Multiparametric Boltzmann sampling and applications

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Random sampling

Problem

Suppose that some implicit description of $\ensuremath{\mathbb{P}}$ is provided.

Let $X \sim \mathbb{P}$, sample X

Framework

- Which descriptions of \mathbb{P} are admitted?
- If \mathbb{P} is parametric, what is pre- and computation complexity?
- What error margin is allowed?

Why random sampling?

Motivations for random sampling

- Art and entertainment
 - T-shirt printing
 - Paintings, decorations, tilings
 - Music composition
 - Artificial intelligence artwork
- Monte-Carlo simulations
 - Property-based software testing (QUICкСнеск, lambda terms)
 - Biology (cell dynamics, RNA structures)
 - Statistical physics (random maps, Bose-Einstein condensate, Ising model, tilings, plane partitions)

Theoretical computer science

- Random permutations, sorting algorithms, cellular automata
- Random graphs and community detection
- Crypto primitives and low-level programming
- Concurrent process analysis, queueing systems
- Automata sampling

Outline of the current talk



Part I. Generating functions and Boltzmann samplers

Generating functions and the symbolic method

Framework

- Discrete objects are represented by words in a finite alphabet.
- The *size* of the object is the number of its letters.
- Let a_n be the number of words of length n

Generating function of the counting sequence:

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







The cartesian product

 $(a_0 + a_1z + a_2z^2 + \dots)(b_0 + b_1z + b_2z^2 + \dots) = c_0 + c_1z + c_2z^2 + \dots$



The convolution rule corresponding to EGF:

$$c_n = \sum_{k=0}^n a_k b_{n-k}$$

Example: lambda terms in de Bruijn notation



Example: lambda terms in de Bruijn notation

$$\mathcal{L} ::= \lambda \mathcal{L} \mid (\mathcal{L}\mathcal{L}) \mid \underline{\mathbf{n}} \qquad \qquad \mathcal{L}(z) = z\mathcal{L}(z) + z\mathcal{L}(z)^2 + \frac{z}{1-z}$$
$$\underline{\mathbf{n}} ::= \underline{\mathbf{0}} \mid \underline{\mathbf{Sn}}. \qquad \qquad \mathcal{T}_n = \mathcal{T}_{n-1} + \sum_{k=1}^n \mathcal{T}_k \mathcal{T}_{n-k-1} + 1$$



Recursive sampling

Algorithm 1: Recursive algorithm for plain lambda terms

Input: Integer n

Output: Plain lambda term of size n

begin

Precompute array $(T_k)_{k=0}^n$ using the recurrence

$$T_n = T_{n-1} + \sum_{k=1}^n T_k T_{n-k-1} + 1$$
, $T_0 = 0$

For each *n*, precompute the probability distribution \mathcal{P}_n :

$$p_{\lambda}^{(n)} = \frac{T_{n-1}}{T_n}, \quad p_k^{(n)} = \frac{T_k T_{n-k-1}}{T_n}, \quad p_{\underline{n}} = \frac{1}{T_n}$$

Function Generate (n): if n = 1 then $\lfloor return \underline{0} // minimal de Bruijn index;$ Sample index k from the probability distribution \mathcal{P}_n ; if $k = \lambda$ then $\lfloor return \lambda Generate(n-1) // abstraction;$ if $k = \underline{n}$ then $\lfloor return \underline{n} // de Bruijn index;$ L := Generate(k); R := Generate(n-k-1);return (LR) // application;

Boltzmann sampling

Algorithm 2: Boltzmann sampler for plain lambda terms

Input: Integer number n

Output: Random term of variable size, target expected size *n* **begin**

Precompute z as a function of n // stay tuned Function Generate(z):

Carefully look at the equation

$$L(z) = zL(z) + zL(z)^{2} + \frac{z}{1-z}$$

Flip a weighted coin $X \in \{\lambda, @, \underline{n}\}$ with weights

$$\mathbb{P}_{\lambda} = \frac{zL(z)}{L(z)}, \quad \mathbb{P}_{@} = \frac{zL^{2}(z)}{L(z)}, \quad \mathbb{P}_{\underline{n}} = \frac{z}{L(z)}$$

if $X = \lambda$ then return λ Generate (n - 1) // abstraction; if X = @ then L := Generate(z); R := Generate(z);return (LR) // application; if $X = \underline{n}$ then return Geom(z) // de Bruijn index;

