

Approximation of Large Probabilistic Networks by Structured Population Protocols^{*}

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Abstract. We consider networks of Markov Decision Processes (MDPs) where each MDP is one of the N nodes of a graph G . The transition probabilities of an MDP depend on the states of its direct neighbors in the graph, and runs operate by selecting a random node and following a random transition in the chosen device MDP. As the state space of all the configurations of the network is exponential in N , classical analysis are unpractical. We study how a polynomial size statistical representation of the system, which gives the densities of the subgraphs of width k , can be used to analyze its behaviors, generalizing the approximate Model Checking of an MDP. We propose a *Structured Population Protocol* as a new Population MDP where states are statistical representations of the network, and transitions are inferred from the statistical structure. Our main results show that when we consider large networks, the distributions of probability of the statistics vectors of the simulation process approximates the distributions of probability of the statistics vectors of the real process. Moreover, when the network has some regularity, both real and approximation processes will converge to the same distributions.

1 Introduction

We consider large networks of probabilistic systems, where each system (or device) is a Markov Decision Process, i.e. a transition system with both non deterministic and probabilistic transitions. The device MDPs are placed at nodes of the graph of the network with N nodes. A policy σ determines the decisions for all device MDPs, and the network itself can be considered as an MDP whose state space is the set of configurations of the network, of size exponential in N . Given a policy and an initial distribution, we observe a stochastic process on the set of configurations by selecting a random node and by following a random transition in the chosen MDP. Sensors networks are typical applications where sensors are nodes of a graph, connected to some neighbors. We consider *Evaluation problems* which predict the global behavior when a policy is fixed, and *Reachability problems* which look for possible policies to ensure predictable behaviors with high probabilities.

Classical Probabilistic Model Checkers such as PRISM [15] answer such questions on simple probabilistic systems. In [7], we presented some techniques to

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approximately decide such questions on a given MDP by associating *frequency vectors* to runs. Given an MDP with n states, we built its *Polytope of frequency vectors* H which represents the k -frequencies of the different states in the runs, in polynomial time. We can then decide if there is a run which *approximately* verifies some Property with high probability with simple geometrical procedures.

Given a network of N device MDPs, the polytope-based method remains exponential in N . In this paper, we introduce a new approximate method based on the statistics on graph neighborhoods of depth k of the network. The crucial point is that the set of k -statistics has size polynomially bounded in N . A *Structured Population Protocol with Decisions* (SPPD) will define a new *Population-MDP* whose states are statistics vectors and where transitions are determined by the graph. If we fix a precision for the values of the statistics densities, say 1%, the number of possible vectors becomes independent of N . The construction of the population-MDP becomes feasible and we can then apply the initial polytope-based method. In this context, the classical problems are:

- *Evaluation problems.* Given a fixed policy σ applied to all the device MDPs and an initial distribution C , can we reach configuration C' with probability greater than λ ? For a property \mathcal{P} on the runs, decide if $\mathbb{P}^{\sigma, C}[\text{a run satisfies } \mathcal{P}] \geq \lambda$ where $\lambda \leq 1$ is a threshold value.
- *Reachability problem.* Is there a policy σ , such that we can reach configuration C' from configuration C with probability greater than λ ? If the device MDPs have two states for example, *dead* and *alive*, we may ask if $\mathbb{P}^{\sigma, C}[\text{more than 80\% of the states are alive in a run}] \geq \frac{1}{2}$?

We map configurations to their statistics, and approach these problems by considering their *approximate* versions on the population MDP. The approximate Evaluation is: given the statistics of the configuration C , can we reach the statistics of configuration C' with probability greater than λ ? The other problems can be formulated in a similar way. The main results of the paper are:

- The k -SPPD associated to a network of MDPs is itself an MDP (definition 4 and proposition 4).
- Bounds on the approximation of the network of MDPs by the k -SPPD (proposition 5 and theorem 1).
- Sufficient conditions for the convergence of the approximate process induced by the k -SPPD towards the limit of the real process (theorem 2)
- The polytope associated to the k -SPPD approximates the polytope of the class of *statistics policies* on the network of MDPs (theorem 3)

In section 2 we present the model of Markov Decision Processes (MDPs) and define the k -statistics on graphs. In section 3 we define our model of network of MDPs. In section 4 we introduce the general model of *k-Structured Population Protocols with Decisions on a graph* (k -SPPD), and we present how to associate a k -SPPD to a network of MDPs. In section 5 we present sufficient conditions for good approximations of networks of MDPs by our k -SPPDs. The conditions rely on a notion of *mixed configurations*. We also study the convergence of the approximate process induced by a k -SPPD, and we present the polytope associated to the set of *statistics policies* on a network of MDPs.

1.1 Comparison with related models

Various theoretical models of networks have been considered in a context of distributed computing and statistical physics. Models for distributed computing [3] also include Petri nets [10], computer networks models [14] and cellular automata [19] which can be seen as a deterministic and synchronous restriction of our model. In statistical physics, spatial models [9] have similar probabilistic transitions associated with physical neighborhoods, in particular the Ising model describing models of spins. These statistical models do not integrate the possibility to take decisions, and the associated processes induce Markov chains on the sets of configurations.

If we restrict to MDPs with no decisions, i.e. to Markov chains, our model lies between the totally non ordered model of *population protocols*, introduced by Angluin et al in [3], and the totally ordered model of *cellular automata*. We differentiate from the population protocol model of [3], as structured graphs neighborhoods are chosen according to some statistics, as opposed to pairs of devices. Our work is closer to [2] where the authors consider devices distributed on the vertex of a graph with non randomized interactions between couples of devices. Cellular automata and dynamical systems consider regular geometries such as linear or square grid graphs (see [19,17]), and update all devices synchronously. In [1], the model is close to our model of SPP since the update function is asynchronous and uniformly random among the devices, with the restriction that the transition functions are deterministic.

2 Preliminaries

We first review the MDP model and its polytope representation, and we introduce a statistical representation of graphs.

2.1 Markov Decision Processes

Let $\mathcal{D}(S)$ be the set of distributions on a set S . A *Markov Decision Process (MDP)* is a triple $\mathcal{S} = (S, \Sigma, P)$ where S is a finite set of *states*, Σ is a set of *actions*, and $P : S \times \Sigma \times S \rightarrow [0, 1]$ is the *transition function*: $P(s, a, t)$, also written $P(t|s, a)$, is the probability to arrive in t in one step when the current state is s and action $a \in \Sigma$ is chosen for the transition. If action a is not allowed from state s , $P(t|s, a) = 0$ for all $t \in S$. A *run* on \mathcal{S} is a finite or infinite sequence of states. Given a run r and $n \in \mathbb{N}$, we write $r_{|n}$ for the sequence of the first $n - 1$ states in r . A *policy* on \mathcal{S} , see [18], is a function $\sigma : S \rightarrow \mathcal{D}(\Sigma)$ which resolves the non determinism of the system by choosing a distribution on the set of available actions for each state of the MDP (we restrict our model to stationary and possibly randomized policies). A policy σ and an initial distribution $\alpha \in \mathcal{D}(S)$ induce a probability distribution $\mathbb{P}^{\sigma, \alpha}$ on the σ -field \mathcal{F} of the set of runs, generated by the cones $C_\rho = \{r \mid r_{|\rho|} = \rho\}$, (see [6,18]). When there is no decision for the MDP, i.e. when $|\Sigma| = 1$, the MDP is in fact a Markov chain. See appendix A for an example of an MDP.

The *frequency vector* $\text{freq}_T(r)$ of the prefix of length T of a run r on \mathcal{S} is the density vector of dimension $|S|$ which measures the proportions of time spent on the different states of the MDP until time T . That is, given $s \in S$,

$$\text{freq}_T(r)[s] = \frac{\text{number of occurrences of } s \text{ in } r|_T}{T}$$

Let σ be a policy on \mathcal{S} and $T \geq 0$, and let \hat{x}^T be the random variable on the set of runs which associates to all r its frequency vector of length T : $\hat{x}^T = \text{freq}_T(r)$. Given an initial distribution α , the *Expected frequency vector* $x_{\sigma,\alpha}^T$ is $\mathbb{E}_{\sigma,\alpha}[\hat{x}^T]$, the expectation of \hat{x}^T . Let $x_{\sigma,\alpha}^\infty$ be the empty set if $x_{\sigma,\alpha}^T$ does not converge as $T \rightarrow +\infty$, and the limit point if $x_{\sigma,\alpha}^T$ converges. We define:

$$\mathcal{H}(\alpha) = \bigcup_{\sigma \text{ policy}} x_{\sigma,\alpha}^\infty$$

If \mathcal{S} is an irreducible Markov chain, then $\mathcal{H}(\alpha)$ is the stationary distribution on the states of the chain. For a general MDP, $\mathcal{H}(\alpha)$ is a convex combination of the set of stationary distributions which can be reached on the Markov chains induced by stationary policies on \mathcal{S} . Generalizing the classical linear characterization of the stationary distribution of an irreducible Markov chain, the authors of [8,16] give linear characterizations of $\mathcal{H}(\alpha)$ [16]. As a consequence, the set $\mathcal{H}(\alpha)$ is a polytope, characterized by a number of linear equation polynomial in the size of the system. This makes possible the evaluation of properties such that: *with high probability, is state s in a run followed by state t ?* [7]. Moreover, H is also the convex hull of the limit frequency vectors associated to non randomized policies. We present in appendix A the polytope H associated to the MDP of appendix A.

