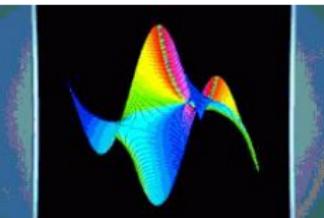


Automatic Analysis of Combinatorial Structures, Old and New

Bruno Salvy

Bruno.Salvy@inria.fr

Algorithms Project, Inria



December 2, 2008

New: recent work and work in progress
with Carine Pivoteau and Michèle Soria

I Introduction

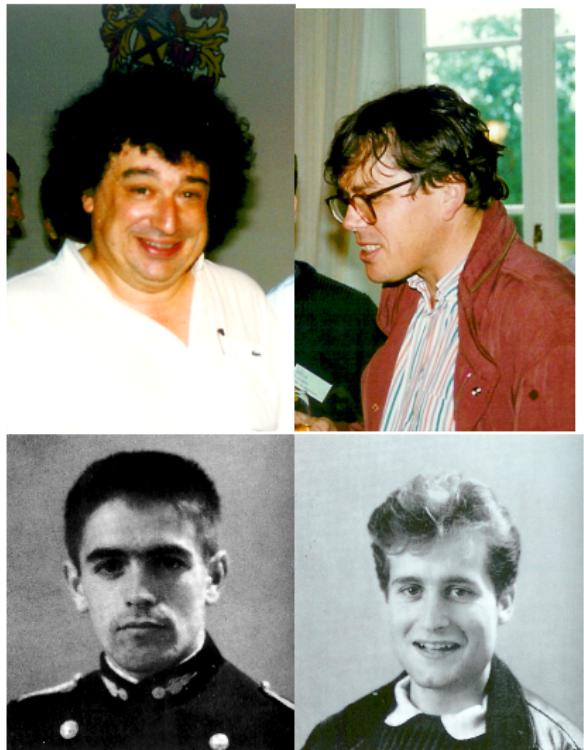
Old: $\Lambda\Omega$ 

Origins: FlajoletSteyaert1981-82.
A complexity calculus for recursive tree algorithms

Old: $\Lambda\Omega$ 

Origins: FlajoletSteyaert1981-82.
*A complexity calculus for
recursive tree algorithms*



Old: $\Lambda\Gamma\Omega$ 

Origins: FlajoletSteyaert1981-82.
A complexity calculus for recursive tree algorithms

The $\Lambda\Gamma\Omega$ system:

Input

```
type bintree = epsilon | product(o, bintree, bintree);
o = atom (1);

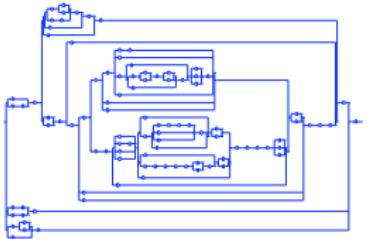
procedure pathlength (t : bintree);
begin
  case t of
    ()           : nil;
    o(u,v)      : begin size(u); size(v);
                     pathlength(u); pathlength(v);
                     end;
    end;
end;
```

Output

$$\text{av_tau_pathlength_n} := \frac{\pi}{4} n^{3/2} + O(n)$$

General Framework

Combinatorial Objects → Equations over Generating Functions



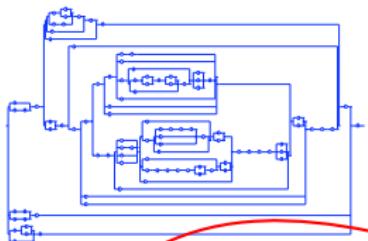
$$Y = Y_1 + Y_2$$

$$Y_1 = (z + Y_2)^2 / (1 - z - Y_2)$$

$$Y_2 = \exp(z + Y_1) - 1 - z - Y_1.$$

General Framework

Combinatorial Objects → Equations over Generating Functions



$$Y = Y_1 + Y_2$$

$$Y_1 = (z + Y_2)^2 / (1 - z - Y_2)$$

$$Y_2 = \exp(z + Y_1) - 1 - z - Y_1.$$

Enumeration

3, 19, 195, 2791, ...

