Trees, Tanglegrams, and Tangled Chains

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Based on joint work with:
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My Definition/Philosophy of Combinatorics

"Combinatorics is the equivalent of nanotechnology in mathematics."

(See also Igor Pak's page `http://www.math.ucla.edu/~pak/hidden/papers/Quotes/Combinatorics-quotes.htm`)

Ravi Vakil's "Three Things Game"

Goal. To learn how to get things out of talks. More info:
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Here is how you win. After the talk, if other people are playing, send each other your things by email or discuss them in person. It is surprisingly enlightening. And there will likely be some follow-up discussion. If you have questions, then ask them to someone (perhaps the speaker over the seminar dinner; or perhaps your advisor or your students or your colleagues). Don't let them drop!

Outline

Background

Formulas for Trees, Tanglegrams and Tangled Chains

Algorithms for random generation

Open Problems

Permutations

Notation. $[n] = \{1, 2, \ldots, n\}$

Defn. A permutation is a bijective function $\pi : [n] \longrightarrow [n]$.

Symmetric Group. S_n = Set of permutations of $[n]$ where multiplication is given by composition $\pi \cdot \sigma(i) = \pi(\sigma(i))$.

Many ways to represent a permutation

$$\begin{bmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 2 & 3 & 4 & 1 \end{bmatrix} = [2341] =$$

1234

2341

$$= s_1 s_2 s_3$$

matrix notation	two-line notation	one-line notation	string diagram	reduced expression

Multiplication of permutations is equivalently determined by matrix multiplication or composition of bijections or stacking of string diagrams.

Many ways to represent a permutation

Cycle Notation. Consider the orbits of $[n]$ under the action of w. These orbits form the cycles of w. Write $w = C_1 C_2 \dots C_k$ as a product of cycles. The cycle type of w is the partition $\lambda = (\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_k)$ given by the sizes of the cycles in decreasing order.

Example. $w = [2,3,4,1]$ means $w(1) = 2,\ w(2) = 3,\ w(3) = 4,\ w(4) = 1$. So, in cycle notation $w = (1 \to 2 \to 3 \to 4)$. So $type(w) = (4)$

Example. $v = [4,5,3,6,1,2,8,7]$ written in cycle notation is $(1 \to 4 \to 6 \to 2 \to 5)(3)(7 \to 8)$. So $type(v) = (5,2,1)$.

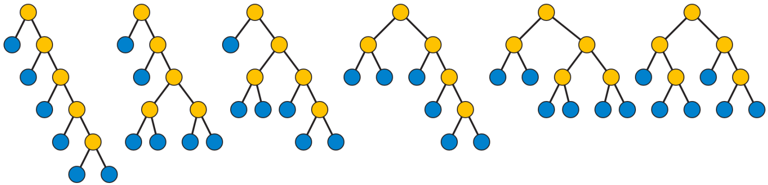
Fact. Two permutations are in the same conjugacy class if and only if they have the same cycle type.

Binary Rooted Trees

Defn. A tree T is a collection of vertices V and edges E connecting pairs of distinct vertices such that there are no cycles and every vertex is connected to every other vertex by a path of edges. A vertex which is incident to exactly one edge is a leaf.

Defn. A binary rooted tree $T = (V, E)$ is a tree with a specified root vertex such that every vertex is either a leaf or it has 2 children.

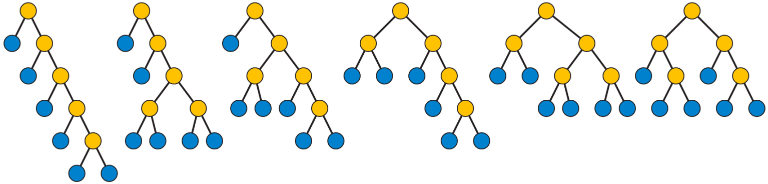
Example: All binary rooted trees with 6 leaves.



credit: `https://en.wikipedia.org/wiki/Wedderburn-Etherington_number`

Binary Rooted Trees

Question. Are the n leaves in those trees distinguishable (like people) or indistinguishable (like electrons)?



