On the Uniform Random Generation of Non deterministic Automata up to Isomorphism

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Abstract

In this paper we address the problem of the uniform random generation of non deterministic automata (NFA) up to isomorphism. First, we show how to use a Monte-Carlo approach to uniformly sample a NFA. Secondly, we show how to use the Metropolis-Hastings Algorithm to uniformly generate NFAs up to isomorphism. Using labeling techniques, we show that in practice it is possible to move into the modified Markov Chain efficiently, allowing the random generation of NFAs up to isomorphism with dozens of states. This general approach is also applied to several interesting subclasses of NFAs (up to isomorphism), such as NFAs having a unique initial states and a bounded output degree. Finally, we prove that for these interesting subclasses of NFAs, moving into the Metropolis Markov chain can be done in polynomial time. Promising experimental results constitute a practical contribution.

1 Introduction

Finite automata play a central role in the field of formal language theory and are intensively used to address algorithmic problems from model-checking to text processing. Many automata-based algorithms have been developed and are still being developed. They propose new approaches and heuristics, even for basic problems like the inclusion problem[1]. Evaluating new algorithms

[1] see `http://www.languageinclusion.org/`

is a challenging problem that cannot be addressed only by the theoretical computation of the worst case complexity. Several other complementary techniques can be used to measure the efficiency of an algorithm: average complexity, generic case complexity, benchmarking, evaluation on hard instances, evaluations on random instances. The first two approaches are hard theoretical problems, particularly for algorithms using heuristics and optmizations. Benchmarks, as well as known hard instances, are not always available. Nevertheless, in practice, random generation of inputs is a good way to estimate the efficiency of an algorithm. Designing uniform random generator for classes of finite automata is a challenging problem that has been addressed mostly for deterministic automata [1, 2, 3, 4] -the interested reader is referred to [5] for a recent survey. However, the problem of uniform random generation of non deterministic automata (NFAs) is more complex, particularly for a random generation up to isomorphism: the size of the automorphism group of a n-state non deterministic automata may vary from 1 to $n!$. For most applications, the complexity of the algorithm is related to the structure of the automata, not to the names of the states: randomly generated NFAs, regardless of the number of isomorphic automata, may therefore lead to an over representation of some isomorphism classes of automata. Moreover, as discussed in the conclusion of [5], the random generation of non deterministic automata has to be done on particular subclasses of automata in order to obtain a better sampler for the evaluation of algorithm (since most of the NFAs, for the uniform distribution, will accept all words).

The random generation of non deterministic automata is explored in [6] using random graph techniques (without considering the obtained distribution relative to automata or to the isomorphism classes). In [7], the random generation of NFAs is performed using bitstream generation. In [8, 9] NFAs are obtained by the random generation of a regular expression and by transforming it into an equivalent automaton using Glushkov Algorithm. The use of Markov chains based techniques to randomly generate finite automata was introduced in [10, 11] for acyclic automata.

1.1 Contributions

In this paper we address the problem of the uniform generation of elements in several classes of non deterministic automata (up to isomorphism) by using Monte-Carlo techniques. We propose this approach for the class of n-state non deterministic automata as well as for (a priori) more interesting

sub-classes. Determining the most interesting subclasses of NFAs for testing practical applications is not the purpose of this paper. We would like to point out that Monte Carlo approaches are very flexible and that the results of this paper can be applied-adapted quite easily for many classes of NFAs. More precisely:

1. We propose in Section 2 several ergodic Markov Chains whose stationary distributions are respectively uniform on the set of n-state NFAs, n-state NFAs with a fixed maximal output degree and n-state NFAs with a fixed maximal output degree for each letter. In addition, these chains can be adapted for these three classes restricted to automata with a fixed single initial state. Moving into these Markov chains can be done in time polynomial in n.

2. The main idea of this paper is exposed in Section 3.1, where we show how to modify these Markov Chains using the Metropolis-Hastings Algorithm in order to obtain stationary distributions that are uniform for the given classes of automata up to isomorphism. Moving into these new Markov chains requires to compute the sizes of the automorphism groups of the occurring NFAs, as explained in Section 3.

3. The main contributions of this paper are given in Section 4 and in Section 5, which can be red independently. In Section 4, we show a theoretical result for the classes with a bounded output degree: moving into the modified Markov chains (for a generation up to isomorphism) can be done in polynomial time.

4. In Section 5, we explain how to use *labelings*, a classical graph technique, to compute in practice the sizes of the automorphism groups. The efficiency of the approach is illustrated with promising experiments in Section 5.2.

1.2 Theoretical Background on NFA

For a general reference on finite automata see [12]. In this paper Σ is a fixed finite alphabet of cardinal $|\Sigma| \geq 2$, and m is an integer satisfying $m \geq 2$.

A *non-deterministic automaton* (NFA) on Σ is a tuple (Q, Δ, I, F) where Q is a finite set of *states*, Σ is a finite alphabet, $\Delta \subseteq Q \times \Sigma \times Q$ is the set of transitions, $F \subseteq Q$ is the set of final states and $I \subseteq Q$ is the set of initial

states. For any state p and any letter a, we denote by $p \cdot a$ the set of states q such that $(p, a, q) \in \Delta$. The set of transitions Δ is *deterministic* if for every pair (p, a) in $Q \times \Sigma$ there is at most one $q \in Q$ such that $(p, a, q) \in \Delta$. Two NFAs are depicted on Fig. 2. A NFA is *complete* if for every pair (p, a) in $Q \times \Sigma$ there is at least one $q \in Q$ such that $(p, a, q) \in \Delta$. A *path* in a NFA is a sequence of transitions $(p_0, a_0, q_0)(p_1, a_1, q_1) \dots (p_k, a_k, q_k)$ such that $q_i = p_{i+1}$. The word $a_0 \dots a_k$ is the *label* of the path and k its *length*. If $p_0 \in I$ and $q_k \in F$ the path is successful. A word is *accepted* by a NFA if it's the label of a successful path. A NFA is *accessible* (resp. *co-accessible*) if for every state q there exists a path from an initial state to q (resp. if for every state q there exists a path from q to a final state). A NFA is *trim* if it is both accessible and co-accessible A *deterministic automaton* is a NFA where $|I| = 1$ and whose set of transitions is deterministic.

Let $\mathfrak{A}(n)$ be the class of finite automata whose set of states is $\{0, \dots, n-1\}$. We are interesting in several subclasses of $\mathfrak{A}(n)$.

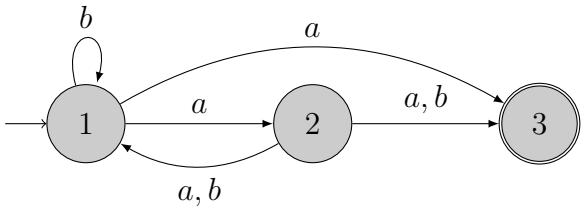
- $\mathfrak{N}(n)$ is the subclass of $\mathfrak{A}(n)$ of trim finite automata.
- $\mathfrak{N}_m(n)$ be the class of finite automata in $\mathfrak{N}(n)$ such that, for each state p, there is at most m pairs (a, q) such that (p, a, q) is a transition: there are at most m transitions outgoing each state.
- $\mathfrak{N}'_m(n)$ be the class of finite automata in $\mathfrak{N}_m(n)$ such that, for each state p and each letter a, there is at most m states q such that (p, a, q) is a transition: for each letter, there are at most m transitions labeled by this letter outgoing each state.
- Finally, for any class $\mathfrak{X}$ of finite automata, we denote by $\mathfrak{X}^\bullet$ the subclass of $\mathfrak{X}$ of automata whose set of initial states is reduced to $\{1\}$.

Examples of automata in One has

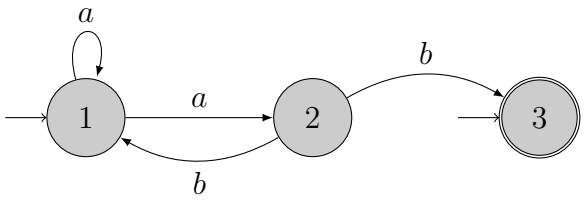
$$\mathfrak{N}_m(n) \subseteq \mathfrak{N}'_m(n) \subseteq \mathfrak{N}(n) \subseteq \mathfrak{A}(n).$$

these classes are depicted on Fig. 1.

