1 2 2 2 2 2 4)	3.3697
(1 1 1 1 1 2 2 3 3 3)	6.0166
(1 1 2 2 2 2 2 2 2 2)	9.8128
(1 1 1 1 2 2 2 2 3 3)	35.4370
(1 1 1 2 2 2 2 2 2 3)	42.1712

APPENDIX B. ACKNOWLEDGEMENTS

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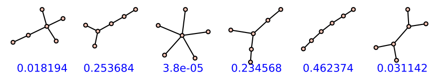

FIGURE 3. Order 6 Tree Frequencies

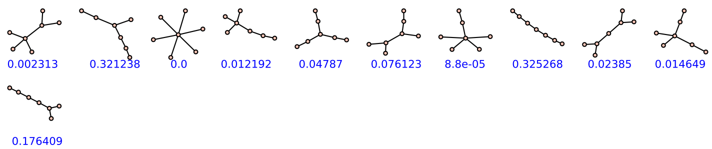

FIGURE 4. Order 7 Tree Frequencies

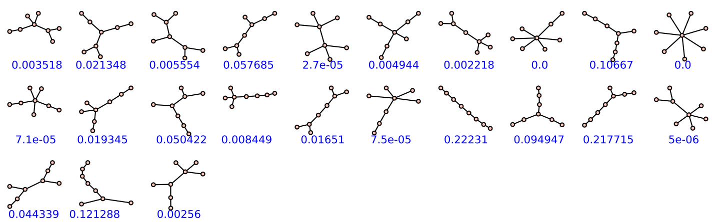

FIGURE 5. Order 8 Tree Frequencies

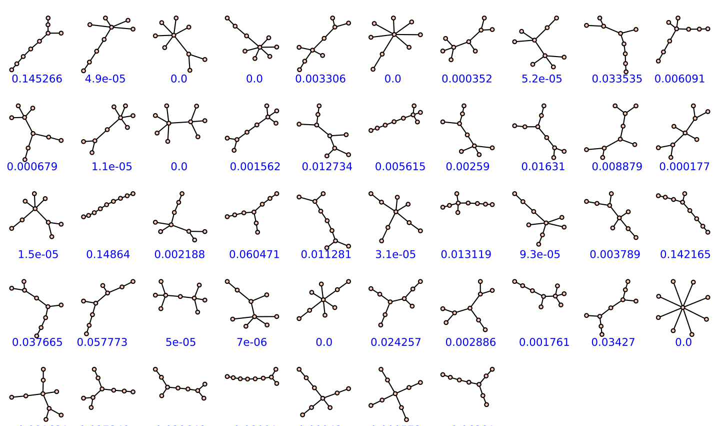

FIGURE 6. Order 9 Tree Frequencies

We also greatly appreciate the advise and collaboration with Bruce Eichinger and Jim Morrow.

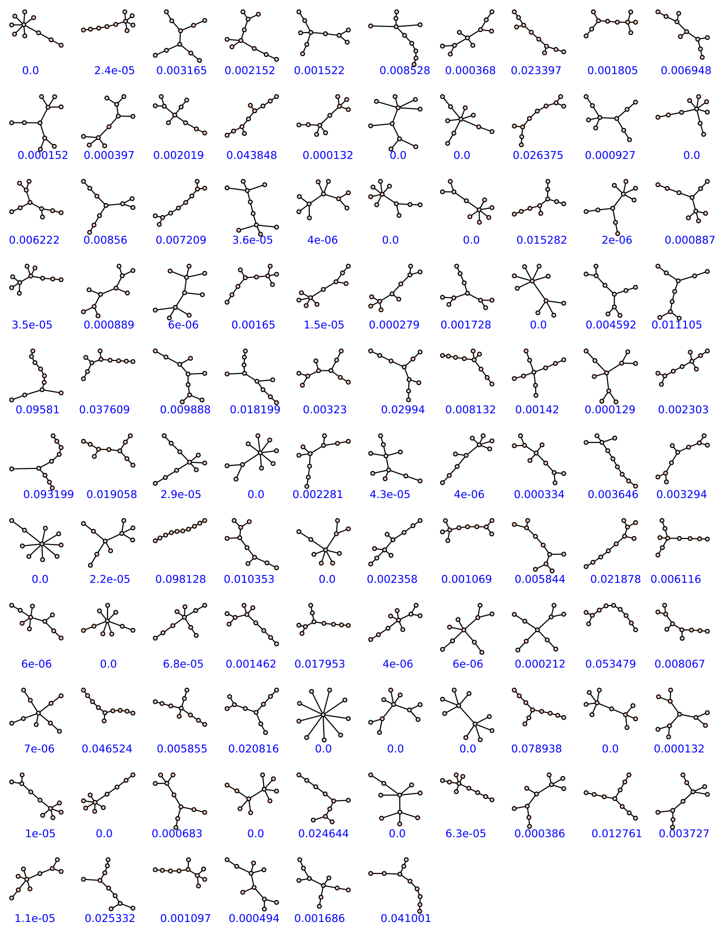

FIGURE 7. Order 10 Tree Frequencies

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