

# Backward Solution of Markov Chains and Markov Regenerative Processes: Formalization and Applications

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## Abstract

In this paper we investigate the computation, and the stochastic interpretation, of backward probabilities of Markov chains (transient and steady-state probabilities derived from backward Kolmogorov equations) and its extension to the case of Markov Regenerative Processes (MRP). The study is then extended to the case of non-ergodic settings, which enlightens a substantial difference between the forward solution process (based on forward Kolmogorov equations) and the backward one.

We shall clarify the role that backward solutions play in computing absorption probabilities and in the model-checking of stochastic logics as CSL and CSL<sup>TA</sup>, which typically require the steady state solution of a non-ergodic CTMC and MRP respectively. Moreover we show that the algorithm for the computation of the whole set of states that satisfy a CSL formula, which is standard practice in CSL model-checkers, can be seen as a case of computation of backward probabilities of Continuous Time Markov Chains (CTMCs). The backward computation of MRP is then inserted in the context of matrix-free solution technique, which allows to deal with MRP of much bigger size than the standard approach based on the computation and solution of the embedded Markov chain.

*Keywords:* Stochastic Model Checking, Forward and Backward, Kolmogorov, MRP

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## 1 Introduction

It is from the very first chapters of any performance evaluation book that we learn about backward and forward Chapman Kolmogorov equations for Discrete Time Markov Chains (DTMC) and Continuous Time Markov Chains (CTMC). But then most of the remaining topics in the books only deal with forward solution (from an initial state towards a target state) and dedicate a very limited attention to the backward case (from a target state back to possible initial states). So we could find no formal setting to deal with backward probabilities for non-ergodic (reducible)

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systems, or for more complex stochastic processes, like Markov Regenerative Processes (MRP).

It is known that the computation of the forward probabilities of reducible CTMCs requires two steps: each recurrent class is solved in isolation, and this solution is normalized using the probability of entering each class from a given initial state or distribution. As we shall show in this paper, backward solution also has the interesting peculiarities of not requiring a two step procedure.

A second question answered in this paper is whether the same approach used for Markov chains can be applied to reducible and irreducible Markov Regenerative Processes (MRP).

The solution of an MRP is usually based on the steady state probabilities of its embedded Discrete Time Markov Chain (EMC) built upon the solution of a number of *subordinated CTMCs*, one per MRP state. This method is often inapplicable because of the cost of building and storing the EMC: indeed even for a very sparse MRP the resulting EMC is usually very dense. A different, matrix-free, approach has been presented in [13], later extended in [7], that does not require the explicit construction of the EMC, at the price of a more complex solution schema. In this paper we shall conclude that we can indeed *go backward* when dealing with MRPs (ergodic and non-ergodic), even in the more complex case of matrix-free solution.

There are some obvious applications of these results, for example for the computation of the absorption probability (probability of reaching, from each state, a set of "final" states) of Stochastic Petri Nets (SPN) [2] or of Deterministic SPN (DSPN) [1,19], which requires, respectively, a CTMC and an MRP solution.

A more recent application comes instead from stochastic model checking (or, more precisely, the model checking of stochastic logics) for Continuous Time Markov Chains (CTMC). Stochastic model checking allows to check whether a state  $s$  satisfies, in probability, a given condition, which is usually defined over the paths that stem from  $s$  in the CTMC, where a (timed) path is a possible (timed) execution of the CTMC process. The most popular of these logics is CSL [8][9]. CSL identifies paths of two fixed types, specified by the NeXt and the Until path operators, with additional conditions on the time constraints that have to be satisfied along the considered paths (timed Until and timed neXt). The computation of timed neXt is pretty immediate, and we shall not consider it in this paper, but to check if a single state  $s$  in a CTMC satisfies a timed Until requires instead the *concatenated* (usually transient) solution of two CTMCs, obtained from the original one by making certain states absorbing (as proved in [9]). *Concatenated* means that the solution of the first one is used as initial distribution of the second CTMC. The approach in [9] is based on the solution at time  $t$  of the forward Kolmogorov equations of the CTMC (*forward solution*).

Solving for one state at a time is not efficient when we need to compute  $Sat(\varphi)$ , the whole *set of states* that satisfy a formula  $\varphi$ , as required in the computation of *nested* CSL formulas, since the same computation has to be repeated with each single state taken as the initial state of the CTMC. In [15] an algorithm is given that computes at the same time the whole set of states that satisfies  $\varphi$  with a procedure

that starts from the "goal" states and computes *backwards* a vector of probabilities, in which the entry for state  $s$  is the probability that  $s$  satisfies the formula.

In this paper we formalize the computation done by the algorithm in [15] as backward Kolmogorov equations for CTMCs, and we write down the equations that allow to prove that backward and forward computation produce the same *Sat* set, but with backward being more efficient when the whole set of satisfying states has to be computed.

MRPs arise instead in the model checking of stochastic logics like  $\text{CSL}^{\text{TA}}$ .  $\text{CSL}^{\text{TA}}$  was defined in [11] as an extension of CSL (and of CSL with actions [14]) to allow a richer characterization of timed paths, identified through a single clock Timed automaton [3]. In [11] it was also shown that the model checking of  $\text{CSL}^{\text{TA}}$  formulas for a CTMC requires the computation of the probability of reaching a set of absorbing states in a (reducible) Markov Regenerative Process. Again, nested formulas require the computation of the whole *Sat* set, and the question then arises on whether we can go backward or not in the solution of a reducible MRP.

## Literature overview.

We could find very little work on backward solutions, apart from the classical backward and forward Kolmogorov equations for irreducible Markov chain. There is a clear relationship with the computation of absorbing probabilities [17], although it is usually not made explicit. We found no extension to the case of reducible DTMCs/CTMCs and no previous work at all on the backward solution of MRPs. Although most of the basic results on backward and forward probabilities for CTMCs have surely already been presented in various books and papers, we could not find a comprehensive treatment of these topics and of their implications on model checking algorithms.

The work in [15] is surely the most relevant previous work for this paper, as it provides the main motivation of this investigation. The paper is mainly devoted to the symbolic (decision diagram based) CSL model-checking. The "faster" (backward) solution of the title is presented as a pseudo-code algorithm, without any formal probabilistic derivation, its correctness being supported by a similar algorithm for the model-checking of the discrete case (PCTL logic for DTMCs), which was certainly adequate for the purpose of the paper, but that was not enough as a basis for an extension to MRPs, as the one we aimed at in this paper. This algorithm in [15] is the one currently implemented in tools like PRISM [18] and MRMC [16].

