Pointing, asymptotics, and random generation in unlabelled classes

Éric Fusy

LIX, École Polytechnique (Paris)

Joint work with Manuel Bodirsky, Mihyun Kang and Stefan Vigerske

Motivations

Automatic methods for

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

in the unlabelled setting.

Motivations

Automatic methods for

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

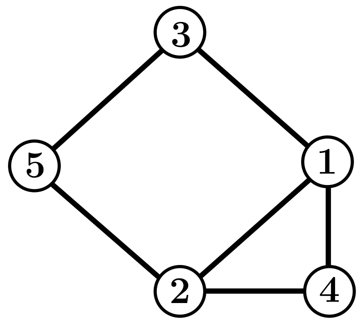
in the unlabelled setting.

References:

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

Labelled/Unlabelled structures

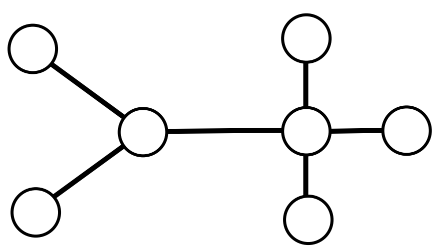
- labelled class $\mathcal{C} = \cup_n \mathcal{C}_n$



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

- Decomposition strategy for labelled structures
  - Pointing + recursive decomp. + gen. functions
  - Examples: trees, planar graphs...

Plan

- Decomposition strategy for labelled structures
  - Pointing + recursive decomp. + gen. functions
  - Examples: trees, planar graphs...
- We adapt the method to the unlabelled setting
  - Difficulties due to symmetries
  - Solution: unbiased pointing + Pólya theory

Plan

- Decomposition strategy for labelled structures
  - Pointing + recursive decomp. + gen. functions
  - Examples: trees, planar graphs...
- We adapt the method to the unlabelled setting
  - Difficulties due to symmetries
  - Solution: unbiased pointing + Pólya theory
- Application to asymptotic enumeration

Plan

- Decomposition strategy for labelled structures
  - Pointing + recursive decomp. + gen. functions
  - Examples: trees, planar graphs...
- We adapt the method to the unlabelled setting
  - 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 $\mathcal{C} = \cup_n \mathcal{C}_n$

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

- 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	$\mathcal{C} = \mathrm{Set}(\mathcal{A})$	$C(x) = \exp(A(x))$
Substitution	$\mathcal{C} = \mathcal{A} \circ \mathcal{B}$	$C(x) = A(B(x))$

Dictionary for EGF

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

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

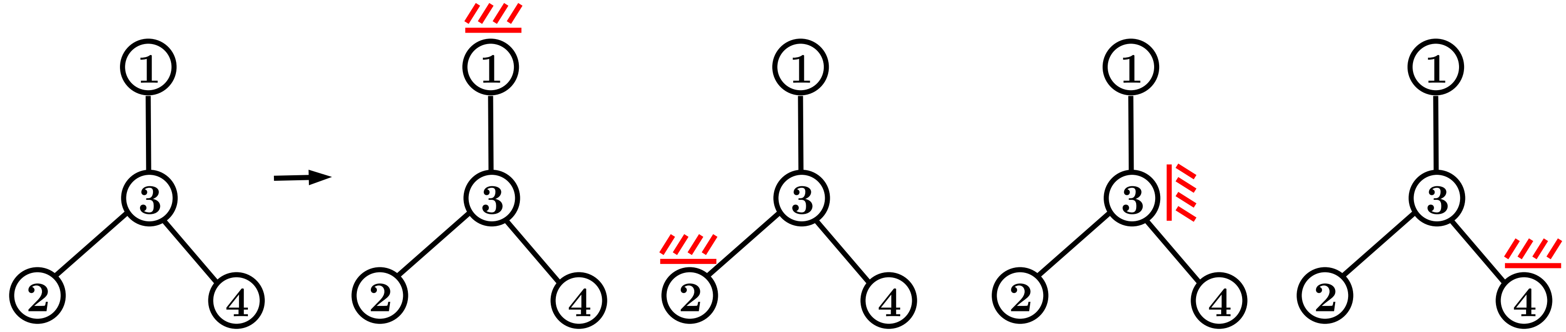
- Simple computation rule for each construction:

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	$\mathcal{C} = \mathrm{Set}(\mathcal{A})$	$C(x) = \exp(A(x))$
Substitution	$\mathcal{C} = \mathcal{A} \circ \mathcal{B}$	$C(x) = A(B(x))$

- **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

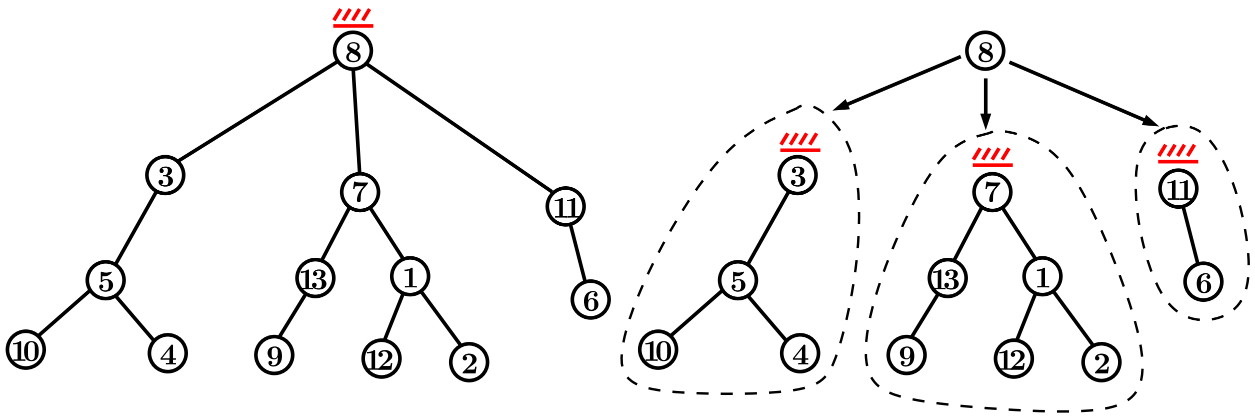


$$\boxed{r_n = n \cdot t_n}$$

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

Rooted trees are decomposable

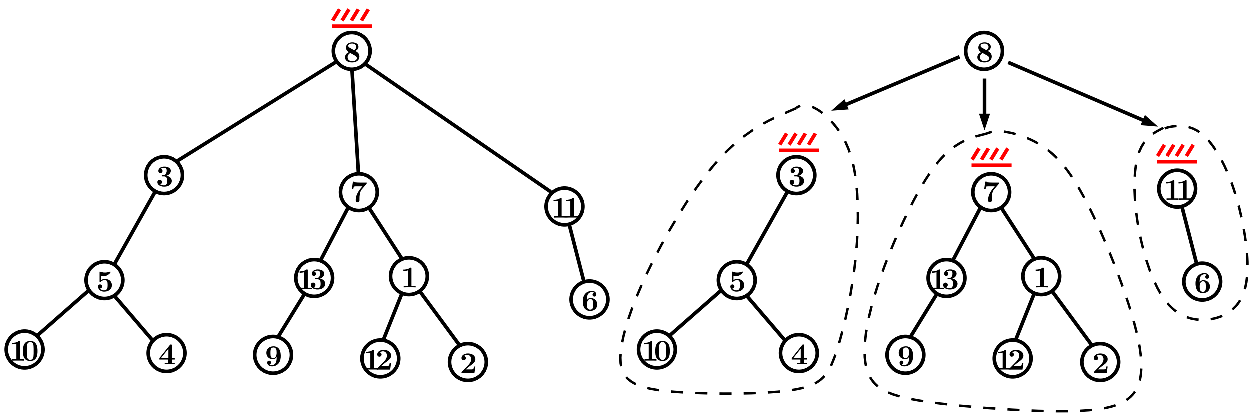
- The class $\mathcal{R}$ of rooted trees satisfies the decomposition



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

Rooted trees are decomposable

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



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

- 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: $t_n = r_n/n$:

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

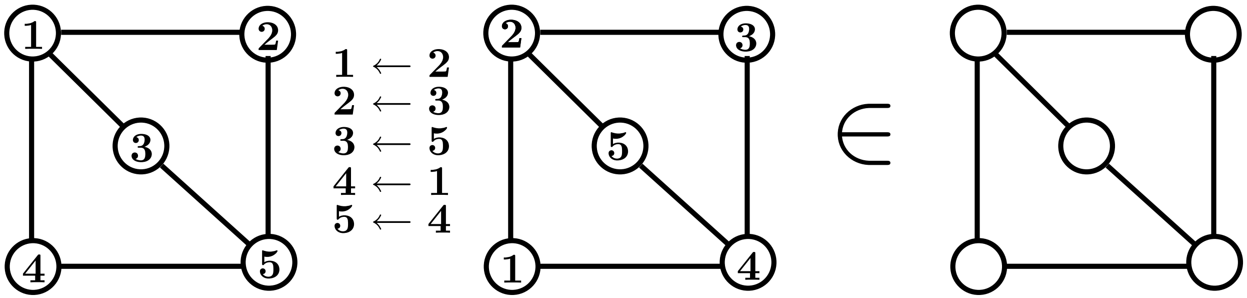
yields $\boxed{t_n = n^{n-2}}$

Same method applies for many classes (planar graphs)

