Random generation of discrete structures

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- **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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- A μ-sampler (μ_n-sampler) is a randomized algorithm that takes no input (n as input) and outputs some random $x \in \mathcal{C}$ according to μ (μ_n).
- 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 μ is "proportional to some weight function" $w : \mathcal{C} \to \mathbb{R}^+$:

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- "Uniform over $\mathcal{C}_n$" as a special case : $w(x) = [|x| = n]$

Rejection principle

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- Special case : $\mathcal{A} \subset \mathcal{C}$, where $\mathcal{C}_n$ is easy to sample from and $|\mathcal{A}_n|/|\mathcal{C}_n|$ is "not too small" ; expected number of trials is $|\mathcal{C}_n|/|\mathcal{A}_n|$

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- $c_n = |\mathcal{C}_n|$

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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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- "Catalan numbers" $c_n = \frac{1}{n+1}\binom{2n}{n}$

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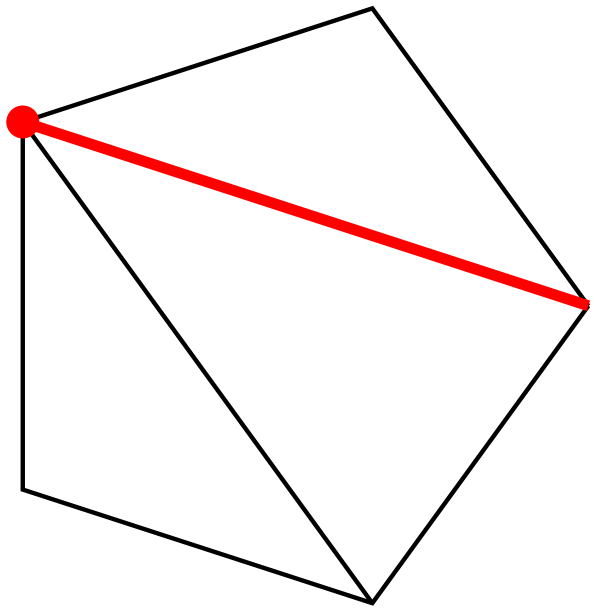
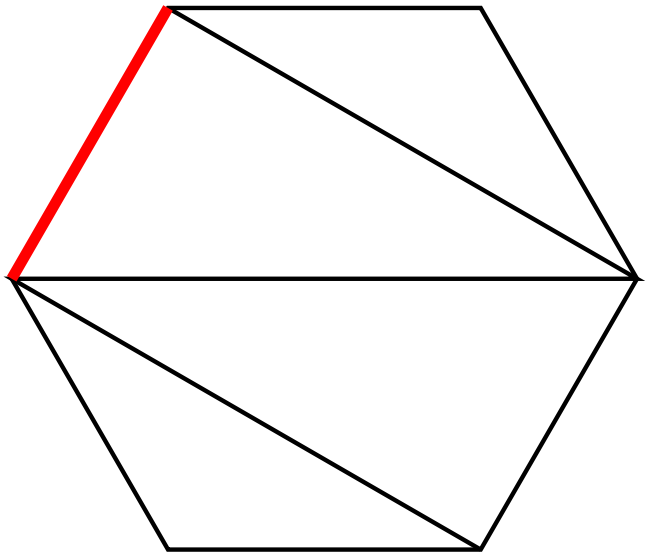
Triangulations : *ad hoc* algorithm

- The Catalan sequence satisfies a simple recursion : $(n+2)c_{n+1} = 2(2n+1)c_n$
- 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)





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- Leads to **uniform, fixed size** sampling algorithm

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 $p_k = c_k c_{n-1-k}/c_n$
Draw $X = \mathrm{GenT}(k)$, $Y = \mathrm{GenT}(n-1-k)$ [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 $\mathcal{C}_n$

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).

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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).

Example 2 : binary (plane, rooted) trees

- 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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- Other conditions on degrees of nodes lead to different recurrences ; the method carries over

