Infinite Boltzmann Samplers and Applications to Branching Processes

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ABSTRACT. In this short note, we extend the Boltzmann model for combinatorial random sampling [8] to allow for infinite size objects; in particular, this extension now fully includes Galton-Watson processes. We then illustrate our idea with two examples, one of which is the generation of prefixes of infinite Cayley trees.

1. INTRODUCTION

Boltzmann sampling, introduced by Duchon, Flajolet, Louchard and Schaeffer [8] in 2001, is an automatic random generation method: it can directly derive random samplers from any combinatorial description, without requiring *ad-hoc* bijections or modifications; and it does so, without precomputations, by evaluating the generating function which enumerates the combinatorial class. The efficiency of this method (it can sample from most classes in time linear with respect to the size of the output) coupled with its genericity have made it fairly popular: since it's inception it has seen many theoretical developments [5, 6, 9, 3], and many practical applications [7, 2, 12].

The concept developed in the original paper nevertheless presents an important restriction: classes must have a combinatorial generating function which is analytic[1] in 0, and the size distribution of the generated objects must remain in $\mathbb{N}$. In other words, the probability of drawing an object of infinite size if always zero. For instance, while binary planar trees constructed by a Boltzmann sampler can be considered in all respects as Galton-Watson processes [1, §1], the infinite-size limitation restricts us to extinction probabilities that are larger than $1/2$—and this limitation seems trite.

In this note, we extend the definition of Boltzmann samplers so as to bypass this restriction. Our approach is quite unique in analytic combinatorics (see [11] for an overview of the topic) as, when considering the equation derived from the combinatorial specification, it no longer restricts itself to the unique combinatorial generating function which is analytic in 0, but instead considers other solutions.

Because of the succinctness of this note, we assume our reader is familiar with the Boltzmann method, as well as with analytic combinatorics.

2. GENERALIZING THE BOLTZMANN MODEL TO INFINITE PROCESSES

In this section, we give an extended definition of the Boltzmann distribution, so that it is now defined on $\mathbb{N} \cup \{\infty\}$. Intuitively, we downscale the existing, traditional distribution to then insert an additional probability, of the object being of infinite size.

We first introduce two technical, commonplace definitions.

Definition. Let $\mathcal{C}$ be a combinatorial class and $C(x)$ its associated generating function. We denote by $E_{\mathcal{C}}(z, C(z))$ the functional equation derived from the recursive[2] specification of the combinatorial class $\mathcal{C}$ and we denote by $V_{\mathcal{C}}$ the 1-manifold associated with the functional equation $E_{\mathcal{C}}$, and defined by

$$V_{\mathcal{C}} := \{(x, y) \mid E_{\mathcal{C}}(x, y) = 0\}.$$

[1]Recent work on random samplers for multiplicative classes [4], which are enumerated by Dirichlet generating functions, has already been confronted with a situation where this is no longer the case.

[2]We only consider infinite size objects resulting from *branching* processes; thus all the combinatorial specifications we consider are *recursive*.

Example. *For instance, for unary-binary trees, the specification is $\mathcal{U} = \mathcal{Z} + \mathcal{ZU} + \mathcal{ZU}^2$, the ordinary generating function is $U(z) = z + zU(z) + zU(z)^2$ and $E_{\mathcal{U}}(z, U(z)) = z + zU(z) + zU(z)^2 - U(z)$ which can be rewritten as a bivariate polynomial $E_{\mathcal{U}}(x, y) = x + xy + xy^2 - y$. Thus, $V_{\mathcal{U}} := \{(x, y) \mid x + xy + xy^2 - y = 0\}$.*

Definition. Let $\mathcal{C}$ be a combinatorial class and $V_{\mathcal{C}}$ be the 1-manifold associated to its functional equation. A point $(x, y) \in V_{\mathcal{C}}$ is called *Boltzmann-valid* if and only if:

- $x \in \mathbb{R}_{>}$;
- $y \in \mathbb{R}_{>}$;
- $y \geqslant C(x)$.

We denote by $T_{\mathcal{C}}$ the set of Boltzmann-valid points.

