Newton's Iteration for Combinatorial Systems and Applications

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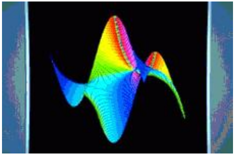
Algorithms Project, Inria

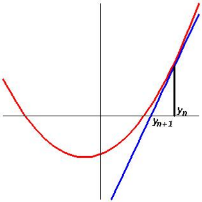


Joint work with Carine Pivoteau and Michèle Soria

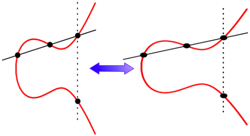
J. Combinatorial Theory Series A. 119 (nov. 2012) 1711–1773.

IMB, Bordeaux, June 24, 2012

I Introduction

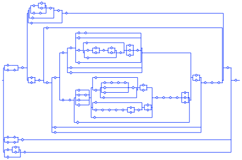


Analysis



Algorithms

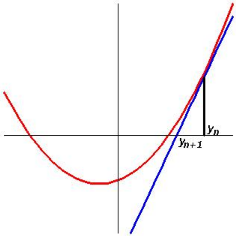
Combinatorics



Main Tool: Newton Iteration

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;
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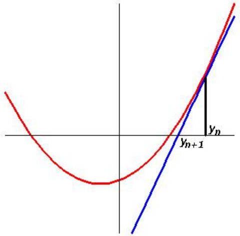


Good case: quadratic convergence if

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

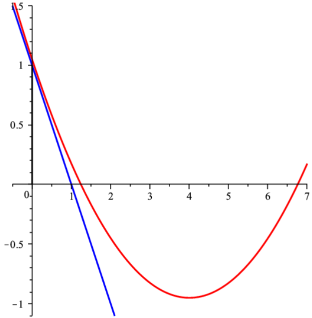
Proof: simple root at ζ

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

Examples of Quadratic Convergence

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

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

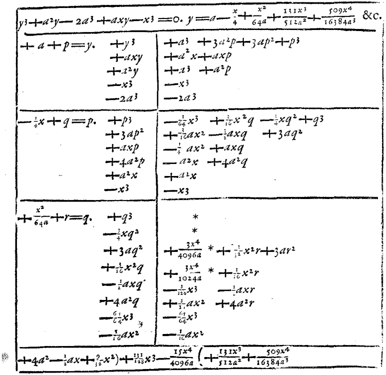


$$y^{[0]} = 0.$$
$$y^{[1]} = 1.0000000000000000000000000$$
$$y^{[2]} = 1.1666666666666666666666666$$
$$y^{[3]} = 1.1715686274509803921568627 5$$
$$y^{[4]} = 1.1715728752506201787474088 4$$
$$y^{[5]} = 1.1715728752538099023966207 5$$

Examples of Quadratic Convergence

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

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



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

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

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

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

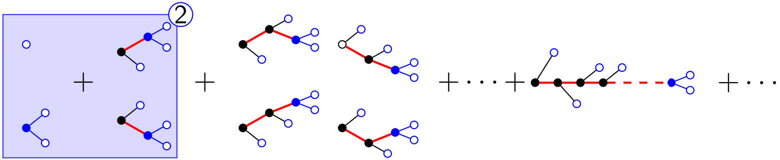
[Newton 1671]

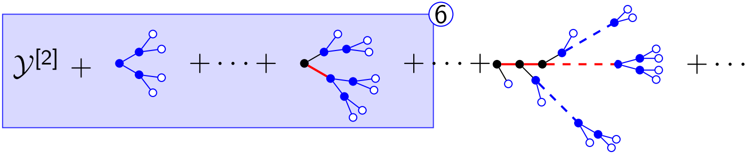
Examples of Quadratic Convergence

$$\phi(\mathcal{Y}) = (\mathcal{E} + \mathcal{Z} \cdot \mathcal{Y}^2) \setminus \mathcal{Y}$$

$$\mathcal{Y}^{[n+1]} = \mathcal{Y}^{[n]} + \mathrm{SEQ}(\mathcal{Z} \cdot \mathcal{Y}^{[n]} \cdot \square + \mathcal{Z} \cdot \square \cdot \mathcal{Y}^{[n]}) \cdot \phi(\mathcal{Y}^{[n]}).$$

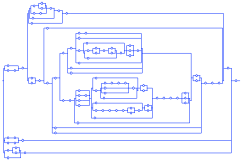
$\mathcal{Y}^{[0]} = \varnothing \qquad \mathcal{Y}^{[1]} = \circ$