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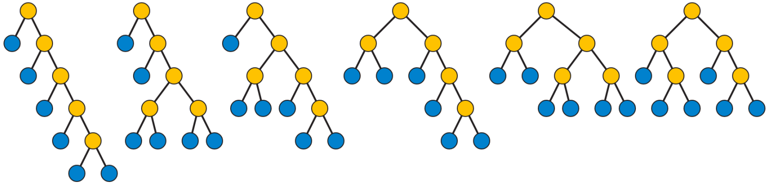

Answer. Count both ways!

1. If we give each leaf a distinct label from 1 to n, there will be many different trees for each one drawn above.
2. The trees above then represent the distinct orbits under the group of permutations on the leaf labels.

Defn. Two trees are inequivalent, if there is no bijection on the leaf labels taking one to the other.

Rooted Binary Trees

- B_n= set of inequivalent binary rooted trees with n leaves
- $|B_n| \longrightarrow 1, 1, 1, 2, 3, 6, 11, 23, 46, 98, \ldots$

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Examples.

- (1), (2), (3) represent the unique rooted binary trees for $n = 1, 2, 3$ respectively.
- $B_4 = \{((1)(3)),\ ((2)(2))\}$,
- $B_5 = \{((1)((1)(3))),\ ((1)((2)(2))),\ ((2)(3))\}$,
- ((1)(((1)((1)((1)(3))))(((2)(2))(((1)(3))((2)(3)))))) is in B_{20}. $|B_{20}| = 293,547$

Catalan objects

- C_n= set of plane rooted binary trees with n leaves
- $|C_n| \longrightarrow 1, 1, 2, 5, 14, 42, \ldots$

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- C_n= set of plane rooted binary trees with n leaves
- $|C_n| \longrightarrow 1, 1, 2, 5, 14, 42, \ldots$ Catalan numbers!

Example.

- ((1)(2)) and ((2)(1)) are distinct as plane trees.

Automorphism Groups of Rooted Binary Trees

- Let $T \in B_n$ rooted binary tree with n leaves.
- $A(T)$ is the subgroup of permutations acting on a fixed labeling of the n leaves which don't change the tree.

Example. $T = ((1)((2)(2)))$ generated by 3 involutions

$$[1,3,2,4,5],\ [1,2,3,5,4],\ [1,4,5,2,3]$$

$$\|\qquad\qquad\|\qquad\qquad\|$$

$$(2\ 3)\qquad\qquad(4\ 5)\qquad\qquad(2\ 4)(3\ 5)$$

$|A(T)| = 2^3 = 8.$

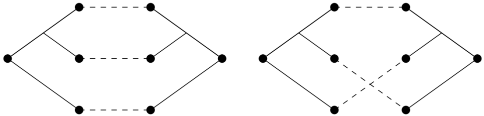
Tanglegrams

Defn. An *(ordered binary rooted) tanglegram* of size n is a triple (T, w, S) where $S, T \in B_n$ and $w \in S_n$.

Two tanglegrams (T, w, S) and (T', w', S') are equivalent provided $T = T'$, $S = S'$ and $w' \in A(T)wA(S)$.

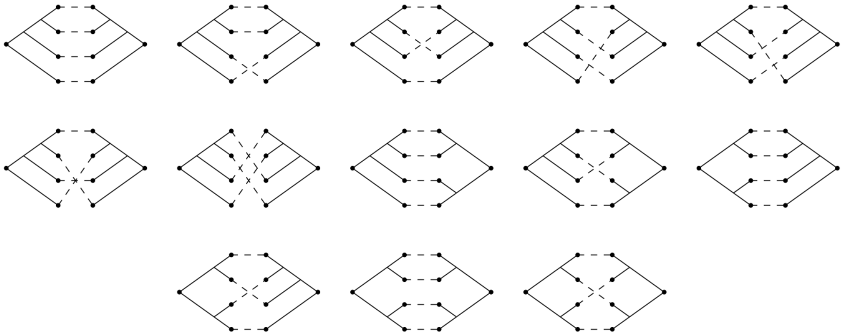
- T_n= set of inequivalent tanglegrams with n leaves
- $t_n = |T_n| \longrightarrow 1, 1, 2, 13, 114, 1509, 25595, 535753, \ldots$