For what concerns  $\text{CSL}^{\text{TA}}$  model checking, the work in [10] uses an iteration scheme that is basically a backward solution of the embedded DTMC, but this obviously requires the construction of the embedded DTMC, which has a time and space cost that we shall avoid with the proposal of a matrix-free backward solution.

The paper is structured as follows. Section 2 and 3 present backward and forward solution of DTMCs and CTMCs respectively. Both irreducible and reducible chains are considered. Section 4 applies the backward and forward solutions to the problem

of CSL model checking, to prove that they are equivalent, in terms of the solution computed, but that backward is faster if the whole *Sat* set is required (as for the algorithm in [15]). Section 5 recalls the definition of Markov Regenerative Processes (MRP) and derives a forward and backward solution for irreducible and reducible MRPs, while Section 6 extends the derivations to the matrix-free solution of MRPs, and Section 7 applies it to CSL<sup>TA</sup>. Section 8 concludes the paper.

## 2 Forward and backward solution of DTMCs

In this section we describe the forward and a backward computation of the transient and steady-state probabilities for irreducible and reducible DTMCs.

We indicate with  $\mathcal{D} = \{Y_n \mid n \in \mathbb{N}\}$  a *time-homogeneous* Discrete Time Markov Chain (DTMC) defined over a finite state space  $\mathcal{S}$ . Let  $\mathbf{P}$  be the stochastic matrix of  $\mathcal{D}$ . The dynamic behavior of a DTMC can be described in terms of *forward* probability or in terms of *backward* probability distributions, based on the forward and backward *Chapman-Kolmogorov* equations [23, p. 342].

Forward probabilities give the behavior of the evolution of the system after  $t$  time units, for a given *initial* fixed state  $i$ . The probability of being in state  $j$  after  $n$  steps, knowing that at time 0 the state was  $i$ , is denoted by:

$$\pi^{\mathcal{D}}(i, j, n) = Pr\{Y_n = j \mid Y_0 = i\} \quad (1)$$

When we consider an initial distribution  $\alpha$  rather than a single initial state, the vector  $\pi^{\mathcal{D}}(\alpha, t)$  of forward state probabilities conditioned by  $\alpha$  becomes:

$$\left[\pi^{\mathcal{D}}(\alpha, n)\right](j) = \sum_{i \in \mathcal{S}} \alpha(i) \cdot \pi^{\mathcal{D}}(i, j, n) \quad (2)$$

Equation (2) is subject to the *forward Chapman-Kolmogorov* equations (for the time-homogeneous case), for  $n \geq 0$ :

$$\pi^{\mathcal{D}}(\alpha, n) = \alpha \cdot \mathbf{P}^n \quad (3)$$

The  $j$ -th element of the vector  $\pi^{\mathcal{D}}(\alpha, n)$  is the probability of reaching state  $j$  in  $n$  steps starting from an initial distribution  $\alpha$ . When we need instead to compute the probability of reaching the fixed state  $j$  in  $n$  steps from *every other state*  $i$ , we need to recompute the above formula  $|\mathcal{S}|$  times, one for each  $\alpha = \mathbf{i}_i$ ,  $\mathbf{i}_i$  being the indicator vector for state  $i$ .

Backward probabilities represent the probability that the system started in state  $i$  at time 0, given that at step  $n$  is observed in a given *destination* state  $j$ :

$$\xi^{\mathcal{D}}(i, j, n) = Pr\{Y_0 = i \mid Y_n = j\} \quad (4)$$

If we now consider a measure vector  $\rho$  over a target set of states at step  $n$ , we can introduce the backward probability vector  $\xi^{\mathcal{D}}(\rho, n)$  that represents the backward probabilities conditioned by the target vector  $\rho$ :

$$\left[\xi^{\mathcal{D}}(\rho, n)\right](i) = \sum_{j \in \mathcal{S}} \rho(j) \cdot \xi^{\mathcal{D}}(i, j, n) \quad (5)$$

Vector  $\xi^{\mathcal{D}}(\rho, n)$  does not represent a probability distribution: indeed it does not sum to one, and each entry is an independent quantity. When  $\rho = \mathbf{i}_j$  then the vector  $\xi^{\mathcal{D}}(\rho, n)$  gives the probability of reaching the fixed state  $j$  in  $n$  steps from *each* possible initial state  $i$ . Equation (5) is governed by the *backward Chapman-Kolmogorov* equation:

$$\xi^{\mathcal{D}}(\rho, n) = \mathbf{P}^n \cdot \rho \quad (6)$$

and it is important to observe that forward and backward probabilities are tied together by the relation:

$$\pi^{\mathcal{D}}(\alpha, n) \cdot \rho = \alpha \cdot \xi^{\mathcal{D}}(\rho, n) \quad (7)$$

which can be easily proven since:  $(\alpha \cdot \mathbf{P}^n) \cdot \rho = \alpha \cdot (\mathbf{P}^n \cdot \rho)$ .

As usual, the stationary behavior is defined as:

$$\pi^{\mathcal{D}}(\alpha) = \lim_{n \rightarrow \infty} \pi^{\mathcal{D}}(\alpha, n) = \alpha \cdot \lim_{n \rightarrow \infty} \mathbf{P}^n \quad (8)$$

$$\xi^{\mathcal{D}}(\rho) = \lim_{n \rightarrow \infty} \xi^{\mathcal{D}}(\rho, n) = \lim_{n \rightarrow \infty} \mathbf{P}^n \cdot \rho \quad (9)$$

and again forward and backward are tied together by:

$$\pi^{\mathcal{D}}(\alpha) \cdot \rho = \alpha \cdot \xi^{\mathcal{D}}(\rho) \quad (10)$$

We recall that for irreducible DTMCs,  $\pi^{\mathcal{D}}(\alpha)$  always exists, it is unique and independent of  $\alpha$  ( $\pi^{\mathcal{D}}(\alpha) = \pi^{\mathcal{D}}(\alpha')$ ). It is less known instead that the vector  $\xi^{\mathcal{D}}(\rho)$  depends on  $\rho$  ( $\xi^{\mathcal{D}}(\rho) \neq \xi^{\mathcal{D}}(\rho')$ ), and that each entry of the vector has the same value  $\xi$  ( $\xi^{\mathcal{D}}(\rho)[k] = \xi^{\mathcal{D}}(\rho)[l]$ ) and  $\xi$  is uniquely dependent on  $\rho$ . Note that when  $\rho = \mathbf{i}_s$  then the value  $\xi$  is exactly  $\pi^{\mathcal{D}}(\alpha) \cdot \mathbf{i}_s$ , so computing the whole vector of steady state probabilities backward has an extra cost of  $|\mathcal{S}|$ .