$\mathcal{Y}^{[2]} =$ 

$\mathcal{Y}^{[3]} =$ 

[Décoste, Labelle, Leroux 1982]

Motivation: Random Generation / Discrete Simulation



$$\mathcal{G} = \mathcal{S} + \mathcal{P},$$
$$\mathcal{S} = \mathrm{Seq}(\mathcal{Z} + \mathcal{P}, \mathrm{card} > 1),$$
$$\mathcal{P} = \mathrm{Set}(\mathcal{Z} + \mathcal{S}, \mathrm{card} > 0).$$

Definition (Generating function)

$Y(z) = y_0 + y_1 z + \cdots + y_n z^n (/n!) + \cdots$ (y_n: nb objects of size n).

Algorithms for uniform random generation in size N use either

- $y_0, \ldots, y_N$ (recursive method);
- $Y(x)$ for some $x > 0$ (Boltzmann sampler).

[Nijenhuis, Wilf 1978; Flajolet, Zimmermann, Van Cutsem 1994; Duchon, Flajolet, Louchard, Schaeffer 2004; Flajolet, Fusy, Pivoteau 2007]

Combinatorial Newton Iteration

Well-Founded Combinatorial Specification

$\Downarrow$

Combinatorial Newton iteration for $\mathcal{Y}$

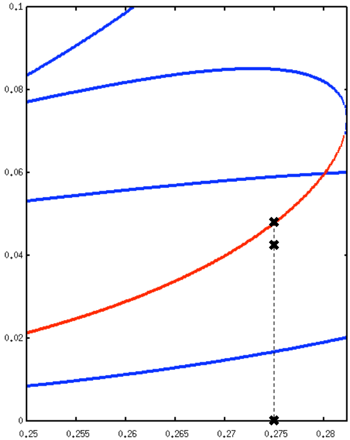
$\Downarrow$

Newton iteration for the gf $Y(z)$

$(y_0, \ldots, y_N)$ fast

$\Downarrow$

Numerical Newton iteration starting from 0 converges to the value of $Y(x)$.



[Labelle *et alii* 80-90] combinatorial part, without $\mathcal{E}$, using species theory

[Pivoteau, S., Soria 2008] labelled case, without $\mathcal{E}$

[2012] general case, using species theory.

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).*

Quasi-optimal wrt size of the result.

Results (2/2): Oracle

1. The egfs and the ogfs of constructible species are convergent in the neighborhood of 0;
2. A numerical iteration converging to $\mathbf{Y}(\alpha)$ in the labelled case (inside the disk);
3. A numerical iteration converging to the sequence $\mathbf{Y}(\alpha), \mathbf{Y}(\alpha^2), \mathbf{Y}(\alpha^3), \ldots$ for $\|\cdot\|_\infty$ in the unlabelled case (inside the disk).

Examples (I): Polynomial Systems

Random generation following given XML grammars

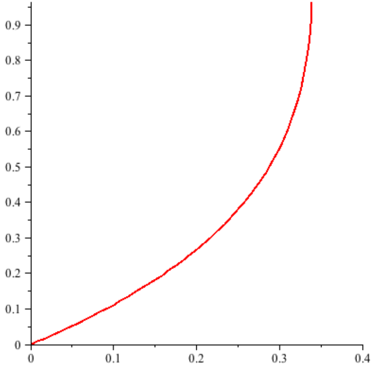
Grammar	nb eqs	max deg	nb sols	oracle (s.)	FGb (s.)
rss	10	5	2	0.02	0.03
PNML	22	4	4	0.05	0.1
xslt	40	3	10	0.4	1.5
relaxng	34	4	32	0.4	3.3
xhtml-basic	53	3	13	1.2	18
mathml2	182	2	18	3.7	882
xhtml	93	6	56	3.4	1124
xhtml-strict	80	6	32	3.0	1590
xmlschema	59	10	24	0.5	6592
SVG	117	10		5.8	$>$1.5Go
docbook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

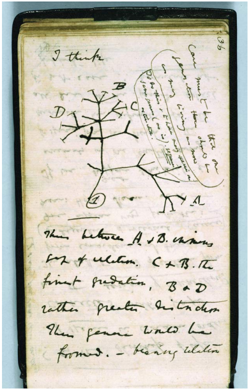
[Darrasse 2008]

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

Unlabelled rooted trees:

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





A Newton iteration driven by combinatorics.

