Combinatorics of increasing trees:

Bijections, asymptotics and algorithms

Mehdi Naima

Under the supervision of Olivier Bodini and Antoine Genitrini In fulfilment of the degree Doctor of Philosophy of Université Sorbonne Paris-Nord

Reviewer[.]

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Jury: F

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- 1. Introduction
- 2. Analytic combinatorics
- 3. Parametrisable evolution process for classes of strict monotonic Schröder trees
- 4. Three particular cases of the evolution process
- 5. Applications
- 6. Conclusion and future works

Introduction

Tree structures are used as abstract data type to represent hierarchical relations between information that it contains. Tree structures appears extensively in computer science:

 In compilation abstract syntax trees represent the abstract syntactic structure of a source code written in a programming language.



Abstract syntax tree

Tree structures

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- In computational linguistics, a parse tree represents the syntactic structure of a string according to some context-free grammar.







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- Lambda terms in lambda calculus are enriched tree structures.





The contemporary structure of the Sri Lankan military health care services. (military-medicine)

 In biology and phylogenetics to represent the evolutionary relationship among species. [Fel03, Ste16]



Diagram of divergence of Taxa 1871. Darwin (On the origin of species)

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Eukaryotes Tree of Life 2020, showing positions of fungi and fungus-like organisms. Tricholome (wikipedia)

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- In philology to construct the family tree (stemma) of preserved copies of ancient manuscript. [NH82]

| AW | 0 | 0 | 0 | 4 | 4 | 4 | 10 | 20 | 38 | 52 | 84 | 124 | 203 | 205 | 225 | 482 | 711 | 726 | 926 |
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| MS | 2 | 5 | 10 | 1 | 8 | 16 | 4 | 6 | П | 12 | 7 | 14 | 17 | 3 | 9 | 15 | 18 | 13 | 15 |

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- Study the number of executions of a parallel process and their synchronisations. This leads to repeated labellings. [BGP16, BGR17]





From [BGR17]

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Both approaches are complementary. It is possible to study random trees and derive similar type of results.

Definition

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- Symbolic method developed in [FS09] is a grammar used to define (specify) combinatorial classes:
 - 1. Elementary constructions are the neutral class and the atomic class.
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Result

Operations in the symbolic method translates directly to operations on generating functions.

- Theorems for automatic asymptotic estimates.
- Theorems for the shape of large random structures.

Ordinary generating functions

For a combinatorial class C we define its *ordinary generating function* (OGF) to be $C(z) = \sum_{n=0}^{\infty} C_n z^n$ where C_n counts the number of objects in C of size n.
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| Atomic class | Z | Class consisting of single object of size 1 | Ζ | |
| $\begin{array}{llllllllllllllllllllllllllllllllllll$ | | Disjoint of objects from ${\mathcal F}$ and ${\mathcal G}$ | F(z) + G(z) | |
| | | Ordered pairs of objects one from ${\mathcal F}$ and one from ${\mathcal G}$ | $F(z) \cdot G(z)$ | |
| Sequence | $\operatorname{Seq} \mathcal{F}$ | Sequences of objects from ${\mathcal F}$ | $\frac{1}{1-F(z)}$ | |
| Substitution | $\mathcal{F}\circ\mathcal{G}$ | Substitute elements of ${\mathcal G}$ for atoms of ${\mathcal F}$ | F(G(z)) | |
| Erasing <i>i</i> atoms | $\mathcal{E}^{i}\mathcal{F}$ | Erase i atoms from objects of ${\cal F}$ | $\frac{F^{(i)}(z)}{i!}$ | |
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The terms are then obtained by coefficient extraction $[z^n]W(z)$ $W(z) = 1 + 3z + 9z^2 + 27z^3 + 81z^4 + 243z^5 + 729z^6 + 2187z^7 + 6561z^8 + 19683z^9 + 59049z^{10} + \dots$

Plane simple trees varieties

Plane simple trees are rooted unlabelled trees

Definition (Weighted degree function)

For a class of trees with ϕ_i colours for *i*-ary nodes, we define its degree function to be $\phi(z) = \sum_{i \ge 0} \phi_i z^i$.

