# Multiparametric Boltzmann sampling and applications 

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## Random sampling

## Problem

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

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

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 (QuiскСнеск, 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

$\underbrace{\text { Multiparametric Boltzmann sampling }}_{\text {Part I }}$ and $\underbrace{\text { applications }}_{\text {Part II }}$

# 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

$$
\left(a_{0}+a_{1} z+a_{2} z^{2}+\ldots\right)\left(b_{0}+b_{1} z+b_{2} z^{2}+\ldots\right)=c_{0}+c_{1} z+c_{2} z^{2}+\ldots
$$

The convolution rule corresponding to EGF:

$$
c_{n}=\sum_{k=0}^{n} a_{k} b_{n-k}
$$

Example: lambda terms in de Bruijn notation

$\lambda x . \lambda y . \lambda z .(x z)(y z) \quad \longrightarrow \quad \lambda \lambda \lambda(\underline{20})(\underline{10})$
Classical notation $\longrightarrow$ de Bruijn notation

Example: lambda terms in de Bruijn notation

$$
\begin{array}{ll}
\mathcal{L}::=\lambda \mathcal{L}|(\mathcal{L L})| \underline{\mathrm{n}} & L(z)=z L(z)+z L(z)^{2}+\frac{z}{1-z} \\
\underline{\mathrm{n}}::=\underline{0} \mid \mathrm{S} \underline{\mathrm{n}} . & T_{n}=T_{n-1}+\sum_{k=1}^{n} T_{k} T_{n-k-1}+1
\end{array}
$$

## Recursive sampling

Algorithm 1: Recursive algorithm for plain lambda terms
Input: Integer $n$
Output: Plain lambda term of size $n$
begin
Precompute array $\left(T_{k}\right)_{k=0}^{n}$ using the recurrence

$$
T_{n}=T_{n-1}+\sum_{k=1}^{n} T_{k} T_{n-k-1}+1, \quad T_{0}=0
$$

For each $n$, precompute the probability distribution $\mathcal{P}_{n}$ :

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

Function Generate ( $n$ ):
if $n=1$ then
return $\underline{0}$ // minimal de Bruijn index;
Sample index $k$ from the probability distribution $\mathcal{P}_{n}$;
if $k=\lambda$ then
return $\lambda$ Generate $(n-1) / /$ abstraction ;
if $k=\underline{\mathrm{n}}$ then
return $\underline{n} / /$ de Bruijn index;
$L:=$ Generate ( $k$ );
$R:=$ Generate $(n-k-1)$;
return $(L R)$ // 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
\[
L(z)=z L(z)+z L(z)^{2}+\frac{z}{1-z}
\]
Flip a weighted coin \(X \in\{\lambda, @, \underline{n}\}\) with weights
\[
\mathbb{P}_{\lambda}=\frac{z L(z)}{L(z)}, \quad \mathbb{P}_{@}=\frac{z L^{2}(z)}{L(z)}, \quad \mathbb{P}_{\underline{n}}=\frac{\frac{z}{1-z}}{L(z)}
\]
if \(X=\lambda\) then
        return \(\lambda\) Generate \((n-1) / /\) abstraction ;
if \(X=@\) then
        \(L:=\) Generate ( \(z\) ) ;
        \(R:=\) Generate ( \(z\) );
        return \((L R) / /\) application ;
    if \(X=\underline{\mathrm{n}}\) then
        return \(\underline{\underline{\operatorname{Geom}(z)} / / \text { de Bruijn index ; }}\)
```


## Boltzmann distribution

## Probability output of the Boltzmann samplers

Let $S(z)$ be the generating function of the language $\mathcal{S}$ :

$$
S(z)=\sum_{n \geqslant 0} a_{n} z^{n}
$$

Consider a distribution $\mathbb{P}_{z}$ on words $w \in \mathcal{S}$ :

- 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:

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

## Multivariate generating functions

Consider a language $\mathcal{S} \subset \Sigma^{*}$ where $\Sigma=\left\{\bullet_{1}, \bullet_{2}, \bullet_{3}, \bullet_{4}\right\}$ is finite. Let $a_{n_{1}, n_{2}, n_{3}, n_{4}}$ count the number of words $w \in \mathcal{S}$ containing

- $n_{1}$ letters $\bullet_{1}$,
$\rightarrow n_{2}$ letters $\bullet_{2}$,
- $n_{3}$ letters $\bullet_{3}$,
- $n_{4}$ letters $\bullet_{4}$;

Its multivariate generating function is

$$
S\left(z_{1}, z_{2}, z_{3}, z_{4}\right)=\sum_{n \geqslant 0} a_{n_{1}, n_{2}, n_{3}, n_{4}} z_{1}^{n_{1}} z_{2}^{n_{2}} z_{3}^{n_{3}} z_{4}^{n_{4}}
$$

Boltzmann distribution

$$
\mathbb{P}\left(n_{1}, n_{2}, n_{3}, n_{4} \mid z_{1}, z_{2}, z_{3}, z_{4}\right)=\frac{a_{n_{1}, n_{2}, n_{3}, n_{4}} z_{1}^{n_{1}} z_{2}^{n_{2}} z_{3}^{n_{3}} z_{4}^{n_{4}}}{S\left(z_{1}, z_{2}, z_{3}, z_{4}\right)}
$$

## Example: lambda terms and their parameters

Abstractions, variables, successors and redexes marked separately:

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



## Multiparametric Recursive sampling