We are now equipped to define the main topic of this paper.

Definition. The *infinite-Boltzmann* distribution associated with $(x, y) \in T_{\mathcal{C}}$, for the random variable $N \in \mathbb{N} \cup \{\infty\}$ is defined as follows,

$$\mathbb{P}[N = n] = \frac{c_n x^n}{y} \qquad \text{and} \qquad \mathbb{P}[N = \infty] = 1 - \frac{C(x)}{y} \qquad \text{with} \qquad C(x) = \sum_{\gamma \in \mathcal{C}} x^{|\gamma|} = \sum_{n=0}^{\infty} c_n x^n.$$

Notice that $C(z)$ (the generating function of the combinatorial class) is the unique solution of $E_{\mathcal{U}}(z, C(z))$ which is analytic in 0 and which has non-negative coefficients; furthermore for $(x, y) \in V_{\mathcal{C}}$ such that $y = C(z)$, we return to the classical Boltzmann distribution, under which $\mathbb{P}[N = \infty] = 0$.

3. Infinite-Boltzmann samplers

This section introduces the concrete rules needed to construct infinite-Boltzmann samplers, and is in divided in two parts: one for unlabeled classes and the other for labeled classes. As usual, much of this will feel redundant to those familiar with the initial paper [8]; to keep this section brief we will use the abbreviated notations used therein, for instance,

$$\begin{aligned} \mathrm{Ber}(p) \Rightarrow A \mid B \qquad &\equiv \qquad \{\ \textbf{if}\ \mathrm{Ber}(p) = 1\ \textbf{then}\ A\ \textbf{else}\ B\ \} \\ \mathrm{Geo}(p) \Rightarrow A \qquad &\equiv \qquad \{\ k = \mathrm{Geo}(p)\,;\ \text{return a } k\text{-tuple of independent calls to } A \} \end{aligned}$$

and this second construction is generalized to Poisson and log-series distributions.

3.1. Infinite-Boltzmann samplers for unlabeled classes. Let $\mathcal{C}$ be an unlabeled combinatorial class, an *infinite-Boltzmann sampler*, denoted by $\Gamma_{(x,y)}$, of parameters $(x, y) \in T_{\mathcal{C}}$ is a random algorithm which draws an objects $\gamma \in \mathcal{C}$ following the distribution $\mathbb{P}[\gamma] = x^{|\gamma|}/y$, where $|\gamma|$ is the size of the object γ. This distribution is the infinite-Boltzmann distribution which we defined in the previous section.

We now wish, as in the original paper, to constructively describe infinite-Boltzmann samplers.

The first bricks are samplers for the neutral class and the atomic class (*i.e.* classes with only one element of size respectively 0 and 1). They just return the unique element in their class.

Disjoint Union. Let $\Gamma_{(x,y_A)}\mathcal{A}$ (resp. $\Gamma_{(x,y_B)}\mathcal{B}$) be an infinite-Boltzmann sampler for unlabeled class $\mathcal{A}$ (resp. $\mathcal{B}$), then the following rule gives an infinite-Boltzmann sampler for the unlabeled class $\mathcal{C} = \mathcal{A} + \mathcal{B}$,

$$\Gamma_{(x,y_A+y_B)}\mathcal{C} := \mathrm{Ber}\left(\frac{y_A}{y_A + y_B}\right) \Rightarrow \Gamma_{(x,y_A)}\mathcal{A} \mid \Gamma_{(x,y_B)}\mathcal{B}.$$

Cartesian Product. Let $\Gamma_{(x,y_A)}\mathcal{A}$ (resp. $\Gamma_{(x,y_B)}\mathcal{B}$) be an infinite-Boltzmann sampler for unlabeled class $\mathcal{A}$ (resp. $\mathcal{B}$), then the following rule gives an infinite-Boltzmann sampler for the unlabeled class $\mathcal{C} = \mathcal{A} \times \mathcal{B}$,

$$\Gamma_{(x,y_A \cdot y_B)}\mathcal{C} := (\Gamma_{(x,y_A)}\mathcal{A}, \Gamma_{(x,y_B)}\mathcal{B}).$$

