

Newton Iteration in Computer Algebra and Combinatorics

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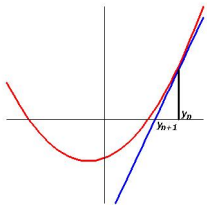
Inria AriC Project, LIP ENS Lyon



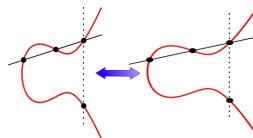
Joint work with Carine Pivoteau and Michèle Soria,
Journal of Combinatorial Theory, Series A **119** (2012), 1711–1773.

Université Paris Diderot, April 2013

I Introduction

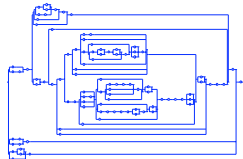


Analysis



Computer Algebra

Combinatorics



Numerical Iteration

$$\phi(y) = 1 + \frac{1}{8}y^2 - y$$

$$y^{[n+1]} = y^{[n]} - \frac{\phi(y^{[n]})}{\phi'(y^{[n]})} = y^{[n]} + \frac{1 + y^{[n]2}/8 - y^{[n]}}{1 - y^{[n]}/4}$$

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

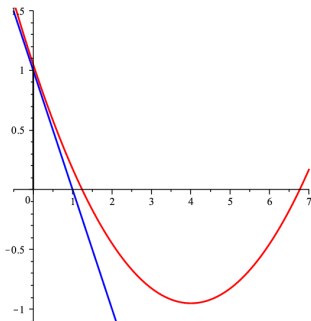
$$y^{[1]} = 1.000000000000000000000000000000$$

$$y^{[2]} = 1.166666666666666666666666666666$$

$$y^{[3]} = 1.17156862745098039215686275$$

$$y^{[4]} = 1.17157287525062017874740884$$

$$y^{[5]} = 1.17157287525380990239662075$$



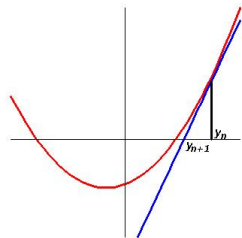
Quadratic Convergence

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

$$y^{[n+1]} = y^{[n]} + u^{[n+1]}, \quad \phi'(y^{[n]})u^{[n+1]} = -\phi(y^{[n]})$$

Good case: **quadratic** convergence if

- the initial point is close enough;
- the root is simple.



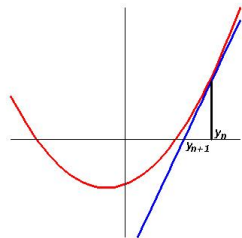
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Proof: simple root at $\zeta \Rightarrow \phi'(\zeta) \neq 0$,

$$\left. \begin{aligned} \phi(y^{[n]}) &= \phi'(\zeta)(y^{[n]} - \zeta) + O((y^{[n]} - \zeta)^2) \\ \phi'(y^{[n]}) &= \phi'(\zeta) + O(y^{[n]} - \zeta) \end{aligned} \right\} \Rightarrow y^{[n]} - \zeta = \frac{\phi(y^{[n]})}{\phi'(y^{[n]})} + O((y^{[n]} - \zeta)^2),$$

$$\Rightarrow y^{[n+1]} - \zeta = O((y^{[n]} - \zeta)^2).$$

Symbolic Iteration

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

$$y^{[n+1]} = y_n + \frac{1 + zy^{[n]2} - y^{[n]}}{1 - 2zy^{[n]}}$$

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

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

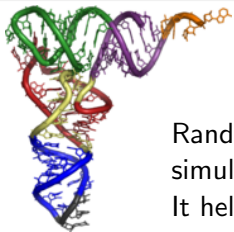
$$y^{[2]} = 1 + z + 2z^2 + 4z^3 + 8z^4 + 16z^5 + 32z^6 + 64z^7 + \dots$$

$$y^{[3]} = 1 + z + 2z^2 + 5z^3 + 14z^4 + 42z^5 + 132z^6 + 428z^7 + \dots$$

[Newton 1671]

$y^3 + az^2y - 2a^2z + axy - x^3 = 0. y = a - \frac{x}{4} + \frac{x^2}{64a} + \frac{111x^3}{512a^2} + \frac{509x^4}{16184a^3} \&c.$	
$+a + p = y.$ $+y^3$ $+axy$ $+x^2y$ $-x^3$ $-2a^2$	$+a^3 + 3a^2p + 3ap^2 + p^3$ $+a^2x + axp$ $+a^3 + a^2p$ $-x^3$ $-2a^3$
$-\frac{1}{2}x + q = p.$ $+p^3$ $+3ap^2$ $+axp$ $+4a^2p$ $+a^2x$ $-x^3$	$-\frac{1}{2}x^3 + \frac{1}{16}x^2q - \frac{1}{2}xq^2 + q^3$ $+\frac{1}{16}ax^2 - \frac{1}{8}axq + \frac{3}{8}aq^2$ $-\frac{1}{2}ax^2 + axq$ $-ax^2 + 4a^2q$ $+a^2x$ $-x^3$
$+\frac{x^2}{64a} + r = q.$ $+q^3$ $-\frac{1}{2}xq^2$ $+3aq^2$ $+\frac{1}{16}x^2q$ $-\frac{1}{8}axq$ $+4a^2q$ $-\frac{6}{64}x^3$ $-\frac{1}{16}ax^2$	$*$ $*$ $+\frac{1x^4}{4096a} + \frac{1}{16}x^2r + 3ar^2$ $+\frac{1x^4}{1024a} + \frac{1}{16}x^2r$ $-\frac{1}{16}x^3 + \frac{1}{16}axr$ $+\frac{1}{16}ax^2 + 4a^2r$ $-\frac{6}{64}x^3$ $-\frac{1}{16}ax^2$
$+\frac{x^2}{64a} + r = q. \dots + \frac{111x^3}{512a^2} + \frac{111x^3}{512a^2} + \frac{509x^4}{16184a^3}$	

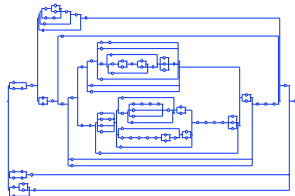
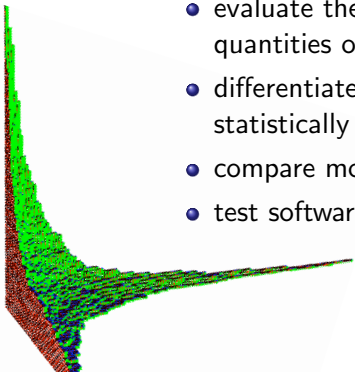
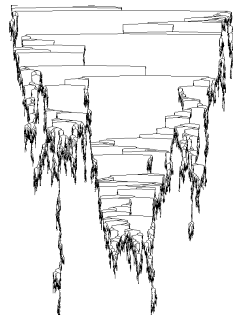
Random Generation in Combinatorics



Random generation of large objects = simulation in the discrete world.