Two NFAs are *isomorphic* if there exists a bijection between their sets of states preserving the sets initial states, final states and transitions. More precisely, let $\mathcal{A} = (Q, \Sigma, \Delta, I, F)$ and let φ be a bijection from Q into a finite set $\varphi(Q)$. We denote by $\varphi(\mathcal{A})$ the automaton $(\varphi(Q), \Sigma, \Delta', \varphi(I), \varphi(F))$,



Automaton in $\mathfrak{N}(3)^\bullet$, $\mathfrak{N}_4(3)^\bullet$, $\mathfrak{N}'_2(3)^\bullet$
and in $\mathfrak{N}(3)$, $\mathfrak{N}_4(3)$, $\mathfrak{N}'_2(3)$.



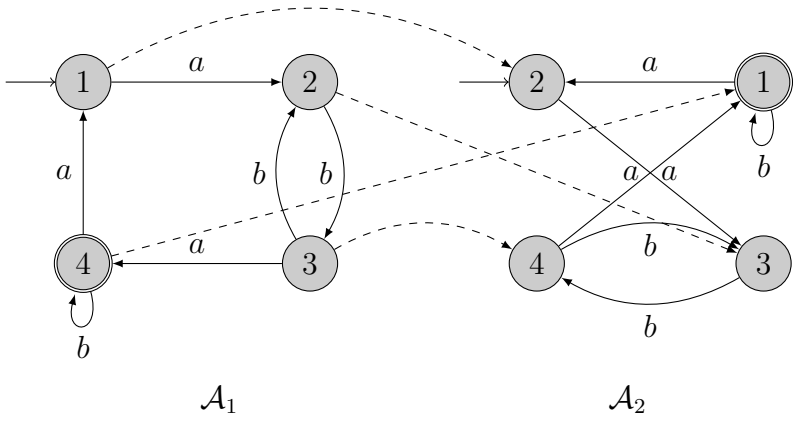
Automaton in $\mathfrak{N}(3)$, $\mathfrak{N}_2(3)$ and $\mathfrak{N}'_2(3)$
but not in any doted class.

Figure 1: Several Classes of Automata.

with $\Delta' = \{(\varphi(p), a, \varphi(q)) \mid (p, a, q) \in \Delta\}$. Two automata $\mathcal{A}_1$ and $\mathcal{A}_2$ are isomorphic if there exists a bijection φ such that $\varphi(\mathcal{A}_1) = \mathcal{A}_2$.

Two isomorphic NFAs have the same number of states and are equal, up to the states names. The relation *is isomorphic to* is an equivalence relation. For instance, the two automata depicted on Fig. 2 are isomorphic.An *automorphism* for a NFA is an isomorphism between this NFA and itself. Given a NFA $\mathcal{A} = (Q, \Sigma, \Delta, I, F)$, the set of automorphisms of $\mathcal{A}$ is a finite group denoted $\mathrm{Aut}(\mathcal{A})$. For $Q' \subseteq Q$, $\mathrm{Aut}_{Q'}(\mathcal{A})$ denotes the subset of $\mathrm{Aut}(\mathcal{A})$ of automorphisms ϕ fixing each element of Q': for each $q \in Q'$, $\phi(q) = q$. Particularly $\mathrm{Aut}_\emptyset(\mathcal{A}) = \mathrm{Aut}(\mathcal{A})$, and $\mathrm{Aut}_Q(\mathcal{A})$ is reduce to the identity. For instance, the automorphism group of the automaton depicted on Fig. 2(a) has two elements, the identity and the isomorphism switching 2 and 3.

The size of the automorphism group of a non deterministic n-state automaton may vary from 1 to $n!$. For instance, any deterministic trim automaton whose states are all final has an automorphism group reduce to the identity. The non deterministic n-state automaton with no transition and



$\varphi(\mathcal{A}_1) = \mathcal{A}_2,\ \varphi(1) = 2,\ \varphi(2) = 3,\ \varphi(3) = 4,\ \varphi(4) = 1.$

Figure 2: Two Isomorphic Automata

where all states are both initial and final has for automorphism group the symmetric group.

The isomorphism problem consists in deciding whether two finite automata are isomorphic. It is investigated for deterministic automata on different alphabet in [13] (with a different definition of isomorphism). It is naturally closed to the same problem for directed graph and the following result [14] will be useful in this paper.

Theorem 1 *Let m be a fixed positive integer. The isomorphism problem for directed graphs with degree bounded by m is polynomial.*

1.3 Theoretical Background on Markov Chains

For a general reference on Markov Chains see [15]. Basic probability notions will not be defined in this paper. The reader is referred for instance to [16].

Let Ω be a finite set. A *Markov chain* on Ω is a sequence $X_0, \ldots, X_t, \ldots$ of random variables on Ω such that $\mathbb{P}(X_{t+1} = x_{t+1} \mid X_t = x_t) = \mathbb{P}(X_{t+1} = x_{t+1} \mid X_t = x_t, \ldots, X_i = x_i, \ldots, X_0 = x_0)$, for all $x_i \in \Omega$. A Markov chain is defined by its *transition matrix* M, which is a function from $\Omega \times \Omega$ into $[0, 1]$ satisfying $M(x, y) = \mathbb{P}(X_{t+1} = y \mid X_t = x)$. The underlying graph of

a Markov chain is the graph whose set of vertices is Ω and there is an edge from x to y if $M(x,y) \neq 0$. A Markov chain is *irreducible* if its underlying graph is strongly connected. It is *aperiodic* if for all node x, the gcd of the lengths of all cycles visiting x is 1. Particularly, if for each x, $M(x,x) \neq 0$, the Markov chain is aperiodic. A Markov chain is *ergodic* if it is irreducible and aperiodic. A Markov chain is symmetric if $M(x,y) = M(y,x)$ for all $x, y \in \Omega$. A distribution π on Ω is a stationary distribution for the Markov Chain if $\pi M = \pi$. It is known that an ergodic Markov chain has a unique stationary distribution [15, Chapter 1]. Moreover, if the chain is symmetric, this distribution is the uniform distribution on Ω.

Given an ergodic Markov chain $X_0, \ldots, X_t, \ldots$ with stationary distribution π, it is known that, whatever is the value of X_0, the distribution of X_t converges to π when $t \to +\infty$: $\max \|M^t(x,\cdot) - \pi\|_{TV} \underset{t\to+\infty}{\to} 0$, where $\|\|_{TV}$ designates the total variation distance between two distributions [15, Chapter 4]. This leads to the Monte-Carlo technique to randomly generate elements of Ω according to the distribution π by choosing arbitrarily X_0, computing $X_1, X_2, \ldots$, and returning X_t for t large enough. The convergence rate is known to be exponential, but computing the constants is a very difficult problem: choosing the step t to stop is a challenging question depending both on how close to π we want to be and on the convergence rate of $M^t(x,\cdot)$ to π. For this purpose, the *ε-mixing time* of an ergodic Markov chain of matrix M and stationary distribution π is defined by $t_{\text{mix}}(\varepsilon) = \min\{t \mid \max_{x\in\Omega} \|P_t(x,\cdot) - \pi\|_{TV} \leq \varepsilon\}$. Computing mixing time bounds is a central question on Markov Chains.

The Metropolis-Hasting Algorithm is based on the Monte-Carlo technique and aims at modifying the transition matrix of the Markov chain in order to obtain a particular stationary distribution [15, Chapter 3]. Suppose that M is an ergodic symmetric transition matrix of a symmetric Markov chain on Ω and ν is a distribution on Ω. The transition matrix P_ν for ν is defined by:

$$P_\nu(x,y) = \begin{cases} \min\left\{1, \frac{\nu(y)}{\nu(x)}\right\} M(x,y) & \text{if } x \neq y, \\ 1 - \sum_{z\neq x} \min\left\{1, \frac{\nu(z)}{\nu(x)}\right\} M(x,z) & \text{if } x = y. \end{cases}$$

The chain defined by P_ν is called *the Metropolis Chain for ν*. It is known [15, Chapter 3] that it is an ergodic Markov chain whose stationary distribution is ν.

2 Random Generation of Non Deterministic Automata using Markov Chain

In this section, we propose families of symmetric ergodic Markov chains on $\mathfrak{A}(n)$, $\mathfrak{N}(n)$, $\mathfrak{N}_m(n)$ and $\mathfrak{N}'_m(n)$, as well as on the respective corresponding doted classes of NFAs. The movement of theses Markov chains are depicted in Fig. 3.