## Reducible DTMCs.

When  $\mathcal{D}$  is reducible, its stochastic matrix  $\mathbf{P}$  can be reordered as an upper triangular block form (the *reducible normal form*):

$$\mathbf{P} = \begin{bmatrix} \mathbf{T} & \mathbf{F}_1 & \cdots & \mathbf{F}_m \\ 0 & \mathbf{R}_1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathbf{R}_m \end{bmatrix}$$

The state space  $\mathcal{S}$  is partitioned into the set of *transient* states  $\mathcal{S}_T$  and  $m$  sets of *recurrent* states  $\mathcal{S}_{R_i}$  (*recurrent classes*). The sub-matrix  $\mathbf{T}$  is the sub-stochastic DTMC of the *transient* states  $\mathcal{S}_T$ . Each rectangular sub-matrix  $\mathbf{F}_i$  is the probability matrix of going into the  $i$ -th recurrent class from  $\mathcal{S}_T$ . Each square sub-matrix  $\mathbf{R}_i$  is the DTMC of the  $i$ -th recurrent class.

We now derive the structure of  $\lim_{n \rightarrow \infty} \mathbf{P}^n$ , as in equations (8) and (9) when  $\mathbf{P}$  is

reducible. The powers of  $\mathbf{P}$  are:

$$\mathbf{P}^0 = \mathbf{I}, \quad \mathbf{P}^n = \begin{bmatrix} \mathbf{T}^n & \mathbf{\Lambda}_1(n) & \cdots & \mathbf{\Lambda}_m(n) \\ 0 & \mathbf{R}_1^n & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathbf{R}_m^n \end{bmatrix}$$

with  $\mathbf{\Lambda}_i(n) = \sum_{k=0}^{n-1} \mathbf{T}^k \mathbf{F}_i \mathbf{R}_i^{n-k-1}$  and  $\mathbf{\Lambda}_i(0) = 0$ .

The  $n$ -th power of  $\mathbf{P}$  reveals the well-known structure of a reducible process after  $n$  steps: the process stays for  $k$  steps ( $k \leq n$ ) in the transient class  $\mathcal{S}_T$ , then a single  $\mathbf{F}_i$  transition occurs and moves the process in the  $i$ -th recurrent class  $\mathcal{S}_{Ri}$ , after which the process remains in  $\mathcal{S}_{Ri}$  for the remaining  $(n-k-1)$  steps.

Transient forward and backward probabilities can then be rewritten from equations (3) and (6) using the expression for  $\mathbf{P}^k$  derived above; it is convenient to separate the part for the recurrent and transient states, to obtain:

$$\begin{aligned} \pi_T^{\mathcal{D}}(\alpha, n) &= \alpha_T \cdot \mathbf{T}^n \\ \pi_{Ri}^{\mathcal{D}}(\alpha, n) &= \alpha_T \cdot \mathbf{\Lambda}_i(n) + \alpha_{Ri} \cdot \mathbf{R}_i^n \\ \xi_T^{\mathcal{D}}(\rho, n) &= \sum_{i=1}^n (\mathbf{\Lambda}_i(n) \cdot \rho_{Ri}) + \mathbf{T}^n \cdot \rho_T \\ \xi_{Ri}^{\mathcal{D}}(\rho, n) &= \mathbf{R}_i^n \cdot \rho_{Ri} \end{aligned} \tag{11}$$

Let  $\mathbf{J} = \sum_{k=0}^{\infty} \mathbf{T}^k$  be a matrix whose entries  $\mathbf{J}(i, j)$  can be interpreted as the mean number of discrete steps from state  $i$  to state  $j$ , without leaving the transient set. Observe that since  $\mathbf{J} = \sum_{k=0}^{\infty} \mathbf{T}^k = (\mathbf{I} - \mathbf{T})^{-1}$ , then it is possible to compute any vector-matrix products with  $\mathbf{J}$  in (12) as the solutions of a linear equation system in  $(\mathbf{I} - \mathbf{T})$ , instead of computing a product with  $\mathbf{J}$  directly, i.e.:

$$\begin{aligned} \mathbf{x} &= \mathbf{b} \cdot \mathbf{J} \quad \Rightarrow \quad \text{solution of: } (\mathbf{I} - \mathbf{T}) \cdot \mathbf{x} = \mathbf{b} \\ \mathbf{x} &= \mathbf{J} \cdot \mathbf{b} \quad \Rightarrow \quad \text{solution of: } \mathbf{x} \cdot (\mathbf{I} - \mathbf{T}) = \mathbf{b} \end{aligned}$$

for any measure vector  $\mathbf{b}$  in the  $\mathbb{R}^{|\mathcal{S}|}$  space.

Considering that  $\lim_{n \rightarrow \infty} \mathbf{T}^n = 0$ , using the definition of  $\mathbf{J}$  we can rewrite the limiting behavior of  $\mathbf{P}^n$  as:

$$\lim_{n \rightarrow \infty} \mathbf{P}^n = \begin{bmatrix} 0 & \mathbf{J} \cdot \mathbf{F}_1 \cdot \lim_{n \rightarrow \infty} \mathbf{R}_1^n & \cdots & \mathbf{J} \cdot \mathbf{F}_m \cdot \lim_{n \rightarrow \infty} \mathbf{R}_m^n \\ 0 & \lim_{n \rightarrow \infty} \mathbf{R}_1^n & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lim_{n \rightarrow \infty} \mathbf{R}_m^n \end{bmatrix}$$

From which the limiting behaviors of (11) result in:

$$\begin{aligned}
 \pi_T^{\mathcal{D}}(\alpha) &= 0 \\
 \pi_{Ri}^{\mathcal{D}}(\alpha) &= (\alpha_T \cdot \mathbf{J} \cdot \mathbf{F}_i + \alpha_{Ri}) \cdot \lim_{n \rightarrow \infty} \mathbf{R}_i^n \\
 \xi_T^{\mathcal{D}}(\rho) &= \mathbf{J} \cdot \sum_{i=1}^m \left( \mathbf{F}_i \cdot \lim_{n \rightarrow \infty} \mathbf{R}_i^n \cdot \rho_{Ri} \right) \\
 \xi_{Ri}^{\mathcal{D}}(\rho) &= \lim_{n \rightarrow \infty} \mathbf{R}_i^n \cdot \rho_{Ri}
 \end{aligned} \tag{12}$$

Observe that therefore the vector  $\pi^{\mathcal{D}}(\alpha)$  is zero in every transient state (as expected since we do not find the system in a transient state in the long run). Moreover, given a recurrent class  $\mathcal{S}_{Ri}$ , since the vector  $\alpha_T \cdot \mathbf{J} \cdot \mathbf{F}_i$  can be interpreted as the probability of entering  $\mathcal{S}_{Ri}$  in the long run, from the set  $\mathcal{S}_T$ , then the probability of the elements of a recurrent classes  $\pi_{Ri}^{\mathcal{D}}(\alpha)$  are obtained by multiplying the steady state solution in isolation of each recurrent class ( $\lim_{n \rightarrow \infty} \mathbf{R}_i^n$ ) by a weighting vector.

