Pointing, asymptotics, and random generation in unlabelled classes

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Motivations

Automatic methods for

- Enumeration (exact/asymptotic)
- Random generation (cf [Flajolet,F,Pivoteau'07])

in the unlabelled setting.

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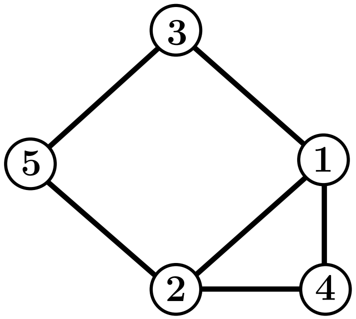
in the unlabelled setting.

References:

- Short version in SODA'07
- Long version written in the framework of "Combinatorial species", cf [Bergeron, Labelle, Leroux'98]

Labelled/Unlabelled structures

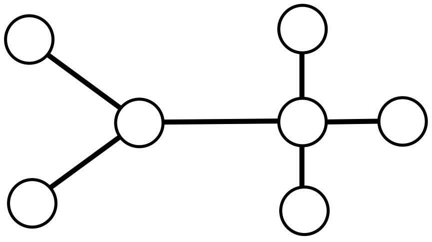
- labelled class $\mathcal{C} = \cup_n \mathcal{C}_n$



Labeled graph of size 5

$$\text{EGF}: \quad C(x) = \sum_n \frac{1}{n!} c_n x^n, \ \text{with } c_n = |\mathcal{C}_n|$$

- Unlabelled class $\widetilde{\mathcal{C}} = \cup_n \widetilde{\mathcal{C}}_n$



Unlabeled tree of size 7

$$\text{OGF}: \quad C(x) = \sum_n \widetilde{c}_n x^n, \ \text{with } \widetilde{c}_n = |\widetilde{\mathcal{C}}_n|$$

Plan

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  - Pointing + recursive decomp. + gen. functions
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  - Examples: trees, planar graphs...
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  - Difficulties due to symmetries
  - Solution: unbiased pointing $+$ Pólya theory
- Application to asymptotic enumeration
- Application to random generation:
  $\Rightarrow$ Boltzmann samplers without rejection

Decomposition strategy for labelled structures

Dictionary for EGF

- labelled class $\mathcal{C} = \cup_n \mathcal{C}_n$

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- Simple computation rule for each construction:

Disjoint union	$\mathcal{C} = \mathcal{A} + \mathcal{B}$	$C(x) = A(x) + B(x)$
Cartesion product	$\mathcal{C} = \mathcal{A} \times \mathcal{B}$	$C(x) = A(x) \cdot B(x)$
Set	$\mathcal{C} = \text{Set}(\mathcal{A})$	$C(x) = \exp(A(x))$
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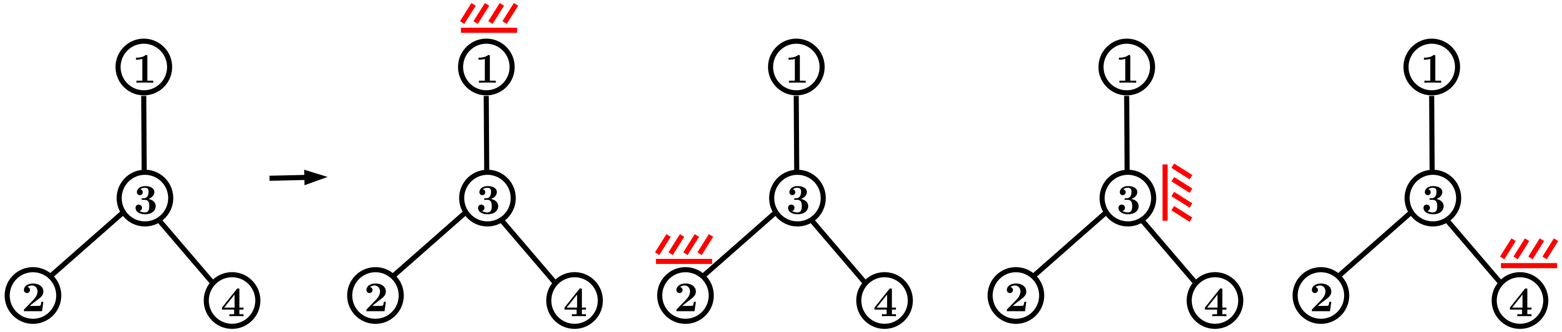
- **Remark.** Substitution rule implies Set rule since the EGF of the class Set is $\exp(z)$ (same for cycle, set, unoriented sequence, etc...)

Decomposition strategy for trees

- **Goal:** find t_n the number of (unrooted) trees of size n
- Important tool: pointing: $\mathcal{A} \mapsto \mathcal{A}^\bullet$
  Let r_n be the number of rooted trees of size n

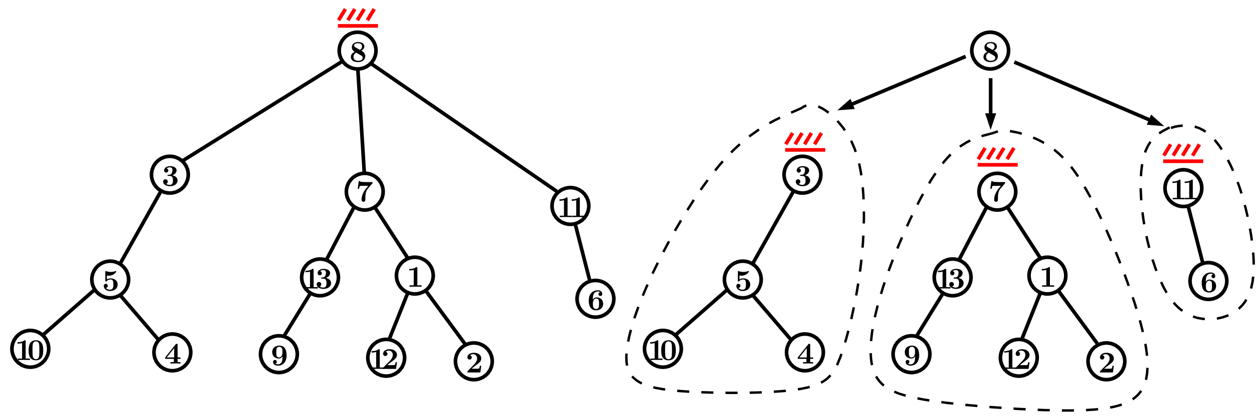


$$r_n = n \cdot t_n$$

$\Rightarrow$ Counting trees reduces to counting rooted trees.

Rooted trees are decomposable

- The class $\mathcal{R}$ of rooted trees satisfies the decomposition



$$\mathcal{R} = \mathcal{Z} \times \text{Set}(\mathcal{R}) \Rightarrow R(x) = x \exp(R(x))$$

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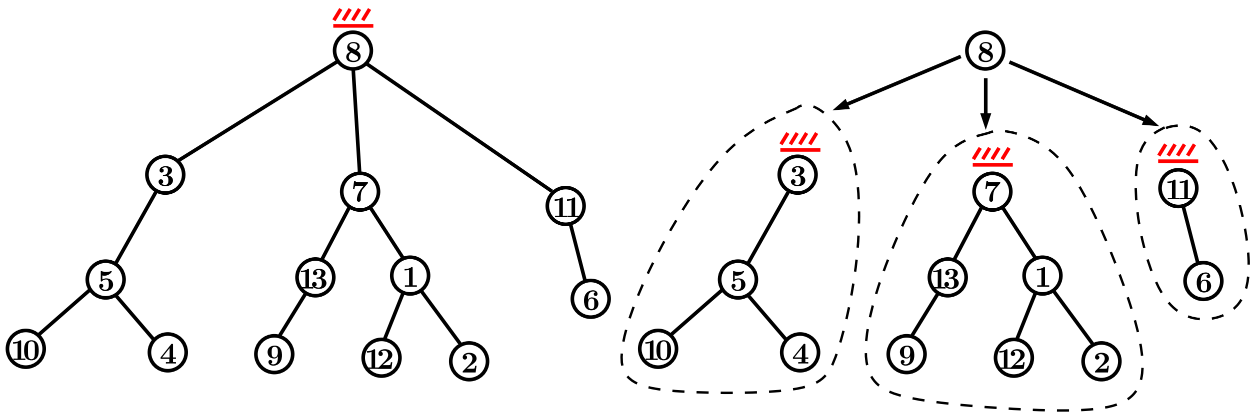


$$\mathcal{R} = \mathcal{Z} \times \mathrm{Set}(\mathcal{R}) \Rightarrow R(x) = x\exp(R(x))$$