Let $\mathcal{A} = (Q, \Sigma, \Delta, I, F)$ be a finite automaton. For any q in Q and any (p, a, q) in $Q \times \Sigma \times Q$, the automata $\mathsf{Ch}_{\mathsf{init}}(\mathcal{A}, q)$, $\mathsf{Ch}_{\mathsf{final}}(\mathcal{A}, q)$ and $\mathsf{Ch}_{\mathsf{trans.}}(\mathcal{A}, (p, a, q))$ are defined as follows:

- If $q \in I$, then $\mathsf{Ch}_{\mathsf{init}}(\mathcal{A}, q) = (Q, \Sigma, \Delta, I \setminus \{q\}, F)$ and $\mathsf{Ch}_{\mathsf{init}}(\mathcal{A}, q) = (Q, \Sigma, \Delta, I \cup \{q\}, F)$ otherwise.
- If $q \in F$, then $\mathsf{Ch}_{\mathsf{final}}(\mathcal{A}, q) = (Q, \Sigma, \Delta, I, F \setminus \{q\})$, and $\mathsf{Ch}_{\mathsf{final}}(\mathcal{A}, q) = (Q, \Sigma, \Delta, I, F \cup \{q\})$ otherwise.
- If $(p, a, q) \in \Delta$, then $\mathsf{Ch}_{\mathsf{trans.}}(\mathcal{A}, (p, a, q)) = (Q, \Sigma, \Delta \setminus \{(p, a, q)\}, I, F)$, and $\mathsf{Ch}_{\mathsf{trans.}}(\mathcal{A}, (p, a, q)) = (Q, \Sigma, \Delta \cup \{(p, a, q)\}, I, F)$ otherwise.

Let ρ_1, ρ_2, ρ_3 be three real numbers satisfying $0 \leq \rho_i \leq 1$ and $\rho_1 + \rho_2 + \rho_3 \leq 1$. Let $\mathfrak{X}$ be a class of automata whose set of states is Q. We define the transition matrix $S^{\mathfrak{X}}_{\rho_1,\rho_2,\rho_3}(x, y)$ on $\mathfrak{X}$ by:

- If there exists q such that $y = \mathsf{Ch}_{\mathsf{init}}(x, q)$, then $S^{\mathfrak{X}}_{\rho_1,\rho_2,\rho_3}(x, y) = \frac{\rho_1}{|Q|}$.
- If there exists q such that $y = \mathsf{Ch}_{\mathsf{final}}(x, q)$, then $S^{\mathfrak{X}}_{\rho_1,\rho_2,\rho_3}(x, y) = \frac{\rho_2}{|Q|}$.
- If there exists $(p, a, q) \in Q \times \Sigma \times Q$ such that $y = \mathsf{Ch}_{\mathsf{trans.}}(x, q)$, then $S^{\mathfrak{X}}_{\rho_1,\rho_2,\rho_3}(x, y) = \frac{\rho_3}{|\Sigma|.|Q|^2}$.
- If y is different of x and has not one of the above forms, $S^{\mathfrak{X}}_{\rho_1,\rho_2,\rho_3}(x, y) = 0$.
- $S^{\mathfrak{X}}_{\rho_1,\rho_2,\rho_3}(x, x) = 1 - \sum_{y \neq x} S^{\mathfrak{X}}_{\rho_1,\rho_2,\rho_3}(x, y)$.

Now for $\mathfrak{X} \in \{\mathfrak{N}(n), \mathfrak{N}_m(n), \mathfrak{N}'_m(n)\}$, and $0 < \rho < 1$ we define the transition matrix $S^{\mathfrak{X}^\bullet}_{\rho}$ on $\mathfrak{X}^\bullet$ by $S^{\mathfrak{X}^\bullet}_{\rho} = S^{\mathfrak{X}}_{0,\rho,1-\rho}$.

Lemma 2 *Let m, n be fixed positive integers, with $m \geq 2$. If $1 > \rho > 0$, $\rho_1 > 0$, $\rho_2 > 0$ and $\rho_3 > 0$, then $S^{\mathfrak{N}(n)}_{\rho_1,\rho_2,\rho_3}$, $S^{\mathfrak{N}_m(n)}_{\rho_1,\rho_2,\rho_3}$ and $S^{\mathfrak{N}'_m(n)}_{\rho_1,\rho_2,\rho_3}$ are irreducible, as well as $S^{\mathfrak{N}(n)^\bullet}_{\rho}$, $S^{\mathfrak{N}_m(n)^\bullet}_{\rho}$ and $S^{\mathfrak{N}'_m(n)^\bullet}_{\rho}$.*

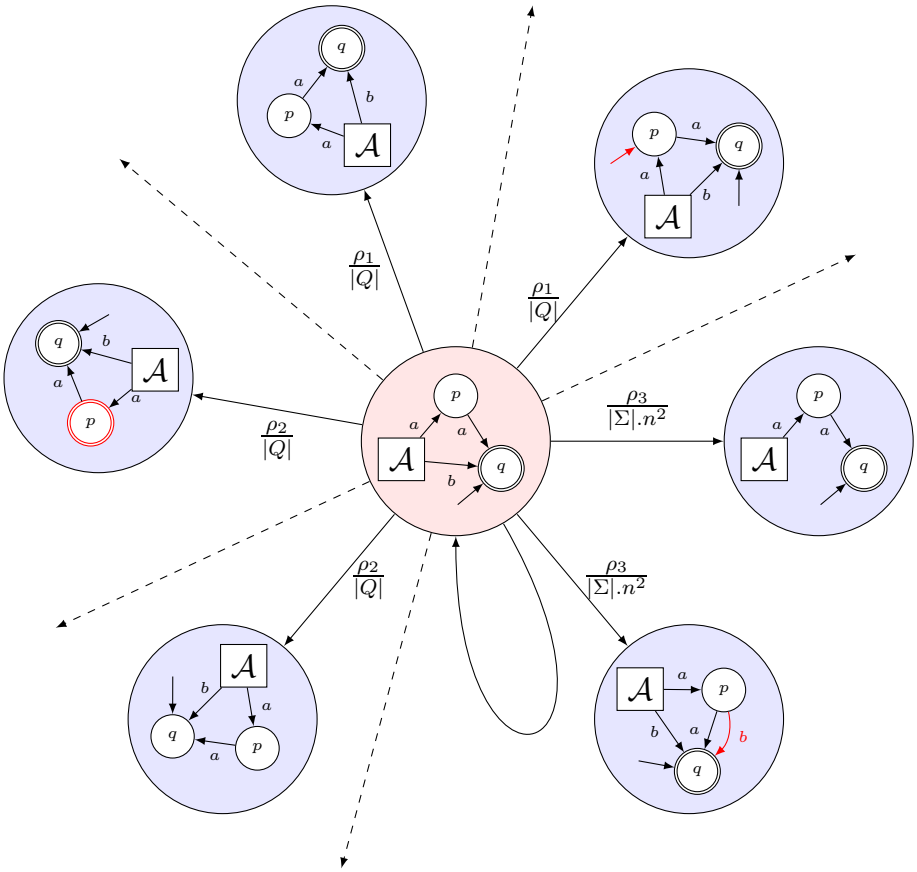


Figure 3: Moves into the Markov Chain. The current state of the Markov Chain is in the center and, around, typical moves. Of course, other moves are possible on other parts of the automaton, which is represented by the dashed arrows.

PROOF. Without loss of generality, we assume that $Q = \{1, \ldots, n\}$. Let $\mathfrak{X} \in \{\mathfrak{N}(n), \mathfrak{N}_m(n), \mathfrak{N}'_m(n)\}$ and $x \in \mathfrak{X}$. We denote by $\mathcal{A}_0$ the automaton $(Q, \Sigma, \emptyset, Q, Q)$. The automaton $\mathcal{A}_0$ is trim and is in $\mathfrak{X}$. We prove there is a path in $\mathfrak{X}$ from x to $\mathcal{A}_0$. Set $x = (Q, \Sigma, \Delta, I, F)$. Since adding initial or final

states to x provides automata that are still in $\mathfrak{X}$, there is a path from x to $y = (Q, \Sigma, \Delta, Q, Q)$ (using $\mathsf{Ch}_{\mathsf{init}}$ and $\mathsf{Ch}_{\mathsf{final}}$). Now, since all states are both initial and final, there is a path from y to $\mathcal{A}_0$ (by deleting all transitions). It follows there is a path in $\mathfrak{X}$ from x to $\mathcal{A}_0$. Since the graph of the Markov chain is symmetric, there is also a path from $\mathcal{A}_0$ to x. Consequently, the Markov chains are irreducible.

We will now consider the bullet classes. The proof is only done for $\mathfrak{N}_m(n)^\bullet$. Proof for others classes are similar. Let a_0 be an arbitrary letter of Σ. Let $x = (\{1, \dots, n\}, \Sigma, \Delta, \{1\}, F) \in \mathfrak{N}_m(n)^\bullet$. Let $\mathcal{A}_1$ be the automaton of $\mathfrak{N}_m(n)^\bullet$ whose set of final states is $\{1, \dots, n\}$ and whose set of transitions is $\{(i, a_0, i+1) \mid 1 \leq i < n\}$. We will prove that there is a path from x to $\mathcal{A}_1$ in the graph of the Markov chain.