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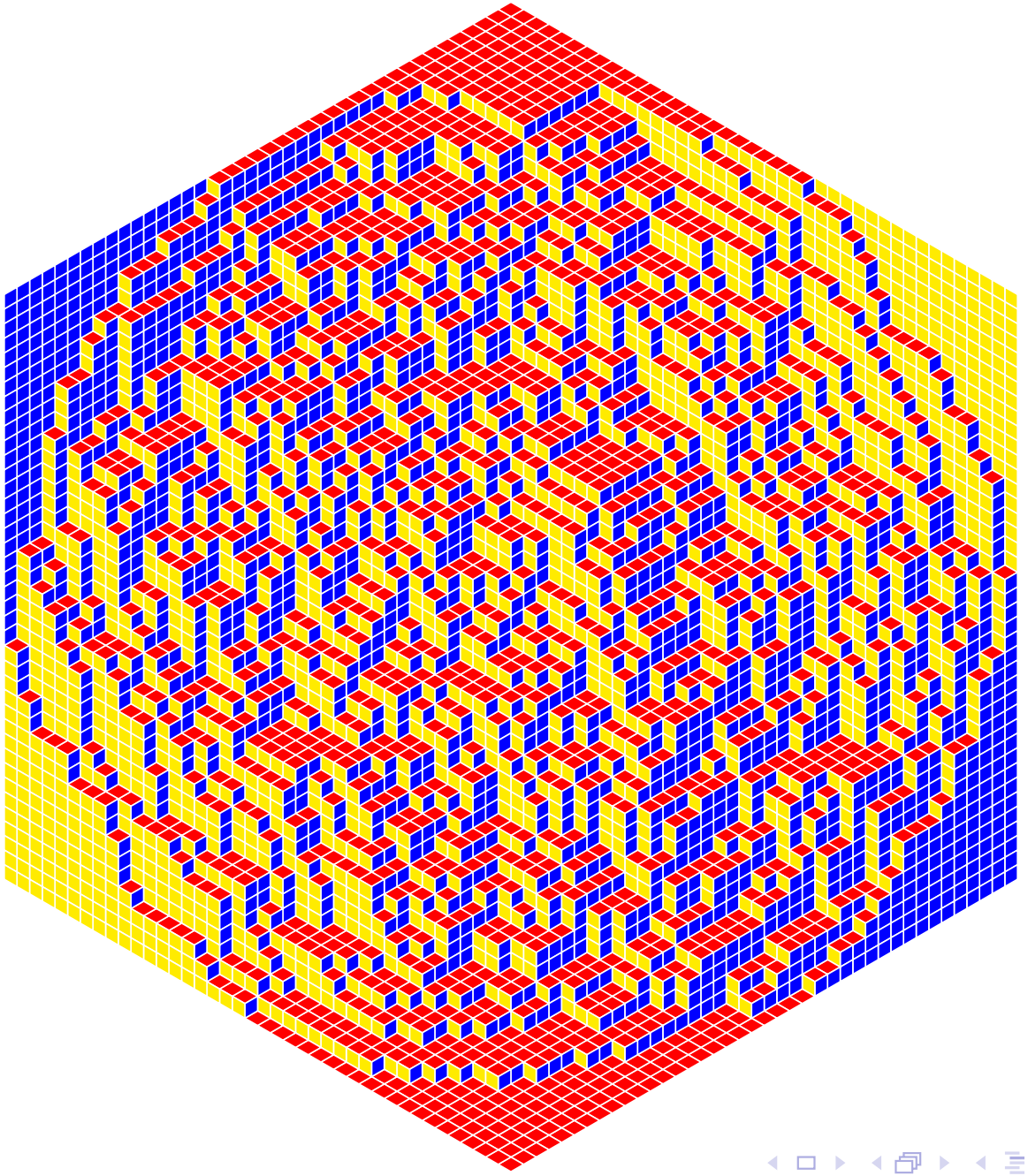
