Random generation of combinatorial structures using Boltzmann samplers

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Plan

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1. Recursive counting and recursive sampling
2. Generating functions and Boltzmann samplers
3. New constructions for Boltzmann samplers
4. Random sampling of plane partitions

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1. **Recursive counting and recursive sampling**
2. Generating functions and Boltzmann samplers
3. New constructions for Boltzmann samplers
   - Multisets
   - Cycles
4. Random sampling of plane partitions

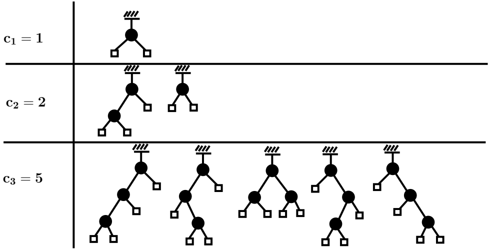
Combinatorial classes

A combinatorial class $\mathcal{C}$ is a set of objects such that

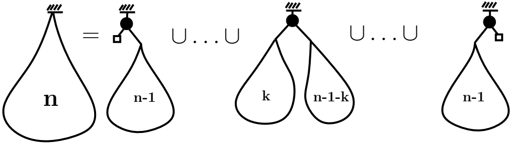
- Each object $\gamma \in \mathcal{C}$ has a size $|\gamma| \in \mathbb{N}$ (e.g. number of vertices in a graph)
- For $n \geq 0$, the number of objects of size n in $\mathcal{C}$ is finite. This number c_n is called the nth coefficient of $\mathcal{C}$

Example: binary trees

- Each inner node has a left son and a right son
- The size is the number of inner nodes



$$c_n = c_0 c_{n-1} + \ldots + c_k c_{n-1-k} + \ldots + c_{n-1} c_0$$

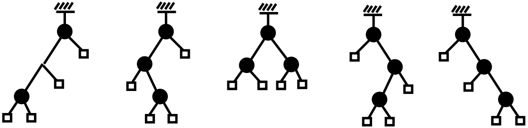


Random generation at a fixed size n

For a given size $n \geq 0$, we want a procedure that picks up an object of size n under the uniform distribution:

$$\Pr(\gamma) = \frac{1}{c_n} \text{ for each } \gamma \in \mathcal{C} \text{ of size } n$$

Binary trees: uniform distribution for $n = 3$

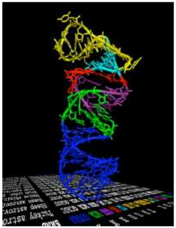


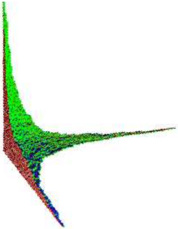
$\Pr = \frac{1}{5}$ $\Pr = \frac{1}{5}$ $\Pr = \frac{1}{5}$ $\Pr = \frac{1}{5}$ $\Pr = \frac{1}{5}$

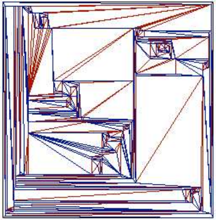
Motivations for random generation

- Observation of asymptotic phenonema

- Generation of structures for experimentation :
  - bio-informatics
  - software testing
  - ...





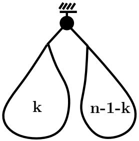


A general procedure: the recursive method

Idea: (Nijenhuis and Wilf'78, Flajolet et al'94) compute the correct probability at the root of the decomposition from the coefficients to have the uniform distribution.

$$\mathbf{c_n = c_0 c_{n-1} + \ldots + c_k c_{n-1-k} + \ldots + c_{n-1} c_0}$$

Proportion of

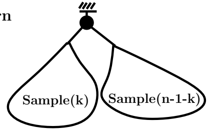


$$= \frac{\mathbf{c_k c_{n-1-k}}}{\mathbf{c_n}}$$

⇒ Recursive algorithm:

Sample(n): 1) choose $k \in \{0, \ldots, n-1\}$ **under the distribution** $\boxed{\Pr(\mathbf{k}) = \frac{\mathbf{c_k c_{n-1-k}}}{\mathbf{c_n}}}$

