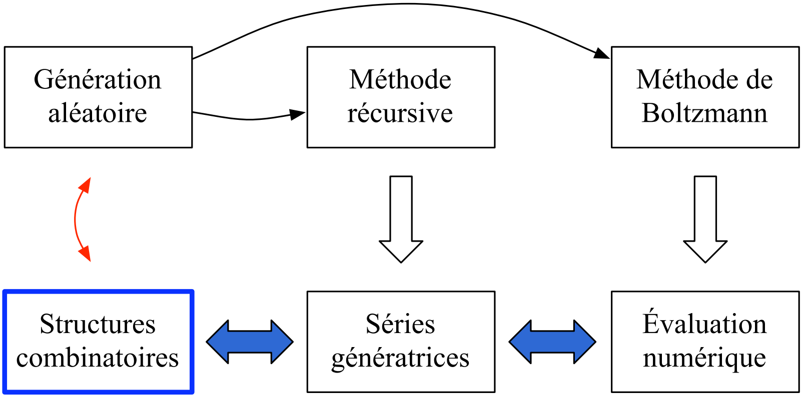
Itération de Newton combinatoire pour le calcul de l'oracle de Boltzmann

Carine Pivoteau

en collaboration avec Bruno Salvy et Michèle Soria

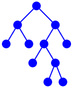
Motivations



Exemples de spécifications combinatoires

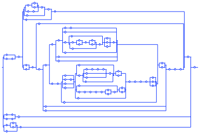
- des arbres binaires planaires :

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



- des circuits série-parallèle :

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



- un langage algébrique :

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

Exemples de spécifications combinatoires

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- un langage algébrique :

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

Exemples de spécifications combinatoires

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- un langage algébrique : pour $z = 0.1$

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

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

```
> 
> [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]

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

```
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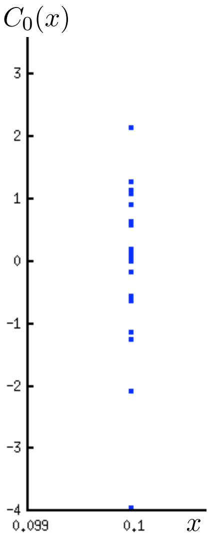