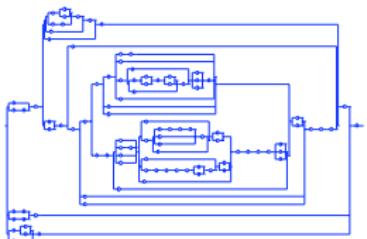
→ Random

generation by the
recursive method

[FIZiVCu94]

General Framework

Combinatorial Objects → Equations over Generating Functions

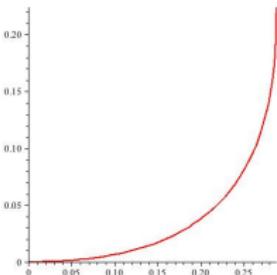


Enumeration

3, 19, 195, 2791, ...

→ Random
generation by the
recursive method
[FIZiVCu94]

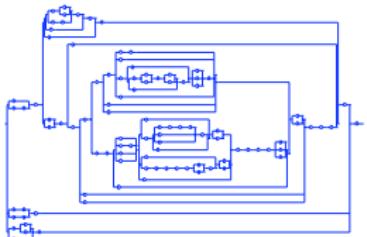
Numerical Values



→ Boltzmann Sampling
[DuFILoSc04, FiFuPi07]
(G. Schaeffer yesterday)

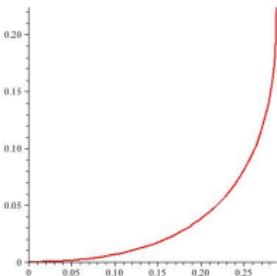
General Framework

Combinatorial Objects → Equations over Generating Functions



Enumeration
3, 19, 195, 2791, ...
→ Random
generation by the
recursive method
[FIZiVCu94]

Numerical Values



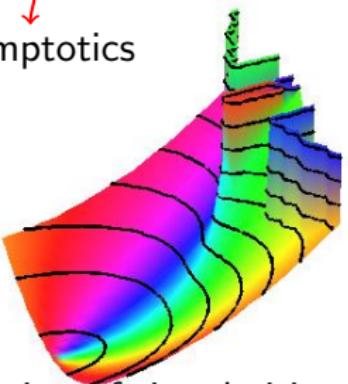
→ Boltzmann Sampling
[DuFiLoSc04, FiFuPi07]
(G. Schaeffer yesterday)

$$Y = Y_1 + Y_2$$

$$Y_1 = (z + Y_2)^2 / (1 - z - Y_2)$$

$$Y_2 = \exp(z + Y_1) - 1 - z - Y_1.$$

Asymptotics



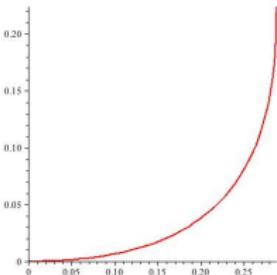
Location of singularities
Singularity analysis
[FlajoletOdlyzko1990]

Computation

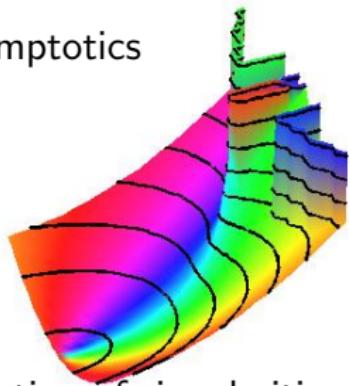
Enumeration

3, 19, 195, 2791, ...

Numerical Values



Asymptotics



Location of singularities
Singularity analysis

Algorithms in $\Lambda\Gamma\Omega$:

- Enumeration: $O(N^2)$;
- Location of singularities: for *explicit* g.f.;
- Local behaviour: *explicit* g.f., no Pólya operator.

→ Numerical values from the truncated g.f.