For backward probabilities we can observe that  $\rho$  values associated to  $\mathcal{S}_T$  ( $\rho_T$ ) have no influence on the probability of neither the transient states ( $\xi_T^{\mathcal{D}}(\rho)$ ) nor for recurrent states ( $\xi_{Ri}^{\mathcal{D}}(\rho)$ ). This is indeed a consequence of the fact that a transient state cannot be encountered as a target on the long run. Moreover the steady state backward probability of a recurrent state can be computed on the recurrent class in isolation (all the quantities in the equation for  $\xi_{Ri}^{\mathcal{D}}(\rho)$  refer only to the recurrent class  $\mathcal{S}_{Ri}$ ). As explained before, all the states of the same recurrent class have the same value of backward probability. More interesting is the case of backward probability of transient states  $\xi_T^{\mathcal{D}}(\rho)$ , in which the probability of each recurrent class is “projected back” to the initial transient states through the multiplication with matrix  $\mathbf{F}_i$  (one step probability of reaching  $\mathcal{S}_{Ri}$  from  $\mathcal{S}_T$ ) and matrix  $\mathbf{J}$  (transient behavior).

The two relations (7) and (10) still hold for reducible Markov chains, which can be proven easily by expanding them with the terms of (12) and (11).

Note that when  $\rho$  is the indicator vector of a set of absorbing states then  $\xi^{\mathcal{D}}(\rho, n)$  is commonly known as “transient absorption probability” [17].

### 3 Forward and backward solution of CTMCs

Given a Continuous Time Markov Chain (CTMC)  $\mathcal{M} = \{X_t \mid t \in \mathbb{R}\}$ , with a finite state space  $\mathcal{S}$  and infinitesimal generator  $\mathbf{Q}$ , its evolution is governed by the forward/backward *Kolmogorov differential equations* [17, th. 2.3]. The probability of being in state  $j$  at time  $t$ , knowing that at time 0 the state was  $i$ , is denoted by:

$$\pi^{\mathcal{M}}(i, j, t) = Pr\{X_t = j \mid X_0 = i\} \tag{13}$$

or, in vector form:

$$\left[ \pi^{\mathcal{M}}(\alpha, t) \right](j) = \sum_{i \in \mathcal{S}} \alpha(i) \cdot \pi^{\mathcal{M}}(i, j, t) \tag{14}$$

with  $\alpha$  a probability distribution at time 0. Vector (14) is the solution of the forward Kolmogorov differential equation:

$$\frac{d\pi^{\mathcal{M}}(\alpha, t)}{dt} = \pi^{\mathcal{M}}(\alpha, t) \cdot \mathbf{Q} \quad (15)$$

with *entrance condition*  $\pi^{\mathcal{M}}(\alpha, 0) = \alpha$ . The solution of (15) for  $t \geq 0$  is:

$$\pi^{\mathcal{M}}(\alpha, t) = \alpha \cdot e^{\mathbf{Q}t} \quad (16)$$

Backward probability gives the probability that  $\mathcal{M}$  was in state  $i$  at time 0, given that at time  $t$  is observed in state  $j$ , is:

$$\xi^{\mathcal{M}}(i, j, t) = Pr\{X_0 = i \mid X_t = j\} \quad (17)$$

or, in vector form:

$$\left[ \xi^{\mathcal{M}}(\rho, v) \right] (i) = \sum_{j \in \mathcal{S}} \rho(j) \cdot \xi^{\mathcal{M}}(i, j, v) \quad (18)$$

with  $\rho$  a measure vector over the target states at time  $t$ . The resulting vector is the solution of the backward Kolmogorov differential equation:

$$\frac{d\xi^{\mathcal{M}}(\rho, t)}{dt} = \mathbf{Q} \cdot \xi^{\mathcal{M}}(\rho, t) \quad (19)$$

with *exit condition*  $\xi^{\mathcal{M}}(\rho, t) = \rho$ . Solution of (19) is:

$$\xi^{\mathcal{M}}(\rho, t) = e^{\mathbf{Q}t} \cdot \rho \quad (20)$$

Forward and backward formulas are tied by the relation:

$$\pi^{\mathcal{M}}(\alpha, t) \cdot \rho = \alpha \cdot \xi^{\mathcal{M}}(\rho, t) \quad (21)$$

which is equivalent to:  $(\alpha \cdot e^{\mathbf{Q}t}) \cdot \rho = \alpha \cdot (e^{\mathbf{Q}t} \cdot \rho)$ , and:

$$\pi^{\mathcal{M}}(\alpha) \cdot \rho = \alpha \cdot \xi^{\mathcal{M}}(\rho) \quad (22)$$

The computation of the transient measures (16) and (20) may be carried out in many ways [21]; the popular uniformization method can be used also for backward probabilities, leading to the two following Taylor series expansion of the solution of the first-order constant coefficients ODE of the Kolmogorov differential equations:

$$\begin{aligned} \pi^{\mathcal{M}}(\alpha, t) &= \alpha \cdot e^{\mathbf{Q}t} = \alpha \cdot \sum_{n=0}^{\infty} \left( \frac{e^{-qt}(qt)^n}{n!} \mathbf{U}^n \right) \\ \xi^{\mathcal{M}}(\rho, t) &= e^{\mathbf{Q}t} \cdot \rho = \sum_{n=0}^{\infty} \left( \frac{e^{-qt}(qt)^n}{n!} \mathbf{U}^n \right) \cdot \rho \end{aligned} \quad (23)$$

with  $q = -\max_{i \in \mathcal{S}} \mathbf{Q}(i, i)$  and  $\mathbf{U} = 1/q \mathbf{Q} + \mathbf{I}$  the *uniformized matrix* of  $\mathbf{Q}$ . As usual,  $\mathbf{U}$  is the stochastic matrix of the mean behavior after a time step of  $1/q$ .

With  $\pi^{\mathcal{M}}(\alpha)$  and  $\xi^{\mathcal{M}}(\rho)$  we denote the stationary forward and backward vectors of the CTMC. Many well-established algorithms exist for the computation of the limiting behavior of a CTMC.