Adaptation to the unlabelled setting

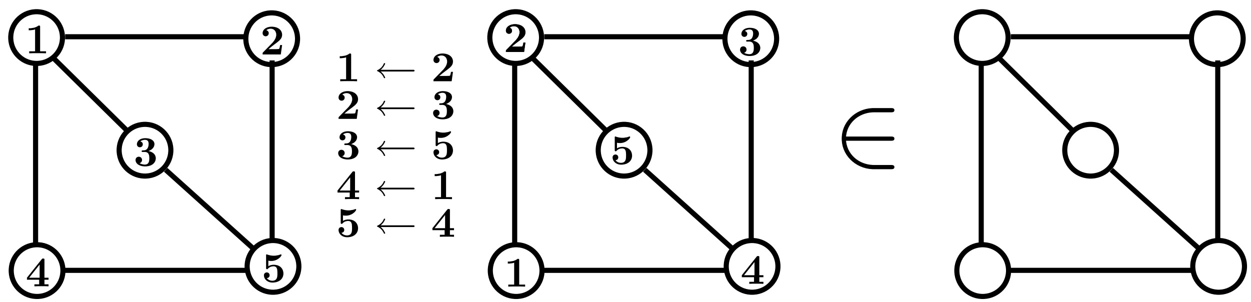
Unlabelled setting

- Unlabelled structures=labelled structures up to relabeling

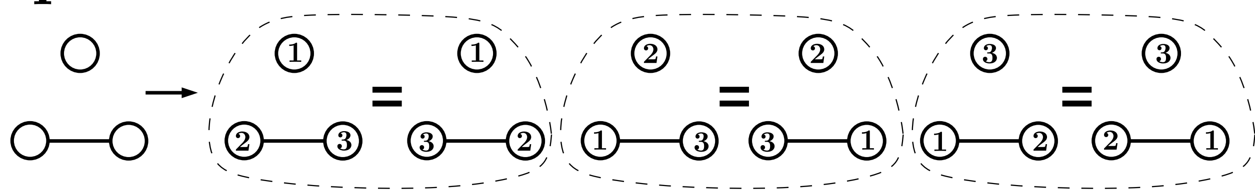


Unlabelled setting

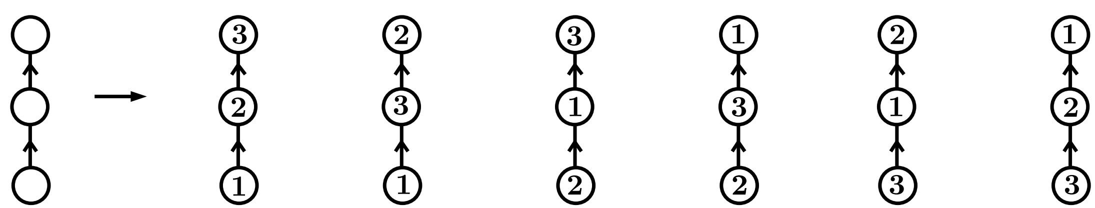
- Unlabelled structures=labelled structures up to relabeling



- **Examples:**



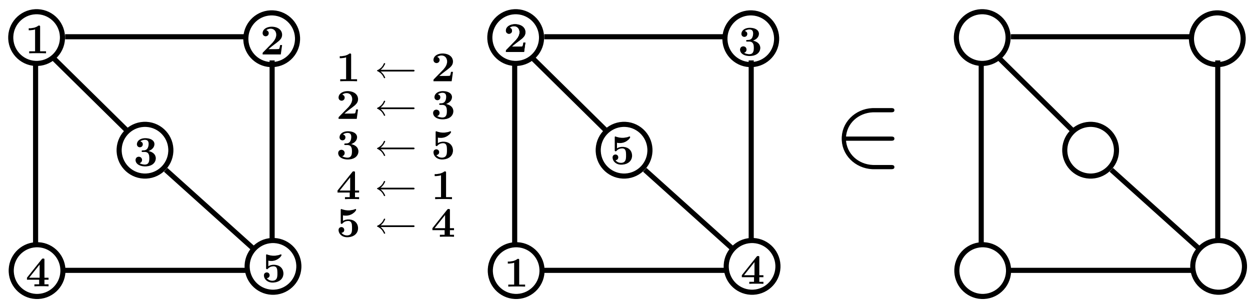
3 labeled objects (instead of $3! = 6$)



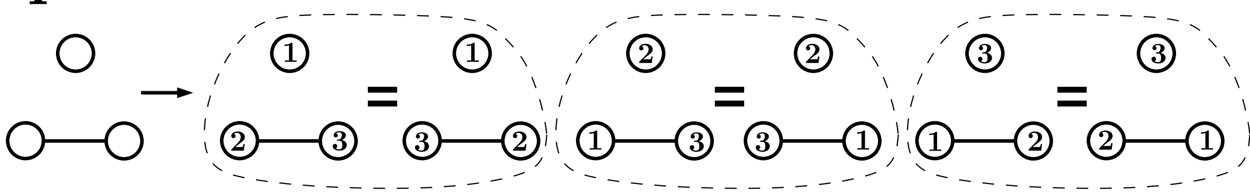
6 labeled objects (no symmetry)

Unlabelled setting

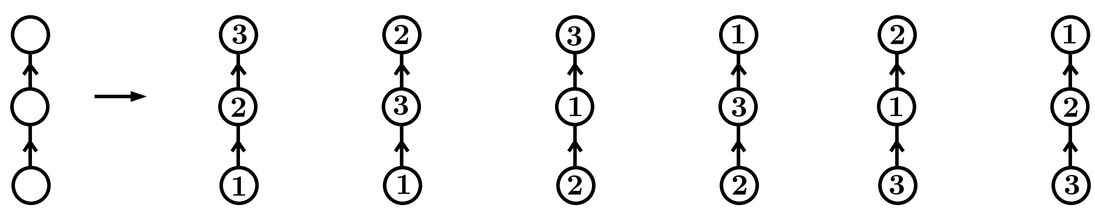
- Unlabelled structures=labelled structures up to relabeling



- **Examples:**



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



6 labeled objects (no symmetry)

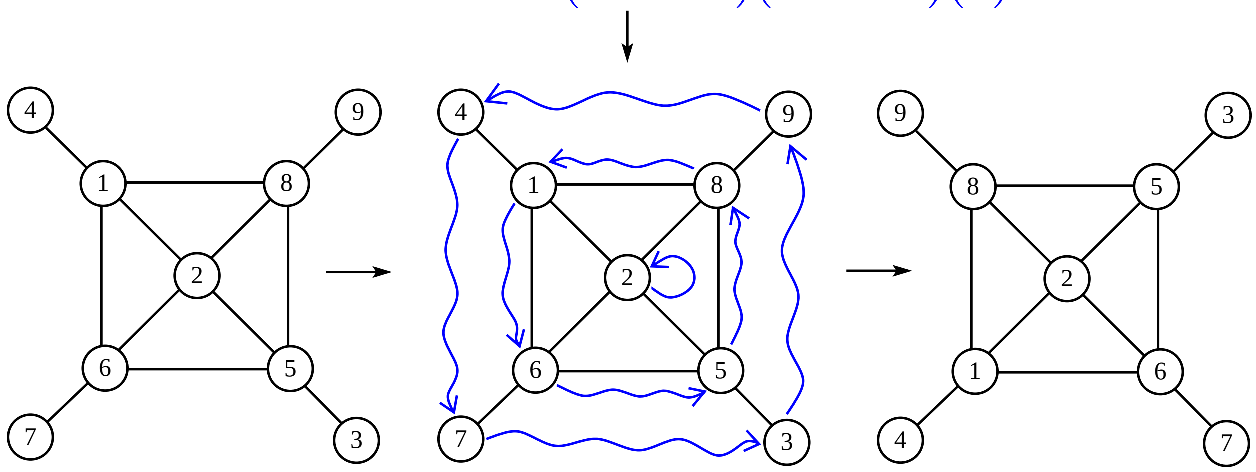
- Unlabelled struct. size $n \longrightarrow$ at most $n!$ labelled structures.
$\Rightarrow \frac{1}{n!} a_n^{\text{label.}} \leq a_n^{\text{unlabel.}} \Rightarrow$ (EGF) $A(x) \preceq \widetilde{A}(x)$ (OGF).

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.

$\sigma = (1\ 6\ 5\ 8)(4\ 7\ 3\ 9)(2)$



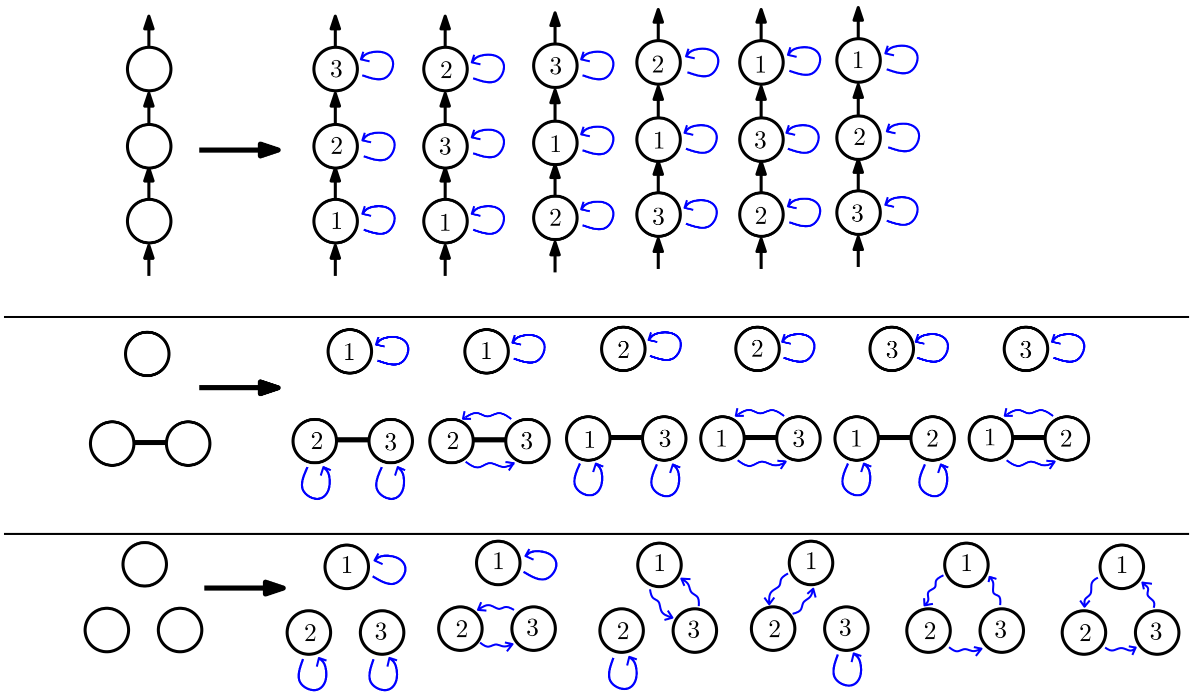
(rotation by $\pi/2$)