Computation

Algorithms in $\Lambda\Omega$:

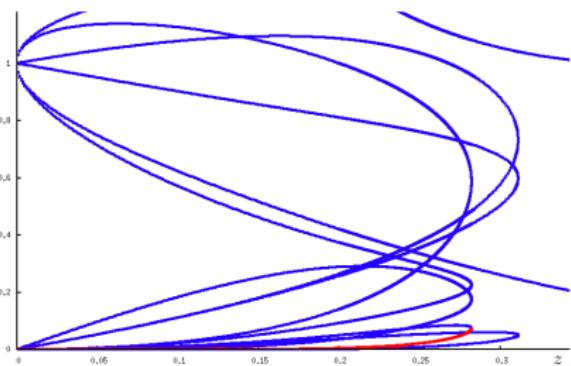
- Enumeration: $O(N^2)$;
- Location of singularities: for *explicit* g.f.;
- Local behaviour: *explicit* g.f., no Pólya operator.

→ Numerical values from the truncated g.f.

New

- Enumeration: $O(M(N))$;
- Numerical evaluation: fast;
- Location of singularities:
directly from a system 

$M(N)$: cost of polynomial multiplication.



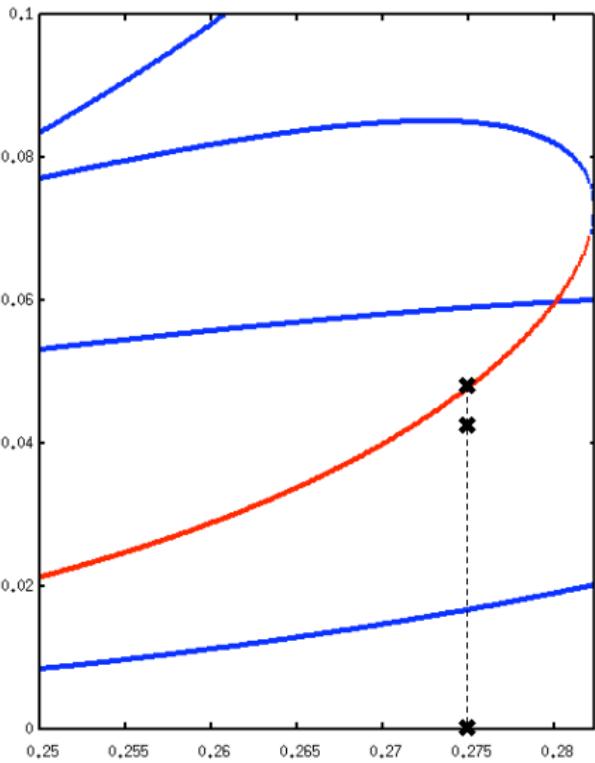
Main Result of (Pivoteau, Salvy, Soria 2008)

Theorem

For all (well-founded) systems of generating series, Newton iteration starting from 0 converges to the desired solution.



Oracle for Boltzmann sampling.



Examples (I): Polynomial Systems (Darrasse 2008)

Random generation following given XML grammars.

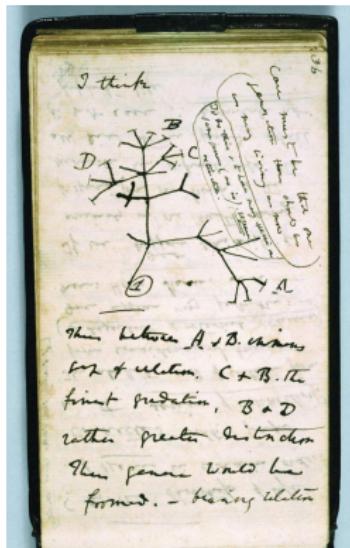
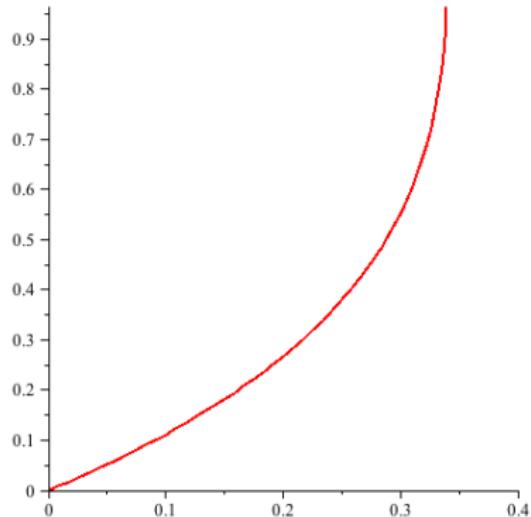
Grammar	nb eqs	max deg	nb sols	oracle (s.)	FGb (s.)
rss	10	5	2	0.02	0.03
PNML	22	4	4	0.05	0.1
xslt	40	3	10	0.4	1.5
relaxng	34	4	32	0.4	3.3
xhtml-basic	53	3	13	1.2	18
mathml2	182	2	18	3.7	882
xhtml	93	6	56	3.4	1124
xhtml-strict	80	6	32	3.0	1590
xmlschema	59	10	24	0.5	6592
SVG	117	10		5.8	>1.5Go
docbook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