- By adding final states, there is a path from x to the automaton $y = (\{1, \dots, n\}, \Sigma, \Delta, \{1\}, \{1, \dots, n\})$.
- Let Δ' be a subset of Δ forming a spanning tree of Δ rooted in 1 (it exists for y is accessible). By removing transitions, there is a path from y to $z = (\{1, \dots, n\}, \Sigma, \Delta', \{1\}, \{1, \dots, n\})$.
- If z there are in z at least two states p and q that have no outgoing transition (p and q are leaves of the spanning tree), then by adding a transition (p, a_0, q) and by removing the unique transition arriving in q, we build a path from z to an automaton inducing a tree on $, \{1, \dots, n\}$ and having strictly less leaves. By repeating this kind of moves, there is a path from z to an automaton of the form

  $$u = (\{1, \dots, n\}, \Sigma, \{(\varphi(i), a_i, \varphi(i+1)) \mid 1 \leq i < n\}, \{1\}, \{1, \dots, n\}),$$

  where φ is a permutation of $\{1, \dots, n\}$ fixing 1.
- Since $m \geq 2$, one can add a transition leaving each state. Therefore, by adding each transition of the form $(i, a_0, i+1)$. Next, one can remove all transitions that are not of the from $(i, a_0, i+1)$, providing a path from u to $\mathcal{A}_1$.

It follows that there is a path from x to $\mathcal{A}_1$ and, since the graph is symmetric, a path from $\mathcal{A}_1$ to x, proving that the Markov chain is irreducible. □

Lemma 3 *Let m, n be two fixed positive integers, with $m \geq 2$. If $1 > \rho > 0$, $\rho_1 > 0$, $\rho_2 > 0$ and $\rho_3 > 0$, then $S^{\mathfrak{N}(n)}_{\rho_1,\rho_2,\rho_3}$, $S^{\mathfrak{N}_m(n)}_{\rho_1,\rho_2,\rho_3}$ and $S^{\mathfrak{N}'_m(n)}_{\rho_1,\rho_2,\rho_3}$ are aperiodic, as well as $S^{\mathfrak{N}(n)^\bullet}_{\rho}$, $S^{\mathfrak{N}_m(n)^\bullet}_{\rho}$ and $S^{\mathfrak{N}'_m(n)^\bullet}_{\rho}$.*

PROOF. With the notations of the proof of Lemma 2, there is a path of length n_x from any $x \in \mathfrak{X}$ to $\mathcal{A}_0$. Therefore there is a cycle of length $2n_x$ visiting x.

Now, $\mathsf{Ch}_{\mathsf{init}}(\mathcal{A}_0, 1) \notin \mathfrak{X}$ since 1 is not accessible in $\mathcal{A}_0$. It follows that $S^{\mathfrak{X}}(\mathcal{A}_0, \mathcal{A}_0) \neq 0$. Therefore, there is also a cycle of length $2n_x + 1$ visiting x. Since the gcd of $2n_x$ and $2n_x + 1$ is 1, the chain is aperiodic.

The proof for $S^{\mathfrak{N}(n)^\bullet}_{\rho}$ is similar: From $\mathcal{A}_1$, if the transition $(1, a_0, 2)$ is picked up (with probability $\frac{(1-\rho)}{|\Sigma|n^2} \neq 0$), then we move from $\mathcal{A}_1$ to $\mathcal{A}_1$. Therefore there is a loop of length 1 from $\mathcal{A}_1$ to $\mathcal{A}_1$ in the graph of the Markov chain, proving that the Markov chain is aperiodic.

One can do as well for $S^{\mathfrak{N}_m(n)^\bullet}_{\rho}$ and $S^{\mathfrak{N}'_m(n)^\bullet}_{\rho}$. □

Proposition 4 *Let m, n be two fixed positive integers, with $m \geq 2$. The Markov chains with matrix $S^{\mathfrak{N}(n)}_{\rho_1,\rho_2,\rho_3}$, $S^{\mathfrak{N}_m(n)}_{\rho_1,\rho_2,\rho_3}$ and $S^{\mathfrak{N}'_m(n)}_{\rho_1,\rho_2,\rho_3}$ are ergodic and their stationary distributions are the uniform distributions.*

PROOF. By lemma 3 and 2, the chain is ergodic. Since the matrix $S^{\mathfrak{N}(n)}_{\rho_1,\rho_2,\rho_3}$, $S^{\mathfrak{N}_m(n)}_{\rho_1,\rho_2,\rho_3}$ and $S^{\mathfrak{N}'_m(n)}_{\rho_1,\rho_2,\rho_3}$ are symmetric, their stationary distributions are the uniform distributions (over the respective family of automata). □

In practice, computing X_{t+1} from X_t is done in the following way: the first step consists in choosing with probabilities ρ_1, ρ_2 and ρ_3 whether we will change either an initial state, a final state or a transition. In a second step and in each case, all the possible changing operations are performed with the same probability. If the obtained automaton is in the corresponding class, X_{t+1} is set to this value. Otherwise, $X_{t+1} = X_t$. Since verifying that an automaton is in the desired class ($\mathfrak{N}(n)$, $\mathfrak{N}_m(n)$ or $\mathfrak{N}'_m(n)$), can be performed in time polynomial in n, computing X_{t+1} from X_t can be done in time polynomial in n.

We define the lazy Markov chain on $\mathfrak{A}(n)$ by $L^{\mathfrak{A}(n)}_{\rho_1,\rho_2,\rho_3}(x, y) = \frac{1}{2} S^{\mathfrak{A}(n)}_{\rho_1,\rho_2,\rho_3}(x, y)$ if $x \neq y$ and $L^{\mathfrak{A}(n)}_{\rho_1,\rho_2,\rho_3}(x, x) = \frac{1}{2} + \frac{1}{2} S^{\mathfrak{A}(n)}_{\rho_1,\rho_2,\rho_3}(x, x)$. It is known that a symmetric Markov chain and its associated lazy Markov chain have similar mixing times.

Proposition 5 *The ε-mixing time $\tau(\varepsilon)$ of $L_{\rho_1,\rho_2,\rho_3}^{\mathfrak{A}(n)}$ satisfies*

$$\tau(\varepsilon) \leqslant \max\left(\left\lceil \frac{n}{\rho_1}\left(\log(n)+\log\left(\frac{1}{\rho_1\varepsilon}\right)\right)\right\rceil, \left\lceil \frac{n}{\rho_2}\left(\log(n),\log\left(\frac{1}{\rho_2\varepsilon}\right)\right)\right\rceil, \left\lceil \frac{|\Sigma|n^2}{\rho_3}\left(\log(|\Sigma|n^2)+\log\left(\frac{1}{\rho_3\varepsilon}\right)\right)\right\rceil\right).$$

Proof.

The proof lies on classical results on random walks int he hypercube.

To each finite automaton $\mathcal{A} = (Q, \Sigma, \Delta, I, F)$ in $\mathfrak{A}(n)$ one can associate a function φ_I from $Q = \{1, \ldots, n\}$ to $\{0, 1\}$ by:

$$\forall q \in Q,\ \varphi_I(q) = \begin{cases} 1 \text{ if } q \in I \\ 0 \text{ otherwise.} \end{cases}$$

In a same way, the functions $\varphi_F : Q \to \{0, 1\}$ and $\varphi_\Delta : Q \times \Sigma \times Q$ are defined as the characteristic function s 1_F and 1_Δ on F and Δ considered as subsets of respectively Q and $Q \times \Sigma \times Q$.

The automaton $\mathcal{A}$ is completely defined by φ_I, φ_F and φ_Δ (since the alphabet is fixed). Therefore, the Markov chain can be decomposed into three random walks : the two first on hypercubes of dimension n and the last one on an hypercube of dimension $n^2|\Sigma|$ (for the transitions). At each step, one moves with probability ρ_1 in the first hypercube, with probability ρ_2 in the second hypercube and with probability ρ_3 in the last hypercube.

The result is then the application of known mixing time results for lazy random walk in the hypercube, see for instance [15, Section 6.5.2, page 81]. □

At this stage, we are not able to compute bounds on the mixing times of the other Markov chains. Practical experiments, with various sizes of alphabets, seems to show that most of the automata generated by the above lazy Markov Chain (using n^3 as mixing bound) are trim. The experimental results are reported in Table 1. This observation leads us to consider, for other experiments, to move n^3 steps to sample automata. Of course, this is not a proof, just an empirical estimation.

