Random generation of discrete structures

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Stochastic geometry - June 25, 2015
- **Topic**: algorithms to generate random (discrete) structures, according to some *prescribed* probability distribution
- Quick overview of two “classes” of methods
  - counting-based methods
  - locally-defined structures, scrambling methods
- Focus on “exact” generation methods, and “geometric” examples
Why random generation?

- to visualize what “typical” (large) structures in a given class look like
- hints to possible limit behaviors
- to provide test cases for algorithms, when a theoretical average-case analysis is unavailable
- sometimes looking for a good random generation algorithm is a good way of “understanding” the objects under consideration
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- Typically, $C$ is endowed with a size function $|.| : C \rightarrow \mathbb{N}$, with the condition that for each integer $n$, $C_n$ (set of $x \in C$ with size $n$) is finite; then $\mu = \mu_n$ can be the uniform distribution over $C_n$. 
Some (finite or countable) family $C$ of “objects” is defined
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the condition that for each integer $n$, $C_n$ (set of $x \in C$ with
size $n$) is finite; then $\mu = \mu_n$ can be the uniform distribution
over $C_n$.
A $\mu$-sampler ($\mu_n$-sampler) is a randomized algorithm that
takes no input ($n$ as input) and outputs some random $x \in C$
according to $\mu$ ($\mu_n$).
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We assume we have access to some perfect source of randomness (independent random bits, independent uniform r.v. over $[0, 1]$).
Picking a distribution

- One practical way of defining $\mu$ is “proportional to some weight function” $w : C \rightarrow \mathbb{R}^+$:

$$\mu(x) := \frac{w(x)}{\sum_{y \in C} w(y)}$$
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- Requires $S_w = \sum_{y \in \mathcal{C}} w(y) < \infty$
- "Uniform over $\mathcal{C}_n$" as a special case: $w(x) = [|x| = n]$
Rejection principle

A simple, but sometimes efficient idea: “try, reject or accept”

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  - Draw random $x$, proportionally to $w'(x)$
  - Draw $U$, uniform on $[0, 1]$
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- On average: $S_{w'}/S_w$ calls to the $w'$ sampler
- Special case: $A \subset C$, where $C_n$ is easy to sample from and $|A_n|/|C_n|$ is “not too small”; expected number of trials is $|C_n|/|A_n|$
Notations

- $C$ : the whole class
- $C_n$ : subclass of objects of size $n$
- $c_n = |C_n|$

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In many situations, we know $c_n$ but we have no obvious (algorithmic) bijection $\Phi_n : \{1, \ldots, c_n\} \to \mathcal{C}_n$
Classical example: triangulations of a convex polygon

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- Consequence: $c_n = \sum_{k=0}^{n-1} c_k c_{n-1-k}$, $c_0 = 1$. 
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“Catalan numbers” $c_n = \frac{1}{n+1} \binom{2n}{n}$
Triangulations: *ad hoc* algorithm

- The Catalan sequence satisfies a simple recursion:

\[(n + 2)c_{n+1} = 2(2n + 1)c_n\]
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Becomes an algorithm for obtaining a uniform triangulation of size \(n + 1\) from one of size \(n\):
- pick an edge at random (including border edge: \(2n + 1\) choices)
- pick an endpoint at random (2 choices)
- inflate the edge into a triangle, splitting the chosen endpoint
- result is a larger triangulation with a marked border edge
- (adapted from a classic algorithm [Rémy, 1985] for binary trees)
Introduction

Counting-based methods

Markov chains for random generation

Coupling from the past
c_0 = 1, c_n = \sum_{k=0}^{n-1} c_k c_{n-1-k}

Allows to compute \((c_1, \ldots, c_n)\) in \(O(n^2)\) arithmetic operations
Triangulations (cont.)

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- Leads to \textbf{uniform, fixed size} sampling algorithm

\textbf{GenT}(n)

[Precompute $c_0, \ldots, c_n$, once]
If $n = 0$ : Return()
Draw a random $k$, $0 \leq k \leq n - 1$, w.p $p_k = \frac{c_k c_{n-1-k}}{c_n}$
Draw $X = \text{GenT}(k)$, $Y = \text{GenT}(n - 1 - k)$ [with indices shifted by $k - 1$]
Return $(\{1, n + 2, k\}, X, Y)$
The “recursive” method

[Flajolet, Zimmermann, Van Cutsem 1994] : for a wide variety of classes, information on how objects are “built” from smaller ones translates into recurrences on the sequence \((c_n)_{n \geq 0}\), from which one can

- compute the first \(n + 1\) terms in the sequence \(c_0, \ldots, c_n\)
- use the counting sequence to sample uniformly from \(C_n\)

The method is widely applicable in a systematic way, and the complexity is \(O(n \log n)\) per sample after a more costly precomputation (\(n\) numbers, typically growing exponentially).
Example: words without consecutives 1’s

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- Generating function is $F(x) = \frac{1+x}{1-x-x^2}$, radius of convergence is positive root of $1 - x - x^2$ (inverse golden ratio).
A binary tree is defined recursively as:
- either a root/leaf, with size 0
- or a root, a left subtree $t_1$ (which is a binary tree), and a right subtree $t_2$ (also a binary tree); size is $|t_1| + |t_2| + 1$
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- The number of binary trees of size $n$ is the Catalan number
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- Other conditions on degrees of nodes lead to different recurrences; the method carries over
Markov chain methods

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Markov chain methods

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- “Hard” to get **estimates of the speed of convergence**
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- **Sometimes** the “Coupling from the past” technique can give **exact** uniform distribution
- A few pictures (uniform via CFTP)…
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- This is **exactly** what a (homogeneous, finite state) Markov chain is.
Transition matrix