Burnside's lemma

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

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

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

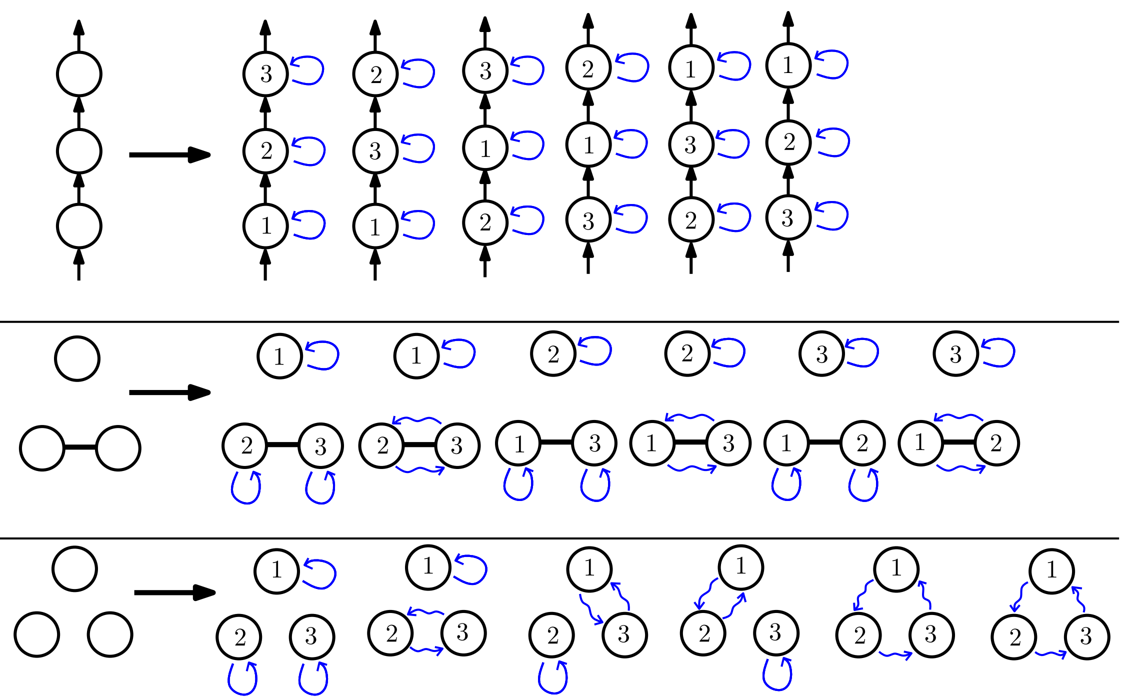


Burnside's lemma

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 $\Rightarrow \text{Sym}(\mathcal{A})_n \simeq n! \times \widetilde{\mathcal{A}}_n$



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

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

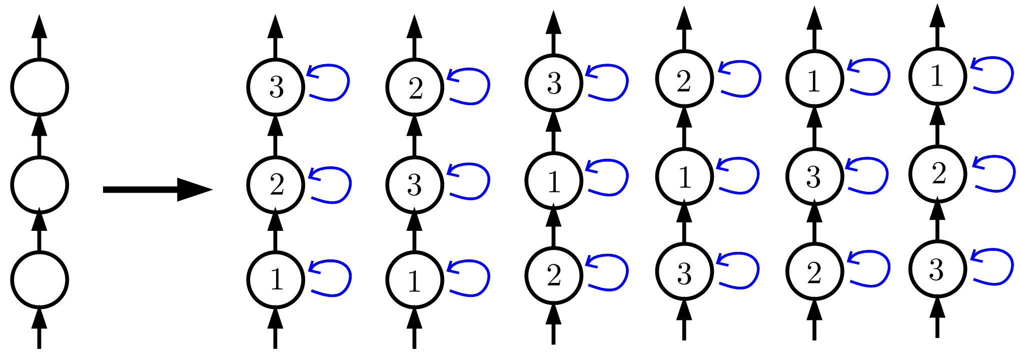
- Cycle index sum of $\mathcal{A}$ (cf Pólya) is the multivariate series

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

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

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

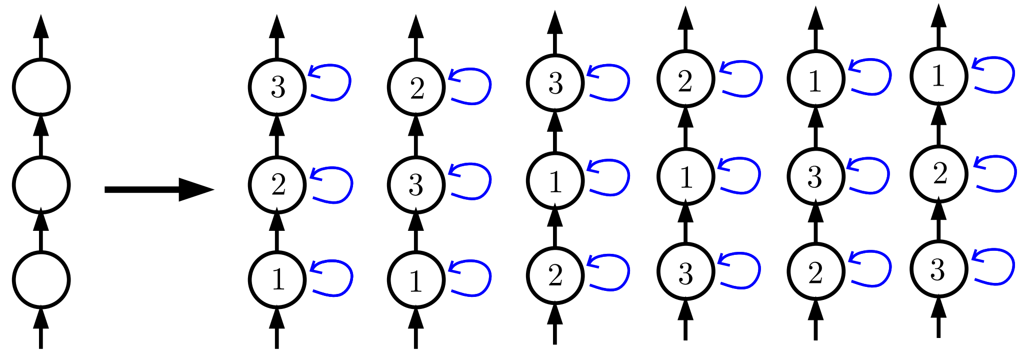
Examples of cycle index sums



$$Z = \frac{1}{6}\, s_1^3 + \frac{1}{6}\, s_1^3 + \frac{1}{6}\, s_1^3 + \frac{1}{6}\, s_1^3 + \frac{1}{6}\, s_1^3 + \frac{1}{6}\, s_1^3$$

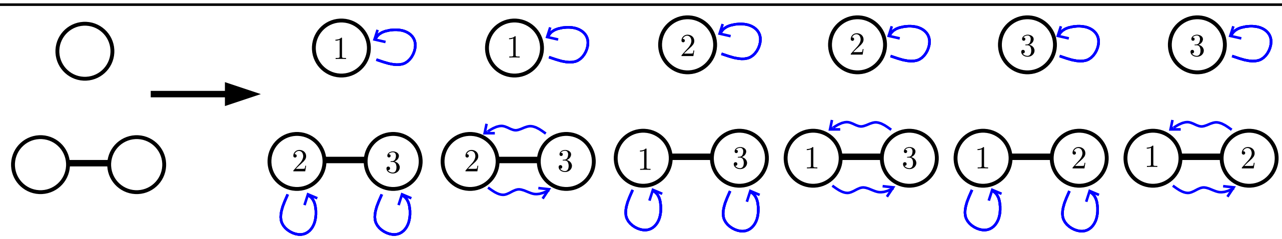
$$= s_1^3$$

Examples of cycle index sums



$$Z = \frac{1}{6}\, s_1^3 + \frac{1}{6}\, s_1^3 + \frac{1}{6}\, s_1^3 + \frac{1}{6}\, s_1^3 + \frac{1}{6}\, s_1^3 + \frac{1}{6}\, s_1^3$$

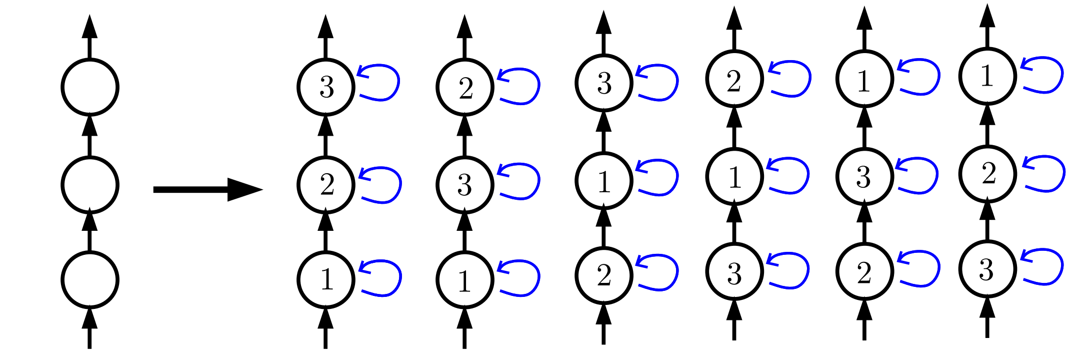
$$= s_1^3$$



$$Z = \frac{1}{6}\, s_1^3 + \frac{1}{6}\, s_1 s_2 + \frac{1}{6}\, s_1^3 + \frac{1}{6}\, s_1 s_2 + \frac{1}{6}\, s_1^3 + \frac{1}{6}\, s_1 s_2$$

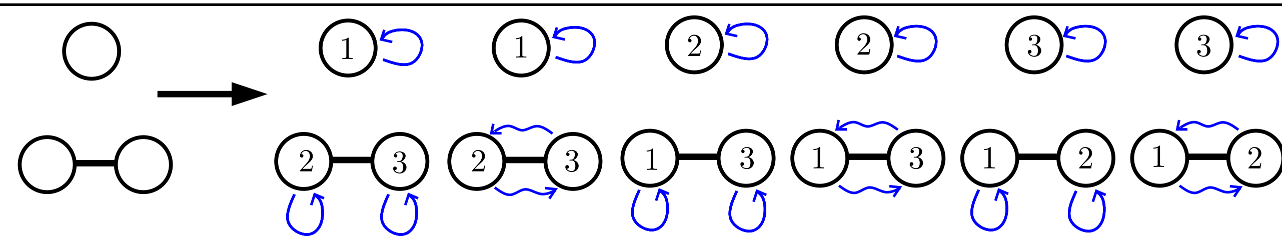
$$= \frac{1}{2}\, s_1^3 + \frac{1}{2}\, s_1 s_2$$

