Combinatorial Newton iteration for Boltzmann oracle

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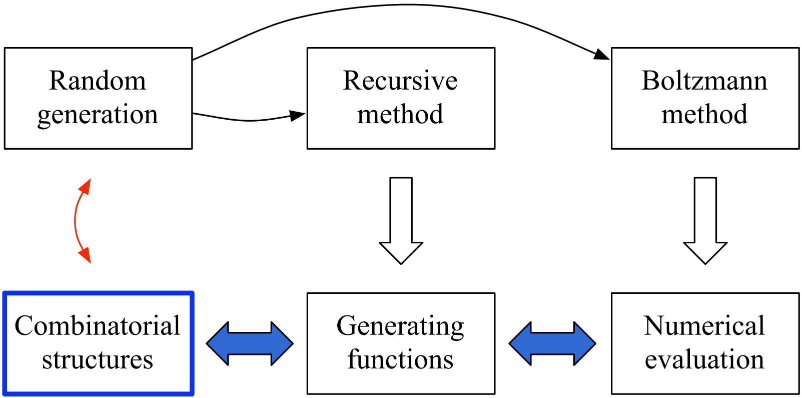
joint work with Bruno Salvy and Michèle Soria

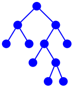
Motivations



Examples of combinatorial specifications

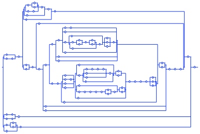
- plane binary trees:

$$\mathcal{B} = \mathcal{Z} + \mathcal{Z} \times \mathcal{B}^2$$



- series-parallel graphs:

$$\begin{aligned} \mathcal{S} &= \textsc{Seq}_{\geq 2}(\mathcal{P} + \mathcal{Z}) \\ \mathcal{P} &= \textsc{MSet}_{\geq 2}(\mathcal{S} + \mathcal{Z}) \end{aligned}$$



- an algebraic language:

$$\begin{aligned} \mathcal{C}_0 &= \mathcal{Z}\mathcal{C}_1\mathcal{C}_2\mathcal{C}_3(\mathcal{C}_1 + \mathcal{C}_2) \\ \mathcal{C}_1 &= \mathcal{Z} + \mathcal{Z}\textsc{Seq}(\mathcal{C}_1^2\mathcal{C}_3^2) \\ \mathcal{C}_2 &= \mathcal{Z} + \mathcal{Z}^2\textsc{Seq}(\mathcal{Z}\mathcal{C}_2^2\textsc{Seq}(\mathcal{Z}))\textsc{Seq}(\mathcal{C}_2) \\ \mathcal{C}_3 &= \mathcal{Z} + \mathcal{Z}(3\mathcal{Z} + \mathcal{Z}^2 + \mathcal{Z}^2\mathcal{C}_1\mathcal{C}_3)\textsc{Seq}(\mathcal{C}_1^2) \end{aligned}$$

Examples of combinatorial specifications

- plane binary trees:

$$\mathcal{B} = \mathcal{Z} + \mathcal{Z} \times \mathcal{B}^2$$

- series-parallel graphs:

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- an algebraic language:

$$\begin{aligned} C_0(z) &= zC_1(z)C_2(z)C_3(z)(C_1(z) + C_2(z)) \\ C_1(z) &= z + z/(1 - C_1(z)^2 C_3(z)^2) \\ C_2(z) &= z + z^2/((1 - zC_2(z)^2/(1 - z))(1 - C_2(z))) \\ C_3(z) &= z + z(3z + z^2 + z^2 C_1(z)C_3(z))/(1 - C_1^2(z)) \end{aligned}$$

Examples of combinatorial specifications

- plane binary trees:

$$\mathcal{B} = \mathcal{Z} + \mathcal{Z} \times \mathcal{B}^2$$

- series-parallel graphs:

$$\begin{aligned} \mathcal{S} &= \textsc{Seq}_{\geq 2}(\mathcal{P} + \mathcal{Z}) \\ \mathcal{P} &= \textsc{MSet}_{\geq 2}(\mathcal{S} + \mathcal{Z}) \end{aligned}$$

- an algebraic language: with $z = 0.1$

$$\begin{aligned} C_0 = C_0(0.1) &= 0.1 C_1 C_2 C_3 (C_1 + C_2) \\ C_1 = C_1(0.1) &= 0.1 + 0.1/(1 - C_1^2 C_3^2) \\ C_2 = C_2(0.1) &= 0.1 + 0.01/((1 - C_2^2/9)(1 - C_2)) \\ C_3 = C_3(0.1) &= 0.1 + 0.1(0.31 + 0.01 C_1 C_3)/(1 - C_1^2) \end{aligned}$$

$$sys := \left[C0 = x\,C1\,C2\,C3\,(C1 + C3),\ Z = x,\ C1 = x + \frac{x}{1 - C1^2\,C3^2},\ C2 = 2\,x + \frac{x}{\left(1 - x\,C1^2\,C2^2\right)\,(1 - C2)},\ C3 = x + \frac{x\left(3\,x + x^2 + x^2\,C1\,C3\right)}{1 - C1^2} \right]$$

```
> 
> [seq(subs(t,C0),t=solve(subs(x=0.1,sys)))];
```

[0.0003125169973, 0.0007429960174, 0.01391132169, -0.01391089776, 0.06534819752, 0.1516695772, 0.5931967039, -0.5909308297, -0.002843524044, -0.006587551424, -0.02496904471, 0.02486320262, 1.016379119, 0.2631789750 + 0.1384080116 I, -0.3391146531, 0.2631789750 − 0.1384080116 I, -0.002894993353, -0.006718005666, -0.02619777844, 0.02609673139, -0.07632515320, -0.1768253273, -0.6704728314, 0.6676342030, 1.015911152, 0.2617092228 + 0.1379131433 I, -0.3359391708, 0.2617092228 − 0.1379131433 I]

$$sys := \left[C0 = x\,C1\,C2\,C3\,(C1 + C3),\ Z = x,\ C1 = x + \frac{x}{1 - C1^2\,C3^2},\ C2 = 2\,x + \frac{x}{\left(1 - x\,C1^2\,C2^2\right)\,(1 - C2)},\ C3 = x + \frac{x\left(3\,x + x^2 + x^2\,C1\,C3\right)}{1 - C1^2} \right]$$