Example. $n = 3$, $t_3 = 2$



Tanglegrams

Case $n = 4,\ t_4 = 13$:



Enumeration of Tanglegrams

Questions.(Matsen) How many tanglegrams are in T_n?
How does t_n grow asymptotically?

First formula.:

$$t_n = \sum_{S \in B_n} \sum_{T \in B_n} \sum_{w \in S_n} \frac{1}{|A(T)wA(S)|}$$

.

This formula allowed us to get data up to $n = 10$. Sequence wasn't in OEIS = Online Encyclopedia of Integer Sequences.

Motivation to study tanglegrams

Cophylogeny Estimation Problem in Biology.: Reconstruct the history of genetic changes in a host vs parasite or other linked groups of organisms.

Tanglegram Layout Problem in CS.: Find a drawing of a tanglegram in the plane with planar embeddings of the left and right trees and a minimal number of crossing (straight) edges in the matching. Eades-Wormald (1994) showed this is NP-hard.

Tanglegrams appear in analysis of software development in CS.

Main Enumeration Theorem

Thm 1. The number of tanglegrams of size n is

$$t_n = \sum_{\lambda} \frac{\prod_{i=2}^{\ell(\lambda)} \left(2(\lambda_i + \cdots + \lambda_{\ell(\lambda)}) - 1\right)^2}{z_\lambda},$$

summed over *binary partitions* of n.

Defn. A *binary partition* $\lambda = (\lambda_1 \geq \lambda_2 \geq \ldots)$ has each part $\lambda_k = 2^j$ for some $j \in \mathbb{N}$.

Defn. $z_\lambda = 1^{m_0} 2^{m_1} 4^{m_2} \cdots (2^j)^{m_j} m_0! m_1! m_2! \cdots m_j!$ for $\lambda = 1^{m_0} 2^{m_1} 4^{m_2} 8^{m_3} \cdots$.

The numbers z_λ are famous!

Defn. More generally, $z_\lambda = 1^{m_1}2^{m_2}3^{m_3}\cdots j^{m_j} m_1! m_2! \cdots m_j!$ for $\lambda = 1^{m_1}2^{m_2}3^{m_3}\cdots$.

Facts.:

1. The number of permutations in S_n of cycle type λ is $\dfrac{n!}{z_\lambda}$.
2. If $v \in S_n$ has cycle type λ, then z_λ is the size of the stabilizer of v under the conjugation of S_n on itself.
3. For fixed $u, v \in S_n$ of cycle type λ,

$$z_\lambda = \#\{w \in S_n \mid wvw^{-1} = u\}.$$

4. The symmetric function $h_n(X) = \sum_\lambda \dfrac{p_\lambda(X)}{z_\lambda}$.

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summed over *binary partitions* of n and z_λ.

Example. The 4 binary partitions of $n = 4$ are

λ :	(4)	(22)	(211)	(1111)
z_λ :	4	$2^2 2!$	$1^2 2^1 2!$	$1^4 4!$

$$t_4 = \frac{1}{4} + \frac{3^2}{8} + \frac{3^2 \cdot 1^2}{4} + \frac{5^2 \cdot 3^2 \cdot 1^2}{24} = 13$$

Corollaries

Cor 1. $t_n = \frac{c_{n-1}^2 n!}{4^{n-1}} \sum_\mu \frac{n(n-1)\cdots(n-|\mu|+1)}{z_\mu \cdot \prod_{i=1}^{\ell(\mu)} \prod_{j=1}^{\mu_i - 1} (2n-2(\mu_1+\cdots+\mu_{i-1})-2j-1)^2}$,
summed is over binary partitions μ with all parts equal to a positive power of 2 and $|\mu| \leq n$.

