Analytic Random Generation of Combinatorial Objects

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I. Introduction

About combinatorial classes, specification generating function, and basic random generation

decomposable combinatorial classes

a class $\mathcal{A}$ is a decomposable combinatorial class if:

- described by symbolic rules (= grammar)

$\mathcal{Z}$, ε	$+$, $\times$, Seq, Set, Cyc, ...
building blocks	ways to combine them

- possible recursive (defined using itself)
- the number a_n of objects of size n is finite

example: binary trees counted by external nodes

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

a binary tree   leaf   or   two subtrees
(each defined recursively in same way)

all binary trees with 4 leaves $(b_4 = 5)$

random generation of combinatorial structures

let $\mathcal{A}$ be a class, with a_n objects of size n, this means drawing an object of size n is uniform:

$$\mathbb{P}_n[\alpha \in \mathcal{A}_n] = \frac{1}{a_n}$$

some methods:

- ad-hoc methods to deal with specific classes: Remy's algorithm (binary trees), Hook formula (Young tableaux), or more generally bijection/rejection methods (random walks, etc.)
- automatic methods to deal with all decomposable classes: **recursive method** [Nijenhuis and Wilf, Flajolet *et al.*], but requires precomputing all enumeration coefficients up until n: a_0, a_1, ..., a_n

some applications:

- **analysis:** study specific properties/statistics of huge objects through simulation
  - generate many random objects, and empirically study properties
  - compare real data with (randomly generated) uniform data: in genetics, in **poetry** [Gasparov 1987]
- **testing:** generate input for algorithm/server to test robustness and ability to withstand heavy loads [Mougenot *et al.* 2009]

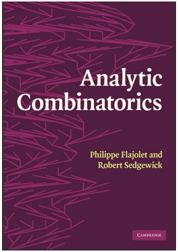
symbolic method [Flajolet & Sedgewick 09]

the **generating function** $A(z)$ of class $\mathcal{A}$ encodes, within a function, the complete enumeration (the number of objects for each size) of the class:

$$A(z) = \sum_{n=0}^{\infty} a_n z^n$$

- in the general case, this generating function (GF) is a formal object; however the GF of decomposable classes is often convergent
- dictionary: correspondence which exactly relates specific. and GF

construction	specification	GF
neutral element	ε	1
atome	$\mathcal{Z}$	z
union	$\mathcal{A} + \mathcal{B}$	$A(z) + B(z)$
Cartesian product	$\mathcal{A} \times \mathcal{B}$	$A(z) \cdot B(z)$
sequence	$\mathrm{Seq}(\mathcal{A})$	$\frac{1}{1-A(z)}$



example: class $\mathcal{B}$ of binary trees

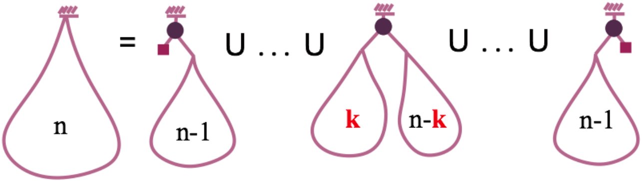
$$\mathcal{B} = \mathcal{Z} + \mathcal{B} \times \mathcal{B} \quad \Rightarrow \quad B(z) = z + B(z) \cdot B(z) = \frac{1 - \sqrt{1-4z}}{2}$$

the "recursive" method

[Nijenhuis & Wilf 1978; Flajolet, Zimmerman & Van Cutsem 1994]

divide and conquer: sample objects of size *n*

by sampling objects of size *1*, ..., *n-1*



uses the recurrences of GF to determine algorithms

efficient and generic for all specifiable classes, exact generation in $O(n \log n)$

Drawbacks

- requires preprocessing b_i for $1 \leqslant i \leqslant n$ and storing coefficients, space $O(n^2)$
- drawing prob. law for k is costly, in $O(k)$

(can be improved with "boustrophedonic" trick)