2) return



Drawback: large auxiliary memory

To sample at size n, we need the coefficients $c_1, \ldots, c_n$
$\Rightarrow$ this requires a quadratic number of bits

n	c_n	n	c_n	n	c_n
1	1	11	58786	21	24466267020
2	2	12	208012	22	91482563640
3	5	13	742900	23	343059613650
4	14	14	2674440	24	1289904147324
5	42	15	9694845	25	4861946401452
6	132	16	35357670	26	18367353072152
7	429	17	129644790	27	69533550916004
8	1430	18	477638700	28	263747951750360
9	4862	19	1767263190	29	1002242216651368
10	16796	20	6564120420	30	3814986502092304

1. Recursive counting and recursive sampling

2. **Generating functions and Boltzmann samplers**

3. New constructions for Boltzmann samplers
   - Multisets
   - Cycles

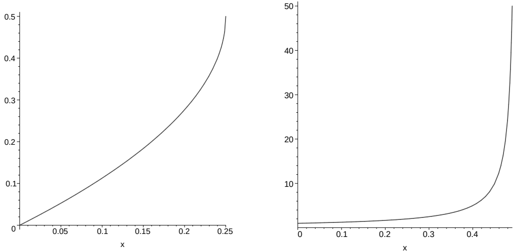
4. Random sampling of plane partitions

Generating functions

The generating function of a class $\mathcal{C}$ is defined as:

$$C(x) := \sum_{\gamma \in \mathcal{C}} x^{|\gamma|} = \sum_{n \geq 0} c_n x^n$$

There is a critical value $\rho > 0$ such that the sum defining the generating function converges for $x < \rho$ and not for $x > \rho$



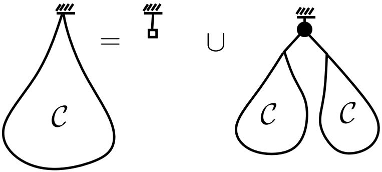
Generating functions: rules of calculations

- Disjoint union: $\boxed{\mathcal{C} = \mathcal{A} \cup \mathcal{B} \Rightarrow C(x) = A(x) + B(x)}$

  Proof: $\sum_{\gamma \in \mathcal{A} \cup \mathcal{B}} x^{|\gamma|} = \sum_{\gamma \in \mathcal{A}} x^{|\gamma|} + \sum_{\gamma \in \mathcal{B}} x^{|\gamma|}$

- Cartesian prod: $\boxed{\mathcal{C} = \mathcal{A} \times \mathcal{B} \Rightarrow C(x) = A(x) \cdot B(x)}$

  Proof: $\sum_{(\gamma_1, \gamma_2) \in \mathcal{A} \times \mathcal{B}} x^{|(\gamma_1, \gamma_2)|} = \sum_{\gamma_1, \gamma_2} x^{|\gamma_1| + |\gamma_2|} = \sum_{\gamma_1 \in \mathcal{A}} x^{|\gamma_1|} \sum_{\gamma_2 \in \mathcal{B}} x^{|\gamma_2|}$



$$\boxed{C(x) = 1 \quad + \quad C(x) x C(x)}$$

simpler than $c_n = c_0 c_{n-1} + \ldots + c_k c_{n-1-k} + \ldots + c_{n-1} c_0.$

Boltzmann samplers

- Introduced by Duchon, Flajolet, Louchard and Schaeffer (2002)
- Relax the constraint of fixed size (cf recursive method) for random generation.
- The distribution is spread over all objects of the class.
- An object is drawn with probability proportional to the exponential of its size (cf statistical physics)

Boltzmann samplers: definition

- Let $\mathcal{C}$ be an unlabelled combinatorial class
  (e.g. binary trees)
  Ordinary generating function:

$$C(x) = \sum_{\gamma \in \mathcal{C}} x^{|\gamma|} = \sum_{n \geq 0} c_n x^n,$$

  where $|\gamma|$ is the size of γ.

- Given $x > 0$ ($x \leq \rho_C$) a fixed real value,
  a Boltzmann sampler $\Gamma C(x)$ is a procedure that draws each object γ of $\mathcal{C}$ with probability:

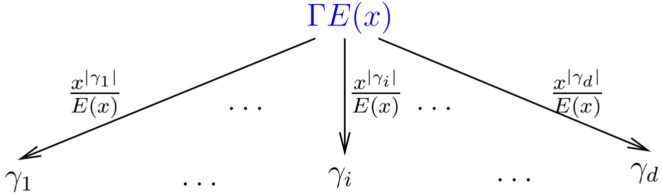
$$\boxed{\Pr(\gamma) = \frac{x^{|\gamma|}}{C(x)}}$$