It helps

- evaluate the order of magnitude of quantities of interest;
- differentiate exceptional values from statistically expected ones;
- compare models;
- test software.



Recursive Method

Binary Trees: $\mathcal{B} = \mathcal{Z} \cup \mathcal{Z} \times \mathcal{B} \times \mathcal{B}$

b_k : nb. binary trees with k nodes (Catalan)



$\text{DrawBinTree}(n) = \{$

 If $n = 1$ return \mathcal{Z}

 Else {

$U := \text{Uniform}([0, 1]); k := 0; S := 0;$

 while $(S < U) \{ k := k + 1; S := S + b_k b_{n-k-1} / b_n; \}$

 return $\mathcal{Z} \times \text{DrawBinTree}(k) \times \text{DrawBinTree}(n - k - 1) \}$

[Nijenhuis and Wilf; Flajolet, Zimmermann, Van Cutsem]

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 return $\mathcal{Z} \times \text{DrawBinTree}(k) \times \text{DrawBinTree}(n - k - 1) \}$

Generalizes to many recursive structures.

Requires b_0, \dots, b_n .

[Nijenhuis and Wilf; Flajolet, Zimmermann, Van Cutsem]

Boltzmann Samplers

Principle (Duchon, Flajolet, Louchard, Schaeffer 2004)

Generate each $t \in \mathcal{T}$ with probability $x^{|t|}/T(x)$, where: $x > 0$ fixed; $T(z) := \sum_{t \in \mathcal{T}} z^{|t|} =$ **generating series** of \mathcal{T} ; $|t| =$ size.

Same size, same probability
 Expected size $xT'(x)/T(x)$ increases with x .

Complexity **linear** in $|t|$ **when the values $T(x)$ are available (oracle).**

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Easy.

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Cartesian Product $\mathcal{C} = \mathcal{A} \times \mathcal{B}$

- Generate $a \in \mathcal{A}$; $b \in \mathcal{B}$;
- Return (a, b) .

Proof. $C(x) = \sum_{(a,b)} x^{|a|+|b|} = A(x)B(x)$; $\frac{x^{|a|+|b|}}{C(x)} = \frac{x^{|a|}}{A(x)} \frac{x^{|b|}}{B(x)}$.

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Disjoint Union $\mathcal{C} = \mathcal{A} \cup \mathcal{B}$

- Draw $b = \text{Bernoulli}(A(x)/C(x))$;
- If $b = 1$ then generate $a \in \mathcal{A}$ else generate $b \in \mathcal{B}$.

Proof. $\frac{x^{|a|}}{C(x)} = \frac{x^{|a|}}{A(x)} \frac{A(x)}{C(x)}$.

Complexity **linear** in $|t|$ when the values $T(x)$ are available (**oracle**).

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Cartesian Product $\mathcal{C} = \mathcal{A} \times \mathcal{B}$

- Generate $a \in \mathcal{A}$; $b \in \mathcal{B}$;
- Return (a, b) .

Use recursively (e.g., binary trees $\mathcal{B} = \mathcal{Z} \cup \mathcal{Z} \times \mathcal{B} \times \mathcal{B}$)

Also: sets, cycles, ...;

Complexity **linear** in $|t|$ **when the values $T(x)$ are available (oracle)**.

Boltzmann Samplers

Principle (Duchon, Flajolet, Louchard, Schaeffer 2004)

Generate each $t \in \mathcal{T}$ with probability $x^{|t|} / T(x) / |t|!$, where: $x > 0$ fixed; $T(z) := \sum_{t \in \mathcal{T}} z^{|t|} / |t|! =$ **generating series** of \mathcal{T} ; $|t| =$ size.

Same size, same probability

Expected size $xT'(x) / T(x)$ increases with x .

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Easy.

Disjoint Union $\mathcal{C} = \mathcal{A} \cup \mathcal{B}$

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- Return (a, b) .

Use recursively (e.g., binary trees $\mathcal{B} = \mathcal{Z} \cup \mathcal{Z} \times \mathcal{B} \times \mathcal{B}$)

Also: sets, cycles, ... ; **labelled case**

Complexity **linear** in $|t|$ **when the values $T(x)$ are available (oracle)**.

Framework: Constructible Species

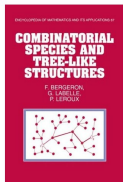
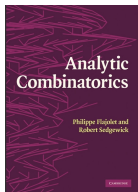
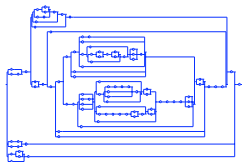
A small set of species

$1, \mathcal{Z}, \times, +, \text{SEQ}, \text{SET}, \text{CYC},$

cardinality constraints that are finite unions of intervals,
used recursively.

Examples:

- Regular languages
- Unambiguous context-free languages
- Trees ($\mathcal{B} = \mathcal{Z} + \mathcal{Z} \times \mathcal{B}^2, \mathcal{T} = \mathcal{Z} \times \text{SET}(\mathcal{T})$)
- Mappings, ...



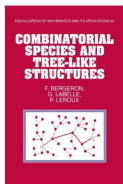
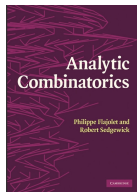
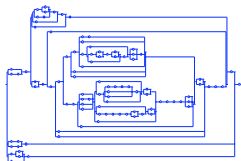
Framework: Constructible Species

A small set of species

$1, \mathcal{Z}, \times, +, \text{SEQ}, \text{SET}, \text{CYC}$,
cardinality constraints that are finite unions of intervals,
used recursively (**when it makes sense**).