GenBinTree(n) :=

draw k following law $\mathbb{P}[K = k] = \dfrac{b_k \cdot b_{n-k}}{b_n}$

return <GenBinTree(k), GenBinTree(n-k)>

b_n := binary trees of size n

II. Analytic samplers

("Boltzmann" samplers)

$$\mathbb{P}_z[N = n] = \frac{f_n z^n}{F(z)}$$

randomly generating objects

by evaluating their GF

analytic random samplers

[Duchon, Flajolet, Louchard & Schaeffer 2002]

approximate-size sampling allows for new approach

let $\mathcal{C}$ be a class, we draw an object $\gamma \in \mathcal{C}$ with probability

$$\mathbb{P}_z[\gamma] = \frac{z^{|\gamma|}}{C(z)}$$

size of object

generat. funct. of comb. class

- uniformity at given size (two obj. same size = same prob. being drawn)

$$\mathbb{P}_z[\gamma \in \mathcal{C} \mid |\gamma| = n] = \frac{1}{c_n}$$

- **idea:** by evaluating GF, get a biased average of coefficients
- the probability distribution ("Power Series Distribution") has all the same good algebraic properties as GF
- later we can see how to control the size

the result is an elegant and simple translation to algorithms
(here for the labeled case)

construction	**algorithm**
$\mathcal{A} = \varepsilon$ or $\mathcal{Z}$	$\Gamma\mathcal{A}(z) :=$ **return** $\square$ or $\blacksquare$
$\mathcal{A} = \mathcal{B} + \mathcal{C}$	$\Gamma\mathcal{A}(z) :=$ **if** $\mathrm{Ber}(B(z)/(B(z)+C(z))) = 1$ **then return** $\Gamma\mathcal{B}(z)$ **else return** $\Gamma\mathcal{C}(z)$
$\mathcal{A} = \mathcal{B} \times \mathcal{C}$	$\Gamma\mathcal{A}(z) :=$ **return** $< \Gamma\mathcal{B}(z); \Gamma\mathcal{C}(z) >$
$\mathcal{A} = \mathrm{Seq}\,(\mathcal{B})$	$\Gamma\mathcal{A}(z) := k \leftarrow \mathrm{Geo}(A(z))$; **return** k indep. $\Gamma\mathcal{B}(z)$
$\mathcal{A} = \mathrm{Set}\,(\mathcal{B})$	$\Gamma\mathcal{A}(z) := k \leftarrow \mathrm{Poi}(A(z))$; **return** k indep. $\Gamma\mathcal{B}(z)$
$\mathcal{A} = \mathrm{Cyc}\,(\mathcal{B})$	$\Gamma\mathcal{A}(z) := k \leftarrow \mathrm{Loga}(A(z))$; **return** k indep. $\Gamma\mathcal{B}(z)$

Definition

An analytic sampler for class $\mathcal{C}$, with generating function $C(z) = \sum c_n z^n$, is an algorithm ΓC which returns any object $\gamma \in \mathcal{C}$ with probability:

$$\mathbb{P}_z[\gamma] = \frac{c_n z^n}{C(z)}.$$

- when $\mathcal{A} = \{\varepsilon\}$ or $\mathcal{A} = \{\mathcal{Z}\}$, $\Gamma\mathcal{A}(z) :=$ **return** $\square$ or $\blacksquare$
  Proof (that it's an analytic sampler): it always returns an element from a singleton (containing a neutral element and atom resp.):

$$\mathbb{P}_z[\square] = \frac{z^0}{z^0} = 1 \qquad \mathbb{P}_z[\blacksquare] = \frac{z^1}{z^1} = 1$$

- when $\mathcal{A} = \mathcal{B} + \mathcal{C}$, $\Gamma\mathcal{A}(z) :=$ **if** $\mathrm{Ber}(B(z)/(B(z) + C(z))) = 1$ **then return** $\Gamma\mathcal{B}(z)$ **else return** $\Gamma\mathcal{C}(z)$
  Proof: prob. of drawing $\beta \in \mathcal{A}$ (when $\beta \in \mathcal{B}$)

$$\mathbb{P}_z[\beta \in \mathcal{A}] = \frac{B(z)}{B(z) + C(z)} \cdot \mathbb{P}_z[\beta \in \mathcal{B}] = \frac{B(z)}{B(z) + C(z)} \cdot \frac{z^{|\beta|}}{B(z)} = \frac{z^{|\alpha|}}{A(z)}$$