2.2 Graph neighborhoods and statistics

Let $\mathcal{G} = (V, E)$ be a graph with vertex set V and edge set E , and S be a finite set of labels. Let $N = |V|$. An *S-labeled graph* on \mathcal{G} is a triple (\mathcal{G}, C, S) where $C : V \rightarrow S$ is a labeling function which associates a label in S to each state in V . We will often write C for the labeled graph (\mathcal{G}, C, S) . We write \mathcal{C} for the set of S -labeled graphs on \mathcal{G} . A *pointed graph* (or *pointed labeled graph*) is a couple (\mathcal{G}, v) where \mathcal{G} is a graph (or a labeled graph) and v is a vertex of \mathcal{G} , called the *center* of the graph. Given two pointed labeled graphs $\mathcal{F} = ((V, E), C, S, v)$ and $\mathcal{F}' = ((V', E'), C', S, v')$, a function $\phi : V \rightarrow V'$ is an *isomorphism* if it is a graph isomorphism between graphs (V, E) and (V', E') , such that $\phi(v) = v'$, and for all $v \in V$, $C(v) = C'(\phi(v))$.

Definition 1 (*k*-neighborhoods in a graph). Let $\mathcal{G} = (V, E)$ be a graph, $v \in V$, and $k \in \mathbb{N}$. The neighborhood of width k around v in \mathcal{G} , or *k-neighborhood* around v in \mathcal{G} , defined up to pointed graph isomorphism, is the pointed graph induced by the set of vertices at distance at most k from v in \mathcal{G} , and whose center is the vertex which corresponds to v .

We write $\mathcal{N}(\mathcal{G}, v, k)$ (resp. $\mathcal{N}(C, v, k)$) for the k -neighborhood around v in \mathcal{G} (resp. (\mathcal{G}, C, S)), and we define:

$$\mathcal{N}_k(\mathcal{G}) = \{\mathcal{N}(\mathcal{G}, v, k) \mid v \in V\} \quad \mathcal{N}_k(\mathcal{C}) = \{\mathcal{N}(C, v, k) \mid v \in V \text{ and } C \in \mathcal{C}\}$$

Given a neighborhood $H \in \mathcal{N}_k(\mathcal{G})$ (resp. $H \in \mathcal{N}_k(\mathcal{C})$), we may write H_v in order to underline the fact that the center of the pointed graph H is v . We generalize the uniform statistics defined on words and trees [11], and define a notion of k statistics on graphs. The k uniform statistics of a word w counts the number of occurrences of all subwords u of length k in w . The role of subwords is played in our context by *graph neighborhoods*.

Definition 2 (k -statistics of graphs). Let $\mathcal{G} = (V, E)$ be a graph with $|V| = N$, and let $k \in \mathbb{N}$. The k -statistics vector $ustat_k(\mathcal{G})$ is the vector in $[0, 1]^{\mathcal{N}_k(\mathcal{G})}$ such that for all $H \in \mathcal{N}_k(\mathcal{G})$ we have:

$$ustat_k(\mathcal{G})[H] = \frac{|\{v \in V \text{ s.t. } \mathcal{N}(\mathcal{G}, v, k) \simeq H\}|}{N}$$

Given an S -labeled graph C on \mathcal{G} , the k -uniform statistics vector $ustat_k(C)$ is the vector in $[0, 1]^{\mathcal{N}_k(\mathcal{C})}$ such that for all $H \in \mathcal{N}_k(\mathcal{C})$ we have:

$$ustat_k(C)[H] = \frac{|\{v \in V \text{ s.t. } \mathcal{N}(C, v, k) \simeq H\}|}{N}$$

That is, the k -statistics vector $ustat_k(\mathcal{G})$ counts the different k -neighborhoods which appear in \mathcal{G} , and the k -statistics vector $ustat_k(C)$ counts the different labeled k -neighborhoods which appear in C .

Proposition 1. Let $k \in \mathbb{N}$. The support of $ustat_k(\mathcal{G})$ (resp. $ustat_k(C)$) has size at most N . Moreover $|\{ustat_k(C) \mid C \in \mathcal{C}\}| \leq N^L$, where $L = |\mathcal{N}_k(\mathcal{C})|$.

Proof. The first assertion follows from the fact that there are at most N k -neighborhoods, one for each $v \in V$. Let $C \in \mathcal{C}$. For each neighborhood $H \in \mathcal{N}_k(\mathcal{C})$, $ustat_k(C)[H]$ counts the number of times H appears in C as the neighbor of a node. The configuration C has N nodes, hence contains at most N different k -neighborhoods. Since there exists $L = |\mathcal{N}_k(\mathcal{C})|$ possible k -neighborhoods, the number of possible $ustat_k(C)$ vectors is at most $N * (N-1) * \dots * (N-L+1) \leq N^L$.

Notice that $|\mathcal{N}_k(\mathcal{C})|$ is uniformly bounded on classes of graphs with degrees uniformly bounded. As a consequence, if we restrict to classes of graphs with uniformly bounded degrees, then $|\{ustat_k(C) \mid C \in \mathcal{C}\}|$ is polynomial in the number of nodes of the graphs.

3 Networks of MDPs

Our network of MDPs is a labeled graph where the set of labels is the set of states of an MDP $\mathcal{S} = (S, \Sigma, P)$. We need to generalize the notion of MDP to make the transitions depend on the environment of a node v . An environment of a node v is a pointed S -labeled graph $((\mathcal{H}, C, S), v)$ where $\mathcal{H} = (V, E)$, $v \in V$,

and each vertex in \mathcal{H} is at distance at most 1 from v . Let \mathcal{N}_1 be the set of such environments. Notice that in particular, given any S -labeled graph \mathcal{F} on a structure \mathcal{G} and v a vertex in \mathcal{F} , the neighborhood $\mathcal{N}_1(\mathcal{F}, v, 1)$ is in \mathcal{N}_1 .

A *device MDP* is a triple $\mathcal{S} = (S, \Sigma, P_D)$ where S is a finite state space, Σ is a finite set of actions, and P_D is the transition function: $P_D : \mathcal{N}_1 \times \Sigma \rightarrow \mathcal{D}(S)$. Given $H \in \mathcal{N}_1$, $s \in S$ and $a \in \Sigma$, $P_D(H, a)(s)$, also written $P_D(s|H, a)$, is the probability that the state of the device MDP is s after the transition, given its environment is H and action a is chosen. The classical definition of an MDP can be retrieved by restricting the transition function P_D so that its values depend only on a and on the label of the pointed node of H .

Definition 3 (Network of MDPs). A network of MDPs is a couple $\mathcal{M} = (\mathcal{G}, \mathcal{S})$, where $\mathcal{G} = (V, E)$ is a graph and $\mathcal{S} = (S, \Sigma, P_D)$ is a device MDP.

A *configuration* on \mathcal{M} is a function $C : V \rightarrow S$ which assigns to each vertex of \mathcal{G} a state of the associated device MDP. We write \mathcal{C} for the set of configurations on \mathcal{M} . A configuration can be seen as an S -labeled graph on \mathcal{G} . We may write C indifferently for the configuration or for the associated S -labeled graph.

3.1 Transitions on a network of MDPs

We define transitions on \mathcal{M} and obtain a new MDP, $\mathcal{S}(\mathcal{M})$. The state space of $\mathcal{S}(\mathcal{M})$ is \mathcal{C} , the set of configurations. The set of actions is Σ , used by each device MDP. For a transition, a random device MDP is chosen and its state is updated according to the transition function P_D . We sample *uniformly at random* a node v (device MDP) to update, as for the *random independent scheme*, a classical model for asynchronous Cellular Automata [12].

Let $C \in \mathcal{C}$, $v \in V$ and $s \in S$. We define $C_{v \rightarrow s}$ as the function from V to S which coincide with C on every $w \in V - \{v\}$, and such that $C_{v \rightarrow s}(v) = s$.

Given v and its 1-neighborhood $H = \mathcal{N}(C, v, 1)$ in the current configuration C , let s be sampled randomly according to distribution $P_D(-|H, a)$, where $a \in \Sigma$ is the chosen action. The configuration is changed to $C' = C_{v \rightarrow s}$. This process defines a transition function P on the MDP $\mathcal{S}(\mathcal{M}) = (\mathcal{C}, \Sigma, P)$ as follows: let $a \in \Sigma$, and let $C, C' \in \mathcal{C}$. Recall that $N = |V|$.

1. If $C \neq C'$ and there exists $v \in V$ and $s \in S$ such that $C' = C_{v \rightarrow s}$, then we define $P(C'|C, a) = \frac{P_D(s|\mathcal{N}(C, v, 1), a)}{N}$
2. If $C = C'$, then we define $P(C'|C, a) = \frac{\sum_{v \in V} P_D(C(v)|\mathcal{N}(C, v, 1), a)}{N}$
3. In the other cases, we define $P(C'|C, a) = 0$.

For all $a \in \Sigma$ and $C \in \mathcal{C}$, $P(-|C, a)$ is indeed a probability distribution on \mathcal{C} , and $\mathcal{S}(\mathcal{M}) = (\mathcal{C}, \Sigma, P)$ is an MDP. Notice that the *policies on $\mathcal{S}(\mathcal{M})$ are global*, i.e. they consider the configurations, not the particular devices.