Boltzmann distribution

Probability output of the Boltzmann samplers

Let S(z) be the generating function of the language S:

$$S(z) = \sum_{n \ge 0} a_n z^n$$

Consider a distribution \mathbb{P}_z on words $w \in S$:

• conditioned on word length |w| = n, the distribution is uniform

length distribution follows Gibbs law

$$\mathbb{P}_z(|w|=n)=\frac{a_n z^n}{S(z)}$$

expected word length:

$$\mathbb{E}_{z}(n) = z \frac{S'(z)}{S(z)}$$

Multivariate generating functions

Consider a language $S \subset \Sigma^*$ where $\Sigma = \{\bullet_1, \bullet_2, \bullet_3, \bullet_4\}$ is finite. Let a_{n_1, n_2, n_3, n_4} count the number of words $w \in S$ containing

- \blacktriangleright *n*¹ letters •₁,
- \blacktriangleright *n*² letters \bullet_2 ,
- \blacktriangleright *n*³ letters •₃,
- \blacktriangleright *n*⁴ letters •⁴;

Its multivariate generating function is

$$S(z_1, z_2, z_3, z_4) = \sum_{n \ge 0} a_{n_1, n_2, n_3, n_4} z_1^{n_1} z_2^{n_2} z_3^{n_3} z_4^{n_4}$$

Boltzmann distribution

$$\mathbb{P}(n_1, n_2, n_3, n_4 \mid z_1, z_2, z_3, z_4) = \frac{a_{n_1, n_2, n_3, n_4} z_1^{n_1} z_2^{n_2} z_3^{n_3} z_4^{n_4}}{S(z_1, z_2, z_3, z_4)}$$

Example: lambda terms and their parameters

Abstractions, variables, successors and redexes marked separately:

$$L(z, \vec{u}) = u_{(abs)} z L(z, \vec{u}) + N(z, \vec{u})$$

$$N(z, \vec{u}) = \frac{u_{(var)} z}{1 - u_{(suc)} z} + u_{(red)} u_{(abs)} z^2 L(z, \vec{u})^2 + z N(z, \vec{u}) L(z, \vec{u}).$$



Multiparametric Recursive sampling

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Algorithm 3: Recursive algorithm for plain lambda terms with parameters
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Input: Target integer parameters N, n<sub>(abs)</sub>, n<sub>(var)</sub>, n<sub>(suc)</sub>, n<sub>(red)</sub>
Output: Random term with target size N, and given parameter values
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va

```
beginPrecompute array (T_{K,k_1,k_2,k_3,k_4})_{k,k_1,k_2,k_3,k_4} using the<br/>recurrence...
```

Complexity

Memory complexity is now $\mathcal{O}(\textit{n}^5)$ and grows exponentially with the number of parameters.

Multiparametric Boltzmann sampling

Plain lambda terms with given portions of abstractions, variables, successors and redexes

$$L(z, \vec{u}) = u_{(abs)} z L(z, \vec{u}) + N(z, \vec{u})$$

$$N(z, \vec{u}) = \frac{u_{(var)} z}{1 - u_{(suc)} z} + u_{(red)} u_{(abs)} z^2 L(z, \vec{u})^2 + z N(z, \vec{u}) L(z, \vec{u})$$

Algorithm 4: Boltzmann sampler for plain lambda terms

Input: Target expectations *N*, *n*_(abs), *n*_(var), *n*_(suc), *n*_(red) **Output:** Random term with target expected size *N*, and given expected parameters

begin

Precompute $(z, u_{(abs)}, u_{(var)}, u_{(suc)}, u_{(red)})$ as functions of $(N, n_{(abs)}, n_{(var)}, n_{(suc)}, n_{(red)})$ // stay tuned; Function $\Gamma L(z, u_{(abs)}, u_{(var)}, u_{(suc)}, u_{(red)})$: Generate $X \in \{0, 1\}$ such that $\mathbb{P}(X = 0) = \frac{u_{(abs)} z L(z, \vec{u})}{L(z, \vec{u})},$ $\mathbb{P}(X = 1) = \frac{N(z, \vec{u})}{L(z, \vec{u})}$