- Lagrange inversion formula
  inverse of $R(x)$ is $R^{(-1)}(y) = y\exp(-y))$
  $\Rightarrow$ Rooted trees: $r_n = n^{n-1} \Rightarrow$ Trees: $c_n = n^{n-2}$

Counting labelled trees: summary

- Decomposition of rooted trees

$$R(x) = x \exp(R(x))$$

yields $r_n = n^{n-1}$ from Lagrange inversion formula

- Pointing relation: $t_n = r_n/n$:

$$R(x) = xT'(x)$$

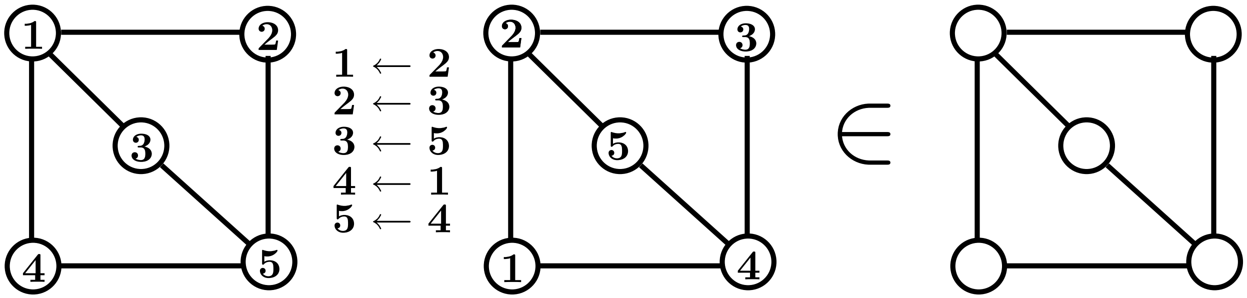
yields $\boxed{t_n = n^{n-2}}$

Same method applies for many classes (planar graphs)

Adaptation to the unlabelled setting

Unlabelled setting

- Unlabelled structures=labelled structures up to relabeling



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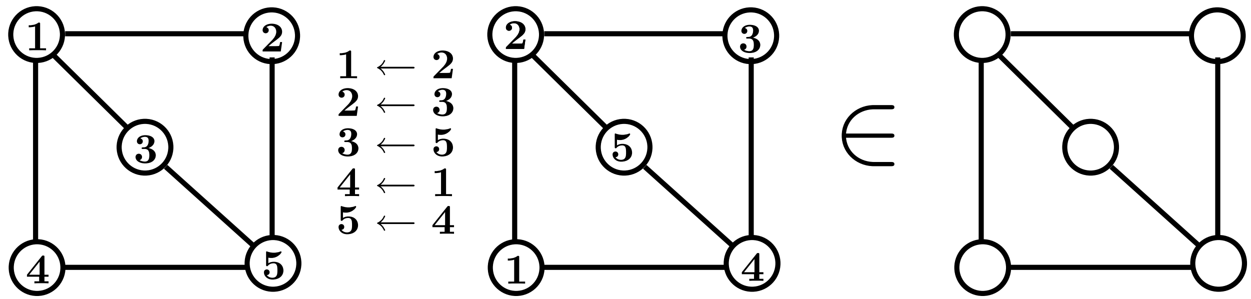
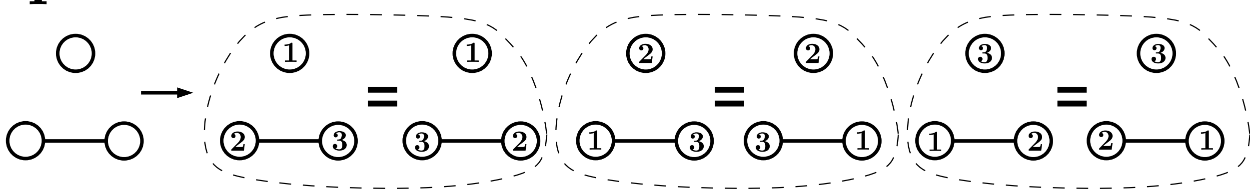
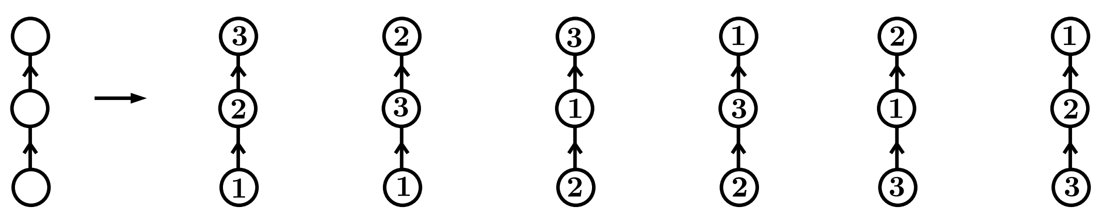


- **Examples:**



3 labeled objects (instead of $3! = 6$)



6 labeled objects (no symmetry)

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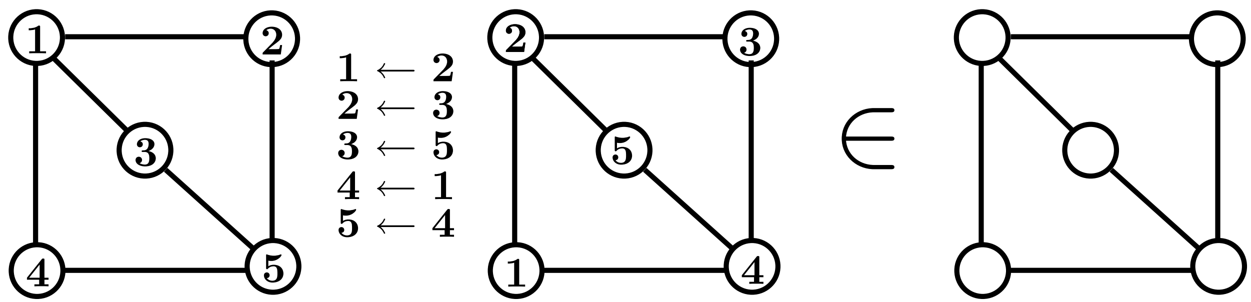

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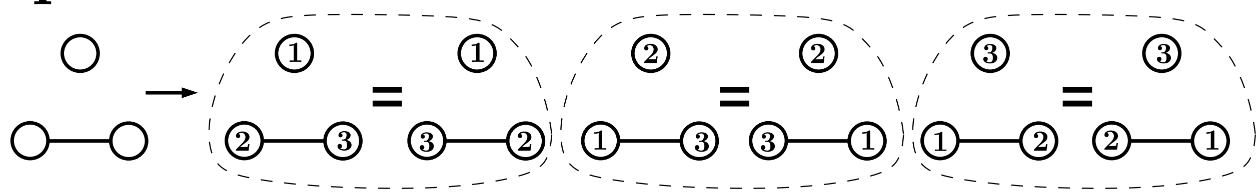

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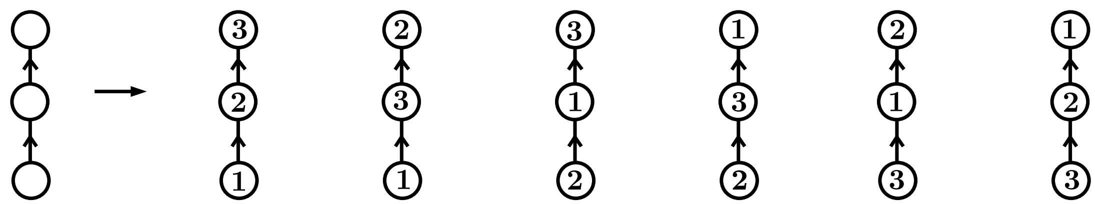


