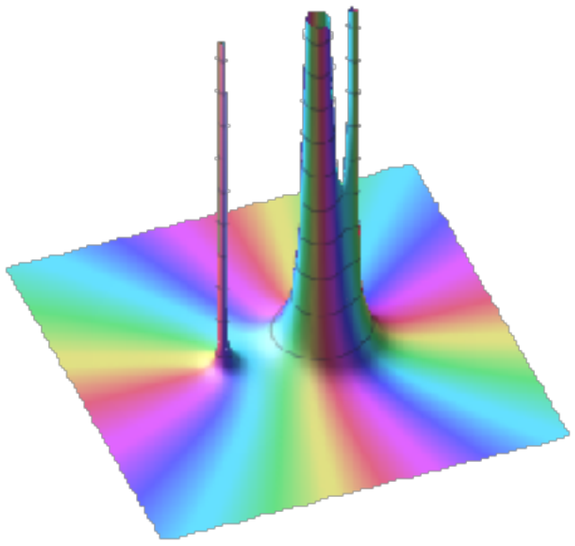
On (Effective) Analytic Combinatorics

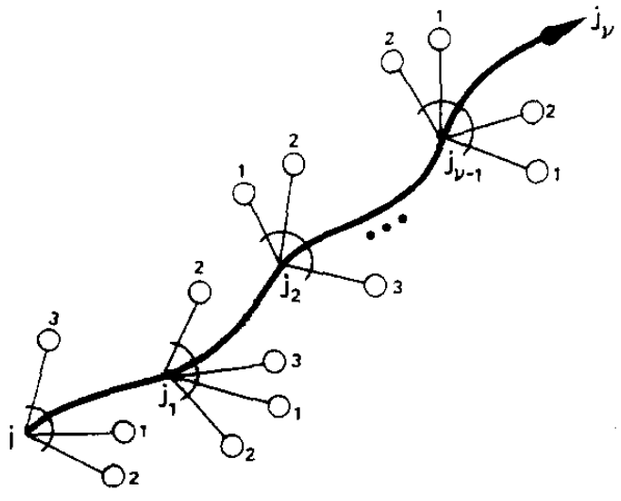


Bruno Salvy

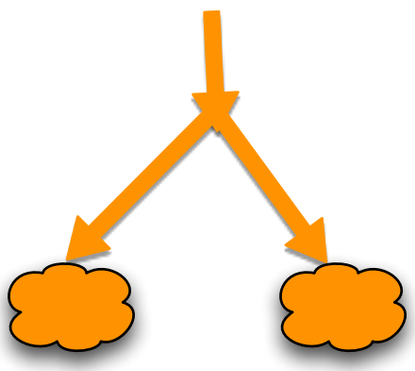
Inria & ENS de Lyon

Séminaire Algorithmes

Dec. 2017



Combinatorics, Randomness and Analysis



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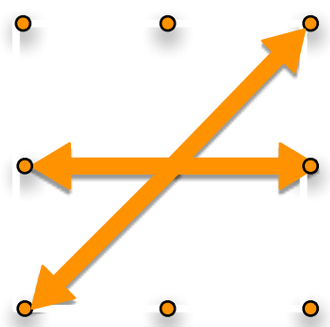
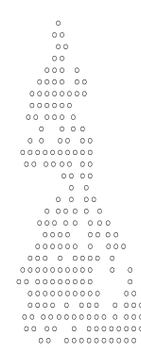
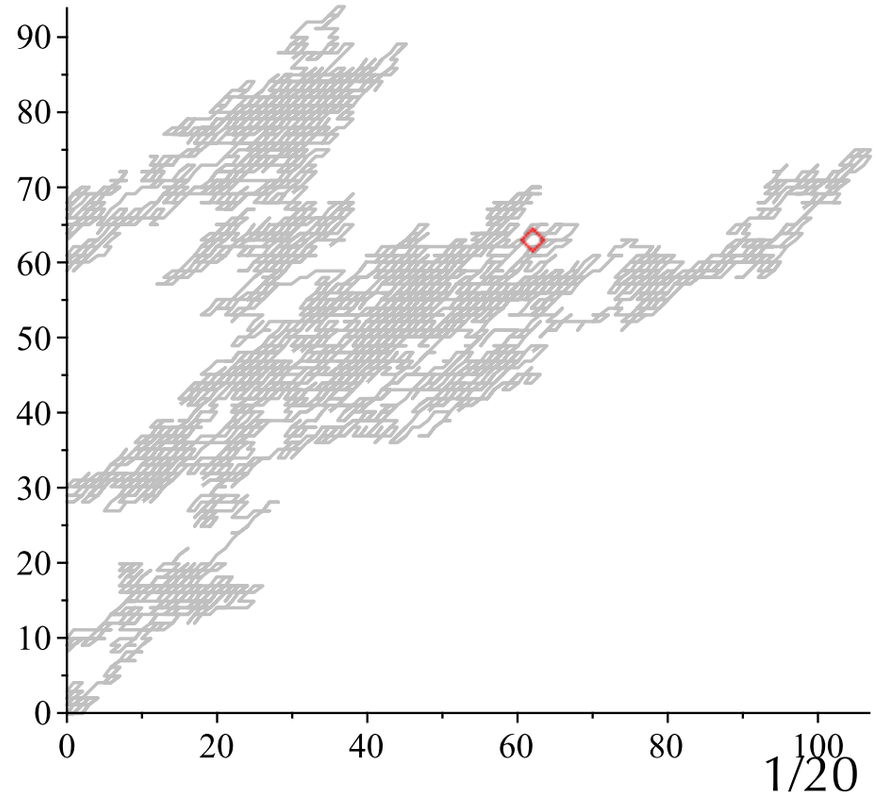




A quest for **universality** in random discrete structures**:**
➡ **probabilistic complexity** of structures and algorithms.

Quantitative results using **complex analysis.**



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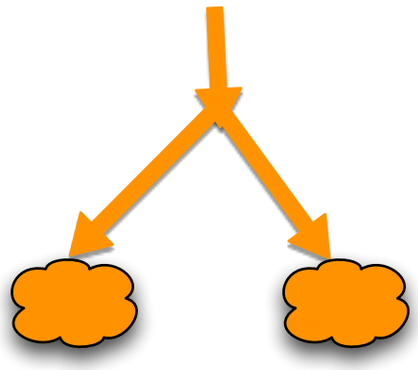

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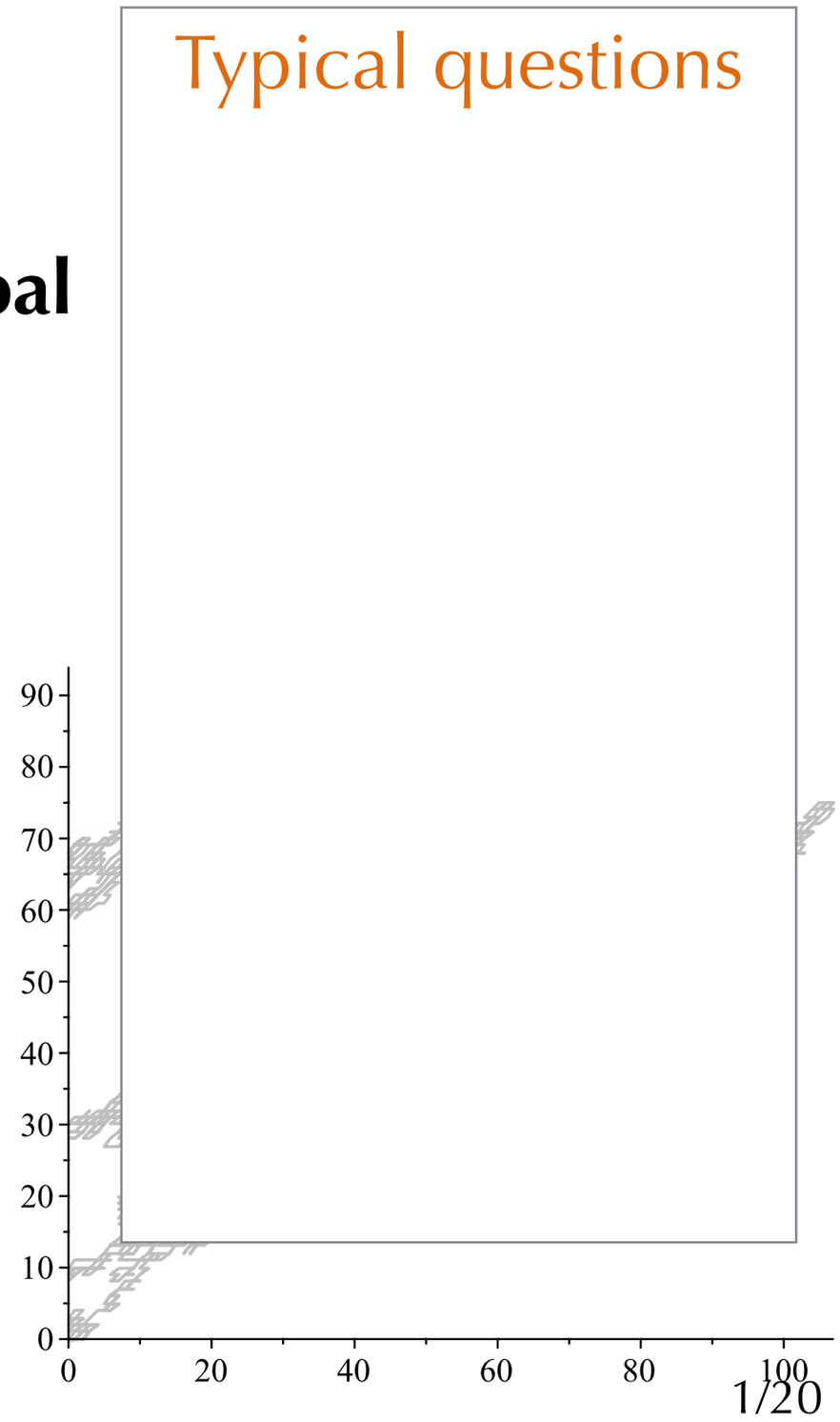

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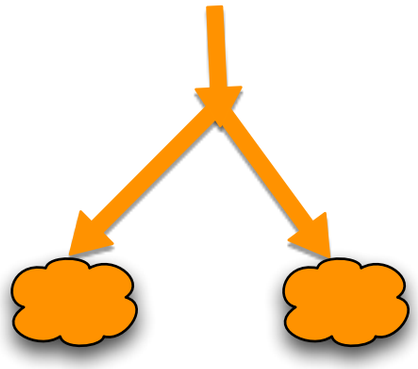

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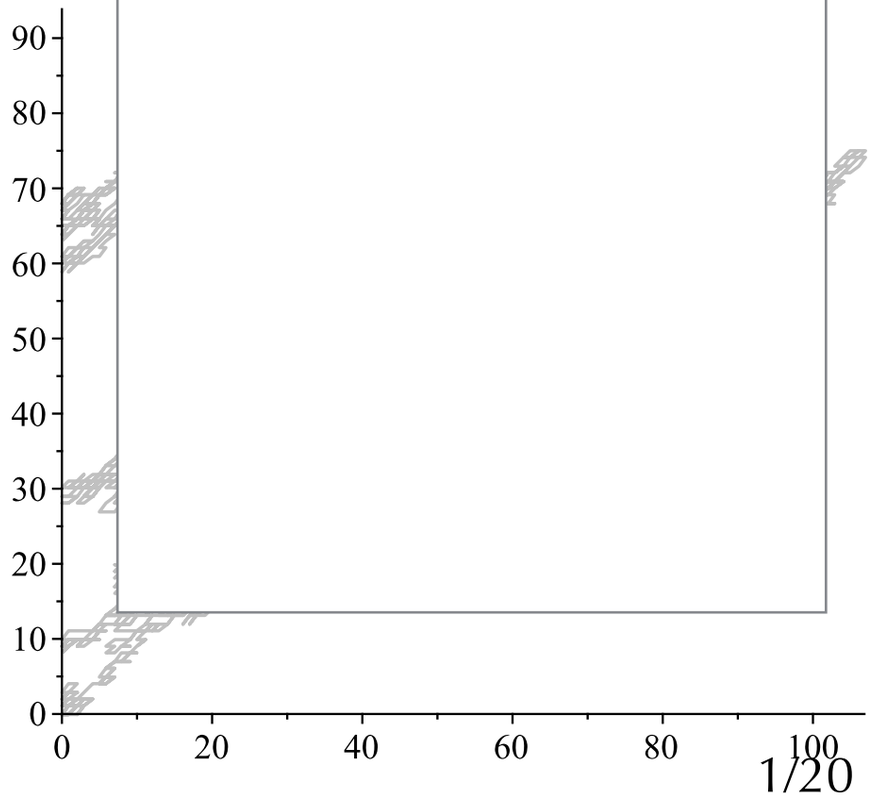

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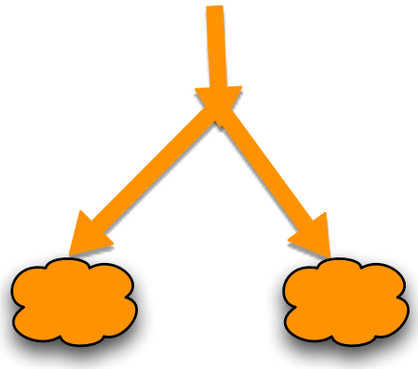

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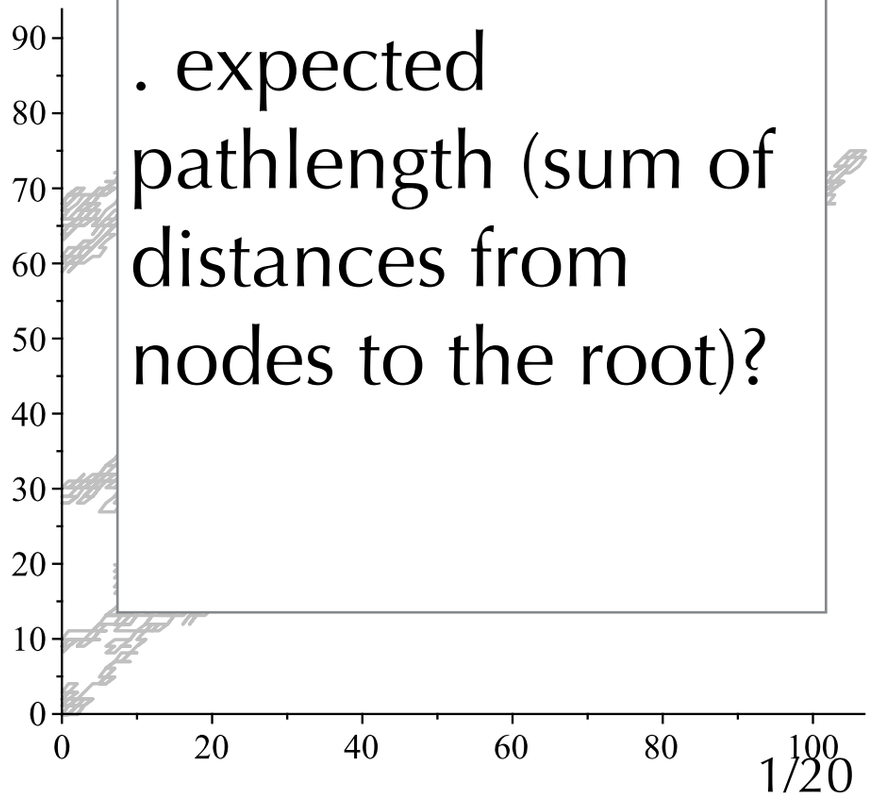

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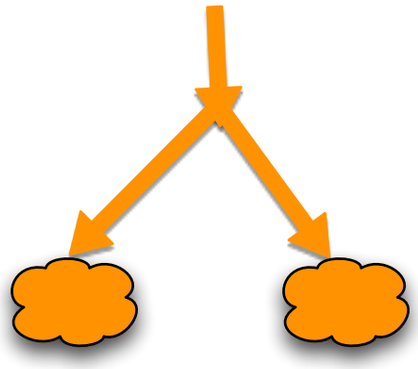

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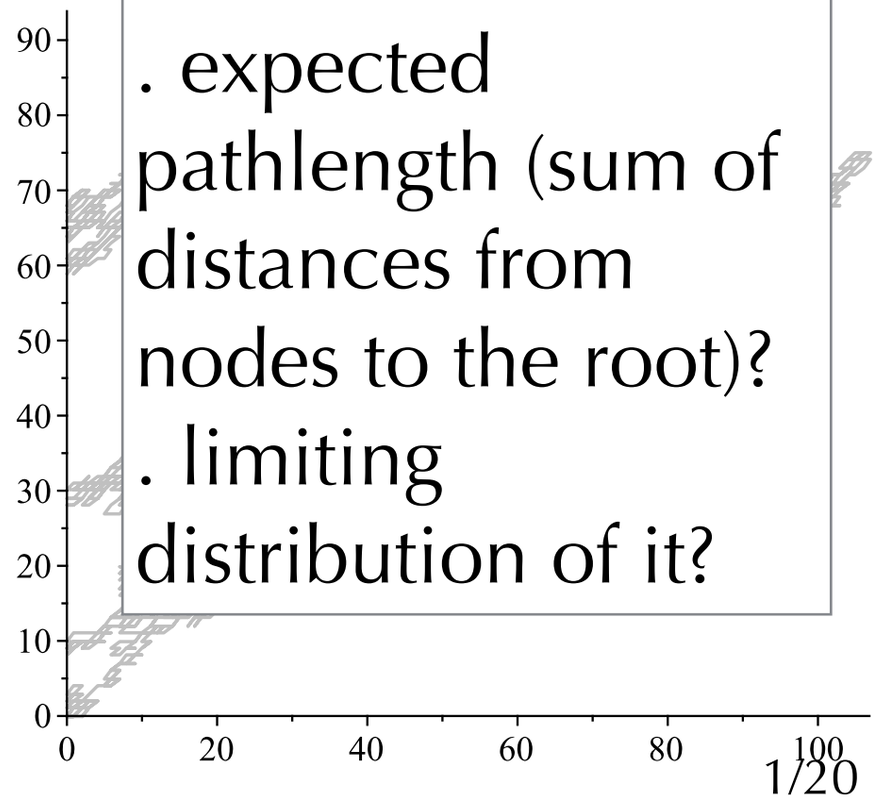
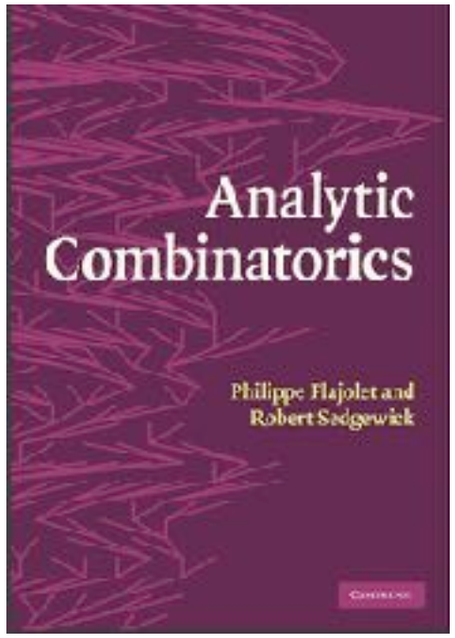
. limiting distribution of it?