Examples of cycle index sums



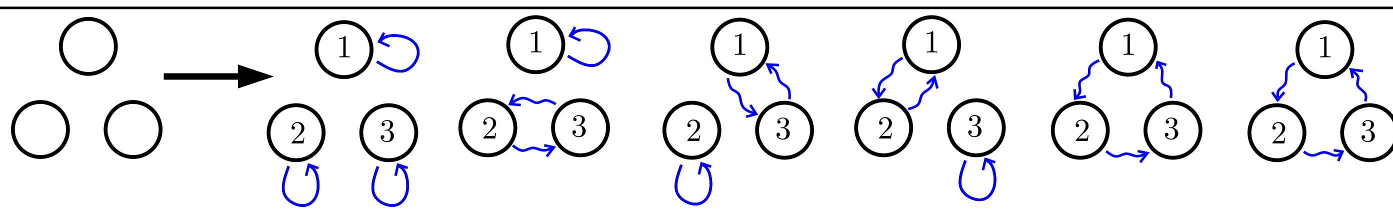
$$Z = \frac{1}{6}\, s_1^3 + \frac{1}{6}\, s_1^3 + \frac{1}{6}\, s_1^3 + \frac{1}{6}\, s_1^3 + \frac{1}{6}\, s_1^3 + \frac{1}{6}\, s_1^3$$

$$= s_1^3$$



$$Z = \frac{1}{6}\, s_1^3 + \frac{1}{6}\, s_1 s_2 + \frac{1}{6}\, s_1^3 + \frac{1}{6}\, s_1 s_2 + \frac{1}{6}\, s_1^3 + \frac{1}{6}\, s_1 s_2$$

$$= \frac{1}{2}\, s_1^3 + \frac{1}{2}\, s_1 s_2$$



$$Z = \frac{1}{6}\, s_1^3 + \frac{1}{6}\, s_1 s_2 + \frac{1}{6}\, s_1 s_2 + \frac{1}{6}\, s_1 s_2 + \frac{1}{6}\, s_3 + \frac{1}{6}\, s_3$$

Dictionary for OGF

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

$$\mathrm{OGF}: \quad \widetilde{C}(x) = \sum_{n \geq 0} \widetilde{c_n} x^n$$

- Dictionary (computation rules):

Disjoint union	$\mathcal{C} = \mathcal{A} + \mathcal{B}$	$\widetilde{C}(x) = \widetilde{A}(x) + \widetilde{B}(x)$
Product	$\mathcal{C} = \mathcal{A} \times \mathcal{B}$	$\widetilde{C}(x) = \widetilde{A}(x)\widetilde{B}(x)$
Set	$\mathcal{C} = \mathrm{Set}(\mathcal{A})$	$\widetilde{C}(x) = \exp\left(\sum_{k \geq 1} \frac{1}{k} \widetilde{A}(x^k)\right)$
Substitution	$\mathcal{C} = \mathcal{A} \circ \mathcal{B}$	$\widetilde{C}(x) \neq \widetilde{A}(\widetilde{B}(x))$

Dictionary for OGF

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

$$\mathrm{OGF}: \quad \widetilde{C}(x) = \sum_{n \geq 0} \widetilde{c_n} x^n$$

- Dictionary (computation rules):

Disjoint union	$\mathcal{C} = \mathcal{A} + \mathcal{B}$	$\widetilde{C}(x) = \widetilde{A}(x) + \widetilde{B}(x)$
Product	$\mathcal{C} = \mathcal{A} \times \mathcal{B}$	$\widetilde{C}(x) = \widetilde{A}(x)\widetilde{B}(x)$
Set	$\mathcal{C} = \mathrm{Set}(\mathcal{A})$	$\widetilde{C}(x) = \exp\left(\sum_{k \geq 1} \frac{1}{k} \widetilde{A}(x^k)\right)$
Substitution	$\mathcal{C} = \mathcal{A} \circ \mathcal{B}$	$\widetilde{C}(x) = Z_{\mathcal{A}}(\widetilde{B}(x), \widetilde{B}(x^2), \ldots)$

Dictionary for OGF

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

$$\mathrm{OGF}: \quad \widetilde{C}(x) = \sum_{n\geq 0} \widetilde{c_n} x^n$$

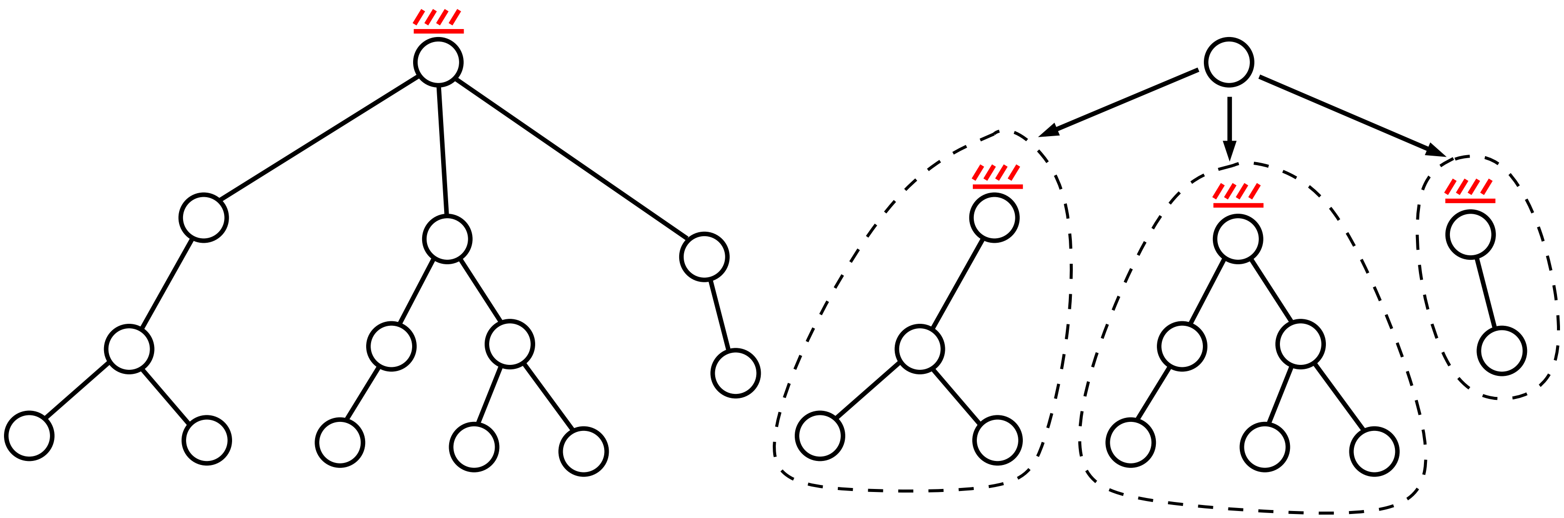
- Dictionary (computation rules):

Disjoint union	$\mathcal{C} = \mathcal{A} + \mathcal{B}$	$\widetilde{C}(x) = \widetilde{A}(x) + \widetilde{B}(x)$
Product	$\mathcal{C} = \mathcal{A} \times \mathcal{B}$	$\widetilde{C}(x) = \widetilde{A}(x)\widetilde{B}(x)$
Set	$\mathcal{C} = \mathrm{Set}(\mathcal{A})$	$\widetilde{C}(x) = \exp\left(\sum_{k\geq 1} \frac{1}{k} \widetilde{A}(x^k)\right)$
Substitution	$\mathcal{C} = \mathcal{A} \circ \mathcal{B}$	$\widetilde{C}(x) = Z_{\mathcal{A}}(\widetilde{B}(x), \widetilde{B}(x^2), \ldots)$

- **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

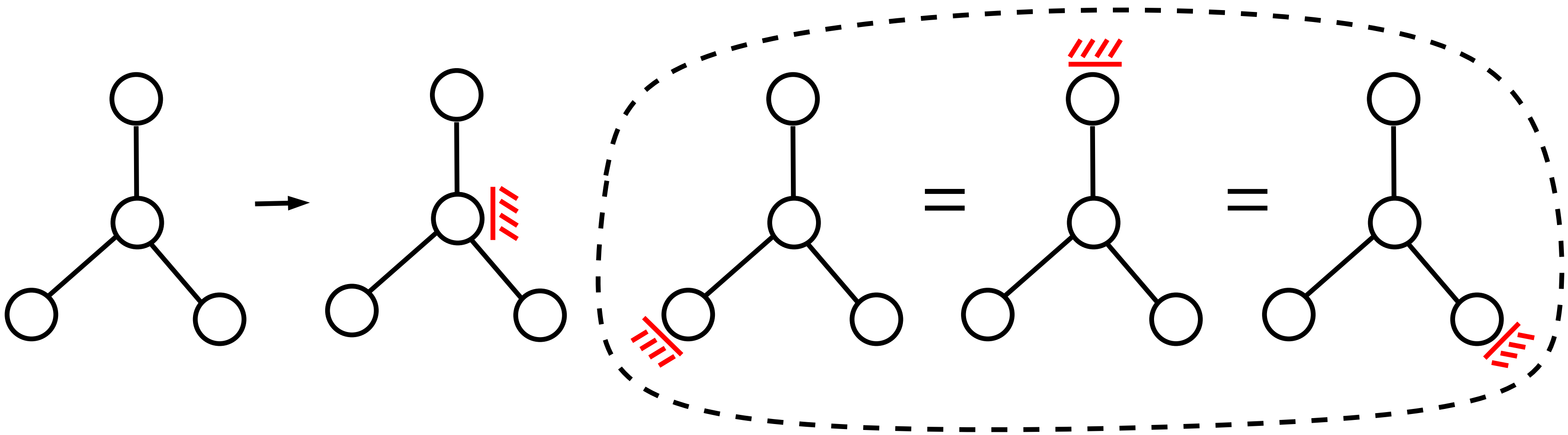
Decomposition at the root:



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

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

Count rooted $\not\Rightarrow$ count unrooted



tree size 4

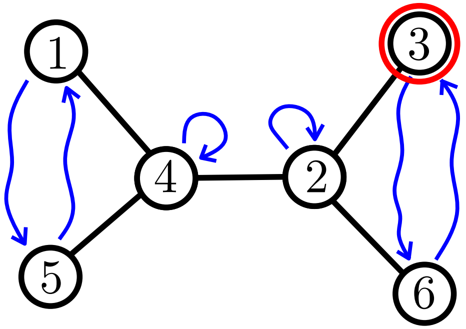
2 rooted trees (instead of 4)