We exploit the combinatorial structure

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 Combinatorics

Combinatorial Specifications

Language and Gen. Fcns (labelled)

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

Examples

- Binary trees: $\mathcal{B} = \mathcal{Z} \cup \mathcal{Z} \times \mathcal{B} \times \mathcal{B}$;

$$B(z) = z + zB(z)^2$$

- General trees: $\mathcal{T} = \mathcal{Z} \times \text{SET}(\mathcal{T})$;

$$T(z) = z \exp(T(z))$$

Combinatorial Specifications

Language and Gen. Fcns (labelled)

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

Examples

- Binary trees: $\mathcal{B} = \mathcal{Z} \cup \mathcal{Z} \times \mathcal{B} \times \mathcal{B};$

$$B(z) = z + zB(z)^2$$

- General trees: $\mathcal{T} = \mathcal{Z} \times \text{SET}(\mathcal{T});$

$$T(z) = z \exp(T(z))$$

System (Σ): $\mathcal{Y} = \mathcal{H}(\mathcal{Z}, \mathcal{Y})$

Definition (Well-founded)

$\mathcal{H}(\emptyset, \emptyset) = \emptyset$ and
 Jacobian $\partial\mathcal{H}/\partial\mathcal{Y}$
 nilpotent at (\emptyset, \emptyset) .

Proposition

If (Σ) well-founded,

- $\mathcal{Y}_{n+1} = \mathcal{H}(\mathcal{Z}, \mathcal{Y}_n)$
 converges to a limit species \mathcal{Y} [Joyal 1981]
- $\mathbf{Y}(z)$ is analytic in a neighborhood of 0.

Combinatorial Specifications

Language and Gen. Fcns (unlabelled)

$$\mathcal{A} \cup \mathcal{B} \quad A(z) + B(z)$$

$$\mathcal{A} \times \mathcal{B} \quad A(z) \times B(z)$$

$$\mathcal{A}' \quad A'(z)$$

$$\text{SEQ}(\mathcal{C}) \quad \frac{1}{1-C(z)}$$

$$\text{PSET}(C) \quad \exp\left(\sum (-1)^i C(z^i)/i\right)$$

$$\text{MSET}(C) \quad \exp\left(\sum C(z^i)/i\right)$$

$$\text{CYC}(C) \quad \sum_{k \geq 1} \frac{\phi(k)}{k} \log \frac{1}{1-C(z^k)}$$

Examples

- Binary trees: $\mathcal{B} = \mathcal{Z} \cup \mathcal{Z} \times \mathcal{B} \times \mathcal{B}$;

$$B(z) = z + zB(z)^2$$

- General trees: $\mathcal{T} = \mathcal{Z} \times \text{SET}(\mathcal{T})$;

$$T(z) = z \exp(T(z) + T(z^2)/2 + \dots)$$

System (Σ): $\mathcal{Y} = \mathcal{H}(\mathcal{Z}, \mathcal{Y})$

Definition (Well-founded)

$\mathcal{H}(\emptyset, \emptyset) = \emptyset$ and
 Jacobian $\partial \mathcal{H} / \partial \mathcal{Y}$
 nilpotent at (\emptyset, \emptyset) .

Proposition

If (Σ) well-founded,

- $\mathcal{Y}_{n+1} = \mathcal{H}(\mathcal{Z}, \mathcal{Y}_n)$ converges to a limit species \mathcal{Y} [Joyal 1981]
- $\mathbf{Y}(z)$ is analytic in a neighborhood of 0.

$\Lambda\Omega$ via attribute grammars

- Attribute grammars: Knuth1968;
- Parameters of trees: DelestFedou1992;
- Decomposable structures: Mishna2003.