Cor 2.: As n gets large, $\frac{t_n}{n!} \sim \frac{e^{\frac{1}{8}} 4^{n-1}}{\pi n^3}$.

Cor 3.: There is an efficient recurrence relation for t_n based on stripping off all copies of the largest part of λ.
We can compute t_{4000} exactly.

Second Enumeration Theorem

Thm 2. The number of binary trees in B_n is

$$b_n = \sum_{\lambda} \frac{\prod_{i=2}^{\ell(\lambda)} \Big(2(\lambda_i + \cdots + \lambda_{\ell(\lambda)}) - 1\Big)}{z_\lambda},$$

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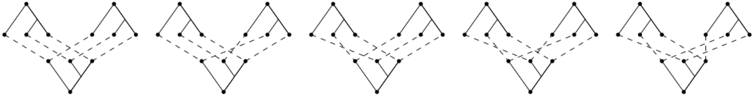
Question. What if the exponent k is bigger than 2?

$$t(k,n) = \sum_{\lambda} \frac{\prod_{i=2}^{\ell(\lambda)} \left(2(\lambda_i + \cdots + \lambda_{\ell(\lambda)}) - 1\right)^k}{z_\lambda}.$$

Tangled Chains

Defn. A *tangled chain* of size n and length k is an ordered sequence of binary trees with complete matchings between the leaves of neighboring trees in the sequence.



Thm 3. The number of tangled chains of size n and length k is

$$t(k,n) = \sum_{\lambda} \frac{\prod_{i=2}^{\ell(\lambda)} \Big(2(\lambda_i + \cdots + \lambda_{\ell(\lambda)}) - 1\Big)^k}{z_\lambda}.$$

Outline of Proof of Theorem 1

$$t_n = \sum_{S \in B_n} \sum_{T \in B_n} \sum_{w \in S_n} \frac{1}{|A(T)wA(S)|}$$

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$$= \sum_{u \in A(T)} \sum_{v \in A(S)} \sum_{w \in S_n} \chi[u = wvw^{-1}]$$

$$= \sum_{\lambda \vdash n} |A(T)_\lambda| \cdot |A(S)_\lambda| \cdot z_\lambda$$

where $A(T)_\lambda = \{w \in A(T) \mid type(w) = \lambda\}$. Only binary partitions occur!

Outline of Proof of Main Theorem

$$t_n = \sum_{S \in B_n} \sum_{T \in B_n} \sum_{w \in S_n} \frac{1}{|A(T)wA(S)|}$$

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To show:

$$\sum_{T \in B_n} \frac{|A(T)_\lambda|}{|A(T)|} = \frac{\prod_{i=2}^{\ell(\lambda)} \left(2(\lambda_i + \cdots + \lambda_{\ell(\lambda)}) - 1\right)}{z_\lambda} =: q_\lambda$$

via the recurrence

$$2q_\lambda = q_{\lambda/2} + \sum_{\lambda^1 \cup \lambda^2 = \lambda} q_{\lambda^1} q_{\lambda^2}$$

Conclusion: $t_n = \sum z_\lambda q_\lambda^2$.

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Random Generation of Tanglegrams

Input: n

Step 1: Pick a binary partition $\lambda \vdash n$ with prob $z_\lambda q_\lambda^2 / t_n$.

Step 2: Choose T and $u \in A(T)_\lambda$ uniformly by subdividing $\lambda = \lambda^1 \cup \lambda^2$ according to the recurrence for q_λ. Similarly, choose S and $v \in A(T)_\lambda$ uniformly by subdividing.

Step 3: Among the z_λ permutations w such that $u = wvw^{-1}$, pick one uniformly.

Output: (T, w, S).

Random Generation of a Permutation in $A(T)$

Input: Binary tree $T \in B_n$ with left and right subtrees T_1 and T_2.

If $n = 1$, set $w = (1) \in A(T)$, unique choice.