## Reducible CTMCs.

When the Markov process  $\mathcal{M}$  is reducible, its infinitesimal generator  $\mathbf{Q}$  can be written in reducible normal form:

$$\mathbf{Q} = \begin{bmatrix} \mathbf{T} & \mathbf{F}_1 & \cdots & \mathbf{F}_m \\ 0 & \mathbf{R}_1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathbf{R}_m \end{bmatrix} \quad (24)$$

As for DTMCs, we derive the structure of  $\lim_{t \rightarrow \infty} e^{\mathbf{Q}t}$  to show how to derive transient and stationary (forward and backward) formulas. The powers of  $\mathbf{Q}$  are:

$$\mathbf{Q}^0 = \mathbf{I}, \quad \mathbf{Q}^n = \begin{bmatrix} \mathbf{T}^n & \mathbf{\Lambda}_1(n) & \cdots & \mathbf{\Lambda}_m(n) \\ 0 & \mathbf{R}_1^n & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathbf{R}_m^n \end{bmatrix}$$

with  $\mathbf{\Lambda}_i(n) = \sum_{k=0}^{n-1} \mathbf{T}^k \mathbf{F}_i \mathbf{R}_i^{n-k-1}$  and  $\mathbf{\Lambda}_i(0) = 0$ . The exponential of  $\mathbf{Q}t$  is then:

$$e^{\mathbf{Q}t} = \sum_{n=0}^{\infty} \frac{\mathbf{Q}^n t^n}{n!} = \begin{bmatrix} e^{\mathbf{T}t} \mathbf{\Theta}_1(t) \cdots \mathbf{\Theta}_m(t) \\ 0 & e^{\mathbf{R}_1 t} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & e^{\mathbf{R}_m t} \end{bmatrix}$$

with the term  $\mathbf{\Theta}_i(t)$  defined as:

$$\mathbf{\Theta}_i(t) = \sum_{n=0}^{\infty} \frac{\mathbf{\Lambda}_i(n) t^n}{n!} = \sum_{n=0}^{\infty} \sum_{k=0}^{n-1} \frac{\mathbf{T}^k \mathbf{F}_i \mathbf{R}_i^{n-k-1} t^n}{n!} = \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} \mathbf{T}^n \mathbf{F}_i \mathbf{R}_i^k \frac{t^{n+k+1}}{(n+k+1)!}$$

The last factor can be rewritten:

$$\frac{t^{n+k+1}}{(n+k+1)!} = \frac{1}{n! k!} \int_0^t x^n (t-x)^k dx$$

so that the term  $\mathbf{\Theta}_i(t)$  can be reformulated:

$$\begin{aligned} \mathbf{\Theta}_i(t) &= \sum_{n=0}^{\infty} \frac{\mathbf{T}^n}{n!} \cdot \mathbf{F}_i \cdot \left( \sum_{k=0}^{\infty} \frac{\mathbf{R}_i^k}{k!} \int_0^t x^n (t-x)^k dx \right) = \\ &= \int_0^t \left( \sum_{n=0}^{\infty} \frac{\mathbf{T}^n x^n}{n!} \right) \cdot \mathbf{F}_i \cdot \left( \sum_{k=0}^{\infty} \frac{\mathbf{R}_i^k (t-x)^k}{k!} \right) dx = \\ &= \int_0^t e^{\mathbf{T}x} \cdot \mathbf{F}_i \cdot e^{\mathbf{R}_i(t-x)} dx \end{aligned} \quad (25)$$

This last equation can be interpreted as follows: the process initially passes  $x$  time units in the transient class  $\mathcal{S}_T$ , then one  $\mathbf{F}_i$  transition occurs, after which the process spends the remaining time  $(t-x)$  in the  $i$ -th recurrent class.

Transient forward and backward equations for  $\mathcal{S}_T$  and  $\mathcal{S}_{Ri}$  state partitions can then be rewritten as:

$$\begin{aligned}\pi_T^{\mathcal{M}}(\alpha, t) &= \alpha_T \cdot e^{\mathbf{T}t} \\ \pi_{Ri}^{\mathcal{M}}(\alpha, t) &= \alpha_T \cdot \Theta_i(t) + \alpha_{Ri} \cdot e^{\mathbf{R}_i t} \\ \xi_T^{\mathcal{M}}(\rho, t) &= \sum_{i=1}^m (\Theta_i(t) \cdot \rho_{Ri}) + e^{\mathbf{T}t} \cdot \rho_T \\ \xi_{Ri}^{\mathcal{M}}(\rho, t) &= e^{\mathbf{R}_i t} \cdot \rho_{Ri}\end{aligned}\tag{26}$$

By defining the term:

$$\mathbf{W} = \int_0^\infty e^{\mathbf{T}x} dx \tag{27}$$

which is the expected sojourn time matrix in the transient states, it is possible to rewrite the limit of  $\Theta_i(t)$  by integration by parts:

$$\begin{aligned}\lim_{t \rightarrow \infty} \Theta_i(t) &= \int_0^\infty e^{\mathbf{T}x} dx \cdot \mathbf{F}_i \cdot \lim_{t \rightarrow \infty} e^{\mathbf{R}_i t} = \\ &= \mathbf{W} \cdot \mathbf{F}_i \cdot \lim_{t \rightarrow \infty} e^{\mathbf{R}_i t}\end{aligned}\tag{28}$$

The term  $\lim_{t \rightarrow \infty} e^{\mathbf{R}_i t}$  is the *stationary* stochastic matrix of the  $i$ -th recurrent class. The limiting behavior of a reducible Markov chain is therefore:

$$\lim_{t \rightarrow \infty} e^{\mathbf{Q}t} = \begin{bmatrix} 0 & \mathbf{W} \cdot \mathbf{F}_1 \cdot \lim_{t \rightarrow \infty} e^{\mathbf{R}_1 t} \cdots \mathbf{W} \cdot \mathbf{F}_m \cdot \lim_{t \rightarrow \infty} e^{\mathbf{R}_m t} \\ 0 & \lim_{t \rightarrow \infty} e^{\mathbf{R}_1 t} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lim_{t \rightarrow \infty} e^{\mathbf{R}_m t} \end{bmatrix}$$

Since  $\mathbf{T}$  has at least one row that has a negative rowsum, then the limiting behavior of  $\lim_{t \rightarrow \infty} e^{\mathbf{T}t}$  tends to 0. Therefore  $\lim_{t \rightarrow \infty} e^{\mathbf{Q}t}$  has the column of  $\mathcal{S}_T$  states zeroed, and the integral (27) is equivalent to:  $\mathbf{W} = -\mathbf{T}^{-1}$ , so that a product with  $\mathbf{W}$  can be computed as the solution of a linear system in  $\mathbf{T}$ .