Specification + attribute grammar → Multivariate g.f.

```

tree:={B=Union(Epsilon,Prod(Z,B,B))}:
path_length:={pl(B)=Union(0,Prod(0,size(B)+pl(B),size(B)+pl(B)))}:
combstruct[agfeqns](tree,path_length,unlabelled,z,[[u,pl]]):

$$[ B(z, u) = 1 + z B(z u, u)^2, Z(z, u) = z u ]$$


```

- Generalizes $\Lambda\Omega$;
- All moments available by differentiating wrt u ;
- Opens the way to the automatic computation of limit laws (e.g., with [DrmotaGittenbergerKlausner2005]).

Combinatorial Newton (Décoste, Labelle, Leroux 1982)

For one equation: $\mathcal{Y} = \mathcal{H}(\mathcal{Z}, \mathcal{Y}) \rightarrow \mathcal{Y}_{n+1} = \mathcal{N}_{\mathcal{H}}(\mathcal{Y}_n)$

$$\mathcal{N}_{\mathcal{H}}(\mathcal{Y}) = \mathcal{Y} \cup \text{SEQ}\left(\frac{\partial \mathcal{H}}{\partial \mathcal{Y}}(\mathcal{Z}, \mathcal{Y})\right) \times (\mathcal{H}(\mathcal{Z}, \mathcal{Y}) - \mathcal{Y}).$$

Contact doubles at each step.

Binary trees:

$$\mathcal{H}(\mathcal{Z}, \mathcal{Y}) = \mathcal{Z} \cup \mathcal{Z} \times \mathcal{Y} \times \mathcal{Y} = \bullet \quad \bullet \stackrel{\mathcal{Y}}{\cdot} \quad \frac{\partial \mathcal{H}}{\partial \mathcal{Y}}(\mathcal{Z}, \mathcal{Y}) = \swarrow \stackrel{\mathcal{Y}}{\cdot} \searrow$$

$$\mathcal{Y}_0 = \emptyset \quad \mathcal{Y}_1 = \bullet \quad \mathcal{H}(\mathcal{Y}_1) - \mathcal{Y}_1 = \mathcal{Z} + \mathcal{Z}\mathcal{Y}_1^2 - \mathcal{Y}_1 = \times \quad \bullet \swarrow \bullet$$

$$\mathcal{Y}_2 = \boxed{\bullet \swarrow \bullet} + \bullet \swarrow \bullet + \bullet \swarrow \bullet + \cdots + \bullet \swarrow \bullet + \cdots$$

The diagram shows the recursive construction of binary trees. A blue box encloses the first two terms of the sum, which are both labeled with a circled '5'. The first term is a tree with a root node connected to two children, each of which has a single child. The second term is a tree with a root node connected to two children, each of which has a single child. The ellipsis indicates that this pattern continues for higher-order terms.

Combinatorial Newton (Décoste, Labelle, Leroux 1982)

For one equation: $\mathcal{Y} = \mathcal{H}(\mathcal{Z}, \mathcal{Y}) \rightarrow \mathcal{Y}_{n+1} = \mathcal{N}_{\mathcal{H}}(\mathcal{Y}_n)$

$$\mathcal{N}_{\mathcal{H}}(\mathcal{Y}) = \mathcal{Y} \cup \text{SEQ}\left(\frac{\partial \mathcal{H}}{\partial \mathcal{Y}}(\mathcal{Z}, \mathcal{Y})\right) \times (\mathcal{H}(\mathcal{Z}, \mathcal{Y}) - \mathcal{Y}).$$

Binary trees:

$$\mathcal{H}(\mathcal{Z}, \mathcal{Y}) = \mathcal{Z} \cup \mathcal{Z} \times \mathcal{Y} \times \mathcal{Y} = \bullet \quad \bullet \stackrel{\mathcal{Y}}{\circ} \quad \frac{\partial \mathcal{H}}{\partial \mathcal{Y}}(\mathcal{Z}, \mathcal{Y}) = \bullet \stackrel{\mathcal{Y}}{\circ}$$