- when $\mathcal{A} = \mathcal{B} \times \mathcal{C}$, $\Gamma\mathcal{A}(z) :=$ **return** $< \Gamma\mathcal{B}(z); \Gamma\mathcal{C}(z) >$
  Proof: let $\alpha \in \mathcal{A}$, $\alpha = (\beta, \gamma)$,

$$\mathbb{P}_z[\alpha] = \mathbb{P}_z[\beta] \cdot \mathbb{P}_z[\gamma] = \frac{z^{|\beta|}}{B(z)} \cdot \frac{z^{|\gamma|}}{C(z)} = \frac{z^{|\beta|+|\gamma|}}{B(z) \cdot C(z)} = \frac{z^{|\alpha|}}{A(z)}$$

first example: binary trees

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

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$$B(z) = z + B(z)^2 = \frac{1 - \sqrt{1 - 4z}}{2}$$

$$\begin{aligned}\Gamma\mathcal{B}(z) := &\ \textbf{if } \mathrm{Ber}(z/B(z)) = 1 \textbf{ then return } \blacksquare \\ &\ \textbf{else return } < \Gamma\mathcal{B}(z); \Gamma\mathcal{B}(z) >\end{aligned}$$

Untitled-1

```
(* Specification:   B = Z + B^2   *)

In[4]:= Solve[B == z + B^2, B]
```

Out[4]= $\left\{\left\{B \to \frac{1}{2}\left(1 - \sqrt{1 - 4 z}\right)\right\}, \left\{B \to \frac{1}{2}\left(1 + \sqrt{1 - 4 z}\right)\right\}\right\}$

In[5]:= B[z_] := $\frac{1}{2}\left(1 - \sqrt{1 - 4 z}\right)$

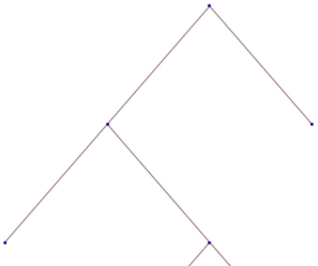
```
In[6]:= AnaBinTree[z_] :=
         If[RandomVariate[BernoulliDistribution[z / B[z]]] == 1,
          (*if*) Return[{}],
          (*else*) Return[{AnaBinTree[z], AnaBinTree[z]}]]

In[7]:= AnaBinTree[0.25]

Out[7]= {{{}, {{}, {}}}, {}}

In[36]:= DrawTree[Out[7]]

Out[36]//TreeForm=
```



RECURSIVE version [Flajolet *et al.* 1994]

RecBT(n) := {
  if $n = 1$ **then** return Leaf
  else
    k from distr. $\mathbb{P}[K = k] = (b_k \cdot b_{n-k})/b_n$
    return Node(RecBT(k), RecBT($n - k$))
}

"BOLTZMANN" vers. [Duchon *et al.* 02]

AnaBT(z) := {
  if $\mathrm{Ber}(z/B(z)) = 1$ **then** return Leaf
  else
    return Node(AnaBT(z), AnaBT(z))
}

Noteworthy, in "Boltzmann"/analytic random sampling, the randomization is **global**: the same law is calculated in all recursive calls.

second example: general trees (any number of children)

$$\mathcal{G} = \mathcal{Z} \times \mathsf{Seq}\,(\mathcal{G})$$

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second example: general trees (any number of children)

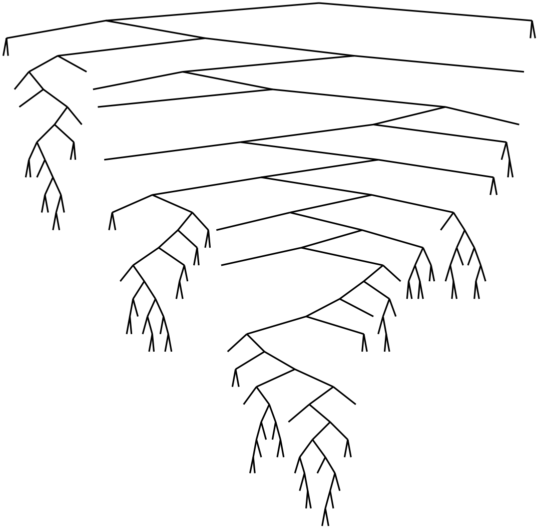
$$\mathcal{G} = \mathcal{Z} \times \mathsf{Seq}\,(\mathcal{G})$$

$$G(z) = \frac{z}{1 - G(z)} = \frac{1 - \sqrt{1 - 4z}}{2}$$

$$\begin{aligned} \Gamma\mathcal{G}(z) &:= \text{let } k = \mathrm{Geo}(G(z)) \\ &\quad \textbf{return} \;\; < \blacksquare; \Gamma\mathcal{G}(z); \ldots; \Gamma\mathcal{G}(z) > \qquad k \text{ times} \end{aligned}$$

