Markov chain algorithms for generating sets uniformly at random

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Abstract

In this paper we tackle the problem of generating uniformly at random two representative types of sets with n elements: transitive sets and weakly transitive sets, that is, transitive sets with atoms. A set is said to be *transitive* if any of its elements is also a subset of it; a set is *weakly transitive* if any of its elements, unless disjoint from it, is also a subset of it. We interpret such sets as (weakly) extensional acyclic digraphs—that is, acyclic digraphs whose (non-sink) vertices have pairwise different out-neighborhoods—and employ a Markov chain technique already given for acyclic digraphs. We thus propose Markov chain-based algorithms for generating uniformly at random (weakly) extensional acyclic digraphs with a given number of vertices. The Markov chain is then refined to generate such digraphs which are also simply connected, and digraphs in which the number of arcs is fixed.

Keywords: Extensional digraph, transitive set, set theory, random generation, Markov chain.

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1   Introduction

Sets are basic mathematical and computational objects, and for this reason one is some-
times interested—in order to perform tests and evaluate benchmarks, collect statistical data,
(dis)prove conjectures, etc.—in generating uniformly at random a set of given size. In this
paper we tackle this problem by building on results originally given in the context of graphs.

   The sets we consider belong to the standard Zermelo-Fraenkel set theory and thus con-
tain only other sets as elements. We focus on two archetypal sets: *transitive* sets and
weakly transitive sets, that is, sets s whose elements are also subsets of s, and sets s whose
elements, unless disjoint from s, are also subsets of s. A weakly transitive set s can be
simply seen as a transitive set with *atoms* (or *ur-elements*), the atoms of s constituting the
collection of elements of s disjoint from s. Zermelo-Fraenkel sets stand at the basis of
programming languages such as SETL [15], or the more recent {log} [3] and CLP($\mathcal{SET}$)
[5], and of the automatic proof-verifier Referee [14].

   Since sets are *nested* structures, they are best represented by digraphs: vertices will
stand for sets, while the arc relation will correspond to the inverse of the membership
relation between them ($\rightarrow \, \equiv \, \ni$). Such digraphs are acyclic, since membership is well-
founded, and *weakly extensional*, in the sense that distinct non-sink vertices have distinct
collections of out-neighbors. This digraph interpretation was exploited in [13] to give a
recurrence relation for the number of weakly transitive sets with n elements, generalizing
the result of [12] for transitive sets with n elements.

   Under this graph-theoretic interpretation, we show in this paper how a Markov chain
based procedure for generating acyclic digraphs, first introduced in [9], can be transferred
to our set-theoretic universe. This Markov chain algorithm was already modified in [10]
to generate simply connected acyclic digraphs. The random generation of elements from
a particular class of acyclic digraphs modeling Bayesian networks was proposed in [6].
Finally, the same approach was used in [2] to generate deterministic acyclic automata.
Each of these examples can be seen as a less basic case than the one tackled here.

   The idea behind this Markov chain technique is to start with an arbitrary weakly exten-
sional acyclic digraph (*w.e.a.* digraph, for short) on n vertices and apply a certain number
T of random local transformations which preserve weak extensionality and acyclicity. The
uniformity of the resulting distribution is basically proved by showing that any w.e.a. di-
graph on n vertices can be thus transformed into any other w.e.a. digraph on n vertices.
Like in the acyclic digraph case, we argue that the transformation rules are symmetric and
always allow reaching a specific digraph among the collection of w.e.a. digraphs with n
vertices. In our case, however, the most natural target digraph for this purpose turns out
to be an acyclic tournament on n vertices, that is, the digraph whose interpretation in the
universe of sets is the von Neumann numeral of n, the unique transitive set with n elements
well-ordered by the membership relation.

   We prove here only 'correctness' and defer to future work computational aspects such
as estimations for the choice of T or an analysis of the mixing time of the Markov chain
[8]. As next research steps we also mention the random generation of hypersets, objects
for which the acyclicity requirement is dropped, and weak extensionality is accordingly
strengthened by an equality criterion based on the notion of bisimulation [1].

   The paper is organized as follows. In Section 2 we give some notation and formally
introduce the above-mentioned notions. In Section 3 we put forward a Markov chain for
generating weakly extensional acyclic digraphs, while in Section 4 we propose a Markov
chain for generating simply connected weakly extensional acyclic digraphs. The latter can

be easily adapted to generate extensional acyclic digraphs. Finally, in Section 5, we present a Markov chain for generating w.e.a. digraphs on n vertices and m arcs, $0 \leqslant m \leqslant \binom{n}{2}$, which can also serve to generate acyclic digraphs with a given number of vertices and of arcs.