Philippe Flajolet, the Father of Analytic Combinatorics

1948-2011

Planned complete works span
7 volumes of approx 600 pp. each.



2009

Combinatorial specification → Generating functions →

- counting;
- random generation;
- asymptotic analysis.

If you can specify, you can analyze.

Constructible Structures

Language: $1, \mathcal{Z}, +, \times$, Seq, Set, Cyc and recursion.

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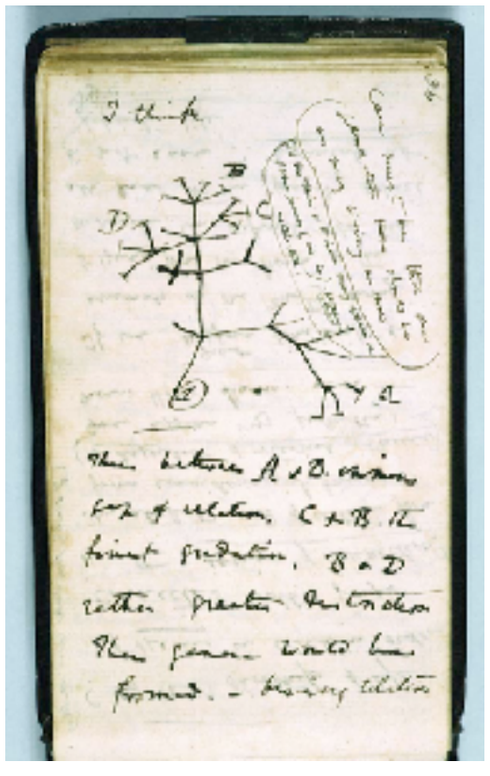

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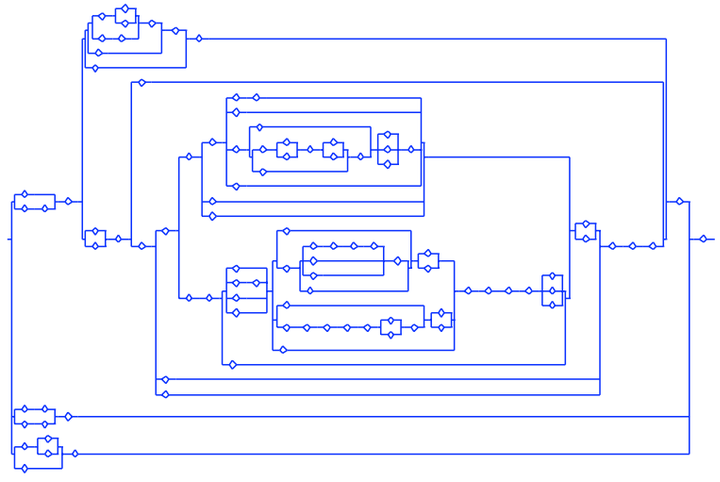

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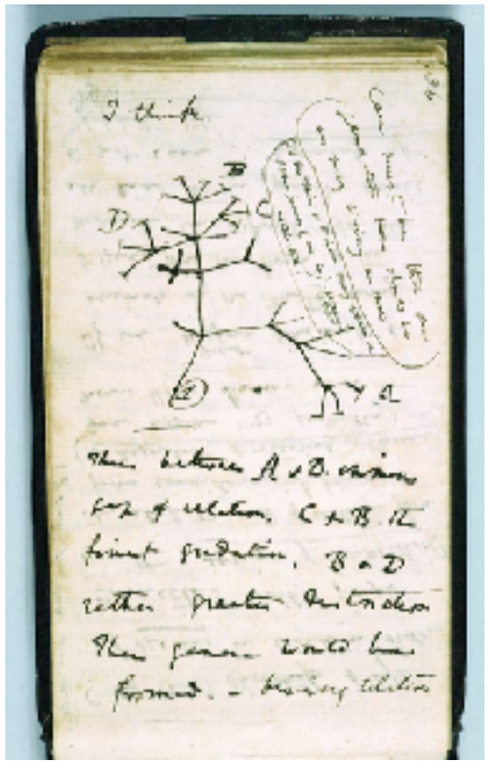

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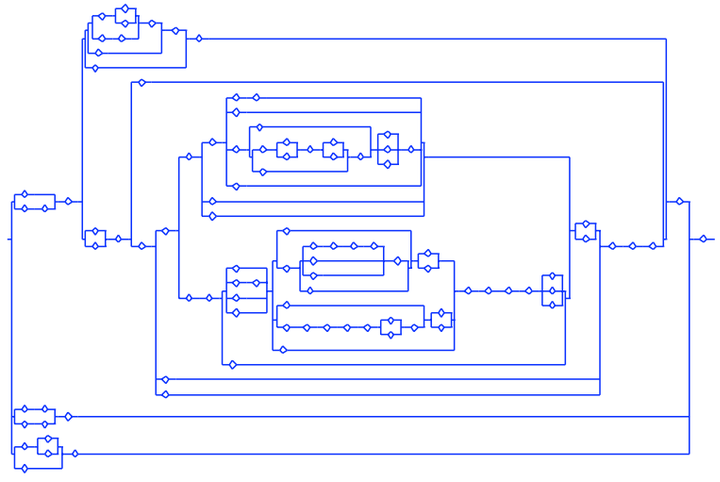
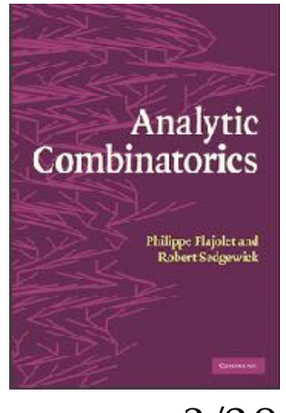
- ...hundreds of examples in “the purple book”.





I. Enumeration and Generating Functions

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Example: Binary Trees

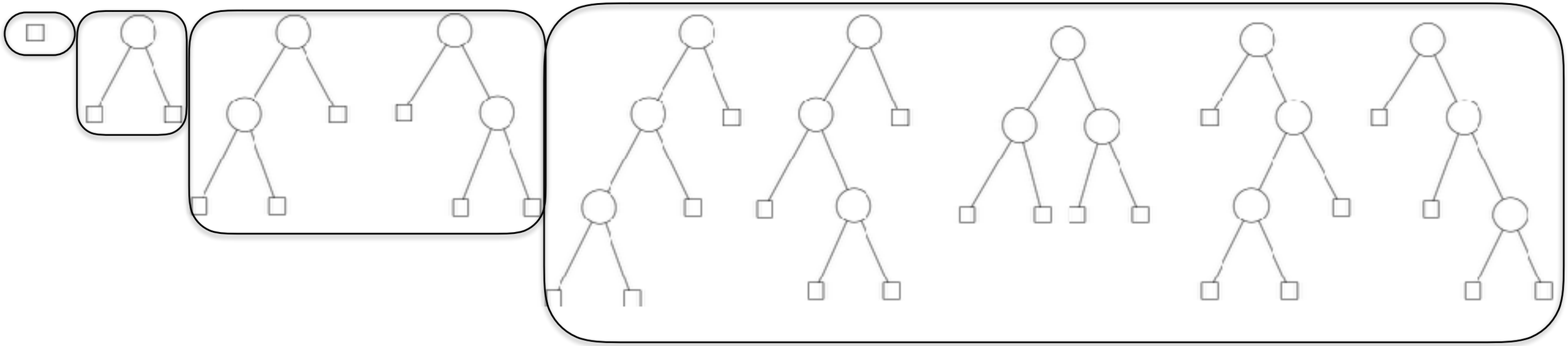
$$\mathscr{B} = 1 + \mathscr{Z} \times \mathscr{B} \times \mathscr{B}$$

$$B(z) = \sum_{n=0}^{\infty} B_n z^n$$

number of binary trees with *n* nodes

(Catalan)

$B_0 = B_1 = 1 \quad B_2 = 2 \qquad B_3 = 5$



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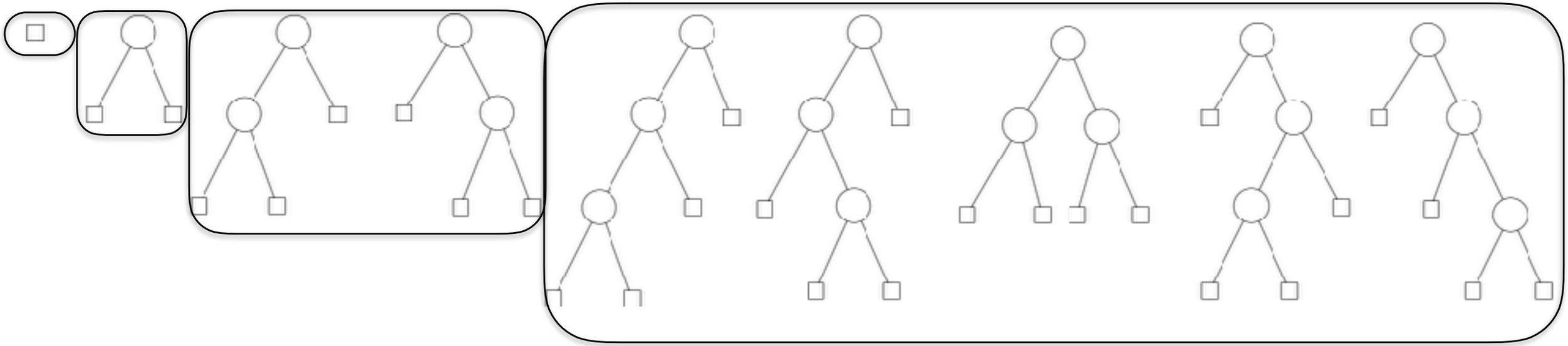

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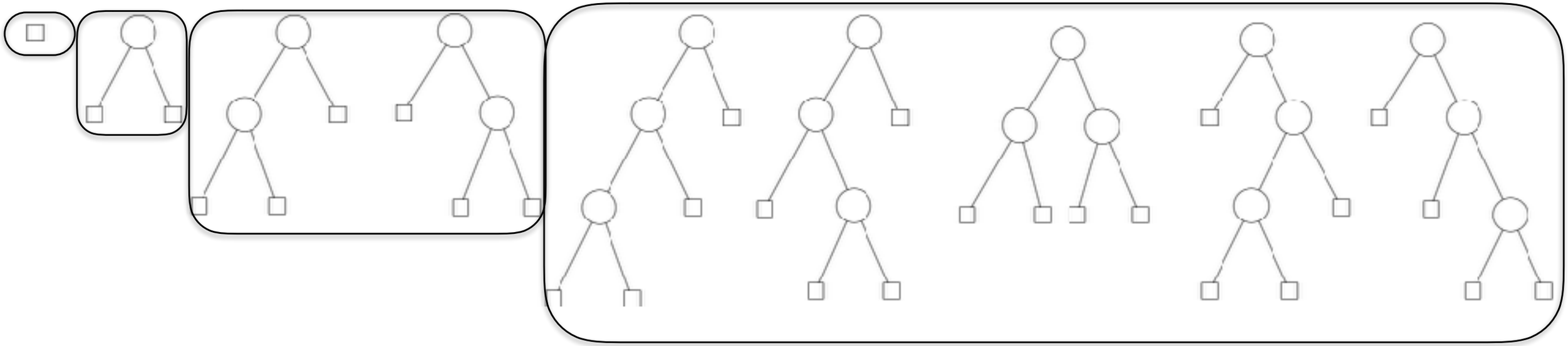

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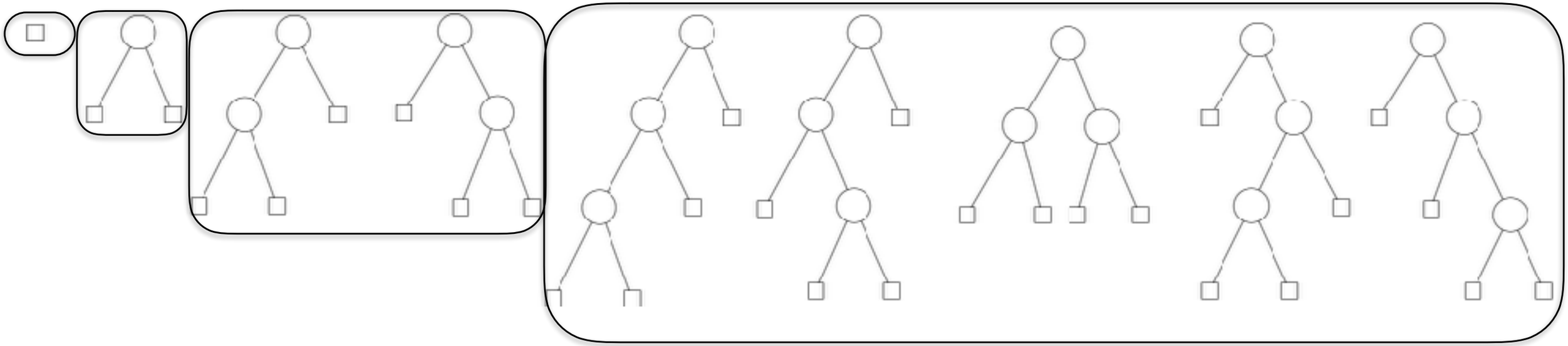

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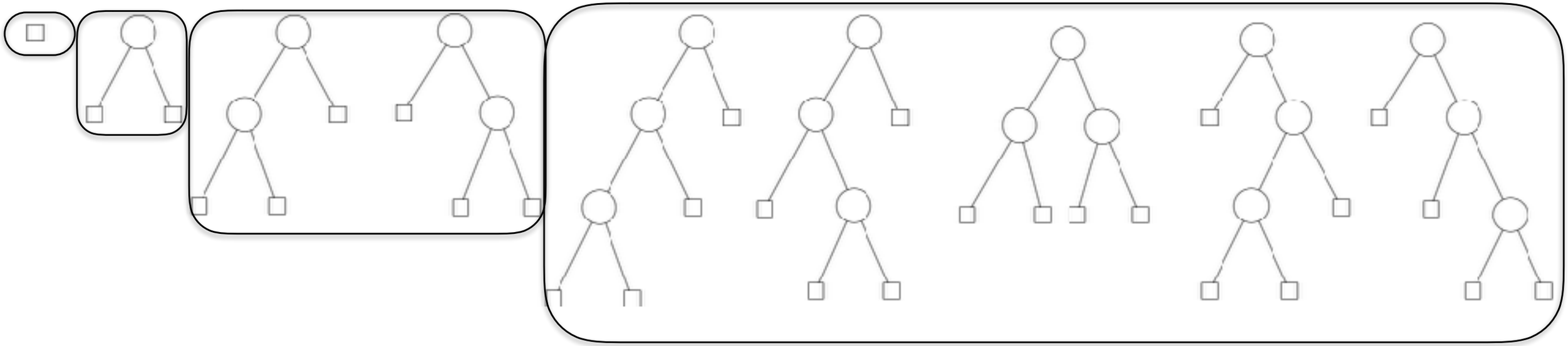