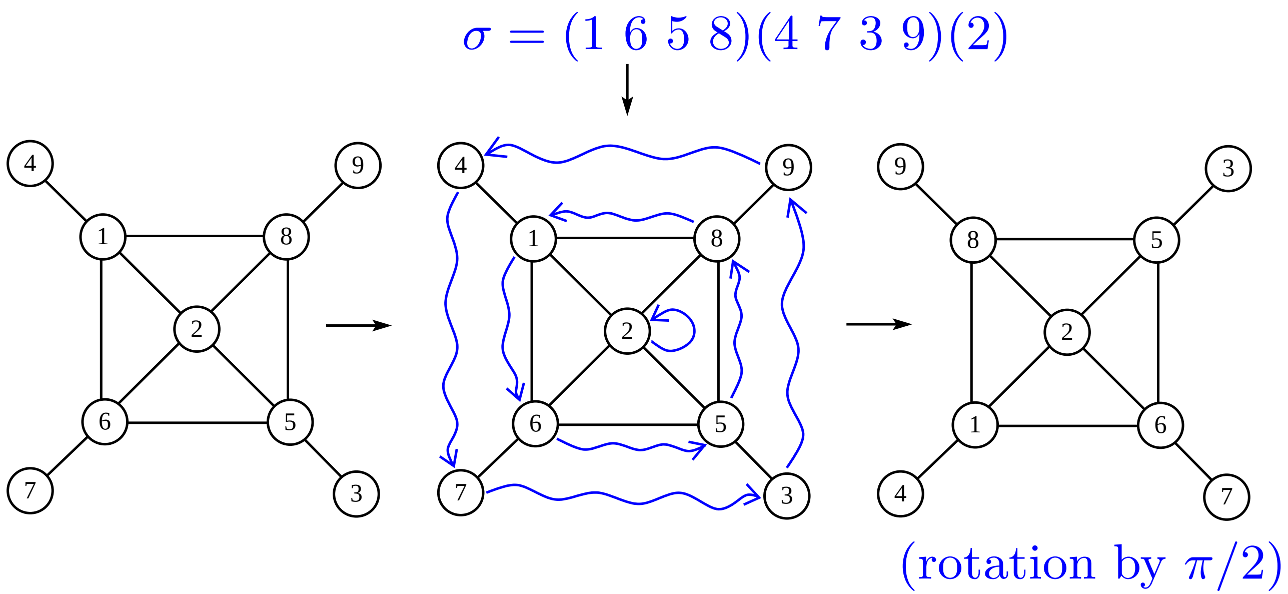
6 labeled objects (no symmetry)

- Unlabelled struct. size $n \longrightarrow$ at most $n!$ labelled structures.
$\Rightarrow \frac{1}{n!} a_n^{\text{label.}} \leq a_n^{\text{unlabel.}} \Rightarrow$ (EGF) $A(x) \preceq \widetilde{A}(x)$ (OGF).

Symmetries

Let $\mathcal{A}$ be a labelled class,

- A symmetry of size n on $\mathcal{A}$ is a pair $(\sigma \in \mathfrak{S}_n, A \in \mathcal{A}_n)$ such that A is fixed by the action of σ.

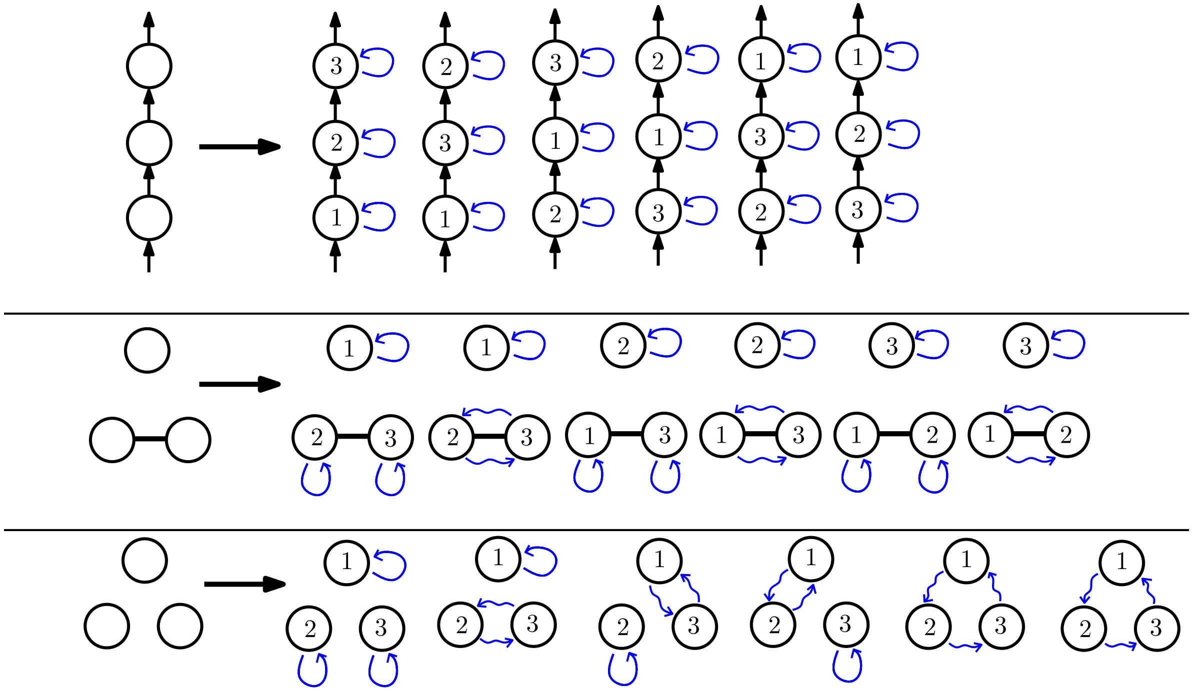


Burnside's lemma

Given $\mathcal{A}$ a labelled class (species of structures) let

$\widetilde{\mathcal{A}} = \mathcal{A}/\text{isomorphisms}, \;\; \text{Sym}(\mathcal{A}) = \{\text{Symmetries from } \mathcal{A}\}$

- Burnside's lemma $\Rightarrow \text{Sym}(\mathcal{A})_n \simeq n! \times \widetilde{\mathcal{A}}_n$



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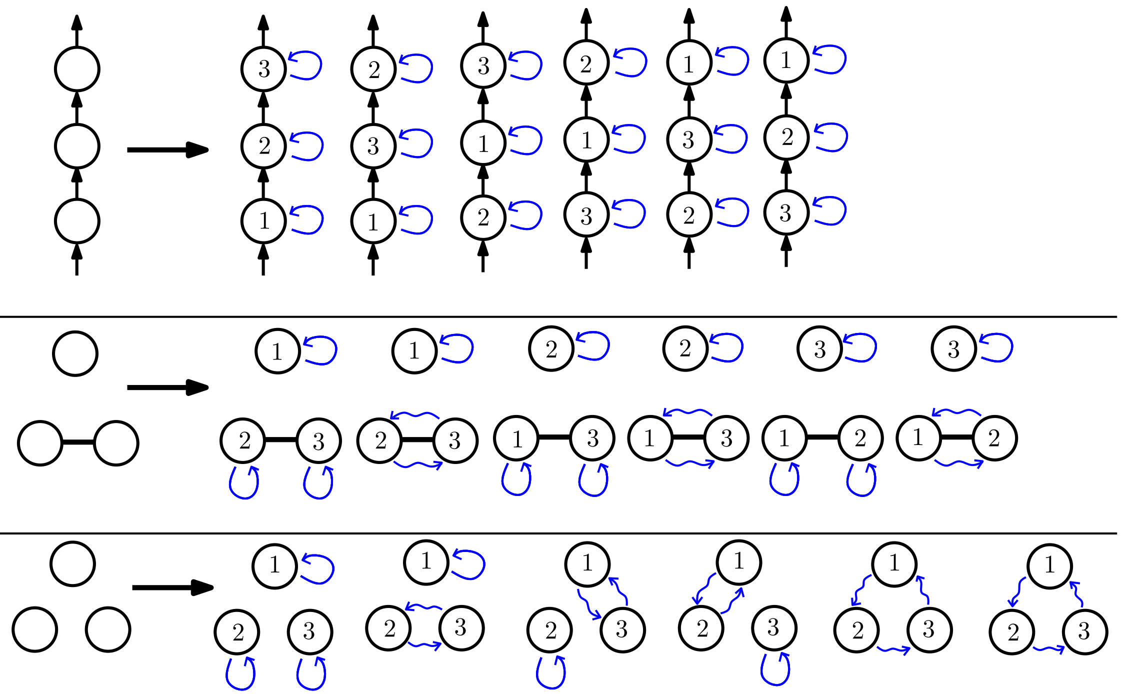


- Hence $\boxed{\text{EGF of Sym}(\mathcal{A}) = \widetilde{A}(x) \text{ (OGF)}}$

Cycle index sum

Let $\mathcal{A}$ be a labelled class, $\mathrm{Sym}(\mathcal{A})$ the symmetry class.