```
Algorithm 3: Recursive algorithm for plain lambda terms with
parameters
Input: Target integer parameters \(N, n_{(\text {abs })}, n_{(\text {var })}, n_{(\text {suc })}, n_{(\text {red })}\)
Output: Random term with target size \(N\), and given parameter
            values
begin
    Precompute array \(\left(T_{K, k_{1}, k_{2}, k_{3}, k_{4}}\right)_{k, k_{1}, k_{2}, k_{3}, k_{4}}\) using the
        recurrence
```


## Complexity

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

## Multiparametric Boltzmann sampling

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

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

```
Algorithm 4: Boltzmann sampler for plain lambda
terms
Input: Target expectations \(N, n_{\text {(abs) }}, n_{\text {(var) }}, n_{\text {(suc) }}, n_{\text {(red) }}\)
Output: Random term with target expected size \(N\), and
    given expected parameters
begin
    Precompute \(\left(z, u_{\text {(abs) }}, u_{(\text {var })}, u_{(\text {suc })}, u_{(\text {(red })}\right)\) as
        functions of ( \(\left.N, n_{(\text {abs })}, n_{(\text {var })}, n_{(\text {suc })}, n_{(\text {red })}\right)\)
    // stay tuned;
    Function \(\Gamma L\left(z, u_{(a b s)}, u_{(\text {var })}, u_{(s u c)}, u_{(\text {red })}\right)\) :
        Generate \(X \in\{0,1\}\) such that
\[
\begin{aligned}
& \mathbb{P}(X=0)=\frac{u_{(\mathrm{abs})} z L(z, \vec{u})}{L(z, \vec{u})}, \\
& \mathbb{P}(X=1)=\frac{N(z, \vec{u})}{L(z, \vec{u})}
\end{aligned}
\]
\[
X=0 \Rightarrow \text { return } \lambda \Gamma L(z, \vec{u}) ;
\]
\[
X=1 \Rightarrow \text { return } \Gamma N(z, \vec{u})
\]
```


## Function

$\Gamma N\left(z, u_{(a b s)}, u_{(\text {var })}, u_{(s u c)}, u_{(\text {red })}\right):$
Generate $X \in\{0,1,2\}$ such that

$$
\begin{aligned}
& \mathbb{P}(X=0)=\frac{\frac{u_{(\mathrm{var})} z^{2}}{1-u_{(\mathrm{suc}} z^{2}}}{N(z, \vec{u})} \\
& \mathbb{P}(X=1)=\frac{u_{(\mathrm{red})} u_{(\mathrm{abs})} z^{2} L(z, \vec{u})^{2}}{N(z, \vec{u})} \\
& \mathbb{P}(X=2)=\frac{z N(z, \vec{u}) L(z, \vec{u})}{N(z, \vec{u})}
\end{aligned}
$$