Analogy with statistical physics

Combinatorics ⟷	**Stat. Phys.**
Structure γ	State s
size n	Energy E
Generating function $C(x) = \sum_\gamma x^{\lvert\gamma\rvert}$	Partition function $Z = \sum_{\mathrm{s}} e^{-\beta E}$
Boltz: $\mathbb{P}(\gamma) = \frac{x^{\lvert\gamma\rvert}}{C(x)}$	Boltz: $\mathbb{P}(s) = \frac{e^{-\beta E}}{Z}$

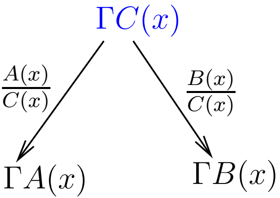
Finite sets

Let $\mathcal{E} = (\gamma_1, \ldots, \gamma_d)$ $\qquad E(x) = \sum_{i=1}^{d} x^{|\gamma_i|}$



The basic construction rules: union

Union: Let $\mathcal{C} = \mathcal{A} \cup \mathcal{B}$. Assume we have Boltzmann samplers $\Gamma A(x)$ for $\mathcal{A}$ and $\Gamma B(x)$ for $\mathcal{B}$. Define $\Gamma C(x)$ as:



Then $\Gamma C(x)$ is a Boltzmann sampler for $\mathcal{A} \cup \mathcal{B}$.

Proof: Let $\gamma \in \mathcal{A} \cup \mathcal{B}$

- If $\gamma \in \mathcal{A}$, then $\Pr(\gamma) = \frac{A(x)}{C(x)} \cdot \frac{x^{|\gamma|}}{A(x)} = \frac{x^{|\gamma|}}{C(x)}$.
- If $\gamma \in \mathcal{B}$, then $\Pr(\gamma) = \frac{B(x)}{C(x)} \cdot \frac{x^{|\gamma|}}{B(x)} = \frac{x^{|\gamma|}}{C(x)}$.

The basic construction rules: product

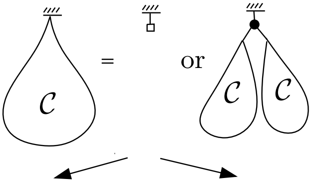
Product: Let $\mathcal{C} = \mathcal{A} \times \mathcal{B}$. Assume we have Boltzmann samplers $\Gamma A(x)$ for $\mathcal{A}$ and $\Gamma B(x)$ for $\mathcal{B}$. Define $\Gamma C(x)$ as:

$$\begin{array}{lll} \Gamma C(x) & : & \gamma_1 \leftarrow \Gamma A(x) \\ & & \gamma_2 \leftarrow \Gamma B(x) \\ & & \text{return } (\gamma_1, \gamma_2) \end{array}$$

Then $\Gamma C(x)$ is a Boltzmann sampler for $\mathcal{A} \cup \mathcal{B}$:
Proof: an object $\gamma = (\gamma_1, \gamma_2)$ has probability:

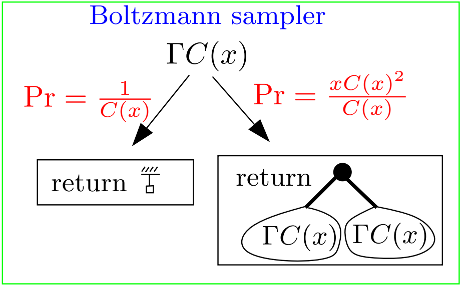
$$\frac{x^{|\gamma_1|}}{A(x)} \frac{x^{|\gamma_2|}}{B(x)} = \frac{x^{|\gamma_1|+|\gamma_2|}}{A(x) \cdot B(x)} = \frac{x^{|\gamma|}}{C(x)}$$

Example: binary trees



Generating function

$$C(x) = 1 + xC(x)^2$$



A first Sampling dictionary

Theorem

A Boltzmann sampler can be designed for any class having a recursive specification with the constructions $\cup$ and $\times$. The complexity is linear in the size of the output object.