3 Metropolis Hastings Approach

In this section we show how to use the Metropolis-Hastings algorithm to uniformly generate NFAs up to isomorphism and that, for this purpose, it

$n \to$	5	10	15	20
$\mathfrak{N}(n)$, 2 letters	0.94	0.95	0.99	1.0
$\mathfrak{N}(n)$, 4 letterers	0.95	0.96	1.0	1.0

Table 1: Observed proportion of trim automata.

suffices to compute the sizes of the automorphism groups of involved NFAs. We prove in Section 3.2 that this computation is polynomially equivalent to testing the isomorphism problem for the involving automata. For the classes $\mathfrak{N}_m(n)$, $\mathfrak{N}_m(n)^\bullet$, $\mathfrak{N}'_m(n)$ and $\mathfrak{N}'_m(n)^\bullet$, we show that it can be done in time polynomial in n (if m is fixed). In Section 5.1 we show how to practically compute the sizes of automorphism group using labelings techniques. Finally, experimental results are given in Section 5.2.

3.1 Metropolis-Hastings Algorithm

For a class $\mathfrak{C}$ of NFAs (closed by isomorphism) and n a positive integer, let $\mathfrak{C}(n)$ be the elements of $\mathfrak{C}$ whose set of states is $\{1, \ldots, n\}$ and let γ_n be the number of isomorphism classes on $\mathfrak{C}(n)$. There are $n!$ possible bijections on $\{1, \ldots, n\}$. If $\mathcal{A} \in \mathfrak{C}(n)$, Let φ_1 and φ_2 be two bijections on $\{1, \ldots, n\}$. One has $\varphi_1(\mathcal{A}) = \varphi_2(\mathcal{A})$ iff $\varphi_2^{-1}\varphi_1(\mathcal{A}) = \mathcal{A}$, iff $\varphi_2^{-1}\varphi_1(\mathcal{A}) \in \mathrm{Aut}(\mathcal{A})$. It follows that the isomorphism classes of $\mathcal{A}$ (in $\mathfrak{C}(n)$) has $\frac{n!}{|\mathrm{Aut}(\mathcal{A})|}$ elements. This leads to the following result.

Proposition 6 *Randomly generates an element x of $\mathfrak{C}(n)$ with probability $\frac{|\mathrm{Aut}(x)|}{\gamma_n n!}$ provides a uniform random generator of the isomorphism classes of $\mathfrak{C}(n)$.*

Proof. Let H be an isomorphism class of $\mathfrak{C}(n)$; H is generated with probability

$$\sum_{x \in H} \frac{|\mathrm{Aut}(x)|}{\gamma_n n!} = \sum_{x \in H} \frac{1}{\gamma_n |H|} = \frac{1}{\gamma_n |H|} \sum_{x \in H} 1 = \frac{|H|}{\gamma_n |H|} = \frac{1}{\gamma_n}.$$

□

In order to compute P_ν it is not necessary to compute γ_n, since $\frac{\nu(x)}{\nu(y)} = \frac{|\mathrm{Aut}(y)|}{|\mathrm{Aut}(x)|}$. A direct use of the Metropolis-Hastings algorithm requires to compute all the neighbors of x and the sizes of theirs automorphism groups to

move from x. Since a n-state automaton has about $|\Sigma|n^2$ neighbors, it can be a quite huge computation for each move. However, practical evaluations show that in most cases the automorphism group of an automaton is quite small and, therefore, the rejection approach exposed in [17] is more tractable. It consists in moving from x to y using $S(x, y)$ (the non-modified chain) and to accept y with probability $\min\left\{1, \frac{\nu(y)}{\nu(x)}\right\}$. If it is not accepted, repeat the process (moving from x to y using S with probability $\min\left\{1, \frac{\nu(y)}{\nu(x)}\right\}$) until acceptance. In practice, we observe a very small number of rejects.

The problem of computing the size of the automorphism group of a NFA is investigated in the next session. Assuming it can be done in a reasonable time, an alternative solution to randomly generate NFAs up to isomorphism may be to use a rejection algorithm: randomly and uniformly generate a NFA $\mathcal{A}$ and keep it with probability $\frac{|\mathrm{Aut}(\mathcal{A})|}{n!}$. This way, each class of isomorphism is picked up with the same probability. However, as we will observe in the experiments (see Table 2), most of automata have a very small group of automorphisms, and the number of rejects will be intractable, even for quite small n's.

3.2 Counting Automorphisms

This section is dedicated to show how to compute $|\mathrm{Aut}(\mathcal{A})|$ by using a polynomial number of calls to the isomorphism problem. It is an adaptation of a corresponding result for directed graphs [18].

Let $\mathcal{A} = (Q, \Sigma, \Delta, I, F)$ be a NFA and $Q' \subseteq Q$. Let σ be an arbitrary bijective function from Q' into $\{1, \ldots, |Q'|\}$, a_0 an arbitrary letter in Σ and $\ell = |Q| + |Q'| + 2$. For each state $r \in Q \backslash Q'$ we denote by $\mathcal{A}_r^{Q'}$ the automaton $(Q_r, \Sigma, \Delta_r, I, F)$ where $Q_r = Q \cup \{(p, i) \mid p \in Q \text{ and } 1 \leq i \leq \ell\}$, and $\Delta_r = \Delta \cup \{(p, a, (p, 1) \mid p \in Q\} \cup \{((p, i), a_0, (p, i + 1)) \mid p \in Q' \text{ and } 1 \leq i < |Q| + 1 + \sigma(p)\} \cup \{((r, i), a_0, (r, i + 1)) \mid 1 \leq i \leq \ell\} \cup \{((p, i), a_0, (p, i + 1)) \mid p \notin Q' \cup \{r\} \text{ and } 1 < i \leq |Q| + 1\}$. Note that the size of $\mathcal{A}_r^{Q'}$ is polynomial in the size of $\mathcal{A}$.

The two next lemma show how to polynomially reduce the problem of counting automorphisms to the isomorphism problem.

Lemma 7 *Let $\mathcal{A} = (Q, \Sigma, \Delta, I, F)$ be a NFA and Q' a non-empty subset of Q. For every $q, q' \in Q \backslash Q'$, there exists $\phi \in \mathrm{Aut}_{Q'}(\mathcal{A})$ such that $\phi(q) = q'$ iff $\mathcal{A}_q^{Q'}$ and $\mathcal{A}_{q'}^{Q'}$ are isomorphic.*

PROOF. In $\mathcal{A}_r$, for any state $p \in Q' \cup \{r\}$, we denote by π_p the path

$$\pi_p = (p, a_0, (p,1))((p,1), a_0, (p,2)) \dots ((p, \ell-1), a_0, (p, \ell)),$$

called the *tail* of p.

Assume that there exists $\phi \in \mathrm{Aut}_{Q'}(\mathcal{A})$ such that $\phi(q) = q'$. Let $\hat{\phi}$ be the function defined from the set of states of $\mathcal{A}_q$ into the set of $\mathcal{A}_{q'}$ by: if $p \in Q$, then $\hat{\phi}(p) = \phi(p)$ and if (p,i) is a state of $\mathcal{A}_q$, then $\hat{\phi}((p,i)) = (\phi(p), i)$. This function is well defined since p and $\varphi(p)$ have tails of the same length. By construction, $\hat{\phi}$ is an isomorphism.

Conversely, assume that there exists an isomorphism Φ from $\mathcal{A}_q$ to $\mathcal{A}_{q'}$. Since isomorphisms preserve accessible and co-accessible states and since $\mathcal{A}$ is trim, $p \in Q$ iff $\Phi(p) \in Q$. Let ϕ be the restriction of Φ to Q. Since Φ is a morphism, ϕ is an automorphism of $\mathcal{A}$. Now, Φ preserves the lengths of the tails. It follows that for any $p \in Q'$, $\Phi(p) = p$. Furthermore, $\Phi(q) = q'$ for the same reason, proving the lemma. □

Lemma 8 *Let $\mathcal{A} = (Q, \Sigma, \Delta, I, F)$ be a NFA and Q' a non-empty subset of Q. For every $q \in Q'$, there exists an integer d such that $|\mathrm{Aut}_{Q'\setminus\{q\}}(\mathcal{A})| = d|\mathrm{Aut}_{Q'}(\mathcal{A})|$. Moreover d can be computed with a polynomial number of isomorphism tests between automata of the form $\mathcal{A}_r^{Q'\setminus\{q\}}$.*

PROOF. Let $d = |\{\phi(q) \mid \phi \in \mathrm{Aut}_{Q'\setminus\{q\}}(\mathcal{A})\}|$. We consider the relation $\sim_q$ on $\mathrm{Aut}_{Q'\setminus\{q\}}(\mathcal{A})$ defined by $\phi_1 \sim_q \phi_2$ iff $\phi_1(q) = \phi_2(q)$. One has $\phi_1 \sim_q \phi_2$ iff $\phi_1\phi_2^{-1} \in \mathrm{Aut}_{Q'}(\mathcal{A})$. Therefore $\sim$ is a group-congruence relation and, therefore, $|\mathrm{Aut}_{Q'\setminus\{q\}}(\mathcal{A})| = d|\mathrm{Aut}_{Q'}(\mathcal{A})|$.