- Refined weight for $(\sigma, A) \in \mathrm{Sym}(\mathcal{A})$

$$W(\sigma, A) := \frac{1}{n!} s_1^{c_1(\sigma)} s_2^{c_2(\sigma)} \cdots s_n^{c_n(\sigma)}$$

  where $c_i(\sigma) = \#\{\text{cycles length } i \text{ in } \sigma\}$

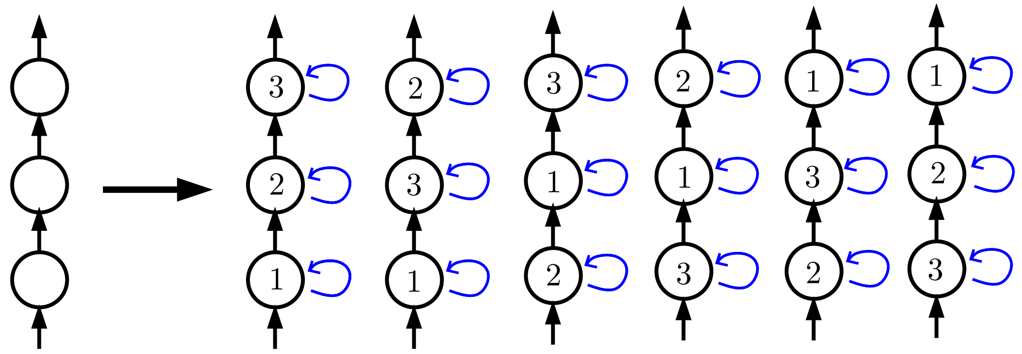
- Cycle index sum of $\mathcal{A}$ (cf Pólya) is the multivariate series

$$Z_{\mathcal{A}}(s_1, s_2, \ldots) = \sum_{\sigma \cdot A = A} W_{(\sigma, A)}$$

$$= \sum_{n \geq 1} \frac{1}{n!} \sum_{\sigma \in \mathfrak{S}_n} s_1^{c_1} \ldots s_n^{c_n} \ \#(\mathrm{Fix}_\sigma)$$

- OGF of $\widetilde{\mathcal{A}}$= EGF of $\mathrm{Sym}(\mathcal{A}) = Z_{\mathcal{A}}(x, x^2, x^3, \ldots)$

Examples of cycle index sums



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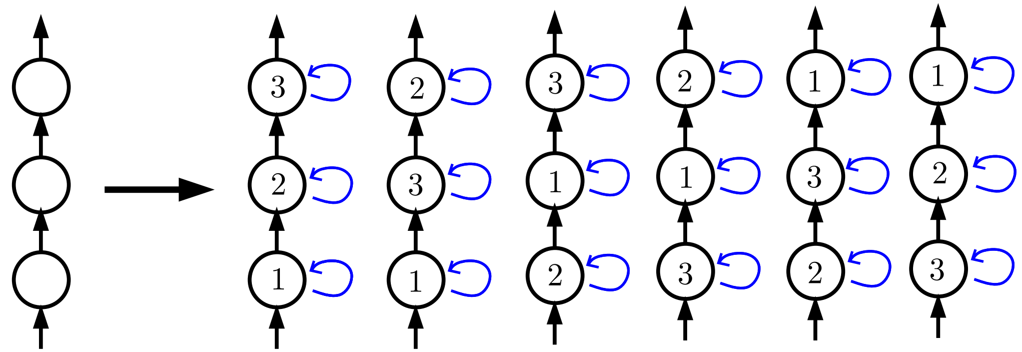

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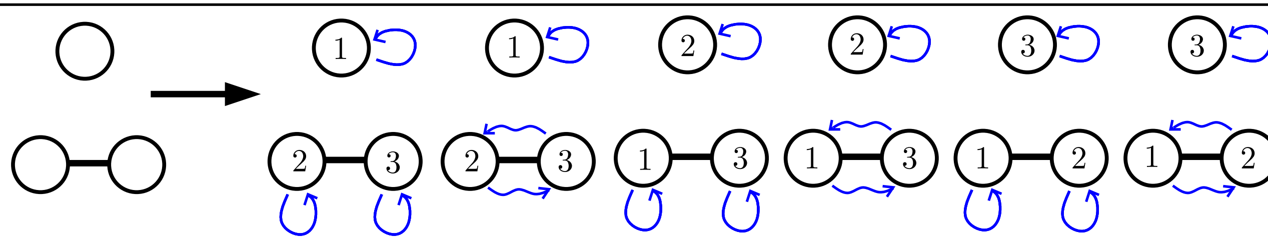

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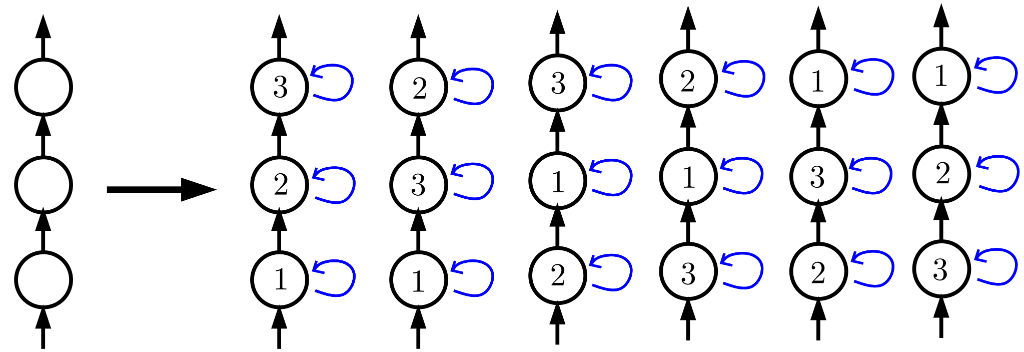

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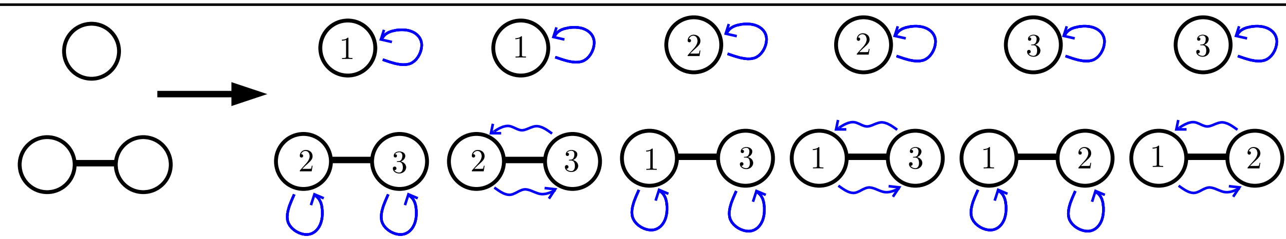

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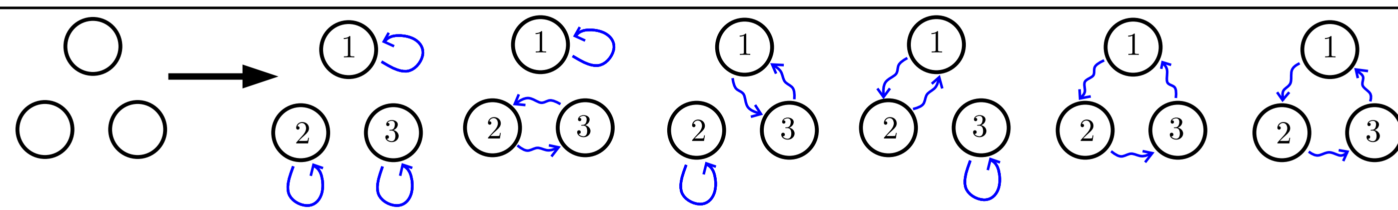

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Dictionary for OGF

- Unlabelled class $\widetilde{\mathcal{C}} = \cup_n \mathcal{C}_n / \mathfrak{S}_n \quad \widetilde{c_n} = \mathrm{Card}(\widetilde{\mathcal{C}_n})$