The whole Markov chain is entirely defined by

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- This is just the (weighted) adjacency matrix!
- The probability distribution for \(X_t\) (state at time \(t\)) is just

\[ \pi^{(t)} = \pi \cdot M^t \]
Possible asymptotic behaviors

Important question: $\pi^{(t)}$ for large $t$; completely described in terms of the graph $G$:

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- (This is all graph-dependent; only the distribution itself depends on the weights!)
Identifying the limit

(Strongly connected case) unique vector (with sum 1) satisfying, for each $u$, the “balance condition”

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**Special special case**: unbiased walk in undirected graph,

$$p(u, v) = 1/\deg(u)$$: $\pi_u$ is proportional to the degree of $u$. (If the graph is bipartite, the walk is periodic)
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- run the chain for a “large” number $t$ of rounds
- output $X_t$: “close” to $\pi$ distribution.
Choosing the graph: adjacences

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You need a property of the form: any object can be reached from any other by a sequence of such moves.
Sufficient moves for tilings (strongly connected regions)
Choosing transition probabilities

A good solution is to look for the detailed balance condition: pick $p(u, v)$ and $p(v, u)$ together, with the condition

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- If $\pi$ is uniform over $\mathcal{C}$: just pick $p(u, v) = p(v, u)$. 

Running the Markov chain

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To simulate the Markov chain for an arbitrary time, you must be able to:

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- Algorithmically simulate one step: given any state $u$,
  - compute the list of its neighbours $v_1, \ldots, v_k$
  - compute transition probabilities $p(u, v_i)$
  - pick next state $v_i$ with probability $p(u, v_i)$
  - (or alternatively, pick $v_i$ with probability $p(u, v_i)$ without actually computing the whole list)
How long is long enough?

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Coupling from the past

**CFTP [Propp-Wilson, 1996]**: a technique to sample from the **exact** distribution $\pi$, with a Markov chain that converges to $\pi$. 
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CFTP [Propp-Wilson, 1996]: a technique to sample from the exact distribution $\pi$, with a Markov chain that converges to $\pi$. No need to estimate the mixing time: the algorithm stops by itself, and when it does, outputs a $\pi$-distributed object.
Generalized coupling

View the simulation of the Markov chain as a two step algorithm:

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- Apply the function: if current state is $x$, next state is $F(x)$. 
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As a byproduct, this defines a “generalized coupling” of the Markov chain: one copy $(X_t^{(u)})_{t \geq 0}$ starting from each state $u$, with the “sticky” property

$$X_t^{(u)} = X_t^{(v)} \Rightarrow \forall t' > t, X_{t'}^{(u)} = X_{t'}^{(v)}.$$
Note on update functions

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For a given transition matrix, one can design many different distributions for transition functions.

- Images can be chosen independently (extremely costly!)
- A “good” design will try to make it more likely that chains starting from different states will reach the same state.
For any integer $t$, here is an exact simulation algorithm for $\pi$:
- Draw $t$ independent update functions $F_1, \ldots, F_n$;
- Compute $G = F_n \circ \cdots \circ F_1$;
- Draw a random initial state $u$ from distribution $\pi$;
- Output $G(u)$. 
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(Useless : if we know how to choose \( u \), we don’t need a more complex algorithm)
But...

If we make the right choice for the distribution of $F$, it is very likely that, for large $t$, the composite function $G$ is a constant function over $V$; then the result does not depend on choice of $u$. 
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- $G \leftarrow I$, $u \leftarrow u_0$
- While $G$ is not constant, $F \leftarrow \text{RandomF}();$ $G \leftarrow F \circ G;$
  $u \leftarrow F(u)$
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This is a forward coupling: after $t$ steps, $G = G_t = F_t \circ \cdots \circ F_1$; $G_t(u) = \text{RandomF}()(G_{t-1}(u))$. 
Backward coupling (from the future)

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**View as**: Take a coupling that has already run for an infinite time, it must have become coalescent at time 0; we are simply looking into its recent past to discover its state at time 0.
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- Forward coupling does **not**, in general, simulate distribution $\pi$;
- Backward coupling does simulate distribution $\pi$, **provided** it has **positive probability** to terminate (this implies probability 1).
Example: walk on a line

\[ V = \{1, \ldots, k\}, \quad p(i, i + 1) = p(i, i - 1) = \frac{1}{2}, \]
\[ p(0, 0) = p(k, k) = \frac{1}{2} \]
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Realize coupling with 2 update functions: \( F^+(i) = \min(k, i + 1) \); \( F^-(i) = \max(1, i - 1) \)
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Forward coupling will always stop with a constant function 1 or k, so will never output any other value!
Why CFTP is correct

Consider a **doubly infinite** sequence of independent random update functions \((F_n)_{n \in \mathbb{Z}}\), and set \((n < m)\)

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G_{n,m} = F_{m-1} \circ F_{m-2} \circ \cdots \circ F_n
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(This is a monotone convergence argument; where forward coupling fails is that we do not have \(G_{0,n'} = G_{0,n}\) as soon as \(G_{0,n}\) is constant and \(n' > n\))
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In particular, if $V$ has a unique minimum and maximum (e.g., a finite distributive lattice), only need to compute $G_{n,0}(\text{max})$ and $G_{n,0}(\text{min})$; (most easy cases are of this type)
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- **binary-backoff CFTP**: compute $G_{-2^k,0}$ for $k = 1, 2, \ldots$, storing all functions $F_n$ so as to be able to reuse them; this way, composition always happen in the natural order.