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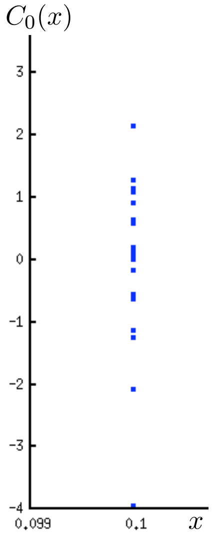
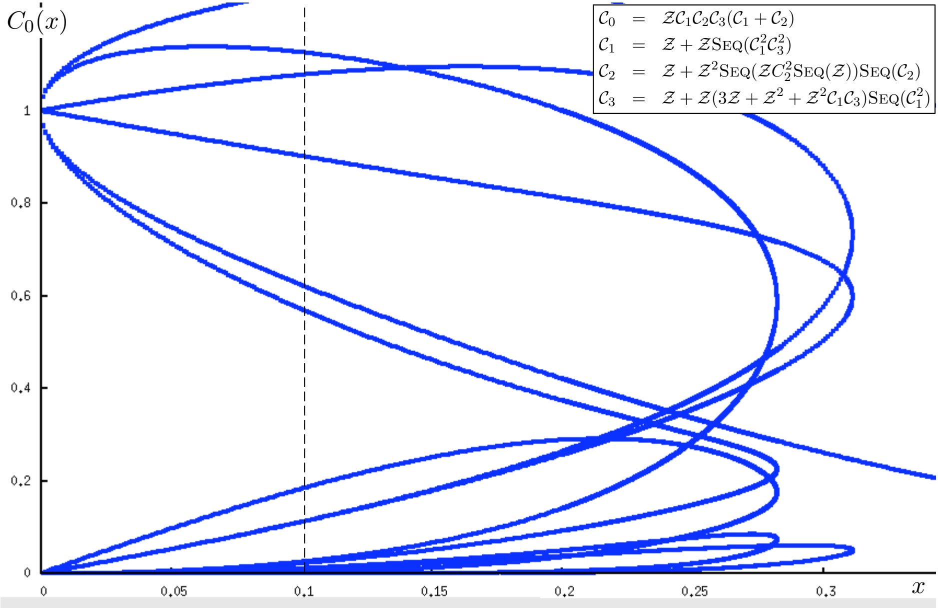
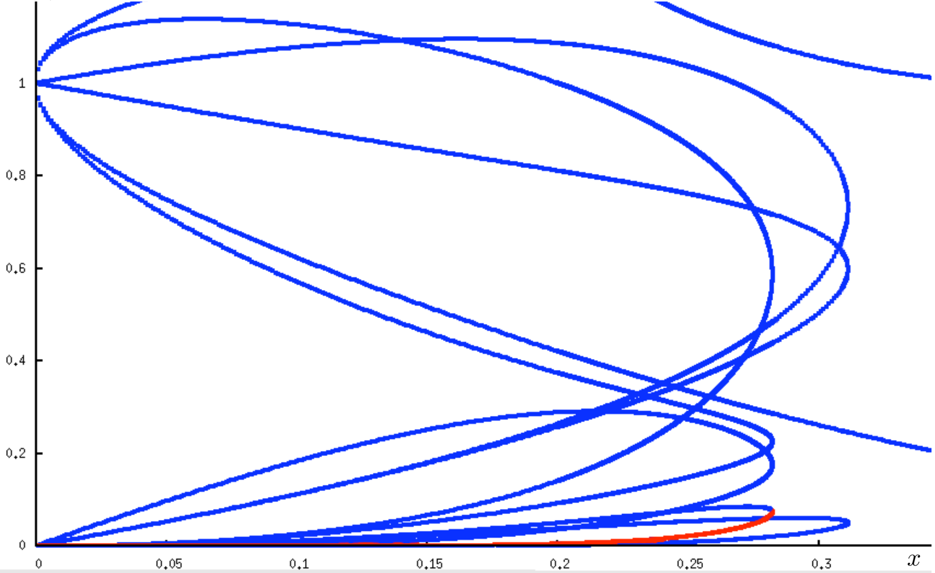
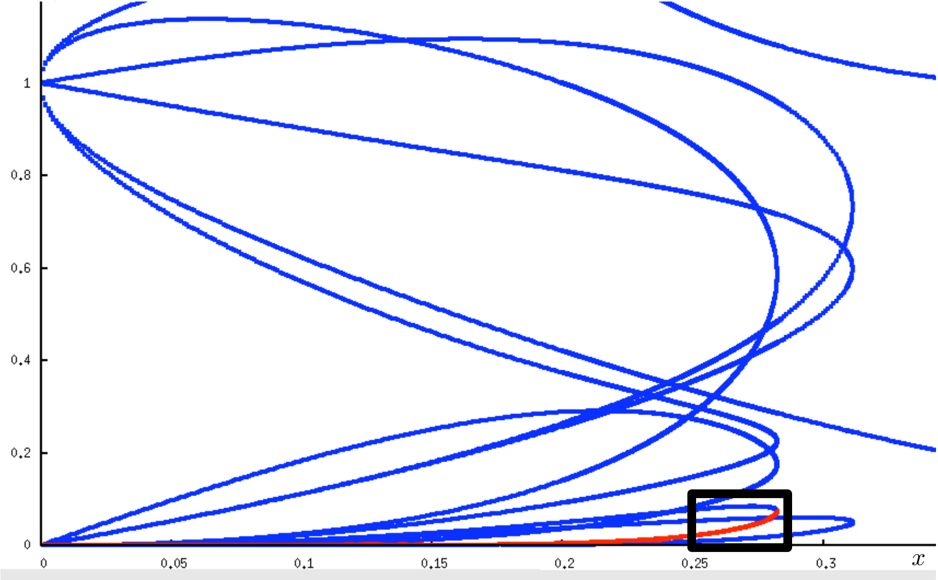



$C_0(x)$
$\mathcal{C}_0 = \mathcal{Z}\mathcal{C}_1\mathcal{C}_2\mathcal{C}_3(\mathcal{C}_1+\mathcal{C}_2)$
$\mathcal{C}_1 = \mathcal{Z}+\mathcal{Z}\textsc{Seq}(\mathcal{C}_1^2\mathcal{C}_3^2)$
$\mathcal{C}_2 = \mathcal{Z}+\mathcal{Z}^2\textsc{Seq}(\mathcal{Z}C_2^2\textsc{Seq}(\mathcal{Z}))\textsc{Seq}(\mathcal{C}_2)$
$\mathcal{C}_3 = \mathcal{Z}+\mathcal{Z}(3\mathcal{Z}+\mathcal{Z}^2+\mathcal{Z}^2\mathcal{C}_1\mathcal{C}_3)\textsc{Seq}(\mathcal{C}_1^2)$
1
0,8
0,6
0,4
0,2
0
0
0,05
0,1
0,15
0,2
0,25
0,3
x

$$C_0(z) = 18z^5 + 90z^6 + 222z^7 + 1032z^8 + 4446z^9 + 23184z^{10} + 126492z^{11} + 732264z^{12} + \ldots$$



$$C_0(z) = 18z^5 + 90z^6 + 222z^7 + 1032z^8 + 4446z^9 + 23184z^{10} + 126492z^{11} + 732264z^{12} + \ldots$$

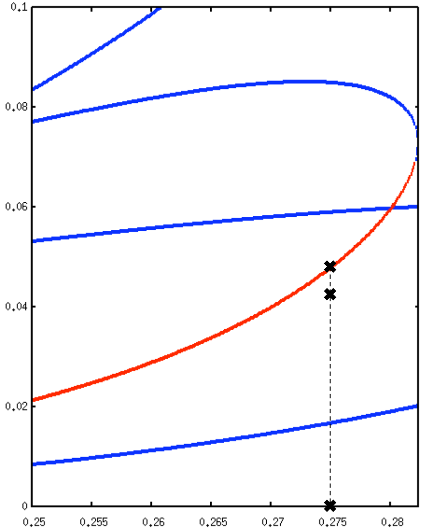


Proposition

Newton iteration converges quadratically to the solution.