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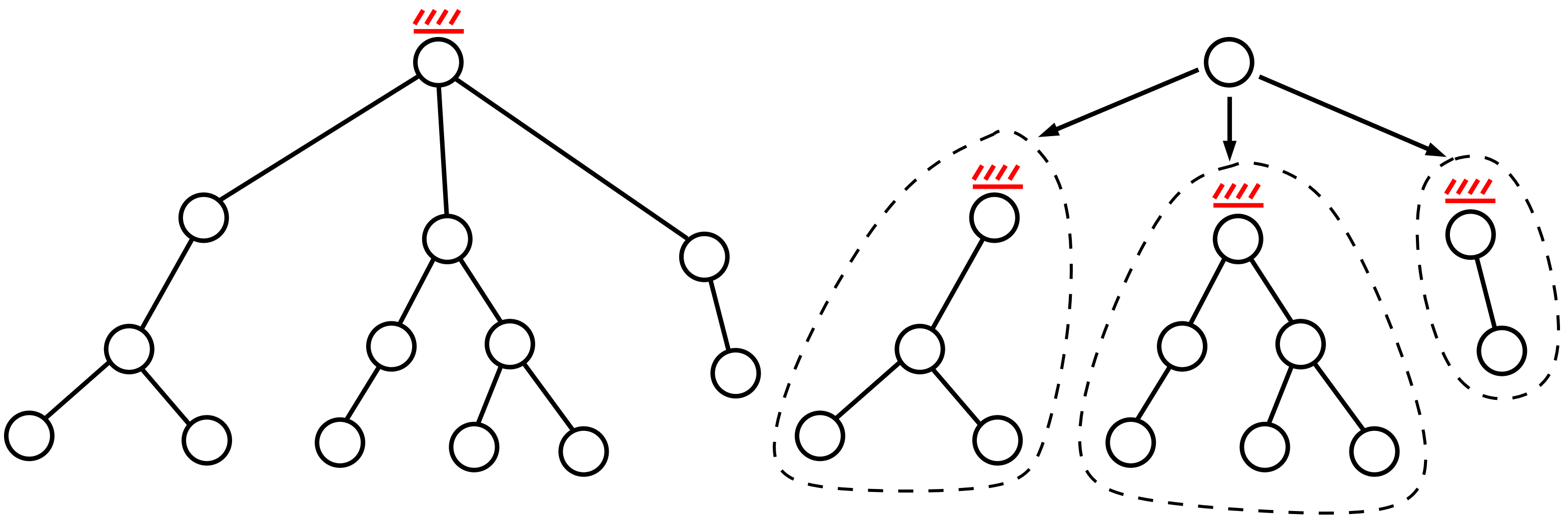
- **Remark:** $\mathrm{Set}(\mathcal{A}) = \mathrm{Set} \circ \mathcal{A}$, computation rule for $\circ$ implies the one for Set using $Z_{\mathrm{Set}} = \exp(\sum_{i \geq 1} s_i/i)$

Example: rooted trees

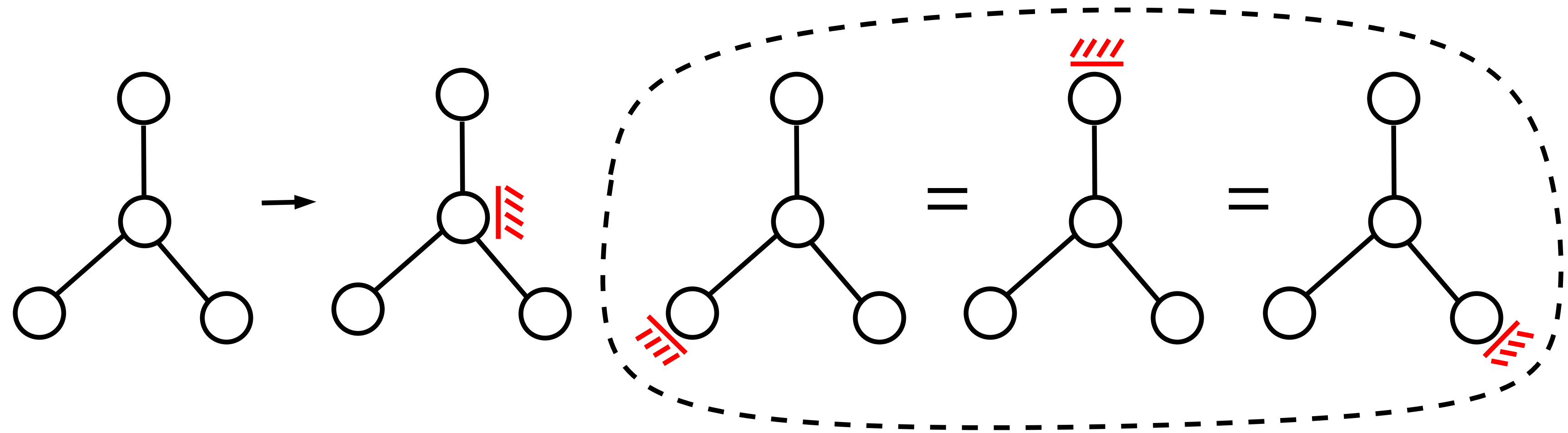
Decomposition at the root:



$$\mathcal{R} = \mathcal{Z} \times \mathrm{Set}(\mathcal{R}) \Rightarrow R(z) = z \exp\Big(\sum_{i \geq 1} \frac{1}{i} R(z^i)\Big)$$

$\Rightarrow$ recurrence formula for $[z^n]R(z)$

Count rooted $\not\Rightarrow$ count unrooted



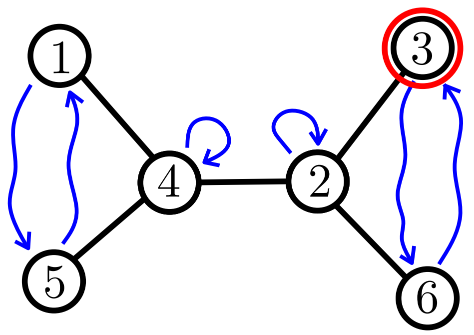
tree size 4 **2 rooted trees (instead of 4)**

In general $n \cdot a_n^{\text{unrooted}} > a_n^{\text{rooted}}$ (symmetries)

Question: $n \cdot a_n^{\text{unrooted}} = ?$

Pointing symmetries

Pointed symmetry = symmetry + marked atom



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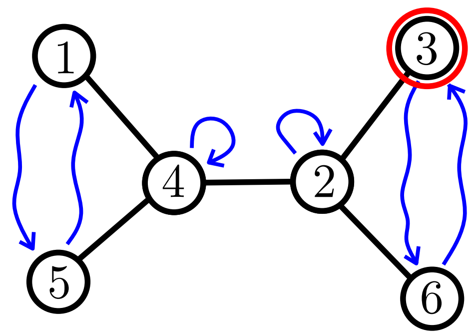

In size n we have

$$\widetilde{\mathcal{A}} \xrightarrow[\times n!]{} \mathrm{Sym}(\mathcal{A}) \xrightarrow{\times n} (\mathrm{Sym}(\mathcal{A}))^{\bullet}$$

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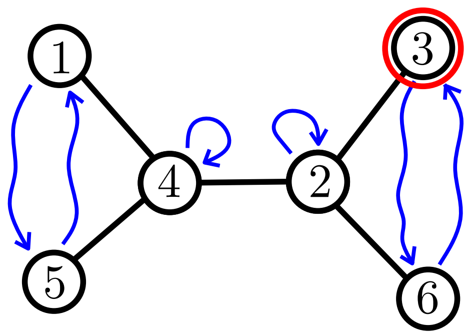

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Look for a class $\mathcal{P}$ such that $\mathrm{Sym}(\mathcal{P}) \simeq (\mathrm{Sym}(\mathcal{A}))^{\bullet}$

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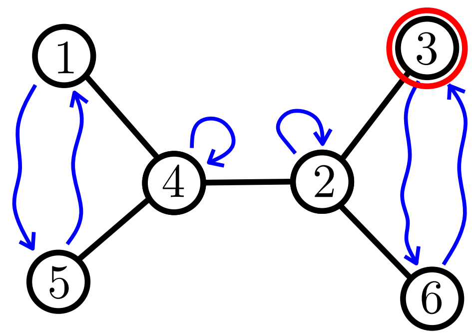

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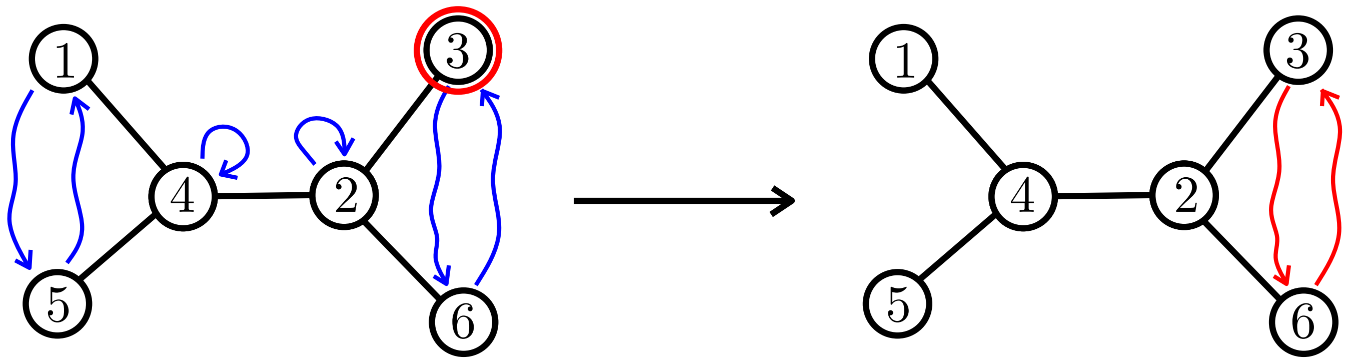
(rk: $\mathrm{Sym}(\mathcal{A}^\bullet) \subseteq (\mathrm{Sym}(\mathcal{A}))^\bullet$)

Cycle-pointed structures

Definition: Cycle-pointed structure=structure A + cycle c such that there exists (at least) one automorphism of A having c as one of its cycles.