Examples:

- Regular languages
- Unambiguous context-free languages
- Trees ($\mathcal{B} = \mathcal{Z} + \mathcal{Z} \times \mathcal{B}^2$, $\mathcal{T} = \mathcal{Z} \times \text{SET}(\mathcal{T})$)
- Mappings, ...



Results (1/2): Fast Enumeration

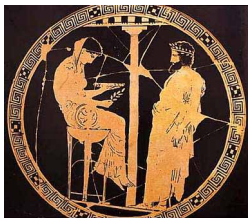
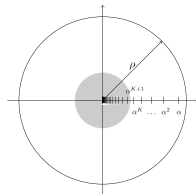
Theorem (Enumeration in Quasi-Optimal Complexity)

First N coefficients of gfs of constructible species in

- ① arithmetic complexity:
 - $O(N \log N)$ (both ogf and egf);
- ② binary complexity:
 - $O(N^2 \log^2 N \log \log N)$ (ogf);
 - $O(N^2 \log^3 N \log \log N)$ (egf).

Results (2/2): Oracle

- 1 A numerical iteration converging to $\mathbf{Y}(\alpha)$ in the labelled case (inside the disk);
- 2 A numerical iteration converging to the sequence $\mathbf{Y}(\alpha), \mathbf{Y}(\alpha^2), \mathbf{Y}(\alpha^3), \dots$ for $\|\cdot\|_\infty$ in the unlabelled case (inside the disk).



Examples (I): Polynomial Systems

Random generation following given XML grammars

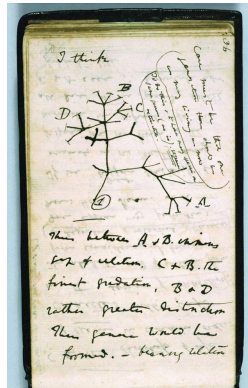
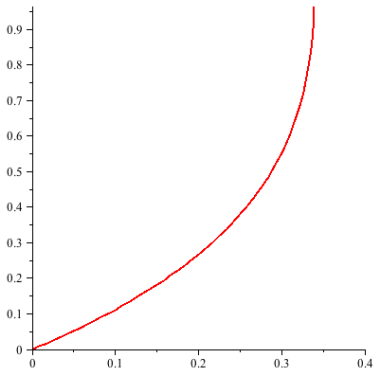
Grammar	nb eqs	max deg	nb sols	oracle (s.)	FGb (s.)
rss	10	5	2	0.02	0.03
PNML	22	4	4	0.05	0.1
xslt	40	3	10	0.4	1.5
relaxng	34	4	32	0.4	3.3
xhtml-basic	53	3	13	1.2	18
mathml2	182	2	18	3.7	882
xhtml	93	6	56	3.4	1124
xhtml-strict	80	6	32	3.0	1590
xmlschema	59	10	24	0.5	6592
SVG	117	10		5.8	>1.5Go
docbook	407	11		67.7	>1.5Go
OpenDoc	500			3.9	

[Darrasse 2008]

Example (II): A Non-Polynomial "System"

Unlabelled rooted trees:

$$f(x) = x \exp(f(x) + \frac{1}{2}f(x^2) + \frac{1}{3}f(x^3) + \dots)$$



II Newton Iteration for Power Series

Symbolic Iteration

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

$$y^{[n+1]} = y_n + \frac{1 + zy^{[n]2} - y_n}{1 - 2zy^{[n]}}$$

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

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

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

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[Newton 1671]

$y^3 + ay^2y - 2a^3 + axy - x^3 = 0. y = a - \frac{x}{4} + \frac{x^2}{64a} + \frac{11x^3}{512a^2} + \frac{509x^4}{161844a^3} \&c.$	
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$-\frac{1}{2}x + q = p.$ $+p^3$ $+3ap^2$ $+axp$ $+4a^2p$ $+a^2x$ $-x^3$	$-\frac{1}{2}x^3 + \frac{1}{16}x^2q - \frac{1}{2}xq^2 + q^3$ $+\frac{3}{16}ax^2 - \frac{1}{4}axq + 3aq^2$ $-\frac{1}{2}ax^2 + axq$ $-axx + 4a^2q$ $+a^2x$ $-x^3$
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Newton Iteration for Power Series has Good Complexity

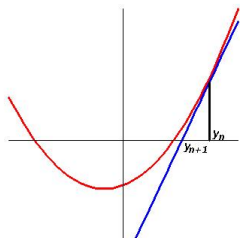
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Quadratic convergence



Divide-and-Conquer



Newton Iteration for Power Series has Good Complexity

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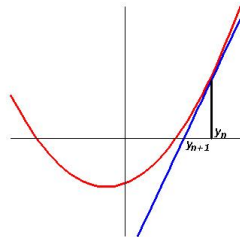
Quadratic convergence



Divide-and-Conquer

To solve at precision N

- 1 Solve at precision $N/2$;
- 2 Compute ϕ and ϕ' there;
- 3 Solve for $u^{[n+1]}$.



$$\text{Cost}(y^{[n]}) = \text{constant} \times \text{Cost}(\text{last step}).$$

Newton Iteration for Power Series has Good Complexity

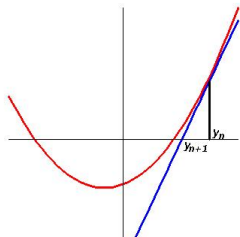
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Divide-and-Conquer



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- 2 Compute ϕ and ϕ' there;
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$$\text{Cost}(y^{[n]}) = \text{constant} \times \text{Cost}(\text{last step}).$$

Useful in conjunction with **fast multiplication** (e.g., FFT):

- power series at order N : $O(N \log N)$ ops on the coefficients;
- N -bit integers: $O(N \log N \log \log N)$ bit ops.

Example: Newton Iteration for Inverses

$$\phi(y) = a - 1/y \Rightarrow 1/\phi'(y) = y^2 \Rightarrow \boxed{y^{[n+1]} = y^{[n]} - y^{[n]}(ay^{[n]} - 1)}.$$

Cost: a small number of multiplications

Works for:

- ① Numerical inversion;
- ② Reciprocal of power series;
- ③ Inversion of matrices.