 $\begin{array}{ll} \mathbf{X} = 0 \; \Rightarrow \; \mathbf{return} \; \lambda \Gamma \mathbf{L}(\mathbf{z}, \vec{\mathbf{u}}); \\ \mathbf{X} = 1 \; \Rightarrow \; \mathbf{return} \; \Gamma \mathbf{N}(\mathbf{z}, \vec{\mathbf{u}}); \end{array}$

Function

$$\begin{split} \Gamma N(z, u_{(abs)}, u_{(var)}, u_{(suc)}, u_{(red)}) : \\ \text{Generate } X \in \{0, 1, 2\} \text{ such that} \\ \mathbb{P}(X = 0) = \frac{\frac{u_{(var)}z}{1 - u_{(suc)}z}}{N(z, \vec{u})}, \\ \mathbb{P}(X = 1) = \frac{u_{(red)}u_{(abs)}z^2L(z, \vec{u})^2}{N(z, \vec{u})}, \\ \mathbb{P}(X = 2) = \frac{zN(z, \vec{u})L(z, \vec{u})}{N(z, \vec{u})}, \\ X = 0 \Rightarrow \text{ return } \underbrace{\text{Geom}(zu_{(suc)});}_{X = 1 \Rightarrow \text{ return }} (\overline{\lambda \Gamma L(z, \vec{u}))\Gamma L(z, \vec{u})}; \\ X = 1 \Rightarrow \text{ return } (\nabla N(z, \vec{u}))\Gamma L(z, \vec{u}); \\ X = 1 \Rightarrow \text{ return } (\nabla N(z, \vec{u}))\Gamma L(z, \vec{u}); \end{split}$$

Why Boltzmann sampling?

Exact multiparametric sampling

Suppose that S_i are defined by an unambiguous context-free grammar

$$S_i \rightarrow \sum_j T_{ij}(S_1, \ldots, S_n, \bullet_1, \bullet_2, \bullet_3, \bullet_d)$$

where $(T_{ij})_{ij}$ are transitions, and $(\bullet_1, \bullet_2, \bullet_3, \bullet_d)$ are alphabet letters.

Problem

Given positive integers $(n_1, n_2, ..., n_d)$, sample a word *w* with n_k literals of color *k* from a context-free grammar uniformly at random;

Complexity

Exact multiparametric sampling from CFG is #*P*-complete, i.e. higher in the complexity hierarchy than NP-complete.

Exact sampling is #P-complete: reduction from #2-SAT [Welsh, Gale '2001] + [Jerrum, Valiant, Vazirani '86] + [Bendkowski, Bodini, D. '2020]

Consider a 2-CNF formula

$$F = \underbrace{(\mathbf{x}_1 \lor \overline{\mathbf{x}}_2)}_{c_1} \underbrace{(\mathbf{x}_1 \lor \overline{\mathbf{x}}_4)}_{c_2} \underbrace{(\overline{\mathbf{x}}_2 \lor \overline{\mathbf{x}}_3)}_{c_3} \underbrace{(\overline{\mathbf{x}}_2 \lor \overline{\mathbf{x}}_4)}_{c_4} \underbrace{(\overline{\mathbf{x}}_3 \lor \mathbf{x}_4)}_{c_5}$$

Construct a system of algebraic equations

$$A(c_1,\ldots,c_5) = (x_1 + \bar{x}_1)\ldots(x_4 + \bar{x}_4)(1+c_1)\ldots(1+c_5)$$

where

 $x_1 = c_1 c_2, \quad \overline{x}_1 = 1, \quad x_2 = 1, \quad \overline{x}_2 = c_1 c_3 c_4, \quad \overline{x}_3 = c_3 c_5, \quad \cdots$

Then, using the notation $[\mathbf{z}^n]F(\mathbf{z}) = \mathbf{n}$ -th coefficient of $F(\mathbf{z})$,

$$#2SAT(F) = [c_1^2 c_2^2 \dots c_5^2]A(c_1, \dots, c_5)$$

Tuning of a multiparametric Boltzmann sampler



" The handles cannot be tuned independently

Multiparametric tuning complexity

Theorem (Bendkowski, Bodini, D. '2020)

For context-free grammars with L states and transitions, d parameters and target size parameter n, there is a tuning algorithm running in time

 $\mathcal{O}(d^{3.5}L\log n)$

based on convex optimisation with barriers.