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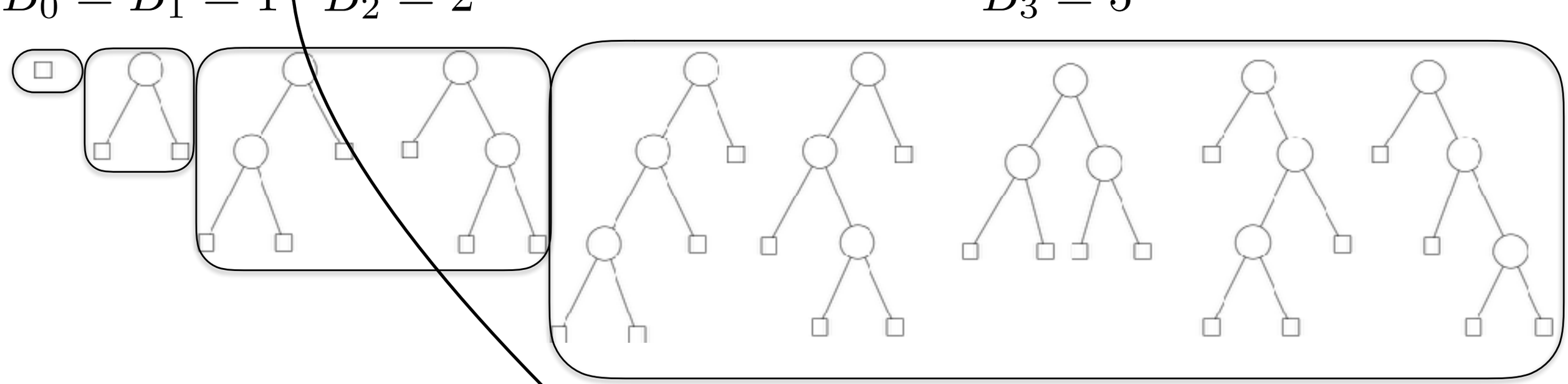

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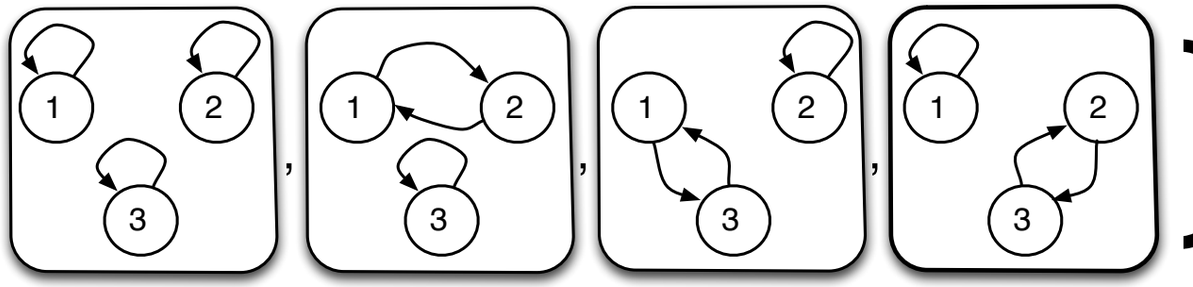
What do we count?

$$\mathrm{Inv}[\{1,2,3\}] = \Big\{$$  $$\Big\}$$

4 involutions;

3 of them permuted by $\mathfrak{S}_3 \to$ 2 *unlabelled structures*.

Exponential generating series (EGF):

$$F(z) = \sum_{n=0}^{\infty} f_n \frac{z^n}{n!}, \quad f_n = \text{nb. labelled structs of size } n. \qquad \mathrm{Inv}_3(z) = \frac{2}{3} z^3$$

Ordinary generating series (OGF):

$$\tilde{F}(z) = \sum_{n=0}^{\infty} \tilde{f}_n z^n, \quad \tilde{f}_n = \text{nb. unlabelled structs of size } n. \qquad \widetilde{\mathrm{Inv}}_3(z) = 2z^3$$

A Dictionary for Generating Series

Language: $1, \mathcal{Z}, +, \times$, SEQ, SET, CYC and recursion.

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Structure	EGF	OGF
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SEQ($\mathscr{A}$)	$\frac{1}{1-A(z)}$	$\frac{1}{1-\tilde{A}(z)}$
SET($\mathscr{A}$)	$\exp(A(z))$	$\exp(\sum \tilde{A}(z^i)/i)$

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CYC($\mathscr{A}$)	$\log\frac{1}{1-A(z)}$	$\sum\frac{\phi(i)}{i}\log\frac{1}{1-\tilde{A}(z^i)}$

Examples

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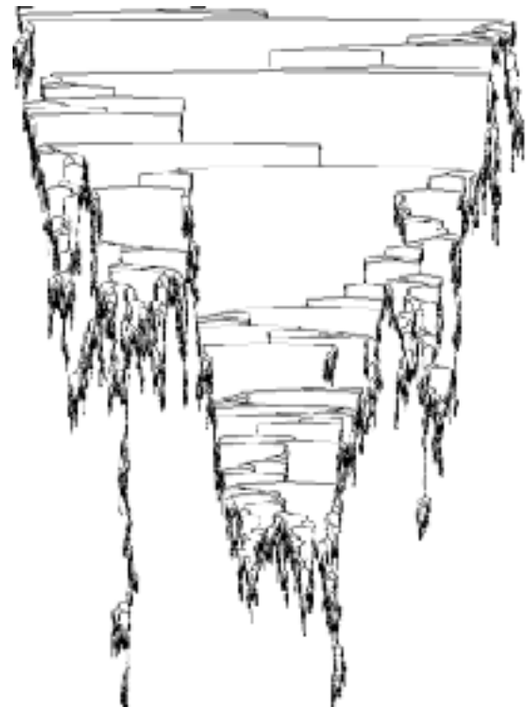
Binary trees: $\mathscr{B}=1+\mathscr{Z}\times\mathscr{B}\times\mathscr{B}$

$$\longrightarrow B(z) = 1 + zB(z)^2 = \tilde{B}(z)$$



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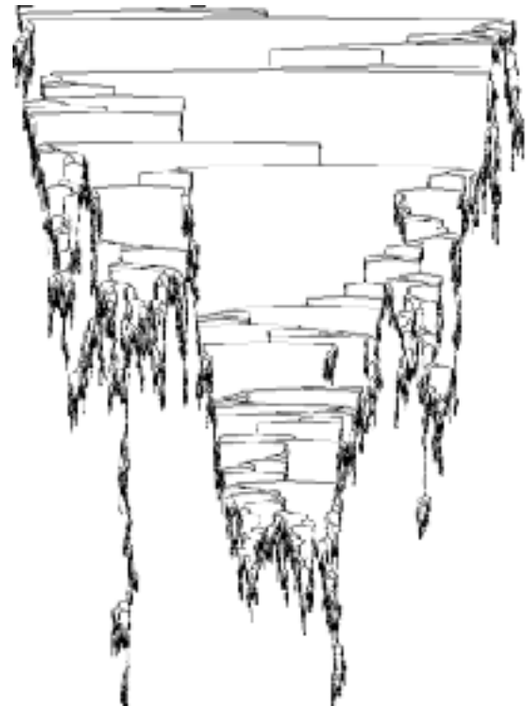

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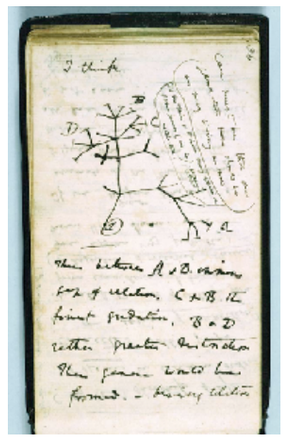

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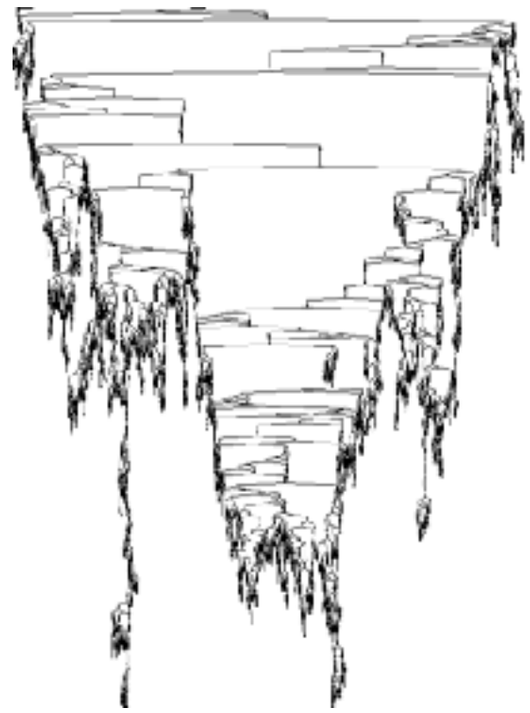

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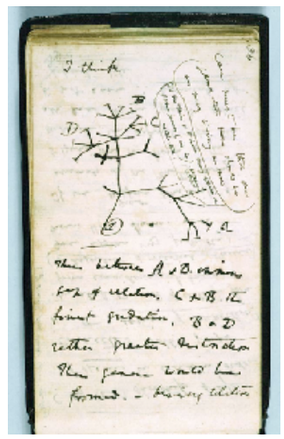

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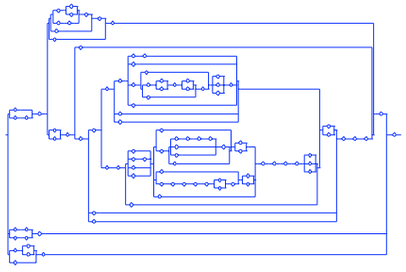
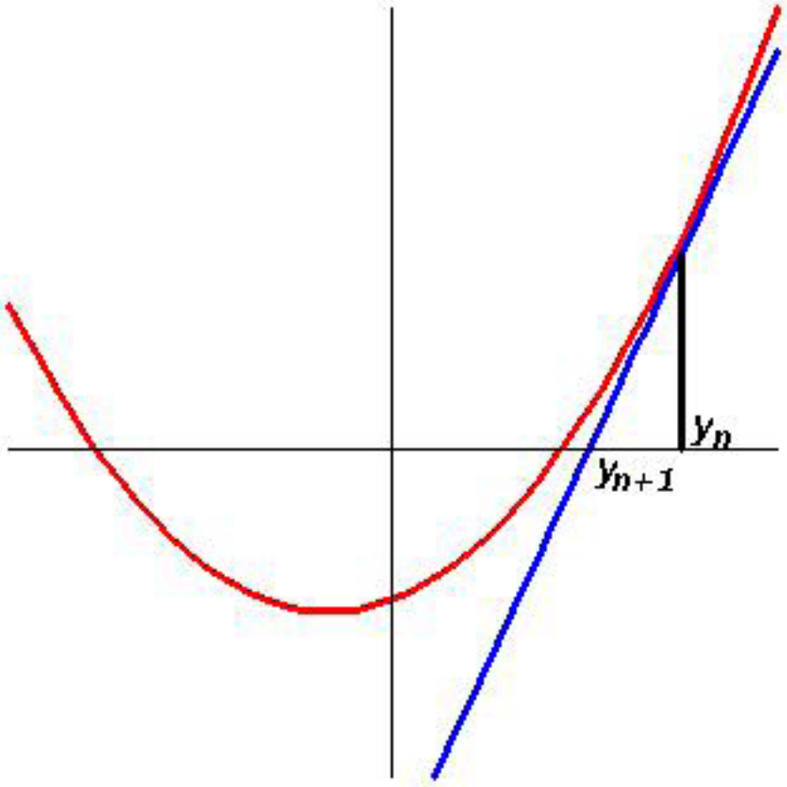


Series-parallel graphs:

$$\mathcal{G} = \mathcal{Z} + \mathcal{S} + \mathcal{P}, \mathcal{S} = \textsc{Seq}_{>0}(\mathcal{Z} + \mathcal{P}), \mathcal{P} = \textsc{Set}_{>0}(\mathcal{Z} + \mathcal{S})$$

$$\longrightarrow \left\{G(z) = z + S(z) + P(z), S(z) = \frac{1}{1 - z - P(z)} - 1, P(z) = e^{z+S(z)} - 1\right\}$$

II. Newton Iteration and Fast Enumeration



$y^3 + a^2y - 2a^3 + axy - x^3 = 0.$ $y = a - \frac{x}{4} + \frac{x^2}{64a} + \frac{131x^3}{512a^2} + \frac{509x^4}{16384a^3}$ &c.

$+a+p=y.$	$+y^3$	$+a^3 +3a^2p+3ap^2+p^3$
	$+axy$	$+a^2x+axp$
	$+x^2y$	$+x^3 +a^2p$
	$-x^3$	$-x^3$
	$-2a^3$	$-2a^3$
$-\frac{1}{4}x+q=p.$	$+p^3$	$-\frac{1}{64}x^3 +\frac{1}{16}x^2q -\frac{1}{8}xq^2+q^3$
	$+3ap^2$	$+\frac{3}{16}ax^2 -\frac{3}{2}axq +3aq^2$
	$+axp$	$-\frac{1}{4}ax^2 +axq$
	$+4a^2p$	$-a^2x +4a^2q$
	$+a^2x$	$+a^2x$
	$-x^3$	$-x^3$
$+\frac{x^2}{64a}+r=q.$	$+q^3$	*
	$-\frac{3}{4}xq^2$	*
	$+3aq^2$	$+\frac{3x^4}{4096a}$ * $+\frac{1}{32}x^2r+3ar^2$
	$+\frac{1}{16}x^2q$	$+\frac{3x^4}{1024a}$ * $+\frac{1}{16}x^2r$
	$-\frac{1}{2}axq$	$-\frac{1}{128}x^3 -\frac{1}{2}axr$
	$+4a^2q$	$+\frac{1}{17}ax^2 +4a^2r$
	$-\frac{61}{64}x^3$	$-\frac{61}{64}x^3$
	$-\frac{1}{16}ax^2$	$-\frac{1}{16}ax^2$

$+4a^2 - \frac{1}{2}ax + \frac{9}{32}x^2) + \frac{133}{128}x^3 - \frac{15x^4}{4096a}$ $(+\frac{131x^3}{512a^2} + \frac{509x^4}{16384a^3}$