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

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

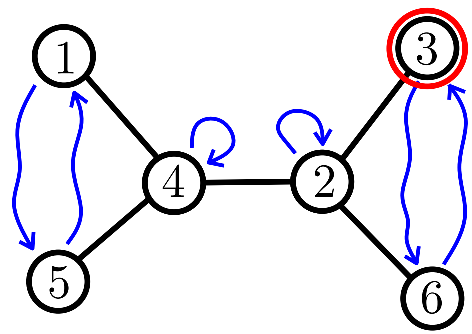
Pointing symmetries

Pointed symmetry $=$ symmetry $+$ marked atom



Pointing symmetries

Pointed symmetry $=$ symmetry $+$ marked atom

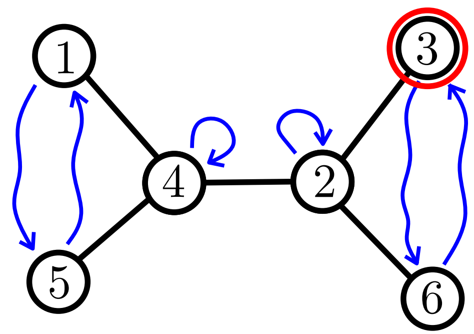


In size n we have

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

Pointing symmetries

Pointed symmetry = symmetry + marked atom



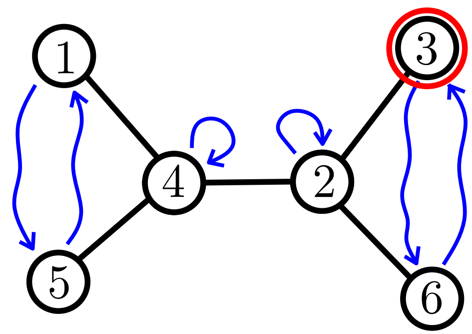
In size n we have

$$\begin{array}{ccc} \widetilde{\mathcal{A}} & \xrightarrow[\times n!]{} & \mathrm{Sym}(\mathcal{A}) \\ & & \Big\downarrow \times n \\ & & (\mathrm{Sym}(\mathcal{A}))^{\bullet} \end{array}$$

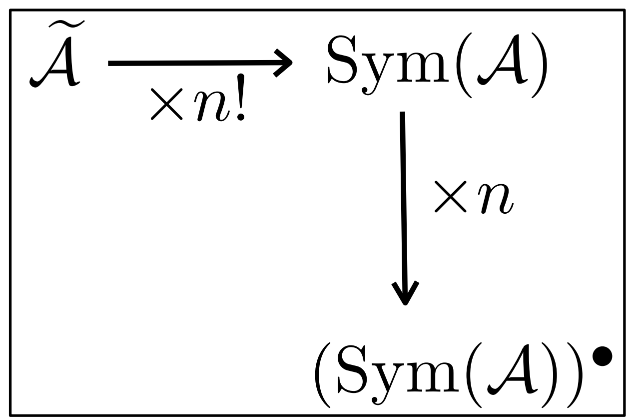
Look for a class $\mathcal{P}$ such that $\mathrm{Sym}(\mathcal{P}) \simeq (\mathrm{Sym}(\mathcal{A}))^{\bullet}$

Pointing symmetries

Pointed symmetry = symmetry + marked atom



In size n we have

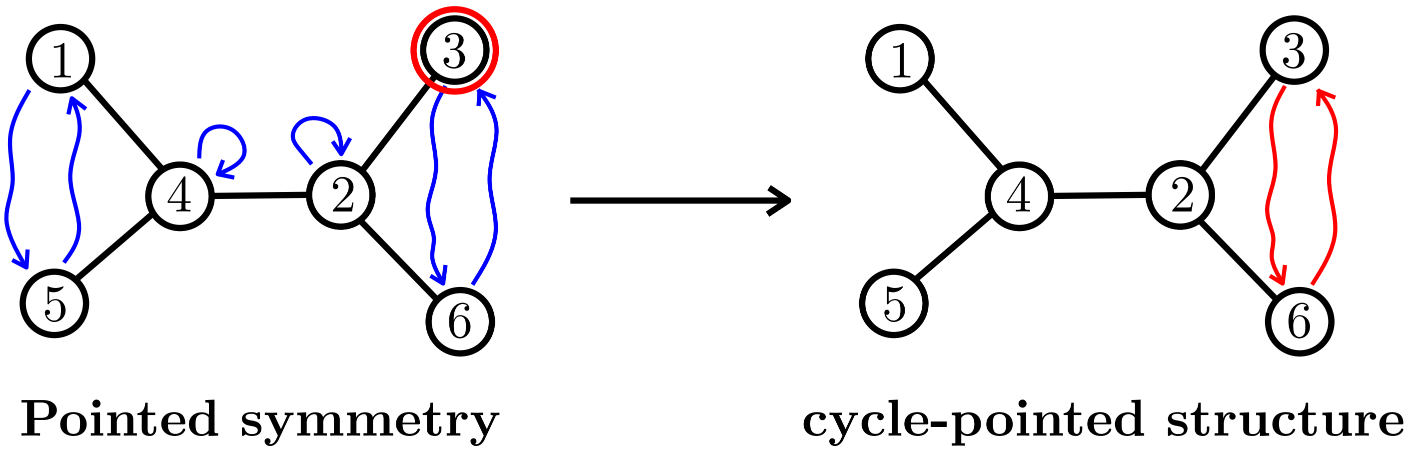


Look for a class $\mathcal{P}$ such that $\mathrm{Sym}(\mathcal{P}) \simeq (\mathrm{Sym}(\mathcal{A}))^{\bullet}$

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

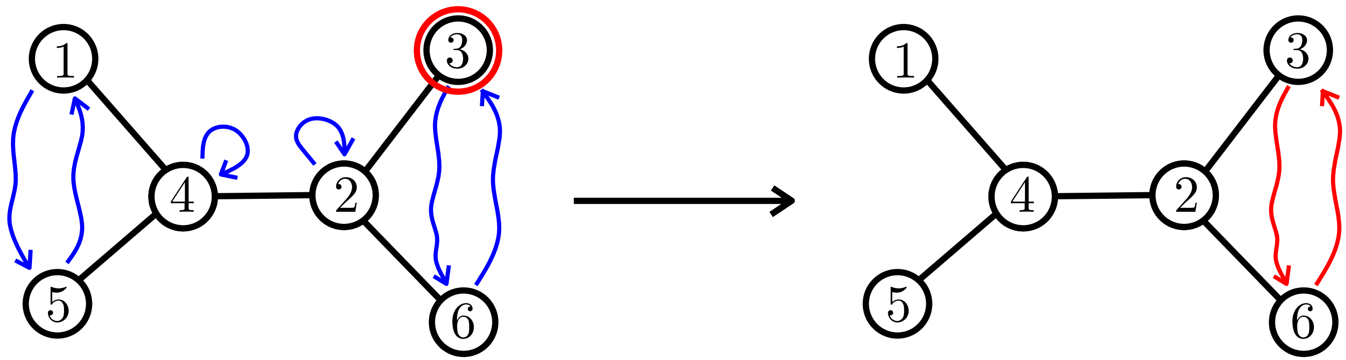
Cycle-pointed structures

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.



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.



Pointed symmetry **cycle-pointed structure**

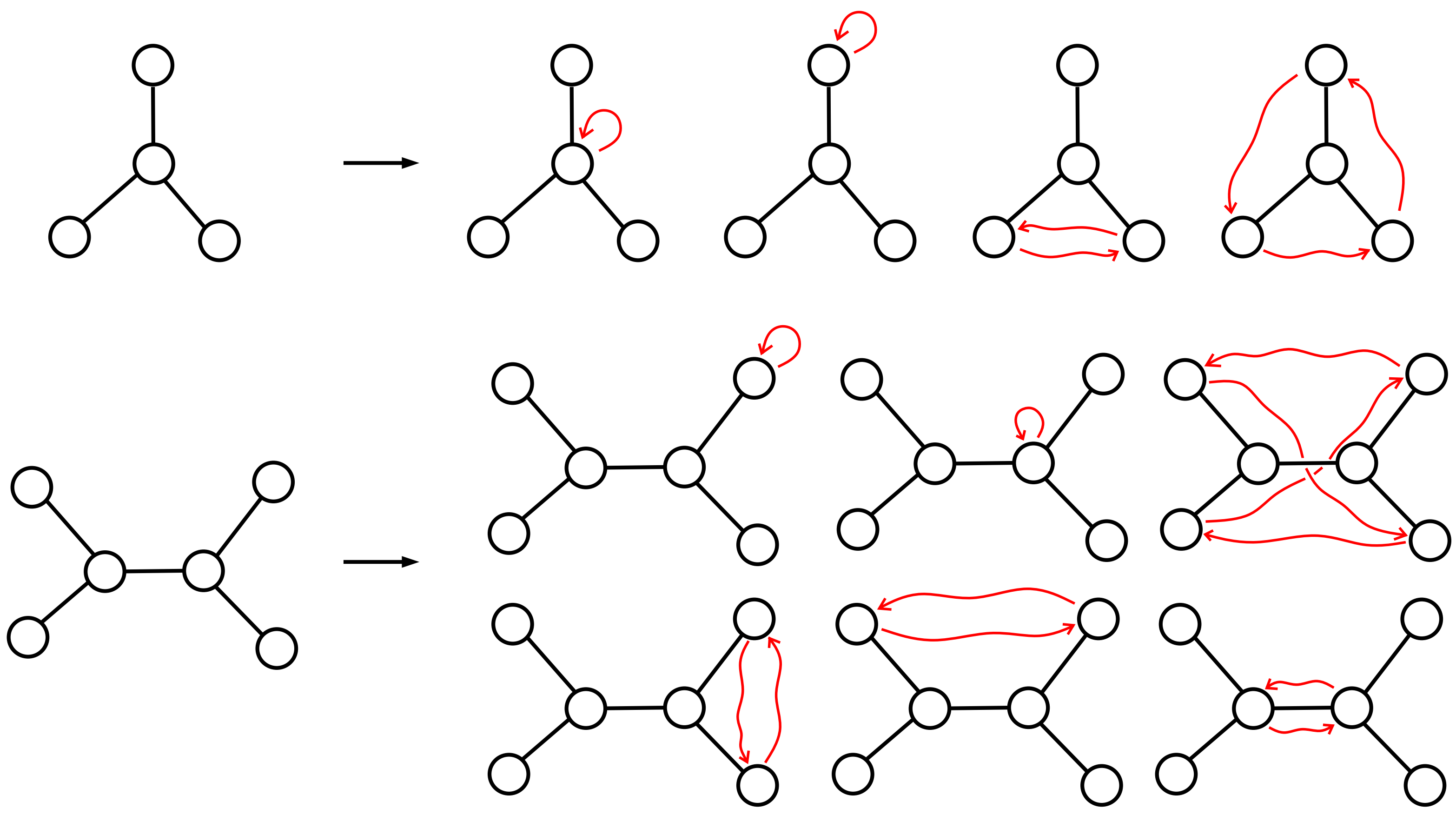
Let $\mathcal{A}^\circ = \{\text{cycle} - \text{pointed structures from } \mathcal{A}\}$. Then