$$\mathcal{Y}_0 = \emptyset \quad \mathcal{Y}_1 = \bullet \quad \mathcal{H}(\mathcal{Y}_1) - \mathcal{Y}_1 = \mathcal{Z} + \mathcal{Z}\mathcal{Y}_1^2 - \mathcal{Y}_1 = \times \quad \bullet \stackrel{\mathcal{Y}}{\circ}$$

$$\mathcal{Y}_3 = \mathcal{Y}_2 + \bullet \stackrel{\mathcal{Y}}{\circ} + \cdots + \bullet \stackrel{\mathcal{Y}}{\circ} + \cdots + \bullet \stackrel{\mathcal{Y}}{\circ} + \cdots + \bullet \stackrel{\mathcal{Y}}{\circ} + \cdots$$

The diagram illustrates the recursive construction of binary trees. A blue box encloses the first term $\bullet \stackrel{\mathcal{Y}}{\circ}$. Above the box is the number 13, indicating the total number of terms in the sum. The terms consist of a black dot followed by a blue circle containing a black dot, representing a node with a single child. Ellipses indicate that there are many more terms. The final part of the equation shows a sequence of terms where each term is a black dot connected by a dashed red line to a blue circle containing a black dot, representing a node with two children.

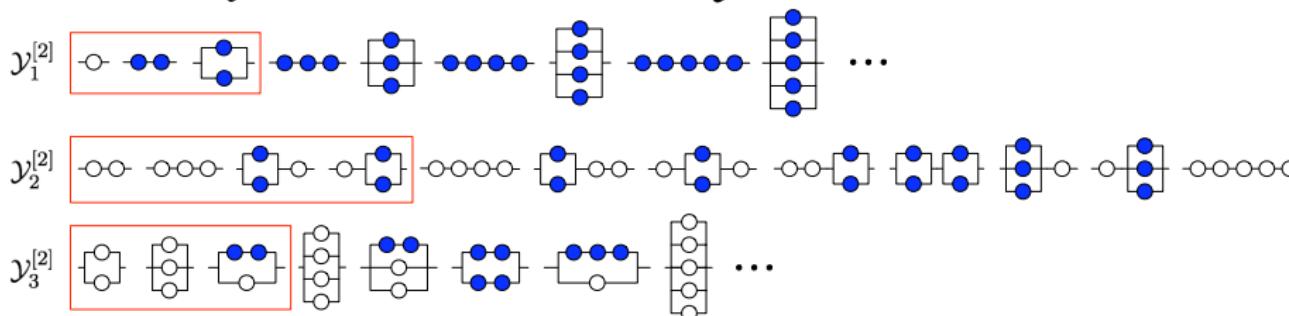
Combinatorial Newton (Décoste, Labelle, Leroux 1982)

For one equation: $\mathcal{Y} = \mathcal{H}(\mathcal{Z}, \mathcal{Y}) \rightarrow \mathcal{Y}_{n+1} = \mathcal{N}_{\mathcal{H}}(\mathcal{Y}_n)$

$$\mathcal{N}_{\mathcal{H}}(\mathcal{Y}) = \mathcal{Y} \cup \text{SEQ}\left(\frac{\partial \mathcal{H}}{\partial \mathcal{Y}}(\mathcal{Z}, \mathcal{Y})\right) \times (\mathcal{H}(\mathcal{Z}, \mathcal{Y}) - \mathcal{Y}).$$

Extension to systems (Pivoteau, Soria, Salvy 2008):

- $\text{SEQ}\left(\frac{\partial \mathcal{H}}{\partial \mathcal{Y}}\right)$ replaced by $\mathcal{U} = \cup_{k \geq 0} \left(\frac{\partial \mathcal{H}}{\partial \mathcal{Y}}\right)^k$ (Labelle's bloomings);



Combinatorial Newton (Décoste, Labelle, Leroux 1982)

For one equation: $\mathcal{Y} = \mathcal{H}(\mathcal{Z}, \mathcal{Y}) \rightarrow \mathcal{Y}_{n+1} = \mathcal{N}_{\mathcal{H}}(\mathcal{Y}_n)$

$$\mathcal{N}_{\mathcal{H}}(\mathcal{Y}) = \mathcal{Y} \cup \text{SEQ}\left(\frac{\partial \mathcal{H}}{\partial \mathcal{Y}}(\mathcal{Z}, \mathcal{Y})\right) \times (\mathcal{H}(\mathcal{Z}, \mathcal{Y}) - \mathcal{Y}).$$