Approach

numerical iteration
converges to the solution
⇑
counting series
evaluation
⇑
combinatorial systems
of equations



Combinatorial structures

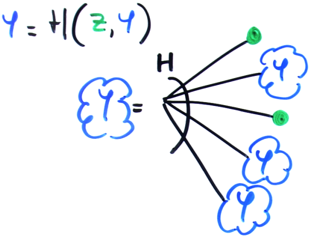
Combinatorial specification

A *combinatorial specification* for an m-tuple $\boldsymbol{\mathcal{Y}} = (\mathcal{Y}_1, \ldots, \mathcal{Y}_m)$ of classes is a system

$$\boldsymbol{\mathcal{Y}} = \boldsymbol{\mathcal{H}}(\mathcal{Z}, \boldsymbol{\mathcal{Y}}) \quad \equiv \quad \begin{cases} \mathcal{Y}_1 = \mathcal{H}_1(\mathcal{Z}, \mathcal{Y}_1, \mathcal{Y}_2, \ldots, \mathcal{Y}_m), \\ \mathcal{Y}_2 = \mathcal{H}_2(\mathcal{Z}, \mathcal{Y}_1, \mathcal{Y}_2, \ldots, \mathcal{Y}_m), \\ \qquad \vdots \\ \mathcal{Y}_m = \mathcal{H}_m(\mathcal{Z}, \mathcal{Y}_1, \mathcal{Y}_2, \ldots, \mathcal{Y}_m), \end{cases}$$

each $\mathcal{H}_i$ denoting a term built from the $\mathcal{Y}_i$'s and the initial class $\mathcal{Z}$ (atomic) using the classical constructions.

construction	notation	$\mathcal{B} = \varnothing$	$\mathcal{B} = \mathcal{E}$
Disjoint union	$\mathcal{A} + \mathcal{B}$	$\mathcal{A}$	$\mathcal{A} + \mathcal{E}$
Cartesian product	$\mathcal{A} \times \mathcal{B}$	$\varnothing$	$\mathcal{A}$
Sequence	$\mathrm{SEQ}(\mathcal{B})$	$\mathcal{E}$	–
Cycle	$\mathrm{CYC}(\mathcal{B})$	$\varnothing$	–
Set	$\mathrm{SET}(\mathcal{B})$	$\mathcal{E}$	–



Well founded specification

Definition

The combinatorial specification $\boldsymbol{\mathcal{Y}} = \boldsymbol{\mathcal{H}}(\mathcal{Z}, \boldsymbol{\mathcal{Y}})$ is *well founded* if and only if, for all $n \geq 0$, it derives only finitely many structures of size n. This is denoted by $|\boldsymbol{\mathcal{Y}}|_n < \infty$.

$\mathcal{Y} = \textsc{Seq}(\mathcal{Z})$ ✓
$1+z+z^2+z^3+z^4+\ldots$

$\mathcal{Y} = \textsc{Seq}(\mathcal{Z}\,\textsc{Seq}(\mathcal{Z}))$ ✓
$1+z+2z^2+4z^3+8z^4+\ldots$

$\mathcal{Y} = \textsc{Seq}(\textsc{Seq}(\mathcal{Z}))$ ✗
$|\mathcal{Y}|_0=\infty$

$\mathcal{Y} = \mathcal{Z}\,\mathcal{Y}$ ✓
0

$\mathcal{Y} = \mathcal{Z} + \mathcal{Z}\,\mathcal{Y}$ ✓
$z+z^2+z^3+z^4+\ldots$

$\mathcal{Y} = \mathcal{Z} + \mathcal{Y}$ ✗
$|\mathcal{Y}|_1=\infty$

$$\begin{cases} \mathcal{Y}_1 = \mathcal{Z} + \mathcal{Y}_2 \\ \mathcal{Y}_2 = \mathcal{Z}\,\mathcal{Y}_1\,\textsc{Seq}(\mathcal{Y}_2) \end{cases}$$ ✓

$Y_1(z)=z+z^2+z^3+2z^4+4z^5+\ldots$

$Y_2(z)=z^2+z^3+2z^4+4z^5+\ldots$

$$\begin{cases} \mathcal{Y}_1 = \mathcal{Z} + \mathcal{Y}_2 \\ \mathcal{Y}_2 = \mathcal{Z} + \mathcal{Y}_1\,\textsc{Seq}(\mathcal{Y}_2) \end{cases}$$ ✗

$|\boldsymbol{\mathcal{Y}}|_1=\infty$

Combinatorial derivative

$\partial\mathcal{H}/\partial\mathcal{T}$: *derivative* of $\mathcal{H}(\mathcal{Z},\mathcal{Y}_1,\dots,\mathcal{Y}_m)$ with respect to $\mathcal{T}$.

$$\mathcal{H}(\mathcal{Z},\mathcal{Y}) = \mathcal{Z}\ \textsc{Seq}(\mathcal{Y}) \qquad \partial\mathcal{H}/\partial\mathcal{Y} = \mathcal{Z}\ \textsc{Seq}(\mathcal{Y})^2$$

$$z/(1-y) \qquad z/(1-y)^2$$

$$\mathcal{H}(\mathcal{Z},\mathcal{Y}_1,\mathcal{Y}_2) = \mathcal{Z}\ \mathcal{Y}_1^2\ \textsc{Cyc}(\mathcal{Y}_2) \qquad \partial\mathcal{H}/\partial\mathcal{Y}_2 = \mathcal{Z}\ \mathcal{Y}_1^2\ \textsc{Seq}(\mathcal{Y}_2)$$

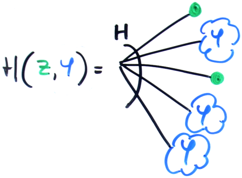
$$zY_1^2\log(1/(1-Y_2)) \qquad zY_1^2/(1-Y_2)$$

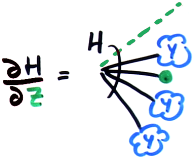
$$zY_1^2\sum_{k\geq 0}\varphi(k)\log(1/(1-Y_2(z^k)))/k$$

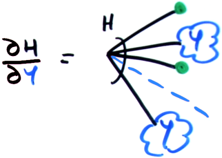
$$\mathcal{H}(\mathcal{Z},\mathcal{Y}_1,\mathcal{Y}_2) = \begin{cases}\mathcal{Z}\ \textsc{Set}(\mathcal{Y}_1)\\ \mathcal{Y}_1^2\ \mathcal{Y}_2\end{cases} \qquad \partial\mathcal{H}/\partial\mathcal{Y}_1 = \begin{cases}\mathcal{Z}\ \textsc{Set}(\mathcal{Y}_1)\\ 2\ \mathcal{Y}_1\ \mathcal{Y}_2\end{cases}$$

$$z\exp(Y_1)\ ,\ Y_1^2Y_2 \qquad z\exp(Y_1)\ ,\ 2Y_1Y_2$$

$$z\exp\Big(\sum_{k\geq 0}Y_1(z^k)/k\Big)\ ,\ Y_1^2Y_2 \qquad z\exp\Big(\sum_{k\geq 0}Y_1(z^k)/k\Big)\ ,\ 2Y_1Y_2$$