Sequence. The sequence operator $\textsc{Seq}$ can be recursively defined from the disjoint union and the Cartesian product—$\mathcal{C} = \textsc{Seq}\,(\mathcal{A}) \equiv \mathcal{C} = 1 + \mathcal{AC}$—we can therefore deduce the correct sampler from the two previous rules,

$$\Gamma_{(x,1/(1-y_A))}\mathcal{C} := \mathrm{Geo}(y_A) \Rightarrow \Gamma_{(x,y_A)}\mathcal{A}.$$

Similarly, we can extend unlabeled Boltzmann samplers given in Flajolet *et al.* [10], such as the cycle and the multiset, by similarly rewriting their rules.

3.2. Infinite-Boltzmann samplers for labeled classes. Consider now labeled combinatorial structures $\mathcal{C}$ in which a labeled object of size n is an object composed of n distinct (labeled) atoms. We can adapt the notion of Boltzmann-validity by considering the point (x, y) verifying the functional equation $E_{\mathcal{C}}(z, C)$ and the three properties: $x \in \mathbb{R}_{>}$, $y \in \mathbb{R}_{>}$, $y \geqslant \hat{C}(x)$ where $\hat{C}(z)$ is the exponential generating function of $\mathcal{C}$.

Let $\mathcal{C}$ be a labeled combinatorial class, the generalized Boltzmann distribution with parameters $(x, y) \in T_{\mathcal{C}}$ for the random variable N with values in $\mathbb{N} \cup \{\infty\}$ is defined as follows:

$$\mathbb{P}[N = n] = \frac{c_n x^n}{n! y} \qquad \text{and} \qquad \mathbb{P}[N = \infty] = 1 - \frac{\hat{C}(x)}{y} \qquad \text{with} \qquad \hat{C}(x) = \sum_{\gamma \in \mathcal{C}} \frac{x^{|\gamma|}}{|\gamma|!} = \sum_{n=0}^{\infty} \frac{c_n x^n}{n!}.$$

As for unlabeled classes, samplers for the neutral class and the atomic class (*i.e.* classes just return the unique element in their class. The rules for the disjoint union, the Cartesian product and the sequence are the same as in the labeled case. Now however, the set and cycle constructions are sufficiently simple that we can give them here.

Set. Let $\Gamma_{(x,y_A)}\mathcal{A}$ be an infinite-Boltzmann sampler for labeled class $\mathcal{A}$, if $\mathcal{C} = \textsc{Set}\,(\mathcal{A})$, then

$$\Gamma_{(x, \exp\,(y_A))}\mathcal{C} := \mathrm{Poi}(y_A) \Rightarrow \Gamma_{(x,y_A)}\mathcal{A}.$$

Cycle. Let $\Gamma_{(x,y_A)}\mathcal{A}$ be an infinite-Boltzmann sampler for labeled class $\mathcal{A}$, if $\mathcal{C} = \textsc{Cyc}\,(\mathcal{A})$, then

$$\Gamma_{(x, \ln(1/(1-y_A)))}\mathcal{C} := \mathrm{Loga}(y_A) \Rightarrow \Gamma_{(x,y_A)}\mathcal{A}.$$

4. Examples

We propose two applications of our extension. The first one consists in showing how we can fully include infinite process in the Boltzmann model. The second one shows a simulation of the prefix of a random infinite Cayley tree.

4.1. Galton-Watson processes. A direct application of the infinite-Boltzmann model is the full integration of branching processes of Galton-Watson [1] in it. Here we will apply the principle in the case of the simplest branching processes: that is, one where each vertex has a probability p of extinction (leaf) and a probability $1 - p$ to have two children.

When $p < 1/2$, one has a nonzero probability of having an infinite process which could not be considered in the classical Boltzmann model. We describe later in this section how thanks to the sampling under infinite-Boltzmann model, it is possible to reproduce the Galton-Walton process even in the infinite case.