2 Notation and preliminaries

We consider only finite *simple* digraphs, that is, without parallel arcs or self-loops. Given a digraph D, we denote by $V(D)$ its vertex set and by $E(D)$ the set of its arcs. For any $v \in V(D)$, $N^+(v)$ stands for the set $\{u \in V(D) \mid (v,u) \in E(D)\}$, which is called the *out-neighborhood* of v in D. Similarly, $N^-(v) = \{u \in V(D) \mid (u,v) \in E(D)\}$ is the *in-neighborhood* of v. We will use $d^+(v) = |N^+(v)|$ and $d^-(v) = |N^-(v)|$. A vertex $v \in V(D)$ such that $d^+(v) = 0$ will be called a *sink*; if $d^-(v) = 0$, it will be called a *source*; we denote by $I(D)$ the set of the sinks of D.

A digraph D is said to be *simply connected* if the underlying (undirected) graph of D is connected. If $(i,j) \in E(D)$, we will employ $D - (i,j)$ as a shorthand for the digraph obtained from D by removing the arc (i,j). Analogously, $D + (i,j)$ is the digraph obtained from D by the addition of the arc (i,j).

Definition 2.1. A digraph D is said to be

- *extensional*, if for any distinct $u, v \in V(D)$ it holds that $N^+(u) \neq N^+(v)$;
- *weakly extensional*, if for any distinct vertices $u, v \in V(D) \setminus I(D)$, it holds that $N^+(u) \neq N^+(v)$.

If u, v are distinct vertices of a digraph D having $N^+(u) = N^+(v)$, we say that u and v *collide*. Note that this is not the case if D is acyclic and there is a directed path from u to v. In particular, in an acyclic tournament there are no collisions (a *tournament* is a digraph D such that for any distinct $u, v \in V(D)$ either $(u,v) \in E(D)$ or $(v,u) \in E(D)$ holds, but not both). Moreover, any e.a. digraph is simply connected.

Under the Zermelo-Fraenkel axioms, each set is uniquely characterized by its elements (Extensionality Axiom), and the membership relation is well-founded (Foundation Axiom). The standard universe of sets is von Neumann's cumulative hierarchy, whose subset of hereditarily finite sets is defined as the union, over all natural numbers i, of $\mathbb{V}_i$, where $\mathbb{V}_0 = \emptyset$, each level $\mathbb{V}_{i+1}$ is $\mathcal{P}(\mathbb{V}_i)$, and $\mathcal{P}(\cdot)$ stands for the power-set operator. For example, $\mathbb{V}_1 = \{\emptyset\}$, $\mathbb{V}_2 = \{\emptyset, \{\emptyset\}\}$, $\mathbb{V}_3 = \{\emptyset, \{\emptyset\}, \{\{\emptyset\}\}, \{\emptyset, \{\emptyset\}\}\}$.
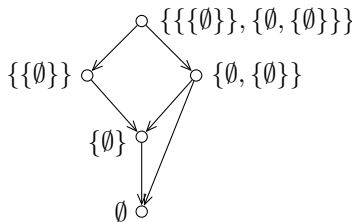

Figure 1: The digraph representation of a transitive set.

To faithfully represent a set x as a digraph, one considers the digraph D_x defined as

$$D_x = (x, \{(u,v) \mid u, v \in x, v \in u\}).$$

See Figure 1 for an example. Since the membership relation between sets is well-founded, such digraphs are acyclic. Moreover, if x is transitive, then D_x is also extensional, while if x is weakly transitive, then D_x is weakly extensional. To see this, observe that if distinct non-sink vertices have the same out-neighborhood, then from the (weak) transitivity assumption they correspond to the same set, contradicting the definition of D_x; see also [13].

Given $n \geqslant 1$, we denote by $\mathcal{W}_n$ the set of all w.e.a. digraphs with vertex set $\{1, \ldots, n\}$, while $\mathcal{W}_n^c$ denotes its subset of simply connected w.e.a. digraphs. Analogously, $\mathcal{W}_{n,m}$ denotes the set of all w.e.a. digraphs with vertex set $\{1, \ldots, n\}$ and m arcs.

Definition 2.2. A *discrete time finite stochastic process* is a sequence $X = (X_t \ : \ t \in \mathbb{N})$, where X_t are $\mathcal{S}$-valued random variables and $\mathcal{S}$ is a finite set, called the *state space* of X. We say that X is a *Markov chain* if

$$\forall t \in \mathbb{N}, \Pr(X_{t+1} = s_{t+1} \mid X_t = s_t, \ldots, X_0 = s_0) = \Pr(X_{t+1} = s_{t+1} \mid X_t = s_t).$$

Moreover, a Markov chain X is said to be *time-homogeneous* if

$$\forall s, s' \in \mathcal{S}, \exists p_{ss'}, \forall t \in \mathbb{N}, \Pr(X_{t+1} = s \mid X_t = s') = p_{ss'}.$$

Definition 2.3. A time-homogeneous Markov chain over the state space $\mathcal{S}$ is said to be:

- *irreducible* iff $\forall s, s' \in \mathcal{S}, \exists t \in \mathbb{N}, \Pr(X_t = s' \mid X_0 = s) > 0$;
- *aperiodic* iff $\forall s \in \mathcal{S}, \gcd\{t \in \mathbb{N} \mid \Pr(X_t = s \mid X_0 = s) > 0\} = 1$;
- *symmetric* iff $\forall s, s' \in \mathcal{S}, \ p_{ss'} = p_{s's}$.