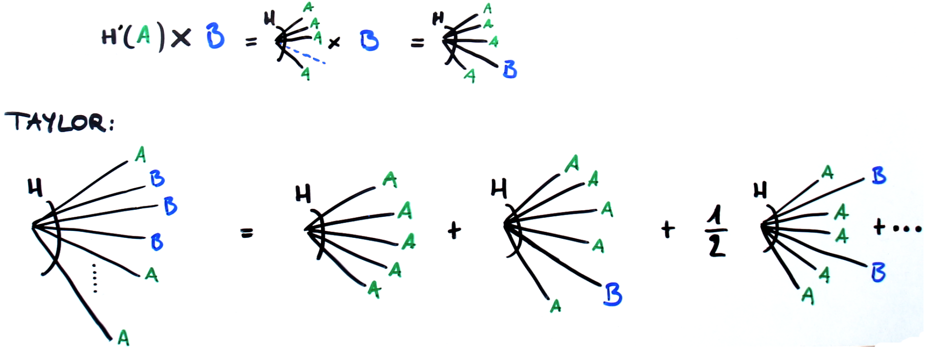




Combinatorial derivative

Cartesian product and Taylor formula (Labelle 90)

$$\mathcal{H}(\mathcal{A}+\mathcal{B}) = \mathcal{H}(\mathcal{A}) + \mathcal{H}'(\mathcal{A}) \times \mathcal{B} + \frac{1}{2}\mathcal{H}''(\mathcal{A}) \times \mathcal{B}^2 + \dots$$



Jacobian matrix

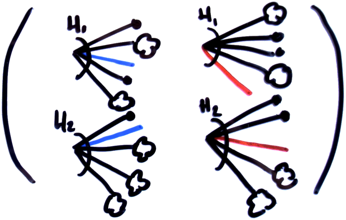
$\partial\boldsymbol{\mathcal{H}}/\partial\boldsymbol{\mathcal{Y}}$: the *Jacobian matrix* of $\boldsymbol{\mathcal{H}}(\mathcal{Z},\boldsymbol{\mathcal{Y}})$ with respect to $\boldsymbol{\mathcal{Y}}$,
its entries are the partial derivatives $\partial\mathcal{H}_i(\mathcal{Z},\boldsymbol{\mathcal{Y}})/\partial\mathcal{Y}_j$.

$$\boldsymbol{\mathcal{H}}_{\mathbf{1}}(\mathcal{Z},\boldsymbol{\mathcal{Y}}) = \begin{cases} \mathcal{Z}\ \textsc{Set}(\mathcal{Y}_1) \\ \mathcal{Y}_1^2\ \mathcal{Y}_2 \end{cases} \qquad \partial\boldsymbol{\mathcal{H}}_{\mathbf{1}}/\partial\boldsymbol{\mathcal{Y}} = \begin{pmatrix} \mathcal{Z}\ \textsc{Set}(\mathcal{Y}_1) & \varnothing \\ 2\ \mathcal{Y}_1\ \mathcal{Y}_2 & \mathcal{Y}_1^2 \end{pmatrix}$$

$$\boldsymbol{\mathcal{H}}_{\mathbf{2}}(\mathcal{Z},\boldsymbol{\mathcal{Y}}) = \begin{cases} \mathcal{Z} + \mathcal{Y}_2 \\ \mathcal{Z}\ \textsc{Seq}(\mathcal{Y}_1) \end{cases} \qquad \partial\boldsymbol{\mathcal{H}}_{\mathbf{2}}/\partial\boldsymbol{\mathcal{Y}} = \begin{pmatrix} \varnothing & \mathcal{E} \\ \mathcal{Z}\ \textsc{Seq}(\mathcal{Y}_1)^2 & \varnothing \end{pmatrix}$$

$$\begin{cases} Y_1 = H_1(Z, Y_1, Y_2) \\ Y_2 = H_2(Z, Y_1, Y_2) \end{cases}$$

$$\frac{\partial H}{\partial Y}(Z, Y_1, Y_2) =$$



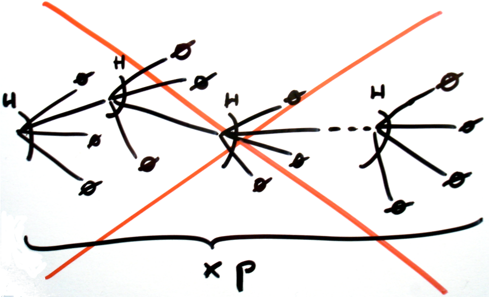
Jacobian matrix

Nilpotent matrix : one of its powers is $\boldsymbol{\varnothing}$ (all its entries are $\varnothing$).

$$\partial \boldsymbol{\mathcal{H}_1} / \partial \boldsymbol{\mathcal{Y}}(\varnothing, \boldsymbol{\varnothing}) = \begin{pmatrix} \varnothing & \varnothing \\ \varnothing & \varnothing \end{pmatrix}$$

$$\partial \boldsymbol{\mathcal{H}_2} / \partial \boldsymbol{\mathcal{Y}}(\varnothing, \boldsymbol{\varnothing}) = \begin{pmatrix} \varnothing & \mathcal{E} \\ \varnothing & \varnothing \end{pmatrix} \qquad (\partial \boldsymbol{\mathcal{H}_2} / \partial \boldsymbol{\mathcal{Y}}(\varnothing, \boldsymbol{\varnothing}))^2 = \begin{pmatrix} \varnothing & \varnothing \\ \varnothing & \varnothing \end{pmatrix}$$

$$\left(\frac{\partial H}{\partial Y}(\varnothing, \varnothing)\right)^p = \varnothing \quad \rightsquigarrow$$



Characterization of well-founded systems

Proposition

A combinatorial specification $\boldsymbol{\mathcal{Y}} = \boldsymbol{\mathcal{H}}(\mathcal{Z}, \boldsymbol{\mathcal{Y}})$ such that $\boldsymbol{\mathcal{H}}(\varnothing, \boldsymbol{\varnothing}) = \boldsymbol{\varnothing}$ is well founded if and only if the Jocabian matrix $\partial\boldsymbol{\mathcal{H}}/\partial\boldsymbol{\mathcal{Y}}(\varnothing, \boldsymbol{\varnothing})$ is nilpotent.

$\Leftarrow$ by contradiction. $(\boldsymbol{\partial\mathcal{H}}/\boldsymbol{\partial\mathcal{Y}}(\varnothing, \boldsymbol{\varnothing}))^p = \boldsymbol{\varnothing}$
$n = \min\{k,\ |\boldsymbol{\mathcal{Y}}|_k = \infty\}$ and $\boldsymbol{\alpha} = \boldsymbol{\mathcal{H}}(\mathcal{Z}, \alpha_1, \ldots, \alpha_m),\ \ |\boldsymbol{\alpha}| = n$.
$\forall i,\ |\alpha_i| < n$ or $\exists i, |\alpha_i| = n$ and $\forall j \neq i,\ |\alpha_j| = 0$.
In the later case: $\partial\boldsymbol{\mathcal{H}}/\partial\boldsymbol{\mathcal{Y}}(\varnothing, \boldsymbol{\varnothing})^q \times \boldsymbol{\beta}$, with $|\boldsymbol{\beta}| = n$ and $q \leq p$.