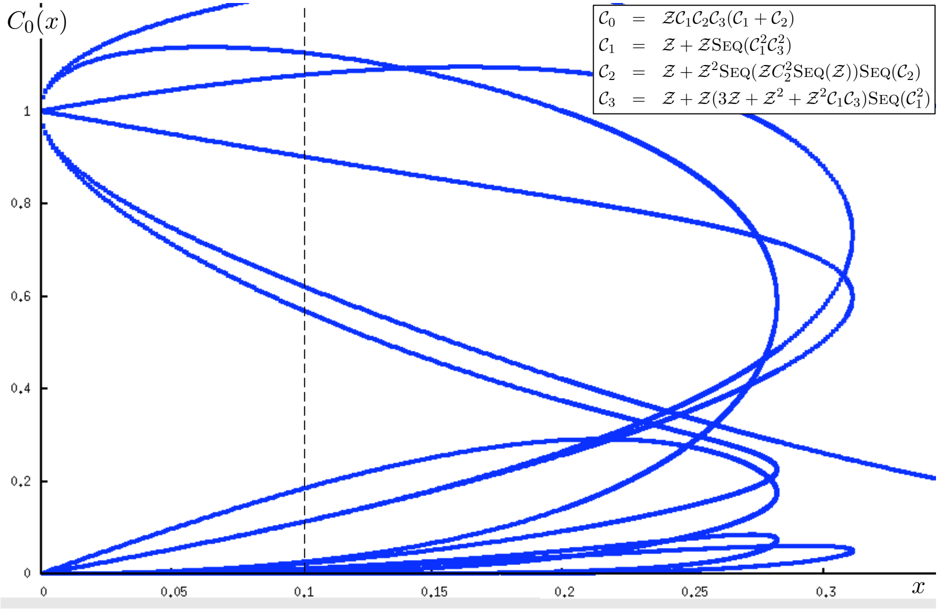
$C_0(x)$
$\mathcal{C}_0 = \mathcal{Z}\mathcal{C}_1\mathcal{C}_2\mathcal{C}_3(\mathcal{C}_1 + \mathcal{C}_2)$
$\mathcal{C}_1 = \mathcal{Z} + \mathcal{Z}\textsc{Seq}(\mathcal{C}_1^2\mathcal{C}_3^2)$
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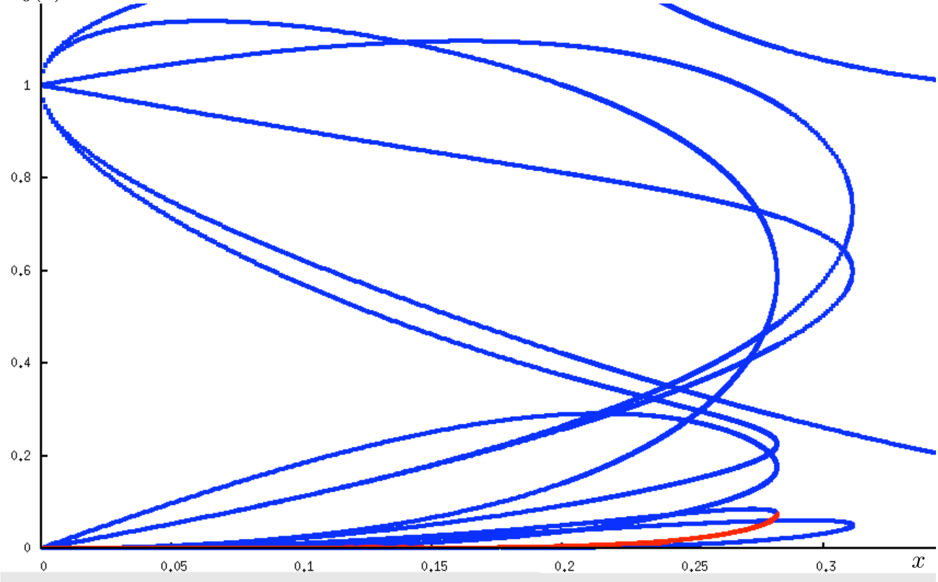
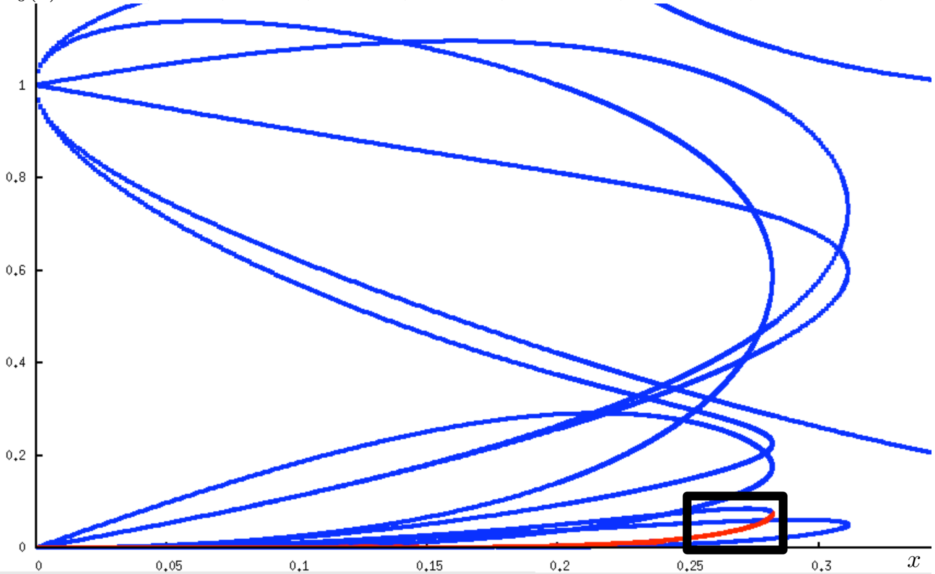
1
0,8
0,6
0,4
0,2
0
0
0,05
0,1
0,15
0,2
0,25
0,3
x

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



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

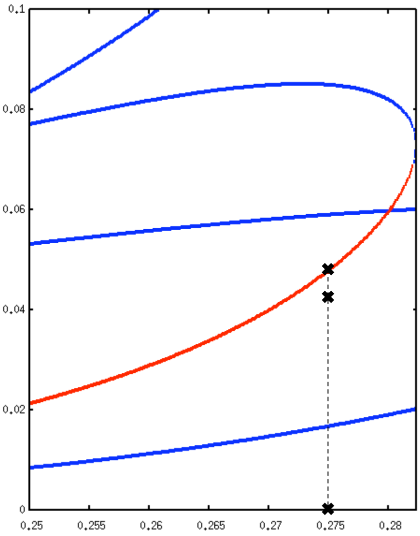


Proposition

L'itération de Newton converge (rapidement) vers la solution.