This branching process immediately returns to the symbolic specification of binary trees which is : $\mathcal{T} = \mathcal{Z} + \mathcal{Z}\mathcal{T}^2$, The set of valid points is $T_{\mathcal{T}} = \{(x, y),\, x \leq 1/2,\, x + xy^2 = y\}$.

So, for every $(x, y) \in T_{\mathcal{T}}$, we have the sampler $\Gamma_{(x,y)}\mathcal{T} := \mathrm{Ber}(x/y) \rightarrow (\blacksquare | [\blacksquare, \Gamma_{(x,y)}\mathcal{T}, \Gamma_{(x,y)}\mathcal{T}])$

Now, the couples $(x, y) \in T_{\mathcal{T}}$ can be partitioned in two classes, couples of the shape $C_1 = \{(\frac{1-\sqrt{1-4\,x^2}}{2x}), \forall 0 \leq x \leq 1/2\}$ and whose of the shape $C_2 = \{(\frac{1+\sqrt{1-4\,x^2}}{2x}), \forall 0 \leq x < 1/2\}$. The class C_1 corresponds to the branching processes with $p \geq 1/2$ and could already be reached with classical Boltzmann sampling. The class C_2 henceforth allows to reach the branching processes with $p < 1/2$. The figure 1 shows the probability that the process does not finish in function to the stop probability p.

Of course, the main interest of this example is to highlight how infinite-Boltzmann sampler can now include the infinite branching processes.

In order to complete our considerations, the next paragraph is dedicated to prove that in the case of simple variety of trees (i.e. when the functional equation is of the shape $t = z\phi(t, z)$ with ϕ a bivariate polynomial) for every α in $]0, 1[$, there exists a unique $(x, y) \in V_{\mathcal{C}}$ such that $\alpha = \frac{x}{y}$. In other words, we want to prove that our new Boltzmann model contains Galton-Watson processes for every probability of death.

First we recall a corollary of the Descartes rule of sign.

Lemma 1. *Let $p = a_0 + \cdots + a_d x^d$ be a univariate polynomial such that for all $i \geq 1, a_i \leq 0$ and p is a non constant polynomial. Then, the equation $p(x) = 0$ has exactly one positive solution if $a_0 > 0$, and no positive solution otherwise.*

Proof. The Descartes lemma ([13, page 121]) states that the number of positive solutions is bounded by the number of sign alternation in the coefficient vector. Moreover, the number of positive solutions has the same parity as the number of sign alternation. If $a_0 > 0$, the number of sign alternation is 1, else, it is 0, hence the result. ☐

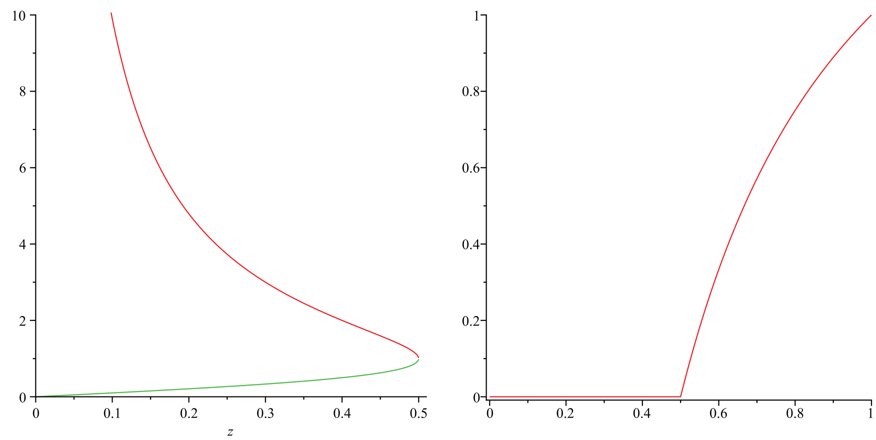


Figure 1. On the left, the curve of the valid points for the class of binary trees. On the right, the probability that the process does not finish according to the death probability.