1671

Numerical Newton Iteration

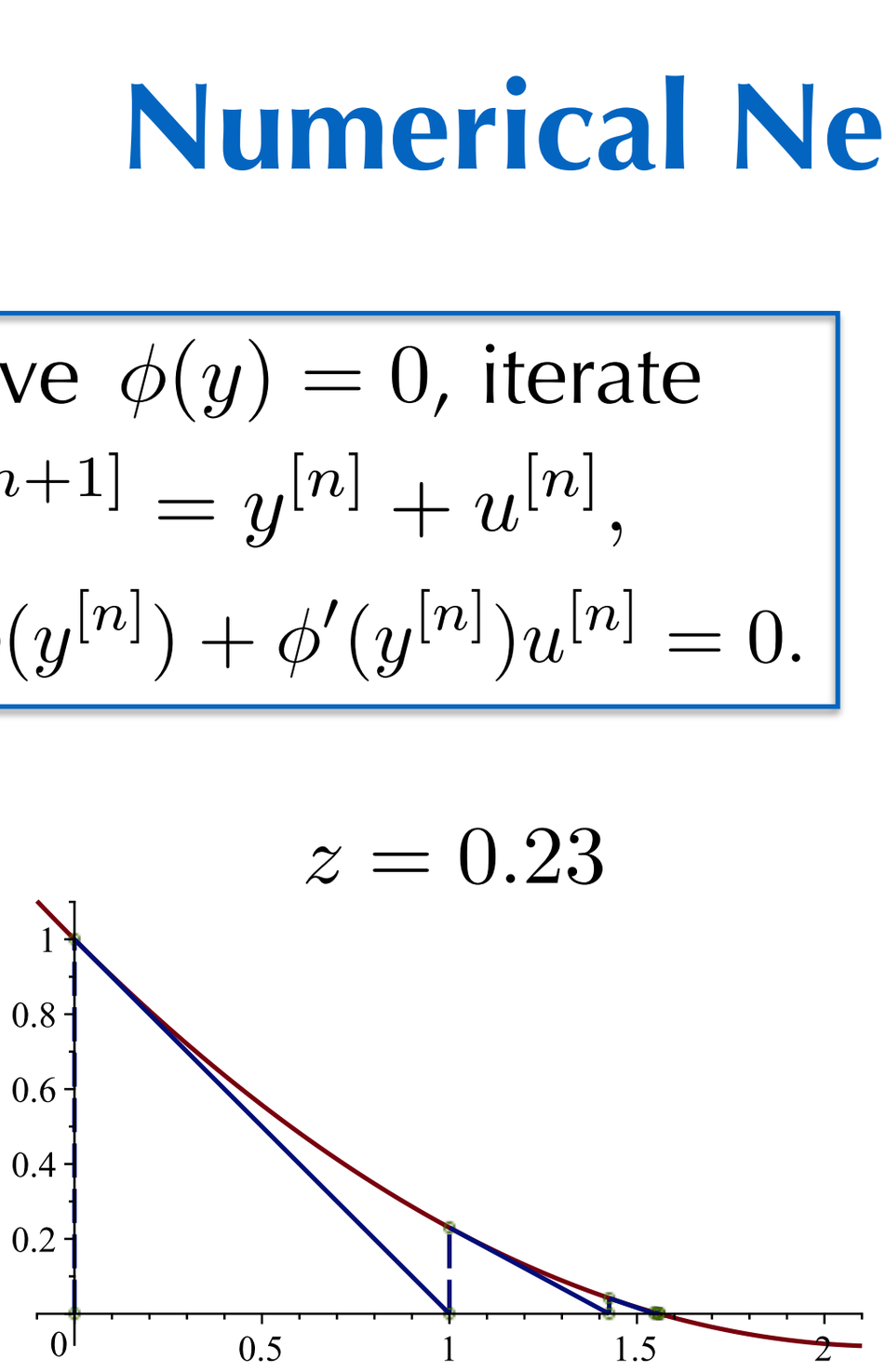
To solve $\phi(y) = 0$, iterate

$$y^{[n+1]} = y^{[n]} + u^{[n]},$$

with $\phi(y^{[n]}) + \phi'(y^{[n]})u^{[n]} = 0.$

$$\phi(y) = 1 + zy^2 - y$$

$$z = 0.23$$



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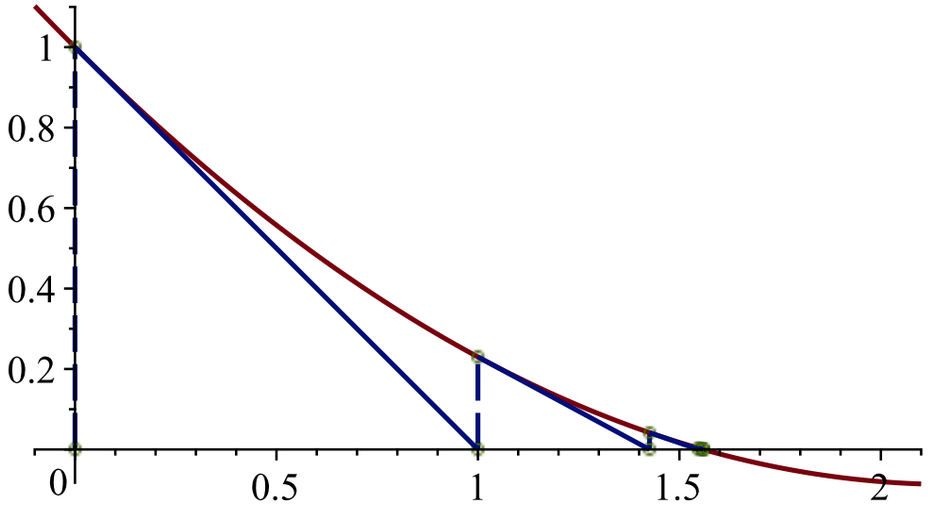

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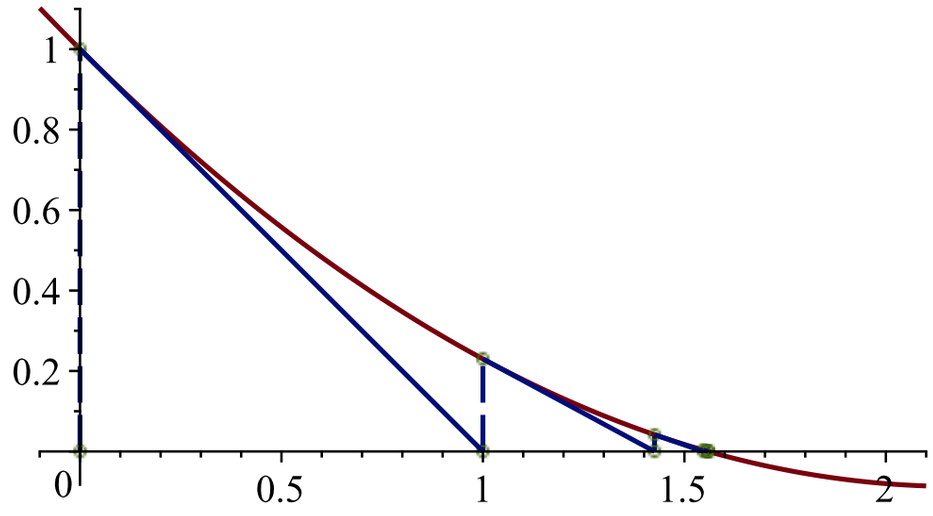

$$y^{[0]} = 0,$$

$$y^{[1]} = 1.000000000000000,$$

$$y^{[2]} \simeq 1.425925925925925,$$

$$y^{[3]} \simeq 1.547193318183630 3,$$

$$y^{[4]} \simeq 1.558925660274882 2,$$

$$y^{[5]} \simeq 1.559037571392659 2,$$

$$y^{[6]} \simeq 1.559037581576915 1$$

Quadratic convergence

Newton Iteration for Power Series

Same Newton Iteration

$$y^{[n+1]} = \mathcal{N}(y^{[n]}) = y^{[n]} + \frac{1 + z{y^{[n]}}^2 - y^{[n]}}{1 - 2zy^{[n]}}$$

Newton Iteration for Power Series

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$$y^{[n+1]} = \mathcal{N}(y^{[n]}) = y^{[n]} + \frac{1 + z{y^{[n]}}^2 - y^{[n]}}{1 - 2zy^{[n]}}$$

$$y^{[0]} = 0$$

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$$y^{[2]} = 1 + z + 2z^2 + 4z^3 + 8z^4 + 16z^5 + 32z^6 + 64z^7 + \cdots$$

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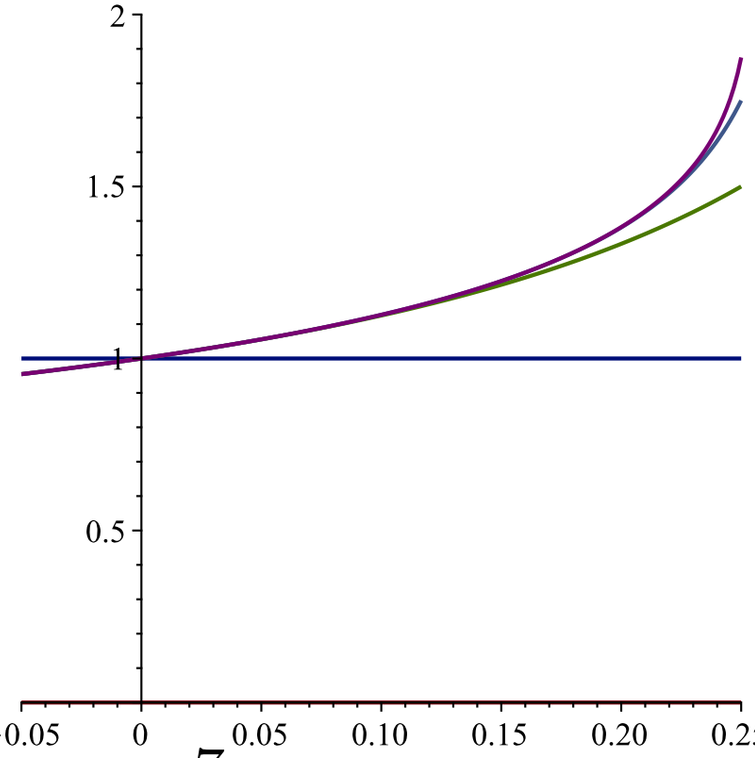

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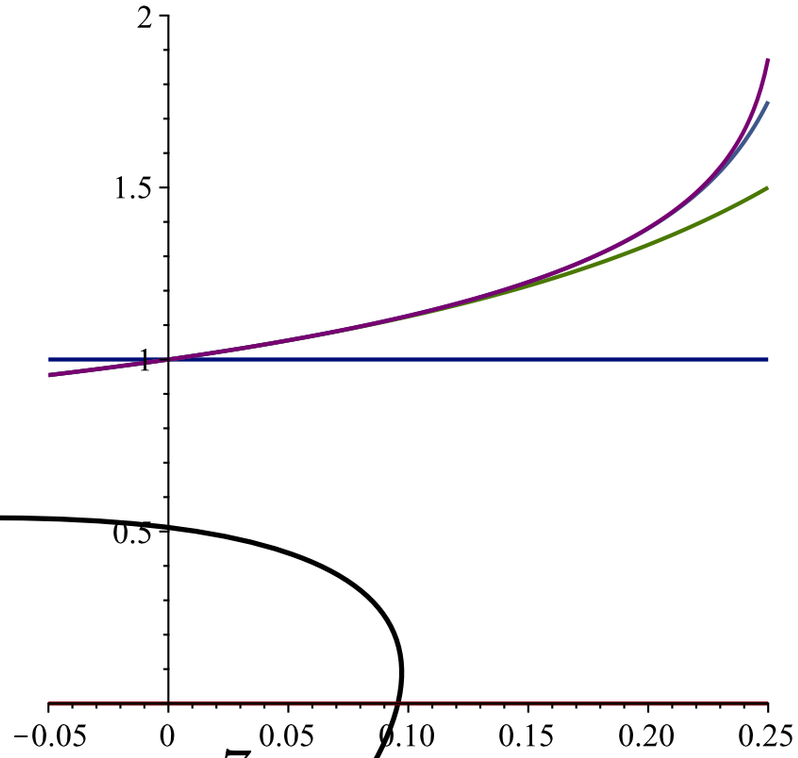
Proving numerical convergence requires control over the tails



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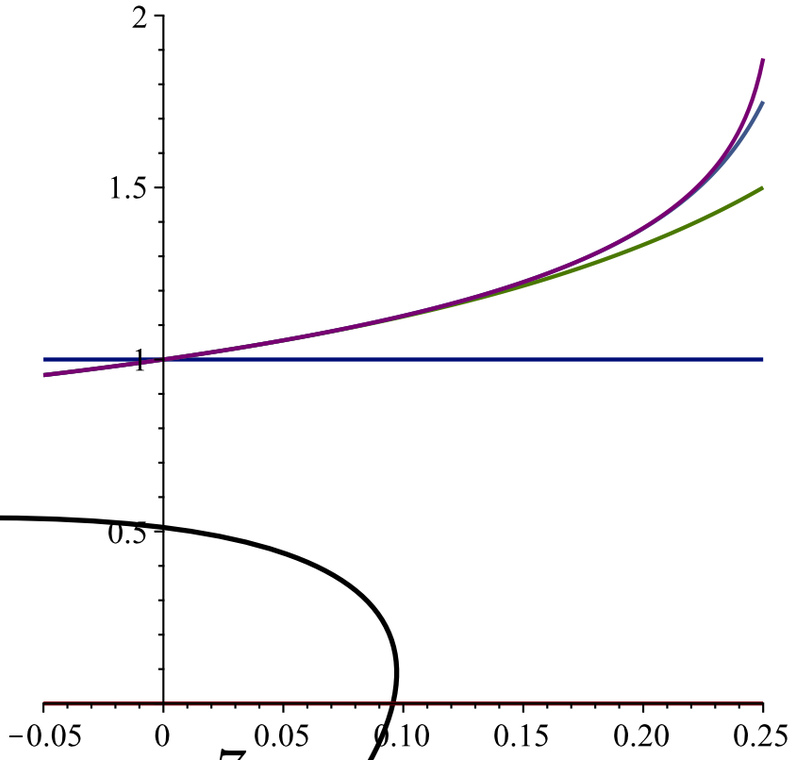

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On power series: $y - y^{[\infty]} = O(z^{m}) \Longrightarrow \mathcal{N}(y) - y^{[\infty]} = O(z^{2m(+1)})$

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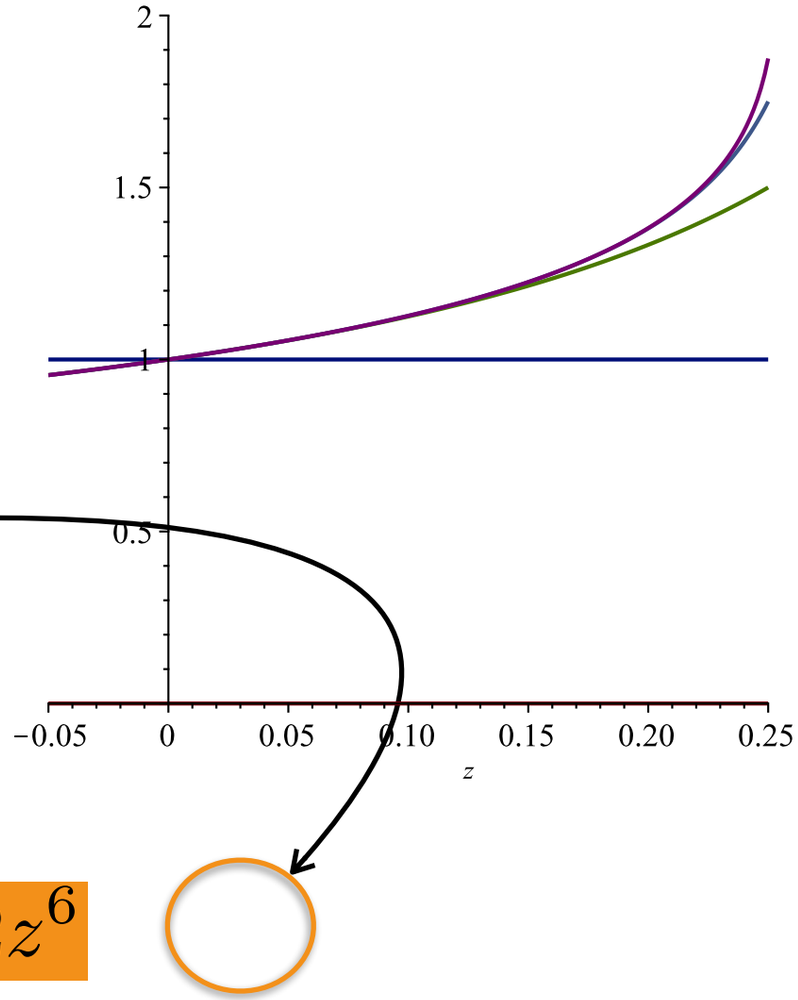

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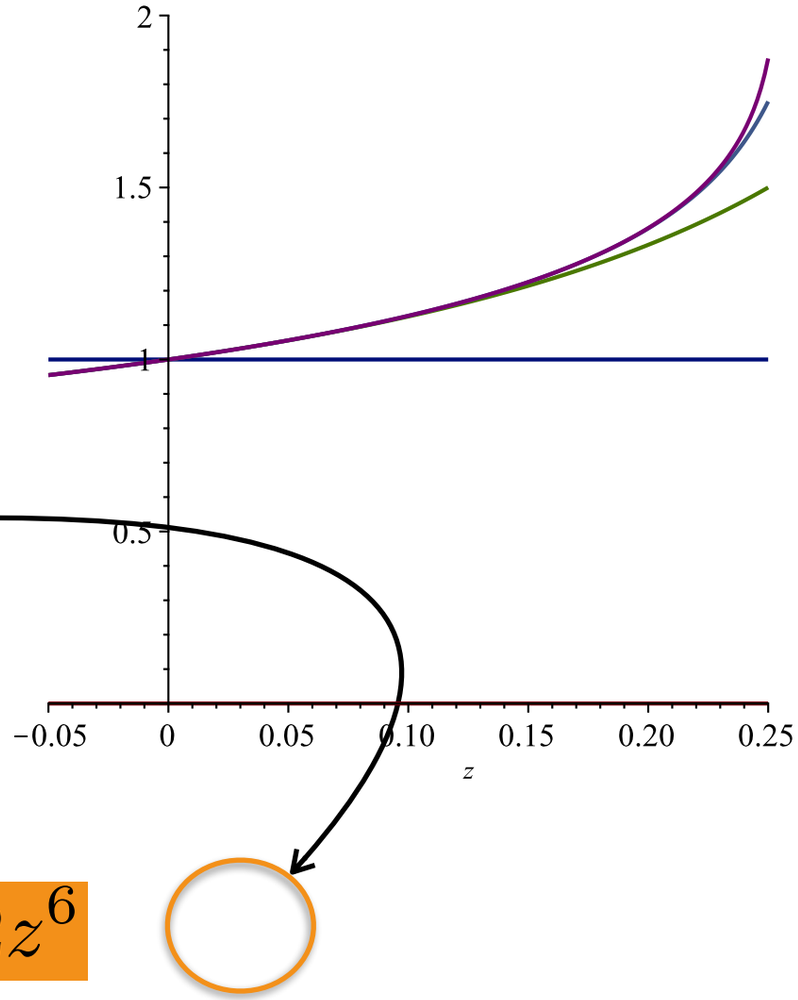