$\Rightarrow$ by contradiction.
$n = \min\{k,\ |\boldsymbol{\mathcal{Y}}|_k \neq 0\}$ and $\boldsymbol{\alpha}$ is a $\boldsymbol{\mathcal{Y}}$-structure of size n.
Suppose that the matrix $\partial\boldsymbol{\mathcal{H}}/\partial\boldsymbol{\mathcal{Y}}(\varnothing, \boldsymbol{\varnothing})$ is not nilpotent.
Then, $\forall q \in \mathbb{N}$, there exist a nonempty structure β_q of size 0 in $(\boldsymbol{\partial\mathcal{H}}/\boldsymbol{\partial\mathcal{Y}}(\varnothing, \boldsymbol{\varnothing}))^q$ such that $\beta_q \cdot \alpha$ is a $\boldsymbol{\mathcal{Y}}$-structure of size n. $\square$

Examples

$\mathcal{Y} = \textsc{Seq}(\mathcal{Z})$ ✓ $\mathcal{H}'(\varnothing) = \varnothing$

$\mathcal{Y} = \textsc{Seq}(\mathcal{Z}\,\textsc{Seq}(Z))$ ✓ $\mathcal{H}'(\varnothing) = \varnothing$

$\mathcal{Y} = \textsc{Seq}(\textsc{Seq}(Z))$ ✗ $\mathcal{H}'(\varnothing)$ not defined!

$\mathcal{Y} = \mathcal{Z}\,\mathcal{Y}$ ✓ $\mathcal{H}'(\varnothing,\varnothing) = \varnothing$

$\mathcal{Y} = \mathcal{Z} + \mathcal{Z}\,\mathcal{Y}$ ✓ $\mathcal{H}'(\varnothing,\varnothing) = \varnothing$

$\mathcal{Y} = \mathcal{Z} + \mathcal{Y}$ ✗ $\mathcal{H}'(\varnothing,\varnothing) = \mathcal{E}$

$$\begin{cases} \mathcal{Y}_1 = \mathcal{Z}\,\mathcal{Y}_2 \\ \mathcal{Y}_2 = \mathcal{Z}\,\mathcal{Y}_1\,\textsc{Seq}(\mathcal{Y}_2) \end{cases} \checkmark$$

$$\left.\begin{pmatrix} \varnothing & \varnothing \\ \mathcal{Z}\,\textsc{Seq}(\mathcal{Y}_2) & \mathcal{Z}\,\mathcal{Y}_1\,\textsc{Seq}(\mathcal{Y}_2)^2 \end{pmatrix}\right|_{\varnothing,\varnothing} = \begin{pmatrix} \varnothing & \varnothing \\ \varnothing & \varnothing \end{pmatrix}$$

$$\begin{cases} \mathcal{Y}_1 = \mathcal{Z} + \mathcal{Y}_2 \\ \mathcal{Y}_2 = \mathcal{Z}\,\mathcal{Y}_1\,\textsc{Seq}(\mathcal{Y}_2) \end{cases} \checkmark$$

$$\begin{pmatrix} \varnothing & \mathcal{E} \\ \varnothing & \varnothing \end{pmatrix}$$

$$\begin{cases} \mathcal{Y}_1 = \mathcal{Z} + \mathcal{Y}_2 \\ \mathcal{Y}_2 = \mathcal{Z} + \mathcal{Y}_1\,\textsc{Seq}(\mathcal{Y}_2) \end{cases} ✗$$

$$\left.\begin{pmatrix} \varnothing & \mathcal{E} \\ \textsc{Seq}(\mathcal{Y}_2) & \mathcal{Y}_1\,\textsc{Seq}(\mathcal{Y}_2)^2 \end{pmatrix}\right|_{\varnothing,\varnothing} = \begin{pmatrix} \varnothing & \mathcal{E} \\ \mathcal{E} & \varnothing \end{pmatrix}$$

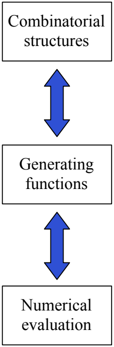
Iteration and Oracle

Result

Theorem (Transfer of Convergence)

Let $\mathcal{Y} = \mathcal{F}(\mathcal{Z}, \mathcal{Y})$ *be* well founded *and* $\mathcal{F}(\varnothing, \varnothing) = \varnothing$.

1. *The iteration* $\mathcal{Y}_{n+1} = \mathcal{F}(\mathcal{Z}, \mathcal{Y}_n)$, *with* $\mathcal{Y}_0 = \varnothing$, *converges to the combinatorial class* $\mathcal{Y}$, *solution of* $\mathcal{Y} = \mathcal{F}(\mathcal{Z}, \mathcal{Y})$.
2. *The iteration* $\mathbf{Y}_{n+1}(z) = \mathbf{F}(z, \mathbf{Y}_n(z))$, *with* $\mathbf{Y}_0(z) = 0$, *converges to the generating series* $\mathbf{Y}(z)$ *of the class* $\mathcal{Y}$.
3. *If* $\mathcal{F}$ *is an analytic specification, then* $\mathbf{Y}$ *has positive radius of convergence* ρ *and for all* α *such that* $|\alpha| < \rho$, *the iteration* $\mathbf{y}_{n+1} = \mathbf{F}(\alpha, \mathbf{y}_n)$, *with* $\mathbf{y}_0 = 0$, *converges to* $\mathbf{Y}(\alpha)$.



$\mathcal{F}(\mathcal{Z}, \mathcal{Y})$ is called *analytic* when the generating series $\boldsymbol{F}(z, \boldsymbol{Y})$ is analytic in $(z, \boldsymbol{Y})$ in the neighborhood of $(0, \mathbf{0})$, with nonnegative coefficients.

Example: binary trees

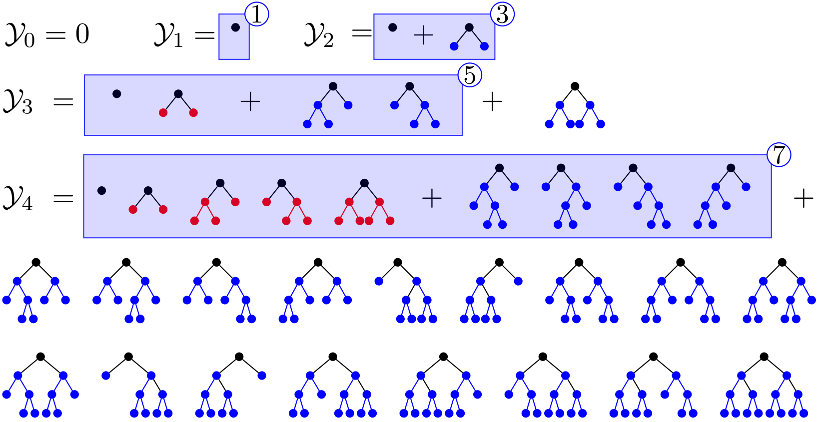
$\mathcal{Y} = \mathcal{Z} + \mathcal{Z} \times \mathcal{Y}^2$