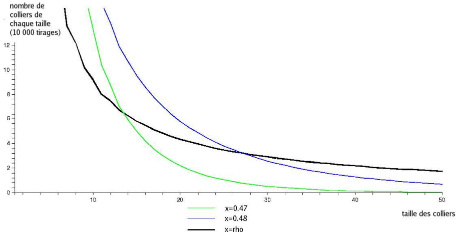
construction	generator
$\mathcal{C} = \varnothing$	$\Gamma C(x) :=$ return $\varnothing$
$\mathcal{C} = \{\bullet\}$	$\Gamma C(x) :=$ return $\{\bullet\}$
$\mathcal{C} = \mathcal{A} + \mathcal{B}$	$\Gamma C(x) := \left(\text{Bern}\ \frac{A(x)}{C(x)} \longrightarrow \Gamma A(x) \mid \Gamma B(x) \right)$
$\mathcal{C} = \mathcal{A} \times \mathcal{B}$	$\Gamma C(x) := (\ \Gamma A(x); \Gamma B(x)\ )$

Choosing x to draw objects around a target-size

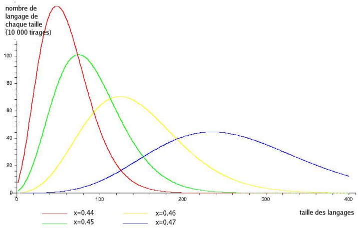
The probability of drawing an object of size n is:

$$\mathbb{P}_x(\text{Size} = n) = \sum_{|\gamma|=n} \frac{x^{|\gamma|}}{C(x)} = \frac{c_n x^n}{C(x)}$$

$\rightarrow$ size distributions for different values of x.



Bicolored necklaces



Finite languages

Boltzmann samplers *vs* the recursive method

	Boltzmann	recursive method
size distribution	$Pr(size = n) = \frac{c_n x^n}{C(x)}$	fixed size n
auxiliary memory	$\mathcal{O}(\log(n))$	$\mathcal{O}(n^2)$
time per generation	$\mathcal{O}(n^2)$ Exact $\mathcal{O}(n)$ Approx	$\mathcal{O}(n \log(n))$ Exact

New constructions for Boltzmann samplers

(with Philippe Flajolet and Carine Pivoteau)

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A first construction: MSet_2

$\textsc{MSet}_2(\mathcal{A}) \cong$ unorderer pairs of objects de $\mathcal{A}$

$$\mathcal{C} = \textsc{MSet}_2(\mathcal{A})$$

$$C(z) = \frac{1}{2}A^2(z) + \frac{1}{2}A(z^2) \qquad \left[\ 2\textsc{MSet}_2(\mathcal{A}) = \mathcal{A}^2 + \Delta\mathcal{A}^2\ \right]$$

Algorithm: $\Gamma C(x)$

if $Bern\left(\frac{1}{2}\frac{A^2(x)}{C(x)}\right) = 1$ **then**
  Return $(\ \Gamma A(x), \Gamma A(x)\ )$
else
  $a \leftarrow \Gamma A(x^2)$;
  Return (a, a);
end if

Proof that the algorithm is correct

Proof.

Let $\gamma = \langle \gamma_1, \gamma_2 \rangle$ be an unordered pair of objects of $\mathcal{A}$. The probability that γ is drawn by $\Gamma C(x)$ is:

1. $\gamma_1 \neq \gamma_2$

$$\mathbb{P}_x(\gamma) = \frac{1}{2} \frac{A(x)^2}{C(x)} \, \frac{x^{|\gamma_1|}}{A(x)} \, \frac{x^{|\gamma_2|}}{A(x)} \times 2 = \frac{x^{|\gamma|}}{C(x)}$$

2. $\gamma_1 = \gamma_2$

$$\mathbb{P}_x(\gamma) = \frac{1}{2} \frac{A(x)^2}{C(x)} \, \frac{x^{|\gamma_1|}}{A(x)} \, \frac{x^{|\gamma_1|}}{A(x)} + \frac{1}{2} \frac{A(x^2)}{C(x)} \, \frac{x^{2|\gamma_1|}}{A(x^2)} = \frac{x^{|\gamma|}}{C(x)}$$

□

Application

Unembedded binary trees
(Otter trees)

$$\mathcal{B} = \mathcal{Z} + \mathrm{MS{\scriptsize ET}}_2(\mathcal{B})$$

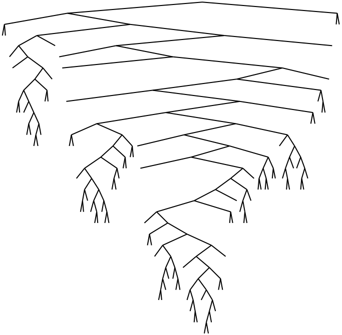
$$B(z) = z + \frac{1}{2}B^2(z) + \frac{1}{2}B(z^2)$$