$X=0 \Rightarrow$ return $\operatorname{Geom}\left(z u_{(s u c)}\right)$;
$X=1 \Rightarrow \operatorname{return} \overline{(\lambda \Gamma L(z, \vec{u})) \Gamma L}(z, \vec{u})$;
$X=1 \Rightarrow \operatorname{return}(\Gamma N(z, \vec{u}) \Gamma L(z, \vec{u}))$;

# Why Boltzmann sampling? 

## Exact multiparametric sampling

Suppose that $S_{i}$ are defined by an unambiguous context-free grammar

$$
S_{i} \rightarrow \sum_{j} T_{i j}\left(S_{1}, \ldots, S_{n}, \bullet_{1}, \bullet_{2}, \bullet_{3}, \bullet_{d}\right)
$$

where $\left(T_{i j}\right)_{i j}$ are transitions, and $\left(\bullet_{1}, \bullet_{2}, \bullet_{3}, \bullet_{d}\right)$ are alphabet letters.

## Problem

Given positive integers $\left(n_{1}, n_{2}, \ldots, n_{d}\right)$, 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 $2-\mathrm{CNF}$ formula

$$
F=\underbrace{\left(x_{1} \vee \bar{x}_{2}\right)}_{c_{1}} \underbrace{\left(x_{1} \vee \bar{x}_{4}\right)}_{c_{2}} \underbrace{\left(\bar{x}_{2} \vee \bar{x}_{3}\right)}_{c_{3}} \underbrace{\left(\bar{x}_{2} \vee \bar{x}_{4}\right)}_{4} c_{5}^{\left(\bar{x}_{3} \vee x_{4}\right)}
$$

Construct a system of algebraic equations

$$
A\left(c_{1}, \ldots, c_{5}\right)=\left(x_{1}+\bar{x}_{1}\right) \ldots\left(x_{4}+\bar{x}_{4}\right)\left(1+c_{1}\right) \ldots\left(1+c_{5}\right)
$$

where

$$
x_{1}=c_{1} c_{2}, \quad \bar{x}_{1}=1, \quad x_{2}=1, \quad \bar{x}_{2}=c_{1} c_{3} c_{4}, \quad \bar{x}_{3}=c_{3} c_{5}, \quad \cdots
$$

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

$$
\# 2 S A T(F)=\left[c_{1}^{2} c_{2}^{2} \ldots c_{5}^{2}\right] A\left(c_{1}, \ldots, c_{5}\right)
$$

## Tuning of a multiparametric Boltzmann sampler

$$
\text { Handles } \boldsymbol{z} \Rightarrow \quad \text { Expectations } \mathbb{E} n_{k}
$$


!! 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

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

based on convex optimisation with barriers.
Proof idea: log-sum-exp with non-negative coefficients is convex

$$
f\left(x_{1}, \ldots, x_{n}\right)=\log \sum_{i=1}^{n} e^{x_{i}}
$$

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