To compute d it suffices to test which elements of $Q \setminus Q'$ are in $\{\phi(q) \mid \phi \in \mathrm{Aut}_{Q'\setminus\{q\}}(\mathcal{A})\}$, whether there exists an automorphism ϕ in $\mathrm{Aut}_{Q'\setminus\{q\}}(\mathcal{A})$ such that $\phi(q) = p$. □

Lemma 8 provides a way to compute sizes of automorphism groups by testing whether two NFAs are isomorphic. Indeed, since $\mathrm{Aut}_Q(\mathcal{A})$ is reduced to the identity, and since $\mathrm{Aut}(\mathcal{A}) = \mathrm{Aut}_\emptyset(\mathcal{A})$, one has, by a direct induction using Lemma 8, $\mathrm{Aut}(\mathcal{A}) = d_1 \dots d_{|Q|}$, where each d_i can be computed by a polynomial number of isomorphism tests. Therefore, the problem of counting automorphism reduces to test whether two automata are isomorphic.

4 Polynomial Time Result for Specific Classes

4.1 Isomorphism Problem for Automata with a Bounded Degree

It is proved (not explicitly) in [13] that the isomorphism problem for deterministic automata (with a different notion of isomorphismsince automata may have different alphabets) is polynomially equivalent to the isomorphism problem for directed finite graphs. We prove (Theorem 9) a similar result for NFAs, by using an encoding preserving some bounds on the output degree. Therefore, combining Theorem 9 and Lemma 8, it is possible to compute the size of the automorphism group of an automaton in $\mathfrak{N}_m(n)$, $\mathfrak{N}'_m(n)$, $\mathfrak{N}_m(n)^\bullet$ and $\mathfrak{N}'_m(n)^\bullet$ in time polynomial in n (assuming that m is a constant).

Theorem 9 *Let m be a fixed integer. The isomorphism problem for automata in $\mathfrak{N}_m$ $\mathfrak{N}'_m$, $\mathfrak{N}_m(n)^\bullet$ and $\mathfrak{N}'_m(n)^\bullet$ can be solved in polynomial time.*

The proof of the theorem is given in appendix and is based on a graph encoding of non deterministic automata and on Theorem 1 [14]. Note that the proof is constructive but the exponents are too huge to provide an efficient algorithm. It will be possible to work on a finer encoding but we prefer, in practice, to use labeling techniques described in the next section and that are practically very efficient on graphs (see [19] for a recent survey).

4.2 Proof of Theorem 9

Let h be an arbitrary bijective function from Σ into $\{1, \ldots, k\}$.

Let $\mathcal{A} = (Q, \Sigma, \Delta, I, F)$ be a finite automaton. We denote by $G_{\mathcal{A}}$ the finite graph (V, E) where:

- $V = Q \cup (I \cap F^c) \times \{1, \ldots, k+1\} \cup (F \cap I^c) \times \{1, \ldots, k+2\} \cup (I \cap F) \times \{1, \ldots, k+3\} \cup \{((p, a, q), i) \mid (p, a, q) \in \Delta \text{ and } 1 \leq i \leq h(a)\} \cup \Delta$.
- $E = \{(p, (p, a, q)) \mid (p, a, q) \in \Delta\} \cup \{((p, a, q)), q) \mid (p, a, q) \in \Delta\} \cup \{((p, a, q), ((p, a, q), 1)) \mid (p, a, q) \in \Delta\} \cup \{(((p, a, q), i), ((p, a, q), j)) \mid (p, a, q) \in \Delta \text{ and } 1 \leq i, j \leq h(a)\} \cup \{((q, i), (q, j)) \mid q \in I \cap F^c \text{ and } 1 \leq i, j \leq k+1\} \cup \{((q, i), (q, j)) \mid q \in F \cap I^c \text{ and } 1 \leq i, j \leq k+2\} \cup \{((q, i), (q, j)) \mid q \in F \cap I \text{ and } 1 \leq i, j \leq k+3\} \cup \{(q, (q, 1)) \mid q \in I \cup F)\}$

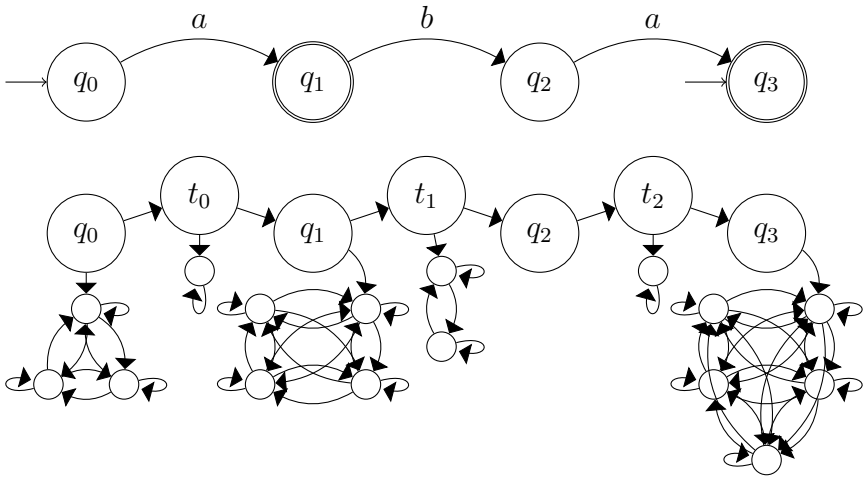


Figure 4: Example $\mathcal{A}$ and $G_{\mathcal{A}}$, $h(a) = 1$ and $h(b) = 2$

Intuitively each transition is first decomposed into two edges, then a complete graph (with a number of edges depending on the letter of the transition) is linked to the middle vertex. A similar construction is done for initial, final or both initial and final states.

For any vertex s of $G_{\mathcal{A}} = (V, E)$, we denote by $d(s)$ the largest possible size of a clique in $G_{\mathcal{A}}$ containing s. More formally, one has

$$d(s) = \max\{|H|,\ H \times H \subseteq E \text{ and } s \in H\}|$$

Note that we may have $d(s) = 0$.

Lemma 10 *For any vertex s of $G_{\mathcal{A}}$, one has $0 \leq d(s) \leq k + 3$.*

Proof. By construction.

Lemma 11 *Let $\mathcal{A}$ be a finite automaton. If there is in $G_{\mathcal{A}}$ an edge of the form (s, t) then,*

1. *If $d(s) = 0$, then s is in $Q \cup \Delta$,*
2. *If $0 < d(s) \leq k$, then s is of the form $((p, \ell, q), i)$, with $(p, \ell, q) \in \Delta$ and $1 \leq i \leq h^{-1}(\ell)$,*

3. *If* $d(s) = k+1$, *then* s *is of the form* (q,i) *with* $q \in I \cap F^c$,

4. *If* $d(s) = k+2$, *then* s *is of the form* (q,i) *with* $q \in F \cap I^c$,

5. *If* $d(s) = k+3$, *then* s *is of the form* (q,i) *with* $q \in F \cap I$.

PROOF. By construction. □

Lemma 12 *Let* $\mathcal{A}$ *be a finite automaton. If there is in* $G_{\mathcal{A}}$ *an edge of the form* (s,t) *with* $s \in Q$, *then*

1. $d(t) \in \{0, k+1, k+2, k+3\}$ *and,*

2. *If* $d(t) = 0$, *then* t *is in* Δ,

3. *If* $d(t) = k+1$, *then* $s \in I \cap F^c$,

4. *If* $d(t) = k+2$, *then* $s \in F \cap I^c$,

5. *If* $d(t) = k+3$, *then* $s \in F \cap I$.

Proposition 13 *Two finite automata* $\mathcal{A}_1$ *and* $\mathcal{A}_2$ *are isomorphic iff* $G_{\mathcal{A}_1}$ *and* $G_{\mathcal{A}_2}$ *are isomorphic too.*

PROOF. By construction if $\mathcal{A}_1$ and $\mathcal{A}_2$ are isomorphic, then $G_{\mathcal{A}_1}$ and $G_{\mathcal{A}_2}$ are isomorphic too.