$\rightarrow$ □

$\rightarrow$ ■$\langle\ \Gamma B(x), \Gamma B(x)\ \rangle$

$\rightarrow$ $ot \leftarrow \Gamma B(x^2)$;

return ■$\langle\ ot, ot\ \rangle$;



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$\rightarrow$ $\blacksquare\langle\, \Gamma B(x), \Gamma B(x)\,\rangle$

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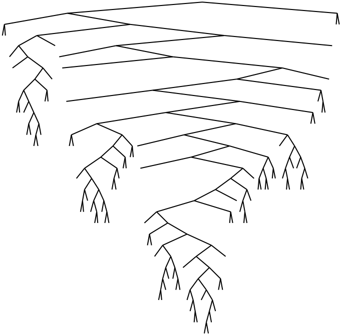

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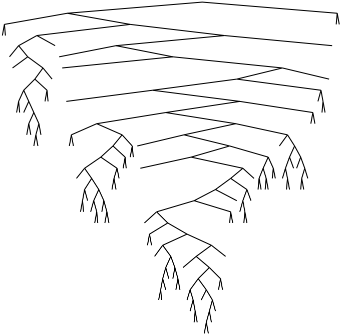

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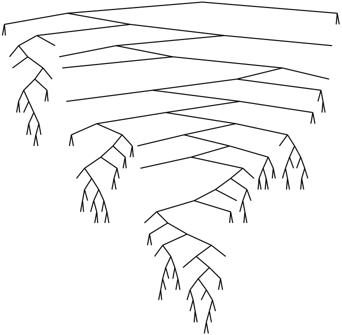

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General MSet

Let $\mathcal{M} := \textsc{MSet}(\mathcal{A})$ be the class of all multisets of objects of $\mathcal{A}$.

$$M(z) = \exp\left(\sum_{k=1}^{\infty} \frac{1}{k} A(z^k)\right) = \prod_{k=1}^{\infty} \exp\left(\frac{1}{k} A(z^k)\right)$$

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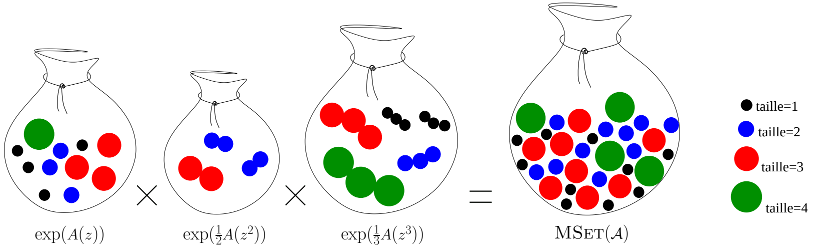

Algorithm for general MSet

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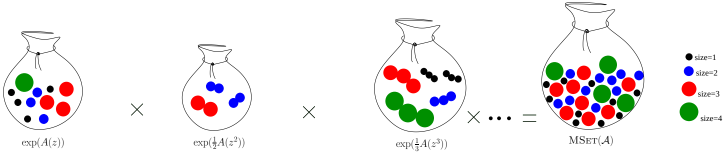

repeat Poiss$(A(x))$ times $\gamma \leftarrow \Gamma A(x)$ add γ	repeat Poiss$(\frac{A(x^2)}{2})$ times $\gamma \leftarrow \Gamma A(x^2)$ add 2 copies of γ	repeat Poiss$(\frac{A(x^3)}{3})$ times $\gamma \leftarrow \Gamma A(x^3)$ add 3 copies of γ

Algorithm for general MSet (2)

Algorithm $\Gamma MSet[\mathcal{A}](x)$

$k \longleftarrow \text{MaxIndex}(x)$;
for i **from** 1 **to** $k-1$ **do** {
  $p \longleftarrow \text{Pois}\left(\frac{1}{i}A(x^i)\right)$;
  repeat p {
    $\gamma \leftarrow \Gamma A(x^i)$;
    Add $\boldsymbol{i}$ copies of γ to the MSet
  }
}
$p \longleftarrow \text{Pois}_{\geq 1}\left(\frac{1}{k}A(x^k)\right)$;
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}