[Schulz 1933; Cook 1966; Sieveking 1972; Kung 1974]

Inverses for Series-Parallel Graphs

$$(G, S, P) = \mathbf{H}(G, S, P).$$

$$\begin{cases} G = S + P, \\ S = (1 - z - P)^{-1} - 1, \\ P = e^{z+S} - 1 - z - S. \end{cases} \quad \frac{\partial \mathbf{H}}{\partial \mathbf{Y}} = \begin{pmatrix} 0 & 1 & 1 \\ 0 & 0 & (1 - z - P)^{-2} \\ 0 & e^{z+S} - 1 & 0 \end{pmatrix}$$

Newton iteration:

$$\mathbf{Y}^{[n+1]} = \mathbf{Y}^{[n]} + (\text{Id} - \frac{\partial \mathbf{H}}{\partial \mathbf{Y}}(\mathbf{Y}^{[n]}))^{-1} \cdot (\mathbf{H}(\mathbf{Y}^{[n]}) - \mathbf{Y}^{[n]}).$$

$$\begin{cases} \mathbf{Y}^{[n+1]} = \mathbf{Y}^{[n]} + U^{[n+1]} \cdot (\mathbf{H}(\mathbf{Y}^{[n]}) - \mathbf{Y}^{[n]}) \bmod z^{2^{n+1}}, \\ U^{[n+1]} = U^{[n]} + U^{[n]} \cdot \left(\frac{\partial \mathbf{H}}{\partial \mathbf{Y}}(\mathbf{Y}^{[n]}) \cdot U^{[n]} + \text{Id} - U^{[n]} \right) \bmod z^{2^n}. \end{cases}$$

Inverses for Series-Parallel Graphs

$$(G, S, P) = \mathbf{H}(G, S, P).$$

$$\begin{cases} G = S + P, \\ S = (1 - z - P)^{-1} - 1, \\ P = e^{z+S} - 1 - z - S. \end{cases} \quad \frac{\partial \mathbf{H}}{\partial \mathbf{Y}} = \begin{pmatrix} 0 & 1 & 1 \\ 0 & 0 & (1 - z - P)^{-2} \\ 0 & e^{z+S} - 1 & 0 \end{pmatrix}$$

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\Rightarrow **Wanted:** efficient exp.

From the Inverse to the Exponential

- ① Logarithm of power series: $\log f = \int (f'/f)$;
- ② exponential of power series: $\phi(y) = a - \log y$.

$$\begin{aligned} e^{[n+1]} &= e^{[n]} + \frac{a - \log e^{[n]}}{1/e^{[n]}} \bmod z^{2^{n+1}}, \\ &= e^{[n]} + e^{[n]} \left(a - \int e^{[n]}'/e^{[n]} \right) \bmod z^{2^{n+1}}. \end{aligned}$$

And $1/e^{[n]}$ is computed by Newton iteration too!

[Brent 1975; Hanrot-Zimmermann 2002]

Application: Power Sums

$$F = t^N + a_{N-1}t^{N-1} + \cdots + a_0 \leftrightarrow S_i = \sum_{F(\alpha)=0} \alpha^i, \quad i = 0, \dots, N.$$

Application: Power Sums

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Fast conversion using the generating series:

$$\frac{\text{rev}(F)'}{\text{rev}(F)} = - \sum_{i \geq 0} S_{i+1} t^i \leftrightarrow \text{rev}(F) = \exp \left(- \sum \frac{S_i}{i} t^i \right).$$

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Application: composed product and sums

$$(F, G) \mapsto \prod_{F(\alpha)=0, G(\beta)=0} (t - \alpha\beta) \quad \text{or} \quad \prod_{F(\alpha)=0, G(\beta)=0} (t - (\alpha + \beta)).$$

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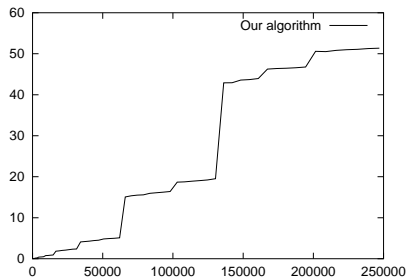
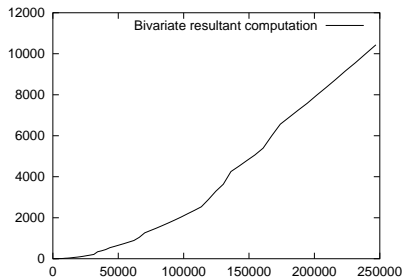
Easy in Newton representation: $\sum \alpha^s \sum \beta^s = \sum (\alpha\beta)^s$ and

$$\sum \frac{\sum (\alpha + \beta)^s}{s!} t^s = \left(\sum \frac{\sum \alpha^s}{s!} t^s \right) \left(\sum \frac{\sum \beta^s}{s!} t^s \right).$$

[Schönhage 1982; Bostan, Flajolet, Salvy, Schost 2006]

Timings

Applications (crypto): over finite fields, degree > 200000 expected.



Timings in seconds vs. output degree N , over \mathbb{F}_p , 26 bits prime p

Conclusion for Series-Parallel Graphs

$$\mathcal{G} = \mathcal{S} + \mathcal{P}, \quad \mathcal{S} = \text{SEQ}_{>0}(\mathcal{Z} + \mathcal{P}), \quad \mathcal{P} = \text{SET}_{>1}(\mathcal{Z} + \mathcal{S})$$

compiles into the Newton iteration:

$$\left\{ \begin{array}{l} i^{[n+1]} = i^{[n]} - i^{[n]}(e^{[n]}i^{[n]} - 1), \\ e^{[n+1]} = e^{[n]} - e^{[n]} \left(1 + \frac{d}{dz} S^{[n]} - \int \left(\frac{d}{dz} e^{[n]} \right) i^{[n]} \right), \\ v^{[n+1]} = v^{[n]} - v^{[n]}((1 - z - P^{[n]})v^{[n]} - 1), \\ U^{[n+1]} = U^{[n]} + U^{[n]} \cdot \left(\begin{array}{ccc} 0 & 1 & 1 \\ 0 & 0 & v^{[n+1]2} \\ 0 & e^{[n+1]} - 1 & 0 \end{array} \right) \cdot U^{[n]} + \text{Id} - U^{[n]}, \\ \begin{pmatrix} G^{[n+1]} \\ S^{[n+1]} \\ P^{[n+1]} \end{pmatrix} = \begin{pmatrix} G^{[n]} \\ S^{[n]} \\ P^{[n]} \end{pmatrix} + U^{[n+1]} \cdot \begin{pmatrix} S^{[n]} + P^{[n]} - G^{[n]} \\ v^{[n+1]} - S^{[n]} \\ e^{[n+1]} - P^{[n]} \end{pmatrix} \pmod{z^{2^{n+1}}}. \end{array} \right.$$

Computation reduced to products and linear ops.