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

Cycle-pointing is unbiased

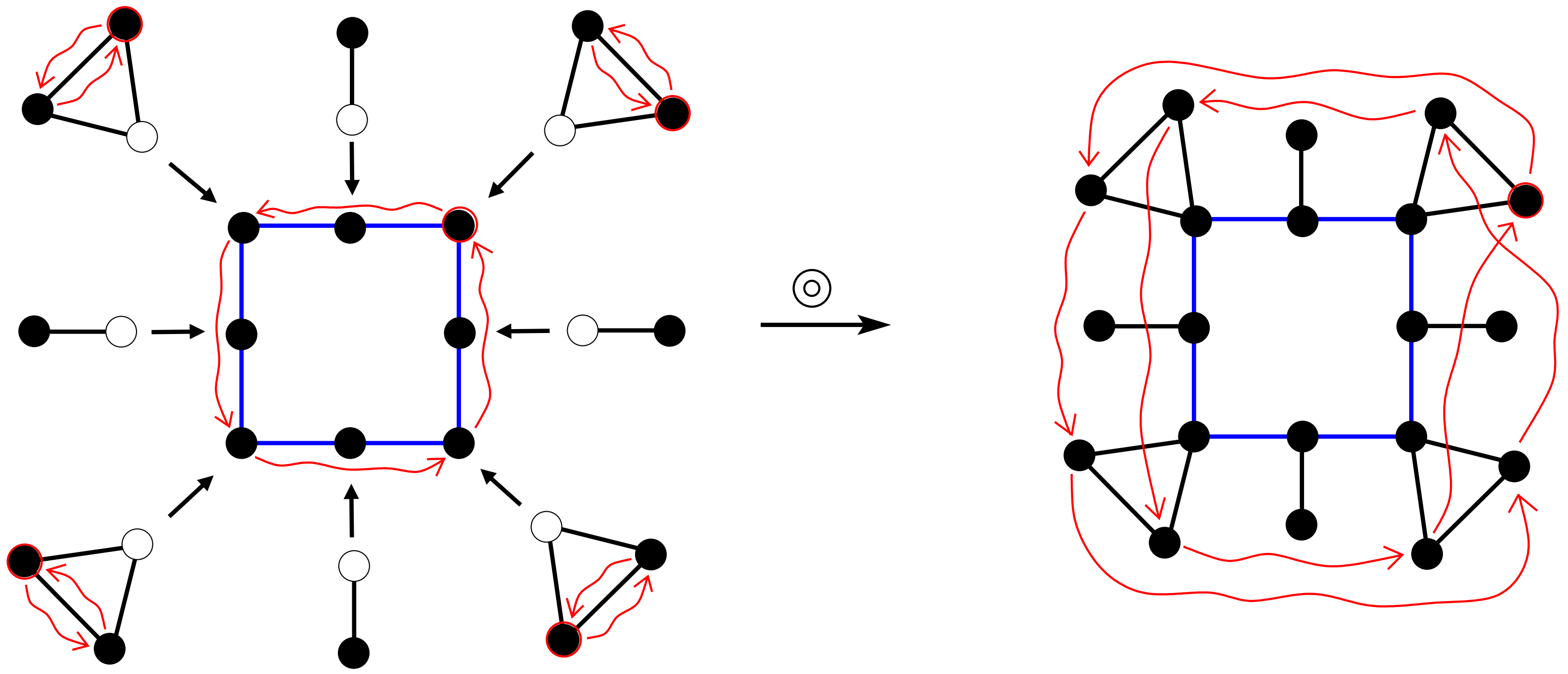
Theorem: An unlabelled structure of size n gives rise to n unlabelled cycle-pointed structures (cf Parker's lemma).

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



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)

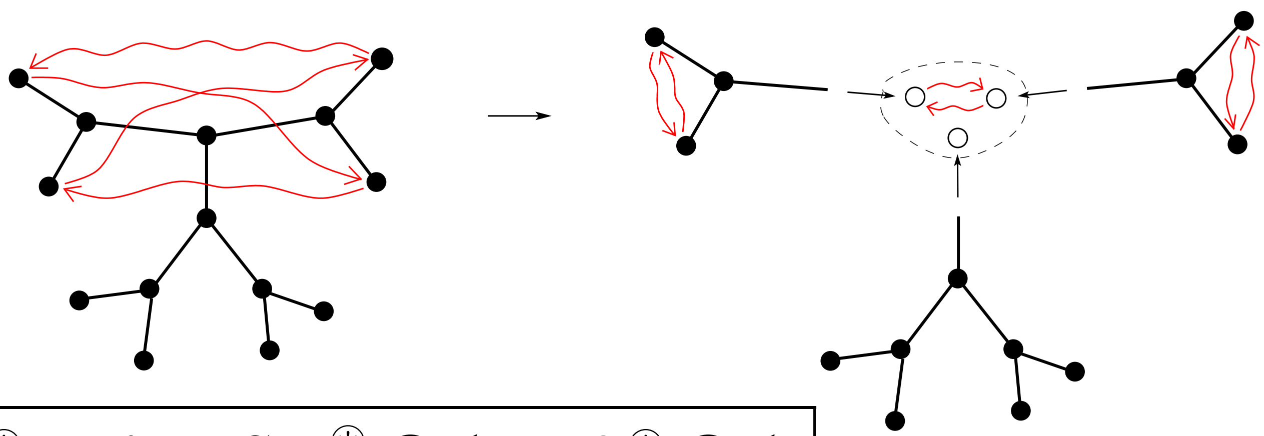
- Dichotomy: pointed cycle has length 1 or ≥ 2:

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

- 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.



$$3)\ \mathcal{T}^{\circledast} = \mathcal{Z} \times \mathrm{Set}^{\circledast} \circledcirc \mathcal{R} + \mathcal{L}^{\circledast} \circledcirc \mathcal{R}$$

Application: counting trees (2)

$$\begin{cases} \mathcal{T}^{\circ} & = & \mathcal{R} + \mathcal{T}^{\circledast} \\ \mathcal{R} & = & \mathcal{Z} \times \mathrm{Set}(\mathcal{R}) \\ \mathcal{T}^{\circledast} & = & \mathcal{Z} \times \mathrm{Set}^{\circledast} \circledcirc (\mathcal{R}) + \mathcal{L}^{\circledast} \circledcirc (\mathcal{R}) \end{cases}$$

↓ **translate to equation system**
(dictionary rules+Pólya operators)

$$\begin{cases} R(x) & = & x \exp\left(\sum_{k \geq 1} \frac{1}{k} R(x^k) \right) \\ xt'(x) & = & R(x) + x^2 R'(x^2) + \sum_{i \geq 2} x^i R'(x^i) R(x) \end{cases}$$

↓ **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
$\widetilde{a_n}$	1	1	1	2	3	6	11	23	47

Application: counting trees (2)

$$\begin{cases} \mathcal{T}^{\circ} & = & \mathcal{R} + \mathcal{T}^{\circledast} \\ \mathcal{R} & = & \mathcal{Z} \times \mathrm{Set}(\mathcal{R}) \\ \mathcal{T}^{\circledast} & = & \mathcal{Z} \times \mathrm{Set}^{\circledast} \circledcirc (\mathcal{R}) + \mathcal{L}^{\circledast} \circledcirc (\mathcal{R}) \end{cases}$$

↓ **translate to equation system**
(dictionary rules+Pólya operators)

$$\begin{cases} R(x) & = & x \exp\left(\sum_{k\geq 1} \frac{1}{k} R(x^k)\right) \\ xt'(x) & = & R(x) + x^2 R'(x^2) + \sum_{i\geq 2} x^i R'(x^i) R(x) \\ & & = xR'(x)(1 - R(x)) + x^2 R'(x^2) \end{cases}$$

↓ **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
$\widetilde{a_n}$	1	1	1	2	3	6	11	23	47

Exact counting results

Theorem: [Bergeron,Labelle,Leroux],

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

- basic classes $\{\mathbf{1}, \mathcal{Z}, \mathrm{Seq}, \mathrm{Cyc}, \mathrm{Set}\}$,
- constructions $\{+, \times, \circ\}$

the counting coefficients $|\widetilde{\mathcal{A}_n}|$ can be computed automatically

Exact counting results

Theorem: [Bergeron,Labelle,Leroux], [Bodirsky et al'07,10]

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

- basic classes $\{\mathbf{1}, \mathcal{Z}, \mathrm{Seq}, \mathrm{Cyc}, \mathrm{Set}\}$,
- constructions $\{+, \times, \circ\}$ and $\circledcirc$,
- cycle-pointing operator $\mathcal{C} \mapsto \mathcal{C}^{\circ}$,

the counting coefficients $|\widetilde{\mathcal{A}_n}|$ can be computed automatically

Exact counting results

Theorem: [Bergeron,Labelle,Leroux], [Bodirsky et al'07,10]