Example. A contamination network. Consider the following network of MDPs \mathcal{M} which illustrates our approach. The device MDPs have only one possible action, and

their state space is $S = \{0, 1\}$. State 1 is the "infected" state, whereas 0 is the "non-infected" state. Non infected devices may become infected with a small probability, and infect their neighbors. The network \mathcal{M} is a circle of N device MDPs. There is no non-determinism in this system, since only one action is allowed.

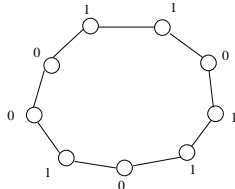


Fig. 1. A circular network of MDPs.

Let $r - s - t \xrightarrow{\delta} s'$ describe a transition of a device in state $s \in S$ with neighbors in state $r \in S$ and $t \in S$, to state s' with probability δ . In other words, notation $r - s - t \xrightarrow{\delta} s'$ holds for $P_D(s'|r - s - t, a) = \delta$. In the following, an $*$ in the notation holds for any state. The transition function of the device MDP is given by:

$$* - 1 - * \xrightarrow{1} 1; \quad * - 0 - 1 \xrightarrow{1} 1; \quad \begin{cases} 0 - 0 - 0 \xrightarrow{\epsilon} 1 \\ 0 - 0 - 0 \xrightarrow{1-\epsilon} 0 \end{cases}$$

This process is a Markov chain since there is no non-determinism. At each step, a device is chosen uniformly at random among the vertices of the network, and updated. The induced Markov chain has a state space of size 2^N , and we can see that all the configurations are reachable from the initial configuration $0 - 0 - \dots - 0$ with non-zero probability. We cannot study the evolution of the chain by using explicit linear equations on the state space if N is larger than 20. We will approximate the distribution at time $\tau \in \mathbb{N}$ of the proportion of infected states, using our statistical approach.

We will use *shift vectors* to quantify the change in the statistics of the configurations induced by the update of the state of one device MDP in the network. Given $C \in \mathcal{C}$, $v \in V$ and $a \in \Sigma$, we define

$$\Delta_k(C, v \rightarrow s) = N \cdot [ustat_k(C_{v \rightarrow s}) - ustat_k(C)]$$

Given $k \in \mathbb{N}$, a *k-statistics shift vector* on \mathcal{G} is a vector $\Delta \in [-N, N]^{\mathcal{N}_k(\mathcal{C})}$ whose components in \mathbb{Z} sum to zero. Clearly, vectors of the type $\Delta_k(C, v \rightarrow s)$ are *k-shift vectors*. The following proposition shows that when the state of one of the vertices of a labeled graph is changed, the variation on the *k-statistics* depends only on bounded neighborhoods around the changed vertex. It can be proven directly by counting the variations which appear on the *k-statistics*.

Proposition 2 (($k, \phi(k)$)-locality). *Let $k \in \mathbb{N}$. Let $\phi : \mathbb{N} \rightarrow \mathbb{N}$ be such that $\phi(0) = 1$ and $\phi(k) = 2 \cdot k$ if $k \geq 1$. Then for all $C \in \mathcal{C}$, $v \in V$ and $s \in S$ we have $\Delta_k(C, v \rightarrow s) = \Delta_k(\mathcal{N}(C, v, \phi(k)), v \rightarrow s)$, i.e. for all $H \in \mathcal{N}_k(\mathcal{C})$ we have:*

$$\Delta_k(C, v \rightarrow s)[H] = N \cdot [ustat_k(\mathcal{N}(C, v, \phi(k))_{v \rightarrow s})[H] - ustat_k(\mathcal{N}(C, v, \phi(k)))[H]]$$

We can generalize this fact to the transition function of a network of MDPs. In the following, given $C \in \mathcal{C}$, we write C' for the random configuration distributed accordingly to the probability distribution $P(-|C, a)$. The following proposition is a direct consequence of proposition 2.

Proposition 3. *Let \mathcal{M} be a network of MDPs, $a \in \Sigma$, $C \in \mathcal{C}$, $k \in \mathbb{N}$, and let Δ_k be a k -statistics shift vector. Then:*

$$\begin{aligned} P(ustat_k(C') = ustat_k(C) + \frac{\Delta_k}{N} \mid C, a) = \\ P(ustat_k(C') = ustat_k(C) + \frac{\Delta_k}{N} \mid ustat_{\phi(k)}(C), a) \end{aligned}$$

In other words, the distribution of the k -order statistics of the configurations after a transition depends only on the $\phi(k)$ -th order statistics of the configuration C before the transition.

4 Structured Population Protocols with Decisions

Let $\mathcal{G} = (V, E)$ be a graph network, and let $N = |V|$. Let S be a finite set of labels, and let \mathcal{C} be the set of S -labeled graphs on \mathcal{G} . Given $k \in \mathbb{N}$, recall that $\mathcal{N}_k(\mathcal{C})$ is the set of all possible k -neighborhoods which can appear in S -labeled graphs on the structure \mathcal{G} . We define a *Structured Population Protocol* which will induce an MDP on the set of statistics vectors. Our model generalizes classical Population Protocols in two ways:

- it uses statistics on graphs neighborhoods, i.e. on a structured domain, as opposed to statistics on sets,
- decisions can be taken on states, using the same decision space Σ as the original device MDPs.

A *Population* of statistics of order k , or k -Population, on \mathcal{G} , is a vector $A \in \mathbb{N}^{\mathcal{N}_k(\mathcal{C})}$ whose components sum to N . We write \mathcal{A}_k for the set of k -Populations. A Population can be seen as a *soup* of neighborhoods, i.e. a multiset of neighborhoods with no structure. Given a neighborhood H in $\mathcal{N}_k(\mathcal{C})$, $A[H]$ is equal to the number of times the neighborhood H appears in the soup of neighborhoods A . A k -Population A induces a distribution $\frac{A}{N}$ on $\mathcal{N}_k(\mathcal{C})$, with $\frac{A}{N}(H) = A[H]/N$. Reciprocally, an $ustat_k$ vector $x = ustat_k(C)$ induces a k -Population $A = N \cdot x$. Typically, a k -Population counts the different k -neighborhoods which appear in an S -labeled graph C on \mathcal{G} . In that case, the probability distribution $\frac{A}{N}(-)$ is equal to $ustat_k(C)(-)$. Notice however that there may exist k -Populations A such that for no S -labeled graph C on \mathcal{G} we have $\frac{A}{N}(-) = ustat_k(C)(-)$. As a consequence of Proposition 1, given $L = |\mathcal{N}_k(\mathcal{C})|$,

$$|\mathcal{A}_k| \leq N^L$$

As in [3], in our approach of Population Protocols, the devices, i.e. the nodes of the graph, will interact locally. The associated transition probabilities will be given by a transition function δ . A *k-Structured Population Protocols with Decisions* on \mathcal{G} is given by a *transition function* δ and a *reconstruction function* R_k . The function R_k will impose the updates to depend on the structure of the underlying graph \mathcal{G} .

Definition 4 (*k-Structured Population Protocols with Decisions*). *Given $k \in \mathbb{N}$, a k -Structured Population Protocols with Decisions, or k -SPPD, on \mathcal{G} , is a triple $\mathcal{O}_k = (\delta, R_k, \Sigma)$ where $\delta : \mathcal{N}_1(\mathcal{C}) \times \Sigma \rightarrow \mathcal{D}(S)$ and $R_k : \mathcal{A}_k \times \mathcal{N}_{\phi(k)}(\mathcal{G}) \rightarrow \mathcal{D}(\mathcal{N}_{\phi(k)}(\mathcal{C}))$.*

Function $\delta : \mathcal{N}_1(\mathcal{C}) \times \Sigma \rightarrow \mathcal{D}(S)$ is the *transition function*. When $|\Sigma| = 1$, the domain of δ is $\mathcal{N}_1(\mathcal{C})$ and the system is called a *k-Structured Population Protocol*, or *k-SPP*. In that case, our model is close to the standard model of Population Protocol, [4]. Given $k \geq 0$ and $\overline{H}_v \in \mathcal{N}_{\phi(k)}(\mathcal{C})$, δ induces a distribution $\delta(-|\overline{H}_v, a)$ on the set of *k-shift vectors*. If Δ_k is a *k-shift vector*, $\delta(\Delta_k|\overline{H}_v, a)$ is the probability that an update of the label of the center node v of \overline{H}_v according to the transition function δ induces a change Δ_k in the *k-statistics*. Formally, let $\delta(\Delta_k|\overline{H}_v, a)$ be defined as:

$$\delta(\Delta_k|\overline{H}_v, a) = \sum_{s \in S \text{ s.t. } \Delta_k(\overline{H}_v, v \rightarrow s) = \Delta_k} \delta(\mathcal{N}(\overline{H}_v, v, 1), a)(s)$$

Function $R_k : \mathcal{A}_k \times \mathcal{N}_{\phi(k)}(\mathcal{G}) \rightarrow \mathcal{D}(\mathcal{N}_{\phi(k)}(\mathcal{C}))$ is a *reconstruction function*: given a *k-Population* A and H_v a $\phi(k)$ -neighborhood of the graph \mathcal{G} , it outputs randomly a valuation in S for the nodes of H_v . In other words, distribution $R_k(A, H_v)(-)$ assigns probabilities to the labellings of H_v .