Linear Differential Equations of Arbitrary Order

Given a linear differential equation with power series coefficients,

$$a_r(t)y^{(r)}(t) + \cdots + a_0(t)y(t) = 0,$$

compute the first N terms of a basis of power series solutions.

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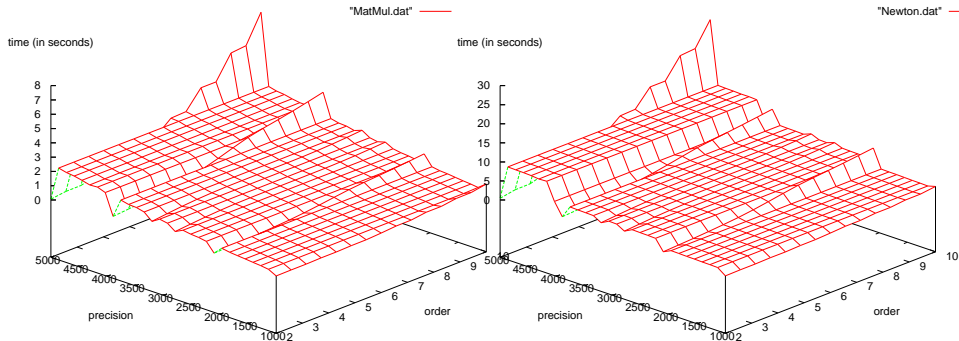
Algorithm

- 1 Convert into a system $\Phi : Y \mapsto Y' - A(t)Y$ ($D\Phi = \Phi$);
- 2 $D\Phi|_Y(U) = \Phi(Y)$ rewrites $U' - AU = Y' - AY$;
- 3 Variation of constants: $U = Y \int Y^{-1}(Y' - AY)$;
- 4 Y^{-1} by Newton iteration too.

Special case: recover good exponential.

[Bostan, Chyzak, Ollivier, Salvy, Schost, Sedoglavic 2007]

Timings

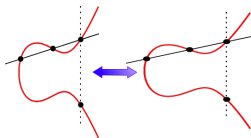


Polynomial matrix multiplication vs. solving $Y' = AY$.

Non-Linear Differential Equations

Example from cryptography:

$$\phi : y \mapsto (x^3 + Ax + B)y'^2 - (y^3 + \tilde{A}y + \tilde{B}).$$



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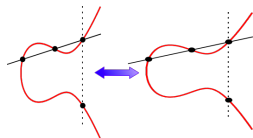
Differential:

$$D\phi|_y : u \mapsto 2(x^3 + Ax + B)y'u' - (3y^2 + \tilde{A})u.$$

Solve the **linear** differential equation

$$D\phi|_y u = \phi(y)$$

at each iteration.



Again, **quasi-linear** complexity.

[Bostan, Morain, Salvy, Schost 2008]

III Combinatorics

Generating Series: a Simple Dictionary

$$\text{ogf} := \sum_{t \in \mathcal{T}} z^{|t|}, \quad \text{egf} := \sum_{t \in \mathcal{T}} \frac{z^{|t|}}{|t|!}.$$

Language and Gen. Fcns (labelled)

$\mathcal{A} \cup \mathcal{B}$	$A(z) + B(z)$
$\mathcal{A} \times \mathcal{B}$	$A(z) \times B(z)$
$\text{SEQ}(\mathcal{C})$	$\frac{1}{1-C(z)}$
\mathcal{A}'	$A'(z)$
$\text{CYC}(\mathcal{C})$	$\log \frac{1}{1-C(z)}$
$\text{SET}(\mathcal{C})$	$\exp(C(z))$

Consequences:

- 1 Newton for EGFs easy;

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$\text{SEQ}(\mathcal{C})$	$\frac{1}{1-C(z)}$	$\frac{1}{1-C(z)}$
\mathcal{A}'	$A'(z)$	—
$\text{CYC}(\mathcal{C})$	$\log \frac{1}{1-C(z)}$	$\sum_{k \geq 1} \frac{\phi(k)}{k} \log \frac{1}{1-C(z^k)}$
$\text{SET}(\mathcal{C})$	$\exp(C(z))$	$\exp(\sum C(z^i)/i)$

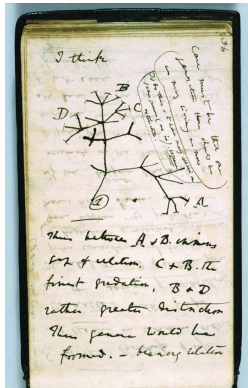
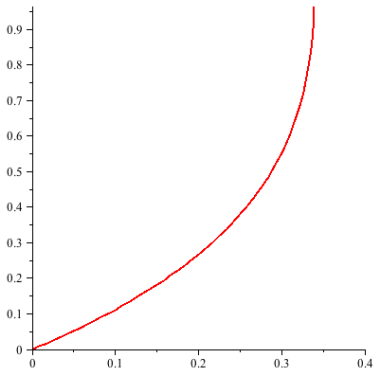
Consequences:

- ① Newton for EGFs easy;
- ② Pólya operators for ogfs;
- ③ Newton iteration more difficult for ogfs.