For example $\phi(z) = 1 + z^2 + 10z^3 + 2z^5.$

Corresponds to a class of trees having:

- One type of leaves.
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Given a weighted degree function $\phi(z)$ such that $\phi_0 > 0$, the variety of plane simple trees parameterised by ϕ is specified in world of OGF by,

$$\mathcal{T} = \mathcal{Z} \times (\phi \circ \mathcal{T})$$

which gives,

$$T(z) = z \phi(T(z))$$

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Binary trees are parameterised by $\phi(z) = 1 + 2z + z^2$, then, $B(z) = z\phi(B(z))$ Solves to, $B(z) = -1 + \frac{(1-\sqrt{1-4z})}{2z}$

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In plane simple trees nodes can be decorated but do not bear labels

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Example: Ordered set partitions. $[\{2,4,5\},\{1,7\},\{3,6\}]$ is an ordered partition of size 7.

$$\mathcal{B} = \operatorname{SEQ}\left(\operatorname{SET}_{\geq 1}(\mathcal{Z})\right) \stackrel{\text{symbolic method}}{\Longrightarrow} B(z) = \frac{1}{1 - (\exp(z) - 1)} = \frac{1}{2 - \exp(z)}$$

The terms are then obtained by $n![z^n]B(z)$ and are called Ordered Bell numbers: $B(z) = 1z + 3z^2 + 13z^3 + 75z^4 + 541z^5 + 4683z^6 + 47293z^7 + 545835z^8 + \dots$

- Labelled structures are naturally specified with EGF since each atom bears an integer label. Then the normalisation ^{zⁿ}/_{n!} insures the generating function to be convergent and analytic methods apply.
- The term increasing trees classically refers to trees such that the labels are strictly increasing along branches and have no label repetitions.[BFS92]

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The boxed product (Greene operator) is defined in the EGF world. That is defined as the label product with the additional constraint that the smallest left has to appear on the left class \mathcal{B} .

$$\mathcal{A} = \mathcal{B}^{\Box} \star \mathcal{C} \to \mathcal{A}(z) = \int_{0}^{z} (\partial_{t} B(t)) \cdot \mathcal{C}(t) dt$$

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Example: Increasing binary trees.

$$\mathcal{B} = \epsilon + \mathcal{Z}^{\Box} \star (\mathcal{B} \star \mathcal{B}) \stackrel{\text{symbolic method}}{\Longrightarrow} B(z) = 1 + \int_{0}^{z} 1 \cdot B^{2}(t) dt$$

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which solves to $B'(z) = B^2(z), B(0) = 1 \implies B(z) = \frac{1}{1-z}$ $B_n = n![z^n]B(z) = n!.$



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Can be modeled using trees such that

- Internal nodes bear integer labels corresponding to the time of differentiation (label repetitions are allowed).
- The size of the tree is its number of leaves.
- Nodes can have different arities.
- Branches are strictly increasing (label repetitions allowed).



Parametrisable evolution process for classes of strict monotonic Schröder trees

Definition (Coloured degree function)

For a class of trees with ϕ_i colours of *i*-ary nodes, we define its coloured degree function to be $\phi(z) = \sum_{i>1} \phi_i z^i$.

Definition (Set of allowed repetitions)

The set $r \subset \mathbb{N}^*$.

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The set $r \subset \mathbb{N}^*$.

For example

$$r = \{2, 3, 5\}.$$

At each iteration step there are either 2, 3 or 5 repetitions of the same label (i.e the number of leaves that evolves at each step is constrained to lie in r).

$$\phi(z)=2z^2+2z^3$$
 and $r=\mathbb{N}^*$

- 1. Choose a non-empty subset L of leaves of the so-far built tree such that $|L| \in r$.
- 2. For each $\ell \in L$ choose an integer k > 1such that $\phi_k > 0$, and one of the $1 \le c \le \phi_k$ colours.
- Replace ℓ with an internal node labelled i with the chosen colour and attach to it k new leaves.