4.1 A *k-SPPD* is an MDP

We associate an MDP $\mathcal{S}_{\mathcal{O}_k}$ to a *k-SPPD* \mathcal{O}_k as follows. The state space of $\mathcal{S}_{\mathcal{O}_k}$ is \mathcal{A}_k , the set of *k-Populations*, and the set of action labels is Σ . We have to define the transition function $P_{\mathcal{O}_k}$. Given a population $A \in \mathcal{A}_k$ and an action a , we first show how to sample a population A' distributed according to the distribution $P_{\mathcal{O}_k}(-|A, a)$. This gives a first definition for the transition function $P_{\mathcal{O}_k}$.

1. First, let $\mu = \text{ustat}_{\phi(k)}(\mathcal{G})$ be the distribution of the $\phi(k)$ -neighborhoods of \mathcal{G} . Sample $H_v \in \mathcal{N}_{\phi(k)}(\mathcal{G})$ according to μ . This is equivalent to sampling a node in \mathcal{G} uniformly at random and defining H_v as its $\phi(k)$ -neighborhood.
2. Sample $\overline{H}_v \in \mathcal{N}_{\phi(k)}(\mathcal{C})$ according to distribution $R_k(A, H_v)(-)$. That is, sample a valuation for the nodes of H_v .
3. Sample $s \in S$ according to distribution $\delta(a, \mathcal{N}(\overline{H}_v, v, 1))(-)$. That is, update the state of device v at the center of the neighborhood \overline{H}_v .
4. Let $\Delta_k = \Delta_k(\overline{H}_v, v \rightarrow s)$. Δ_k represents the change in the statistics of order k induced by the update.
5. Define $A' = A + \Delta$.

The transition function $P_{\mathcal{O}_k}$ on $\mathcal{S}_{\mathcal{O}_k}$ can also be defined formally as follows: given Δ_k a k -shift vector,

$$P_{\mathcal{O}_k}(A' = A + \Delta_k | A, a) = \sum_{H \in \mathcal{N}_{\phi(k)}(\mathcal{C}), F \in \mathcal{N}_{\phi(k)}(\mathcal{G})} \delta(\Delta_k | H, a) \cdot R_k(A, F)(H) \cdot \text{ustat}_{\phi(k)}(\mathcal{G})[F]$$

The following proposition can be proved directly by probability conditioning.

Proposition 4. *The two previous definitions of $P_{\mathcal{O}_k}$ coincide.*

4.2 The k -SPPD associated to a network of MDPs

Let $\mathcal{M} = (\mathcal{G}, \mathcal{S})$ be a network of MDPs, with $\mathcal{G} = (V, E)$ and $\mathcal{S} = (S, \Sigma, P_D)$. Let $\mathcal{S}(\mathcal{M}) = (\mathcal{C}, \Sigma, P)$ be the MDP associated to \mathcal{M} . Given $k \in \mathbb{N}$, we want to define a k -SPPD $\mathcal{O}_k(\mathcal{M}) = (\delta, R_k, \Sigma')$ on \mathcal{G} such that the associated MDP $\mathcal{S}_{\mathcal{O}_k}$ mimics the transitions of $\mathcal{S}(\mathcal{M})$ on the set of k -statistics vectors.

The set of actions on $\mathcal{O}_k(\mathcal{M})$ will be Σ , the same as for \mathcal{M} . The state space of $\mathcal{O}_k(\mathcal{M})$ will be \mathcal{A}_k , the set of k -Populations on \mathcal{G} , which can also be seen as the set of k -statistics of configurations on \mathcal{M} . The transition function δ of $\mathcal{O}_k(\mathcal{M})$ will be equal to the transition function P_D of the device MDPs of \mathcal{M} . The point is to define a relevant reconstruction function R_k . The role of the function R_k is, given a k -Population A and a $\phi(k)$ -neighborhood $H \in \mathcal{N}_k(\mathcal{G})$, to guess valuations for the nodes in H . Ideally, we would like, given $C \in \mathcal{C}$ and $H \in \mathcal{N}_{\phi(k)}(\mathcal{G})$, the distributions $R_k(N \cdot \text{ustat}_k(C), H)(-)$ and $(\text{ustat}_{\phi(k)}(C)|H)(-)$ to be equal. That is, the reconstruction of size $\phi(k)$ of the k -statistics of a configuration is the $\phi(k)$ statistics of the configuration. This is not possible in general, but we give an algorithm to compute the function R_k which will give good approximations on a restricted class of *mixed configuration*, defined in the next subsection. The following is the algorithm that we will use to define functions R_k .

Algorithm 1 (Sampling from R_k)

Input: A Population $A \in \mathcal{A}_k$, $H \in \mathcal{N}_{\phi(k)}(\mathcal{G})$.

Output: $\overline{H} = (H, C) \in \mathcal{N}_{\phi(k)}(\mathcal{C})$ an S -valuation of the nodes of H .

Method: We define C incrementally on the set of nodes of H . Until a valuation for all the node of H is defined to the following:

1: Sample a node v uniformly at random among the nodes in H whose k -neighborhood contains unlabeled nodes, and which is at distance at most k from the center of H .

2: Sample $K \in \mathcal{N}_k(\mathcal{C})$ according to distribution $(\frac{A}{N}|C)(-)$. That is, sample K according to the distribution $\frac{A}{N}$ conditioned to the partial valuation C defined so far. (See section 5.1 for a precise definition of this conditional probability). This corresponds to sampling labels for a neighborhood of size k in H . For all $w \in K$, define $C(w) = K(w)$.

Return $\overline{H} = (H, C)$.

Finally, given $\mathcal{M} = (\mathcal{G}, \mathcal{S})$ the network of MDPs, using the algorithm 1 for the construction of R_k , we have a k -SPPD $\mathcal{O}_k(\mathcal{M}) = (\delta, R_k, \Sigma)$ on \mathcal{G} , with state

space \mathcal{A}_k . In appendix B, we present the construction of the 1-SPP associated to the contamination network of section 3.1.

Now, given a policy on the MDP \mathcal{M} , how can we build a related policy on \mathcal{O}_k ? Since the state space of \mathcal{M} has size exponential in the state space of \mathcal{O}_k , we cannot associate a policy on \mathcal{O}_k to each policy on \mathcal{M} . We will have to restrict the class of policies that we consider on \mathcal{M} : a policy on \mathcal{M} must satisfy certain compatibility properties to be transferable on \mathcal{O}_k . A natural condition is the fact that it depends only on the k -statistics of the configurations. We call *statistical policies* such policies on \mathcal{M} :

Definition 5 (Statistical Policies). *A policy σ on \mathcal{M} is k -statistical if:*

$$\forall C, C' \in \mathcal{C}, \text{ustat}_k(C) = \text{ustat}_k(C') \Rightarrow \sigma(C) = \sigma(C')$$

Let $SR^k(\mathcal{M})$ be the set of k -Statistical and Randomized policies. For instance, a policy which takes its decisions according to the 0-statistic of the configurations, i.e. according to the proportions of the different states among the devices, is k -statistical for all $k \in \mathbb{N}$. A policy $\sigma \in SR^k(\mathcal{M})$ induces trivially a policy σ on \mathcal{O}_k , since σ can be defined on the set of ustat_k vectors, hence on \mathcal{A}_k .

5 Approximations on Networks of MDPs.

Let \mathcal{M} be a network of MDPs as before, with state space \mathcal{C} and transition function P , and let \mathcal{O}_k be the associated k -SPPD, with state space \mathcal{A}_k and transition function $P_{\mathcal{O}_k}$. In this section we show that we can bound the difference in the evolutions of the statistics of the real process induced by \mathcal{M} , and the evolution of the approximation process induced by \mathcal{O}_k . More precisely, we show that we can define a notion of *mixed configurations*, quantified by a *mixing parameter*, such that the reconstruction function R_k defined by algorithm 1 on the Population Protocol approximates \mathcal{M} .

5.1 Mixed configurations

A *partially labeled graph* is a graph such that labels are associated only to a subset of nodes. In particular, a graph $H = (V, E)$ can be seen as a partially labeled graph, where no valuation is defined for any node. We write $\mathcal{N}_k(\mathcal{C}_p)$ for the set of k -neighborhoods of partially labeled graphs on \mathcal{G} . Given F, F' two partially labeled graphs on the same domain \mathcal{G} , F and F' are said to be *compatible* if there exists no node of \mathcal{G} to which F and F' assign different labels. Given C_H a partially labeled graph on a graph H , we define $\mathcal{L}(C_H)$ as the set of labeled graphs on H compatible with C_H . We need to condition probability distributions by a structure: given a distribution μ on $\mathcal{N}_k(\mathcal{C})$, given $H \in \mathcal{N}_k(\mathcal{G})$ and given C_H a partially labeled graph on H such that $\mu(\mathcal{L}(C_H)) > 0$, the distribution $(\mu|_{C_H})(-)$ on $\mathcal{N}_k(\mathcal{C})$ is defined as follows: for all $K \in \mathcal{N}_k(\mathcal{C})$,

$$(\mu|_{C_H})(K) = 0 \text{ if } K \notin \mathcal{L}(C_H) \text{ and else } (\mu|_{C_H})(K) = \frac{\mu(K)}{\mu(\mathcal{L}(C_H))}$$

We now want to quantify the quality of the reconstruction function R_k . As we said before, ideally, given a configuration $C \in \mathcal{C}$ and $H \in \mathcal{N}_{\phi(k)}(\mathcal{G})$, the distributions $R_k(N \cdot \text{ustat}_k(C), H)(-)$ and $(\text{ustat}_{\phi(k)}(C)|H)(-)$ should be equal. However, this is not possible in general, since there may exist configurations $C, C' \in \mathcal{C}$ such that $\text{ustat}_k(C) = \text{ustat}_k(C')$ but $\text{ustat}_{\phi(k)}(C) \neq \text{ustat}_{\phi(k)}(C')$. We present a class of configurations for which there exist good reconstruction functions, i.e. functions R_k such that the distributions $R_k(N \cdot \text{ustat}_k(C), H)(-)$ and $(\text{ustat}_{\phi(k)}(C)|H)(-)$ are close. Such configurations can be seen as "mixed" configurations, and we define a *mixing coefficient*.