Now let $\mathcal{A}_1 = (Q_1, A, \Delta_1, I_1, F_1)$ and $\mathcal{A}_2 = (Q_2, A, \Delta_2, I_2, F_2)$ be two NFAs such that $G_{\mathcal{A}_1}$ and $G_{\mathcal{A}_2}$ are isomorphic. One can note that for every vertex s of $G_{\mathcal{A}_1}$, $d(\varphi(s)) = d(s)$. It follows that, $d(s) = 0$ iff $d(\varphi(s)) = 0$. Therefore, by Lemma 11, φ induces a bijective map from Q_1 to Q_2. In the following we prove that the restriction of φ to Q_1 is an isomorphism from Q_1 to Q_2.

- If $q \in I_1 \cap F_1^c$, then $d((q,1)) = k+1$. Therefore $d(\varphi((q,1))) = k+1$. Since $(q,(q,1))$ is an edge of $G_{\mathcal{A}_1}$, $(\varphi(q), \varphi((q,1)))$ is an edge of $G_{\mathcal{A}_2}$. Using the Assertion 3. of Lemma 12, $\varphi(q) \in I_2 \cap F_2^c$.

- If $q \in I_1^c \cap F_1$, then $d((q,1)) = k+2$. Therefore $d(\varphi((q,1))) = k+2$. Since $(q,(q,1))$ is an edge of $G_{\mathcal{A}_1}$, $(\varphi(q), \varphi((q,1)))$ is an edge of $G_{\mathcal{A}_2}$. Using the Assertion 4. of Lemma 12, $\varphi(q) \in I_2 \cap F_2^c$.

- If $q \in I_1 \cap F_1$, then $d((q,1)) = k+3$. Therefore $d(\varphi((q,1))) = k+3$. Since $(q,(q,1))$ is an edge of $G_{\mathcal{A}_1}$, $(\varphi(q), \varphi((q,1)))$ is an edge of $G_{\mathcal{A}_2}$. Using the Assertion 5. of Lemma 12, $\varphi(q) \in I_2 \cap F_2^c$.

- If $(p,a,q) \in \Delta_1$, then $d((p,a,q)) = 0$). Consequently $d(\varphi((p,a,q))) = 0$). Since $(p,(p,a,q))$ is an edge in $G_{\mathcal{A}_1}$, $(\varphi(p), \varphi((p,a,q)))$ is an edge in $G_{\mathcal{A}_2}$. By Assertion 2. of Lemma 12, $\varphi((p,a,q)) \in \Delta_2$. Set $\varphi((p,a,q)) = (s,b,t)$, with $s,t \in Q_2$. The only ongoing edge in (s,b,t) in $G_{\mathcal{A}_2}$ is $(s,(s,b,t))$. Since φ is an isomorphism, $(\varphi^{-1}(s),(p,a,q))$ is an edge of $G_{\mathcal{A}_1}$. It follows that $\varphi^{-1}(s) = p$. There are two outgoing edges from (s,b,t) in $G_{\mathcal{A}_2}$: $((s,b,t),(1,(s,b,t))$ and $((s,b,t),t)$. The two outgoing edges from (p,a,q) in $G_{\mathcal{A}_1}$ are $((p,a,q),1,(p,a,q))$ and $((p,a,q),q)$. Since $d(q) = 0$, $d(t) = 0$, $d((1,(p,a,q))) = h(a)$ and $d(((s,b,t),t)) = h(b)$, one necessarily has $\varphi(q) = t$ and $h(a) = h(b)$ (and therefore $a = b$). In conclusion, we proved that if $(p,a,q) \in \Delta_1$, then $(\varphi(p),a,\varphi(q)) \in \Delta_2$. The same proof can be made using φ^{-1}, proving the proposition.

□

Proposition 14 *The size of $G_{\mathcal{A}}$ is polynomial in the size of $\mathcal{A}$. Moreover, if there is at most m outgoing transitions from a state of $\mathcal{A}$, the degree of $G_{\mathcal{A}}$ is bounded by* $\max\{m+1, k+3\}$.

PROOF. By construction, the size of $G_{\mathcal{A}}$ is polynomial in the size of $\mathcal{A}$. Let s be a vertex of $G_{\mathcal{A}}$. The following cases arise:

- If $s \in Q \cap I^c \cap F^c$, then the edges in G_A starting from s are all of the form (s,t) where $t \in \Delta$ starts from s (as a transition in $\mathcal{A}$).
  Therefore there are at most m outgoing edges from s.

- If $s \in I \cup F$, then the edges in G_A starting from s are those of the form (s,t) where $t \in \Delta$ starts from s (as a transition in $\mathcal{A}$), and the one from s to $(s,(s,1))$.
  Therefore there are at most $m+1$ outgoing edges from s.

- If $s \in \Delta$, then there are two outgoing edges from s.

- If $s = (q,i)$, with $q \in Q$, then there are at most $k+3$ outgoing edges from (q,i).

- If $s = (t, i)$, with $t \in \Delta$, then there are at most k outgoing edges from (t, i), depending on the letter labeling t, proving the Proposition.

□

Theorem 9 is a consequence of Proposition 14, Proposition 13 and Theorem 1.

5 Practical Approach using Labelings

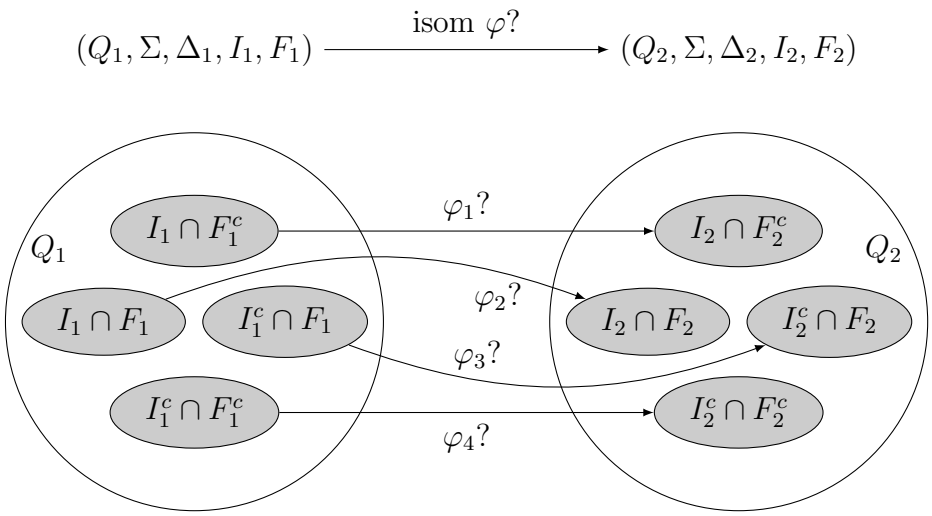


Figure 5: Labelings Technique

5.1 Practical Computation using Labelings

For testing graph isomorphism (or to count the number of automorphisms), the most efficient currently used approach is based on labeling [19] and it works practically for large graphs. It can be naturally adapted for NFAs. Intuitively, to illustrate the approach, one can note that if two n-state automata are isomorphic, then they have the same number of initial states and of final states. Rather than testing potential $n!$ possible bijections from the automata to point out an isomorphism, it suffices to test $n_1!n_2!n_3!n_4!$ where n_1 is the number of states that are both initial and final, n_2 the number of

final states (that are not initial), n_3 the number of initial states (that are not final), and n_4 is the number of states that are neither initial, nor final. With an optimal distribution, the number of tests falls from $n!$ to $[(n/4)!]^4$. Of course, if all states are both initial and final, there are still $n!$ bijection to test. This idea is illustrated in Fig. 5.

Input: $\mathcal{A}$, a n-state automaton, τ a labelling with image $D = \{\alpha_1, \ldots, \alpha_\ell\}$.
Output: $|\mathrm{Aut}(\mathcal{A})|$

$res = 0$
For $\alpha \in D$
    $C[\alpha] = \emptyset$
EndFor
For $i \in \{1, \ldots, n\}$
    $C[\tau(\mathcal{A}, i)] = C[\tau(\mathcal{A}, i)] \cup \{i\}$
EndFor
Foreach permutation σ_1 of $\tau^{-1}(\alpha_1)$
    Foreach permutation σ_2 of $\tau^{-1}(\alpha_2)$
        $\vdots$
        Foreach permutation σ_ℓ of $\tau^{-1}(\alpha_\ell)$
            If $\sigma = \sigma_1 \ldots \sigma_\ell \in \mathrm{Aut}(\mathcal{A})$, **Then**
                $res = res + 1$
            EndIf
        EndForeach
        $\vdots$
    EndForeach
EndForeach
Return res