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```
Expand(N) = {
   res=Expand(N/2);
   a=ϕ(res); b=ϕ'(res);
   u=Solve(a+bx,x);
   return res+u; }
```

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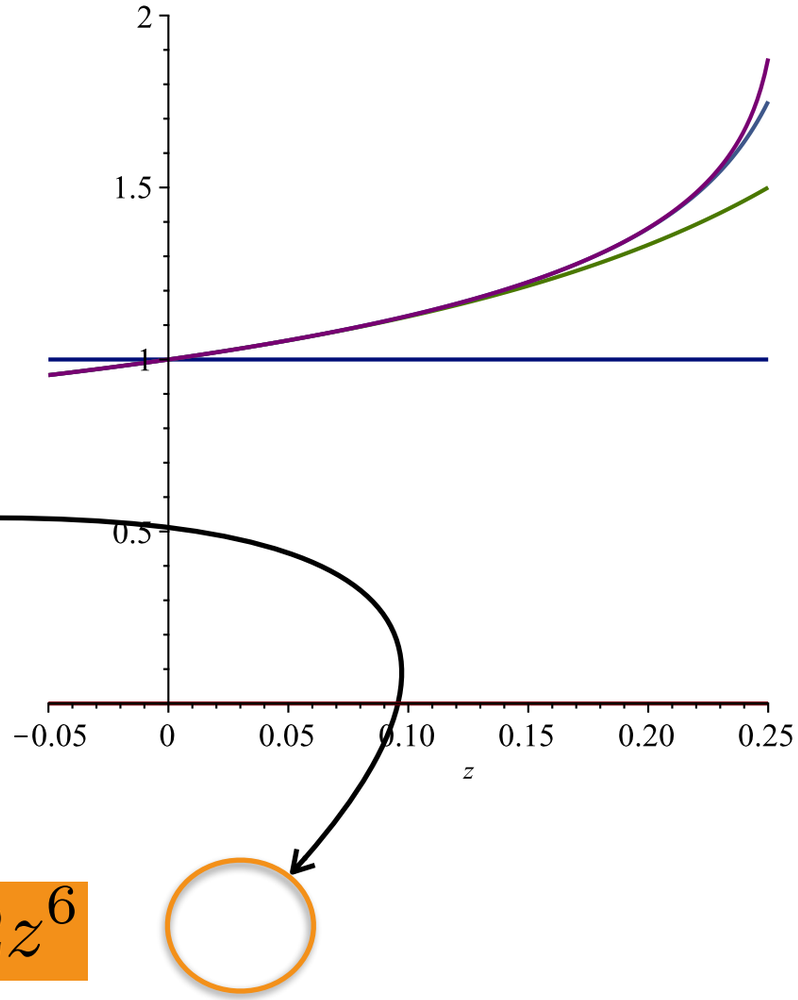

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```

Cost(N) ≤ ct x Cost(last step)

Fast Enumeration

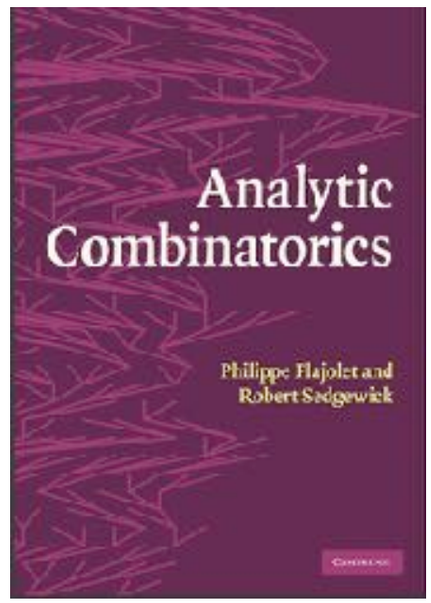
Thm. First N coefficients of GFs of all *constructible* structures:

1. arithmetic complexity $O(N \log N)$ (both ogf & egf);

2. bit complexity

$O(N^2 \log^2 N \log\log N)$ (ogf); $O(N^2 \log^3 N \log\log N)$ (egf).

Ingredients: Newton iteration & FFT.



[Pivoteau-S-Soria 2012]

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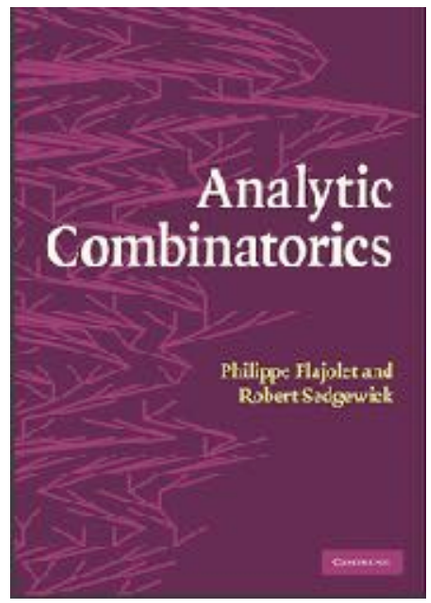
Ingredients: Newton iteration & FFT.