Let $C \in \mathcal{C}$, let v be a node in C and let $H = \mathcal{N}(C, v, k)$. Let K be a partial labeling of $\mathcal{N}(\mathcal{G}, v, \phi(k))$ such that the partial labeling K_H induced by K on $\mathcal{N}(\mathcal{G}, v, k)$ is compatible with H . Let P_C be the probability distribution $\text{ustat}_k(C)(-)$. We define the following conditional probabilities: $P_C[H|H \cap K]$ is the probability, among the k -neighborhoods of C , of the neighborhood H , given the partial valuation K_H is given. $P_C[H|K]$ is the probability, among the $\phi(k)$ -neighborhoods of C , of the neighborhood which contains H around its center, given the partial valuation K is given. Formally:

$$P_C[H|H \cap K] = \frac{|\{u \in V \text{ s.t. } \mathcal{N}(C, u, k) \simeq H\}|}{|\{u \in V \text{ s.t. } \mathcal{N}(C, u, k) \in \mathcal{L}(K_H)\}|}$$

$$P_C[H|K] = \frac{|\{u \in V \text{ s.t. } \mathcal{N}(C, u, k) \simeq H \wedge \mathcal{N}(C, u, \phi(k)) \in \mathcal{L}(K)\}|}{|\{u \in V \text{ s.t. } \mathcal{N}(C, u, \phi(k)) \in \mathcal{L}(K)\}|}$$

If K is not compatible with C , let $P_C[H|H \cap K] = P_C[H|K] = 0$.

Definition 6 (Mixing coefficient ϵ_k). Let $C \in \mathcal{C}$ be a configuration. The k -mixing coefficient of C is defined as:

$$\epsilon_k(C) = \text{Max}_{H=\mathcal{N}(C, u, k), K \in \mathcal{N}_{\phi(k)}(C_p)} \{|P_C[H|H \cap K] - P_C[H|K]|\}$$

Intuitively, $\epsilon_k(C)$ is small if the distribution of the k -neighborhoods does not depend on their environment. We say that C is *well mixed* if $\epsilon_k(C)$ is small. The following proposition, proved in appendix D, shows that if configuration C is well mixed, the function R_k defined by the algorithm 1 is a good reconstruction function. We measure the distance between the distributions using the $\|\cdot\|_\infty$ -norm: given $v \in \mathbb{R}^n$, $\|v\|_\infty = \max_{i \in [1; n]} |v_i|$. As a consequence, if C is well mixed, we can find a good approximation of $\text{ustat}_{\phi(k)}(C)$ from $\text{ustat}_k(C)$. This is exactly what the function R_k is supposed to do. In appendix C we present an example of statistics for the circular network.

Proposition 5. Let $C \in \mathcal{C}$ be a configuration, and let R_k be defined by algorithm 1. Then for all $H \in \mathcal{N}_{\phi(k)}(\mathcal{G})$ we have:

$$\|R_k(N \cdot \text{ustat}_k(C), H)(-) - (\text{ustat}_{\phi(k)}(C)|H)(-)\|_\infty \leq \epsilon_k(C)$$

We now use the mixing coefficient to give bounds on approximation of the behavior of networks of MDPs by our k -SPPDs. In [13], the authors approximate

the short term evolution of large Markov chains by using a “sliding windows” approach. As in [13], we try to bound the deviation between our approximation and the real process as time goes on. Given $C \in \mathcal{C}$ and $a \in \Sigma$, we write C' for the random configuration induced by the probability distribution $P(-|C, a)$. Given $C \in \mathcal{C}$ and $A = N \cdot \text{ustat}_k(C)$, define the distributions $\mu_{C,a}^k$ and $\nu_{A,a}^k$ on \mathcal{A}_k as follows: given $A' \in \mathcal{A}_k$, let:

$$\mu_{C,a}^k(A') = P(N \cdot \text{ustat}_k(C') = A' | C, a), \quad \text{and} \quad \nu_{A,a}^k(A') = P_{\mathcal{O}_k}(A' | A, a)$$

In other words, $\mu_{C,a}^k(-)$ is the distribution of the k -statistics of configurations after a transition from the configuration C , on the network of MDPs \mathcal{M} . On the other hand, $\nu_{A,a}^k(-)$ is the distribution of the k -statistics after a transition from the population $N \cdot \text{ustat}_k(C)$, on \mathcal{O}_k . The following theorem measures the quality of the approximation of the network of MDPs by the k -SPPD, on the set of k -statistics. It is proved in appendix D.

Theorem 1. $\|\mu_{C,a}^k - \nu_{A,a}^k\|_\infty \leq \|\text{ustat}_k(C)(-) - \frac{A}{N}(-)\|_\infty + \epsilon_k(C)$

5.2 Approximation for Markov Chains: The Evaluation Problem.

For this subsection, we assume that the process induced on the set of configurations by \mathcal{M} is a Markov chain. This is the case when there is no non-determinism on \mathcal{M} , or when a stationary policy has been fixed and resolves the non-determinism of \mathcal{M} . Let $\{X_n\}_{n \in \mathbb{N}}$ be the Markov chain induced on \mathcal{C} , given an initial configuration $C_0 \in \mathcal{C}$ is fixed. Let \mathcal{O}_k be the associated k -SPP on state space \mathcal{A}_k , and let $\{U_n^k\}_{n \in \mathbb{N}}$ be the Markov chain induced by \mathcal{O}_k on \mathcal{A}_k .

We compare the evolutions of the distributions on the set of statistics vectors induced by $\{\text{ustat}_k(X_n)\}_{n \in \mathbb{N}}$ and $\{U_n^k\}_{n \in \mathbb{N}}$. The question is the following: in case of convergence of X_n to a configuration $C \in \mathcal{C}$, does the approximate process U_n^k converges also to a limit close to $N \cdot \text{ustat}_k(C)$? Moreover, in case of multiple stationary configurations for X_n , does process U_n^k converge to close limits with close probabilities?

We show that the answer is positive in the context of the circular contamination graph. However, a consequence of the lower bound on the computational complexity of the reachability problem for Cellular Automata is that the reachability problem for network of MDPs is PSPACE complete. This can be proved by a slight generalization of theorem 4.2 of [5] to the context of asynchronous Cellular Automata. As a consequence, the evaluation problem for X_n and $\text{ustat}_k(X_n)$ are computationally intractable, hence we cannot expect the approximation U_n^k to always match closely the process $N \cdot \text{ustat}_k(X_n)$.

Theorem 2. *If configuration $C \in \mathcal{C}$ is a fixpoint for the chain $\{X_n\}_{n \in \mathbb{N}}$, i.e. a configuration such that $\mathbb{P}[X_{n+1} = C' | X_n = C] = 1$ if $C' = C$ and 0 if $C' \neq C$, then for all $k \geq 1$, $N \cdot \text{ustat}_k(C) \in \mathcal{A}_k$ is a fixpoint for the chain $\{U_n^k\}_{n \in \mathbb{N}}$.*

Proof. If C is a fixpoint, all neighborhoods in $\mathcal{N}_1(C)$ which appear in C are stable for the transition function δ . All the neighborhoods of $\mathcal{N}_1(C)$ centered in

the neighborhoods that we sample from the distributions $R_k(N \cdot \text{ustat}_k(C), H)$ are also stable, i.e. $\mathbb{P}[U_{n+1}^k = U_n^k | U_n^k = N \cdot \text{ustat}_k(C)] = 1$, hence $N \cdot \text{ustat}_k(C)$ is a fixpoint for the chain $\{U_n^k\}_{n \in \mathbb{N}}$.

In appendix E.1, show that the converse of theorem 2 does not hold: there may exist fixpoints for the chain $\{U_n^k\}_{n \in \mathbb{N}}$ which do not correspond to the ustat_k vector of any configuration. We prove that in the contamination model, such fixpoints of $\{U_n^k\}_{n \in \mathbb{N}}$ are not reachable from an initial state which corresponds to the ustat_k vector of a configuration. In appendix E.2, we prove that theorem 2 does not hold for $k = 0$: the transition function of the approximation process $\{U_n^0\}_{n \in \mathbb{N}}$ is too weak since it does not consider overlappings of neighborhoods.