Approche

convergence de
l'itération numérique
$\Uparrow$
évaluation des séries
de dénombrement
$\Uparrow$
système d'équations
combinatoires

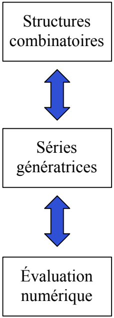


Résultat

Théorème (2008)

Pour tout système combinatoire $\boldsymbol{Y} = \boldsymbol{H}(\mathcal{Z}, \boldsymbol{Y})$ bien fondé, *l'itération de Newton :*

- *converge quadratiquement vers l'espèce solution,*
- *calcule les suites d'énumération en complexité quasi optimale par rapport au nombre de coefficients,*
- *fournit un oracle numérique dont la convergence est asymptotiquement quadratique.*



★ bonus : itération de Newton optimisée.

Calculer la solution par itération

Cadre combinatoire

Théorème (Espèces implicites, Joyal 81)

Le système combinatoire

$$\begin{array}{rcl} Y_1 & = & H_1(Z, Y_1, Y_2, \ldots, Y_m) \\ Y_2 & = & H_2(Z, Y_1, Y_2, \ldots, Y_m) \\ \vdots & & \vdots \\ Y_m & = & H_m(Z, Y_1, Y_2, \ldots, Y_m) \end{array}$$

admet une unique solution dès que :

- *la matrice jacobienne* $\frac{\partial H}{\partial \mathbf{Y}}(0, \mathbf{0})$ *est nilpotente*
- $H(0, \mathbf{0}) = 0$.

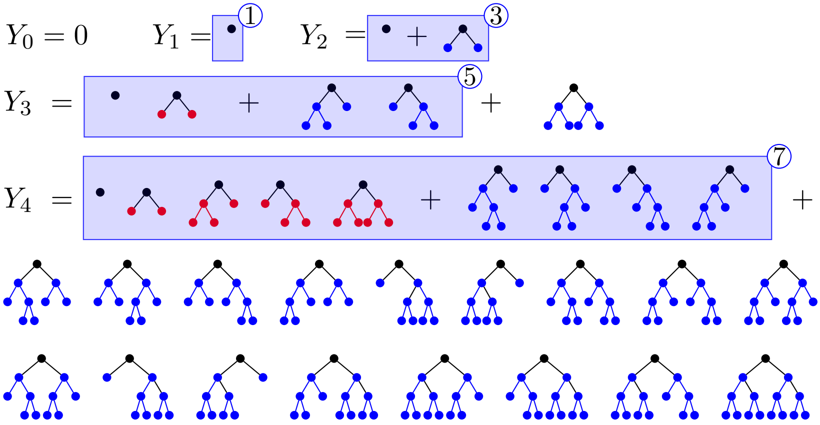
Exemple : les arbres binaires

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

$\boxed{Y = H(\mathcal{Z}, Y)}$

$Y_{k+1} = \mathcal{Z} + \mathcal{Z} \times Y_k^2$

Itération : $Y_{k+1} = H(\mathcal{Z}, Y_k)$



Séries génératrices

$$Y(z) = z + z\widehat{Y}^2(z)$$

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

$$\widehat{Y}_{k+1}(z) = z + z\widehat{Y}_k(z)^2$$

Itération : $\widehat{Y}_{k+1}(z) = H(z, \widehat{Y}_k(z))$

$$\begin{aligned}
\widehat{Y}_0(z) &= \mathbf{0} \\
\widehat{Y}_1(z) &= \boldsymbol{z} \\
\widehat{Y}_2(z) &= \boldsymbol{z + z^3} \\
\widehat{Y}_3(z) &= \boldsymbol{z + z^3 + 2z^5} + z^7 \\
\widehat{Y}_4(z) &= \boldsymbol{z + z^3 + 2z^5 + 5z^7} + 6z^9 + 6z^{11} + 4z^{13} + z^{15} \\
\widehat{Y}_5(z) &= \boldsymbol{z + z^3 + 2z^5 + 5z^7 + 14z^9} + 26z^{11} + 44z^{13} + 69z^{15} \\
\widehat{Y}(z) &= \boldsymbol{z + z^3 + 2z^5 + 5z^7 + 14z^9} + 42z^{11} + 132z^{13} + 429z^{15} + \dots
\end{aligned}$$