Otter tree

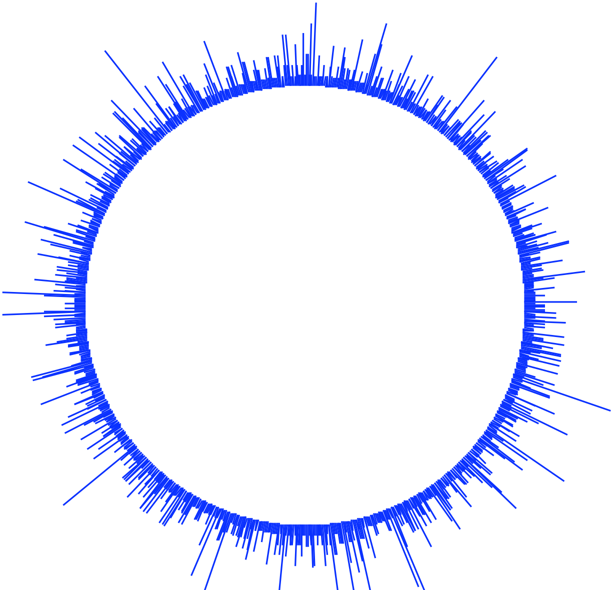
$$\mathcal{O} = Z + \mathrm{MSet}_2(\mathcal{O})$$



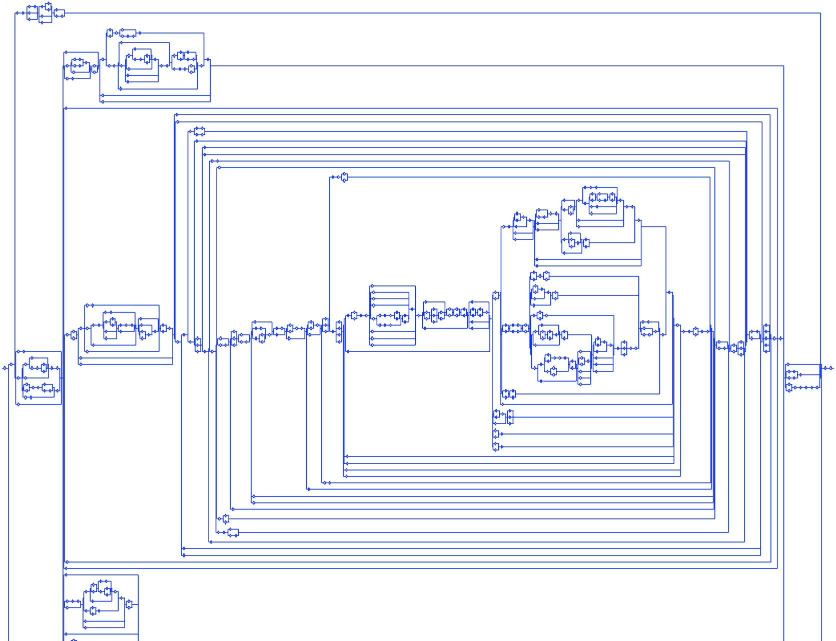
picture by Carine Pivoteau

Circular composition (size about 2000)

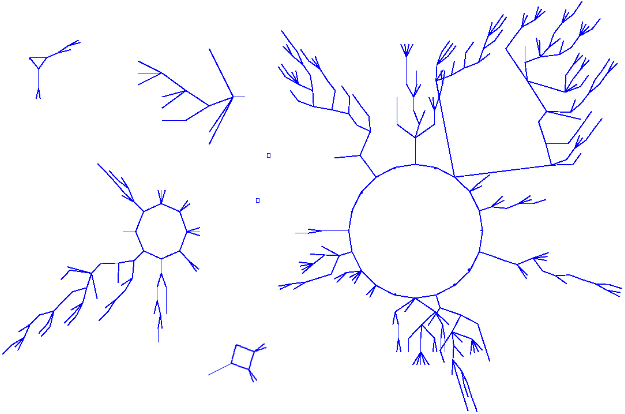
$$\mathcal{C} = \mathrm{Cyc}\left(\mathrm{Seq}\left(\mathcal{Z}\right)\right)$$



Series-parallel graphs (size about 500)



Functional graph



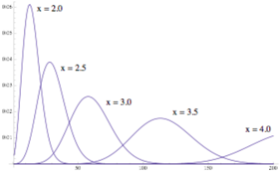
III. Size matters

Analytic samplers efficiently draw objects
but following some "arbitrary" distribution

How to make this useful?