$\mathcal{Y} = F(\mathcal{Z}, \mathcal{Y})$

$\mathcal{Y}_{k+1} = \mathcal{Z} + \mathcal{Z} \times \mathcal{Y}_k^2$

Iteration: $\mathcal{Y}_{k+1} = F(\mathcal{Z}, \mathcal{Y}_k)$

$\mathcal{Y}_0 = 0$



Generating functions

$Y(z) = z + zY^2(z)$

$Y(z) = F(z, Y(z))$

$Y_{k+1}(z) = z + zY_k(z)^2$

Iteration: $Y_{k+1}(z) = F(z, Y_k(z))$

$$
\begin{aligned}
Y_0(z) &= \mathbf{0} \\
Y_1(z) &= \boldsymbol{z} \\
Y_2(z) &= \boldsymbol{z} + \boldsymbol{z}^{\mathbf{3}} \\
Y_3(z) &= \boldsymbol{z} + \boldsymbol{z}^{\mathbf{3}} + \mathbf{2}\boldsymbol{z}^{\mathbf{5}} + z^7 \\
Y_4(z) &= \boldsymbol{z} + \boldsymbol{z}^{\mathbf{3}} + \mathbf{2}\boldsymbol{z}^{\mathbf{5}} + \mathbf{5}\boldsymbol{z}^{\mathbf{7}} + 6z^9 + 6z^{11} + 4z^{13} + z^{15} \\
Y_5(z) &= \boldsymbol{z} + \boldsymbol{z}^{\mathbf{3}} + \mathbf{2}\boldsymbol{z}^{\mathbf{5}} + \mathbf{5}\boldsymbol{z}^{\mathbf{7}} + \mathbf{14}\boldsymbol{z}^{\mathbf{9}} + 26z^{11} + 44z^{13} + 69z^{15} \\
Y(z) &= \boldsymbol{z} + \boldsymbol{z}^{\mathbf{3}} + \mathbf{2}\boldsymbol{z}^{\mathbf{5}} + \mathbf{5}\boldsymbol{z}^{\mathbf{7}} + \mathbf{14}\boldsymbol{z}^{\mathbf{9}} + 42z^{11} + 132z^{13} + 429z^{15} + \ldots
\end{aligned}
$$

convergence for structures $\Rightarrow$ convergence for series

Numerical iteration

$Y(\alpha) = \alpha + \alpha Y^2(\alpha)$

$Y(\alpha) = F(\alpha, Y(\alpha))$

$Y_{k+1} = 0.2 + 0.2 Y_k^2$

Iteration: $Y_{k+1}(\alpha) = F(\alpha, Y_k(\alpha))$

$$
\begin{aligned}
Y_0 &= Y_0(0.2) = \mathbf{0} \\
Y_1 &= Y_1(0.2) = \mathbf{0.2} \\
Y_2 &= Y_2(0.2) = \mathbf{0.208} \\
Y_3 &= Y_3(0.2) = \mathbf{0.208}6528 \\
Y_4 &= Y_4(0.2) = \mathbf{0.2087}07198189568\ldots \\
Y_5 &= Y_5(0.2) = \mathbf{0.20871}17389152279\ldots \\
Y &= Y(0.2) = \mathbf{0.20871}21525220799\ldots
\end{aligned}
$$

- for any value of $\alpha < \rho$
- numerical iteration $\Leftrightarrow$ evaluation of the series at α.

Proof idea

1. **Combinatorial convergence**

   Consequence of Joyal's proof of his Implicit Species theorem ($\boldsymbol{\mathcal{Y}}_n =_k \boldsymbol{\mathcal{Y}}_{n+1} \Rightarrow \boldsymbol{\mathcal{Y}}_{n+p} =_{k+1} \boldsymbol{\mathcal{Y}}_{n+p+1}$).

   Note that $\boldsymbol{\mathcal{Y}}_n \subset \boldsymbol{\mathcal{Y}}_{n+1}$ for all n.

   Two combinatorial classes $\mathcal{F}$ and $\mathcal{G}$ have *contact* of order k, denoted by $\mathcal{F} =_k \mathcal{G}$, when their structures of size up to k are identical.

2. **Power series**

   Symbolic method. $\boldsymbol{Y}_n(z)$ are the generating series of the classes $\boldsymbol{\mathcal{Y}}_n$: $\mathrm{val}(\boldsymbol{Y}_n(z) - \boldsymbol{Y}(z)) \rightarrow \infty$.

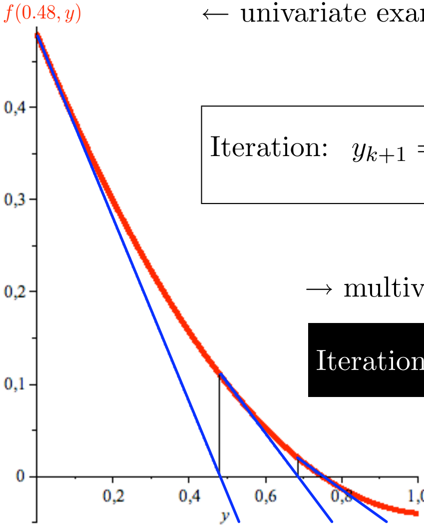
3. **Numerical values** ($|\alpha| < \rho$)

   $\boldsymbol{Y}$ is analytic at 0 (implicit function theorem).

   - $\boldsymbol{Y}_n(\alpha)$ converges to $\boldsymbol{Y}(\alpha)$.
   - $\boldsymbol{y}_n = \boldsymbol{Y}_n(\alpha)$.

Newton iteration

Principle of Newton iteration



← univariate example: $y(x) = x + xy^2(x)$

$f(x, y) = x + xy^2 - y$

$$\text{Iteration:} \quad y_{k+1} = y_k - \frac{f(x, y_k)}{\frac{\partial f}{\partial y}(x, y_k)}$$

→ multivariate:

$$\text{Iteration:} \quad y_{k+1} = y_k - \left(\frac{\partial f}{\partial y}(x, y_k)\right)^{-1} f(x, y_k)$$

Result

Theorem (Newton Oracle)

Let $\boldsymbol{\mathcal{Y}} = \boldsymbol{\mathcal{H}}(\mathcal{Z}, \boldsymbol{\mathcal{Y}})$ be a well-founded analytic specification with $\boldsymbol{\mathcal{H}}(\varnothing, \boldsymbol{\varnothing}) = \boldsymbol{\varnothing}$. Let α be inside the disk of convergence of the generating series $\mathbf{Y}(z)$ of $\boldsymbol{\mathcal{Y}}$. Then the iteration

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \left(\mathbf{I} - \frac{\partial \mathbf{H}}{\partial \mathbf{Y}}(\alpha, \mathbf{y}_n)\right)^{-1} \cdot (\mathbf{H}(\alpha, \mathbf{y}_n) - \mathbf{y}_n), \qquad \mathbf{y}_0 = \mathbf{0}$$

converges to $\mathbf{Y}(\alpha)$.

★ bonus: optimized Newton iteration.