Proof idea: log-sum-exp with non-negative coefficients is convex

$$f(x_1,\ldots,x_n) = \log \sum_{i=1}^n e^{x_i}$$

generating functions are reduced to log-sum-exp by variable change

Part II. Applications

Boltzmann Brain + Paganini

Grammar example: Motzkin trees with non-uniform weights



$$M(z) = z + uz^2 M(z) + z^2 M^2(z)$$

Applications and examples

- 1. Polyomino tilings
- 2. Software testing using lambda calculus
- 3. Models of random trees
- 4. RNA folding design
- 5. Bose-Einstein condensate in quantum harmonic oscillator
- 6. Permutation classes

Application 1. Tilings and performance benchmarks

Tiling example, practical benchmark



Tiling example, practical benchmark

Tilings $9 \times n$ form a regular grammar with

- 1022 tuning parameters
- 19k states
- 357k transitions

We tune for a uniform distribution for tile frequency. This results in **few hours** of tuning. Application 2. Software testing using lambda calculus

Application 2: software testing

Goal: finding bugs in optimising compilers using **corner-case** random sampling of simply typed lambda terms

The C	Glasgow Haskell	Compiler	U
			Вики Хроно
	#5557 closed	bug (fixed)	
	Code using see	q has wrong strictness	(too lazy)
	Сообщил:	michal.palka	Владелец:
	Приоритет:	high	Этап разработки:
	Компонент:	Compiler	Версия:
	Ключевые слова:	seq strictness strict lazy	Копия:
	Operating System:	Unknown/Multiple	Architecture:
	Type of failure:	Incorrect result at runtime	Test Case:

Application 2: software testing



- Plain lambda terms: Motzkin trees whose leaves contain non-negative integers.
- Closed lambda terms: Plane lambda terms whose leaf values do not exceed their unary height.
- Holy grail: simply typed lambda terms (in progress)

Application 2: software testing

Tuning uniform leaf index frequencies from 0 to 8:

TABLE 3. Empirical frequencies (with respect to the term size) of index distribution.

Index	<u>0</u>	1	2	<u>3</u>	<u>4</u>	<u>5</u>	<u>6</u>	7	<u>8</u>
Tuned frequency	8.00%	8.00%	8.00%	8.00%	8.00%	8.00%	8.00%	8.00%	8.00%
Observed frequency	7.50%	7.77%	8.00%	8.23%	8.04%	7.61%	8.53%	7.43%	9.08%
Default frequency	21.91%	12.51%	5.68%	2.31%	0.74%	0.17%	0.20%	0.07%	

Can be also tuned:

- number of atomic nodes of distinguished colors
- number of redexes (i.e. patterns necessary to perform a computation step in lambda calculus)
- number of head abstractions
- number of closed subterms
- number of any tree-like patterns

Application 3. Models of random trees

Application 3. Models of random trees

Model 1: Multi-partite rooted labelled trees

Target expectation tuning $\left(0.01, 0.03, 0.05, 0.07, 0.09, 0.11, 0.13, 0.15, 0.17, 0.19\right)$

$$T_{1}(z, u_{1}, \dots, u_{d}) = zu_{1}e^{T_{2}(z, u_{1}, \dots, u_{d})}$$
$$T_{2}(z, u_{1}, \dots, u_{d}) = zu_{2}e^{T_{3}(z, u_{1}, \dots, u_{d})}$$
$$\vdots$$
$$T_{d}(z, u_{1}, \dots, u_{d}) = zu_{d}e^{T_{1}(z, u_{1}, \dots, u_{d})}$$