```
-- Motzkin trees
MotzkinTree = Leaf
    | Unary MotzkinTree (2) [0.3]
    | Binary MotzkinTree MotzkinTree (2).
```


## 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 Glasgow Haskell Compiler

## \#5557 closed bug (fixed)

## Code using seq has wrong strictness (too lazy)

| Сообщил: | michal.palka | Владелеи: |
| :--- | :--- | :--- |
| Приоритет: | high | Этап разработки: |
| Компонент: | Compler | Версия: |
| Ключевые слова: | seq strictness strict lazy | Копия: |
| Operating System: | Unknown/Multiple | Architecture: |
| Type of fallure: | Incorrect result at runtime | Test Case: |

## Application 2: software testing

$$
\lambda x, \lambda y, \lambda z \cdot x z(y z)
$$

- 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 | $\underline{0}$ | $\underline{1}$ | $\underline{2}$ | $\underline{3}$ | $\underline{4}$ | $\underline{5}$ | $\underline{6}$ | $\underline{7}$ | $\underline{8}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 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 ( $0.01,0.03,0.05,0.07,0.09,0.11,0.13,0.15,0.17,0.19)$

$$
\begin{gathered}
T_{1}\left(z, u_{1}, \ldots, u_{d}\right)=z u_{1} e^{T_{2}\left(z, u_{1}, \ldots, u_{d}\right)} \\
T_{2}\left(z, u_{1}, \ldots, u_{d}\right)=z u_{2} e^{T_{3}\left(z, u_{1}, \ldots, u_{d}\right)} \\
\vdots \\
T_{d}\left(z, u_{1}, \ldots, u_{d}\right)=z u_{d} e^{T_{1}\left(z, u_{1}, \ldots, u_{d}\right)}
\end{gathered}
$$



| $z$ | $u_{1}$ | $u_{2}$ | $u_{3}$ | $u_{4}$ | $u_{5}$ | $u_{6}$ | $u_{7}$ | $u_{8}$ | $u_{9}$ | $u_{10}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 0.3 | 0.009 | 1.88 | 1.37 | 1.29 | 1.26 | 1.25 | 1.24 | 1.23 | 1.23 | 3.52 |

Table 1: Numerical values for arguments


## Application 3. Models of random trees

Model 2: Otter trees with coloured leaves

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

$$
\begin{aligned}
T\left(z, u_{1}, \ldots, u_{d}\right) & =z \sum_{i=1}^{d} u_{i}+\operatorname{MSet}_{2}\left(T\left(z, u_{1}, \ldots, u_{d}\right)\right) \\
\operatorname{MSet}_{2}\left(T\left(z, u_{1}, \ldots, u_{d}\right)\right) & =\frac{T\left(z, u_{1}, \ldots, u_{d}\right)^{2}+T\left(z^{2}, u_{1}^{2}, \ldots, u_{d}^{2}\right)}{2}
\end{aligned}
$$

| $u_{1} z$ | $u_{2} z$ | $u_{3} z$ | $u_{4} z$ | $u_{5} z$ | $u_{6} z$ | $u_{7} z$ | $u_{8} z$ | $u_{9} z$ | $u_{10} z$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 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



Application 4. RNA folding design

## Application 4: RNA folding design

[Hammer, Ponty, Wang, Will '2019]


- Problem. Given the set of allowed secondary structures $\left(s_{1}, \cdots, s_{k}\right)$, sample uniformly at random RNA satisfying each of those structures.
- Proposition. The problem is equivalent to enumerating independent sets in bipartite graphs


## Application 4: RNA folding design

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

Step 1: construct a graph based on secondary structures


## Application 4: RNA folding design

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

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



$$
m_{\{u g e\} \rightarrow\{p g u\}}\left(x_{g}, x_{u}\right)=\sum_{\text {allowed } x_{e}}\left(m_{\{u e a\} \rightarrow\{u g e\}}\left(x_{u}, x_{e}\right)\right)\left(m_{\{e s\} \rightarrow\{u g e\}}\left(x_{e}\right)\right)
$$

## Application 4: RNA folding design

image taken from [Hammer, Ponty, Wang, Will '2019]
Step 3: add the parameters

- each secondary structure energy (marked by $u_{c}$ )
- letter frequency




$$
m_{u \rightarrow v}(x)=\sum_{\widetilde{x}} \prod_{w \rightarrow u} m_{w \rightarrow u}(x, \widetilde{x}) \times u_{c}^{- \text {energy of added edge }}
$$

## Application 4: RNA folding design

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


Application 5: Bose-Einstein condensate in quantum harmonic oscillator

## 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 |
| :---: |
| temperature |