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We have two colours of binary nodes (w,g) and two colours of ternary nodes (w,g).

Start at step 0 with a leaf; at each step $i \ge 1$ do:



- 1. Choose a non-empty subset L of leaves of the so-far built tree such that $|L| \in r$.
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Let $\phi(z)$ a coloured degree function, $r \subset \mathbb{N}^*$ a set of allowed repetitions and $m = \min(r)$, then

$$\mathcal{B} = \mathcal{Z}^m + \sum_{i \in r} \left(\mathcal{E}^i \mathcal{B} \right) \times \left(\phi^i \backslash (\phi_1 \mathcal{Z})^i \right).$$

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Which translates to,

$$B(z) = z^{m} + \sum_{i \in r} \frac{1}{i!} B^{(i)}(z) \left(\phi(z)^{i} - (\phi_{1} z)^{i} \right).$$

 $\frac{B^{(i)}(z)}{i!}$ corresponds to erasing *i* leaves.

 Increasing trees [BFS92].
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 Two increasing labellings where all arities are allowed.
- Families of monotonic trees [BGNS20].

A general asymptotic for cases where the number of repetitions allowed is not bounded.



| r | $\phi(z)$ | Name | References |
|----------------|-----------------------|--|------------|
| $\{1\}$ | z ^d | Plane <i>d</i> -ary increasing | [BFS92] |
| $\{1\}$ | $\frac{z^2}{1-z}$ | Increasing Schröder | [BGN19] |
| \mathbb{N}^* | z^2 | Strict monotonic binary | [BGGW20] |
| \mathbb{N}^* | $\frac{z^2}{1-z}$ | Strict monotonic Schröder | [BGN19] |
| \mathbb{N}^* | $\frac{z}{1-z}$ | Strict monotonic general Schröder | [BGMN20] |
| \mathbb{N}^* | plane <i>d</i> -ary | Monotonic <i>d</i> -ary trees | [BGNS20] |
| $\{1,2\}$ | <i>z</i> ² | Supertrees | [SDH+04] |
| { <i>d</i> } | <i>z</i> ² | Increasing binary with d label repetitions | |

Table 1: Some of examples of tree classes covered by the evolution process

Three particular cases of the evolution process

Corresponds to the parameters $\phi(z) = \frac{z^2}{1-z}$ and $r = \{1\}$. Therefore, a single leaf can evolve at each iteration step.



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- Number of trees is $\frac{n!}{2}$.
- Bijections with half permutations that preserves several parameters. Number of internal nodes and the depth of the leftmost leaf are related to the the number of cycles in a permutation.



This tree with 8 leaves Corresponds to the permutation (1,4,5)(2)(3)(6,8)(7) it has 8+1-5=4 internal nodes.

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- Typical parameters are:

| | | | 1 | Mean | Va | riance | L | imit law | |
|--------------------------|--------------|----------|----------|----------------|--------------|-------------|----------------|-----------------|----------------------|
| | Internal n | odes | n | — In <i>n</i> | I | n <i>n</i> | | Normal | |
| Dept | h of the lef | tmost le | af | ln n | I | n <i>n</i> | | Normal | |
| | Height of th | ie tree | e | (In <i>n</i>) | | | | | |
| [| Degree of th | ie root | 2 | e – 3 | 14 e - | $4 e^2 - 4$ | 8 Mod | ified Poiss | on |
| | | | | | | | | | |
| | 2-ary | 3-ary | 4-ary | 5-ary | 6-ary | 7-ary | 8-ary | 9-ary | 10-a |
| $\mathbb{E}C_n^{(\ell)}$ | n — 2 ln n | ln n | 23 90 | $\frac{1}{32}$ | 107 25200 | 47 86400 | 101 1587600 | 229 33868800 | <u>659</u> 100590 |



Corresponds to the parameters $\phi(z) = \frac{z^2}{1-z}$ and $r = \mathbb{N}^*$. Any number of repetitions is allowed and the node degrees can be anything ≥ 2 .