5.3 Approximations for Markov Decision Processes.

Now, we extend our approach to networks of MDPs with non-determinism. Given \mathcal{M} , the associated polytope H (see section 2.1) is a subset of \mathbb{R}^C . The k -SPPD \mathcal{O}_k associated to \mathcal{M} is also an MDP, and its polytope lies in $\mathbb{R}^{\mathcal{A}_k}$. How can we relate these two polytopes?

We consider the set of the limit points associated to stationary statistics policies on \mathcal{M} , and we prove that it is also a polytope. We obtain a natural approximation of $H_{stat}^k(\mathcal{M})$ by the polytope $H(\mathcal{O}_k)$ associated to all the stationary policies on \mathcal{O}_k .

Theorem 3. *The set $H_{stat}^k(\mathcal{M}) = \{N \cdot \text{ustat}_k(x_{\sigma, \alpha}^\infty) \mid \sigma \in SR^k\}$ is a polytope of $\mathbb{R}^{\mathcal{A}_k}$, with a number of extremal points polynomial in N .*

Proof. First, notice that a convex combination of k -statistical policy is clearly a statistical policy. Thus, $H_{stat}^k(\mathcal{M})$ is convex. Next, any statistical policy is a convex combination of "deterministic" statistical policies which assign Dirac distribution to statistic vectors of configurations. (i.e. policies σ such that, given $A \in \mathcal{A}_k$, $\sigma(A) \in \Sigma$). This proves that $H_{stat}^k(\mathcal{M})$ is a polytope, and it is the convex hull of the limit frequency vectors associated to deterministic statistical policies. We can conclude using the fact that since there exists only a polynomial number of ustat_k vectors of configurations in \mathcal{A}_k , there exists only a polynomial number of "deterministic" statistical policies, hence of extremal points of the polytope.

6 Conclusion

We have studied how to approximate the evolution of large probabilistic networks of MDPs. Given a network \mathcal{M} of N device MDPs, we defined a k -Structured Population Protocol with Decisions \mathcal{O}_k , which is also an MDP, whose states are statistics vectors. From an exponential number of configurations, we obtain a polynomial number of statistics. This allows the use of standard evaluation methods on the approximation system, and we gave a sufficient condition, using a mixing parameter ϵ_k , to guarantee a good approximation. If we discretize the

statistics vectors up to a coefficient γ , the size of the set of configurations of the approximation process becomes independent of N : it depends only on δ , k , and the degree of the underlying graph. In appendix F, we present the values of the sizes of the state spaces of the real and the approximation processes for various parameters, underlying the efficiency of the discretization model.

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A A Simple MDP and its polytope

Let $\mathcal{S} = \{s, t, u, w\}$, $\Sigma = \{a, b, c\}$ and the transitions given by the Figure 2. Nodes s, u are deterministic, node t, w are non deterministic, node t is also probabilistic: $P(s|b, t) = .5$ and $P(u|b, t) = .5$. A policy specifies the decision a or b in state t , and the decisions b or c in state w . If the original distribution α specifies the state s with probability 1, a possible run is s, t, u, w, u . The 4 stationary strategies $\sigma_1, \sigma_2, \sigma_3, \sigma_4$ are: $\sigma_1(t) = a; \sigma_1(w) = b$, $\sigma_2(t) = a; \sigma_2(w) = c$, $\sigma_3(t) = b; \sigma_3(w) = b$, and $\sigma_4(t) = b; \sigma_4(w) = c$. Let us now construct $H(\mathcal{S})$,

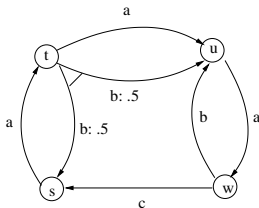


Fig. 2. An MDP with 4 states: nodes t, w are non deterministic, i.e. the transitions are specified by a policy σ .

the polytope of order 1 for the MDP of Figure 1. We consider the frequency vectors, which are distributions on $\{s, t, u, w\}$. By simple calculations on the Markov chains, we get the following limit frequency vectors associated to the stationary strategies $\sigma_1, \sigma_2, \sigma_3, \sigma_4$: $y_1 = (0; 0; 1/2; 1/2)$, $y_2 = (1/4; 1/4; 1/4; 1/4)$, $y_3 = (2/6; 2/6; 1/6; 1/6)$, and $y_4 = (0; 0; 1/2; 1/2)$.

The polytope $H(\mathcal{S})$ is represented partially in Figure 3, using a projection on two dimension: the interpretation is that the limit frequency vector associated to any policy lies in the polytope. We can then decide given a run and its frequency vector y of order k if there is a policy σ which will witness runs ε -close to y , using the *Edit distance with moves* as a distance between runs seen as sequences of letters [7] when $k = \frac{1}{\varepsilon}$. In Figure 3, y is the frequency vector of some run, which is at distance d from $H(\mathcal{S})$. The closest point y' is the limit frequency vector of the randomized policy $\sigma' = \frac{1}{3}.\sigma_1 + \frac{2}{3}.\sigma_2$, i.e. $\sigma'(t) = a$ and $\sigma'(w) = b : \frac{1}{3}, \sigma'(w) = c : \frac{2}{3}$.

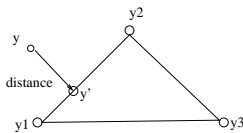


Fig. 3. The polytope $H(\mathcal{S})$ for the MDP of Figure 1.

B The 1-SPP associated to the contamination network

Let $\mathcal{O}_1 = (\delta, R_1, \Sigma)$ be the 1-SPP associated to \mathcal{M} , the circular contamination network of section 3.1. The state space of \mathcal{O}_1 is \mathcal{A}_1 , the set of 1-Populations. We know that:

$$|\mathcal{A}_1| \leq N^{|\mathcal{N}_1(\mathcal{C})|}$$

Since $\mathcal{N}_1(\mathcal{C}) = \{b_1 - b_2 - b_3 \mid b_1, b_2, b_3 \in \{0, 1\}\}$ and since the neighborhoods are taken up to labeled graph isomorphism, we get $|\mathcal{A}_1| \leq N^6$, which allows large N in practice. The set of labels Σ for \mathcal{O}_i is the same as for \mathcal{M} , hence it is reduced to only one label.

We present an example of a sampling from the function R_1 , i.e. we present an execution of algorithm 1 on an input A, H . We have $k = 1$, hence $\phi(k) = 2$. We have $\mathcal{N}_{\phi(1)}(\mathcal{G}) = \{\cdot - \cdot - \cdot - \cdot - \cdot\}$, hence $H = \cdot - \cdot - \cdot - \cdot - \cdot$. Suppose for instance that

$$\begin{aligned} \frac{A}{N} = & (000 : 0.10; 001 : 0.1; 010 : 0.10; 011 : 0.10; \\ & 100 : 0.15; 101 : 0.16; 110 : 0.40; 111 : 0.24) \end{aligned}$$

We want to output \overline{H} , a valuation for the five nodes of H . We use the method of the algorithm 1.

- 1: we sample a node v uniformly at random among the nodes in H , at distance at most 1 from the center of H . Suppose for instance that we sample the center node.
- 2: we sample $K \in \mathcal{N}_k(\mathcal{C})$ according to distribution $\frac{A}{N}$ conditioned to the partial labeling C defined so far. Since no partial labeling have been defined so far, this is equivalent to sampling $K \in \mathcal{N}_k(\mathcal{C})$ according to $\frac{A}{N}$. Suppose for instance that we sample $K = 1 - 0 - 0$. For all $w \in K$, let $C(w) = K(w)$.
- So far, we have defined the partial valuation $\cdot - 1 - 0 - 0 - \cdot$ on H .
- 1bis: we sample a node v uniformly at random among the nodes in H whose k -neighborhood contains unlabeled nodes, and which is at distance at most 1 from the center of H . Suppose for instance that we sample the node on the right of the center.
- 2bis: we sample $K \in \mathcal{N}_k(\mathcal{C})$ according to distribution $\frac{A}{N}$ conditioned to the partial labeling C defined so far. We have $\mathcal{N}(v, C, 1) = 0 - 0 - \cdot$, hence, by definition of the probability conditioning we sample $K = a_1 - a_2 - a_3 \in \mathcal{N}_1(\mathcal{C})$ with probability 0 if $a_1 - a_2 \neq 0 - 0$, and else with probability

$$\frac{A}{N}(K|0 - 0 - \cdot) = \frac{A[a_1 - a_2 - a_3]}{A[0 - 0 - *]}$$

For instance, if $K = 0 - 0 - 1$, since $A[0 - 0 - 1] = 0.1$ and $A[0 - 0 - 0] + A[0 - 0 - 1] = 0.1 + 0.1 = 0.2$, the probability to sample K is $\frac{0.1}{0.2} = \frac{1}{2}$. Suppose we sample indeed $0 - 0 - 1$.

- So far, we have defined the partial valuation $\cdot - 1 - 0 - 0 - 1$ on H .
- In another execution of steps 1 and 2, we may finally get the valuation $\overline{H} = 0 - 1 - 0 - 0 - 1$ on H .