Example (II): A Non-Polynomial "System"

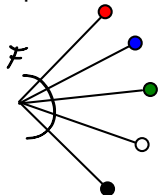
Unlabelled rooted trees:

$$f(x) = x \exp(f(x) + \frac{1}{2}f(x^2) + \frac{1}{3}f(x^3) + \dots)$$



Mini-Introduction to Species Theory

- Species \mathcal{F} :

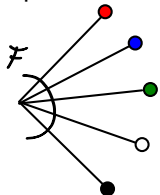


Examples:

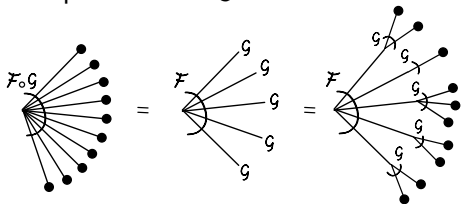
- $0, \mathbb{Z}, 1$;
- SET;
- SEQ, CYC.

Mini-Introduction to Species Theory

- Species \mathcal{F} :



- Composition $\mathcal{F} \circ \mathcal{G}$:

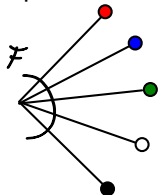


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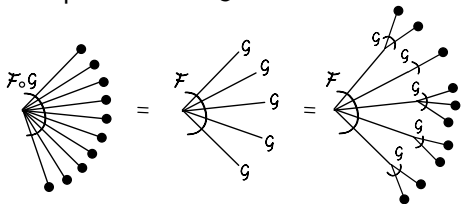
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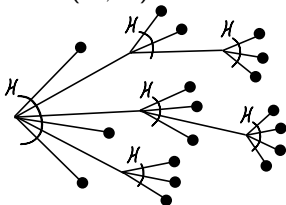
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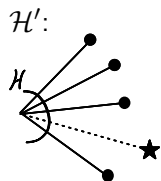
Examples:

- $0, \mathcal{Z}, 1$;
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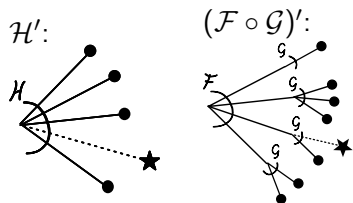
- $\mathcal{Y} = \mathcal{H}(\mathcal{Z}, \mathcal{Y})$



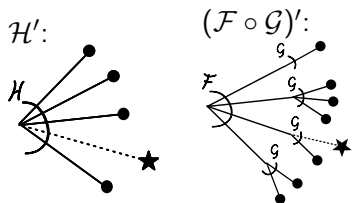
Derivative



Derivative

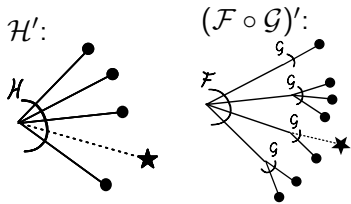


Derivative



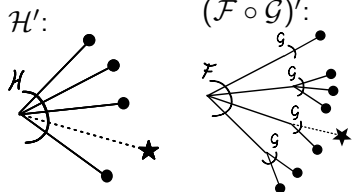
Huet's zipper

Derivative



species	derivative
$\mathcal{A} + \mathcal{B}$	$\mathcal{A}' + \mathcal{B}'$
$\mathcal{A} \cdot \mathcal{B}$	$\mathcal{A}' \cdot \mathcal{B} + \mathcal{A} \cdot \mathcal{B}'$
$\text{SEQ}(\mathcal{B})$	$\text{SEQ}(\mathcal{B}) \cdot \mathcal{B}' \cdot \text{SEQ}(\mathcal{B})$
$\text{CYC}(\mathcal{B})$	$\text{SEQ}(\mathcal{B}) \cdot \mathcal{B}'$
$\text{SET}(\mathcal{B})$	$\text{SET}(\mathcal{B}) \cdot \mathcal{B}'$

Derivative



Example:

species	derivative
$A + B$	$A' + B'$
$A \cdot B$	$A' \cdot B + A \cdot B'$
$\text{SEQ}(B)$	$\text{SEQ}(B) \cdot B' \cdot \text{SEQ}(B)$
$\text{CYC}(B)$	$\text{SEQ}(B) \cdot B'$
$\text{SET}(B)$	$\text{SET}(B) \cdot B'$

$$\mathcal{H}(G, S, P) := (S + P, \text{Seq}_{>0}(Z + P), \text{Set}_{>1}(Z + S)).$$

$$\frac{\partial \mathcal{H}}{\partial \mathcal{Y}} = \begin{pmatrix} \emptyset & 1 & 1 \\ \emptyset & \emptyset & \text{Seq}(Z + P) \cdot 1 \cdot \text{Seq}(Z + P) \\ \emptyset & \text{Set}_{>0}(Z + S) \cdot 1 & \emptyset \end{pmatrix}$$

Joyal's Implicit Species Theorem

Theorem

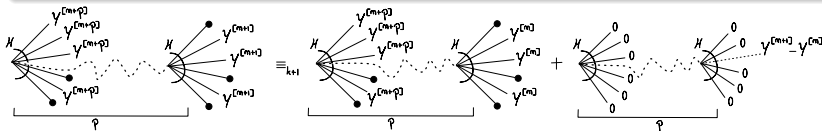
If $\mathcal{H}(0,0) = 0$ and $\partial\mathcal{H}/\partial\mathcal{Y}(0,0)$ is nilpotent, then $\mathcal{Y} = \mathcal{H}(\mathcal{Z}, \mathcal{Y})$ has a unique solution, limit of

$$\mathcal{Y}^{[0]} = 0, \quad \mathcal{Y}^{[n+1]} = \mathcal{H}(\mathcal{Z}, \mathcal{Y}^{[n]}) \quad (n \geq 0).$$

Def. $\mathcal{A} =_k \mathcal{B}$ if they coincide up to size k (contact k).

Key Lemma

If $\mathcal{Y}^{[n+1]} =_k \mathcal{Y}^{[n]}$, then $\mathcal{Y}^{[n+p+1]} =_{k+1} \mathcal{Y}^{[n+p]}$, ($p = \text{dimension}$).



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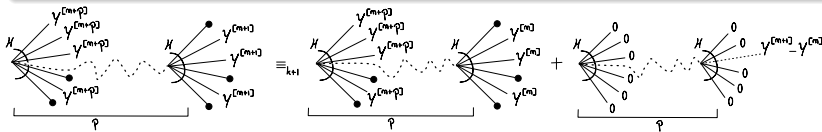
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We prove an **iff** when no 0 coordinate.