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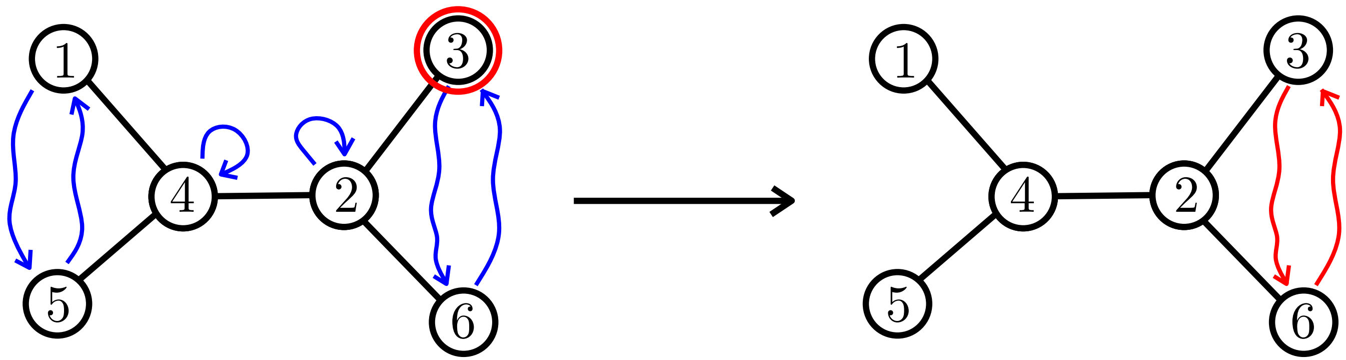


Pointed symmetry **cycle-pointed structure**

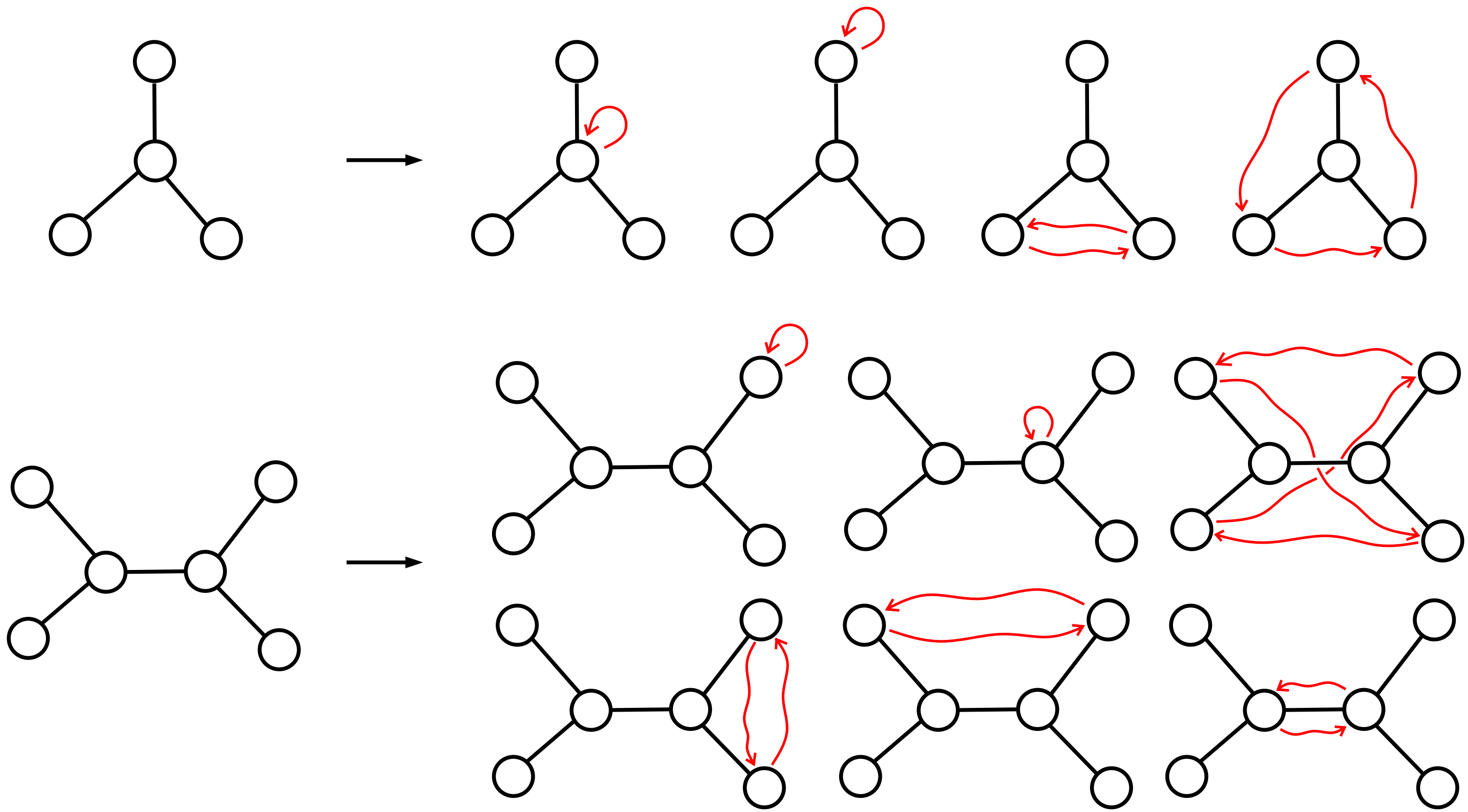
Let $\mathcal{A}^\circ = \{\text{cycle} - \text{pointed structures from } \mathcal{A}\}$. Then

$$\mathrm{Sym}(\mathcal{A}^\circ) \simeq (\mathrm{Sym}(\mathcal{A}))^\bullet$$

Cycle-pointing is unbiased

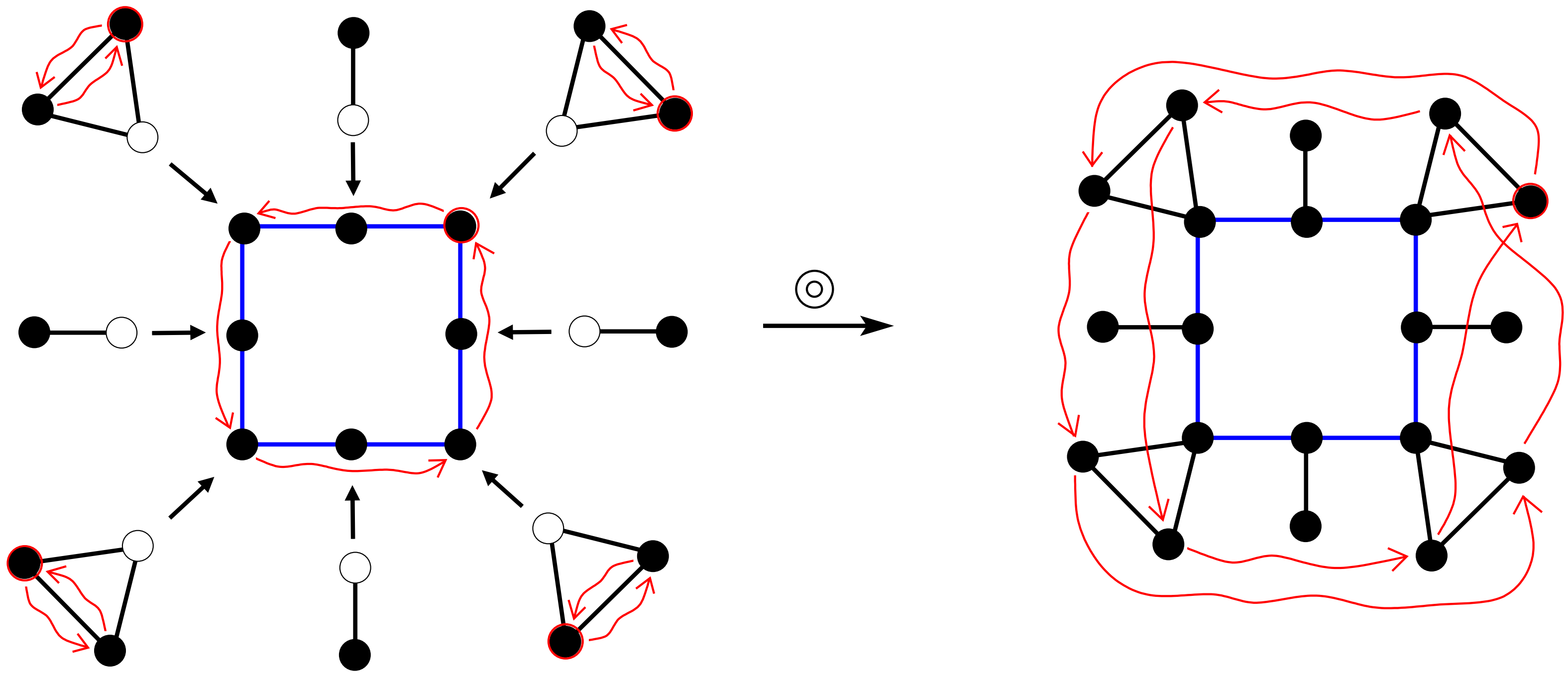
Theorem: An unlabelled structure of size n gives rise to n unlabelled cycle-pointed structures (cf Parker's lemma).