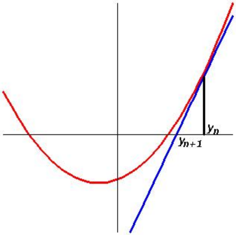
II Newton Iteration for Power Series

Newton Iteration for Power Series has Good Complexity

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

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

Quadratic convergence
$\Updownarrow$
Divide-and-Conquer



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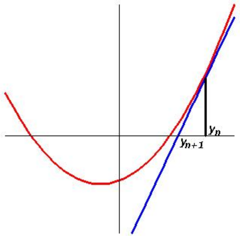

To solve at precision N

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

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

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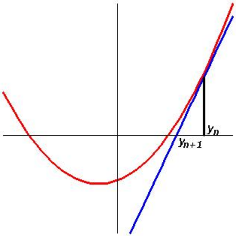

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Useful in conjunction with fast multiplication (quasi-linear):

- 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.

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.

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$$\Phi(Y+U) = \Phi(Y) + \underbrace{Y^{-1}UY^{-1}}_{D\Phi|_Y U} + O(U^2),$$

$$D\Phi|_Y U = \Phi(Y) \Rightarrow U = Y(A - Y^{-1})Y.$$

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

Inverses for Series-Parallel Graphs

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

Newton iteration solving $\mathbf{Y} = \mathbf{H}(z, \mathbf{Y})$:

$$\mathbf{Y}^{[n+1]} = \mathbf{Y}^{[n]} - \left(\frac{\partial \mathbf{H}}{\partial \mathbf{Y}}(z, \mathbf{Y}^{[n]}) \right)^{-1} \cdot \mathbf{H}(z, \mathbf{Y}^{[n]}).$$

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

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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: $\phi(y) = a - \log y$.

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

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

[Brent 1975]

Application: Power Sums

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

Application: Power Sums

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Fast conversion using the generating series:

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

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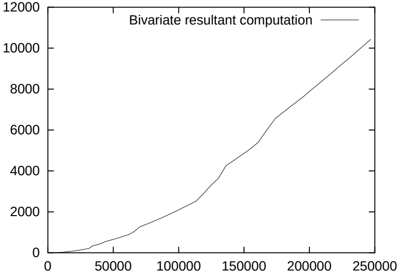
Easy in Newton representation: $\sum \alpha^s \sum \beta^s = \sum (\alpha\beta)^s$ and

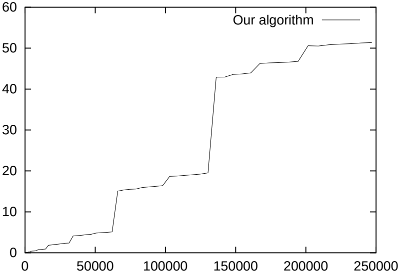
$$\sum \frac{\sum(\alpha+\beta)^s}{s!}t^s = \left(\sum \frac{\sum \alpha^s}{s!}t^s\right)\left(\sum \frac{\sum \beta^s}{s!}t^s\right).$$

[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

Exponential for Series-Parallel Graphs

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

compiles into the Newton iteration:

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

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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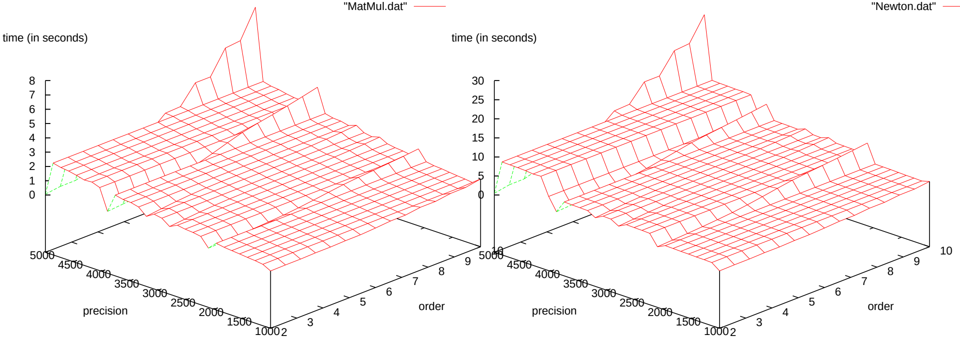
Algorithm

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

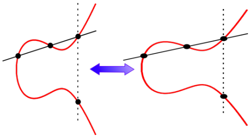


Polynomial matrix multiplication vs. solving $Y' = AY$.