Otherwise, recursively find $w_1 \in A(T_1)$ and $w_2 \in A(T_2)$ at random.

- If $T_1 \neq T_2$, set $w = w_1 w_2$.
- If $T_1 = T_2$, choose either $w = w_1 w_2$ or $w = \pi w_1 w_2$ with equal probability.

Here $\pi = (1\ k)(2\ (k+1))(3\ (k+3)) \cdots (k\ n)$ where $k = n/2$ flips the labels on the leaves of the two subtrees.

Output: Permutation $w \in A(T)$.

Random Generation of Tanglegrams:Step 2

Step 2: Choose T and $u \in A(T)_\lambda$ uniformly by subdividing $\lambda = \lambda^1 \cup \lambda^2$ according to the recurrence for q_λ.

Input: $\lambda \vdash n$.

- If $n = 1$, output $T = \bullet$, $u = (1) \in A(T)$, unique choice.
- Otherwise, pick a subdivision of λ from two types

$$\{(\lambda/2, \lambda/2)\} \bigcup \{(\lambda^1, \lambda^2) : \lambda^1 \cup \lambda^2 = \lambda\}$$

  with probability proportional to

$$q_{\lambda/2} + \sum q_{\lambda^1} q_{\lambda^2} = 2q_\lambda.$$

Random Generation of Tanglegrams:Step 2

Step 2: Choose T and $u \in A(T)_\lambda$ uniformly by subdividing $\lambda = \lambda^1 \cup \lambda^2$ according to the recurrence for q_λ.

- Type 1: $(\lambda/2, \lambda/2)$. Use the algorithm recursively to compute $T_1 \in B_{n/2}$ and a permutation $u_2 \in A(T_1)_{\lambda/2}$. Uniformly at random, generate another permutation $u_1 \in A(T_1)$. Set

$$T = (T_1, T_1),\ u = \pi u_1 \pi u_1^{-1} \pi u_2.$$

- Type 2: (λ^1, λ^2). Use the algorithm recursively to compute trees T_1, T_2 and permutations $u_1 \in A(T_1)_{\lambda^1}$ $u_2 \in A(T_2)_{\lambda^2}$. Switch if necessary so $T_1 \leq T_2$. Set

$$T = (T_1, T_2),\ u = u_1 u_2.$$

Output: (T, u).

Random Generation of Tanglegrams:Step 2

Example If $\lambda = (6, 4)$, then $|\lambda| = 10$, $\lambda/2 = (3, 2)$ and $\pi = (1\ 6)(2\ 7)(3\ 8)(4\ 9)(5\ 10)$. If

$$w_1 = (1\ 4)(2\ 5)(3) \text{ and } w_2 = (6\ 9\ 7)(8\ 10)$$

then

$$w = \pi w_1 \pi w_1^{-1} \pi w_2 = (6\ 1\ 9\ 5\ 7\ 4)(8\ 2\ 10\ 3),$$

all in cycle notation.

Review: Random Generation of Tanglegrams

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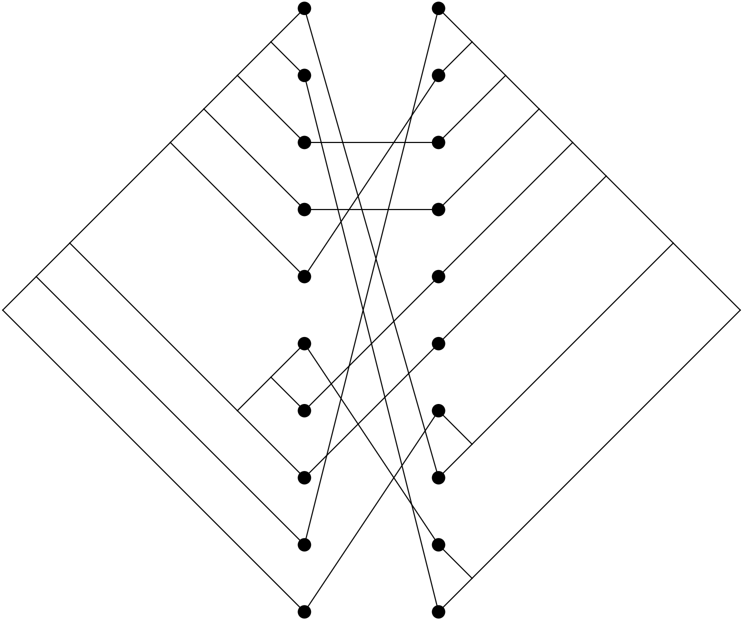
Random Tanglegrams: n=10