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

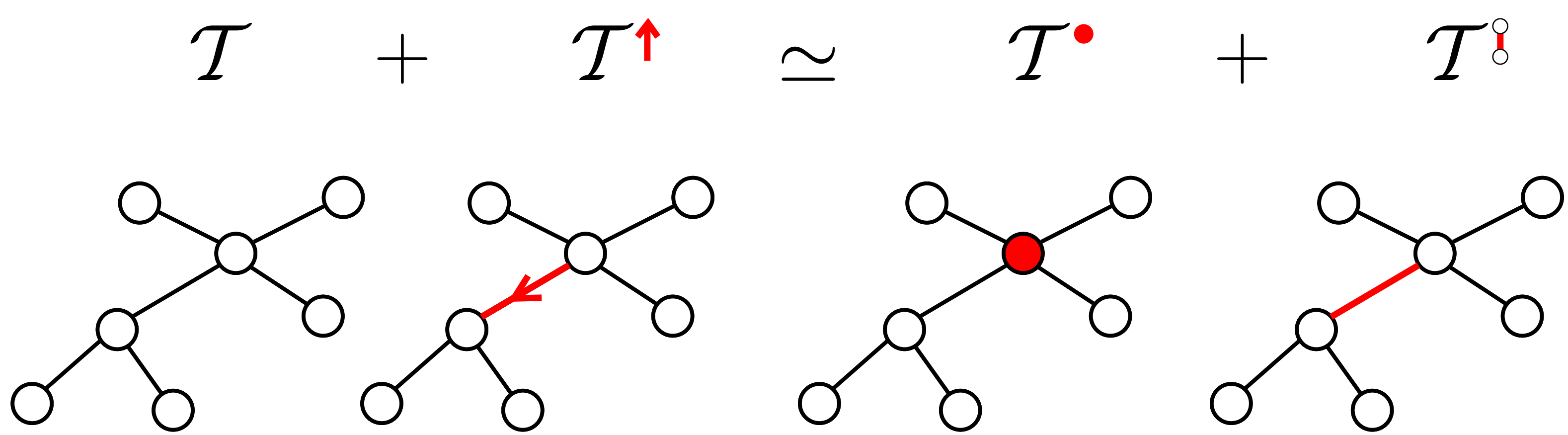
- basic classes $\{\mathbf{1}, \mathcal{Z}, \mathrm{Seq}, \mathrm{Cyc}, \mathrm{Set}\}$,
- constructions $\{+, \times, \circ\}$ and $\circledcirc$,
- cycle-pointing operator $\mathcal{C} \mapsto \mathcal{C}^{\circ}$,

the counting coefficients $|\widetilde{\mathcal{A}_n}|$ can be computed automatically

(includes tree families, outerplanar graphs,...)

Another approach

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

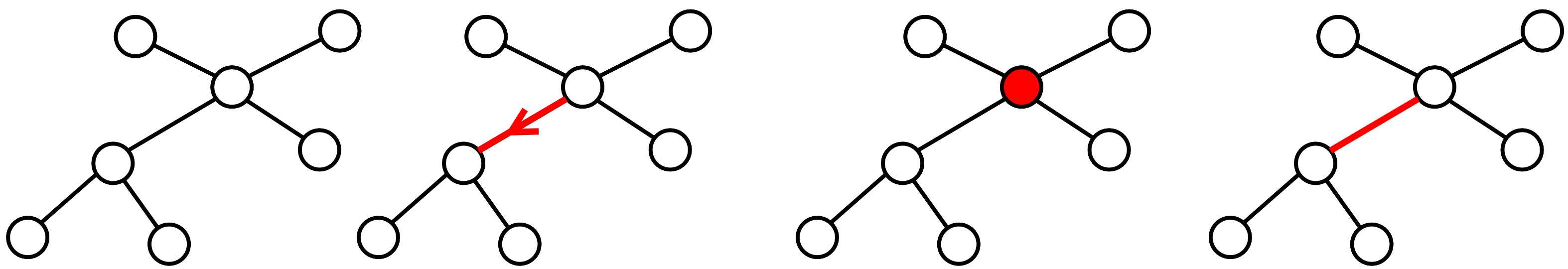


$$\mathbf{t}(\mathbf{x}) = \mathbf{t}^{\bullet}(\mathbf{x}) + \mathbf{t}^{\circ\!-\!\circ}(\mathbf{x}) - \mathbf{t}^{\uparrow}(\mathbf{x})$$

Another approach

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

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



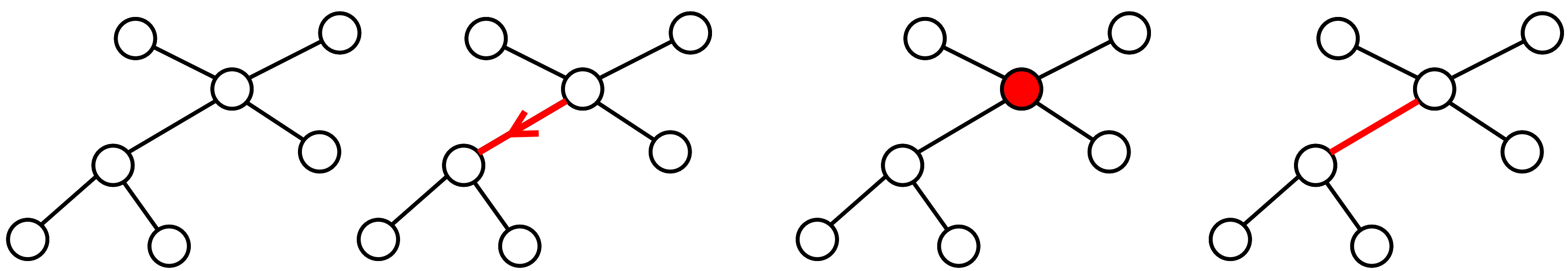
$$\boxed{\mathbf{t}(\mathbf{x}) \;=\; \mathbf{t}^{\bullet}(\mathbf{x}) + \mathbf{t}^{\circ\!-\!\circ}(\mathbf{x}) - \mathbf{t}^{\uparrow}(\mathbf{x})}$$

$\Rightarrow \; t(x) = R(x) - (R(x)^2 - R(x^2))$ with $R(x) = \exp(\sum_{i\geq 1} \frac{1}{i} R(x^i))$

Another approach

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

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



$$\boxed{\mathbf{t}(\mathbf{x}) \ = \ \mathbf{t}^{\bullet}(\mathbf{x}) + \mathbf{t}^{\circ\!-\!\circ}(\mathbf{x}) - \mathbf{t}^{\uparrow}(\mathbf{x})}$$

$\Rightarrow \ t(x) = R(x) - (R(x)^2 - R(x^2))$ with $R(x) = \exp(\sum_{i\geq 1} \frac{1}{i} R(x^i))$

(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

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

for "any" unrooted "tree-like" family $\mathcal{A}$

Asymptotic scheme

Main result: "universality" of asymptotic behaviour

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

for "any" unrooted "tree-like" family $\mathcal{A}$

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] $\Rightarrow$ $|\widetilde{\mathcal{A}^\circ_n}| \sim c\,\gamma^n n^{-3/2}$
- Pointing relation: $|\widetilde{\mathcal{A}_n}| = \frac{1}{n}|\widetilde{\mathcal{A}^\circ_n}| \sim c\,\gamma^n n^{-5/2}$

Illustration on trees

- Rooted labelled trees: $y = L(z)$ satisfies
$$y = z\exp(y)$$
Inverse is $g(y) = y\exp(-y)$,
$g'(y) = 0 \Rightarrow y = 1 \Rightarrow z = 1/e \Rightarrow L(z) = 1 - c\sqrt{1 - ze} + \cdots$

Illustration on trees

- Rooted labelled trees: $y = L(z)$ satisfies
$$y = z\exp(y)$$
Inverse is $g(y) = y\exp(-y)$,
$g'(y)=0 \Rightarrow y=1 \Rightarrow z=1/e \Rightarrow L(z)=1-c\sqrt{1-ze}+\cdots$
- Rooted unlabelled trees: $y = R(z)$ satisfies
$$y = z\exp(y + A(z)), \quad \text{where } A(z) = \sum_{i\geq 2}\frac{1}{i}R(z^i)$$

Illustration on trees

- Rooted labelled trees: $y = L(z)$ satisfies
$$y = z\exp(y)$$
Inverse is $g(y) = y\exp(-y)$,
$g'(y)=0 \Rightarrow y=1 \Rightarrow z=1/e \Rightarrow L(z)=1-c\sqrt{1-ze}+\cdots$
- Rooted unlabelled trees: $y = R(z)$ satisfies
$$y = z\exp(y + A(z)), \quad \text{where } A(z) = \sum_{i\geq 2} \frac{1}{i} R(z^i)$$
Hence $R(z) = L(A(z)) = 1 - c'\sqrt{1 - z/\rho} + \cdots$
where ρ satisfies $A(\rho) = 1/e$

Illustration on trees

- Rooted labelled trees: $y = L(z)$ satisfies
$$y = z\exp(y)$$
Inverse is $g(y) = y\exp(-y)$,
$g'(y)=0 \Rightarrow y=1 \Rightarrow z=1/e \Rightarrow L(z)=1-c\sqrt{1-ze}+\cdots$
- Rooted unlabelled trees: $y = R(z)$ satisfies
$$y = z\exp(y + A(z)), \quad \text{where } A(z) = \sum_{i\geq 2}\frac{1}{i}R(z^i)$$
Hence $R(z) = L(A(z)) = 1 - c'\sqrt{1 - z/\rho} + \cdots$
where ρ satisfies $A(\rho) = 1/e$
- Cycle-pointed trees
$$zt'(z) = \underbrace{z^2R'(z^2)}_{\text{analytic at } \rho} + \underbrace{(1 + \sum_{i\geq 2} z^iR'(z^i))}_{G(z) \text{ analytic at } \rho} \cdot R(z)$$