C Probability conditioning

Consider the Circular Network of the contamination model, presented in section 3.1. Let $k = 1$, hence $\phi(k) = 2$. In the following, we write \cdot to denote a node of a partially labeled graph whose label is not defined. As before, a $*$ may hold for any label. Hence, for instance, we write $\cdot - \dots - \cdot$ for a linear graph with n nodes with no valuation defined, and $a_1 - \dots - a_3 - \cdot$ is the linear graph with four nodes with two of them labeled a_1 and a_3 . In the contamination model, we have:

$$\mathcal{N}_1(\mathcal{G}) = \{\cdot - \dots - \cdot\}; \text{ and } \mathcal{N}_2(\mathcal{G}) = \{\cdot - \dots - \dots - \cdot\}$$

In fact, we have

$$\begin{aligned} \mathcal{N}_1(\mathcal{C}_p) &= \{b_1 - b_2 - b_3 \mid b_1, b_2, b_3 \in \{0, 1, \cdot\}\} \\ \text{and } \mathcal{N}_2(\mathcal{C}_p) &= \{b_1 - b_2 - b_3 - b_4 - b_5 \mid b_1, \dots, b_4 \in \{0, 1, \cdot\}\} \end{aligned}$$

To illustrate our notion of conditional probabilities, we consider two types of neighborhoods.

First, let:

$$K = \cdot - \dots - \dots - 1, \quad \text{and} \quad H = a_2 - a_3 - a_4, \quad \text{with } a_2, a_3, a_4 \in \{0, 1\}$$

We have $K \in \mathcal{N}_{\phi(k)}(\mathcal{C}_p)$, and $H \in \mathcal{L}(\mathcal{N}(K, v, k))$. By definition, given a configuration $C \in \mathcal{C}$, we have:

$$P_C[H|H \cap K] = \frac{|\{u \in V \text{ s.t. } \mathcal{N}(C, u, k) \simeq H\}|}{|\{u \in V \text{ s.t. } \mathcal{N}(C, u, k) \in \mathcal{L}(K_H)\}|}$$

Since $K = \cdot - \dots - \dots - 1$ and the center of K is the third node, we have $K_H = \cdot - \dots - \cdot$, hence any configuration in $\mathcal{N}_1(\mathcal{C})$ is an extension of K_H . In other words, $\mathcal{L}(K_H) = \mathcal{N}_1(\mathcal{C})$. Hence, we get

$$P_C[H|H \cap K] = \frac{|\{u \in V \text{ s.t. } \mathcal{N}(C, u, k) \simeq H\}|}{|V|} = \text{ustat}_k(C)[H]$$

This means that the conditional probability of H conditioned to $H \cap K$ is in fact the probability of H to appear as neighborhood in C . This is coherent with the intuition that $H \cap K$ should not interfere with the probability of K , since the partial valuation K forces no valuations for nodes in H . With analogous calculations, we have:

$$P_C[H|K] = \frac{\#_C * - a_2 - a_3 - a_4 - 1}{\#_C * - * - * - * - 1}$$

Where $\#_C * - a_2 - a_3 - a_4 - 1$ is the number of neighborhoods of width 2 in C which are of the form $* - a_2 - a_3 - a_4 - 1$, where $*$ = 0 or 1, and $\#_C * - * - * - * - 1$ is the number of neighborhoods of the form $* - * - * - * - 1$ in C . In other words, $\#_C(H) = N \cdot \text{ustat}_k(C)[H]$.

Hence, $|P_C[H|H \cap K] - P_C[H|K]|$ is small if the proportion of neighborhoods $a_2 a_3 a_4$ among the 1-neighborhoods of C is close to the proportion of the neighborhoods of the form $* - a_2 - a_3 - a_4 - 1$ among the 2-neighborhoods of C of the form $* - * - * - * - 1$. This is coherent with the intuition of a "mixing configuration": the probability to have a 1 on the right does not depend on the center of the neighborhood.

Second, let $K' \in \mathcal{N}_{\phi(k)}(\mathcal{C}_p)$ be $\cdot - \cdot - \cdot - 1 - 1$. Then, given a configuration $C \in \mathcal{C}$, we have $P_C[H|H \cap K'] = 0$ if $a_4 \neq 1$, and else

$$P_C[H|H \cap K'] = \frac{\#_C a_2 - a_3 - 1}{\#_C * - * - 1}$$

Which is different from $ustat_k(C)[H]$ in general. Also, we have:

$$P_C[H|K'] = \frac{\#_C * - a_2 - a_3 - 1 - 1}{\#_C * - * - * - 1 - 1}$$

The typical example of a perfectly mixed configuration, i.e. for which $\epsilon_1(C) = 0$, for 1-statistics in the contamination model network, is a configuration where there is a majority of 0 states, except some 1's which are repartited such that no couple of 1's are separated by less than two 0 states.

D Proofs for section 5

Proposition 5. Let $C \in \mathcal{C}$ be a configuration, and let R_k be defined by algorithm 1. Then for all $H \in \mathcal{N}_{\phi(k)}(\mathcal{G})$ we have:

$$\|R_k(N \cdot ustat_k(C), H)(-) - (ustat_{\phi(k)}(C)|H)(-)\|_{\infty} \leq \epsilon_k(C)$$

Proof. Let $A = ustat_k(C)$. We write μ for the distribution $R_k(N \cdot ustat_k(C), H)(-)$, and ν for the distribution $(ustat_{\phi(k)}(C)|H)(-)$, both on $\mathcal{N}_{\phi(k)}(\mathcal{C})$. Let $\overline{H} \in \mathcal{N}_{\phi(k)}(\mathcal{C})$.

First, if $\overline{H} \notin \mathcal{L}(H)$, then by definition of R_k we have $R_k(N \cdot ustat_k(C), H)(\overline{H}) = 0$, and by definition of the conditional probability $(ustat_{\phi(k)}(C)|H)(-)$, we have $(ustat_{\phi(k)}(C)|H)(\overline{H}) = 0$.

Let $\overline{H} \in \mathcal{L}(H)$. For this proof, we fix an input $N \cdot ustat_k(C), H$ for the algorithm 1. A step of the algorithm 1 is an execution of the points 1 and 2. The algorithm 1 is randomized, and always stops after at most $|H|$ steps. Let Γ be the set of possible executions on input $N \cdot ustat_k(C), H$, which is a finite set. Given $\gamma \in \Gamma$, let i_{γ} be the number of steps of the execution. Given $\gamma \in \Gamma$ and $j \in [1; i_{\gamma}]$, let H_j^{γ} be the partially labeled graph defined on H after j iterations, and let $K_j \in \mathcal{N}_k(\mathcal{C})$ be the neighborhood which is sampled at the point 2 of the j -th step. We define $H_0 = H$.

Let Ω be the set of finite sequence H_0, \dots, H_i of partially labeled graph on H such that $H_0 = H$, $H_i = \overline{H}$, and for all $j \in [0; i - 1]$, H_{j+1} is an extension of H_j (i.e. H_{j+1} defines more labels for nodes than H_j , and the labels of H_{j+1} are compatible with the labels of H_j).

Given $j \in \mathbb{N}$, let \mathbb{P}_j be the distribution of probability on executions associated to the algorithm after j steps, on input $N \cdot \text{ustat}_k(C), H$. For instance, given $K_j \in \mathcal{N}_k(C)$, $\mathbb{P}_j[K_j|H_j]$ is the probability to sample K_j at point 2 of the second step of the algorithm, given partially labeled graph H_j has been defined so far. Then, by conditional probability, we have:

$$R_k(N \cdot \text{ustat}_k(C), H)(\overline{H}) = \sum_{H_0, \dots, H_i \in \Omega} \prod_{j=0}^{i-1} \mathbb{P}_j[H_{j+1}|H_j]$$

Now, given $H_0, \dots, H_i \in \Omega$ and $j \in [0; i-1]$,

$$\mathbb{P}_j[H_{j+1}|H_j] = \sum_{K_j \in \mathcal{N}_k(C)} \mathbb{P}_j[H_{j+1}|H_j \wedge K_j] \cdot \mathbb{P}_j[K_j|H_j]$$

Given $K_j \in \mathcal{N}_k(C)$, by the definition of the algorithm, we have

$$\mathbb{P}_j[K_j|H_j] = (\text{ustat}_k(C)(-)|H_j \cap K_j)(K_j)$$

That is,

$$\mathbb{P}_j[K_j|H_j] = P_C[K_j|H_j \cap K_j] \quad (1)$$

Indeed, the sample in the point 2 of the algorithm is done conditionally to the neighborhoods of width k .

On the other hand, since if $H_0, \dots, H_i \in \Omega$ all the H_j in H_0, \dots, H_i are compatible with \overline{H} , we have:

$$(\text{ustat}_{\phi(k)}(C)|H)(\overline{H}) = \sum_{H_0, \dots, H_i \in \Omega} \prod_{j=0}^{i-1} P_C(H_{j+1}|H_j)$$

Now,

$$P_C(H_{j+1}|H_j) = \sum_{K_j \in \mathcal{N}_k(C)} P_C[H_{j+1}|H_j \wedge K_j] \cdot P_C[K_j|H_j]$$

We have $\mathbb{P}_C[H_{j+1}|H_j \wedge K_j] = \mathbb{P}_j[H_{j+1}|H_j \wedge K_j]$. All we have to do is to bound

$$|P_C[K_j|H_j] - \mathbb{P}_j[K_j|H_j]|$$

But, by equation 1,

$$|P_C[K_j|H_j] - \mathbb{P}_j[K_j|H_j]| = |P_C[K_j|H_j] - P_C[K_j|H_j \cap K_j]| \leq \epsilon_k(C)$$

Which gives the result.