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- Bijection with ordered set partitions (Ordered Bell numbers) with the number of iteration steps corresponding to the number of subsets in the partitions.
- $g_n = B_{n-1} \stackrel{=}{=} \frac{(n-1)!}{2(\ln 2)^n}$, $(B_n \text{ is the } n\text{-th ordered Bell number}).$



This tree with 8 leaves Corresponds to the ordered set partition $({3, 4}, {1, 5, 7}, {2, 6}).$ The tree has 3 distinct labels and the partition 3 subsets. Corresponds to the parameters $\phi(z) = \frac{z^2}{1-z}$ and $r = \mathbb{N}^*$. Any number of repetitions is allowed and the node degrees can be anything ≥ 2 .

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- $g_n = B_{n-1} \stackrel{=}{=} \frac{(n-1)!}{2(\ln 2)^n}$, $(B_n \text{ is the } n\text{-th ordered Bell number}).$
- Typical parameters are:

| | Mean | Variance | Limit law |
|----------------------------|-----------------------|----------------------------------|--------------------------------|
| Internal nodes | n — ln 2 ln n | | |
| Distinct labels | $\frac{1}{2 \ln 2} n$ | $\frac{(1-\ln 2)}{(2\ln 2)^2} n$ | Normal |
| Degree of the root | $2 \ln 2 + 1$ | $-2 \ln 2 (\ln 2 - 1)$ | Shifted zero-truncated Poisson |
| Depth of the leftmost leaf | ln n | ln n | Normal |



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- Typical parameters are:

| | Mean |
|----------------------------|---------------|
| Internal nodes | $\Theta(n^2)$ |
| Distinct labels | $\Theta(n)$ |
| Unary nodes | $\Theta(n^2)$ |
| Depth of the leftmost leaf | $\Theta(n)$ |
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Remark

Unary nodes change significantly the number of trees and its typical shape.

| | Number of trees | Number of internal nodes |
|---------------------------------|---------------------------------|--------------------------|
| Increasing Schröder trees | n!/2 | $n - \ln n$ |
| Strict monotonic Schröder trees | $(n-1)!/(2(\ln 2)^n)$ | n — ln 2 ln n |
| Strict monotonic general trees | $c \ 2^{(n-1)(n-2)/2} \ (n-1)!$ | $\Theta(n^2)$ |

Remark

For all three models, it seems that typical large trees have nodes that are mostly from the first allowed arity, and little from the second allowed arity while other arities appear very rarely.

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Remark

For all three models, it seems that typical large trees have nodes that are mostly from the first allowed arity, and little from the second allowed arity while other arities appear very rarely.



This idea is developed in the next theorems in the form of asymptotic enumeration.

Let $r \subset \mathbb{N}^*$ and m = min(r). Let $\phi(z)$ be a coloured degree function and such that $\phi_1 = 0$, $\phi_2 \ge 1$ and $\phi_n \underset{n \to \infty}{=} O\left(\frac{n!}{m!^{n/m}n^{m+4}}\right)$.

Let $B_n^{\phi,r}$ be the number of trees of size *n* built via the evolution process

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Theorem

Let $\phi(z)$ be a coloured degree function as in the condition, and $r \subset \mathbb{N}^*$, with $r \neq \emptyset$. Let $m = \min(r)$, then as n tends to infinity and is of the form $n \equiv 0 \mod m$,

$$B_n^{r,\phi} \underset{n \to \infty}{\sim} \kappa \ n! \ \left(\frac{\phi_2}{\rho}\right)^n \ n^{-1+\frac{\rho \ \phi_3}{\phi_2^2} - \frac{\rho \ f''(\rho)}{f'(\rho)}},$$

where κ is a constant that depends on $\phi(z)$ and r. Let $f(z) = \sum_{i \in r} \frac{z^i}{i!}$, then ρ is the smallest positive real of the equation f(z) - 1 = 0.

Let $\phi(z)$ be a coloured degree function and such that $\phi_1 \ge 1$, $\phi_2 \ge 1$ and $\phi_n = O\left(\frac{n!}{n^5}\right)$.