A well-known result (see, e.g., [8]) states that any finite, irreducible, aperiodic and symmetric time-homogeneous Markov chain converges toward the uniform distribution on its state space. Therefore, all the Markov chains presented here will be shown to satisfy these three properties.

3   A Markov chain algorithm for generating w.e.a. digraphs

Let M be a Markov chain over $\mathcal{W}_n$, defined in Figure 2. Observe that M differs from the Markov chain of [9] for generating arbitrary acyclic digraphs in the fact that arc deletions and additions are done only provided that the resulting digraph is w.e.a.

Notice that for any $t \in \mathbb{N}$ and any two distinct states $s, s' \in \mathcal{W}_n$, $\Pr(X_{t+1} = s \mid X_t = s') > 0$ if and only if $\Pr(X_{t+1} = s' \mid X_t = s) > 0$. To be more precise, the probability of passing from a state $s \in \mathcal{W}_n$ to any other state $s' \neq s$ is either 0 or $1/n^2$, hence M is symmetric. Moreover, for every $s \in \mathcal{W}_n$ the probability of remaining in s at any $t > 0$ is positive, for example by choosing diagonal pairs (i, i), with $i \in \{1, \ldots, n\}$. Therefore, if M turns out to be irreducible, then it will also be aperiodic.

The initial state of this Markov chain and of the ones given in the next section can be taken to be a linear digraph consisting of a directed path $(n, n-1, \ldots, 1)$. The acyclicity of a digraph on n vertices and m arcs can be established by a depth-first visit, in time $O(n+m)$. To test whether a digraph is (weakly) extensional, the algorithm in [4, Sec. 4] can be used, taking time $O(n+m)$.

Let X_t denote the state of the Markov chain at time t. Suppose a couple of integers (i, j) has been drawn uniformly at random from the set $\{1, \ldots, n\} \times \{1, \ldots, n\}$.

($\mathbf{T}_1$) **if** $(i, j) \in E(X_t)$ **and**

        $X_t - (i, j)$ is w.e., **then** $X_{t+1} = X_t - (i, j)$

   else $X_{t+1} = X_t$.

($\mathbf{T}_2$) **if** $(i, j) \notin E(X_t)$ **and**

        $X_t + (i, j)$ is w.e.a., **then** $X_{t+1} = X_t + (i, j)$

   else $X_{t+1} = X_t$.

Figure 2: A Markov chain algorithm for generating w.e.a. digraphs.

Lemma 3.1. *Let D be a w.e.a. digraph with $E(D) \neq \emptyset$. There exists an arc $(u, v) \in E(D)$ such that the digraph $D - (u, v)$ is w.e.a.*

Proof. Observe first that there exists $u \in V(D)$ such that $\emptyset \neq N^+(u) \subseteq I(D)$. If this were not the case, then for all u in $V(D)$ with $N^+(u) \neq \emptyset$, there would exist a vertex u' in D with $N^+(u') \neq \emptyset$ such that $(u, u') \in E(D)$. Since the same property holds for u' as well, and as the number of vertices of D is finite, we can find a finite directed cycle, contradicting hence the acyclicity of D.

Let now $U(D)$ be the set of vertices of D with the above property, that is, $U(D) \overset{\text{def}}{=} \{u \in V(D) \mid \emptyset \neq N^+(u) \subseteq I(D)\}$. Let $u_0 \in U(D)$ be a vertex of minimum out-degree, i.e., $d^+(u_0) = \min\{d^+(u) : u \in U(D)\}$. Since $N^+(u_0) \neq \emptyset$, let v_0 be an element of $N^+(u_0)$. The arc (u_0, v_0) can be removed and the resulting digraph remains w.e.a. Indeed, since u_0 is among the vertices of minimum out-degree in $U(D)$, in $D - (u_0, v_0)$ it will either be a sink, or it will be the only vertex in $U(D - (u_0, v_0))$ with out-degree $d^+(u) - 1$, hence having its out-neighborhood different from that of any other vertex of $D - (u_0, v_0)$. $\qquad\square$

Theorem 3.2 (Irreducibility of M). *Let M be the Markov chain defined over the space $\mathcal{W}_n$ together with the transition rules $\mathbf{T}_1$ and $\mathbf{T}_2$. Given two distinct digraphs D and H in $\mathcal{W}_n$, there exists in M a sequence of transitions $D = D_0 \to D_1 \to \cdots \to D_{p-1} \to D_p = H$, where $p \geqslant 1$ and $D_i \in \mathcal{W}_n$, for all $0 \leqslant i \leqslant p$. Such a sequence exists with length at most $n^2 - n$.*

Proof. Since M is symmetric, it suffices to show that there exists a sequence of transitions from any given w.e.a. digraph $D \in \mathcal{W}_n$ to a fixed element O in $\mathcal{W}_n$. For our purpose here, we will choose O to be the unique totally disconnected digraph, that is, having $E(O) = \emptyset$.