Theorem 1. $\|\mu_{C,a}^k - \nu_{A,a}^k\|_\infty \leq \|\text{ustat}_k(C)(-) - \frac{A}{N}(-)\|_\infty + \epsilon_k(C)$

Proof. This is a consequence of the proposition 5. By $(k, \phi(k))$ locality, give a k -shift vector Δ_k , we have:

$$\mu_{C,a}^k(A+\Delta_k) = \sum_{H \in \mathcal{N}_{\phi(k)}, \overline{H} \in \mathcal{L}(H)} \text{ustat}_{\phi(k)}(\mathcal{G})[H] \cdot (\text{ustat}_{\phi(k)}(C)(-)|H)[\overline{H}] \cdot \delta(\Delta_k|\overline{H}, a)$$

On the other hand, if $A = \text{ustat}_k(C)$, we have:

$$\nu_{A,a}^k(A+\Delta_k) = P_{\mathcal{O}_k}(A+\Delta_k|A, a) = \sum_{H \in \mathcal{N}_{\phi(k)}, \overline{H} \in \mathcal{L}(H)} R_k(A, H)(\overline{H}) \cdot \delta(\Delta_k|\overline{H}, a)$$

This proves the result since by proposition 5,

$$\|\text{ustat}_{\phi(k)}(\mathcal{G})[H] \cdot (\text{ustat}_{\phi(k)}(C)(-)|H)[-] - R_k(A, H)(\overline{H})\|_{\infty} \leq \epsilon_k(C)$$

E Remarks on Theorem 2.

E.1 The converse of theorem 2 does not hold

We consider the order 1 statistics of the circle contamination model of appendix C. Given $A \in \mathcal{A}_1$ and $a, b \in \{0, 1\}$, we write $A[*-a-b]$ for $A[0-a-b] + A[1-a-b]$: the symbol $*$ holds for a projection on the associated component. Then, it is not difficult to see that all the fixpoints of the chain $\{U_n^1\}_{n \in \mathbb{N}}$ are exactly the $A \in \mathcal{A}_1$ such that $A[*-0-*] = 0$. Indeed, if the state of the center device of any neighborhood of width 1 is one, then there is no change when we make an update, and A is a fixpoint. However, there exists $A \in \mathcal{A}_1$ such that $A[*-0-*] = 0$ and which corresponds to no ustat_1 of configuration in \mathcal{C} .

We prove that these fixpoint are in fact unreachable from any initial configuration which corresponds to the ustat_1 vector of a configuration. We prove the result by induction: for all $n \in \mathbb{N}$ we have $U_n^1[*-0-*] > 0$, or $U_n^1[1-1-1] = 1$. In fact, we prove the following: for all $n \in \mathbb{N}$, $U_n^1[*-0-*] = U_n^1[*-* - 0] = U_n^1[0-*-*]$.

- The base case is $U_0^1 = N \cdot \text{ustat}_1(C_0)$, where C_0 the initial configuration is in \mathcal{C} . Then the results follows directly from the fact that the underlying graph is a circle.
- Suppose the result true for U_n^1 , $n \in \mathbb{N}$. Then we remark that the change in the statistics of order two that the transition makes respects the property: for instance, if algorithm 1 guesses a neighborhood $y = [0-1-0-0-1]$ and the state of the center device is updated to 1, then the shift vector Δ is such that $\Delta[*-0-*] = -1 = \Delta[*-* - 0] = \Delta[0-*-*]$.

Now, if for all $n \in \mathbb{N}$ we have $U_n^1[*-0-*] = U_n^1[*-* - 0] = U_n^2[0-*-*]$, then $U_n^1[*-0-*] = 0$ implies $U_n^1[1-1-1] = N$, i.e. A is the ustat_1 vector of the stationary configuration for $\{X_n\}_{n \in \mathbb{N}}$ where all devices are in state 1.

E.2 Theorem 2 does not hold for $k = 0$

Consider a circular network analogous to the contamination model, where the transition function of the device MDPs has been changed to:

$$1 - 0 - 1 \xrightarrow{1} 0; \quad 1 - 1 - * \xrightarrow{1} 1; \quad \begin{cases} 0 - 1 - 1 \xrightarrow{\epsilon} 0 \\ 0 - 1 - 1 \xrightarrow{1-\epsilon} 1 \end{cases}$$

Suppose that N the number of device MDPs in the circular network is even, and let $C = \dots 0 - 1 - 0 - 1 - 0 - 1 \dots$ be the circular configuration which is an alternating sequence of 0's and 1's. Then by definition of the transition function of the device MDPs, C is a fixpoint of the process induced on the set of configuration by the network of MDPs. Now, let \mathcal{O}_0 be the 0-SPP associated to the network of MDPs, and let $A = N \cdot \text{ustat}_0(C) \in \mathcal{A}_0$ be the population associated to C . Notice that we have

$$R_0(A, \cdot - \cdot - \cdot)(011) > 0$$

Indeed, we have $R_0(A, \cdot - \cdot - \cdot)(011) \geq \frac{A}{N}[0] * \frac{A}{N}[1] * \frac{A}{N}[1]$. As a consequence, since $\delta(0 - 1 - 1, a)(1) > 0$ and $\delta(0 - 1 - 1, a)(0) > 0$, we have:

$$P_{\mathcal{O}_0}(A'[1] = A[1] + 1 | A, a) > 0 \text{ and } P_{\mathcal{O}_0}(A'[1] = A[1] | A, a) > 0$$

or

$$P_{\mathcal{O}_0}(A'[1] = A[1] - 1 | A, a) > 0 \text{ and } P_{\mathcal{O}_0}(A'[1] = A[1] | A, a) > 0$$

In both cases, this proves that A is not a fixpoint for the chain U_n^0 .

F Practical bounds on the Structured Population Protocols

The goal is to apply our approach to the study of real systems, such as large sensor networks. In the following we give bounds on the sizes of the state spaces of Structured Population Protocols associated to various classes of networks, and corresponding to statistics of order 0, 1 or 2. We see that the size of the systems are reasonable for statistics of order 0 or 1, 1 being the most interesting case. Using discretization, we see that we can easily consider networks with up to 10000 nodes.

In the following table we consider various networks of MDPs on device MDPs for which $|S| = 2$. We present the size of the state spaces of these networks, and the sizes of the associated k -SPPDs. We consider two different parameters for the networks: d is the degree of the underlying graphs (for instance 2 in the circular contamination model), and N is the number of nodes of the graph. In the table, $\# \text{ network}$ is the number of configurations on the network of MDPs, and given $k \in \mathbb{N}$, $\# k\text{-SPPD}$ is the size of the of the associated k -SPPDs. We have $\#k\text{-SPPD} \sim N^{|\mathcal{N}_k(\mathcal{C})|}$, hence we have to compute the values of the $|\mathcal{N}_k(\mathcal{C})|$,

which can be done easily since we consider small graphs, with $k \in \{0, 1, 2\}$. Remark that for all d , we have $|\mathcal{N}_0(\mathcal{C})| = 2$, since the 0-neighborhoods correspond to the node of the graphs and $|\Sigma| = 2$. Hence for all d , $\#0 - SPPD = N^2$. A network of N device MDPs has size $\#network \sim 2^N$. Finally, the size of the 5% discretized k -SPPD has size less than $20^{|\mathcal{N}_2(\mathcal{C})|}$.

N	d	$ \mathcal{N}_1(\mathcal{C}) $	$ \mathcal{N}_2(\mathcal{C}) $	# network	# 0-SPPD	# 1-SPPD	# 2-SPPD	# 2-SPPD 5%
10	2	6	20	1024	100	≤ 1024	≤ 1024	≤ 1024
20	2	6		$\sim 10^6$	400	$\leq 10^6$	$\leq 10^6$	$\leq 10^6$
1000	2	6		$\geq 10^{50}$	10^6	$\sim 10^{20}$	$\sim 10^8$	$\sim 10^8$
10000	2	6		$\geq 10^{50}$	10^{10}	$\sim 10^{24}$	$\geq 10^{50}$	$\sim 10^8$
10	3	8	10^9	1024	100	≤ 1024	≤ 1024	≤ 1024
20	3	8	10^9	$\sim 10^6$	400	$\leq 10^6$	$\leq 10^6$	$\leq 10^6$
1000	3	8	10^9	$\geq 10^{50}$	10^6	$\sim 10^{20}$	$\geq 10^{50}$	$\sim 10^{10}$
10000	3	8	10^9	$\geq 10^{50}$	10^{10}	$\sim 10^{32}$	$\geq 10^{50}$	$\sim 10^{10}$
10	4	10	$\geq 10^{50}$	1024	100	≤ 1024	≤ 1024	≤ 1024
20	4	10	$\geq 10^{50}$	$\sim 10^6$	400	$\leq 10^6$	$\leq 10^6$	$\leq 10^6$
1000	4	10	$\geq 10^{50}$	$\geq 10^{50}$	10^6	$\sim 10^{30}$	$\geq 10^{50}$	$\sim 10^{13}$
10000	4	10	$\geq 10^{50}$	$\geq 10^{50}$	10^{10}	$\sim 10^{40}$	$\geq 10^{50}$	$\sim 10^{13}$