Table 1: Numerical values forarguments



Application 3. Models of random trees

Model 2: Otter trees with coloured leaves

Target expectation tuning (0.01, 0.03, 0.05, 0.07, 0.09, 0.11, 0.13, 0.15, 0.17, 0.19)

$$T(z, u_1, \dots, u_d) = z \sum_{i=1}^d u_i + \mathsf{MSet}_2(T(z, u_1, \dots, u_d))$$
$$\mathsf{MSet}_2(T(z, u_1, \dots, u_d)) = \frac{T(z, u_1, \dots, u_d)^2 + T(z^2, u_1^2, \dots, u_d^2)}{2}$$



u_1z	u ₂ z	u ₃ z	u_4z	u ₅ z	u ₆ z	u7z	u ₈ z	u ₉ z	$u_{10}z$
0.005	0.015	0.025	0.035	0.044	0.054	0.063	0.072	0.081	0.09

Table 2: Numerical values for arguments



[Hammer, Ponty, Wang, Will '2019]



- Problem. Given the set of allowed secondary structures (s₁, · · · , s_k), sample uniformly at random RNA satisfying each of those structures.
- Proposition. The problem is equivalent to enumerating independent sets in bipartite graphs

image taken from [Hammer, Ponty, Wang, Will '2019]

Step 1: construct a graph based on secondary structures





image taken from [Hammer, Ponty, Wang, Will '2019]

Step 2: construct a suitable tree decomposition and a context-free grammar



$$m_{\{uge\} \to \{pgu\}}(x_g, x_u) = \sum_{\text{allowed } x_e} \left(m_{\{uea\} \to \{uge\}}(x_u, x_e) \right) \left(m_{\{es\} \to \{uge\}}(x_e) \right)$$

image taken from [Hammer, Ponty, Wang, Will '2019]

Step 3: add the parameters

- each secondary structure energy (marked by u_c)
- letter frequency



$$m_{u
ightarrow v}(x) = \sum_{\widetilde{x}} \prod_{w
ightarrow u} m_{w
ightarrow u}(x, \widetilde{x}) imes u_c^{- ext{energy of added edge}}$$

image taken from [Hammer, Ponty, Wang, Will '2019]

Conclusion:

- The energies of the secondary structures and letter frequencies can be tuned
- This can be subsequently refined to energies of adjacent pairs in RNA sequence, triples, etc.
- Empirically observed energy distributions are Gaussian



Bianconi-Barabási model

An evolving network can be compared to a diluted gas at low temperature



Bose-Einstein condensation in evolving networks Bianconi-Barabási model

Bose gas	network evolution
temperature	temperature
energy	energy
particle	half-edge
number of energy levels	\leqslant number of nodes
Bose-Einstein condensation	topological phase transition



In this model, the number of particles on the energy level ε follows the Bose statistics $n(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)}-1}$ which also represents the number of edges linking to nodes with energy ε .

Application 5: Bose–Einstein condensate in quantum harmonic oscillator [Bernstein, Fahrbach, Randall], [Bendkowski, Bodini, D.]

Integer partitions \leftrightarrow 1-dimensional quantum oscillator



 $partitions = multiset(\mathbb{N}) = multiset(multiset(1))$

[Bernstein, Fahrbach, Randall], [Bendkowski, Bodini, D.]

 $\textbf{Coloured partitions} \leftrightarrow \textbf{d-dimensional quantum oscillator}$

coloured partitions = multiset
$$\binom{\mathbb{N} + d - 1}{\mathbb{N}} = \mathsf{MSet}(\mathsf{MSet}(d \cdot 1))$$



[Bernstein, Fahrbach, Randall], [Bendkowski, Bodini, D.]

 $\textbf{Coloured partitions} \leftrightarrow \textbf{d-dimensional quantum oscillator}$

Weighted partition	Random particle assembly
Sum of numbers	Total energy
Number of colours	Dimension (<i>d</i>)
Row of Young table	Particle
Number of rows	Number of particles
Number of squares in the row	Energy of a particle (λ)
Partition limit shape	Bose-Einstein condensation
$\binom{d+\lambda-1}{\lambda}$	Number of particle states

Problem: generate random assemblies with given numbers of colours (n_1, n_2, \ldots, n_d) .