Extension to systems (Pivoteau, Soria, Salvy 2008):

- $\text{SEQ}\left(\frac{\partial \mathcal{H}}{\partial \mathcal{Y}}\right)$ replaced by $\mathcal{U} = \cup_{k \geq 0} \left(\frac{\partial \mathcal{H}}{\partial \mathcal{Y}}\right)^k$ (Labelle's bloomings);
- this union \mathcal{U} itself is computed by Newton iteration:

$$\begin{aligned}\mathcal{U}_{n+1} &= \mathcal{U}_n + \mathcal{U}_n \mathcal{T}_{n+1} \\ \mathcal{T}_{n+1} &= \beta_n \mathcal{U}_n + \mathcal{T}_n^2 \\ \beta_n &= \frac{\partial \mathcal{H}}{\partial \mathcal{Y}}(\mathcal{Z}, \mathcal{Y}_n) - \frac{\partial \mathcal{H}}{\partial \mathcal{Y}}(\mathcal{Z}, \mathcal{Y}_{n-1})\end{aligned}$$

At iteration \mathcal{Y}_n , perform a **single step** of the calculation of \mathcal{U} .

III Enumeration Sequences

Combinatorial Iteration → Iteration for Generating Series

- Same iteration in labelled & unlabelled universes:

Example: General trees

$$\mathcal{Y} = \mathcal{H}(\mathcal{Y}) = \mathcal{Z} \times \text{SET}(\mathcal{Y}) \rightarrow \mathcal{N}_H(Y) = Y + \frac{H(Y) - Y}{1 - H(Y)}.$$

$$Y(z) = z \exp(Y(z) + Y(z^2)/2 + \dots)$$

$$Y_0(z) = 0$$

$$Y_1(z) = z$$

$$Y_2(z) = z + z^2 + 2z^3 + 3z^4 + 5z^5 + 7z^6 + 11z^7 + 15z^8 + 22z^9 + \dots$$

$$Y_3(z) = z + z^2 + 2z^3 + 4z^4 + 9z^5 + 20z^6 + 48z^7 + 114z^8 + 280z^9 + \dots$$

$$Y_4(z) = z + z^2 + 2z^3 + 4z^4 + 9z^5 + 20z^6 + 48z^7 + 115z^8 + 286z^9 + \dots$$

Combinatorial Iteration → Iteration for Generating Series

- Same iteration in labelled & unlabelled universes:

Example: General trees

$$\mathcal{Y} = \mathcal{H}(\mathcal{Y}) = \mathcal{Z} \times \text{SET}(\mathcal{Y}) \rightarrow \mathcal{N}_H(Y) = Y + \frac{H(Y) - Y}{1 - H(Y)}.$$

- Small arithmetic complexity:

first N coefficients in $O(M(N))$ operations

($M(N)$: cost of multiplying two series).

→ fast enumeration,

→ fast random generation by the recursive method.

Combinatorial Iteration → Iteration for Generating Series

- Same iteration in labelled & unlabelled universes:

Example: General trees

$$\mathcal{Y} = \mathcal{H}(\mathcal{Y}) = \mathcal{Z} \times \text{SET}(\mathcal{Y}) \rightarrow \mathcal{N}_H(Y) = Y + \frac{H(Y) - Y}{1 - H(Y)}.$$

- Small arithmetic complexity:

first N coefficients in $O(M(N))$ operations

($M(N)$: cost of multiplying two series).

→ fast enumeration,

→ fast random generation by the recursive method.

- Small bit complexity:

exact enumeration in quasi-optimal time.