convergence pour les structures $\Rightarrow$ convergence pour les séries

Itération numérique

$$Y(x) = x + xY^2(x)$$

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

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

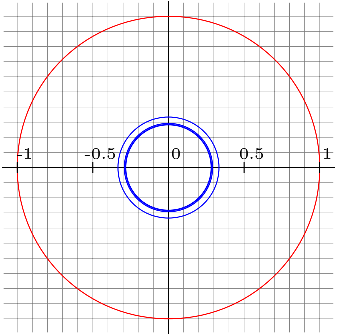
Itération : $Y_{k+1}(x) = H(x, Y_k(x))$

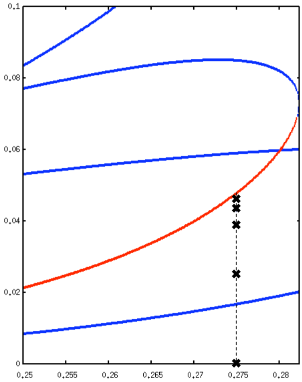
$$\begin{array}{lclcl}
Y_0 & = & \widehat{Y}_0(0.2) & = & \mathbf{0} \\
Y_1 & = & \widehat{Y}_1(0.2) & = & \mathbf{0.2} \\
Y_2 & = & \widehat{Y}_2(0.2) & = & \mathbf{0.208} \\
Y_3 & = & \widehat{Y}_3(0.2) & = & \mathbf{0.2086}528 \\
Y_4 & = & \widehat{Y}_4(0.2) & = & \mathbf{0.2087}07198189568\ldots \\
Y_5 & = & \widehat{Y}_5(0.2) & = & \mathbf{0.20871}17389152279\ldots \\
Y & = & \widehat{Y}(0.2) & = & \mathbf{0.20871}21525220799\ldots
\end{array}$$

- pour toute valeur de $x < \rho$
- itération numérique $\Leftrightarrow$ évaluer la série solution en x.

Structures combinatoires $\Longleftrightarrow$ Séries génératrices $\Longleftrightarrow$ Évaluation numérique

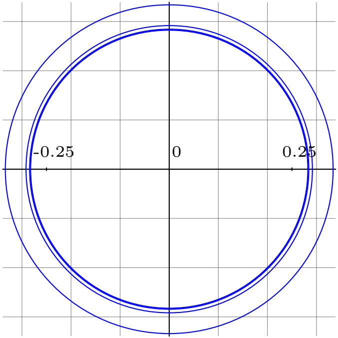
Y_0
Y_1
Y_2
Y_3
Y_4
Y_5
$\vdots$

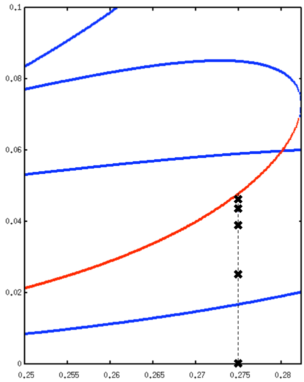




Structures combinatoires $\Longleftrightarrow$ Séries génératrices $\Longleftrightarrow$ Évaluation numérique