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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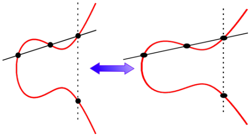

Differential:

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

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)

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

Consequences:

1. EGFs by Newton iteration; also for solutions of $\mathbf{Y}=\mathbf{H}(z,\mathbf{Y})$; also numerically;

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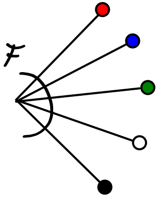
$\mathcal{A}\times\mathcal{B}$	$A(z)\times B(z)$	$A(z)\times B(z)$
$\textsc{Seq}(\mathcal{C})$	$\frac{1}{1-C(z)}$	$\frac{1}{1-C(z)}$
$\mathcal{A}'$	$A'(z)$	—
$\textsc{Cyc}(\mathcal{C})$	$\log\frac{1}{1-C(z)}$	$\sum_{k\ge1}\frac{\phi(k)}{k}\log\frac{1}{1-C(z^k)}$
$\textsc{Set}(\mathcal{C})$	$\exp(C(z))$	$\exp(\sum C(z^i)/i)$

Consequences:

1. EGFs by Newton iteration; also for solutions of $\mathbf{Y}=\mathbf{H}(z,\mathbf{Y})$; also numerically;
2. Pólya operators for ogfs, more difficulties.

Mini-Introduction to Species

- Species $\mathcal{F}$:



Examples:

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

[Joyal 1981, Bergeron-Labelle-Leroux 1998]

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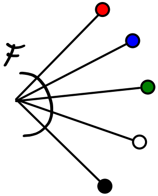

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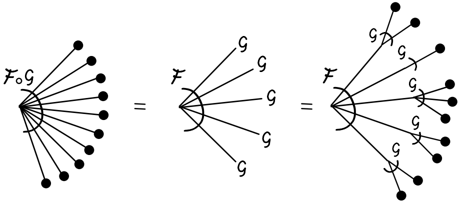

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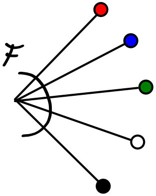

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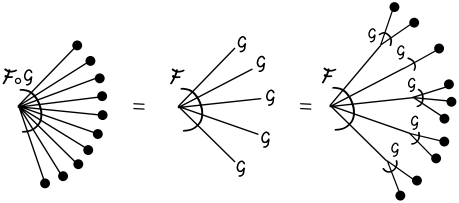

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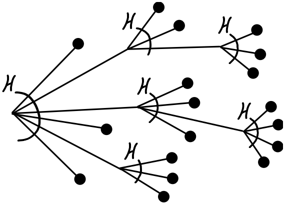
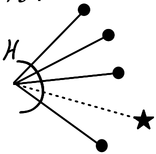


Derivative

$\mathcal{H}'$:



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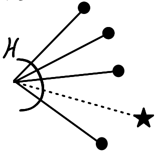

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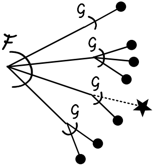

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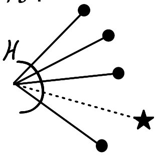

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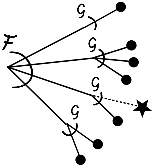

species	derivative
$\mathcal{A}+\mathcal{B}$	$\mathcal{A}'+\mathcal{B}'$
$\mathcal{A}\cdot\mathcal{B}$	$\mathcal{A}'\cdot\mathcal{B}+\mathcal{A}\cdot\mathcal{B}'$
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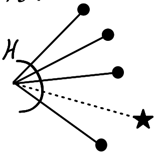

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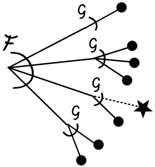

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Example:

$$\boldsymbol{\mathcal{H}}(\mathcal{G},\mathcal{S},\mathcal{P}) := (\mathcal{S}+\mathcal{P}, \mathsf{Seq}(\mathcal{Z}+\mathcal{P}), \mathsf{Set}(\mathcal{Z}+\mathcal{S}))\,.$$

$$\frac{\partial\boldsymbol{\mathcal{H}}}{\partial\boldsymbol{\mathcal{Y}}} = \begin{pmatrix} \varnothing & 1 & 1 \\ \varnothing & \varnothing & \mathsf{Seq}(\mathcal{Z}+\mathcal{P})\cdot 1\cdot\mathsf{Seq}(\mathcal{Z}+\mathcal{P}) \\ \varnothing & \mathsf{Set}(\mathcal{Z}+\mathcal{S})\cdot 1 & \varnothing \end{pmatrix}$$