Newton Iteration for Binary Trees

$$\mathcal{Y} = 1 \cup \mathcal{Z} \times \mathcal{Y} \times \mathcal{Y}$$

Newton Iteration for Binary Trees

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

$$\mathcal{Y}_2 = \begin{array}{c} \text{②} \\ \begin{array}{c} \circ \\ \circ \end{array} + \begin{array}{c} \circ \\ \circ \end{array} + \begin{array}{c} \circ \\ \circ \end{array} + \begin{array}{c} \circ \\ \circ \end{array} + \dots + \begin{array}{c} \circ \\ \circ \end{array} + \dots \end{array}$$

$$\mathcal{Y}_3 = \mathcal{Y}_2 + \begin{array}{c} \circ \\ \circ \end{array} + \dots + \begin{array}{c} \circ \\ \circ \end{array} + \dots + \begin{array}{c} \circ \\ \circ \end{array} + \dots$$

[Décoste, Labelle, Leroux 1982]

Symbolic Iteration

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

$$y^{[n+1]} = y_n + \frac{1 + zy^{[n]2} - y^{[n]}}{1 - 2zy^{[n]}}$$

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

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

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

$$y^{[3]} = 1 + z + 2z^2 + 5z^3 + 14z^4 + 42z^5 + 132z^6 + 428z^7 + \dots$$

[Newton 1671]

$y^3 + az^2y - 2a^2z + axy - x^3 = 0. \quad y = a - \frac{x}{4} + \frac{x^2}{64a} + \frac{11xz^2}{512a^2} + \frac{509x^4}{161844a^3} \&c.$	
$+a + p = y.$ $+y^3$ $+axy$ $+x^2y$ $-x^3$ $-2a^2$	$+a^3 + 3a^2p + 3ap^2 + p^3$ $+a^2x + axp$ $+a^3 + a^2p$ $-x^3$ $-2a^3$
$-\frac{1}{2}x + q = p.$ $+p^3$ $+3ap^2$ $+axp$ $+4a^2p$ $+a^2x$ $-x^3$	$-\frac{1}{2}x^3 + \frac{1}{16}x^2q - \frac{1}{2}xq^2 + q^3$ $+\frac{1}{16}ax^2 - \frac{1}{8}axq + \frac{3}{8}aq^2$ $-\frac{1}{2}ax^2 + axq$ $-axx + 4a^2q$ $+a^2x$ $-x^3$
$+\frac{x^2}{64a} + r = q.$ $+q^3$ $-\frac{1}{2}xq^2$ $+3aq^2$ $+\frac{1}{16}x^2q$ $-\frac{1}{8}axq$ $+4a^2q$ $-\frac{6}{64}x^3$ $-\frac{1}{16}ax^2$	$*$ $*$ $+\frac{1x^2}{4096a} * + \frac{1}{16}x^2r + 3ar^2$ $+\frac{1x^2}{1024a} * + \frac{1}{16}x^2r$ $-\frac{1}{128}x^3 * - \frac{1}{16}axr$ $+\frac{1}{16}ax^2 + 4a^2r$ $-\frac{6}{64}x^3$ $-\frac{1}{16}ax^2$
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Numerical Iteration

$$\phi(y) = 1 + \frac{1}{8}y^2 - y$$

$$y^{[n+1]} = y^{[n]} - \frac{\phi(y^{[n]})}{\phi'(y^{[n]})} = y^{[n]} + \frac{1 + y^{[n]2}/8 - y^{[n]}}{1 - y^{[n]}/4}$$

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

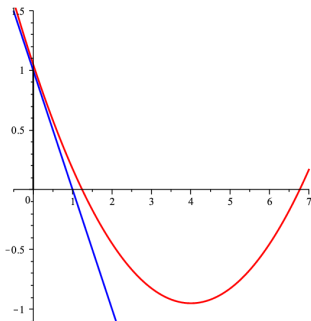
$$y^{[1]} = 1.000000000000000000000000000000$$

$$y^{[2]} = 1.166666666666666666666666666666$$

$$y^{[3]} = 1.17156862745098039215686275$$

$$y^{[4]} = 1.17157287525062017874740884$$

$$y^{[5]} = 1.17157287525380990239662075$$



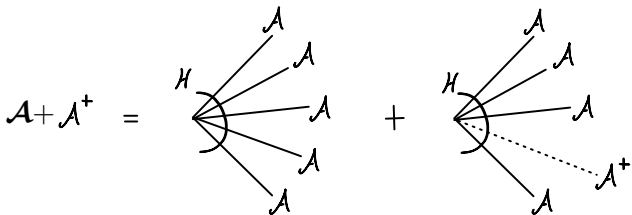
Combinatorial Newton Iteration

Theorem (essentially Labelle)

For any well-founded system $\mathcal{Y} = \mathcal{H}(\mathcal{Z}, \mathcal{Y})$, if \mathcal{A} has contact k with the solution and $\mathcal{A} \subset \mathcal{H}(\mathcal{Z}, \mathcal{A})$, then

$$\mathcal{A} + \sum_{i \geq 0} \left(\frac{\partial \mathcal{H}}{\partial \mathcal{Y}}(\mathcal{Z}, \mathcal{A}) \right)^i \cdot (\mathcal{H}(\mathcal{Z}, \mathcal{A}) - \mathcal{A})$$

has contact $2k + 1$ with it.