```
> with(NewtonGF):
> BinTrees:={B=Union(Epsilon,Prod(Z,B,B))}:
> GFSeries(BinTrees,labelled,z,21)[2];
```

$$B = 1 + z + 2z^2 + 5z^3 + 14z^4 + 42z^5 + 132z^6 + 429z^7 + 1430z^8 + 4862z^9 + 16796z^{10} + 58786z^{11} + 208012z^{12} + 742900z^{13} + 2674440z^{14} + 9694845z^{15} + 35357670z^{16} + 129644790z^{17} + 477638700z^{18} + 1767263190z^{19} + 6564120420z^{20} + O(z^{21})$$

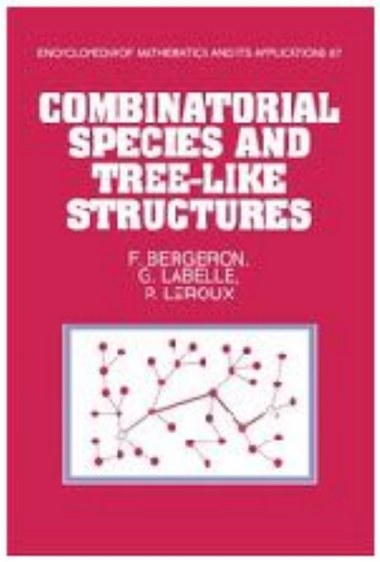


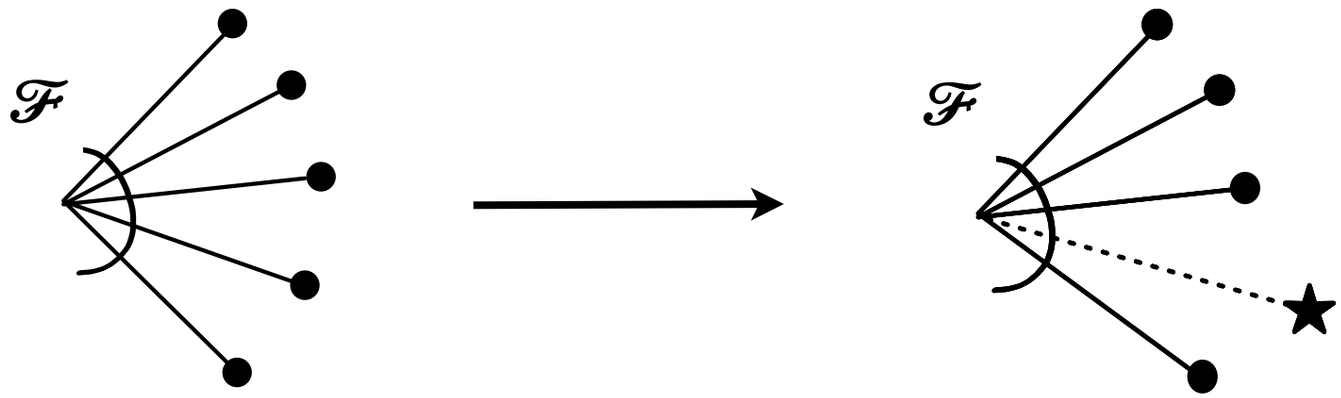
[Pivoteau-S-Soria 2012]

Demo
NewtonGF

Derivative of Combinatorial Structures

(origin: species theory)





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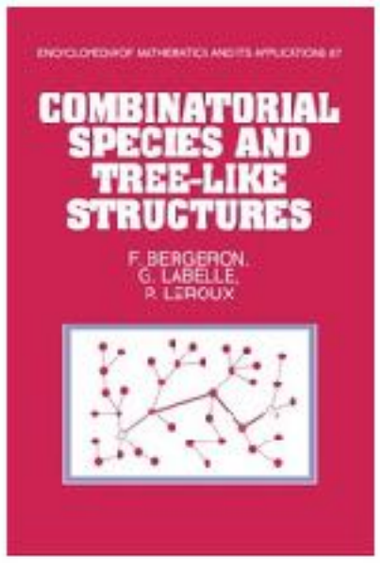

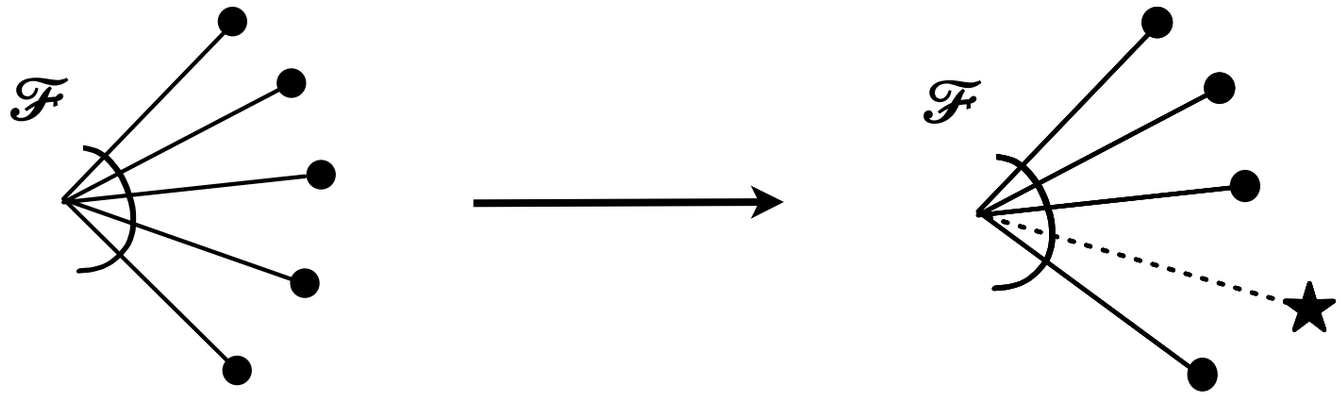

- $(\mathscr{F}+\mathscr{G})'=\mathscr{F}'+\mathscr{G}'; (\mathscr{F}\times\mathscr{G})'=\mathscr{F}'\times\mathscr{G}+\mathscr{F}\times\mathscr{G}';$

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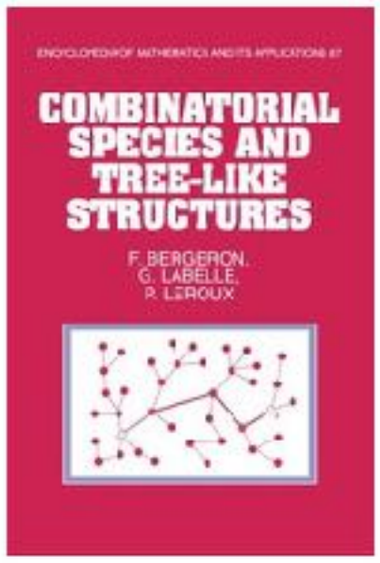

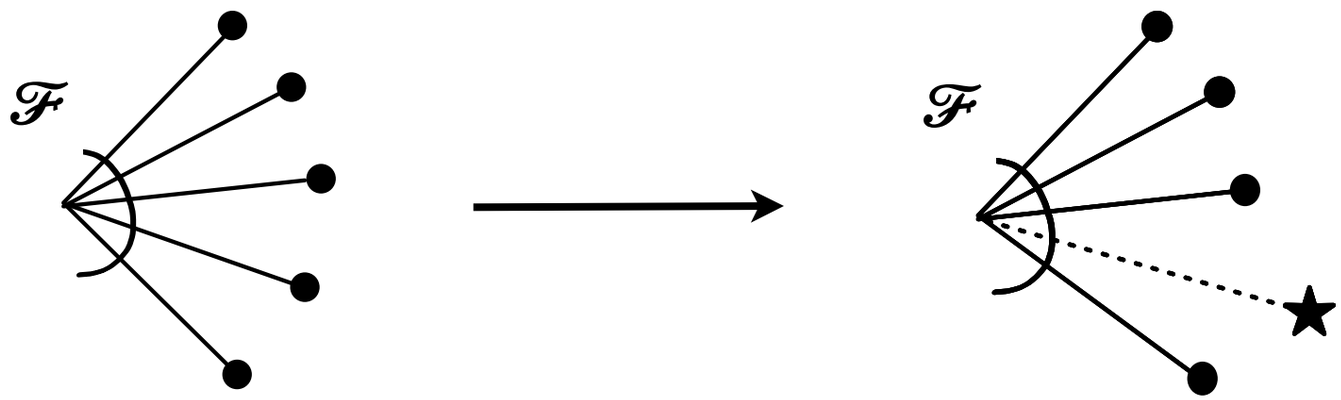

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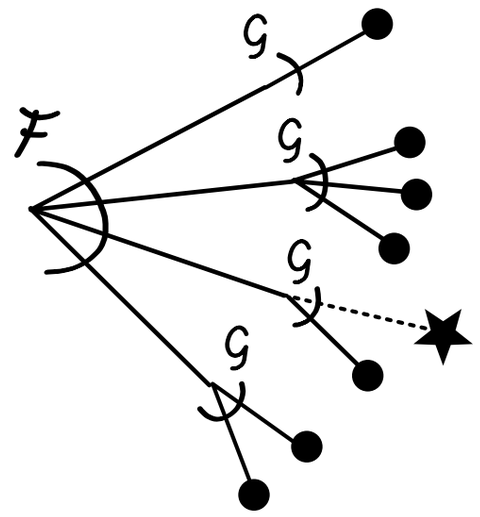
- $\mathscr{F}(\mathscr{G})'=\mathscr{F}'(\mathscr{G})\times\mathscr{G}';$



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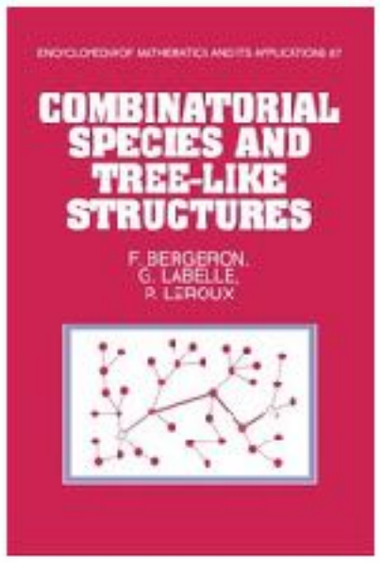
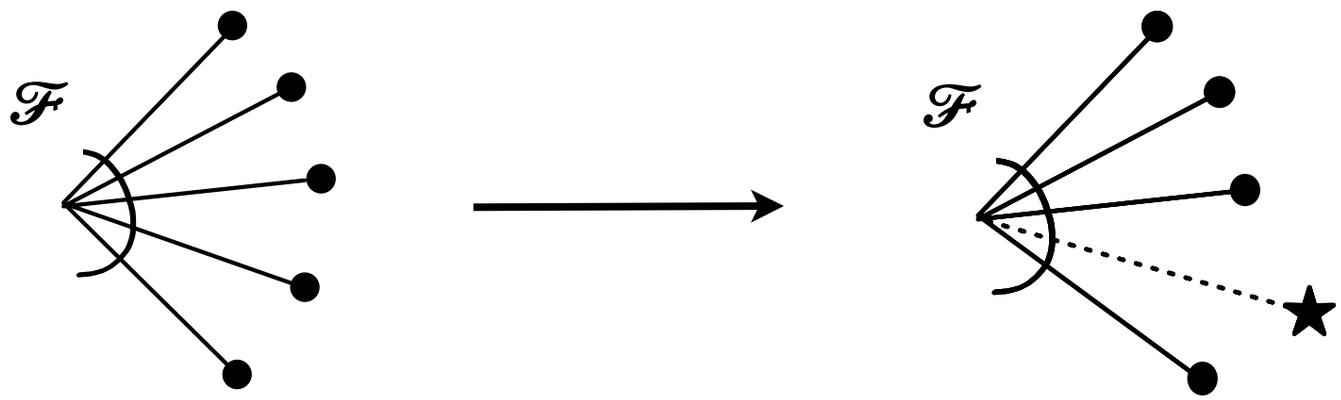
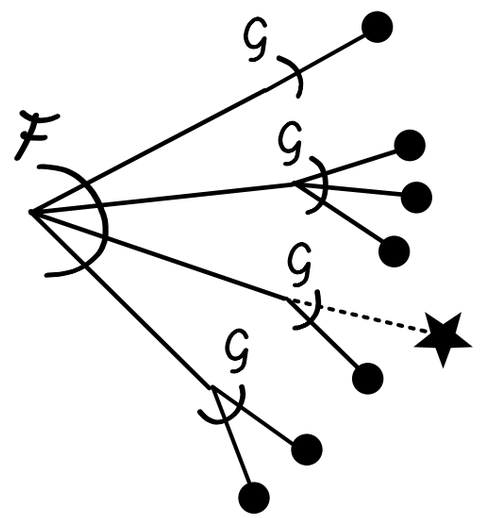




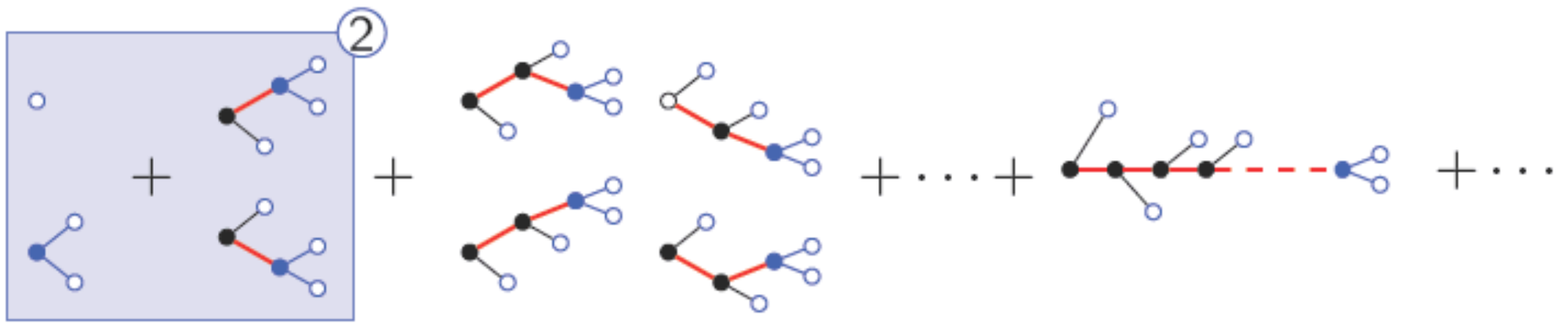
- $(\mathscr{F}+\mathscr{G})'=\mathscr{F}'+\mathscr{G}'$; $(\mathscr{F}\times\mathscr{G})'=\mathscr{F}'\times\mathscr{G}+\mathscr{F}\times\mathscr{G}'$;
- $\mathscr{F}(\mathscr{G})'=\mathscr{F}'(\mathscr{G})\times\mathscr{G}'$;
- $0'=1'=0$; $\mathscr{Z}'=1$;
  $\textsc{Set}'=\textsc{Set}$; $\textsc{Cyc}'=\textsc{Seq}$; $\textsc{Seq}'=\textsc{Seq}\times\textsc{Seq}$.

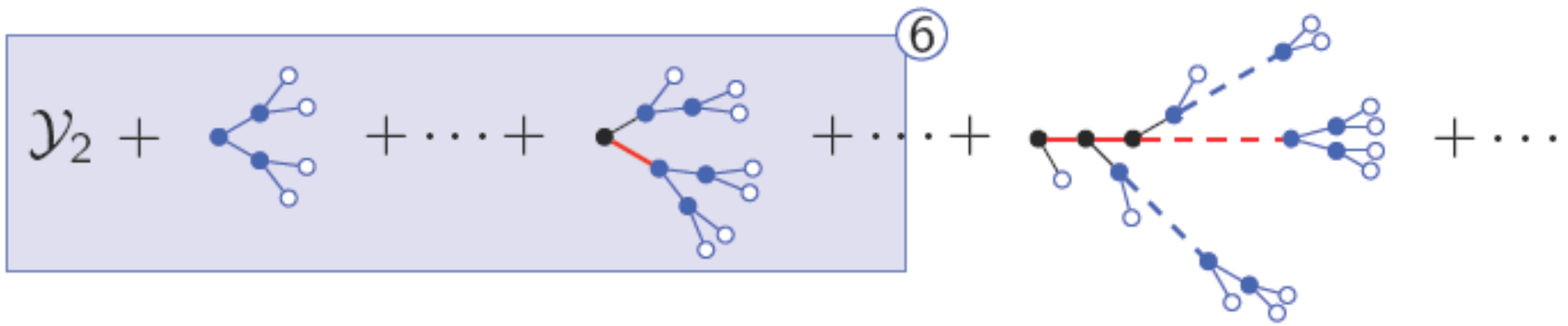


Combinatorial Newton Iteration

$$\mathcal{Y} = 1 + \mathcal{Z} \times \mathcal{Y} \times \mathcal{Y} =: \mathcal{H}(\mathcal{Z}, \mathcal{Y})$$

$\mathcal{Y}_0 = \varnothing$ $\quad$ $\mathcal{Y}_1 = \circ$

$\mathcal{Y}_2 =$ 

$\mathcal{Y}_3 =$ 

[Décoste, Labelle, Leroux 1982]

Combinatorial Newton Iteration

$$\mathcal{Y} = 1 + \mathcal{Z} \times \mathcal{Y} \times \mathcal{Y} =: \mathcal{H}(\mathcal{Z}, \mathcal{Y})$$

$$\mathcal{Y}^{[n+1]} = \mathcal{Y}^{[n]} + \textsc{Seq}(\mathcal{Z} \cdot \mathcal{Y}^{[n]} \cdot \star + \mathcal{Z} \cdot \star \cdot \mathcal{Y}^{[n]}) \cdot ((1 + \mathcal{Z} \cdot \mathcal{Y}^{[n]} \cdot \mathcal{Y}^{[n]}) \setminus \mathcal{Y}^{[n]}).$$

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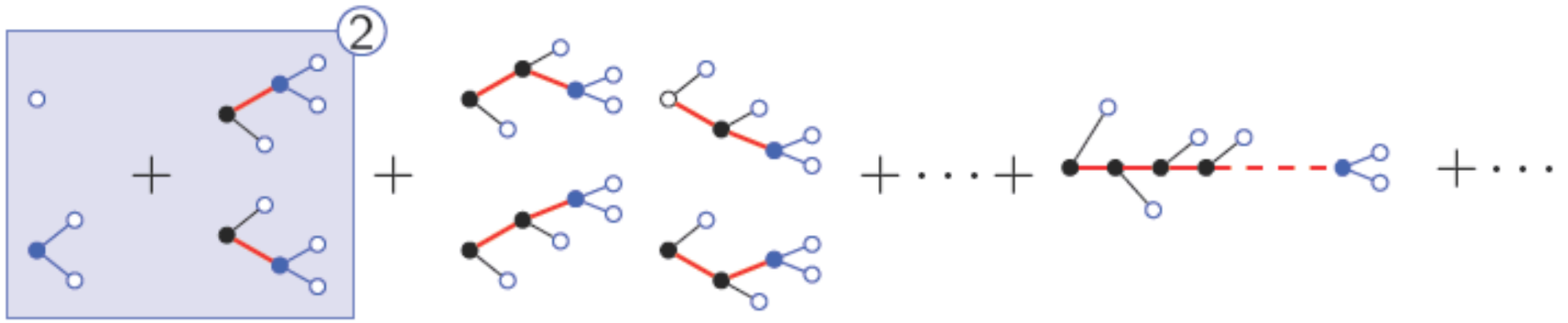
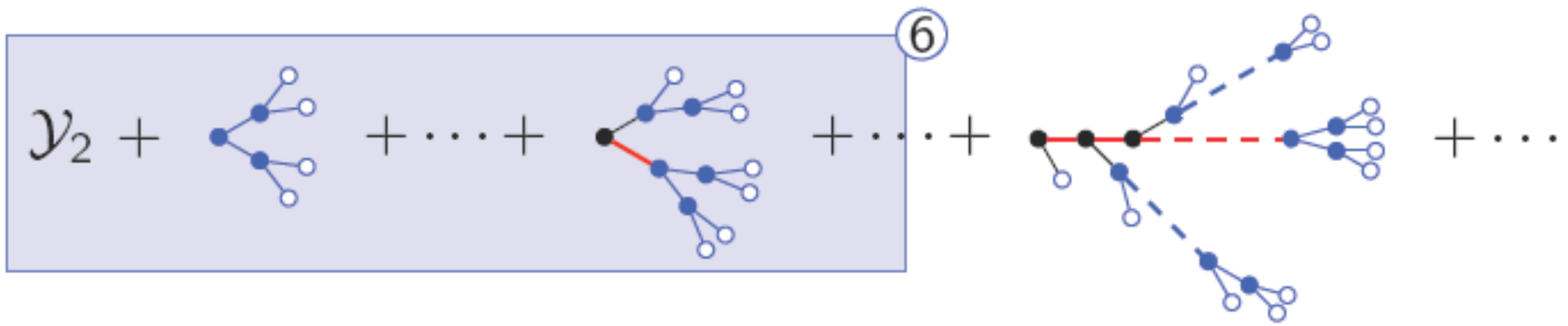
$\mathcal{Y}_2 =$ 

$\mathcal{Y}_3 =$ 

[Décoste, Labelle, Leroux 1982]

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$$\left(\mathrm{Id} - \frac{\partial \mathcal{H}}{\partial \mathcal{Y}}(\mathcal{Z}, \mathcal{Y}^{[n]})\right)^{-1}$$

$\mathcal{Y}_0 = \varnothing$ $\quad$ $\mathcal{Y}_1 =$ ∘

$\mathcal{Y}_2 =$ (2) + + + ⋯ + + ⋯

$\mathcal{Y}_3 =$ $\mathcal{Y}_2$ + (6) + ⋯ + + ⋯ + + ⋯

[Décoste, Labelle, Leroux 1982]

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$$\mathcal{Y} = 1 + \mathcal{Z} \times \mathcal{Y} \times \mathcal{Y} =: \mathcal{H}(\mathcal{Z}, \mathcal{Y})$$

$$\mathcal{Y}^{[n+1]} = \mathcal{Y}^{[n]} + \textsc{Seq}(\mathcal{Z} \cdot \mathcal{Y}^{[n]} \cdot \star + \mathcal{Z} \cdot \star \cdot \mathcal{Y}^{[n]}) \cdot ((1 + \mathcal{Z} \cdot \mathcal{Y}^{[n]} \cdot \mathcal{Y}^{[n]}) \setminus \mathcal{Y}^{[n]}).$$

$$\left(\mathrm{Id} - \frac{\partial \mathcal{H}}{\partial \mathcal{Y}}(\mathcal{Z}, \mathcal{Y}^{[n]})\right)^{-1}$$

$\mathcal{Y}_0 = \varnothing$ $\quad$ $\mathcal{Y}_1 =$ ∘

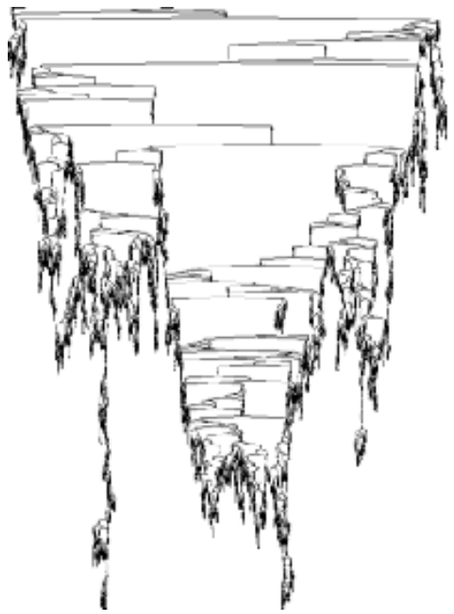
$\mathcal{Y}_2 =$ (2) $+ \cdots +$ $\mathcal{Y}_3 =$ (6) $\mathcal{Y}_2 + \cdots + \cdots + \cdots$

[Décoste, Labelle, Leroux 1982]

Ccl: numerical convergence of the Newton iteration starting from 0.

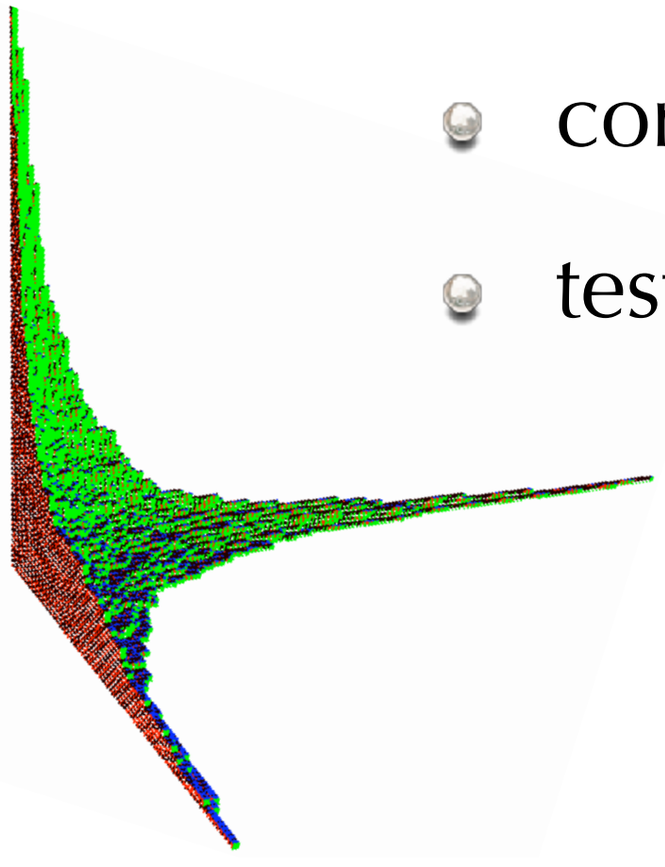
III. Random Generation

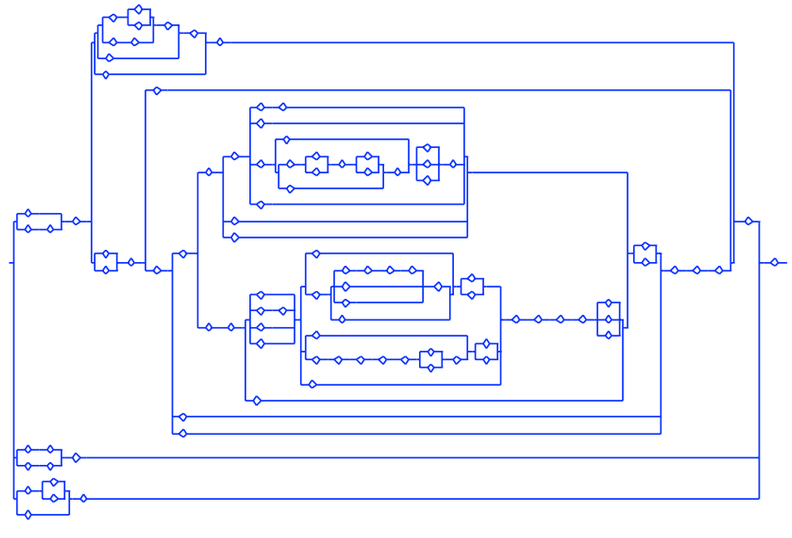
Why Random Generation?



Simulation in the discrete world; helps

- evaluate parameters;
- compare/refine models;
- test software.





Boltzmann Sampling

$$\text{Proba}(t) = \frac{x^{|t|}}{T(x)} \quad \text{with} \quad T(x) = \sum_{t \in \mathcal{T}} x^{|t|} = \sum_{n} T_n x^n$$

x is a parameter of the algorithm

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Expected size:

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```
Generate(h∈𝒦) = {
  if 𝒦=1 return 1;
  if 𝒦=𝒵 return 𝒵;
  if 𝒦=ℱx𝒢 {
     Generate(f∈ℱ);
     Generate(g∈𝒢);
     return (f,g); }
  if 𝒦=ℱ+𝒢 {
     b:=Bernoulli(F(x)/H(x));
     if b=1 return Generate(f∈ℱ);
     else return Generate(g∈𝒢);
  if 𝒦=Set(ℱ) {
     …
```

[Duchon, Flajolet, Louchard, Schaeffer 2002-04]

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F(x),H(x) by Newton iteration

[Duchon, Flajolet, Louchard, Schaeffer 2002-04]

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     return (f,g); }
  if ℋ=ℱ+ℊ {
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$$\mathcal{B}=1+\mathcal{I}\times\mathcal{B}\times\mathcal{B}$$

with 1/B(.23)≃1/1.559≃.6414

Coin: 0,0,1,0,1,1,1,1,0,1,…

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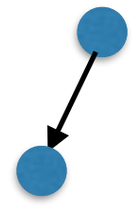

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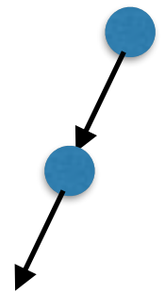

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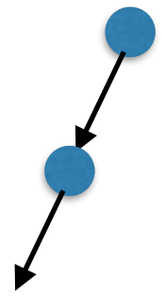

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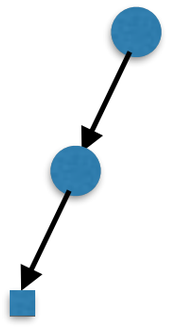

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  if 𝒳=ℤ return ℤ;
  if 𝒳=𝒴x𝒵 {
     Generate(f∈𝒴);
     Generate(g∈𝒵);
     return (f,g); }
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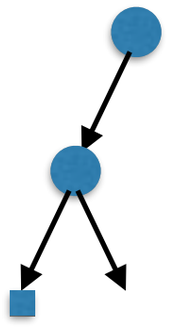