Joyal's Implicit Species Theorem

Theorem

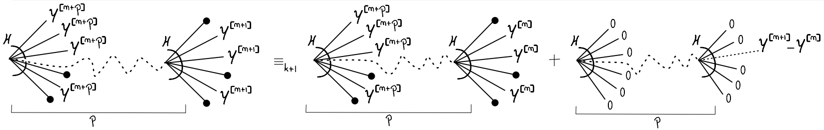
If $\mathcal{H}(0,0)=0$ *and* $\partial\mathcal{H}/\partial\mathcal{Y}(0,0)$ *is nilpotent, then* $\mathcal{Y}=\mathcal{H}(\mathcal{Z},\mathcal{Y})$ *has a unique solution, limit of*

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

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



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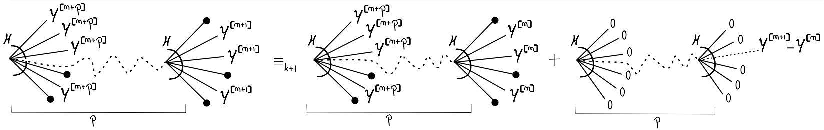


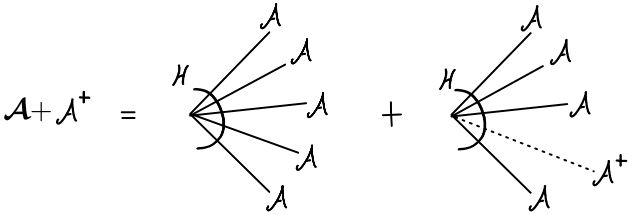
Combinatorial Newton Iteration

Theorem (essentially Labelle)

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

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

has contact $2k+1$ with it.



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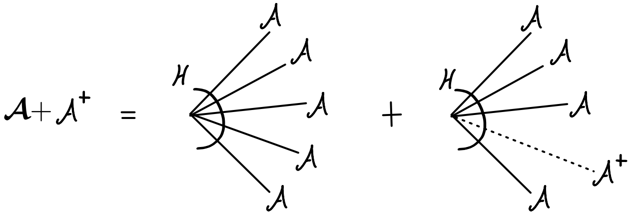
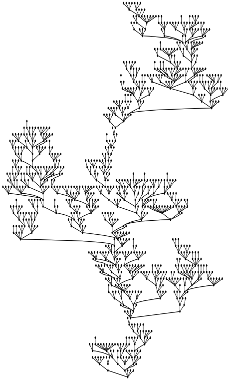


Generation by increasing Strahler numbers.

Unlabelled Rooted Trees: $\mathcal{Y} = \mathcal{Z} \cdot \textsc{Set}(\mathcal{Y}) =: \mathcal{H}(\mathcal{Z}, \mathcal{Y})$

1. Combinatorial Newton iteration:

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



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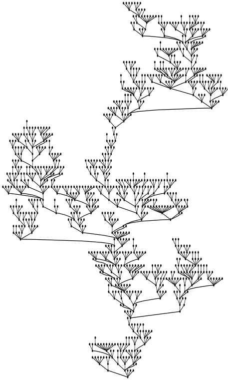

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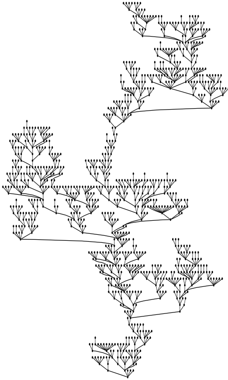

$0,$

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

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

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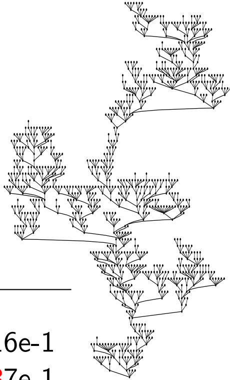

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4. Numerical iteration:

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

IV Conclusion

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  - Newton iteration has good complexity;
  - Oracle: numerical Newton iteration that gives the values of ...
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  - Majorant species;
  - Combinatorial differential systems and linear species
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THE END