Illustration on trees

- Rooted labelled trees: $y = L(z)$ satisfies
$$y = z\exp(y)$$
Inverse is $g(y) = y\exp(-y)$,
$g'(y)=0 \Rightarrow y=1 \Rightarrow z=1/e \Rightarrow L(z)=1-c\sqrt{1-ze}+\cdots$
- Rooted unlabelled trees: $y = R(z)$ satisfies
$$y = z\exp(y + A(z)), \quad \text{where } A(z) = \sum_{i\geq 2} \frac{1}{i} R(z^i)$$
Hence $R(z) = L(A(z)) = 1 - c'\sqrt{1 - z/\rho} + \cdots$
where ρ satisfies $A(\rho) = 1/e$
- Cycle-pointed trees
$$zt'(z) = \underbrace{z^2 R'(z^2)}_{\text{analytic at } \rho} + \underbrace{(1 + \sum_{i\geq 2} z^i R'(z^i))}_{G(z) \text{ analytic at } \rho} \cdot R(z)$$

(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, $t(z) \text{“} \leq \text{”} (1 - z/\rho)^{3/2}$

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

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):

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

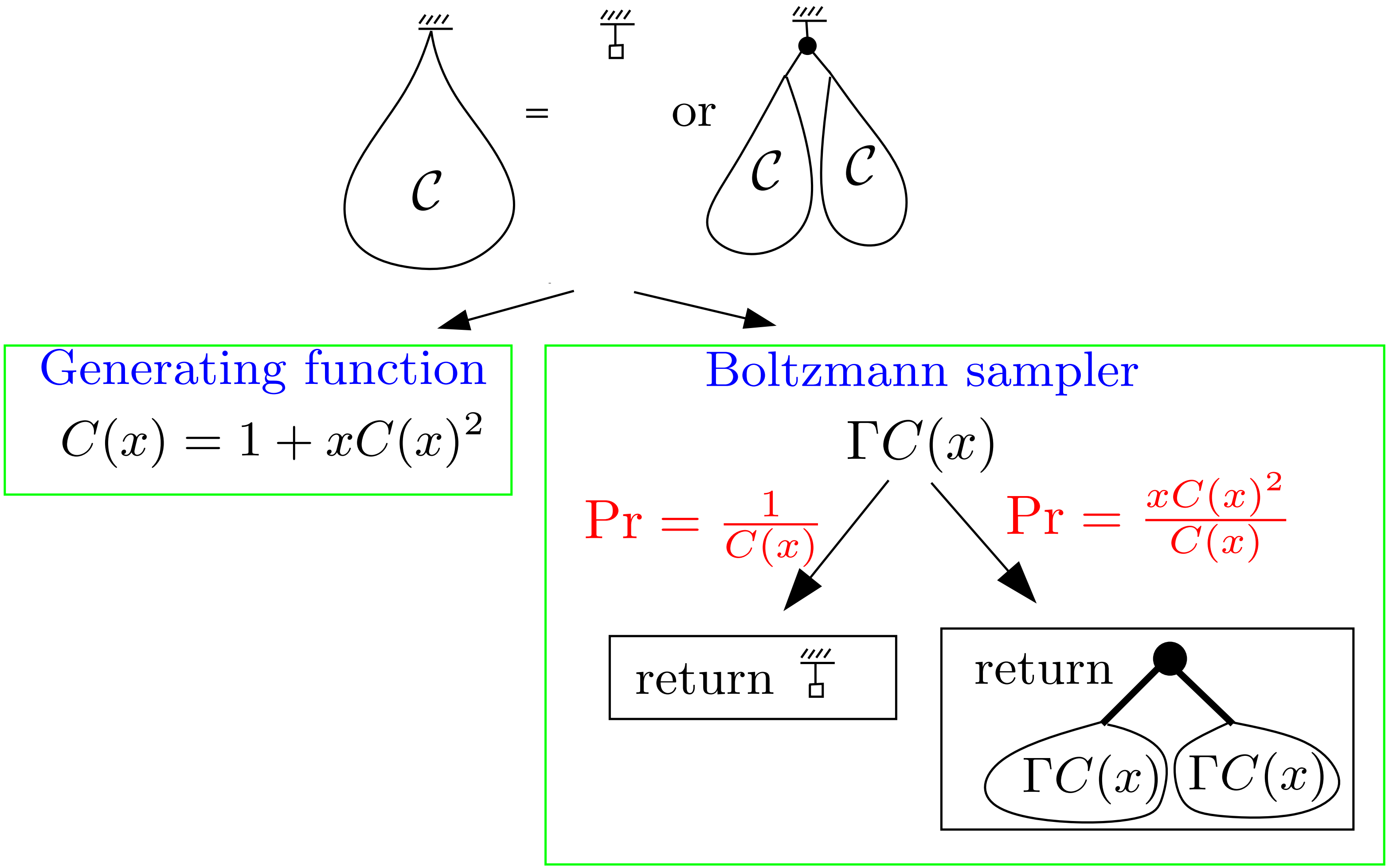
  - Based on coefficients:
    $\mathcal{C} = \mathcal{A} + \mathcal{B} \Rightarrow \mathbb{P}(\gamma \in \mathcal{A}_n) = \frac{a_n}{c_n}$

- 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

- basic classes $\{\mathbf{1}, \mathcal{Z}\}$
- constructions $\{+, \times, \mathrm{Seq}, \mathrm{Cyc}, \mathrm{Set}\}$,

there is a linear-time Boltzmann sampler $\Gamma\widetilde{\mathcal{A}}(x)$.

Theorem: [Bodirsky et al'07,10] For any class $\mathcal{A}$ decomposable in terms of

- basic classes $\{\mathbf{1}, \mathcal{Z}, \mathrm{Seq}, \mathrm{Cyc}, \mathrm{Set}\}\}$,
- constructions $\{+, \times, \circ\}$

there is a linear time Boltzmann sampler $\Gamma\widetilde{\mathcal{A}}(x)$

Results

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

- basic classes $\{\mathbf{1}, \mathcal{Z}\}$
- constructions $\{+, \times, \mathrm{Seq}, \mathrm{Cyc}, \mathrm{Set}\}$,

there is a linear-time Boltzmann sampler $\Gamma\widetilde{\mathcal{A}}(x)$.

Theorem: [Bodirsky et al'07,10] For any class $\mathcal{A}$ decomposable in terms of

- basic classes $\{\mathbf{1}, \mathcal{Z}, \mathrm{Seq}, \mathrm{Cyc}, \mathrm{Set}\}$,
- constructions $\{+, \times, \circ\}$ and $\circledcirc$,
- cycle-pointing operator $\mathcal{C} \mapsto \mathcal{C}^{\circ}$,

there is a linear time Boltzmann sampler $\Gamma\widetilde{\mathcal{A}}(x)$ (or $\Gamma\widetilde{\mathcal{A}^{\circ}}(x)$).

Pólya-Boltzmann samplers

- Ordinary Boltzmann samplers:

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

Pólya-Boltzmann samplers

- Ordinary Boltzmann samplers:

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

- Pólya-Boltzmann samplers:

$$Z_{\mathcal{A}} = \sum_{\sigma \cdot \gamma = \gamma} W_{(\sigma,\gamma)} \;\Rightarrow\; \mathbb{P}(\sigma,\gamma) = \frac{W_{(\sigma,\gamma)}}{Z_{\mathcal{A}}}$$

Pólya-Boltzmann samplers

- Ordinary Boltzmann samplers:

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

- Pólya-Boltzmann samplers:

$$Z_{\mathcal{A}} = \sum_{\sigma\cdot\gamma=\gamma} W_{(\sigma,\gamma)} \;\Rightarrow\; \mathbb{P}(\sigma,\gamma) = \frac{W_{(\sigma,\gamma)}}{Z_{\mathcal{A}}}$$

- Sampling rules $\{+, \times, \circ\}$ // computation rules for $Z_{\mathcal{A}}$:

$$\mathcal{C} = \mathcal{A} + \mathcal{B} \Rightarrow \begin{cases} Z_{\mathcal{C}} = Z_{\mathcal{A}} + Z_{\mathcal{B}} \\ \Gamma Z_{\mathcal{C}} : \mathrm{Bern}\left(\frac{Z_{\mathcal{A}}}{Z_{\mathcal{C}}} \middle| \frac{Z_{\mathcal{B}}}{Z_{\mathcal{C}}}\right) \to \Gamma Z_{\mathcal{A}} | \Gamma Z_{\mathcal{B}} \end{cases}$$

Pólya-Boltzmann samplers

- Ordinary Boltzmann samplers:

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

- Pólya-Boltzmann samplers:

$$Z_{\mathcal{A}} = \sum_{\sigma \cdot \gamma = \gamma} W_{(\sigma,\gamma)} \Rightarrow \mathbb{P}(\sigma, \gamma) = \frac{W_{(\sigma,\gamma)}}{Z_{\mathcal{A}}}$$

- Sampling rules $\{+, \times, \circ\}$ // computation rules for $Z_{\mathcal{A}}$:

$$\mathcal{C} = \mathcal{A} + \mathcal{B} \Rightarrow \begin{cases} Z_{\mathcal{C}} = Z_{\mathcal{A}} + Z_{\mathcal{B}} \\ \Gamma Z_{\mathcal{C}} : \mathrm{Bern}\left(\frac{Z_{\mathcal{A}}}{Z_{\mathcal{C}}} \middle| \frac{Z_{\mathcal{B}}}{Z_{\mathcal{C}}}\right) \to \Gamma Z_{\mathcal{A}} | \Gamma Z_{\mathcal{B}} \end{cases}$$

- 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

$$xt'(x) = \underbrace{R(x)}_{\text{rooted}} + \underbrace{x^2 R'(x^2)}_{\substack{\text{centre symmetry} \\ \text{is edge}}} + \underbrace{\sum_{i \geq 2} x^i R'(x^i) R(x)}_{\substack{\text{centre symmetry} \\ \text{is vertex}}}$$

into a Boltzmann sampler for $\widetilde{\mathcal{T}^{\circ}}$.

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

$$xt'(x) = \underbrace{R(x)}_{\text{rooted}} + \underbrace{x^2 R'(x^2)}_{\substack{\text{centre symmetry} \\ \text{is edge}}} + \underbrace{\sum_{i \geq 2} x^i R'(x^i) R(x)}_{\substack{\text{centre symmetry} \\ \text{is vertex}}}$$

into a Boltzmann sampler for $\widetilde{\mathcal{T}^\circ}$.

(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].