Lemma 2. *Let p be a bivariate polynomial of the form $p(x,y) = y - xq(x,y)$, where q is a polynomial non-constant, with non-negative coefficients, and such that $q(0,0) = 1$. Let V be the set of real positive points $(x,y) \in (\mathbb{R}^{*+})^2$ solution of $p(x,y) = 0$. Then the map:*

$$f: \begin{array}{ccc} V & \to &]0,1[\\ (x,y) & \mapsto & \frac{x}{y} \end{array}$$

is a bijection.

Proof. Let d be the total degree of $q(x,y)$. First, we introduce the new polynomial Q such that $(\frac{y}{x})^d Q(x, \frac{x}{y}) = q(x,y)$. If q_{ij} denotes the coefficient of $x^i y^j$ in $q(x,y)$, then Q is defined explicitly as:

$$\begin{aligned} Q(x,\alpha) &:= \sum_{\substack{0\leq k\leq d\\ d-k\leq l\leq d}} q_{k+l-d,d-l} x^k \alpha^l \\ &= q_{00}\alpha^d + \underbrace{\sum_{\substack{1\leq k\leq d\\ d-k\leq l\leq d}} q_{k+l-d,d-l} x^k \alpha^l}_{r(\alpha,x)} \end{aligned}$$

where $r(x,\alpha)$ is a polynomial whose all monomials have a degree greater or equal to 1 in x. Thus, for all $x > 0, y > 0$, the equation $y - xq(x,y) = 0$ is equivalent to:

$$(\frac{x}{y})^{d-1} - Q(x, \frac{x}{y}) = 0$$

In particular, if we denote $\frac{x}{y}$ by α, then, x is the solution of the polynomial equation:

$$s_\alpha(x) := \alpha^{d-1} - q_{00}\alpha^d - r(\alpha,x) = 0$$

By hypothesis, $x > 0$ and $y > 0$, thus $\alpha > 0$. Also, $q(0,0) = 1$ and q is non-constant, thus $q_{00} = 1$ and s_α is non-constant. According to Lemma 1, the polynomial equation $s_\alpha(x) = 0$ has a positive solution if and only if $\alpha^{d-1} - \alpha^d > 0$, which implies that $\alpha \in]0,1[$. This ensures that $f(V) \subset]0,1[$. Moreover, if $\alpha \in]0,1[$, Lemma 1 states that the positive solution of $s_\alpha(x)$ is unique. This ensures that f is bijective. □

4.2. Simulation of the prefix of infinite Cayley trees. The second application we present is the simulation of the prefix of a random infinite Cayley tree $\mathcal{T}$, which are a labelled trees such that each vertex has a finite number of children. Therefore the specification of Cayley trees is $\mathcal{T} = \mathcal{Z} \times \textsc{Set}(\mathcal{T})$.

By applying the rules given previously, the infinite-Boltzmann sampler is:

$$\Gamma_{(x,x\cdot e^y)}\mathcal{T} = (\mathcal{Z}, \left[\text{Poi}(y) \Longrightarrow \Gamma_{(x,y)}\mathcal{T}\right]).$$

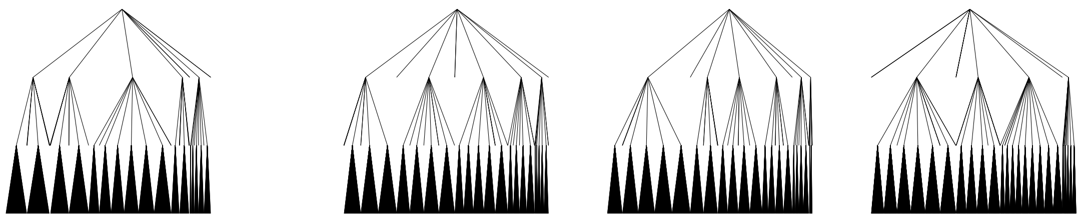
We are interested in generating the prefix of a height H of an infinite Cayley tree, which is the set of vertices of the tree from the root to the height H. To obtain this prefix, we construct the tree $\mathcal{T}$ in depth, which allows us to control the development of its branches.