Numerical convergence

$Y(\alpha) = \alpha + \alpha Y^2(\alpha)$

$Y(\alpha) = H(\alpha, Y(\alpha))$

Iteration: $Y_{k+1} = Y_k + (I - \frac{\partial H}{\partial Y}(\alpha, Y_k))^{-1}(H(\alpha, Y_k) - Y_k)$

for $\alpha = 0.48, \quad Y_{k+1} = Y_k + \frac{1}{1-0.96Y_k}(0.48 + 0.48Y_k^2 - Y_k)$

$$
\begin{aligned}
Y_0 &= \mathbf{0}\\
Y_1 &= \mathbf{0}.48\\
Y_2 &= \mathbf{0}.685103857566765578635014836795 25\ldots\\
Y_3 &= \mathbf{0.74}40942953173578506931541165958 9\ldots\\
Y_4 &= \mathbf{0.7499}4139686483588184679391778624\ldots\\
Y_5 &= \mathbf{0.7499999}41137642045942008051107 7\ldots\\
Y_4 &= \mathbf{0.749999999999999}4060382090306852\ldots\\
Y_5 &= \mathbf{0.7499999999999999999999999999999}7\ldots
\end{aligned}
$$

asymptotically quadratic convergence

Newton on series

$$Y = z + zY^2(z)$$

$$\boxed{Y(z) = H(z, Y)}$$

Iteration: $Y_{k+1} = Y_k + (I - \frac{\partial H}{\partial Y}(z, Y_k))^{-1}(H(z, Y_k) - Y_k)$

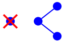
$$Y_{k+1} = Y_k + \frac{1}{1-2zY_k}(z + zY_k^2 - Y_k)$$

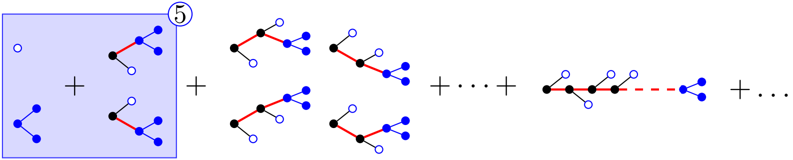
$$Y_0 = \mathbf{0}$$
$$Y_1 = \boldsymbol{z}$$
$$Y_2 = \boldsymbol{z} + \boldsymbol{z^3} + \boldsymbol{2z^{\boxed{5}}} + 4z^7 + 8z^9 + 16z^{11} + 32z^{13} + 64z^{15} + \ldots$$
$$Y_3 = \boldsymbol{z} + \boldsymbol{z^3} + \boldsymbol{2z^5} + \boldsymbol{5z^7} + \boldsymbol{14z^9} + \boldsymbol{42z^{11}} + \boldsymbol{132z^{\boxed{13}}} + 428z^{15} + \ldots$$
$$Y_4 = \boldsymbol{z} + \boldsymbol{z^3} + \boldsymbol{2z^5} + \boldsymbol{5z^7} + \cdots + \boldsymbol{2674440z^{\boxed{29}}} + 9694844z^{31} + \ldots$$

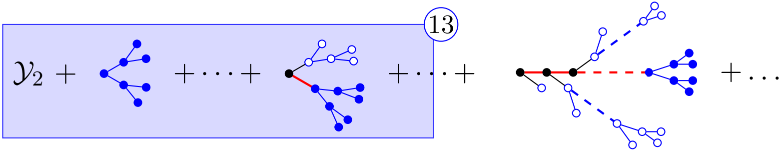
Combinatorial Newton for a single equation
(Bergeron, Décoste, Labelle, Leroux 82/98)

Iteration: $\mathcal{Y}_{k+1} = \mathcal{Y}_k + \textsc{Seq}(\mathcal{H}'(\mathcal{Z},\mathcal{Y}_k))(\mathcal{H}(\mathcal{Z},\mathcal{Y}_k) - \mathcal{Y}_k)$

$$\mathcal{Y}_{k+1} = \mathcal{Y}_k + \textsc{Seq}(2\mathcal{Z}\mathcal{Y}_k)(\mathcal{Z} + \mathcal{Z}\mathcal{Y}_k^2 - \mathcal{Y}_k)$$

$\mathcal{Y}_0 = 0$ $\quad \mathcal{Y}_1 = \bullet$ $\quad \mathcal{H}(Y_1) - \mathcal{Y}_1 = \mathcal{Z} + \mathcal{Z}\mathcal{Y}_1^2 - \mathcal{Y}_1 =$ 

$\mathcal{Y}_2 =$ 

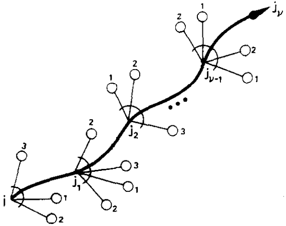
$\mathcal{Y}_3 =$ 

Newton for a system

$$\text{Iteration: } \mathcal{Y}_{k+1} = \mathcal{Y}_k + \boxed{(I - \frac{\partial \mathcal{H}}{\partial \mathcal{Y}}(\mathcal{Z}, \mathcal{Y}_k))^{-1}} (\mathcal{H}(\mathcal{Z}, \mathcal{Y}_k) - \mathcal{Y}_k)$$

- one single equation → sequence
- many equations → combinatorial bloomings (Labelle 85)

$$\left(\mathbf{I} - \frac{\partial \boldsymbol{\mathcal{H}}}{\partial \boldsymbol{\mathcal{Y}}}(\mathcal{Z}, \boldsymbol{\mathcal{Y}})\right)^{-1} = \sum_{k \geq 0} \left(\frac{\partial \boldsymbol{\mathcal{H}}}{\partial \boldsymbol{\mathcal{Y}}}(\mathcal{Z}, \boldsymbol{\mathcal{Y}})\right)^k$$



Contact for vectors is componentwise contact.

Proof idea

Proposition

Let $\mathcal{Y} = \mathcal{H}(\mathcal{Z}, \mathcal{Y})$ be a well-founded specification with $\mathcal{H}(\varnothing, \varnothing) = \varnothing$. Let $\mathcal{N}_{\mathcal{H}}$ be the operator defined by

$$\mathcal{N}_{\mathcal{H}}(\mathcal{Z}, \mathcal{Y}) = \mathcal{Y} + \left(\mathbf{I} - \frac{\partial \mathcal{H}}{\partial \mathcal{Y}}(\mathcal{Z}, \mathcal{Y})\right)^{-1} \times (\mathcal{H}(\mathcal{Z}, \mathcal{Y}) - \mathcal{Y}).$$

Then the sequence defined by $\mathcal{Y}_0 = \varnothing$, $\mathcal{Y}_{n+1} = \mathcal{N}_{\mathcal{H}}(\mathcal{Z}, \mathcal{Y}_n)$ $(n \geq 0)$ converges to $\mathcal{Y}$. Moreover this convergence is quadratic.

1. The iteration is well defined

The subtraction is possible only if $\mathcal{Y}_n \subset \mathcal{H}(\mathcal{Z}, \mathcal{Y}_n)$. by induction.