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  if 𝓗=𝓩 return 𝓩;
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     Generate(f∈𝓕);
     Generate(g∈𝓖);
     return (f,g); }
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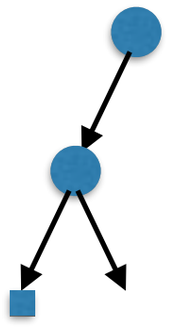

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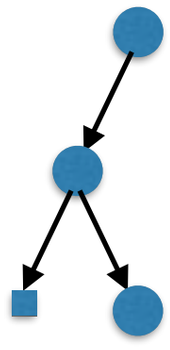

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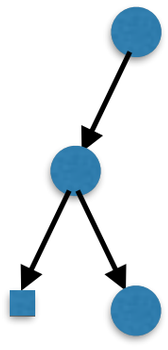

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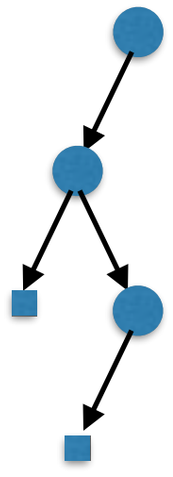

[Duchon, Flajolet, Louchard, Schaeffer 2002-04]

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$$\text{Proba}(t)=\frac{x^{|t|}}{T(x)} \quad \text{with} \quad T(x)=\sum_{t\in\mathcal{T}} x^{|t|}=\sum_n T_n x^n$$

Expected size:
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x is a parameter of the algorithm

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F(x),H(x) by Newton iteration

Example: binary trees

$$\mathscr{B}=1+\mathscr{Z}\times\mathscr{B}\times\mathscr{B}$$

with 1/B(.23)≃1/1.559≃.6414

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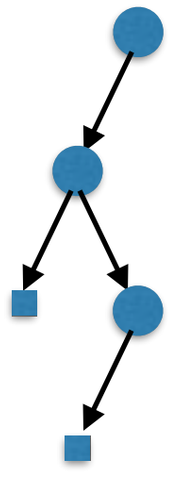

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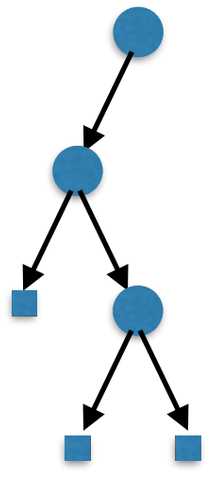

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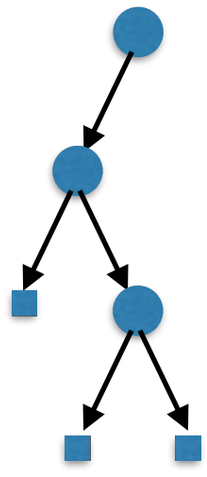

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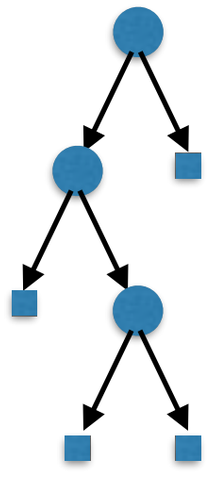

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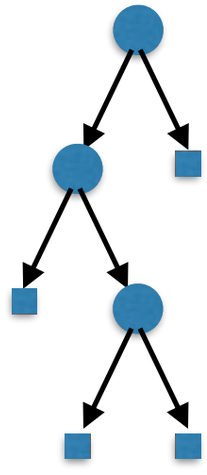
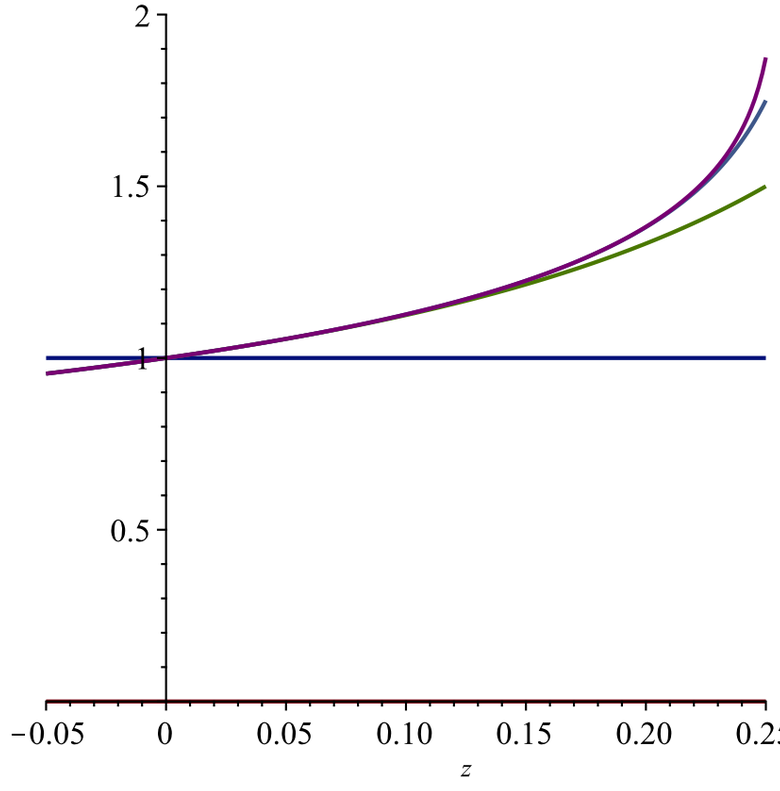


Exp. size
$$\sim\frac{1}{2\sqrt{1-4x}}$$

[Duchon, Flajolet, Louchard, Schaeffer 2002-04]

Example: XML-trees

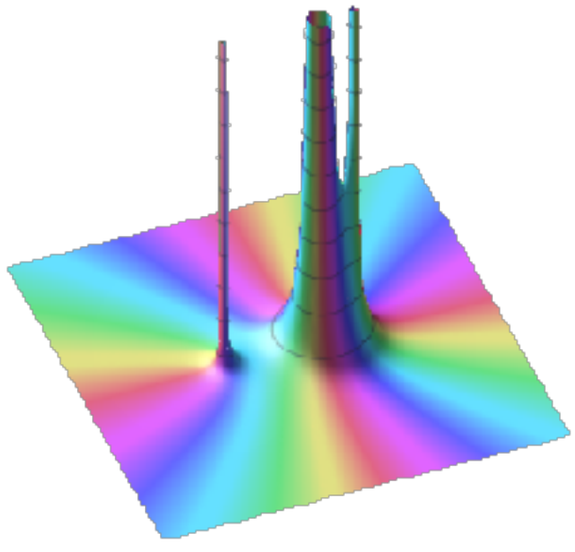
Grammar	File size	#eq.	Newton
rss	9.5k	16	0.02s.
Relax NG	124k	114	0.10s.
XSLT	168k	122	0.12s.
XHTML Basic	284k	96	0.32s.
SVG	6.3M	232	0.23s.
OpenDocument	2.8M	814	0.34s.
DocBook	11M	977	23s.



Time for x s.t. E(size)=10,000

[Darrasse2010]

IV. Asymptotic Analysis



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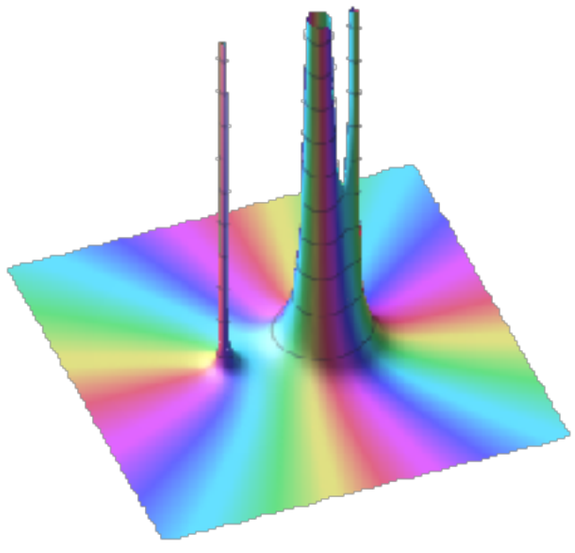

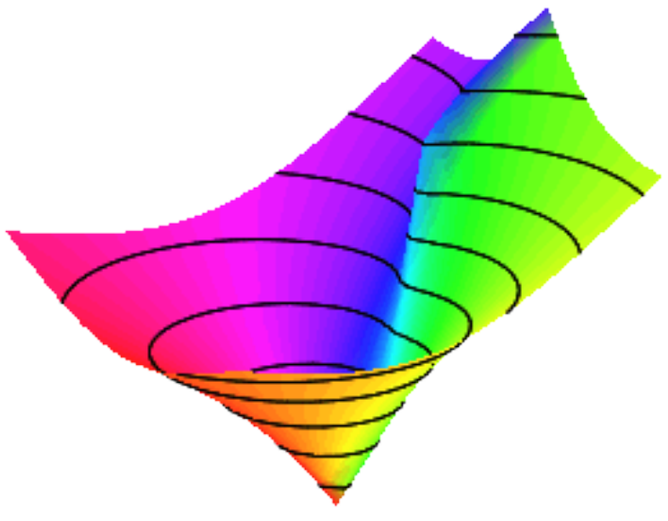

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Singularity Analysis

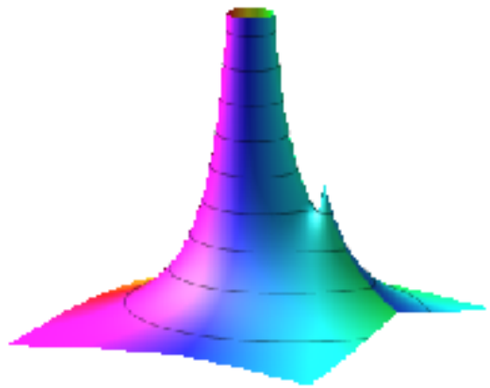
counts the number of objects of size *n*

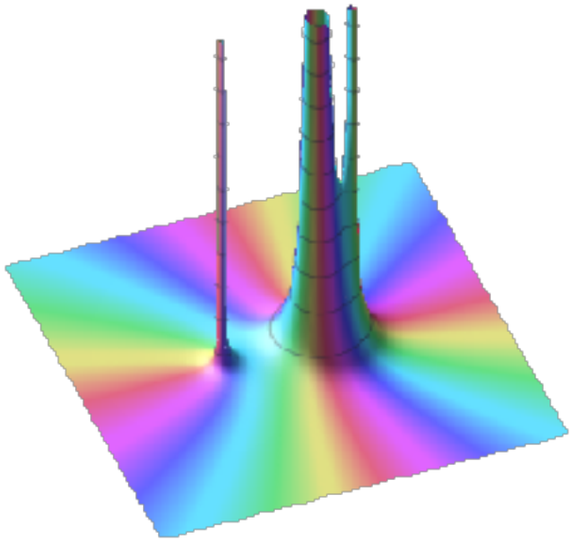
$$(a_n) \mapsto A(z) := \sum_{n \geq 0} a_n z^n$$

captures some structure

A 3-Step Method:

$$a_n = \frac{1}{2\pi i} \oint \frac{A(z)}{z^{n+1}}\, dz$$





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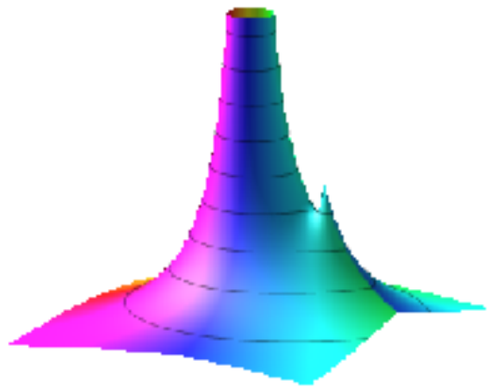

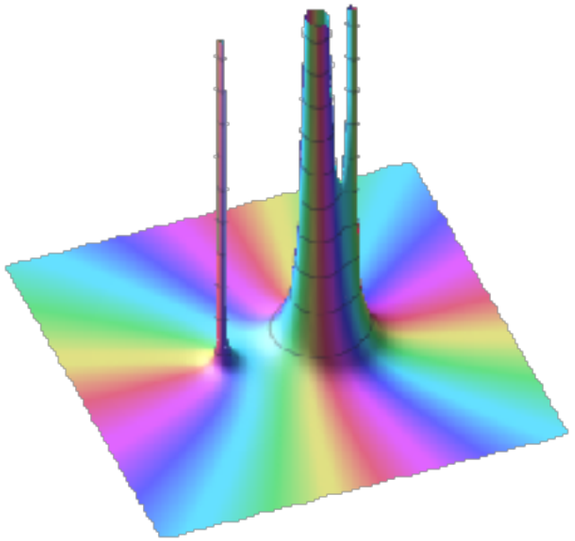

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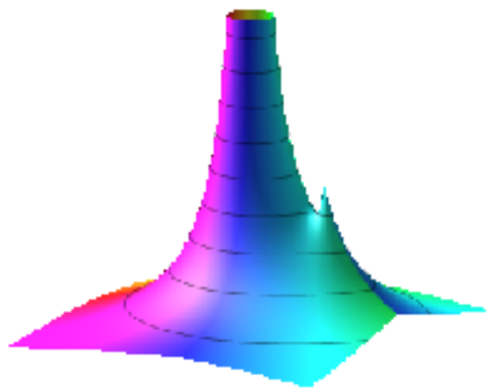

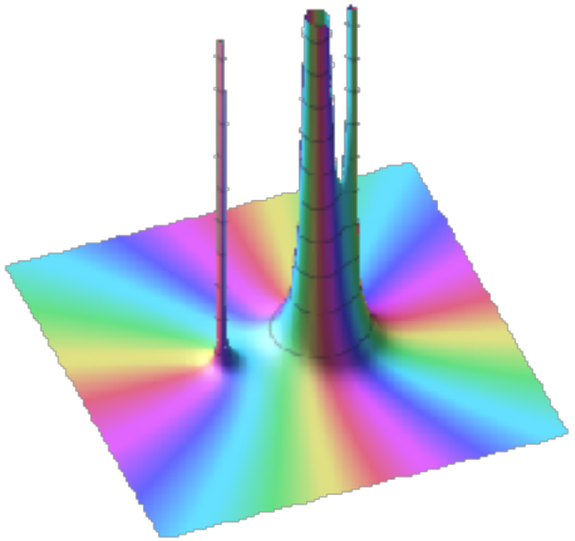

$$A(z) \underset{z \to \rho}{\sim} c \left(1 - \frac{z}{\rho}\right)^{\alpha} \log^m \frac{1}{1 - \frac{z}{\rho}}$$

$$a_n \underset{n \to \infty}{\sim} c\, \rho^{-n} \frac{n^{-\alpha-1}}{\Gamma(-\alpha)} \log^m n \qquad (\alpha \notin \mathbb{N})$$

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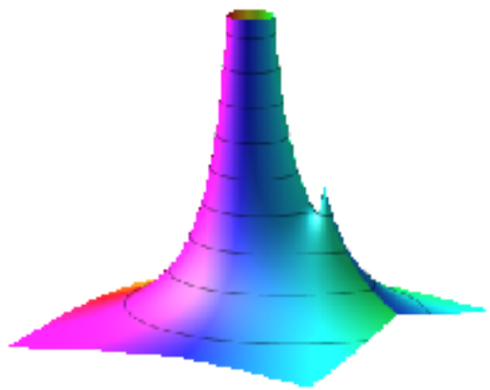

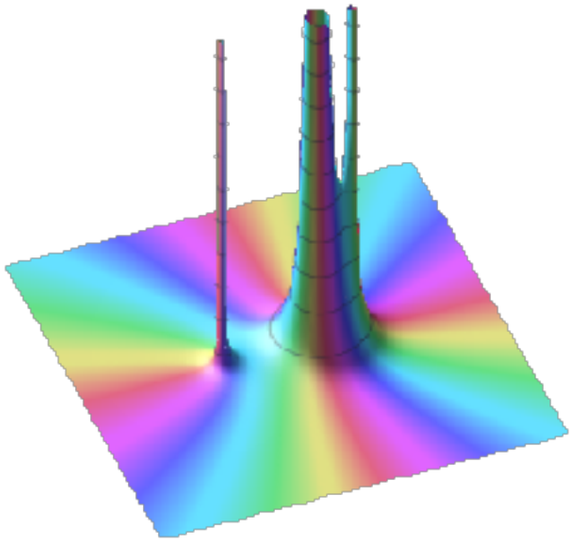

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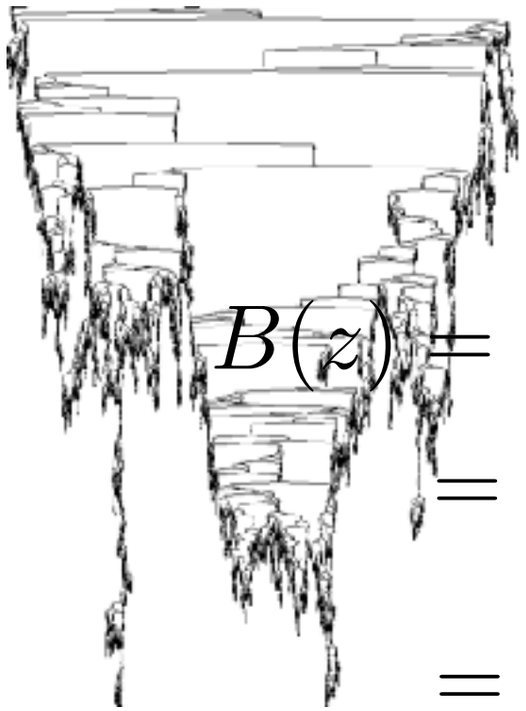
full asymptotic expansion available