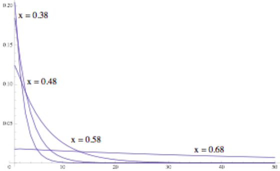
size control: rejection & its cost (for typical classes)

"bumpy"



$$P(z) = e^{e^z - 1}$$

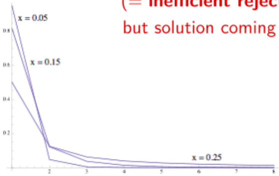
"flat"



$$S(z) = \frac{1}{1 - (e^z - 2)}$$

"peaked"

(= **inefficient rejection**
but solution coming up)



$$B(z) = \frac{1 - \sqrt{1 - 4z}}{2}$$

- solve/approximate expected value to find z targeting size

$$\mathbb{P}_z[N = n] = \frac{f_n z^n}{F(z)} \quad \Rightarrow \quad \mathbb{E}_z[N] = z\frac{F'(z)}{F(z)} \quad \Rightarrow \quad z_n = \ldots$$

- size distribution of samplers depends on *type of singularity* of generating function

$$f(z) \underset{z \to \rho}{\sim} P(z) + c_0(1 - z/\rho)^{-\alpha} + o((1 - z/\rho)^{-\alpha}), \quad \alpha \in \mathbb{R} \setminus \{0, -1, -2, \ldots\}$$

ρ : radius of convergence $\qquad \alpha$: singular exponent

- ⚠ size distribution affects *rejection complexity*; for "bumpy" and "flat" approx. in **O(1) loops** and exact in **O(n) loops**

approximate-size rejection

loop
obj $:= \Gamma B(z)$
while $|\text{size}(\text{obj}) - n| > \epsilon$

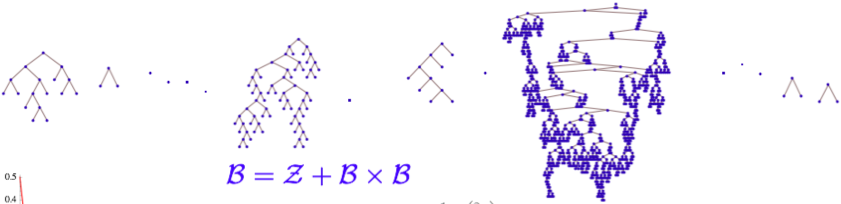
exact-size rejection

loop
obj $:= \Gamma B(z)$
while $\text{size}(\text{obj}) \neq n$

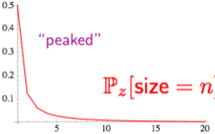
for target size n and tolerance $\epsilon = \ldots\%$

ex.: size distribution of sampler for binary trees

9, 2, 1, 1, 1, 1, 36, 1, 6, 1, 449, 1, 1, 1, 2, 2,



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



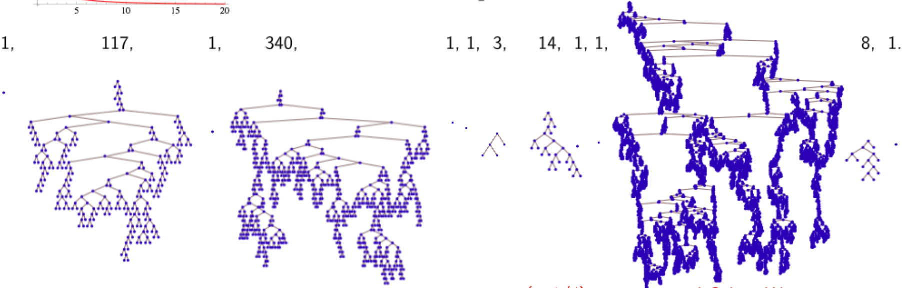
$$\mathbb{P}_z[\text{size} = n] = \frac{b_n z^n}{B(z)}$$

$$b_{n+1} := \frac{1}{n+1}\binom{2n}{n}$$

$$B(z) := \frac{1 - \sqrt{1-4z}}{2}$$

3107,

1, 117, 1, 340, 1, 1, 3, 14, 1, 1, 8, 1.