2. The iteration is not ambiguous

All the structures of $\mathcal{N}_{\mathcal{H}}(\mathcal{Z}, \mathcal{Y}_n)$ are distinct. by induction, using the fact that the final grafting of an element of $\mathcal{H}(\mathcal{Z}, \mathcal{Y}_n) - \mathcal{Y}_n$ cannot occur anywhere else in a structure built on $\mathcal{Y}_n$'s only.

Proof idea

3. Convergence and its quadratic behaviour

$$\boldsymbol{\mathcal{Y}}_{n-1} =_k \boldsymbol{\mathcal{Y}}_n \Rightarrow \boldsymbol{\mathcal{Y}}_n =_{2k+1} \boldsymbol{\mathcal{Y}}_{n+1}$$

The limit is the solution of $\boldsymbol{\mathcal{Y}} = \boldsymbol{\mathcal{H}}(\mathcal{Z}, \boldsymbol{\mathcal{Y}})$:

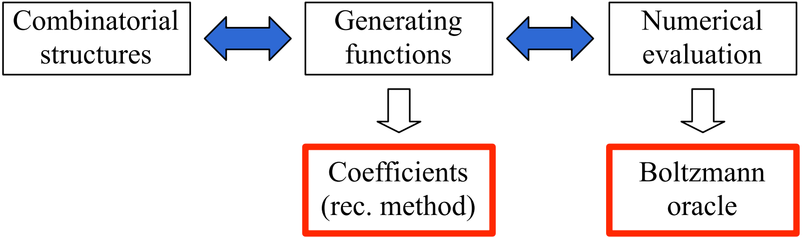
$$\boldsymbol{\mathcal{H}}(\mathcal{Z}, \boldsymbol{\mathcal{Y}}_n) - \boldsymbol{\mathcal{Y}}_n + \frac{\partial \boldsymbol{\mathcal{H}}}{\partial \boldsymbol{\mathcal{Y}}}(\mathcal{Z}, \boldsymbol{\mathcal{Y}}_n) \cdot (\boldsymbol{\mathcal{Y}}_{n+1} - \boldsymbol{\mathcal{Y}}_n) = \boldsymbol{\mathcal{Y}}_{n+1} - \boldsymbol{\mathcal{Y}}_n$$

since $\boldsymbol{\mathcal{Y}}_{n+1} - \boldsymbol{\mathcal{Y}}_n$ converges to $\boldsymbol{\varnothing}$, so does $\boldsymbol{\mathcal{H}}(\mathcal{Z}, \boldsymbol{\mathcal{Y}}_n) - \boldsymbol{\mathcal{Y}}_n$.

Proof of Newton Oracle Theorem

The limit of $\boldsymbol{\mathcal{Y}}_{n+1} = \boldsymbol{\mathcal{N}}_{\boldsymbol{\mathcal{H}}}(\mathcal{Z}, \boldsymbol{\mathcal{Y}}_n)$ is the solution of $\boldsymbol{\mathcal{Y}} = \boldsymbol{\mathcal{H}}(\mathcal{Z}, \boldsymbol{\mathcal{Y}})$, which is well founded, thus there are only finitely many elements in $\boldsymbol{\mathcal{Y}}_n$ of any size in $\boldsymbol{\mathcal{Y}}$. Then, $\boldsymbol{\mathcal{Y}} = \boldsymbol{\mathcal{N}}_{\boldsymbol{\mathcal{H}}}(\mathcal{Z}, \boldsymbol{\mathcal{Y}})$ is well founded too. It is analytic by the analyticity of $\boldsymbol{\mathcal{H}}$. The proof is completed by the Transfer of Convergence Theorem with $\boldsymbol{\mathcal{F}} = \boldsymbol{\mathcal{N}}_{\boldsymbol{\mathcal{H}}}$.

Summary


Combinatorial structures
Generating functions
Numerical evaluation
Coefficients (rec. method)
Boltzmann oracle

Optimized Newton

★ Optimisation:

- combinatorial Newton to compute $\boldsymbol{U} = (I - \frac{\partial H}{\partial Y}(\mathcal{Z}, Y_k))^{-1}$

$$\begin{aligned} \boldsymbol{U}_{k+1} &= \boldsymbol{U}_k + \boldsymbol{U}_k \boldsymbol{T}_{k+1} \\ \boldsymbol{T}_{k+1} &= \boldsymbol{\beta}_k \boldsymbol{U}_k + \boldsymbol{T}_k^2 \\ \boldsymbol{\beta}_k &= \frac{\partial H}{\partial Y}(\mathcal{Z}, Y_k) - \frac{\partial H}{\partial Y}(\mathcal{Z}, Y_{k-1}) \end{aligned}$$

- at iteration Y_k, perform a single step of the calculation of $\boldsymbol{U}$.

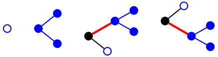
★ experimental gain: 2 times faster.

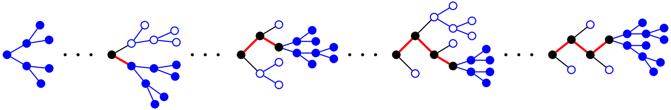
Optimized Newton: example

$$\begin{aligned}
Y_{k+1} &= Y_k + U_{k+1}(\mathcal{Z} + \mathcal{Z}Y_k^2 - Y_k) \\
U_{k+1} &= U_k + U_k T_{k+1} \\
T_{k+1} &= \beta_k U_k + T_k^2 \\
\beta_k &= 2\mathcal{Z}(Y_k - Y_{k-1})
\end{aligned}$$

$$\begin{aligned}
&Y_k + U_{k+1}(H(Y_k) - Y_k) \\
&U_k + U_k T_{k+1} \\
&\beta_k U k + T_k^2 \\
&\frac{\partial H}{\partial Y}(\mathcal{Z}, Y_k) - \frac{\partial H}{\partial Y}(\mathcal{Z}, Y_{k-1})
\end{aligned}$$

$Y_0 = 0 \quad Y_1 =$ 

$Y_2 =$ 

$Y_3 = Y_2 +$ 

Applications

Maple prototype:

- → library (maple and/or other language)
- random grammars,
- XML grammars, $\sim 10^3$ equations (A. Darrasse),
- software random testing (J. Oudinet),
- others?

# equations	4	10	50		100		500
# constructions/eqn	10	10	10	50	10	50	50
avg size largest scc	2.47	3.42	7.95	18.62	10.93	67.18	339.1
time (0.99ρ)	0.05	0.11	0.17	0.47	0.23	7.29	61.73
time (0.999999ρ)	0.08	0.16	0.19	0.56	0.25	8.11	61.86
avg expected size	$4.1\,10^{14}$	$1.4\,10^7$	$2.2\,10^5$	$1.0\,10^5$	$1.2\,10^6$	$5.0\,10^4$	$3.3\,10^4$

in seconds, using Maple 11 on an Intel processor at 3.2 GHz with 2 GB of memory.

Future work

- work in progress...
  - unlabelled set and cycles,
  - extension to $\boldsymbol{\mathcal{H}}(\varnothing, \boldsymbol{\varnothing}) \neq \boldsymbol{\varnothing}$,
  - substitution.
- next steps
  - convergence acceleration,
  - singularities,
  - tuning of Boltzmann parameter according to expected size.