[Bernstein, Fahrbach, Randall], [Bendkowski, Bodini, D.]

Challenge: express the inner generating function

$$MSET(\bullet_1, \bullet_2, \cdots, \bullet_{\ell}) = \frac{1}{1-z_1} \cdot \frac{1}{1-z_2} \cdot \cdots \cdot \frac{1}{1-z_{\ell}} - 1$$

in DCP rules using only polynomial number of additions and multiplications.

Solution: convexity proof of length $\Theta(\ell^2)$ using dynamic programming.



Application 6: Substitution-closed permutation classes

Simple permutations and inflations

Simple permutation: does not contain intervals

$$\{a, a+1, ..., b\} \rightarrow \{c, c+1, ..., d\}$$

of length strictly between 1 and *n*. Permutation from the figure is not simple because it contains an interval $\{1, 2, 3\} \rightarrow \{5, 6, 7\}$. *Inflation* is obtained by replacing each entry by interval



Substitution-closed classes

Theorem (Albert, Atkinson '2005)

Let C be substitution-closed and contain 12 and 21. Let S be the class of all simple permutations contained in C. Then, C satisfies

$$\mathcal{C} = \{\bullet\} + 12[\mathcal{C}^+, \mathcal{C}] + 21[\mathcal{C}^-, \mathcal{C}] + \sum_{\pi \in \mathcal{S}} \pi[\mathcal{C}, \mathcal{C}, \dots, \mathcal{C}]$$
$$\mathcal{C}^+ = \{\bullet\} + 21[\mathcal{C}^-, \mathcal{C}] + \sum_{\pi \in \mathcal{S}} \pi[\mathcal{C}, \mathcal{C}, \dots, \mathcal{C}]$$
$$\mathcal{C}^- = \{\bullet\} + 12[\mathcal{C}^+, \mathcal{C}] + \sum_{\pi \in \mathcal{S}} \pi[\mathcal{C}, \mathcal{C}, \dots, \mathcal{C}].$$

Remark

Algorithm for computing specifications of permutation classes containing finitely many simple permutations is given in [Bassino, Bouvel, Pierrot, Pivoteau, Rossin '2017]

Substitution-closed classes

Expected number of simple permutations $\pi \in \mathcal{S}$

$$\mathcal{C} = \{\bullet\} + 12[\mathcal{C}^+, \mathcal{C}] + 21[\mathcal{C}^-, \mathcal{C}] + \sum_{\pi \in \mathcal{S}} u_\pi \pi[\mathcal{C}, \mathcal{C}, \dots, \mathcal{C}]$$
$$\mathcal{C}^+ = \{\bullet\} + 21[\mathcal{C}^-, \mathcal{C}] + \sum_{\pi \in \mathcal{S}} u_\pi \pi[\mathcal{C}, \mathcal{C}, \dots, \mathcal{C}]$$
$$\mathcal{C}^- = \{\bullet\} + 12[\mathcal{C}^+, \mathcal{C}] + \sum_{\pi \in \mathcal{S}} u_\pi \pi[\mathcal{C}, \mathcal{C}, \dots, \mathcal{C}].$$

By tuning the expectations attached to $(u_{\pi})_{\pi \in S}$, we can alter the expected frequencies of inflation used during the construction of a permutation.

Conclusion

Conclusion

- 1. Boltzmann sampler is a fundamental tool for multiparametric sampling. The tuning procedure is very natural in many contexts.
- 2. Context-free unambiguous grammars are ubiquitous in many areas of mathematics, physics and computer science.
- 3. Behind the scenes:
 - An O(n^{d/2}) algorithm with O(log n) memory for exact multiparametric sampling
 - The tuning algorithm can be interpreted in terms of Maximum Likelihood Estimation for combinatorial objects
 - Other frameworks: unlabelled structures and finite differential equations
 - Other applications: multiclass queues, hidden parameter estimation, random graphs with weighted degrees and patterns
 - Theory of self-concordant barriers for interior-point optimisation
 - Precise expected complexity and fine-tuning for rejections

Thank you for your attention