$z = \rho \ (= 1/4) \quad \Rightarrow \quad$ critical Galton Watson process

efficient rejection for "peaked" classes

Pointing: if $\mathcal{A}$ is a class, then $\mathcal{C} = \mathcal{A}^\bullet$ is the class obtained from all possible ways to *distinguish one atom* of objects of $\mathcal{A}$.

$$c_n = n \cdot a_n \qquad C(z) = z\frac{\mathrm{d}}{\mathrm{d}z}A(z)$$

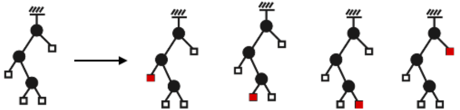
improve the prevalence of larger objects in size distr.

- reshapes size distribution while **preserving uniformity at given size**
- changes profile from "peaked" (inefficient) to "flat" (efficient)

$$\mathcal{B} = \mathcal{Z} + \mathcal{B} \times \mathcal{B} \quad \Longrightarrow \quad \begin{cases} \mathcal{B} & = \quad \mathcal{Z} + \mathcal{B} \times \mathcal{B} \\ \mathcal{B}^\bullet & = \quad \mathcal{Z} + \mathcal{B}^\bullet \times \mathcal{B} + \mathcal{B} \times \mathcal{B}^\bullet. \end{cases}$$

1, 1, 3, 9, 1, 1, 1, 5, 12, 1, 1, 1108, 1, 1, 1, 4, 1, 42, 5, 4, 16, 3, 1, 1, 2, 1, 1, 2, 3, 1, 1, 341, 1, 2, 18, 8, 1, 14, 30, 1, 2, 1, 114, 1, 1, 4, 3, 2, 2, 1, 2, 4, 1, 1, 1, 360, 1, 1, 3, 1, 2, 3, 1, 1, 1, 417, 1, 3, 3, 429, 1, 16, 1, 1, 1, 1, 1, 1, 1, 55, 38, 1, 1, 1, 1, 1, 2, 1, 1, 4, 1, 1, 14, 3, 2, 1, 3, 3, 1, 1

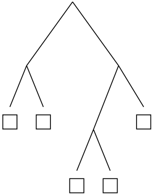
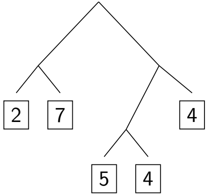
2995, 4, 18, 575, 191, 6, 2697, 2656, 665, 503, 1, 488, 433, 250, 7458, 165, 32, 368, 1384, 1487, 756, 636, 50, 1520, 4974, 866, 1346, 14, 6289, 9, 3775, 85, 687, 79, 6228, 947, 1325, 8, 1, 65, 1, 375, 307, 31, 12, 32, 184, 1094, 2824, 3282, 383, 188, 1435, 277, 1340, 52, 4659, 2089, 3423, 244, 17, 396, 23, 5, 2129, 1330, 9760, 2403, 520, 197, 1816, 9, 249, 867, 799, 59, 62, 1758, 19, 4393, 1783, 1, 373, 146, 363, 5154, 2494, 114, 1137, 1, 1887, 136, 43, 87, 79, 67, 21, 867, 72, 2



a tree of size 4
is "copied" 4 times

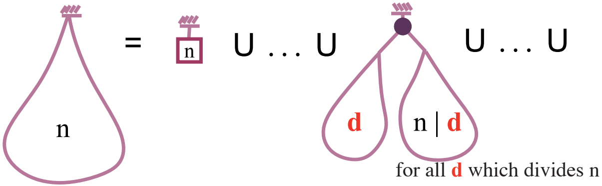
IV. Advanced example: Dirichlet sampling

Multiplicative object that cannot be generated any other way

ADDITIVE (traditional objects)	MULTIPLICATIVE[1]
$\alpha \in \mathcal{A},\ \beta \in \mathcal{B}\ \ \lvert(\alpha,\beta)\rvert = \lvert\alpha\rvert + \lvert\beta\rvert$	$\alpha \in \mathcal{A},\ \beta \in \mathcal{B}\ \ \lvert(\alpha,\beta)\rvert = \lvert\alpha\rvert \cdot \lvert\beta\rvert$
unique atom $\mathcal{Z}$ of unit size 1	**infinity** of atoms, $\mathcal{Z}_m$ $(m \in \mathbb{Z}_{>0})$
$\mathcal{A} = \mathcal{Z} + \mathcal{A} \times \mathcal{A}$	$\mathcal{M} = \mathcal{I} \setminus \mathcal{Z}_1 + \mathcal{M} \times \mathcal{M}$
	