Figure 6: Counting automorphisms using labelings

This idea can be generalized by the notion of labeling; the goal is to point out easily computable criteria that are stable by isomorphism to get a partition of the set of states and to reduce the search. The approach can be directly adapted for finite automata. A *labeling* is a computable function τ from $\mathfrak{N}(n) \times \{1, \ldots, n\}$ into a finite set D, such that for $\mathcal{A}_1 = (Q, \Sigma, E_1, I_1, F_1)$ and $\mathcal{A}_2 = (Q, \Sigma, E_2, I_2, F_2)$, if φ is an isomorphism from $\mathcal{A}_1$ to $\mathcal{A}_2$, then, for every $i \in \{1, \ldots, n\}$, $\tau(\mathcal{A}_1, i) = \tau(\mathcal{A}_2, \varphi(i))$. The algorithm consists in looking for functions φ preserving τ. If there exists $\alpha \in D$ such that

$|\{i \mid \tau(\mathcal{A}_1, i) = \alpha\}| \neq |\{i \mid \tau(\mathcal{A}_2, i) = \alpha\}|$, then the two automata are not isomorphic. Otherwise, all possible bijections preserving the labeling are tested. In the worst case, there are $n!$ possibilities (the labeling doesn't provide any refinement), but in practice, it works very well. Note that if τ_1 and τ_2 are two labelings, then $\tau = (\tau_1, \tau_2)$ is a labeling to, allowing the combination of labeling. In our work, we use the following Labelings: the labeling testing whether a state is initial, the one testing whether a state is final, the one testing whether a state is both initial and final, the one returning, for each letter a, the number of outgoing transitions labeled by a, the similar one with ongoing transitions, the one returning the minimal word (in the lexical order) from the state to a final state and the one returning the minimal word (in the lexical order) from an initial state to the given state.

Note that if the set of states is portioned into p classes with n/p elements en each classes, then one has to performed $t_n = ((n/p)!)^p$ rahter than $n!$. A direct application of Stirling formula show that

$$\frac{n!}{((n/p)!)^p} \sim \sqrt{\frac{p^p}{(2n\pi)^{p-1}}} \cdot p^n,$$

pointing out a significant theoretic complexity improvement.

Using these Labelings the practical computation of the sizes of automorphism groups can be done quite efficiently, using the algorithm depicted in Fig. 6: first the set of states of the automaton is partitioned into several subclasses according τ. Since an automorphism has to preserve these classes, one only explore this kind of automorphisms. Note that if D is large, the algorithm can be easily adapted to work on α's such that $C[\alpha] \neq 0$.

We have computed sizes of automorphism using Markov chains. Computation is very fast: labelings approaches allows to provides partitions of states into subsets which are mostly singletons. Table 2 reports the results which are obtain, for each line, in less than a second. One can also notice that most of generated automata have a small (compared to $n!$) automorphism group.

5.2 Experiments

The experiments have been done on a personal computer with processor `IntelCore i3-4150 CPU 3.50GHz x 4`, `7,7 Go` of memory and running on a 64 bits Ubuntu 14.04 OS. The implementation is a non optimized prototype written in Python.

Class	av. size	maximal size
$\mathfrak{N}_2(5)$	1.023	6
$\mathfrak{N}_2(8)$	1.012	6
$\mathfrak{N}_2(10)$	1.015	2
$\mathfrak{N}_2(15)$	1.007	2
$\mathfrak{N}_2(20)$	1.001	2
$\mathfrak{N}_3(5)$	1.031	6
$\mathfrak{N}_3(8)$	1.015	2
$\mathfrak{N}_3(10)$	1.015	2
$\mathfrak{N}_3(15)$	1.005	2
$\mathfrak{N}_3(20)$	1	1
$\mathfrak{N}(5)$	1.022	2
$\mathfrak{N}(8)$	1.01	2
$\mathfrak{N}(10)$	1.018	2
$\mathfrak{N}(15)$	1.005	2
$\mathfrak{N}(20)$	1.002	2

Table 2: Sizes of automorphisms group, using a n^3 mixing time, 1000 tests for each line, $|\Sigma| = 2$.

The first experimentation consists in measuring the time required to move into the Metropolis chains for $\mathfrak{N}(n)$ and $\mathfrak{N}_m(m)$. Results are reported in Table 3. The labelings used are those described in Section 5.1. These preliminary results show that using a 2 or 3-letter alphabet does not seem to have a significant influence. For each generation, the n^3-th elements of the walk is returned, with an arbitrary start. Moreover, bounding or not the degree does not seem to be relevant for the computation time. Note that we do not use any optimization: several computations on labelings may be reused when moving into the chain. Moreover, Python is not an efficient programming language (compared to C or Java). In practice, for directed graphs, the isomorphism problem is tractable for large graphs (see for instance [20]). Note that the number of moves (n^3) is the major factor for the increasing computation time (relatively to n): the average time for moving a single step is multiplied by about (only) 10 from $n = 20$ to $n = 90$.

For the last experience, we propose to compare our generation for $\mathfrak{N}'_2(n)^\bullet$ with the generator proposed in [6] with a density of a-transitions of 2 and

n	10	20	50	70	90
$\|A\| = 2$	0.02	0.43	32.5	166.1	569.9
$\|A\| = 3$	0.02	0.56	47.1	248.4	848.1

n	10	20	50	70	90
$m = 2, \|A\| = 2$	0.2	0.43	32.5	166.1	566.8
$m = 2, \|A\| = 3$	0.2	0.57	47.0	246.7	847.2
$m = 3, \|A\| = 2$	0.2	0.43	33.0	167.8	561.9
$m = 3, \|A\| = 3$	0.2	0.57	47.2	248.6	851.3

Table 3: Average Time (s) to Sample a NFA in $\mathfrak{N}(n)$ (left) and in $\mathfrak{N}'_m(n)$ (right).

$\sigma = 2$, $n =$	5	8	11	14	17	20
s	1.3	3.0	4.8	5.1	4.5	4.0
$\sigma = 3$, $n =$	5	8	11	14	17	20
s	2.8	4.8	4.7	3.8	3.4	3.0

$\mathfrak{N}'_2(n)^\bullet$, $n =$	5	8	11	14	17	20
s	3.7	6.1	7.9	10.0	11.5	13.9

Table 4: Average sizes of deterministic and minimal automata corresponding to automata sampling using [6] and in $\mathfrak{N}'_2(n)^\bullet$.

3. The parameter of the algorithm is a probability p_f for final states and a density σ on a-transitions: the set of states of the automaton is $\{1, \ldots, n\}$, only 1 is the initial state, each state is final with a probability p_f and for each p and each a, (p, a, q) is a transition with a probability $\frac{\sigma}{n}$. Therefore for each state and each letter, the expected number of outgoing transitions labeled by this letter is σ. We run this algorithm with $p_f = 0.2$ and $\sigma \in \{2, 3\}$. For each size, we compute the average size s of the corresponding minimal automata. We use a two letter alphabet and the average sizes (number of states) are obtained by sampling 1000 automata for each case. Results are reported in Table 4.

One can observe that the generator provides quite different automata. With the Markov chain approach the sizes of the related minimal automata are greater, even if there is no blow-up in both cases.

	$p_i = 0.2$ $p_f = 0.2$ $\sigma = 2$	$p_i = 0.5$ $p_f = 0.5$ $\sigma = 2$	$p_i = 0.8$ $p_f = 0.8$ $\sigma = 2$	$p_i = 0.2$ $p_f = 0.2$ $\sigma = 3$	$p_i = 0.5$ $p_f = 0.5$ $\sigma = 3$	$p_i = 0.8$ $p_f = 0.8$ $\sigma = 3$
n= 5	26	6	25	21	6	24
n=8	2345	112	2213	2254	102	2441
n=10	86 500	1343	71472	83072	1303	79203

Table 5: Observed average sizes of automata generated by [6], obtained with 1000 tests on a two letter alphabet.

Finally, also to compare the proposed generator with [6], we have computed the sizes of the automorphisms groups. Results are reported in Table 2 and in Table 5 and points out significant differences.

6 Conclusion

In this paper we proposed a Markov Chain approach to randomly generate non deterministic automata (up to isomorphism) for several classes of NFAs. We showed that moving into these Markov chains can be done quite quickly in practice and, in some interesting cases, in polynomial time. Experiments have been performed within a non optimized prototype and, following known experimental results on group isomorphism, they allow us to think that the approach can be used on much larger automata. Implementing such techniques using an efficient programming language is a challenging perspective. Moreover, the proposed approach is very flexible and can be applied to various classes of NFAs. An interesting research direction is to design particular subclasses of NFAs that look like NFAs occurring in practical applications, even if this last notion is hard to define. We think that the classes $\mathfrak{N}'_m(n)^\bullet$ and $\mathfrak{N}_m(n)^\bullet$ constitute first attempts in this direction. Theoretically -as often for Monte-Carlo approach-, computing mixing and strong stationary times are crucial and difficult questions we plan to investigate more deeply.

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