Stationary expressions for  $\pi^{\mathcal{M}}(\alpha)$  and  $\xi^{\mathcal{M}}(\rho)$  are:

$$\begin{aligned}\pi_T^{\mathcal{M}}(\alpha) &= 0 \\ \pi_{Ri}^{\mathcal{M}}(\alpha) &= (\alpha_T \cdot \mathbf{W} \cdot \mathbf{F}_i + \alpha_{Ri}) \cdot \lim_{t \rightarrow \infty} e^{\mathbf{R}_i t} \\ \xi_T^{\mathcal{M}}(\rho) &= \mathbf{W} \cdot \sum_{i=1}^m (\mathbf{F}_i \cdot \lim_{t \rightarrow \infty} e^{\mathbf{R}_i t} \cdot \rho_{Ri}) \\ \xi_{Ri}^{\mathcal{M}}(\rho) &= \lim_{t \rightarrow \infty} e^{\mathbf{R}_i t} \cdot \rho_{Ri}\end{aligned}\tag{29}$$

and the considerations done for their discrete counterparts (12) hold also for (29).

## 4 Application to CSL model checking

We now show the role that backward and forward probabilities of CTMCs plays in the CSL model-checking of CTMCs. For the purpose of this paper we concentrate

on the key operator *Until*.

An Until formula of CSL has the form  $\mathcal{P}_{\bowtie\lambda}(\Phi \mathcal{U}^{[t,t']}\Psi)$ ; this formula is true for a state  $s$  of a CTMC  $\mathcal{M}$  if the probability of the set of paths of  $\mathcal{M}$  that starts in  $s$  ( $Paths^{\mathcal{M}}(s)$ ) and satisfies  $\Phi \mathcal{U}^{[t,t']}\Psi$  is  $\bowtie \lambda$ , where  $\bowtie \in \{<, \leq, \geq, >\}$  is a comparison operator. A timed path of  $\mathcal{M}$  satisfies  $\Phi \mathcal{U}^{[t,t']}\Psi$  if it is in a  $\Psi$ -state at time  $u \in [t, t']$ , and  $\forall u' \in [0, u)$  the path passes only through  $\Phi$ -states.

Model-checking of a formula  $\theta$  comes in two variations: given a state  $s$ , to determine if that state satisfies the formula  $\theta$  (written  $s \models \theta$ ), or to identify the set  $Sat(\theta) \subseteq \mathcal{S}$  of states that satisfy  $\theta$ .

Given a timed Until formula  $\varphi = (\Phi \mathcal{U}^{[t,t']}\Psi)$ , a state  $s$  satisfies the CSL formula  $\mathcal{P}_{\bowtie\lambda}(\varphi)$  if  $Prob^{\mathcal{M}}(s, \varphi) \bowtie \lambda$ , where  $Prob^{\mathcal{M}}(s, \varphi) = Pr\{\sigma \in Paths^{\mathcal{M}}(s) \mid \sigma \models \varphi\}$  is the probability measure of all paths  $\sigma$  that start in  $s$  and satisfy  $\varphi$ . Therefore the model checking of CSL Until formula for CTMC reduces to the computation of the probability of a set of paths starting from a given state.

In [8] the quantity  $Prob^{\mathcal{M}}(s, \varphi)$  was shown to be measurable, while [9] showed that the computation of  $Prob^{\mathcal{M}}(s, \varphi)$  can be done with a (transient/steady state) solution of at most two CTMCs, derived from the original model  $\mathcal{M}$  by making certain states absorbing.

Central to the solution method is the idea of *modified CTMC*, obtained through the *Sat*-based filtering operator  $\mathcal{M}[\Phi]$  for a certain CSL formula  $\Phi$ . The labeled CTMC  $\mathcal{M}[\Phi]$  is obtained by making absorbing all the states that satisfy  $\Phi$  in  $\mathcal{M}$ .

The formula for the *Sat*-set computation depends on the shape of the time interval  $I$  of  $\Phi \mathcal{U}^I \Psi$ . The interval  $I$  can be  $I = [0, t]$ ,  $I = [t, t]$ , or  $I = [t, t']$ , with  $0 < t < t'$ . We first review the computation based on the forward approach, since it is more intuitive, and then we move to backward.

The classical formulas of the Until given in [9] are forward formulas, and we can express them as:

$$\begin{aligned} Prob^{\mathcal{M}}(s, \Phi \mathcal{U}^{[0,t]}\Psi) &= \mathbf{i}_{\Psi} \cdot \pi^{\mathcal{M}[\neg\Phi \vee \Psi]}(\mathbf{i}_s, t) \\ Prob^{\mathcal{M}}(s, \Phi \mathcal{U}^{[t,t]}\Psi) &= \mathbf{i}_{\Phi \wedge \Psi} \cdot \pi^{\mathcal{M}[\neg\Phi]}(\mathbf{i}_s, t) \\ Prob^{\mathcal{M}}(s, \Phi \mathcal{U}^{[t,t']}\Psi) &= \mathbf{i}_{\Psi} \cdot \pi^{\mathcal{M}[\neg\Phi \vee \Psi]}(\mathbf{I}^{\Phi} \cdot \pi^{\mathcal{M}[\neg\Phi]}(\mathbf{i}_s, t), t' - t) \end{aligned}$$

The vectors  $\mathbf{i}_{\Psi}$ ,  $\mathbf{i}_{\Phi \wedge \Psi}$  and  $\mathbf{i}_s$  are 1 in the states of  $Sat(\Psi)$ ,  $Sat(\Phi \wedge \Psi)$  and  $\{s\}$ , respectively, and 0 in every other state. The  $\mathbf{I}^{\Phi}$  is the identity matrix where rows corresponding to states that do not satisfy  $\Phi$  are set to zero.

The intuition behind is simple. The probability  $Prob^{\mathcal{M}}(s, \Phi \mathcal{U}^{[0,t]}\Psi)$  is computed as the probability of being, at time  $t$ , in any  $\Psi$ -state on the modified CTMC  $\mathcal{M}[\neg\Phi \vee \Psi]$ . In the modified chain the  $\Psi$  states are absorbing, so even if a  $\Psi$  state is reached before  $t$ , the chain will still be in that state at time  $t$ , the time horizon for the transient probability computation. Similarly, if a  $\neg\Phi$ -state  $s'$  is encountered before a  $\Psi$  state is reached, the modified chain stays trapped in  $s'$ , and that path will not be counted (unless  $s'$  is also a  $\Psi$ -state). Note the use of the inner product with  $\mathbf{i}_{\Psi}$  to sum over all possible  $\Psi$  states, and that the computation of the transient probability assumes the modified chain is in state  $s$  at time 0 (initial vector  $\mathbf{i}_s$ ). The more complicated case of  $I = [t, t']$  requires the path to stay in  $\Phi$ -states during

the time interval  $[0, t]$ , and then to behave as a path that satisfies  $\Phi \mathcal{U}^{[0, (t'-t)]} \Psi$ . This requires the transient solution of two modified CTMCs: at time  $t$ , assuming we start in  $s$  at time 0, for the chain  $\pi^{\mathcal{M}[\neg\Phi]}$  and at time  $t' - t$ , assuming we start at time 0 with a probability vector which is the result of the previous computation, for the chain  $\pi^{\mathcal{M}[\neg\Phi \vee \Psi]}$ . Note that the result of the first computation is filtered out using the  $\mathbf{I}^\Phi$  vector, to put to zero the probability of all states which are not  $\Phi$  states: as a consequence the second transient analysis starts from an initial vector that does not necessarily sum up to one.