From Lemma 3.1, we get that there exists an arc $(u, v) \in E(D)$ such that $D - (u, v)$ is w.e.a. Using rule ($\mathbf{T}_1$), we can step from D to $D - (u, v)$. Repeating the above argument a finite number of steps, we arrive at O. The number of transitions from D to O is at most $n(n - 1)/2$, and this is obtained when D is a tournament. $\qquad\square$

4   A Markov chain algorithm for generating e.a. digraphs

Instead of generating e.a. digraphs, we place ourselves in a more general setting, that of generating simply connected w.e.a. digraphs. Afterwards, we will argue that, with minor

changes, the proposed Markov chain can generate e.a. digraphs. Let M^c be the Markov chain over $\mathcal{W}_n^c$ whose transitions between states are given in Figure 3. This Markov chain is adapted from [10], with the difference that arc deletions, additions, or reversals are done only if the resulting digraph is simply connected and w.e.a. This simple modification, however, requires a totally new and more involved proof of irreducibility.

Just as in the previous section, the probability of passing from a state $s \in \mathcal{W}_n^c$ to any other state $s' \neq s$ is either 0 or $1/n^2$, implying that M^c is symmetric. Likewise, the aperiodicity of M^c will be implied by its irreducibility and by the fact that for every state in $\mathcal{W}_n^c$ there is a positive probability to remain in that state (by choosing diagonal pairs (i, i)). Even if the two transition rules of M^c are not entirely specular, one can think of M^c as having three basic transitions: (1) removal of an arc, (2) reversal of an arc, (3) addition of an arc. According to this view, M^c is entirely symmetric.
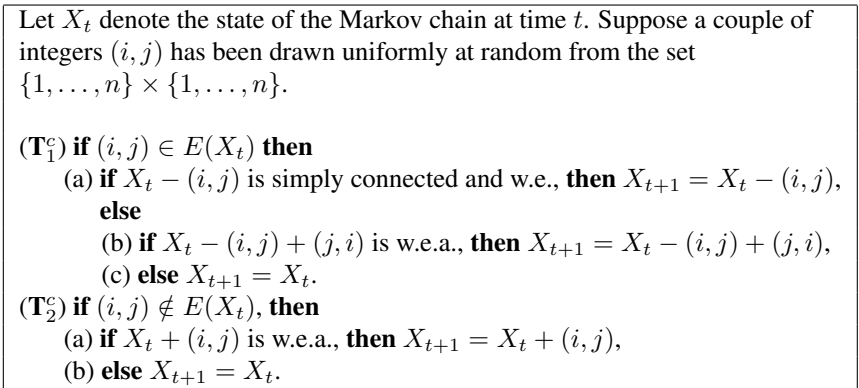

Let X_t denote the state of the Markov chain at time t. Suppose a couple of integers (i, j) has been drawn uniformly at random from the set $\{1, \ldots, n\} \times \{1, \ldots, n\}$.

($\mathbf{T}_1^c$) **if** $(i, j) \in E(X_t)$ **then**
    (a) **if** $X_t - (i, j)$ is simply connected and w.e., **then** $X_{t+1} = X_t - (i, j)$,
    else
        (b) **if** $X_t - (i, j) + (j, i)$ is w.e.a., **then** $X_{t+1} = X_t - (i, j) + (j, i)$,
        (c) **else** $X_{t+1} = X_t$.
($\mathbf{T}_2^c$) **if** $(i, j) \notin E(X_t)$, **then**
    (a) **if** $X_t + (i, j)$ is w.e.a., **then** $X_{t+1} = X_t + (i, j)$,
    (b) **else** $X_{t+1} = X_t$.

Figure 3: A Markov chain algorithm for generating simply connected w.e.a. digraphs.

To show the irreducibility of the Markov chain M^c, it is useful to partition the vertices of an acyclic digraph according to the maximum length of a directed path to a sink of the digraph. Complying with standard set-theoretic notation, we will make use of the following notion.

Definition 4.1. Given an acyclic digraph D, the *rank* of a vertex $v \in V(D)$ is recursively defined as
$$\mathsf{rk}(v) = 1 + \max\{\mathsf{rk}(u) \, : \, (v, u) \in E(D)\},$$
where $\mathsf{rk}(v) = 0$ if v is a sink.

Clearly, the following lemma holds.

Lemma 4.2. *Given an acyclic digraph D, if $v, u \in V(D)$ and $\mathsf{rk}(v) \neq \mathsf{rk}(u)$, then $N^+(v) \neq N^+(u)$ holds.*

Throughout the subsequent two proofs we employ the following notation: given an acyclic digraph D and a vertex v of D,
$$R(v) \stackrel{\text{def}}{=} \{u \in V(D) \mid u \neq v \text{ and } \mathsf{rk}(u) \leqslant \mathsf{rk}(v)\}.$$