The generator of a prefix at height less than or equal to H of a Cayley tree of infinite size is given by the following algorithm:

Algorithme 1: $\Gamma_{(x, x \cdot e^y)} \mathcal{T}$

Input : parameters x, y, H
Output : prefix of height $\leq H$ of infinite Cayley tree
while *($h \leq H$)* **do**
  For any vertex v of height h do: $k = \mathrm{Poi}(y)$, add k sons to v
  $h = h + 1$
return tree

Simulation of the algorithm 1 for different values of the parameters (x, y, H) gives the following prefix of infinite Cayley trees :



$(0.5, 0.3, 4)$: Standard Boltzmann sampler $\quad (0.24, 0.34, 4) \quad (0.16, 0.20, 4) \quad (0.35, 0.80, 4)$.

Remark. Note that this algorithm is iterative—as opposed to recursive like all Boltzmann samplers—because as we perhaps wish to increase the size of the height during the course of the algorithm, it is a more natural way to write the algorithm; in this form, it also bears a striking resemblance with the definition of branching processes.

That said however, it would be equivalent to write this as a regular recursive Boltzmann sampler, with an additional parameter H recursively tracking the height and only making recursive calls if it is not past the desired height.

5. Complexity analysis

It is natural to ask whether our extension can be applied efficiently in practice. Specifically, two questions may come to mind. First, what is the complexity for generating the prefix of a possibly infinite tree (which, in fact, can also be considered as the "beginning of a branching process)? In this case, the answer is straightforward and is an immediate consequence of the proof given in the seminal paper [8].

Proposition 5.1. *At each step of the computation, an infinite-Boltzmann sampler's complexity (measured in the number of real-arithmetic operations) is linearly proportional to the number of atoms which have been outputted.*

The second question we can ask ourselves is whether the ability to generate infinite trees can be diverted to advantageously generate large (but finite) approximate-size trees.

Currently in the Boltzmann model, the best way to generate approximate-size trees is to choose a control parameter near the dominant singularity, and to generate and discard trees until one is obtained which is within the desired size interval. It well-known that although of a constant order, the number of discarded trees is large, with many small trees sampled before a satisfyingly large one is produced. If we target infinite trees however, we can expect to discard fewer trees. However this is counterbalanced by the fact that the trees with are then discarded (with *anticipated rejection*, which consists in interrupting the construction of the tree as soon as it becomes larger than the target interval, see [4, §1.4] for a practical application of this concept) are much larger on average. This is summarized in the following proposition essentially proved in [8].

Proposition 5.2. *The probability generating function $F(u)$ for the cost of an interrupted infinite-Boltzmann sampler targeting objects of size within $[n_1, n_2]$*

$$F(u) = \frac{1}{1 - \left(\sum_{n<n_1} \frac{a_n x^n u^n}{y} + u^{n_2} \sum_{n<n_2} \frac{a_n x^n}{y}\right)} \sum_{n \le n_1 \le n_2} \frac{a_n x^n u^n}{y},$$

where $F(u) := \sum_k \mathbb{P}[Cost = k]\, u^k$.

The mean of the cost is done by $\mathbb{E}(Cost) = \frac{\partial}{\partial u} F(u)|_{u=1}$, and A full analysis can be done to prove that the average cost is linear when then combinatorial class is given by a recursive specification which is irreducible and aperiodic.
Remark. The alternate idea of building large trees by truncating, in some way, infinite trees seems like it would be much too complicated with our current tools—indeed the problem of how to truncate the tree so that overall the distribution is still uniform is non-trivial.

6. Conclusion

While the Boltzmann sampling method usually involves evaluating generating series, in this note, we use instead the functional equation related to the specification. This slight extension (which is derived from the symbolic method, and hence makes an underlying use of generating functions) allows us to efficiently simulate unbounded branching processes in a new way, while remaining in the Boltzmann framework.

Whether this method has any practical advantages over traditional ways of simulating branchings processes remains to be seen. However, our main interest resides in the fact that this new approach seems very promising with regards to the optimization of Boltzmann samplers. Indeed, in work in progress, we pursue a further extension of this idea which allows us to circumvent the main problem of Boltzmann sampling which is the calculation of the oracle (in contrast with previous approaches that sought to efficiently calculate the oracle).

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