To check if a formula  $\varphi$  is true for a (single) given state  $s$ , can be particularly inefficient in case of nested formulas: to verify that  $s$  satisfies the nested formula:  $\mathcal{P}_{\bowtie \lambda_1}(\mathcal{X}(\mathcal{P}_{\bowtie \lambda_2}(\Phi \mathcal{U} \Psi)))$  requires the computation of the *Sat*-set of the inner formula ( $\mathcal{P}_{\bowtie \lambda_2}(\Phi \mathcal{U} \Psi)$ ) for *each state*  $s' \in S$ , which leads to a multiplicative factor of  $|S|$  in the time complexity. The work in [15] shows that it is actually possible to compute in a single step the whole *Sat*-set for a  $\mathcal{U}$  formula, using a different computational scheme, derived from the one already used for PCTL that starts from the goal states and goes back to the initial ones.

Starting from the observation that the solution in [15] is actually a case of backward probability computation, we can write the formulas in terms of the backward operator  $\xi^{\mathcal{M}}(\rho, v)$  and prove that forward/backward formulas are equivalent.

Using backward probabilities it is indeed possible to compute at the same time the vector of probabilities  $\underline{Prob}^{\mathcal{M}}(\Phi \mathcal{U}^{[t, t']} \Psi)$ , which allows to identify the probability of all the elements in the whole *Sat* set. We can then formalize the solution proposed in [15] by writing three equations in vector form for the three cases of the Until, based on the backward equation (17):

$$\begin{aligned} \underline{Prob}^{\mathcal{M}}(\Phi \mathcal{U}^{[0, t]} \Psi) &= \xi^{\mathcal{M}[\neg\Phi \vee \Psi]}(\mathbf{i}_\Psi, t) \\ \underline{Prob}^{\mathcal{M}}(\Phi \mathcal{U}^{[t, t]} \Psi) &= \xi^{\mathcal{M}[\neg\Phi]}(\mathbf{i}_{\Phi \wedge \Psi}, t) \\ \underline{Prob}^{\mathcal{M}}(\Phi \mathcal{U}^{[t, t']} \Psi) &= \xi^{\mathcal{M}[\neg\Phi]}(\mathbf{I}^\Phi \cdot \xi^{\mathcal{M}[\neg\Phi \vee \Psi]}(\mathbf{i}_\Psi, t' - t), t) \end{aligned}$$

The  $\underline{Prob}$  formulas based on the backward  $\xi^{\mathcal{M}}(\rho, v)$  probabilities are specular to the ones based on the forward  $\pi^{\mathcal{M}}(\alpha, t)$  ones: the interval Until case is still computed in two steps, but the order in which the two modified chains are solved is reversed in the backward approach.

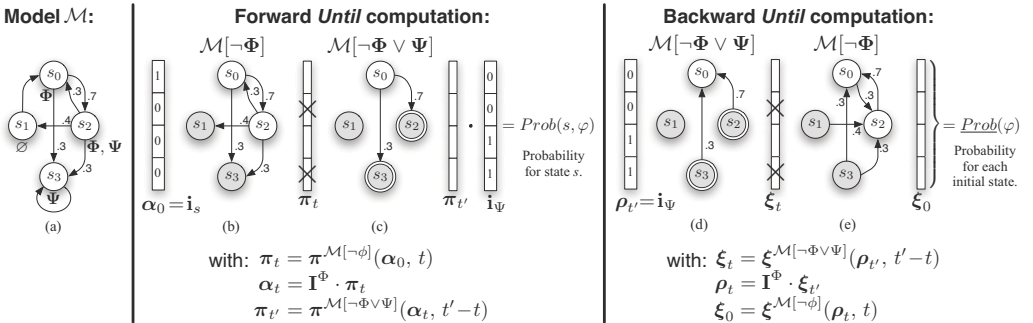


Figure 1. Numerical analysis of the CSL formula  $\varphi = \Phi \mathcal{U}^{[t, t']} \Psi$  on a simple model.

To better explain the relationship between the backward and forward approach, Figure 1 illustrates the numerical analysis based on the  $\pi^M$  and  $\xi^M$  approaches for the until formula  $\varphi = \Phi \mathcal{U}^{[t,t']} \Psi$ . The initial CTMC is shown on the left (a). The central portion of Figure 1 illustrates the forward computation of  $Prob(s, \varphi)$  for an initial state  $s$ : a transient analysis at time  $t$  on the modified CTMC  $\mathcal{M}[\neg\Phi]$  is done (b), then the probability of being in  $(\neg\Phi)$ -states is set to zero and the resulting vector is used as the initial distribution for the transient analysis (c) at time  $t' - t$  of the chain  $\mathcal{M}[\neg\Phi \vee \Psi]$ . The computed probability is then summed-up over all  $\Psi$  states by the cross product with  $\mathbf{i}_\Psi$ . Looking along the time axis we can observe that the use of the behavior at time  $t$  as initial vector for the transient solution at time  $t' - t$  leads to the computation of the behavior of the system at time  $t'$ , and to the consequent choice of calling  $\pi_{t'}$  the vector resulting from the solution of (c). The right portion of Figure 1 illustrates the computation of the entire  $Prob(\varphi)$  vector at once with the backward formula. The model checker starts by computing the backward probabilities for time  $t' - t$  on the goal vector  $\mathbf{i}_\Psi$ , considered as the state at time  $t'$ , in the modified CTMC  $\mathcal{M}[\neg\Phi \vee \Psi]$  (d). In the resulting vector  $\xi_t$  the  $\neg\Phi$  states are zeroed, to produce the measure vector  $\rho_t$ . Finally a backward probability analysis at time  $t$  is carried out on  $\mathcal{M}[\neg\Phi]$  (e), using  $\rho_t$  as exit condition, leading to a vector  $\xi_0$ . The set of states that satisfies the formula is then built by taking all states whose corresponding entry in  $\xi_0$  is  $\bowtie \lambda$ . It is then easy to link the forward and backward model checking through the following theorem