$$\boxed{\widetilde{\mathcal{A}_n^{\circ}} \simeq n \times \widetilde{\mathcal{A}_n}}$$



Pointing the classical constructions

- $(\mathcal{A} + \mathcal{B})^\circ = \mathcal{A}^\circ + \mathcal{B}^\circ$
- $(\mathcal{A} \times \mathcal{B})^\circ = \mathcal{A}^\circ \times \mathcal{B} + \mathcal{A} \times \mathcal{B}^\circ$
- $(\mathcal{A} \circ \mathcal{B})^\circ = \mathcal{A}^\circ \circledcirc \mathcal{B}$



Application: counting trees (1)

Decomposition of cycle-pointed trees (3 lines)

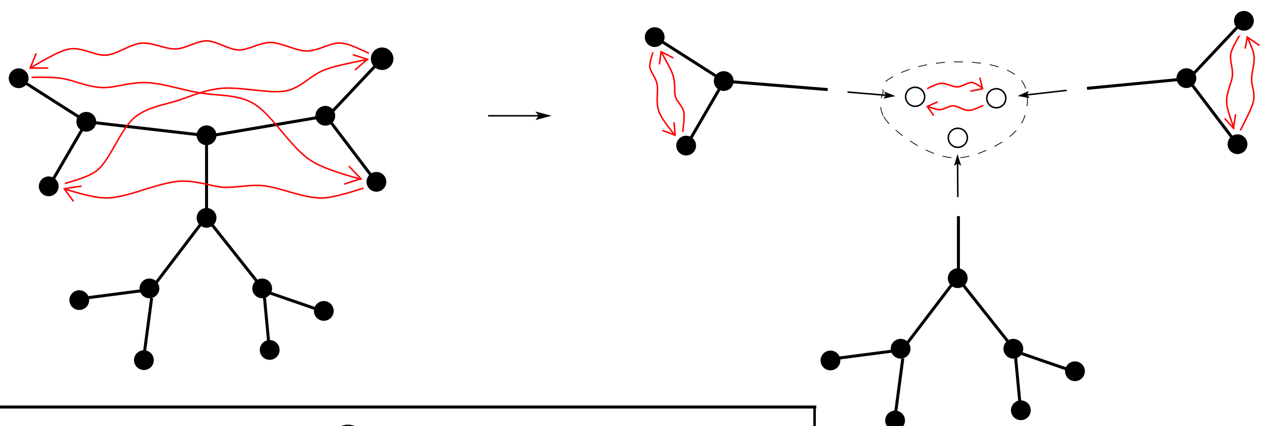
- Dichotomy: pointed cycle has length 1 or ≥ 2:

$$1)\ \mathcal{T}^{\circ} = \mathcal{R} + \mathcal{T}^{\circledast}$$

- Rooted trees ($\mathcal{R}$) are decomposed at the root

$$2)\ \mathcal{R} = \mathcal{Z} \times \mathrm{Set}(\mathcal{R})$$

- Symmetric cycle-pointed trees ($\mathcal{T}^{\circledast}$) are decomposed at a centre of symmetry.



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translate to equation system
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extract coefficients

n	1	2	3	4	5	6	7	8	9
$\widetilde{a_n^{\circ}}$	1	2	3	8	15	36	77	184	423
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Exact counting results

Theorem: [Bergeron,Labelle,Leroux],

For any class $\mathcal{A}$ decomposable in terms of

- basic classes $\{\mathbf{1}, \mathcal{Z}, \mathrm{Seq}, \mathrm{Cyc}, \mathrm{Set}\}$,
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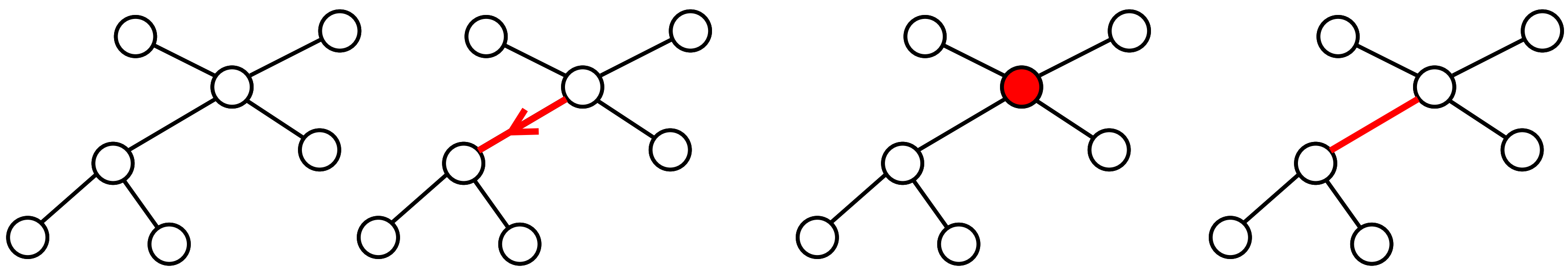
(includes tree families, outerplanar graphs,...)

Another approach

- Dissimilarity characteristic formula (Otter)
- Dissymmetry theorem (Robinson, Leroux):

$$\mathcal{T} \quad + \quad \mathcal{T}^{\uparrow} \quad \simeq \quad \mathcal{T}^{\bullet} \quad + \quad \mathcal{T}^{\circ\!-\!\circ}$$



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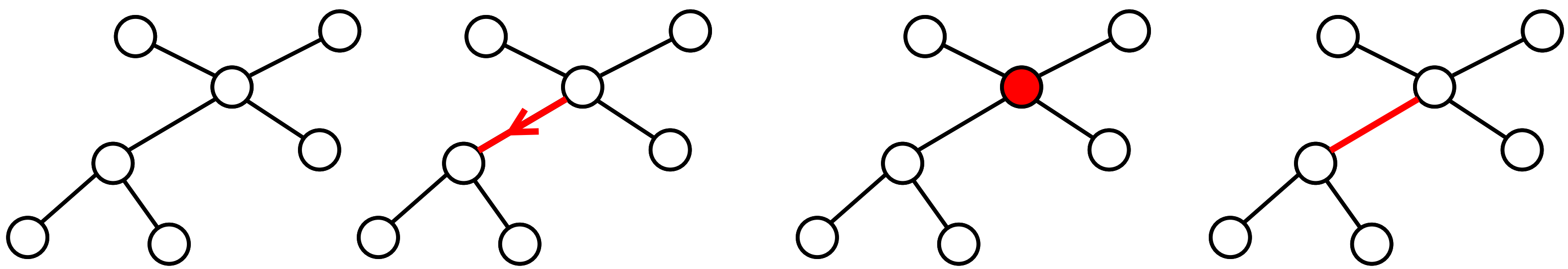

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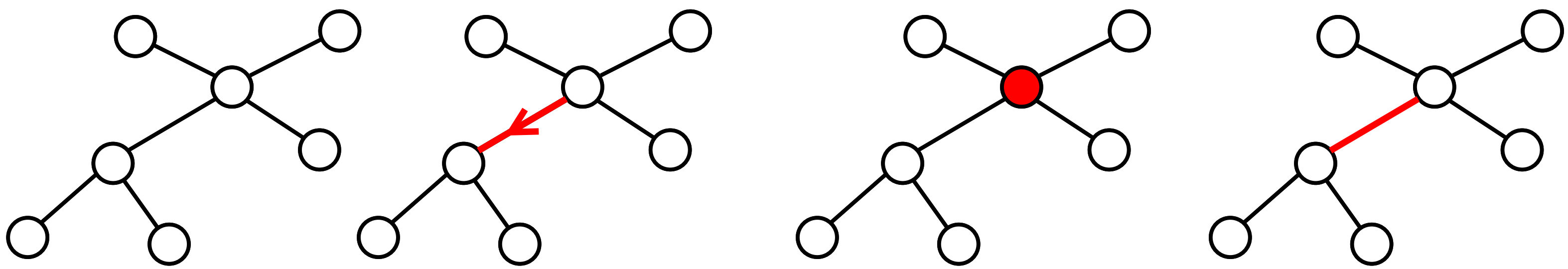