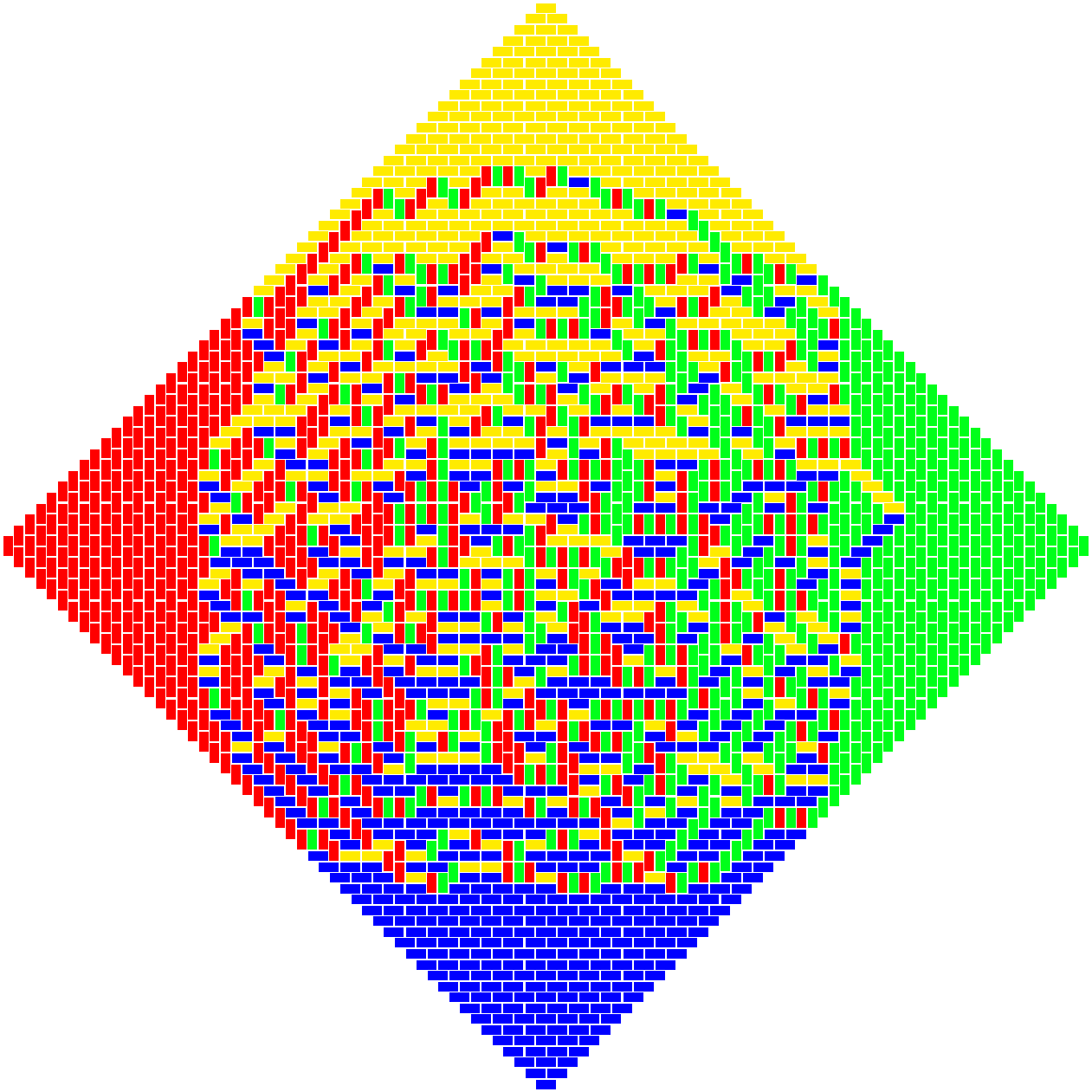
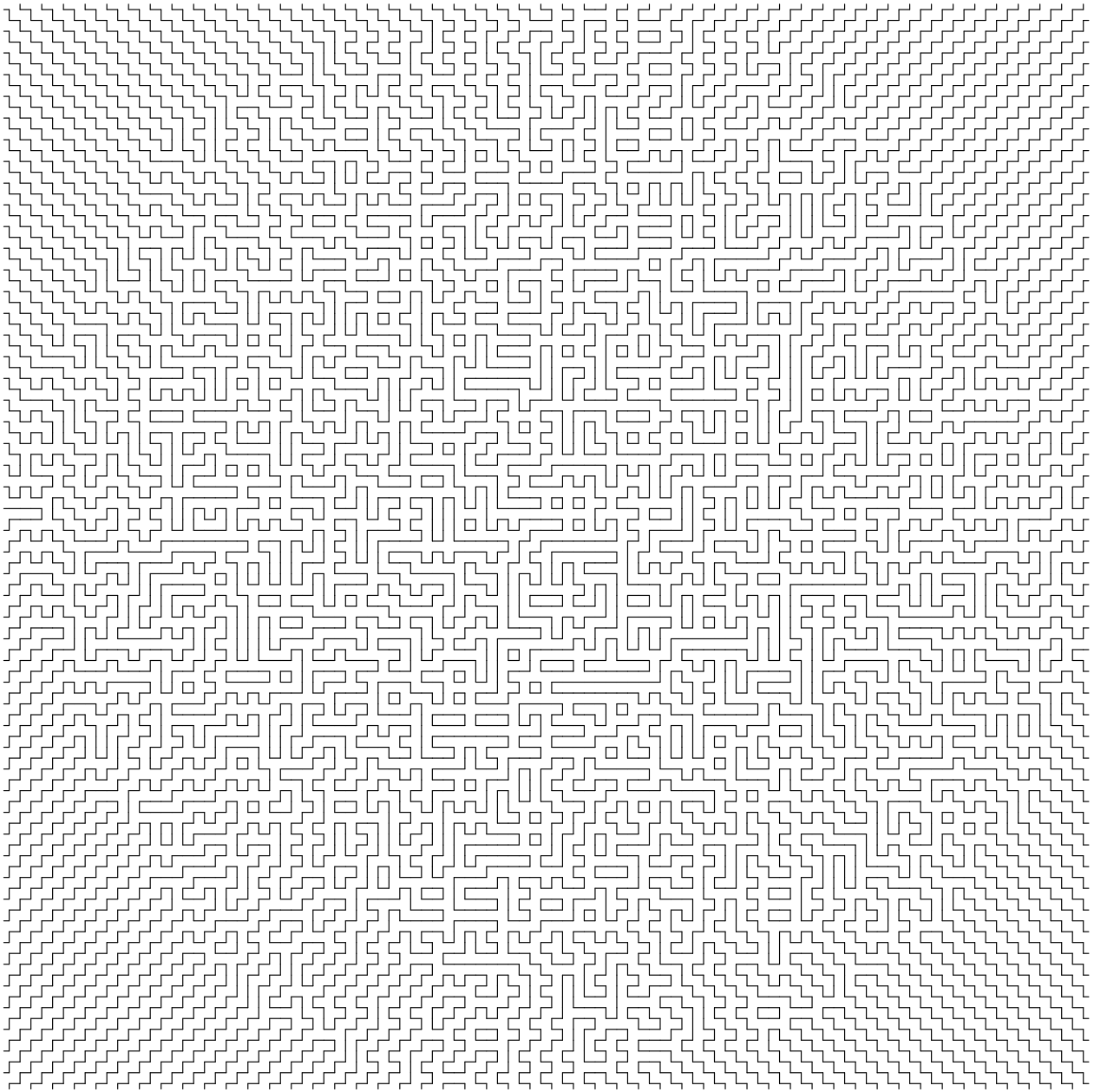
- A few pictures (uniform via CFTP)...