Example: Binary Trees (Again!)



$$B(z) = 1 + zB(z)^2$$
$$= 1 + z + 2z^2 + 5z^3 + \cdots$$
$$= \frac{1 - \sqrt{1-4z}}{2z}$$

A 3-Step Method:

1. Locate dominant singularities;
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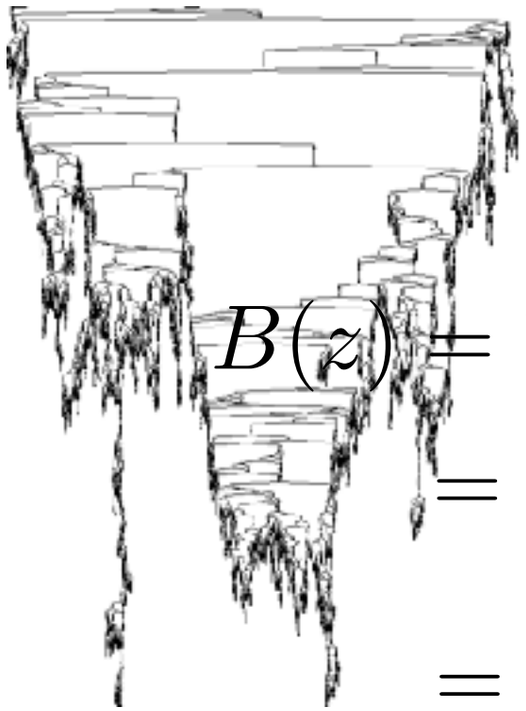

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Probability that a leaf is a child of the root?

$$\frac{[z^n]2zB(z)}{B_n} = \frac{1}{2} + \frac{3}{4n} + O\left(\frac{1}{n^2}\right)$$

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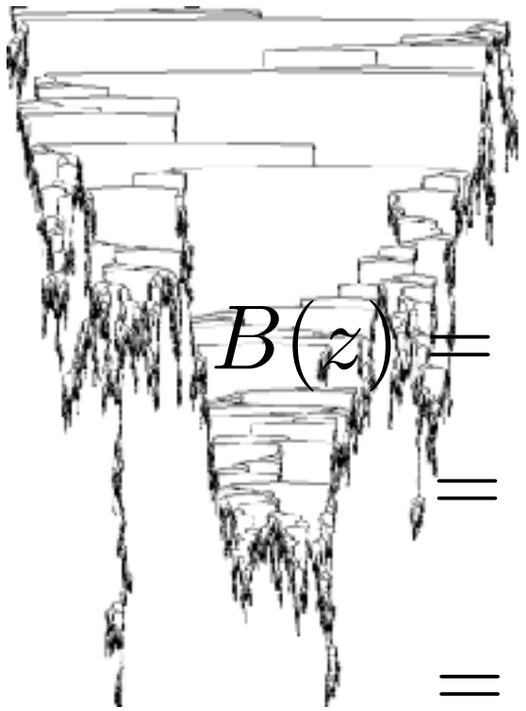

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Demo.

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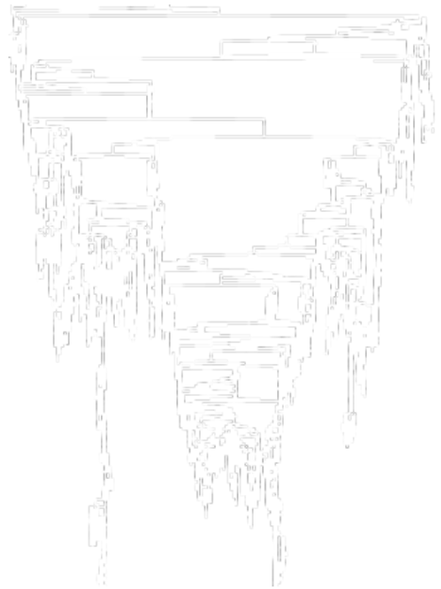

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- Equations over combinatorial structures + parameters

Ex.: path length in binary trees

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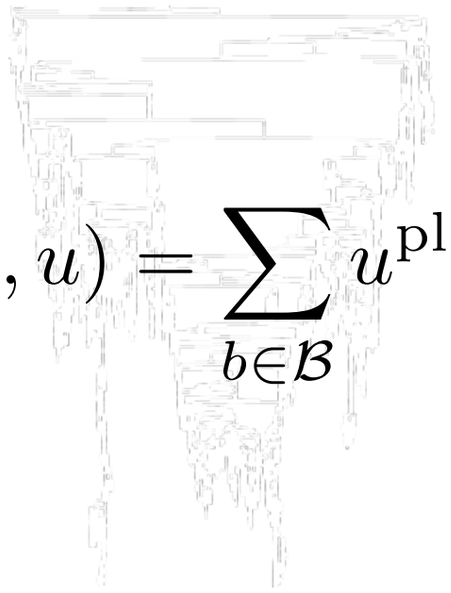

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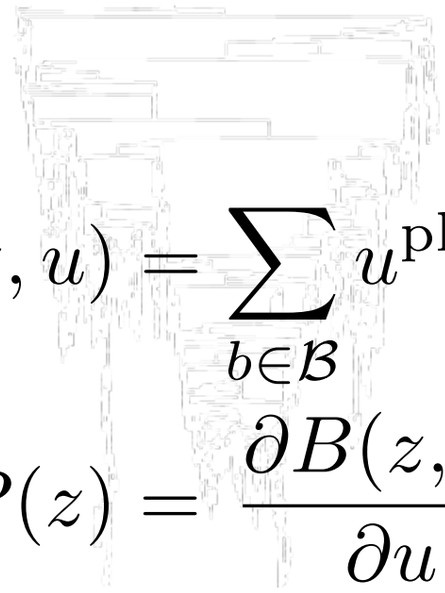

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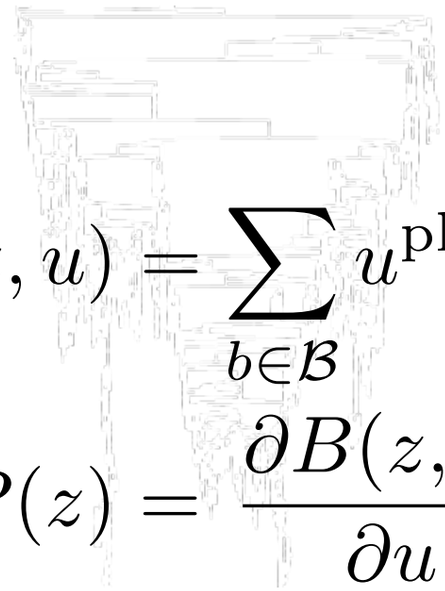

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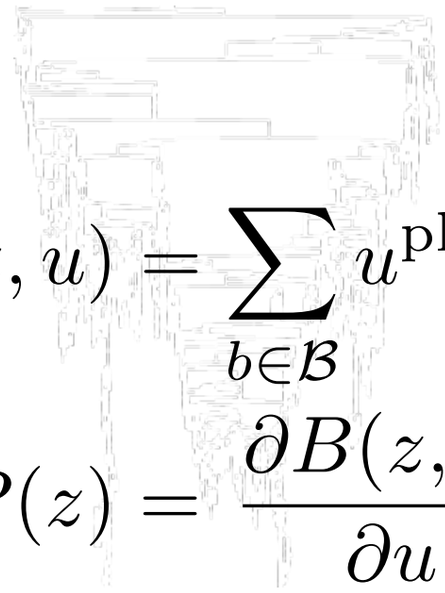

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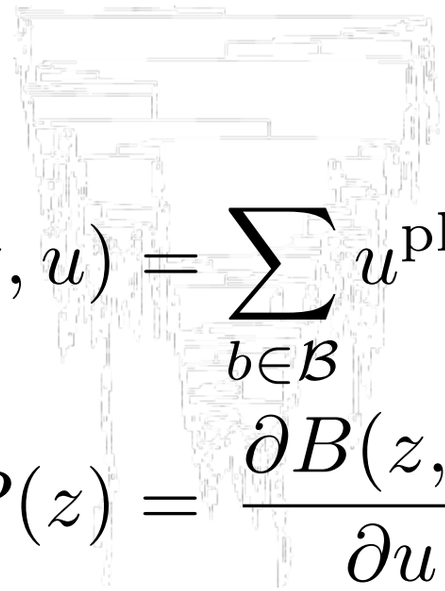

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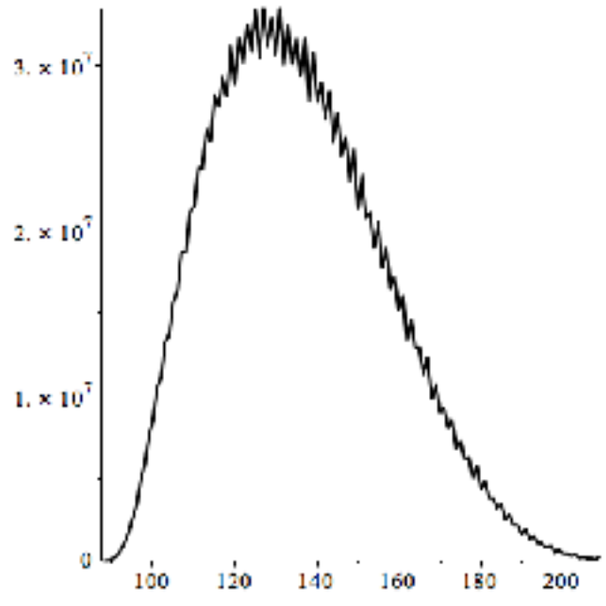

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- Equations over combinatorial structures + parameters
- Multivariate generating series

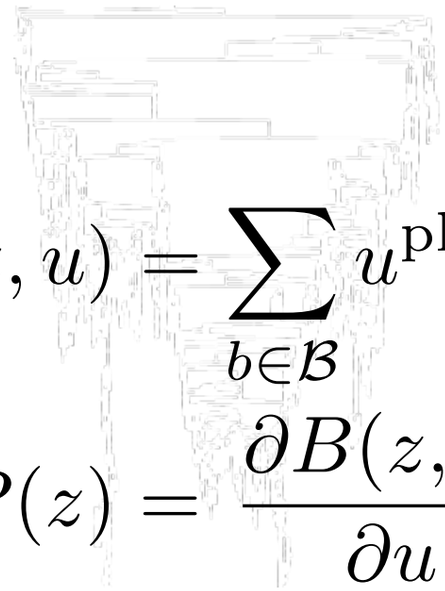
$$F(z,u) = \sum_{n,k} f_{n,k} u^k z^n$$

- Complex analysis

$$f_{n,k} \sim \cdots, n \to \infty$$

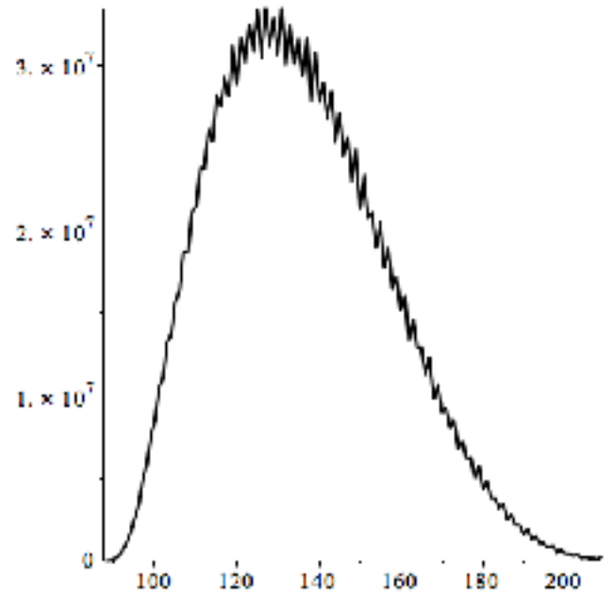
- Limiting distribution

Ex.: path length in binary trees



$$B(z,u) = \sum_{b \in \mathcal{B}} u^{\mathrm{pl}(b)} z^{|b|}$$

$$P(z) = \left. \frac{\partial B(z,u)}{\partial u} \right|_{u=1}$$



$$\frac{P_n}{nB_n} \sim \sqrt{\pi n}$$

Demo.

If you can specify it, you can analyze it!

Permutations
Mappings
Words
Strings
Urns
Trees

Languages
Integers
Compositions
Partitions
...

+ *parameters*

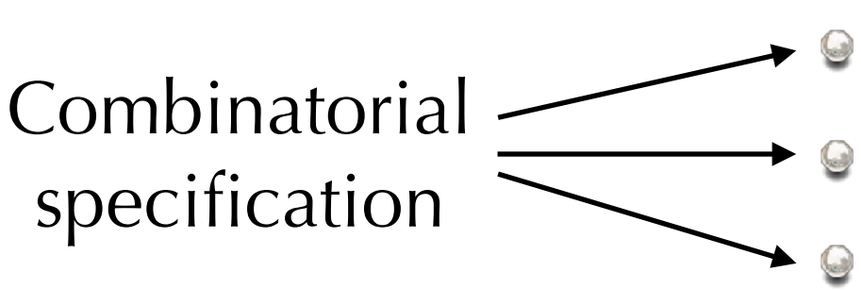
Universality phenomena:

Ex.: # trees of various types $\longrightarrow$ $K\rho^n n^{-3/2}$ $\longrightarrow$ pathlength in $n^{1/2}$

Summary & Conclusion

Summary & Conclusion

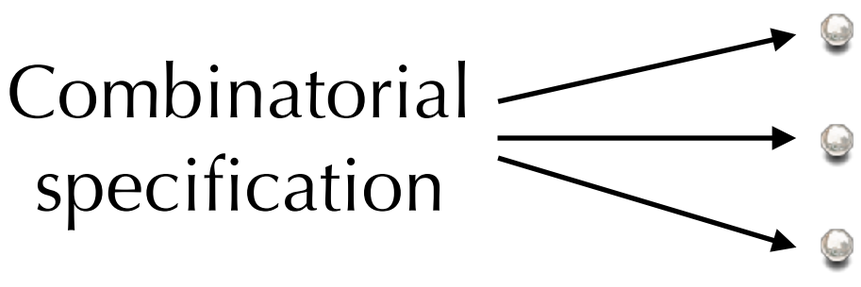
What we have:



	Automated?
counting;	✓
random generation;	✓
asymptotic analysis.	✗ (not fully)

Summary & Conclusion

What we have:



	Automated?
counting;	✓
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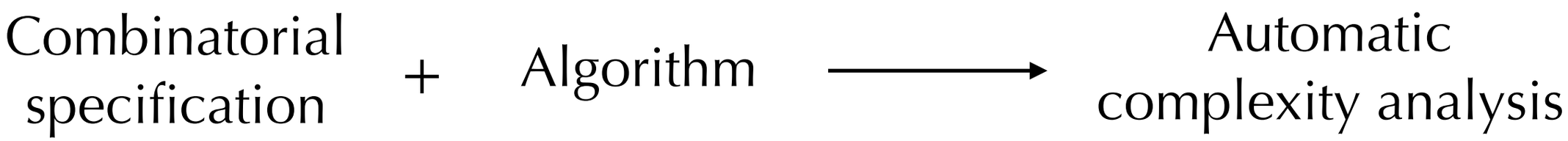
Ultimate (dream) goal:



Summary & Conclusion

What we have:

Automated?

Combinatorial specification

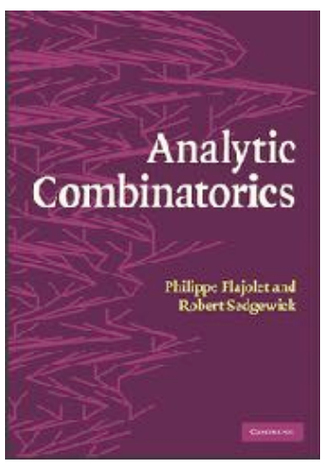
- counting; ✓
- random generation; ✓
- asymptotic analysis. ✗ (not fully)

Ultimate (dream) goal:

Combinatorial specification + Algorithm ⟶ Automatic complexity analysis

Where to learn more:

On-line course by R. Sedgewick at
http://ac.cs.princeton.edu/online/



Summary & Conclusion

What we have:

Combinatorial specification		Automated?
→	counting;	✓
→	random generation;	✓
→	asymptotic analysis.	✗ (not fully)

Ultimate (dream) goal:

Combinatorial specification + Algorithm ⟶ Automatic complexity analysis

The End

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