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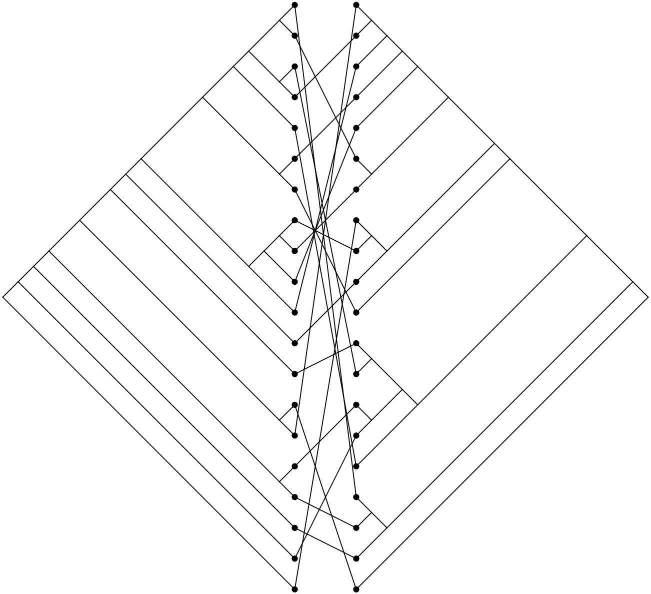
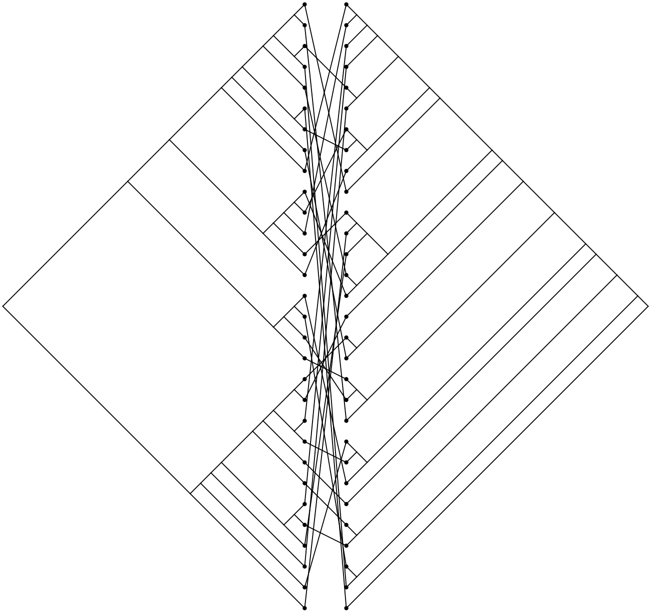
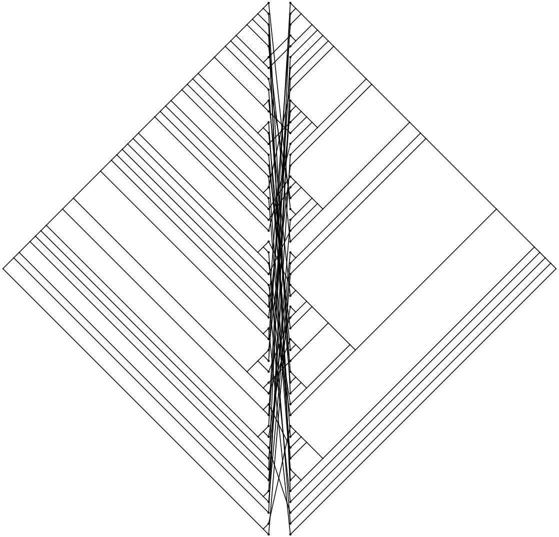