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- This is **exactly** what a (homogeneous, finite state) Markov chain is.

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

$$\pi^{(t)} = \pi . M^t$$

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

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(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, $p(u,v) = 1/\deg(u)$: π_u is **proportional to the degree of** u. (If the graph is bipartite, the walk is periodic)

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- output X_t : "close" to π distribution.

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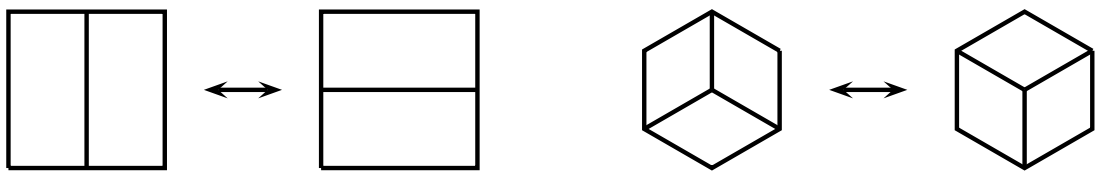
Typically, choose a symmetric graph where two states (objects) are adjacent if they differ by some "small, local change".
You need a property of the form : any object can be reached from any other by a sequence of such moves.

Sufficient moves for tilings (strongly connected regions)



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

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- Pick a starting state (can you construct **one** object from your class ?)
- 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)

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- Any inequality bounding the **second largest eigenvalue** away from 1 is useful.

How long is long enough ?

- Usually the most difficult question : we want to output X_t, and must choose t such that $\pi^{(t)}$ is close to π.
- This is the problem of **mixing time evaluation** :

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- For an overview of bounding techniques : **Jerrum** in **Probabilistic Methods for Algorithmic Discrete Mathematics (Springer, 1998)**

Coupling from the past

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Generalized coupling

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

- Draw a *random update function* $F : V \to V$ from some appropriate distribution
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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

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

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- 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.

Exact, but useless, simulation algorithm

For any integer t, here is an exact simulation algorithm for π :

- Draw t independent update functions $F_1, \ldots, F_n$;
- Compute $G = F_n \circ \cdots \circ F_1$;
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(Useless : if we know how to choose u, we don't need a more complex algorithm)

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Warning : there is a trap

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This is a forward coupling : after t steps, $G = G_t = F_t \circ \cdots \circ F_1$; $G_t(u) = \text{RandomF}()(G_{t-1}(u))$.

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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 π ;
- Backward coupling does simulate distribution π, **provided** it has **positive probability** to terminate (this implies probability 1).

Example : walk on a line

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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 $(n < m)$

$$G_{n,m} = F_{m-1} \circ F_{m-2} \circ \cdots \circ F_n$$

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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 $G_{n,0}(\max)$ and $G_{n,0}(\min)$; (most easy cases are of this type)
- **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.