$1+1+1+1+1=5$	$2 \times 7 \times 5 \times 4 \times 4 = 1120$
Ordinary GF or Exponential GF	Dirichlet GF
$\sum_{k=0}^{\infty} a_k z^k \qquad \sum_{k=0}^{\infty} \frac{a_k}{k!} z^k$	$\sum_{k=1}^{\infty} a_k \frac{1}{k^s}$

[1] First considered from a symbolic/combinatoric perspective by Hwang (1994).

recursive method: not efficient for multiplicative objects



$$b_n = 1 + \sum_{\substack{d|n \\ 1<d<n}} b_d \cdot b_{n|d}$$

PROBLEMS of efficiency

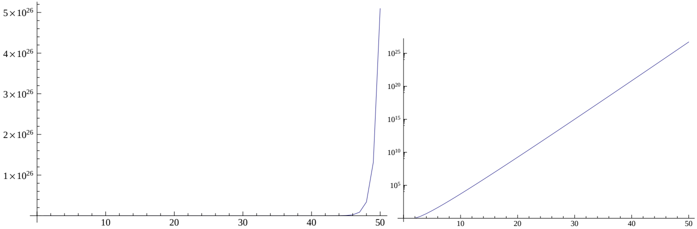
- sizes (wrt. number of "nodes") exponentially larger than for additive objects
- requires **factor decomposition** which is (too) costly

PROBLEMS of quality

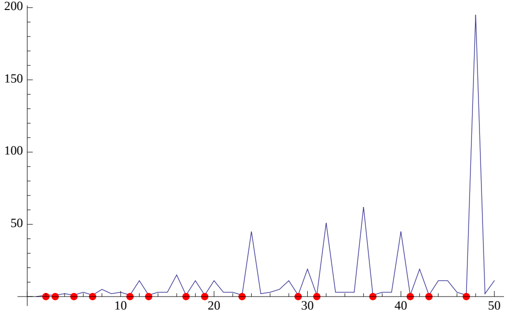
- size distribution is highly irregular

size distributions (# obj. of given size)

additive binary trees (plot then logplot)



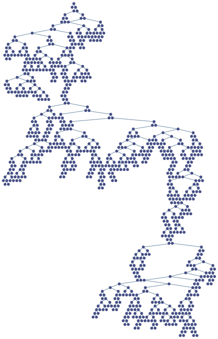
multiplicative (binary) branching factorizations



extending the idea to multiplicative objects

Theorem [Bodini & L. 2012]. Let $\mathcal{C}$ be a multiplicative combinatorial class described with: disjoint union, cartesian product, sequence, well-founded recursion, etc.

Under some hypotheses on the generating function, a Dirichlet sampler for $\mathcal{C}$ can generate an object of size n, with some error $\varepsilon \in (0,1)$, in $O(\log(n)^2)$ worst-case time complexity.



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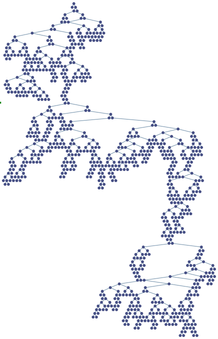
- Zeta-distributed atoms sampled in $O(1)$ [Devroye 1986]
- resorts to analytic number theory: specifically Delange's Tauberian theorem, as equivalent of Flajolet-Odlyzko transfer theorem in additive combinatorics
- tuning of control parameter completely different: in additive analytic ("Boltzmann") sampling, direct inversion of expected value; here expected value is infinite and requires *ad-hoc* tuning informed from theorem



ordered factorizations, $\mathcal{F} := \mathsf{Seq}\left(\mathcal{I} \setminus \mathcal{Z}_1\right)$