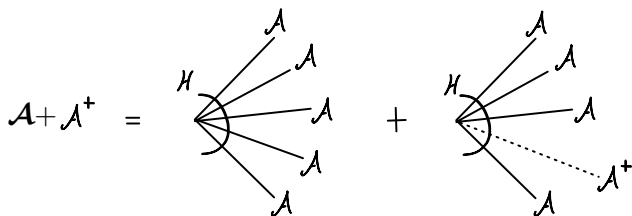
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Theorem (essentially Labelle)

For any well-founded system $\mathcal{Y} = \mathcal{H}(\mathcal{Z}, \mathcal{Y})$, if \mathcal{A} has contact k with the solution and $\mathcal{A} \subset \mathcal{H}(\mathcal{Z}, \mathcal{A})$, then

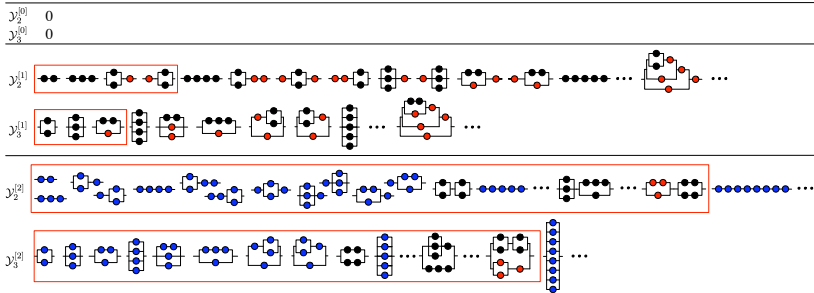
$$\mathcal{A} + \sum_{i \geq 0} \left(\frac{\partial \mathcal{H}}{\partial \mathcal{Y}}(\mathcal{Z}, \mathcal{A}) \right)^i \cdot (\mathcal{H}(\mathcal{Z}, \mathcal{A}) - \mathcal{A})$$

has contact $2k + 1$ with it.



Generation by increasing Strahler numbers.

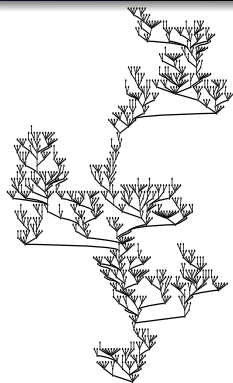
Newton Iteration for Series-Parallel Graphs



$$\begin{pmatrix} \mathcal{S}^{[n+1]} \\ \mathcal{P}^{[n+1]} \end{pmatrix} = \begin{pmatrix} \mathcal{S}^{[n]} \\ \mathcal{P}^{[n]} \end{pmatrix} + \left(\sum_{k \geq 0} \begin{pmatrix} 0 & \text{SEQ}^2(\mathcal{Z} + \mathcal{P}^{[n]} - 1)^k \\ \text{SET}_{>0}(\mathcal{Z} + \mathcal{S}^{[n]}) & 0 \end{pmatrix} \right) \begin{pmatrix} \text{SEQ}_{>1}(\mathcal{Z} + \mathcal{P}^{[n]} - \mathcal{S}^{[n]}) \\ \text{SET}_{>0}(\mathcal{Z} + \mathcal{S}^{[n]} - \mathcal{P}^{[n]}) \end{pmatrix}.$$

Example: Unlabelled Rooted Trees

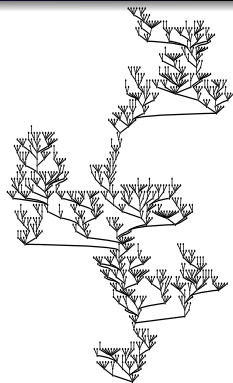
① Combinatorial equation: $\mathcal{Y} = \mathcal{Z} \cdot \text{SET}(\mathcal{Y}) =: \mathcal{H}(\mathcal{Z}, \mathcal{Y});$



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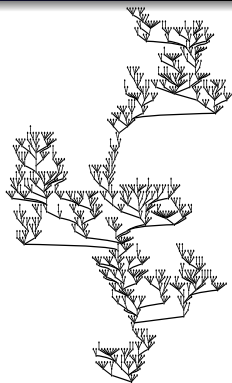
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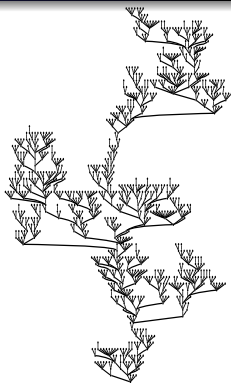
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0,

$$z + z^2 + z^3 + z^4 + \dots,$$

$$z + z^2 + 2z^3 + 4z^4 + 9z^5 + 20z^6 + \dots$$



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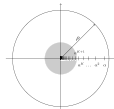
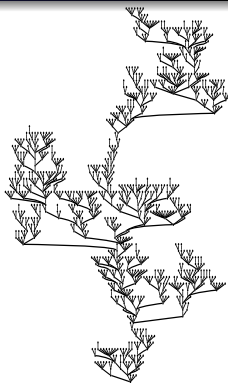
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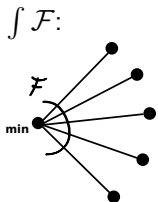
5 Numerical iteration:

n	$\tilde{Y}^{[n]}(0.3)$	$\tilde{Y}^{[n]}(0.3^2)$	$\tilde{Y}^{[n]}(0.3^3)$
0	0	0	0
1	.43021322639	0.99370806338e-1	0.27759817516e-1
2	.54875612912	0.99887132154e-1	0.27770629187e-1
3	.55709557053	0.99887147197e-1	0.27770629189e-1
4	.55713907945	0.99887147198e-1	0.27770629189e-1
5	.55713908064	0.99887147198e-1	0.27770629189e-1



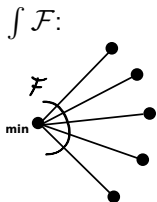
Linear Species and Ordered Structures

The underlying sets are ordered



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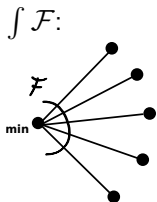


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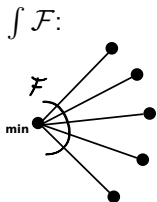
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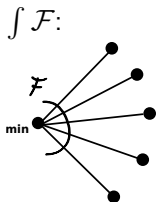
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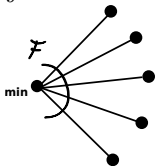
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Theorem (Enumeration in Quasi-Optimal Complexity)

First N coefficients of the solution of

$$\mathcal{Y}(\mathcal{Z}) = \mathcal{H}(\mathcal{Z}, \mathcal{Y}(\mathcal{Z})) + \int_0^{\mathcal{Z}} \mathcal{G}(T, \mathcal{Y}(T)) dT$$

with \mathcal{H} and \mathcal{G} constructible, in $O(N \log N)$ operations.

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THE END