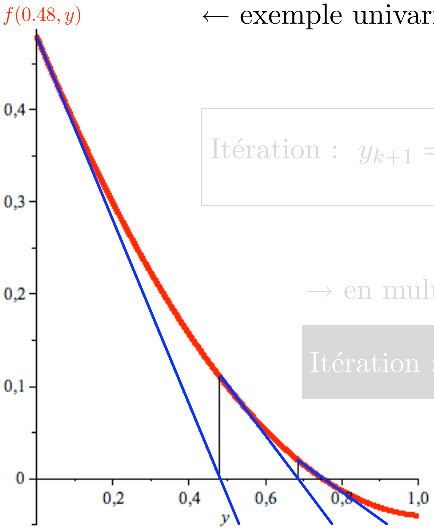
Y_0
Y_1
Y_2
Y_3
Y_4
Y_5
$\vdots$





Itération de Newton

Principe de l'itération de Newton



← exemple univarié : $y(x) = x + xy^2(x)$

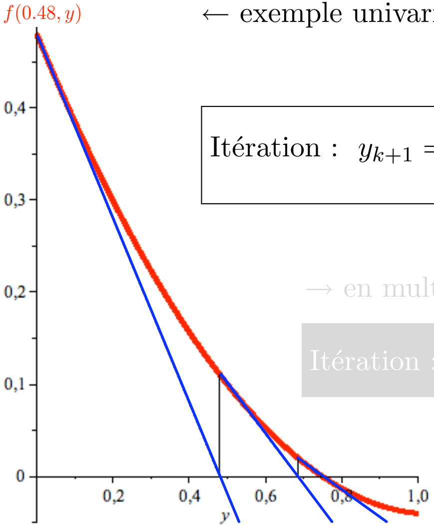
$f(x, y) = x + xy^2 - y$

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

→ en multivarié :

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

Principe de l'itération de Newton



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

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

→ en multivarié :

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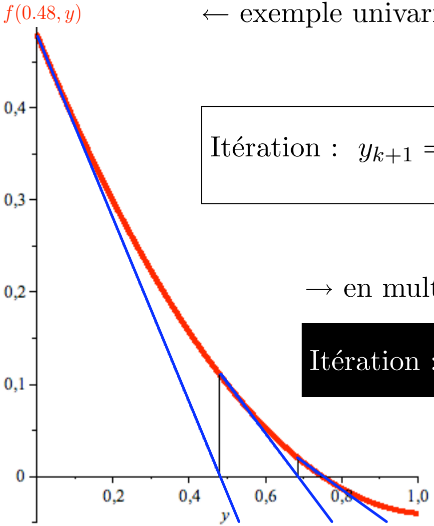
Principe de l'itération de Newton



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→ en multivarié :

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

Convergence numérique

$Y(x) = x + xY^2(x)$ $\qquad$ $\boxed{Y(x) = H(x, Y(x))}$

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

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

$$
\begin{aligned}
Y_0 &= \mathbf{0}\\
Y_1 &= \mathbf{0}.48\\
Y_2 &= \mathbf{0}.685103857566765578635014836795 25\ldots\\
Y_3 &= \mathbf{0.74}40942953173578506931541165 9589\ldots\\
Y_4 &= \mathbf{0.7499}41396864835881846793917786 24\ldots\\
Y_5 &= \mathbf{0.7499999}41137642045942008051107 7\ldots\\
Y_4 &= \mathbf{0.74999999999999}40603820903068 52\ldots\\
Y_5 &= \mathbf{0.7499999999999999999999999999999}7\ldots
\end{aligned}
$$

convergence asymptotiquement quadratique

Newton sur les séries

$\widehat{Y} = z + z\widehat{Y}^2(z)$

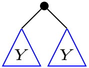
$\boxed{\widehat{Y}(z) = H(z, \widehat{Y})}$

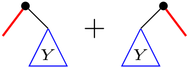
Itération : $\widehat{Y}_{k+1} = \widehat{Y}_k + (I - \frac{\partial H}{\partial \widehat{Y}}(z, \widehat{Y}_k))^{-1}(H(z, \widehat{Y}_k) - \widehat{Y}_k)$

$\widehat{Y}_{k+1} = \widehat{Y}_k + \frac{1}{1-2z\widehat{Y}_k}(z + z\widehat{Y}_k^2 - \widehat{Y}_k)$

$$
\begin{aligned}
\widehat{Y}_0 &= \mathbf{0} \\
\widehat{Y}_1 &= \boldsymbol{z} \\
\widehat{Y}_2 &= \boldsymbol{z + z^3 + 2z^{\boxed{5}}} + 4z^7 + 8z^9 + 16z^{11} + 32z^{13} + 64z^{15} + \ldots \\
\widehat{Y}_3 &= \boldsymbol{z + z^3 + 2z^5 + 5z^7 + 14z^9 + 42z^{11} + 132z^{\boxed{13}}} + 428z^{15} + \ldots \\
\widehat{Y}_4 &= \boldsymbol{z + z^3 + 2z^5 + 5z^7 + \cdots + 2674440z^{\boxed{29}}} + 9694844z^{31} + \ldots
\end{aligned}
$$