| energy |
| particle |
| number of energy levels |
| Bose-Einstein condensation |

network evolution
temperature
energy
half-edge
$\leqslant$ number of nodes
topological phase transition
In this model, the number of particles on the energy level
$\varepsilon$ 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 $\varepsilon$.

# Application 5: Bose-Einstein condensate in quantum harmonic oscillator <br> [Bernstein, Fahrbach, Randall], [Bendkowski, Bodini, D.] 

Integer partitions $\leftrightarrow$ 1-dimensional quantum oscillator

$$
16=1+3+3+4+5
$$


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

## Application 5: Bose-Einstein condensate in quantum

 harmonic oscillator[Bernstein, Fahrbach, Randall], [Bendkowski, Bodini, D.]
Coloured partitions $\leftrightarrow \mathbf{d}$-dimensional quantum oscillator coloured partitions $=\operatorname{multiset}\binom{\mathbb{N}+d-1}{\mathbb{N}}=\operatorname{MSet}(\operatorname{MSet}(d \cdot 1))$


# Application 5: Bose-Einstein condensate in quantum harmonic oscillator <br> [Bernstein, Fahrbach, Randall], [Bendkowski, Bodini, D.] 

Coloured partitions $\leftrightarrow \mathbf{d}$-dimensional quantum oscillator
Weighted partition Random particle assembly

Sum of numbers
Number of colours
Row of Young table
Number of rows
Number of squares in the row
Partition limit shape

$$
\binom{d+\lambda-1}{\lambda}
$$

Total energy
Dimension (d)
Particle
Number of particles
Energy of a particle ( $\lambda$ )
Bose-Einstein condensation
Number of particle states

Problem: generate random assemblies with given numbers of colours ( $n_{1}, n_{2}, \ldots, n_{d}$ ).

## Application 5: Bose-Einstein condensate in quantum

 harmonic oscillator[Bernstein, Fahrbach, Randall], [Bendkowski, Bodini, D.]
Challenge: express the inner generating function

$$
\operatorname{MSET}\left(\bullet_{1}, \bullet_{2}, \cdots, \bullet_{\ell}\right)=\frac{1}{1-z_{1}} \cdot \frac{1}{1-z_{2}} \cdots \cdot \frac{1}{1-z_{\ell}}-1
$$

in DCP rules using only polynomial number of additions and multiplications.
Solution: convexity proof of length $\Theta\left(\ell^{2}\right)$ using dynamic programming.

(A) $[5,10,15,20,25]$

(в) $[4,4,4,4,10,20,30,40]$

(c) $[80,40,20,10,9,8,7,6,5]$

## Application 6: Substitution-closed permutation classes

## Simple permutations and inflations

- Simple permutation: does not contain intervals

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

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

$$
\begin{aligned}
\mathcal{C} & =\{\bullet\}+12\left[\mathcal{C}^{+}, \mathcal{C}\right]+21\left[\mathcal{C}^{-}, \mathcal{C}\right]+\sum_{\pi \in \mathcal{S}} \pi[\mathcal{C}, \mathcal{C}, \ldots, \mathcal{C}] \\
\mathcal{C}^{+} & =\{\bullet\}+21\left[\mathcal{C}^{-}, \mathcal{C}\right]+\sum_{\pi \in \mathcal{S}} \pi[\mathcal{C}, \mathcal{C}, \ldots, \mathcal{C}] \\
\mathcal{C}^{-} & =\{\bullet\}+12\left[\mathcal{C}^{+}, \mathcal{C}\right]+\sum_{\pi \in \mathcal{S}} \pi[\mathcal{C}, \mathcal{C}, \ldots, \mathcal{C}] .
\end{aligned}
$$

## 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 $\pi \in \mathcal{S}$

$$
\begin{aligned}
\mathcal{C} & =\{\bullet\}+12\left[\mathcal{C}^{+}, \mathcal{C}\right]+21\left[\mathcal{C}^{-}, \mathcal{C}\right]+\sum_{\pi \in \mathcal{S}} u_{\pi} \pi[\mathcal{C}, \mathcal{C}, \ldots, \mathcal{C}] \\
\mathcal{C}^{+} & =\{\bullet\}+21\left[\mathcal{C}^{-}, \mathcal{C}\right]+\sum_{\pi \in \mathcal{S}} u_{\pi} \pi[\mathcal{C}, \mathcal{C}, \ldots, \mathcal{C}] \\
\mathcal{C}^{-} & =\{\bullet\}+12\left[\mathcal{C}^{+}, \mathcal{C}\right]+\sum_{\pi \in \mathcal{S}} u_{\pi} \pi[\mathcal{C}, \mathcal{C}, \ldots, \mathcal{C}] .
\end{aligned}
$$

By tuning the expectations attached to $\left(u_{\pi}\right)_{\pi \in S}$, 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 $\mathcal{O}\left(n^{d / 2}\right)$ algorithm with $\mathcal{O}(\log n)$ 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 

