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Random Generation from Boltzmann Principles

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Abstract

This talk proposes a new framework for random generation of combinatorial configurations based on Boltzmann models. The idea is to perform random generation of possibly complex structured objects by placing an appropriate measure on the whole of a combinatorial class. The resulting algorithms often operate in linear time. This talk refers to a joint work with P. Duchon, G. Louchard, and G. Schaeffer, to appear in ACM STOC 2002.

1. Introduction

The problem considered here is that of generating samples of structured combinatorial objects of a certain size. In the usual setting of combinatorics, the objects should be drawn uniformly at random from the family of all objects of the same size (see, e.g., [1, 2]).

The basic principle of Boltzmann method is to relax the constraint of generating objects of a strictly fixed size, and prefer to draw objects with a somewhat randomly fluctuating size. The algorithms developed make use of a continuous control parameter $x > 0$. One can tune the value of x in order to draw objects of a size in some vicinity of a target size n.

2. Boltzmann Models

Let $\mathcal{C}$ be a combinatorial class, where each object γ has a size denoted by $|\gamma|$, and $\mathcal{C}_n$ the subclass of objects of size n. The class $\mathcal{C}$ is represented by the ordinary generating function $C(x) = \sum_{\gamma\in\mathcal{C}} x^{|\gamma|}$ in the case of unlabelled objects, and in the case of labelled objects, by the exponential generating function $C(x) = \sum_{\gamma\in\mathcal{C}} \frac{x^{|\gamma|}}{|\gamma|!}$. Only coherent values of x are to be considered, that is $0 < x < \rho_C$ where ρ_C is the radius of convergence of C.

Definition 1. The *Boltzmann model* of parameter x assigns to any object $\gamma \in \mathcal{C}$ the probability $\mathbf{P}_x(\gamma) = x^{|\gamma|}/C(x)$. A *Boltzmann generator* $\Gamma C(x)$ for a class $\mathcal{C}$ is a process that produces objects from $\mathcal{C}$ according to a Boltzmann model.

Let us point out that the Boltzmann model of parameter x, conditioned by the fact that the size of the object drawn equals n, obviously coincides with the uniform model on $\mathcal{C}_n$. Given a Boltzmann generator $\Gamma C(x)$, we thus have a rejection algorithm $\mu C(n)$, sampling uniformly over $\mathcal{C}_n$, which simply writes as: `repeat` $\gamma := \Gamma C(x)$ `until` $|\gamma| = n$. Random generation of "approximate size" is obtained by weakening the halting condition of the "repeat" loop. For instance, we refer to $\mu C(n, \varepsilon)$, where ε is a certain tolerance, for the sampler halting with condition $|\gamma| \in \big[n(1-\varepsilon), n(1+\varepsilon)\big]$.

3. Constructions for Boltzmann Generators

Let us first deal with unlabelled objects and ordinary counting generating functions. We consider combinatorial classes, constructed from finite classes by means of disjoint union, cartesian product, and sequence construction. It is well known that the corresponding functional operations on generating functions are sum, product, and quasi-inverse.

- If $\mathcal{C} = \mathcal{A} + \mathcal{B}$, a Boltzmann generator for $\mathcal{C}$ is built by calling a Boltzmann generator, either for $\mathcal{A}$ (with probability $A(x)/C(x)$) or for $\mathcal{B}$ (with probability $B(x)/C(x)$).
- If $\mathcal{C} = \mathcal{A} \times \mathcal{B}$, a Boltzmann generator for $\mathcal{C}$ generates a pair of independent elements, the first one drawn by a Boltzmann generator for $\mathcal{A}$, and the second by a Boltzmann generator for $\mathcal{B}$.
- If $\mathcal{C} = \mathrm{Seq}(\mathcal{A})$ then $\mathcal{C}$ is the solution to the symbolic equation $C = 1 + \mathcal{AC}$ which recursively involves the operations of union and product mentioned above. Equivalently, a Boltzmann generator for $\mathcal{C}$ can be built by drawing K randomly according to the geometric distribution with parameter $A(x)$ and then drawing K independent elements with a Boltzmann generator for $\mathcal{A}$.

Theorem 1. *A Boltzmann generator constructed from specifications and rules above:*

1. *draws correctly from Boltzmann model;*
2. *halts with probability 1 with finite expected time;*
3. *has a complexity linear in the size of output object.*

In the case of labelled objects and exponential generating functions, the exponential Boltzmann generator is built according to similar rules, and even extended to cycle and set combinatorial constructions and the analogue of Theorem 1 holds.

4. Efficiency

Since the size N of the object produced by a Boltzmann model of parameter x has mean value $\mathbf{E}_x(N) = x\frac{C'(x)}{C(x)}$, the tuning parameter is set to the solution x_n of the equation $n = x\frac{C'(x)}{C(x)}$.

Theorem 2. *Under some technical conditions on $C(x)$, the rejection sampler $\mu C(n, \varepsilon)$, equipped with the value $x = x_n$, succeeds in one trial with probability tending to 1 as $n \to \infty$.*

Sometimes, although the technical conditions are not satisfied, drawing with approximate size can still be done in linear-time complexity with adapted halting condition. Let us mention the case of generators of supercritical sequences (a sequence $\mathcal{C} = \mathrm{Seq}(\mathcal{A})$ is said to be supercritical if $\rho_A > \rho_C$).

Theorem 3. *For supercritical sequences, the adapted singular Boltzmann generator produces a random object of size $n + O(1)$ in one trial, with high probability. And it hits n exactly in $A'(\rho_C)$ trials on average.*

Bibliography

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