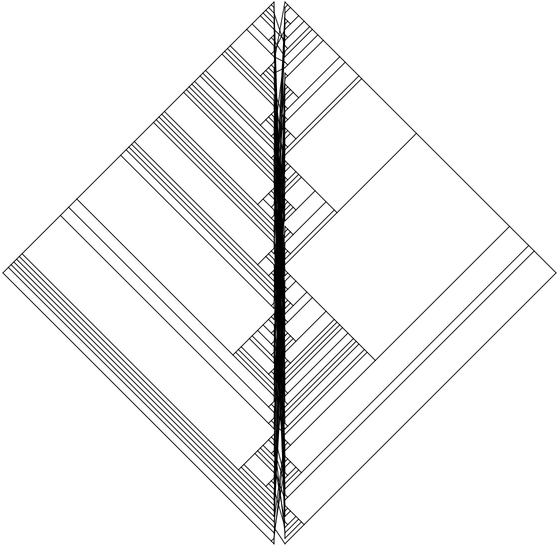
Random Tanglegrams: n=30



Random Tanglegrams: n=50



Random Tanglegrams: n=100



Positivity and symmetric functions
go hand in hand with enumeration.

This is a story that began with an enumeration question and via work of Gessel now connects to symmetric functions, plethysm of Schur functions, and Kronecker coefficients.

Open Problems

Conjecture 1.[Amdeberhan-Konvalinka] For all positive integer n and k, and q a prime number, let

$$t_q(k,n) = \sum_{\lambda} \frac{\prod_{i=2}^{\ell(\lambda)} \left(q(\lambda_i + \cdots + \lambda_{\ell(\lambda)}) - 1 \right)^k}{z_\lambda}$$

summed over all partitions whose parts are powers of q. Then, $t_q(k,n)$ is an integer.

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Conjecture 1.[Amdeberhan-Konvalinka] For all positive integer n and k, and q a prime number, let

$$t_q(k,n) = \sum_{\lambda} \frac{\prod_{i=2}^{\ell(\lambda)} \Big(q(\lambda_i + \cdots + \lambda_{\ell(\lambda)}) - 1\Big)^k}{z_\lambda}$$

summed over all partitions whose parts are powers of q. Then, $t_q(k,n)$ is an integer.

Conjecture 2.[Gessel] For all positive integer n, q a prime number and $1 \leq s < q$,

$$t_q(k,n) = \sum_{\lambda} p_\lambda \frac{\prod_{i=2}^{\ell(\lambda)} \Big(q(\lambda_i + \cdots + \lambda_{\ell(\lambda)}) - s\Big)}{z_\lambda}$$

is a nonnegative integer linear combination of Schur functions.

More Open Problems

1. Is there a closed form or functional equation for $T(x) = \sum t_n x^n$ like there is for binary trees $B(x)$?

$$B(x) = x + \frac{1}{2}\left(B(x)^2 + B(x^2)\right)$$

2. Is there an efficient algorithm for depth first search on tanglegrams?

3. Can one describe the lex minimal permutations in the double cosets $A(T)\backslash S_n/A(S)$ for $S, T \in B_n$?

References

- "On the enumeration of tanglegrams and tangled chains" by Sara Billey, Matjaž Konvalinka, Frederick A Matsen IV (http://arxiv.org/pdf/1507.04976.pdf)
- "On Symmetries In Phylogenetic Trees" Eric Fusy (http://arxiv.org/pdf/1602.07432v1.pdf)
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- "Inducibility in binary trees and crossings in random tanglegrams" Eva Czabarka, László A. Székely, Stephan Wagner (http://arxiv.org/abs/1601.07149)
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