Can we use perfect simulation for non-monotonic Markovian systems?

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Perfect Simulation. Simulation approaches are alternative methods to estimate the stationary behavior of stochastic systems by providing samples distributed according to the stationary distribution, even when it is impossible to compute this distribution numerically. Propp and Wilson used a backward coupling [4] to derive a simulation algorithm providing perfect sampling (*i.e.* which distribution is exactly stationary) of the state of *discrete time finite Markov chains*. Here, we adapt their algorithm by showing that, under mild assumptions, backward coupling can be used over two simulation trajectories only.

Let $\{X_n\}_{n\in\mathbb{N}}$ be an irreducible and aperiodic discrete time Markov chain with a finite state space $\mathcal{S}$ and a transition matrix $P = (p_{i,j})$. The evolution of the Markov chain can always be described by a stochastic recurrence sequence $X_{n+1} = \phi(X_n, U_{n+1})$, with X_n the state of the chain at time n and $\{U_n\}_{n\in\mathbb{Z}}$ an independent and identically distributed sequence of real random variables, uniformly distributed over $[0,1]$. The transition function $\phi : \mathcal{S} \times [0,1] \to \mathcal{S}$ verifies the property that $\mathbb{P}(\phi(i,U) = j) = p_{i,j}$ for every pair of states $(i,j) \in \mathcal{S}\times\mathcal{S}$ and for any U, a real random variable, uniformly distributed over $[0,1]$.

Let $\phi^n : S \times [0,1]^n \to \mathcal{S}$ denote the function whose output is the state of the chain after n iterations and starting in state $s \in S$. That is, $\phi^n(s, u_{1\to n}) = \phi(\dots\phi(\phi(s,u_1),u_2),\dots,u_n)$. This notation can be extended to set of states. So for a set of states $A \subset \mathcal{S}$, we denote $\phi^n(A, u_{1\to n}) = \{\phi^n(s, u_{1\to n}), s \in A\}$. In the following, $|X|$ denotes the size of set X.

Theorem 1 ([4]). *There exists $\ell \in \mathbb{N}$ such that $\lim_{n\to\infty} |\phi^n(\mathcal{S}, U_{-n+1\to 0})| = \ell$ almost surely. The system couples if $\ell = 1$. In that case, the value of $\phi^n(\mathcal{S}, U_{-n+1\to 0})$ is steady state distributed. Furthermore, given an irreducible transition matrix $P = (p_{i,j})$, it is possible to construct a transition function ϕ that couples so that the Perfect Sampling Algorithm 1 (PSA) can always be constructed.*

Algorithm 1: Perfect Simulation Algorithm (PSA) of Markov chains

Data: A coupling representation ϕ of an ergodic finite Markov chain: $X_{n+1} = \phi(X_n, U_{n+1})$, and an infinite sequence $U_0, U_{-1}, U_{-2}, \dots$ of i.i.d. r.v. uniformly distributed over $[0,1]$.
Result: A state $X \in \mathcal{S}$ generated according to the stationary distribution of the Markov chain X_n.
begin
  $m := 1$;
  repeat
    forall *state* $s \in \mathcal{S}$ **do**
      Compute $X_{n+1} = \phi(X_n, U_{n+1})$, starting at time $-m$ with initial state $X_{-m} = s$, up to time 0 using the random variables $U_{-m+1}, \cdots, U_0$.
    $m := m + 1$;
  until *all simulations end up in the same state (X)* ;
  return X
end

The main drawback of Algorithm 1 is the fact that one needs to simulate the MC starting with all states in $\mathcal{S}$, which could be too large for Algorithm 1 to be used in practice.

Several approaches have been used to overcome this problem. The main one is already present in [4]. When the state space $\mathcal{S}$ is partially ordered and when the function $\phi(\cdot, u)$ is monotonic for all u, then it is possible to generate a steady state by starting Algorithm 1 with maximal and

minimal states only. This technique has been successfully used in [5] to construct PSA for network of queues. When $\phi(\cdot, u)$ is not monotonic, one can still use monotonic bounds, as in [3]. In [1], it is shown that extremal states can also be found for perfect simulations of a special class of closed non-monotonic Petri nets.

Envelopes. The approach proposed here generalizes what has been done in [2] to simulate non-monotonic Markov chains. Its main advantage is that it does not need any preliminary assumption on the structure of the Markov chain. If $\mathcal{S}$ is a lattice, then consider a new transition function $\Gamma = (\mathcal{U}, \mathcal{L}) : \mathcal{S} \times \mathcal{S} \times [0,1] \to \mathcal{S} \times \mathcal{S}$ with $\mathcal{U}(M, m, u) \stackrel{\text{def}}{=} \sup_{m \le s \le M} \Phi(s, u)$ and $\mathcal{L}(M, m, u) \stackrel{\text{def}}{=} \inf_{m \le s \le M} \Phi(s, u)$.

Let us call $T \stackrel{\text{def}}{=} \sup \mathcal{S}$ (resp . $B \stackrel{\text{def}}{=} \inf \mathcal{S}$) the top (resp. bottom) element of $\mathcal{S}$. The upper envelope $Y_n \stackrel{\text{def}}{=} \mathcal{U}^n(T, B, U_{1 \to n})$ is not a Markov chain, neither is the lower one, $Z_n \stackrel{\text{def}}{=} \mathcal{L}^n(T, B, U_{1 \to n})$ However, the couple (Y_n, Z_n) is a Markov chain over the state space $\mathcal{S} \times \mathcal{S}$.

Theorem 2. *Assume that the Markov chain $S_n = (Y_n, Z_n)$ hits the diagonal (i.e. states of the form (x, x)) in finite time, $K \stackrel{\text{def}}{=} \min\{n : \mathcal{U}(T, B, U_{-n+1}, \ldots, U_0) = \mathcal{L}(T, B, U_{-n+1}, \ldots, U_0)\}$. Then K is a backward coupling time of the Markov chain S, so that $\Phi(s, U_{-n+1}, \ldots, U_0)$ has a steady state distribution of X, for all initial state s.*

The proof simply uses the fact that $Y_n \ge X_n \ge Z_n$ for all initial conditions for the chain X. Consider a stationary initial condition X_{-K}. Then, $X_0 = \Phi(X_{-K}, U_{-K+1}, \ldots, U_0)$ is also steady state distributed by stationarity and $Y_0 = X_0 = Z_0$ by definition of K.

Now, Algorithm 1 can be adapted to the envelope simulation: start the simulation with only two states: T and B and iterate using the bi-dimensional function Γ.

In general, this approach may not gain over the general non-monotonic coupling techniques because of three problems:

(P_1) The assumption that S_n hits the diagonal may not be verified.
(P_2) Even if Theorem 2 applies, the coupling time can become prohibitively large.
(P_3) The time needed to compute $\mathcal{U}(M, m, u)$ and $\mathcal{L}(M, m, u)$ might depend on the number of states between m and M which amounts to simulating all trajectories.

Some applications. The envelopes can be used to simulate efficiently rather general classes of queueing networks. For example networks of N finite queues (of capacity C) with general index routing (as in [6]) and batch arrivals (which break the monotonicity property). In that case, envelopes always couple w.p.1 (Problem (P_1)). Problem (P_2) is solved by using a partial split of the trajectories when the states reached by the lower and upper envelopes get close in a queue. Problem (P_3) is solved by constructing an algorithm computing ϕ with complexity $O(N \log(C))$.

Other examples are networks of N finite queues with negative customers and/or with fork and join nodes, which are not monotonic.

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