Theorem 4.3 (Irreducibility of M^c). *Let M^c be the Markov chain defined over the space $\mathcal{W}_n^c$ together with the transition rules $\mathbf{T}_1^c$ and $\mathbf{T}_2^c$. Given two distinct digraphs D and H in $\mathcal{W}_n^c$, there exists in M^c a sequence of transitions $D = D_0 \rightarrow D_1 \rightarrow \cdots \rightarrow D_{p-1} \rightarrow D_p = H$, where $p \geqslant 1$ and $D_i \in \mathcal{W}_n^c$, for all $0 \leqslant i \leqslant p$. Such a sequence exists with length at most $(3n^2 - 7n + 4)/2$.*

Proof. As before, first we will show that there exists a sequence of transitions from any given w.e.a. digraph $D \in \mathcal{W}_n^c$ to an element $T(D)$ in $\mathcal{W}_n^c$, where $T(D)$ is an acyclic tournament, with the additional property that whenever $\mathsf{rk}(v) > \mathsf{rk}(u)$ in D, $\mathsf{rk}(v) > \mathsf{rk}(u)$ also holds in $T(D)$. Then, given any D and H in $\mathcal{W}_n^c$, we will show that there is a sequence of transitions from $T(D)$ to $T(H)$, completing hence the proof.

To show the former claim, we proceed as follows. Pick a vertex $v \in V(D)$, in decreasing order of rank (when more vertices of the same maximum rank exist, pick an arbitrary one). Apply rule ($\mathbf{T}_2^c$) and add arcs from v to all the vertices $u \in R(v) \setminus N^+(v)$, in decreasing order on the rank of the elements of $R(v) \setminus N^+(v)$. Note that this is possible, first of all, because the addition of an arc (v, u) does not create a cycle in the resulting digraph. Second, observe that the subdigraph of D induced by the vertices $V(D) \setminus R(v)$ is an acyclic tournament. Therefore, an arc addition would create a collision only between v and a vertex $w \in R(v)$. This is however not the case, since after the first addition of such an arc, $\mathsf{rk}(v)$ becomes strictly greater than $\mathsf{rk}(w)$, for all $w \in R(v)$, and Lemma 4.2 guarantees the absence of collisions.

Denote by $T(D)$ the acyclic tournament obtained at the end of this process. Since for any vertex v we have added arcs only to those vertices of rank less than or equal to v, we also have that whenever $\mathsf{rk}(v) > \mathsf{rk}(u)$ in D, the same holds in $T(D)$.[1]

Passing on to the latter point, observe that for any w.e.a. digraph D, since $T(D)$ is a tournament, there are no two distinct elements of the same rank in $T(D)$, and thus $\{\mathsf{rk}(v) : v \in V(T(D))\} = \{0, \ldots, n-1\}$. Hence, to each digraph $T(D)$ we can uniquely associate a linear order $\prec_{T(D)}$ on $V(D)$ defined in the following way: for all $u, v \in V(T(D))$

$$u \prec_{T(D)} v \text{ iff } \mathsf{rk}(u) < \mathsf{rk}(v) \text{ in } T(D).$$

We now show that given two orders $x_0 \prec_{T(D)} x_1 \prec_{T(D)} \cdots \prec_{T(D)} x_{n-1}$ and $y_0 \prec_{T(H)} y_1 \prec_{T(H)} \cdots \prec_{T(H)} y_{n-1}$, where $\{x_i : 0 \leqslant i \leqslant n-1\} = \{y_i : 0 \leqslant i \leqslant n-1\} = \{1, \ldots, n\}$, we can transform $T(D)$ in $T(H)$, applying rule ($\mathbf{T}_1^c$).

Observe first that for any two consecutive elements $x_i \prec_{T(D)} x_{i+1}$ ($0 \leqslant i < n-1$) it holds that $N^+(x_{i+1}) = N^+(x_i) \cup \{x_i\}$. Therefore, applying rule ($\mathbf{T}_1^c$) on $T(D)$, the arc (x_i, x_{i+1}) cannot be removed (by (a)), but can be reversed (by (b)). In the resulting acyclic tournament $T(D')$, x_i and x_{i+1} have swapped positions, i.e., $x_{i+1} \prec_{T(D')} x_i$. Starting from position $i = 0$ all the way to $i = n-1$, apply the following procedure. If $y_i = x_j$, ($i < j \leqslant n-1$), then bring x_j to position i by iteratively reversing the arcs (x_j, x_{j-1}), (x_j, x_{j-2}), ...,(x_j, x_i).

The maximum number of transitions to pass from D to $T(D)$ is $\binom{n}{2} - (n-1) = (n^2 - 3n + 2)/2$, number obtained when the underlying graph of D is a tree, thus having $n - 1$ edges. To pass from $T(D)$ to $T(H)$, $\binom{n}{2}$ transitions are required at most, when all the arcs of $T(D)$ have to be reversed. Hence, to pass between two arbitrary D and H in $\mathcal{W}_n^c$, we need at most $(3n^2 - 7n + 4)/2$ transitions. □

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[1] However, the converse in general does not hold.

Let us denote by $\mathcal{E}_n$ the set of all e.a. digraphs with vertex set $\{1, \dots, n\}$. The Markov chain illustrated in Figure 3 can be transformed into an irreducible, aperiodic and symmetric Markov chain, M^e, for the generation of digraphs from $\mathcal{E}_n$. The transitions between two states in M^e are given in Figure 4. The analogue of Theorem 4.3 holds for M^e as well.