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Theorem

Let $\phi(z)$ be a coloured degree function as in the condition, let $r \subset \mathbb{N}^*$, $r \neq \emptyset$, and $r \neq \{1\}$, then as n tends to infinity,

$$\mathcal{B}_n^{r,\phi} \underset{n \to \infty}{\sim} \kappa \ (n-1)! \ \phi_2^{n-1} \ \prod_{k=1}^{n-1} \left(\sum_{i=1,i \in r}^{n-k} \phi_1^{i-1} \binom{n-k-1}{i-1} \right)$$

where κ is a constant that depends on $\phi(z)$ and r.

The condition on ϕ_2 can be relaxed and a similar result holds.

Applications

Increasing binary trees with *d* repetitions

- \mathcal{B}^d be the class of increasing binary trees with *d* label repetitions at each iteration step.
- At each iteration step exactly *d* leaves are chosen to expand (we start with a single root that has *d* leaves).

Increasing binary trees with d repetitions

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- At each iteration step exactly *d* leaves are chosen to expand (we start with a single root that has *d* leaves).
- Specification with $\phi(z) = z^2$ and $r = \{d\}$.

| d | Asymptotics | References |
|---|---------------------------------|-------------|
| 1 | (n-1)! | EIS A000142 |
| 2 | $c_2 n! (2^{1/2})^{-n} n^{-2}$ | EIS A000680 |
| 3 | $c_3 n! (3!^{1/3})^{-n} n^{-3}$ | EIS A014606 |
| 4 | $c_4 n! (4!^{1/4})^{-n} n^{-4}$ | EIS A014608 |

Table 2: Asymptotic behaviour for B_n^d for $d \in \{1, 2, 3, 4\}$ when $n \equiv 0 \mod d$. The sequences in OEIS appear shifted (without periodicities).



Simulation for $n \in \{10, 200\}$ of B_n^d divided by their expected asymptotic behaviour with $d \in \{1, 2, 3, 4\}.$

Take $\phi(z)$ to be unlabelled binary trees (or Catalan trees)

 $\phi(z) = cat(z) - z = z^2 + 2z^3 + 5z^4 + \dots$ and $r = \mathbb{N}^*$

- 1. Choose a non-empty subset L of leaves of the so-far built tree such that $|L| \in r$.
- 2. For each $\ell \in L$ choose an integer k > 1such that $\phi_k > 0$, and one of the $1 \le c \le \phi_k$ possible unlabelled trees with k leaves.
- Replace ℓ with the chosen unlabelled tree, labelling all its internal nodes i.

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Increasing labellings of binary trees

As a result we propose new **increasing labellings models** on trees which allow label repetitions:



- Using different values of ϕ and r we can specify and enumerate trees (counted by their leaves) with the different increasing labellings.
- Theorem I applies to give the asymptotic behaviours.

Comparison of binary trees increasing labellings

| | r | $\phi(z)$ | Asymptotics | References |
|-------------------------------|----------------|----------------|--|---------------------|
| Increasing | $\{1\}$ | z ² | (n-1)! | [FS09], Theorem I |
| Connected monotonic | $\{1\}$ | (cat(z) - z) | c3 n! n | Theorem I |
| Strict monotonic | \mathbb{N}^* | z ² | $c_4(n-1)! (\frac{1}{\ln 2})^n n^{-\ln 2}$ | [BGGW20], Theorem I |
| Monotonic (weakly increasing) | \mathbb{N}^* | (cat(z) - z) | $c_5(n-1)! (\frac{1}{\ln 2})^n n^{\ln 2}$ | Theorem I |

 Table 3: Comparison of the asymptotic behaviour of labelled binary trees under different labelling models.



Simulation for $n \in \{1, 100\}$ of binary trees with different increasing labellings divided by their expected asymptotic first order.