Dérivée combinatoire et matrice jacobienne

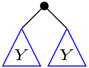
$H(\mathcal{Z},Y) = \bullet +$ 

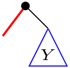
$\frac{\partial H}{\partial Y}(\mathcal{Z},Y) =$ 

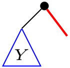
$H(\mathcal{Z},Y) = (H_1(\mathcal{Z},Y), H_2(\mathcal{Z},Y)) = \Big(\bullet +$

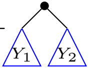
$$\frac{\partial H}{\partial Y} = \begin{pmatrix} \frac{\partial H_1}{\partial Y_1} & \frac{\partial H_1}{\partial Y_2} \\ \frac{\partial H_2}{\partial Y_1} & \frac{\partial H_2}{\partial Y_2} \end{pmatrix} =$$

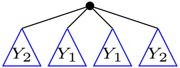
Dérivée combinatoire et matrice jacobienne

$H(\mathcal{Z}, Y) = \bullet +$ 

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

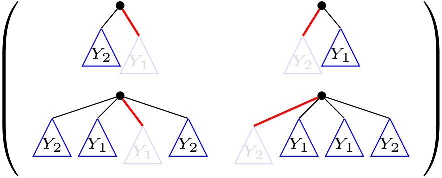
$+$ 

$H(\mathcal{Z}, Y) = (H_1(\mathcal{Z}, Y), H_2(\mathcal{Z}, Y)) = (\ \bullet +$ 

$,$ 

$)$

$$\frac{\partial H}{\partial Y} = \begin{pmatrix} \frac{\partial H_1}{\partial Y_1} & \frac{\partial H_1}{\partial Y_2} \\ \frac{\partial H_2}{\partial Y_1} & \frac{\partial H_2}{\partial Y_2} \end{pmatrix} =$$



Newton combinatoire pour une seule équation
(Bergeron, Décoste, Labelle, Leroux)

$$\text{Itération} : Y_{k+1} = Y_k + (I - \frac{\partial H}{\partial Y}(\mathcal{Z}, Y_k))^{-1}(H(Y_k) - Y_k)$$

$$Y_{k+1} = Y_k + \textsc{Seq}(2\mathcal{Z}Y_k)(\mathcal{Z} + \mathcal{Z}Y_k^2 - Y_k)$$

$Y_0 = 0 \qquad Y_1 = \bullet \qquad H(Y_1) - Y_1 = \mathcal{Z} + \mathcal{Z}Y_1^2 - Y_1 =$

Newton combinatoire pour une seule équation
(Bergeron, Décoste, Labelle, Leroux)

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

$$Y_{k+1} = Y_k + \mathrm{SEQ}(2\mathcal{Z}Y_k)(\mathcal{Z} + \mathcal{Z}Y_k^2 - Y_k)$$

$Y_0 = 0 \qquad Y_1 = \bullet \qquad H(Y_1) - Y_1 = \mathcal{Z} + \mathcal{Z}Y_1^2 - Y_1 =$

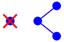
$Y_2 =$

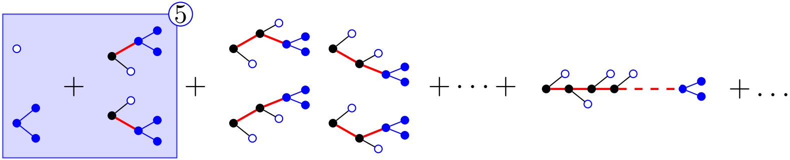
$Y_3 =$

Newton combinatoire pour une seule équation
(Bergeron, Décoste, Labelle, Leroux)

$$\text{Itération : } Y_{k+1} = Y_k + \left(I - \frac{\partial H}{\partial Y}(\mathcal{Z}, Y_k)\right)^{-1}(H(Y_k) - Y_k)$$

$$Y_{k+1} = Y_k + \textsc{Seq}(2\mathcal{Z}Y_k)(\mathcal{Z} + \mathcal{Z}Y_k^2 - Y_k)$$

