Trees, Tanglegrams, and Tangled Chains

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Based on joint work with:
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Positivity and symmetric functions
go hand in hand with enumeration.

Outline

Background

Formulas for Trees, Tanglegrams and Tangled Chains

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Algorithms for random generation

Open Problems

Rooted Binary Trees

- B_n= set of rooted inequivalent binary trees with n leaves
- $|B_n| \longrightarrow 1, 1, 1, 2, 3, 6, 11, 23, 46, 98, \ldots$
- $A(T)$ is the automorphism group of T given a canonical labeling of its leaves.

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Examples.

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- $B_4 = \{((1)(3)),\ ((2)(2))\}$,
- $B_5 = \{((1)((1)(3))),\ ((1)((2)(2))),\ ((2)(3))\}$,
- $((1)(((1)((1)((1)(3))))(((2)(2))(((1)(3))((2)(3))))))$ is in B_{20}. $|B_{20} = 293, 547|$

Catalan objects

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

Example.

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

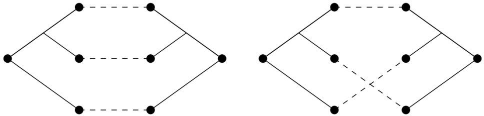
Tanglegrams

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 $w' \in A(T)wA(S)$.

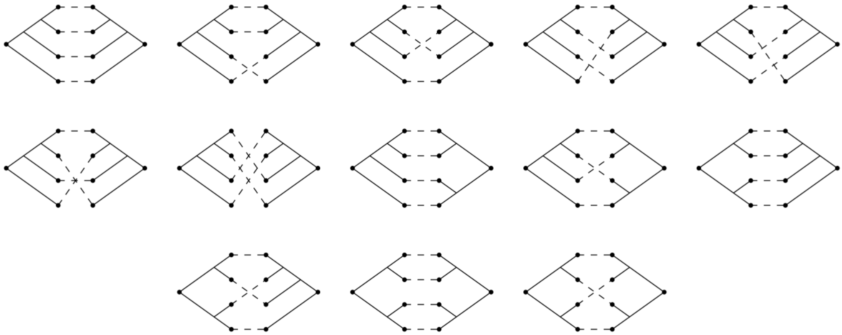
- T_n= set of inequivalent tanglegrams with n leaves
- $t_n = |T_n| \longrightarrow 1, 1, 2, 13, 114, 1509, 25595, 535753, \ldots$

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.

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

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

The numbers z_λ

Defn. More generally, $z_\lambda = 1^{m_1} 2^{m_2} 3^{m_3} \cdots j^{m_j} m_1! m_2! m_2! \cdots m_j!$ 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 $\frac{n!}{/} z_\lambda$.
2. If v has cycle type λ, the 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. $h_n(X) = \sum_\lambda \frac{p_\lambda(X)}{z_\lambda}$

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summed over *binary partitions* of n and z_λ.

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

$$\begin{array}{lcccc} \lambda: & (4) & (22) & (211) & (1111) \\ z_\lambda: & 4 & 2^2 2! & 1^2 2^1 2! & 1^4 4! \end{array}$$

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

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}.

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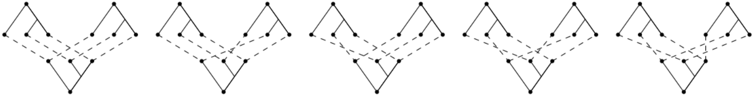
Question. What if the exponent k is bigger than 2?

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

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 Main Theorem

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

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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!

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To show:

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

via the recurrence

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

Conclusion: $t_n = \sum_{\lambda} z_\lambda q_\lambda^2$.

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).

Open Problems

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

2. Is there an efficient 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 $S, T \in B_n$?