Let X_t denote the state of the Markov chain at time t. Suppose a couple of integers (i, j) has been drawn uniformly at random from the set $\{1, \dots, n\} \times \{1, \dots, n\}$.

($\mathbf{T}_1^e$) **if** $(i, j) \in E(X_t)$ **then**
    (a) **if** $X_t - (i, j)$ is extensional, **then** $X_{t+1} = X_t - (i, j)$,
    else
      (b) **if** $X_t - (i, j) + (j, i)$ is e.a., **then** $X_{t+1} = X_t - (i, j) + (j, i)$,
      (c) **else** $X_{t+1} = X_t$.
($\mathbf{T}_2^e$) **if** $(i, j) \notin E(X_t)$, **then**
    (a) **if** $X_t + (i, j)$ is e.a., **then** $X_{t+1} = X_t + (i, j)$,
    (b) **else** $X_{t+1} = X_t$.

Figure 4: A Markov chain algorithm for generating e.a. digraphs.

5 A Markov chain algorithm for generating w.e.a. digraphs with a given number of arcs

A Markov chain M^a for generating w.e.a. digraphs with vertex set $\{1, \dots, n\}$ and m arcs is given in Figure 5. It will immediately follow from the proof of its irreducibility—Theorem 5.1 below—that M^a can also generate uniformly at random acyclic digraphs with a given number of vertices and a fixed number of arcs, by simply swapping two arcs if the resulting digraph is acyclic. Note that controlling the number of arcs was already considered in the literature: [9] proposed generating acyclic digraphs with a bounded number of arcs, or whose vertices have a bounded degree; [7] proposed generating acyclic digraphs with bounded *induced width*, a complexity measure arising from artificial intelligence.

The probability of passing from a state $s \in \mathcal{W}_{n,m}$ to any other state $s' \neq s$ is either 0 or $1/n^4$, implying that M^a is symmetric. As previously, for any state $s \in \mathcal{W}_{n,m}$ there is a positive probability to remain in s. Our next theorem shows that M^a is indeed irreducible. If $m < n - 1$, the initial state of the Markov chain can be a digraph whose arcs form a directed path of length m. Otherwise, the initial state can be a directed path $(n, n-1, \dots, 1)$ together with $m - (n - 1)$ arbitrary arcs of the form (i, j), where $i > j$.

Theorem 5.1 (Irreducibility of M^a)**.** *The Markov chain M^a is irreducible.*

Proof. First, if $m = 0$, $\mathcal{W}_{n,m}$ consists only of the totally disconnected digraph. Assuming that $m > 0$, we show that any digraph $D \in \mathcal{W}_{n,m}$ can be transformed, by transitions of M^a, into a digraph $K(D) \in \mathcal{W}_{n,m}$, satisfying the following two properties:

  i) for all $v \in V(D)$ such that $\mathsf{rk}(v) > 1$ in $K(D)$, it holds that $N^+(v) = R(v)$ in $K(D)$;

  ii) there is only one $v \in V(D)$ such that $\mathsf{rk}(v) = 1$ in $K(D)$.

Let X_t denote the state of M^a at time t. Suppose two pairs of integers (i_1, j_j) and (i_2, j_2) have been drawn uniformly at random and independently from the set $\{1, \ldots, n\} \times \{1, \ldots, n\}$.

if $(i_1, j_1) \in E(X_t)$ **and** $(i_2, j_2) \notin E(X_t)$, **then**
    if $X_t - (i_1, j_1) + (i_2, j_2)$ is w.e.a., **then** $X_{t+1} = X_t - (i_1, j_1) + (i_2, j_2)$,
    else $X_{t+1} = X_t$.

Figure 5: A Markov chain algorithm for generating w.e.a. digraphs on n vertices and m arcs.

To show this, we argue as in the proof of Theorem 4.3, paying particular attention to preserving m arcs at each intermediate step. Observe that if D fails to satisfy i) or ii), then it must own a vertex v such that $N^+(v) \subsetneq R(v)$. Indeed, first note that $N^+(v) \subseteq R(v)$ holds for any vertex v, since D is acyclic. If D does not satisfy i) and $v \in V(D)$ is a vertex with $\mathsf{rk}(v) > 1$ and $N^+(v) \neq R(v)$, then $N^+(v) \subsetneq R(v)$ immediately follows. If D owns two distinct vertices v' and v'' of rank 1, then $v'' \in R(v') \setminus N^+(v')$.

Therefore, as long as D fails to satisfy one of the above conditions i) or ii), apply the following transformation to it. Pick a vertex $v \in V(D)$ inclusion-maximal among the vertices of maximum rank having $N^+(v) \subsetneq R(v)$, and consider all the elements $u \in R(v) \setminus N^+(v)$, in decreasing order on rank. Take $t \in V(D)$ a vertex whose out-neighborhood is inclusion-minimal among the vertices of rank 1. Arguing as in the proof of Lemma 3.1, any arc (t, s) leading from t to an arbitrary sink $s \in V(D)$ can be removed without disrupting the weak extensionality of D. Replace arc (t, s) with arc (v, u) by a transition of M^a.