$Y_0 = 0 \qquad Y_1 = \bullet \qquad H(Y_1) - Y_1 = \mathcal{Z} + \mathcal{Z}Y_1^2 - Y_1 =$ 

$Y_2 =$ 

$Y_3 =$

Newton combinatoire pour une seule équation
(Bergeron, Décoste, Labelle, Leroux)

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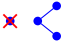
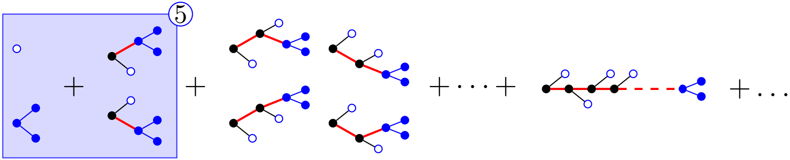
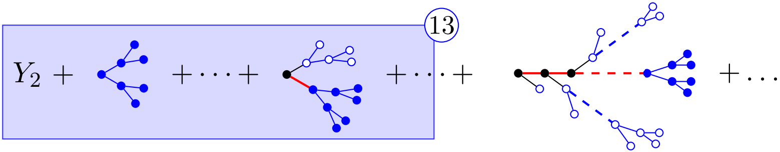
$Y_0 = 0 \qquad Y_1 = \bullet \qquad H(Y_1) - Y_1 = \mathcal{Z} + \mathcal{Z}Y_1^2 - Y_1 =$ 

$Y_2 =$ 

$Y_3 =$ 

Newton pour un système

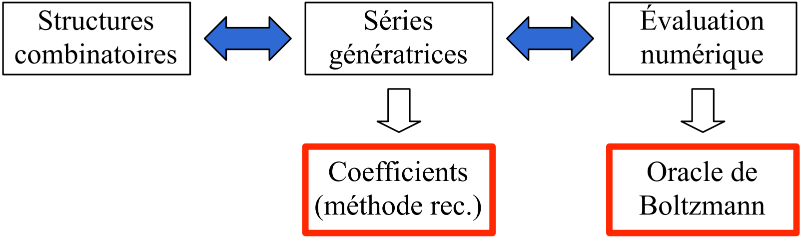
Itération : $Y_{k+1} = Y_k + \boxed{(I - \frac{\partial H}{\partial Y}(\mathcal{Z}, Y_k))^{-1}}(H(Y_k) - Y_k)$

- une seule équation $\rightarrow$ séquence
- plusieurs équations $\rightarrow$ éclosions combinatoires (Labelle)

Newton pour un système

Itération : $Y_{k+1} = Y_k + \boxed{\left(I - \frac{\partial H}{\partial Y}(\mathcal{Z}, Y_k)\right)^{-1}}(H(Y_k) - Y_k)$

- une seule équation $\longrightarrow$ séquence
- plusieurs équations $\longrightarrow$ éclosions combinatoires (Labelle)



Newton optimisé

★ Optimisation :

- Newton combinatoire pour calculer $\boldsymbol{U} = (I - \frac{\partial H}{\partial Y}(\mathcal{Z}, Y_k))^{-1}$

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

- à l'itération Y_k, faire une seule étape du calcul de $\boldsymbol{U}$.

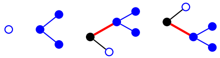
★ Gain expérimental : 2 fois plus rapide.

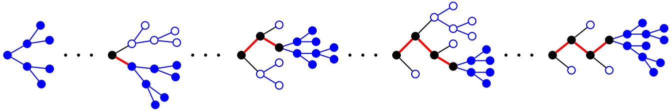
Newton optimisé sur l'exemple

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

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

$Y_0 = 0 \qquad Y_1 = \bullet$

$Y_2 =$ 

$Y_3 = Y_2 +$ 

Expérimentations – Extensions – Perspectives

- prototype en maple
  - $\rightarrow$ bibliothèque (maple et/ou autre langage)
  - grammaires jouet,
  - grammaires XML, $\sim 10^3$ équations (A. Darrasse),
  - tests (cf. exposé A. Denise),
  - autre ?
- en cours...
  - extension aux $\mathcal{E}$,
  - substitution,
  - autres opérateurs.
- prochaines étapes
  - accélération de convergence,
  - calcul de singularité,
  - choix du paramètre en fonction de la taille visée.