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(agrees with $xt'(x) = xR'(x)(1 - R(x)) + x^2 R'(x^2)$)

Application to asymptotic enumeration

Asymptotic scheme

Main result: "universality" of asymptotic behaviour

$$|\widetilde{\mathcal{A}_n}| \sim c\,\gamma^n n^{-5/2}$$

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Scheme:

- Decompose cycle-pointed class $\mathcal{A}^\circ$
  $\Rightarrow$ Equation for $\widetilde{A^\circ}(x)$
- Drmota-Lalley-Woods $\Rightarrow \widetilde{A^\circ}(x)$ has square-root sing.
- Transfer theorem [Flajolet-Odlyzko] $\Rightarrow |\widetilde{\mathcal{A}_n^\circ}| \sim c\,\gamma^n n^{-3/2}$
- Pointing relation: $|\widetilde{\mathcal{A}_n}| = \frac{1}{n}|\widetilde{\mathcal{A}_n^\circ}| \sim c\,\gamma^n n^{-5/2}$

Illustration on trees

- Rooted labelled trees: $y = L(z)$ satisfies

$$y = z\exp(y)$$

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(Rk: $\mathbb{E}_n$(#dissimilar vertices in tree) $\sim n/G(\rho)$)

Asymptotic using dissym. theorem

$$t(z) = R(z) - \frac{1}{2}(R(z)^2 - R(z^2))$$

Square-root expansion: $R(z) = 1 - *\sqrt{1 - z/\rho} + \cdots$

$\Rightarrow$ square-root terms cancel out, $t(z)$ " $\leq$ " $(1 - z/\rho)^{3/2}$

But $zt'(z) \geq R(z)$, so $t(z)$ " $\geq$ " $(1 - z/\rho)^{3/2}$

Hence (transfer theorem):

$$[z^n]t(z) \sim c\,\rho^{-n} n^{-5/2}$$

(Rk: Cancellation proof uneasy if "big" functional equation)

Application to random generation

General methods

Two sampling methods giving uniform distribution

- Recursive method (Nijenhuis-Wilf'78):

$$\mathbb{P}(\gamma \in \mathcal{C}_n) = \frac{1}{c_n} \quad \text{[Fixed size]}$$

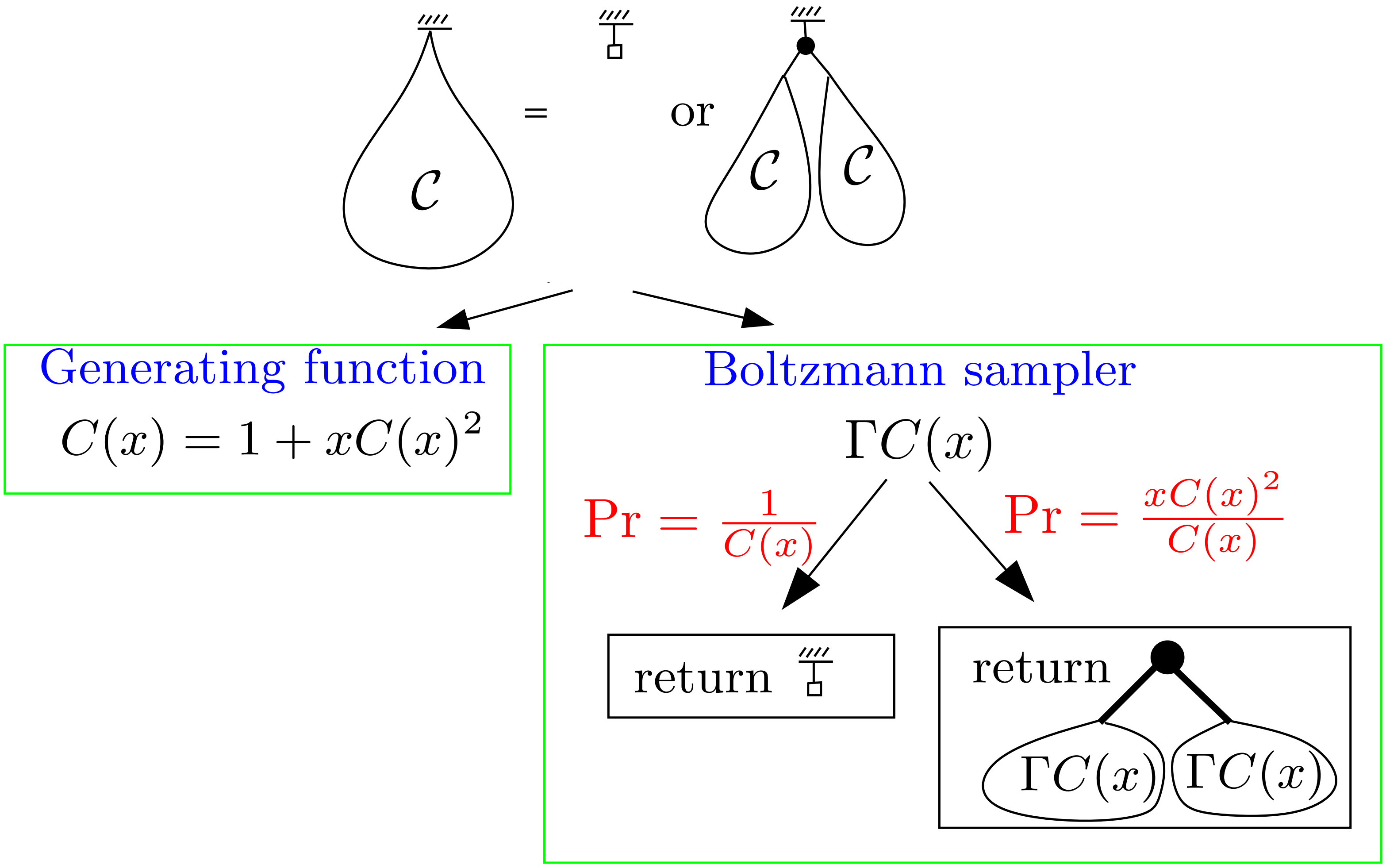
  - Based on coefficients:
    $\mathcal{C} = \mathcal{A} + \mathcal{B} \Rightarrow \mathbb{P}(\gamma \in \mathcal{A}_n) = \frac{a_n}{c_n}$

- Boltzmann samplers (Duchon, Flajolet, Louchard, Schaeffer'02)

$$\mathbb{P}(\gamma \in \mathcal{C}) = \frac{x^{|\gamma|}}{C(x)} \quad \text{[Whole class]}$$

  - Based on gen. funct.
    $\mathcal{C} = \mathcal{A} + \mathcal{B} \Rightarrow \mathbb{P}(\gamma \in \mathcal{A}) = \frac{A(x)}{C(x)}$

Boltzmann samplers: example



Results

Theorem: [Duchon et al'02], [Flajolet et al'07]
For any class $\mathcal{A}$ decomposable in terms of

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Pólya-Boltzmann samplers

- Ordinary Boltzmann samplers:

$$\widetilde{A}(x) = \sum_{\gamma \in \widetilde{\mathcal{A}}} x^{|\gamma|} \;\Rightarrow\; \mathbb{P}(\gamma) = \frac{x^{|\gamma|}}{\widetilde{A}(x)}$$

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- Recover ordinary Boltzmann sampler using specialization

$$Z_{\mathcal{C}}(x, x^2, \ldots) = C(x) \;\Rightarrow\; \Gamma Z_{\mathcal{C}}(x, x^2, \ldots) = \Gamma \widetilde{C}(x)$$

Sampler for trees

Let $t(x)$ be the OGF of (unrooted) trees.

1) Translate the equation

$$R(x) = \exp(\sum_{i\geq 1} \frac{1}{i} R(x^i))$$

into a Boltzmann sampler for $\widetilde{\mathcal{R}}$ cf [Flajolet et al'07] (superposition of Poisson laws)

2) Translate the equation

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(Also recursive sampler by Wilf using "centre of gravity")

Open problems

- Refined complexity analysis of Pólya-Boltzmann samplers, cf [Pivoteau, Salvy, Soria'08]
- Boltzmann sampling with catalytic variables
- For which recursive specification can we determine the growth rate automatically ?
- Use Boltzmann samplers to study random unlabelled structures, cf [Panagiotou, Steger].