This is possible, since, on the one hand, the addition of the arc (v, u) does not create a cycle in the resulting digraph. On the other hand, as before, the subdigraph of D induced by the vertices $V(D) \setminus R(v)$ is an acyclic tournament. Therefore, one such arc addition can create a collision only between v and some vertex $w \in R(v)$. This is not the case, since after the first addition of an arc from v to a maximum rank vertex in $R(v)$, $\mathsf{rk}(v)$ becomes strictly greater than $\mathsf{rk}(w)$, for all $w \in R(v)$, and Lemma 4.2 guarantees the absence of collisions. It should be clear that the above procedure stops after a finite number of steps, and that the final digraph satisfies conditions i) and ii).

It remains to show that, given two digraphs D and H in $\mathcal{W}_{n,m}$, there exists a sequence of transitions in M^a from $K(D)$ to $K(H)$. To any acyclic digraph K whose vertices of positive rank have pairwise distinct ranks we can associate a partial order $\prec_K$ in the following way: for all $u, v \in V(K)$,

$$u \prec_K v \text{ iff } \mathsf{rk}(u) < \mathsf{rk}(v) \text{ in } K.$$

For expository purposes, assume that we also order the sinks of K is an arbitrary way so that $\prec_K$ is a linear order on the vertices of K. Therefore, we have to show that we can transform any order $x_0 \prec_{K(D)} x_1 \prec_{K(D)} \cdots \prec_{K(D)} x_{n-1}$ into $y_0 \prec_{K(H)} y_1 \prec_{K(H)} \cdots \prec_{K(H)} y_{n-1}$, where $\{x_i : 0 \leqslant i \leqslant n-1\} = \{y_i : 0 \leqslant i \leqslant n-1\} = \{1, \ldots, n\}$.

Like in the proof of Theorem 4.3, given a digraph $K(D)$ satisfying i) and ii), we show that we can obtain, by transitions of M^a, a digraph $K(D')$, still satisfying i) and ii), and in which a given pair of consecutive elements $x_i \prec_{K(D)} x_{i+1}$, $0 \leqslant i < n-1$, have swapped positions. If such consecutive elements x_i and x_{i+1} are both sinks, then since

their order has been imposed arbitrarily, they can be swapped without changing the digraph. Otherwise, we have to consider two cases.

If $\mathsf{rk}(x_{i+1}) > 1$, then $N^+(x_{i+1}) = N^+(x_i) \cup \{x_i\}$. The arc (x_{i+1}, x_i) can be reversed, by the application of the transition of M^a on the arcs (x_{i+1}, x_i) and (x_i, x_{i+1}). Indeed, the resulting digraph K' remains acyclic; K' is also w.e. since, on the one hand, vertices $x_i, x_{i+1}, \ldots, x_{n-1}$ induce an acyclic tournament in K', by conditions i) and ii). On the other hand, any non-sink x_j, $0 \leq j < i$, is an out-neighbor of both x_i and x_{i+1}. Moreover, if $\mathsf{rk}(x_{i+1})$ was equal to 2 in $K(D)$ (and hence $\mathsf{rk}(x_i) = 1$), then in K' we may have $N^+(x_i) \neq R(x_i)$. However, it suffices to swap arcs out-going from x_{i+1}, the unique vertex of rank 1 in K', to x_i. The digraph obtained after these transformations satisfies conditions i) and ii), thus is equal to some $K(D')$; the vertices of $K(D')$ have the same ranks as in $K(D)$, with the exception of x_i and x_{i+1} which have swapped ranks.

When however $\mathsf{rk}(x_{i+1}) = 1$, we have that $\mathsf{rk}(x_i) = 0$. Since x_{i+1} is the unique vertex of rank 1, there must be an arc from x_{i+1} to a sink s (s can even be x_i) which can be removed in order to add the arc (x_i, x_{i+1}). After this first arc swap, continue changing all arcs (x_{i+1}, s) into (x_i, s), with s an arbitrary sink. The resulting digraph K' satisfies conditions i) and ii) and is equal to some $K(D')$; moreover, the vertices of $K(D')$ have the same ranks as in $K(D)$, with the exception of x_i and x_{i+1} which, as before, have swapped ranks.

In order to transform $K(D)$ into $K(H)$, apply the following procedure, starting from position $i = 0$ all the way to $i = n - 1$. If $y_i = x_j$, $(i < j \leqslant n - 1)$, then bring x_j to position i by iteratively reversing the arcs (x_j, x_{j-1}), (x_j, x_{j-2}), …, (x_j, x_i). Finally, change the out-going arcs of the unique vertex of rank 1 so that it has precisely the same out-neighborhood as it has in $K(H)$. □

Figure 6 illustrates the transitions indicated by the above proof in order to pass between two digraphs in $\mathcal{W}_{5,6}$.