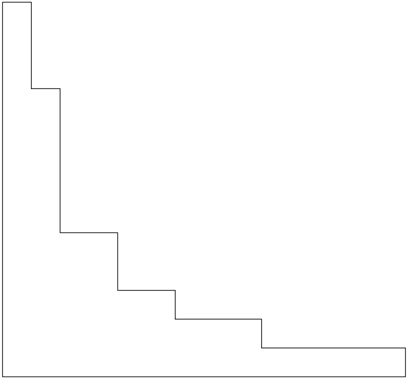
Result

Theorem

If we have a Boltzmann sampler $\Gamma A(x)$ *for* $\mathcal{A}$, *then* $\Gamma MSet[\mathcal{A}](x)$ *is a Boltzmann sampler for* $\textsc{MSet}(\mathcal{A})$.

Generation of a partition (multiset of integers)

$\boldsymbol{k} = 3;$
$p_1 = 5;$
$p_2 = 3;$
$p_3 = 1;$



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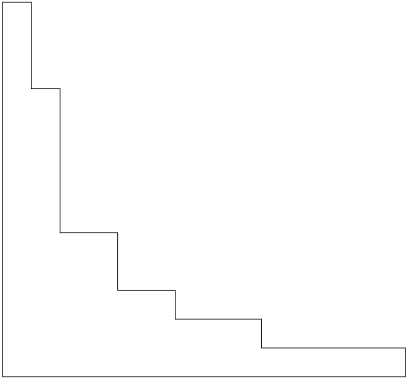
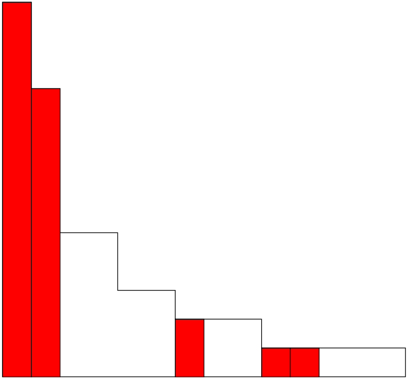


Generation of a partition (multiset of integers)

$\boldsymbol{k} = 3;$
$p_1 = 5;$
$p_2 = 3;$
$p_3 = 1;$

$\rightarrow 13,\ 10,\ 2,\ 1,\ 1$



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$\boldsymbol{k} = 3;$
$p_1 = 5;$
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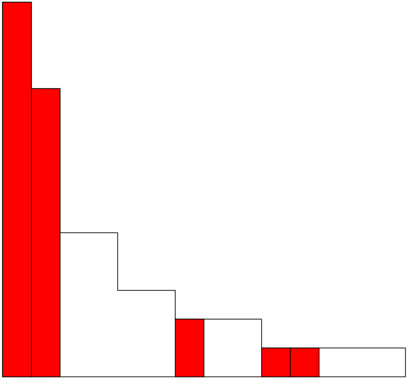
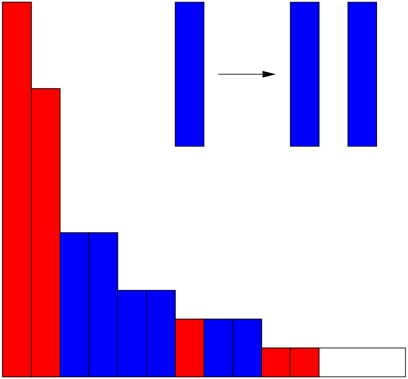


Generation of a partition (multiset of integers)

$\boldsymbol{k} = 3;$
$p_1 = 5;$
$p_2 = 3;$
$p_3 = 1;$

$\rightarrow 5,\ 3,\ 2$



Generation of a partition (multiset of integers)

$\boldsymbol{k} = 3;$

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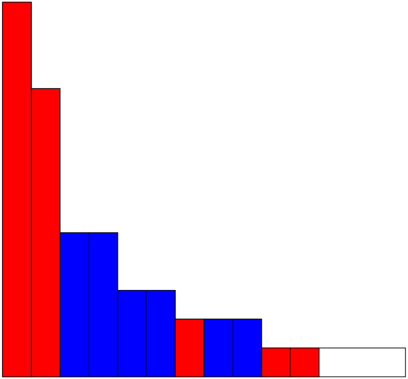

Generation of a partition (multiset of integers)