$$
\begin{array}{l}
\Gamma\mathrm{D}_s\left[\mathcal{F}\right] := \{ \\
\qquad \lambda \leftarrow \zeta(s) - 1; \\
\qquad K \in \mathrm{Geo}(\lambda); \\
\qquad \text{return } \big(\underbrace{\Gamma\mathrm{D}_s\left[\mathcal{I} \setminus \mathcal{Z}_1\right], \ldots, \Gamma\mathrm{D}_s\left[\mathcal{I} \setminus \mathcal{Z}_1\right]}_{K \text{ times}}\big) \\
\}
\end{array}
$$

```
OrderedFactorization[10^200, 0.5] // AbsoluteTiming

{17.002826, {598,
  94 315 438 343 755 964 449 064 464 145 270 360 907 587 302 431 535 020 906 407 \
   589 438 865 191 662 481 620 456 946 846 202 450 914 444 733 710 252 639 029 \
   394 242 922 918 929 394 271 546 094 283 086 276 198 942 107 362 365 753 807 \
   339 520 000 000 000 000 000 000 000,
  {4, 3, 5, 131, 2, 9, 5, 3, 4, 3, 4, 3, 51, 5, 2, 7, 3, 3, 3, 2, 2, 2, 4,
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   2, 12, 7, 2, 2, 4, 2, 3, 2, 54, 2, 27, 9, 18, 2, 3, 41, 8, 2, 44, 2,
   3, 2, 4, 2, 3, 2, 3, 2, 4, 17, 4, 5, 2, 5, 2, 53, 8, 2, 40, 2, 2, 4,
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   33, 3, 4, 3, 7, 523, 3, 10, 3, 3, 2, 12, 3, 86, 67, 4, 2, 2, 2, 2}}}
```
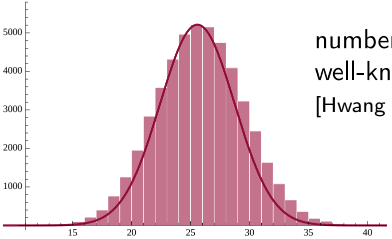
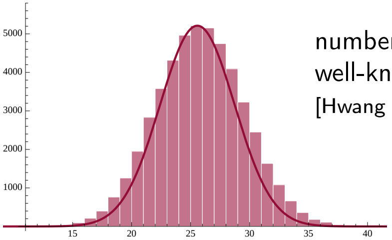

ordered factorizations, $\mathcal{F} := \mathrm{Seq}(\mathcal{I} \setminus \mathcal{Z}_1)$



number of factors in random ordered factorizations well-known to be **normally distributed**

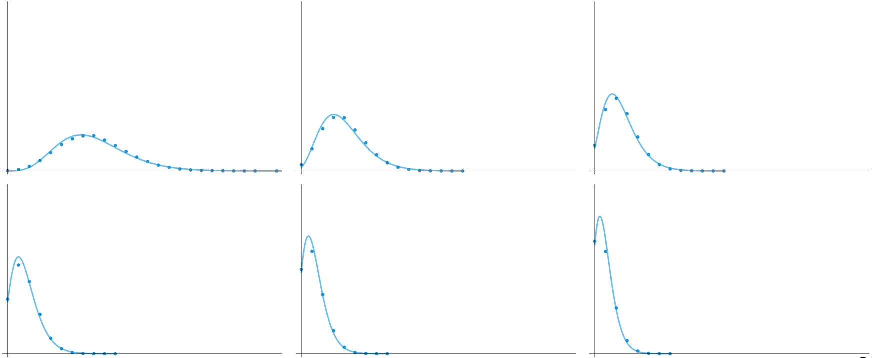
[Hwang 1999] [Hwang and Janson 2009]

ordered factorizations, $\mathcal{F} := \mathrm{Seq}\,(\mathcal{I} \setminus \mathcal{Z}_1)$



number of factors in random ordered factorizations
well-known to be **normally distributed**
[Hwang 1999] [Hwang and Janson 2009]

\# of factors equal to $m = 2, 3, \ldots$ is **gamma distributed** (conjectured then proven)



other developments

other developments

Expressivity

- colored objects [Bodini, Jacquot 2006]
- multi-dimensional generation [Bodini, Ponty 2010; Bodini, L., Ponty 2014]
- holonomic specification [Bacher, Bodini, Jacquot 2013]
- planar graphs [Fusy et al. 2008]

Implementation

- oracle evaluation [Pivoteau, Salvy, Soria, 2008]
- bit complexity [Flajolet, Pelletier, Soria, 2011]
- approximate-evaluation-rejection [Bodini, Lumbroso 2014]

Other

- use the samplers as a proof model [Steger, Panagiotou] conclusion