6   Critical remarks and future work

Although the Markov chains M, M^c and M^e are similar to the Markov chains of [9, 10], the proofs of their irreducibility are different and more involved. In the case of M, the fixed element which can be reached by a chain of transitions from every element D of $\mathcal{W}_n$ is the same as in [9], namely the totally disconnected digraph. However, the arcs of D must be removed in a particular order, respecting the weak extensionality of D. Second, on the one hand, in [10] the fixed element is an arbitrary digraph having a path as underlying graph, which cannot be the case for M^c or M^e since (weak) extensionality would be violated. On the other hand, our proof takes this fixed element to be an acyclic tournament on n vertices, ensuring that the proof proposed here can also show the irreducibility of (a slightly modified version of) the chain of [10]. Lastly, as already noted, the Markov chain M^a can be easily adapted to generate uniformly at random acyclic digraphs on a given number of labeled vertices and a given number of arcs, a result which we have not found in the literature.

Given this dual usability of the Markov chains considered here, and the fact that the acyclic tournament on n vertices (that is, the digraph isomorphic to the von Neumann numeral of n) is a rich structure in which many types of digraphs can be embedded, it would be interesting to give a general characterization of the classes of digraphs whose elements can be generated uniformly at random by these Markov chains.

We regard the generation of digraphs on n vertices, possibly having directed cycles,

(a) $(4,5) \leftrightarrow (3,5)$

(b) $(2,4) \leftrightarrow (3,4)$

(c) $2 \prec 4 \prec \mathbf{5} \prec \mathbf{1} \prec 3$
$(1,5) \leftrightarrow (5,1)$
$(1,4) \leftrightarrow (5,4)$

(d) $1 \prec 2 \prec 4 \prec \mathbf{5} \prec \mathbf{3}$
$(3,5) \leftrightarrow (5,3)$
$(3,2) \leftrightarrow (5,2)$

(e) $1 \prec 2 \prec \mathbf{4} \prec \mathbf{3} \prec 5$
$(3,4) \leftrightarrow (4,3)$
$(3,1) \leftrightarrow (4,1)$
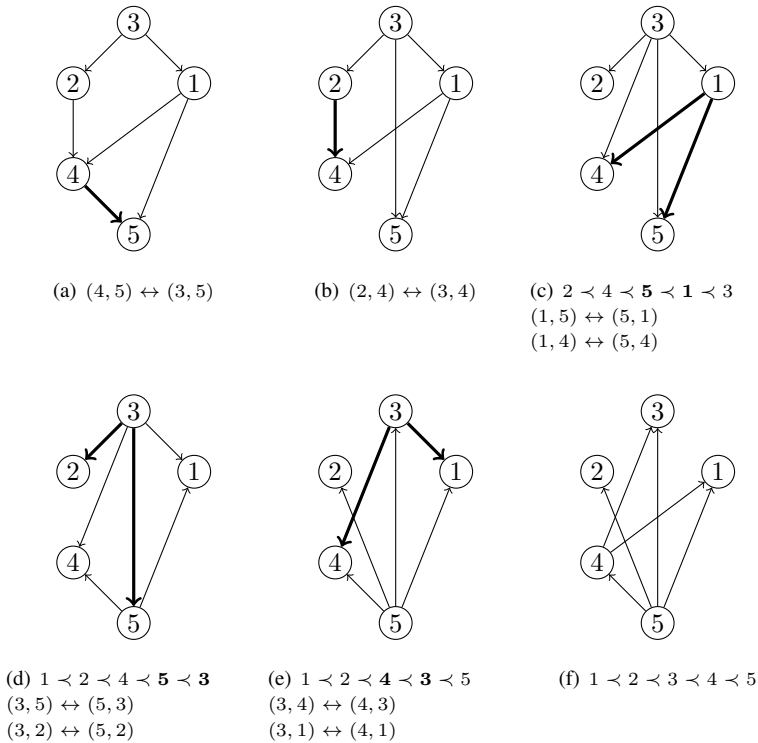
(f) $1 \prec 2 \prec 3 \prec 4 \prec 5$

Figure 6: The sequence of transitions of M^a that transforms $D \in \mathcal{W}_{5,6}$ (Fig. (a)) into $K(D) \in \mathcal{W}_{5,6}$ (Fig. (c)), and then into a digraph $K(H) \in \mathcal{W}_{5,6}$ (Fig. (f))

but deprived of distinct *bisimilar* vertices (the standard interpretation of a *hyperset* [1]) as the next natural step to take. It is interesting to study whether a Markov chain algorithm consisting of three basic operations: addition of an arc, removal of an arc, move of an arc, is irreducible for the class of such digraphs.

As already mentioned in the introduction, the problem of analyzing the mixing times [8] of our proposed Markov chains remains open; this is important from a practical viewpoint.

Finally, since a peculiarity of the sets treated in this paper is to be sets whose elements are themselves sets, it would be interesting to investigate what role our results can play in the theory of random sets ([11], elements taking as values subsets of some space), for example as a tool to generate such objects uniformly.

Acknowledgements

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