$\boldsymbol{k} = 3;$
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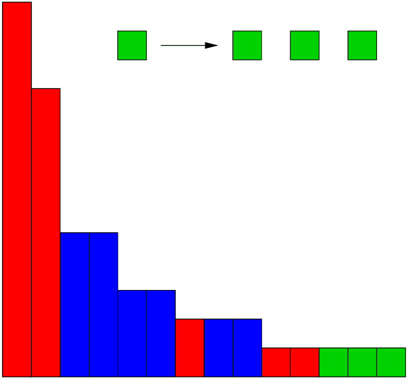
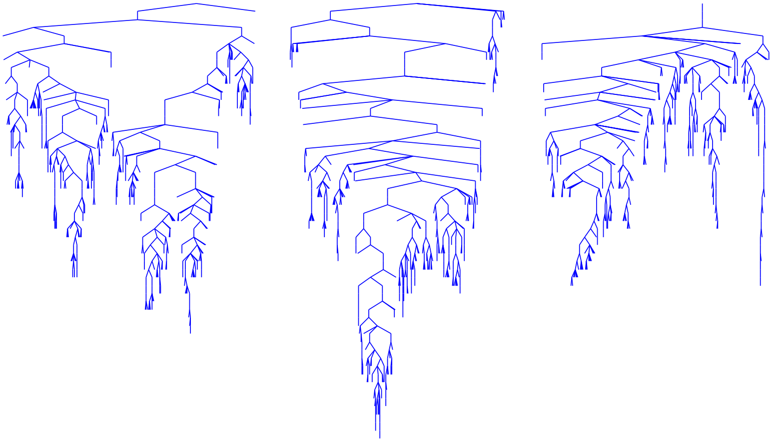
$\rightarrow 1$



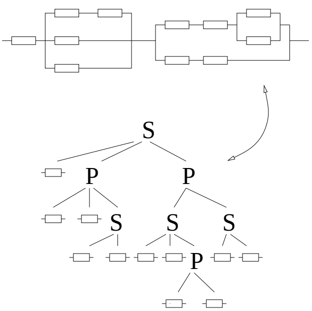
General unembedded trees

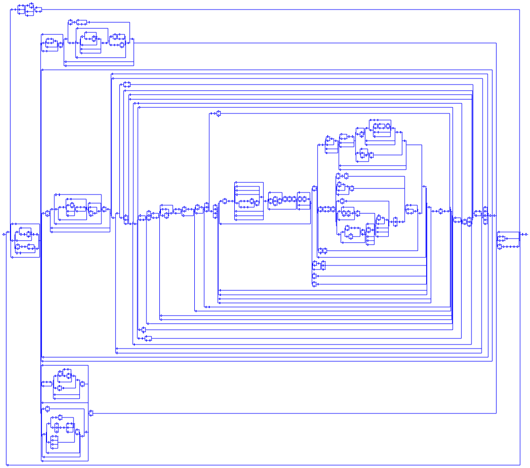
$$\mathcal{T} = \mathcal{Z} \times \mathrm{MS{\small ET}}(\mathcal{T})$$



Series-parallel circuits

$$\mathcal{C} = \mathcal{P} + \mathcal{S} + \mathcal{Z}$$
$$\mathcal{S} = \mathrm{SEQ}_{\geq 2}(\mathcal{P} + \mathcal{Z})$$
$$\mathcal{P} = \mathrm{MSET}_{\geq 2}(\mathcal{S} + \mathcal{Z})$$

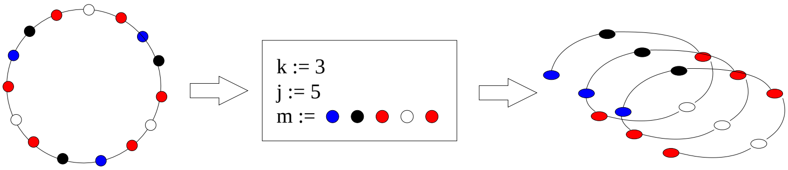




1. Recursive counting and recursive sampling
2. Generating functions and Boltzmann samplers
3. New constructions for Boltzmann samplers
   - Multisets
   - Cycles
4. Random sampling of plane partitions

Generating function for cycles

$$\mathcal{C} = \textsc{Cyc}(\mathcal{A}) \quad \Rightarrow \quad C(z) = \sum_{k \geq 1} \frac{\varphi(k)}{k} \log \frac{1}{1 - A(z^k)}$$