On Schröder trees the different increasing labellings give:



Comparison of Schröder trees under different increasing labellings

| | r | $\phi(z)$ | Asymptotics | References |
|-----------------------------|----------------|-------------------|--|--------------------|
| Increasing Schröder trees | $\{1\}$ | $\frac{z^2}{1-z}$ | $\frac{1}{2}$ n! | [BGN19], Theorem I |
| C. M. Schröder trees | $\{1\}$ | (S(z) - z) | $\alpha n! n^2$ | Theorem I |
| Strictly monotonic Schröder | \mathbb{N}^* | $\frac{z^2}{1-z}$ | $\frac{1}{2}(n-1)! (\frac{1}{\ln 2})^n$ | [BGN19], Theorem I |
| Monotonic Schröder | \mathbb{N}^* | (S(z) - z) | $\kappa(n-1)! (\frac{1}{\ln 2})^n n^{2 \ln 2}$ | Theorem I |

Table 4: Comparison of the asymptotic behaviour of families of labelled Schröder trees. S(z) is the GF of Schröder trees.



Simulation for $n \in \{1, 100\}$ of Schröder trees with different increasing labellings divided by their expected asymptotic first order.

Conclusion and future works

- We studied a general parametrisable evolution process and showed general asymptotic enumeration formulas.
- We also studied three cases separately with their typical parameters → Sample uniformly and efficiently large trees.
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 Uniform random generation for any φ and r is hard in the general case (it relies on the generation of integer partitions).



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- In the three cases presented simplifications occur and trees of large sizes (up to 1000 leaves) can be uniformly sampled.



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- We developed a generic method to compute the compaction rate of increasing trees.
- We applied it on increasing binary trees and get the average compaction rate is $\Theta\left(\frac{n}{\ln n}\right)$ and on recursive tree to get $O\left(\frac{n}{\ln n}\right)$.

Publications and preprints

| O. Bodini, A. Genitrini, M. Naima | "Ranked Schröder trees". In Proceedings of the Sixteenth Workshop on Analytic Algorithmics and Combinatorics (ANALCO), 2019. |
|--|---|
| O. Bodini, A. Genitrini, M. Naima, A. Singh | "Families of Monotonic Trees: Combinatorial Enumeration and Asymptotics". In Proceedings of the 15th International Computer Science Symposium in Russia (CSR), 2020. |
| O. Bodini, A. Genitrini, C. Mailler, M. Naima | "Strict monotonic trees arising from evolutionary processes: combinatorial and probabilistic study". Submitted to a journal. Available on https://hal.sorbonne-universite.fr/hal-02865198 |
| O. Bodini, A. Genitrini, B. Gittenberger, I. Larcher, M. Naima | "Compaction for two models of logarithmic-depth trees: Analysis and Experiments" Submitted to a journal. Available on https://arxiv.org/abs/2005.12997 |

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Increasing labellings

We obtained results on different increasing labellings of tree structures counted by their number of leaves. What about trees in which we count all nodes as it is mostly the case?



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 Another interesting equation related to trees is their optimal representation memory.



Figure 1: (left) A binary tree of size 17. (right) Its compacted version that has size 5.

- Another interesting equation related to trees is their optimal representation memory.
- The idea is that in a single tree, some subtrees can be isomorphic and therefore when compressing the tree we can keep only one occurrence of a repeated subtree and put pointers to it.



Figure 1: (left) A binary tree of size 17. (right) Its compacted version that has size 5.

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- We found a generic method to obtain the average compaction rate of classes of increasing trees based on a perturbed generating function.
- We applied our approach to rederive known results on binary increasing trees and to obtain an upper bound on recursive trees $O(n/\ln n)$. We have reasons to believe that this bound is already sharp.

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- For the general case, the speciation is not convergent (Boltzmann sampling can not be applied).
- But we have a general recurrence that relies on integer partitions (Recursive generation and unranking can be applied).
- But the complexity of the recursive generation corresponds to the one of generating integer partitions.

Improved algorithms for the three particular cases

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 For the model of increasing Schröder trees (φ(z) = z/(1 - z) and r = {1}) we have an incremental process (no recursive generation or operations on big numbers).

Simulation of some parameters



Figure 3: The number of *d*-ary nodes and the number of iteration steps. (up left) Increasing Schröder trees. (up right) Strict monotonic Schröder trees. (down) general monotonic Schröder trees.