IV Numerical values for Boltzmann Samplers

Numerical Values

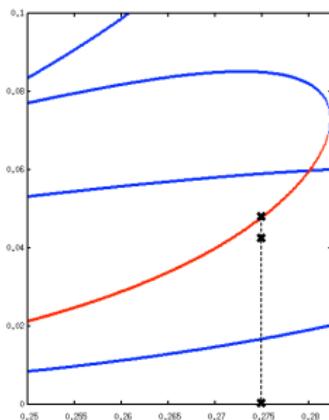
Combinatorics

- $\mathcal{Y} = \mathcal{H}(\mathcal{Z}, \mathcal{Y})$
- $\mathcal{Y}_{n+1} = \mathcal{N}_{\mathcal{H}}(\mathcal{Z}, \mathcal{Y}_n)$
- $\emptyset = \mathcal{Y}_0 \subset \mathcal{Y}_1 \subset \dots \subset \mathcal{Y}$



Generating Series

- $\mathbf{Y}(z) = \mathbf{H}(z, \mathbf{Y}(z))$
(analytic in $|z| < r$ for some $r > 0$)
- $\mathbf{Y}_{n+1}(z) = \mathcal{N}_{\mathbf{H}}(z, \mathbf{Y}_n(z))$
- coeffs ≥ 0 and increasing \Rightarrow
 - ① \mathbf{Y}_n analytic in $|z| < r$;
 - ② $\mathbf{Y}_n(x) \leq \mathbf{Y}_{n+1}(x)$ for $0 \leq x < r$;
 - ③ $\mathbf{Y}_n(z) \rightarrow \mathbf{Y}(z)$ for $|z| < r$.



Numerical Values

Generating Series

- $\mathbf{Y}(z) = \mathbf{H}(z, \mathbf{Y}(z))$
(analytic in $|z| < r$ for some $r > 0$)
- $\mathbf{Y}_{n+1}(z) = \mathcal{N}_{\mathbf{H}}(z, \mathbf{Y}_n(z))$
- coeffs ≥ 0 and increasing \Rightarrow
 - ① \mathbf{Y}_n analytic in $|z| < r$;
 - ② $\mathbf{Y}_n(x) \leq \mathbf{Y}_{n+1}(x)$ for $0 \leq x < r$;
 - ③ $\mathbf{Y}_n(z) \rightarrow \mathbf{Y}(z)$ for $|z| < r$.

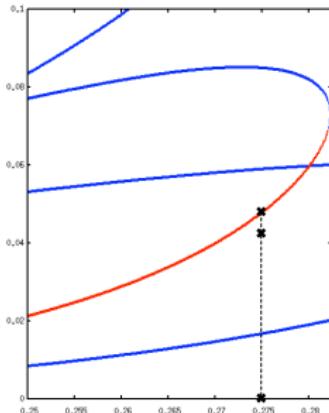


Proposition

For $0 \leq x < r$, define

$$\alpha_0 := 0 \text{ and } \alpha_{n+1} := \mathcal{N}_{\mathbf{H}}(x, \alpha_n).$$

Then, $\alpha_n = \mathbf{Y}_n(x) \rightarrow \mathbf{Y}(x)$.



(Technical point: prove that \mathbf{H} is analytic there.)

Example (II): Unlabelled Rooted Trees

- Combinatorial Newton iteration:

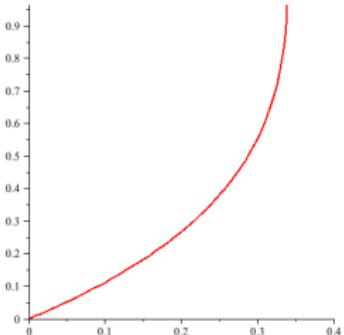
$$\mathcal{Y} = \mathcal{H}(\mathcal{Y}) = \mathcal{Z} \times \text{SET}(\mathcal{Y})$$

$$\rightarrow \mathcal{N}_H(Y) = Y + \frac{H(Y) - Y}{1 - H(Y)}.$$

$$H(Y) = z \exp(Y(z) + Y(z^2)/2 + \dots).$$

- Numerical evaluation at $z = 0.3$:

n	$Y_n(0.3)$	$Y_n(0.3^2)$	$Y_n(0.3^3)$
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



V Conclusion

Conclusions

- More info at Carine Pivoteau's defense tomorrow at LIP6;
- **Next:** extend to \mathcal{E} 's (use multivariate g.f.);
- **Next:** use Schröder iteration at $x = r$
(exploit Drmota-Lalley-Woods);
- **Next:** singularity analysis of these systems
(see also Bousquet-Mélou & Fusy).