Algorithm

$\Gamma Cyc[\mathcal{A}](x)$

$k \longleftarrow \text{ReplicationOrder}(x);$ # how many copies of s

$j \longleftarrow \text{Loga}\left(A(x^k)\right);$ length of s

$s \longleftarrow \underbrace{\Gamma A(x^k), \ldots, \Gamma A(x^k)}_{j\ times};$ sequence

Return $(\underbrace{m, \ldots, m}_{k\ times});$

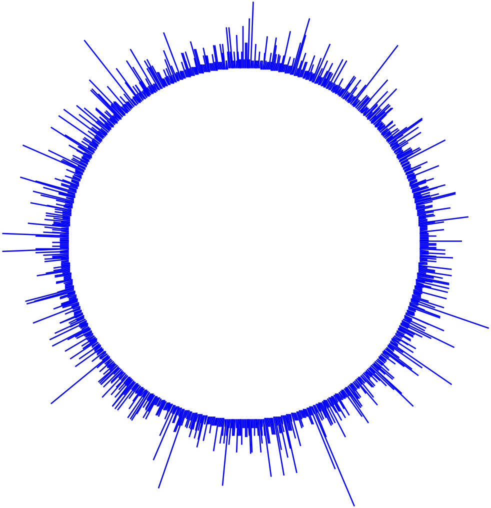
Definition: X follows a Loga law of parameter λ if:

$$\mathbb{P}(X = j) = \frac{1}{\log(1-\lambda)^{-1}} \frac{\lambda^j}{j}$$

Cycles of integers

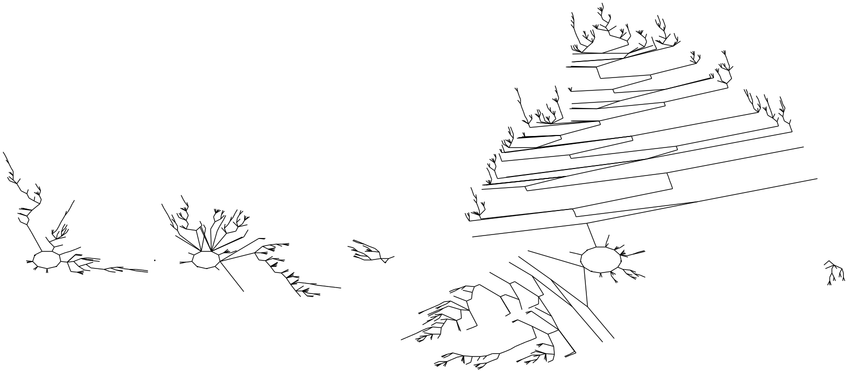
$$\mathcal{C} = \textsc{Cyc}(\mathcal{Z} \times \textsc{Seq}(\mathcal{Z}))$$

$$C(z) = \sum_{k=1}^{\infty} \frac{\varphi(k)}{k} \log \frac{1}{1 - \frac{z^k}{1-z^k}}$$



Functional graphs

$$\begin{array}{rcl} \mathcal{M} & = & \text{MSet}(\mathcal{C}) \\ \mathcal{C} & = & \text{Cyc}(\mathcal{G}) \\ \mathcal{G} & = & \mathcal{Z} \times \text{MSet}(\mathcal{G}) \end{array}$$



Result

Theorem

- *If a combinatorial class $\mathcal{C}$ has a recursive specification with the constructions*

$$\{\cup, \times, \text{Seq}, \text{MSet}, \text{Cyc}\}$$

then a **Boltzmann sampler** *can be designed for $\mathcal{C}$.*

- *This list of constructions can be completed by constructions with cardinality restrictions (e.g.* MSet_2*)*

This applies for several classes:

- partitions, compositions, necklaces,...
- trees,
- regular languages,
- functional graphs,...

Result

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- regular languages,
- functional graphs,...

Complexity

Theorem

By choosing a suitable value for the parameter x, one has the following complexities for approximate size and fixed size:

Integer partitions of size n	$O(\sqrt{n}\log n)$	$O(n)$
Unembedded trees of size n	$O(n)$	$O(n^2)$
Necklaces, circular compositions of size n	$O(n)$	$O(n)$
Mobiles of size n	$O(n)$	$O(n^2)$
Functional graphs of size n	$O(n)$	$O(n\sqrt{n})$

Random sampling of plane partitions

(with Olivier Bodini and Carine Pivoteau)