**Theorem 4.1** *Forward and backward computations of the probability of paths satisfying  $\mathcal{P}_{\bowtie\lambda}(\Phi \mathcal{U}^{[t,t']} \Psi)$ , for a given initial state  $s$ , lead to the same result.*

**Proof** To prove this theorem, it is sufficient to reformulate each  $Prob$  formula with the relation of (21), which connect forward and backward probabilities:

$$\begin{aligned}
 Prob^M(s, \Phi \mathcal{U}^{[0,t]} \Psi) &= \mathbf{i}_\Psi \cdot \pi^M[\neg\Phi \vee \Psi](\mathbf{i}_s, t) = \xi^M[\neg\Phi \vee \Psi](\mathbf{i}_\Psi, t) \cdot \mathbf{i}_s = \\
 &= \underline{Prob}^M(\Phi \mathcal{U}^{[0,t]} \Psi) \cdot \mathbf{i}_s \\
 Prob^M(s, \Phi \mathcal{U}^{[t,t]} \Psi) &= \mathbf{i}_{\Phi \wedge \Psi} \cdot \pi^M[\neg\Phi](\mathbf{i}_s, t) = \xi^M[\neg\Phi](\mathbf{i}_{\Phi \wedge \Psi}, t) \cdot \mathbf{i}_s = \\
 &= \underline{Prob}^M(\Phi \mathcal{U}^{[t,t]} \Psi) \cdot \mathbf{i}_s \\
 Prob^M(s, \Phi \mathcal{U}^{[t,t']} \Psi) &= \mathbf{i}_\Psi \cdot \pi^M[\neg\Phi \vee \Psi](\mathbf{I}^\Phi \cdot \pi^M[\neg\Phi](\mathbf{i}_s, t), t' - t) = \\
 &= \pi^M[\neg\Phi](\mathbf{i}_s, t) \cdot (\mathbf{I}^\Phi \cdot \xi^M[\neg\Phi \vee \Psi](\mathbf{i}_\Psi, t' - t)) = \\
 &= \xi^M[\neg\Phi](\mathbf{I}^\Phi \cdot \xi^M[\neg\Phi \vee \Psi](\mathbf{i}_\Psi, t' - t), t) \cdot \mathbf{i}_s = \\
 &= \underline{Prob}^M(\Phi \mathcal{U}^{[t,t']} \Psi) \cdot \mathbf{i}_s
 \end{aligned}$$

which proves the relation for each initial state  $s$ . □

## 5 Forward and backward solution of MRPs

We now consider the forward and backward stationary analysis for *Markov Regenerative Processes* (MRP). MRPs are stochastic processes where firing times can have a *general* distribution (*general events*). Events with an exponentially distributed firing times are called *exponential events*. A *renewal time* is a point in time where the value of every random variable  $g$  that accounts for the age of the (enabled) gen-

eral events are zero. States of the process encountered at renewal times are called *regeneration points*. When general events are restricted to be enabled at most one per state, the stochastic process is a *Markov Regenerative Process*, which can be described upon a *Markov Renewal Sequence* (MRS).

**Definition 5.1 [Markov renewal sequence]** Let  $\mathcal{S}$  be a finite discrete state space of the MRP. A sequence of bivariate random variables  $\{\langle Y_n, T_n \rangle \mid n \in \mathbb{N}\}$  is called a *Markov renewal sequence with regeneration points*  $Y_n \in \mathcal{S}$  encountered at *renewal times*  $T_n \in \mathbb{R}_{\geq 0}$  iff:

- $0 = T_0 < T_1 < T_2 < \dots$
- $Pr\{Y_{n+1}=j, T_{n+1}-T_n \leq t \mid Y_n=i, T_n \dots Y_0, T_0\} = Pr\{Y_1=j, T_1 \leq t \mid Y_0=i\}$

The process  $Y_n$  is a DTMC, called the *embedded Markov chain* (EMC).

**Definition 5.2 [Markov regenerative process]** A stochastic process  $\mathcal{R} = \{X_t \mid t \geq 0\}$  is a *Markov regenerative process* if there exists an MRS  $\{\langle Y_n, T_n \rangle \mid n \in \mathbb{N}\}$  such that all the conditional finite dimensional distributions of  $\{X_{T_n+t} \mid t \geq 0\}$  given  $\{X_u \mid 0 \leq u \leq T_n, Y_n = i\}$  are the same of  $\{X_t \mid t \geq 0\}$  given  $Y_0 = i$ , so that:

$$Pr\{X_{T_n+t} = j \mid X_u, 0 \leq u \leq T_n, Y_n = i\} = Pr\{X_t = j \mid X_0 = i\}$$

The process behavior  $\{X_t \mid T_n \leq t < T_{n+1}\}$  between two regeneration points  $Y_n$  and  $Y_{n+1}$  is described by a continuous time process, called the *subordinated process* of  $Y_n$ , that we assume to be a CTMC.

We use the notation of [12]. Let  $G$  be the set of random variables that describe the ages of the general events. Given  $g \in G$ , we denote with  $F^g(x)$  the *firing time distribution*, and with  $f^g(x)$  the *density function* of  $g$ .

The set  $\mathcal{S}^E \subseteq \mathcal{S}$  is the *exponential state subset*, where no general event is enabled;  $\mathcal{S}^g$  is the set of states where  $g$  is enabled, and  $\mathcal{S}^G \equiv \bigcup_{g \in G} \mathcal{S}^g$  is the *general state subset*. State transitions are classified into three *kinds*:

- (i) Transition due to a general event completion (*firing*).
- (ii) Exponential event whose firing has no effect on the age of the enabled general transition (*non-preemptive*).
- (iii) Exponential event whose firing resets the age of the currently enabled general transition (*preemptive*).

Events of the first and of the third type may only happen in a general state  $i \in \mathcal{S}^G$ . The next state  $j$  depends on the current state  $i$  and on the age of the currently enabled general event  $g$  (if any), but not on the past history. We assume a *preemptive repeat different* policy for general events.

A sample dynamic of an MRP is depicted in Figure 2.

In Figure 2 the MRP process  $X_t$  passes through various states: from state  $x_1$  to state  $x_4$  a general event  $g$  is enabled, and this enabling ends with the firing event of  $g$  (denoted with a  $\delta$  arc). The same happens from state  $x_4$  to  $x_6$ , where the enabling of  $g$  ends due to an exponential event that disables  $g$  (denoted with a  $\bar{q}$  arc). The age of  $g$  is not 0 in states  $x_2$ ,  $x_3$  and  $x_5$ , therefore these states are not regeneration points, and do not appear in the embedded process  $Y_n$ .

An MRP can be described [12] by 3 matrices  $\mathbf{Q}$ ,  $\bar{\mathbf{Q}}$  and  $\Delta$ :

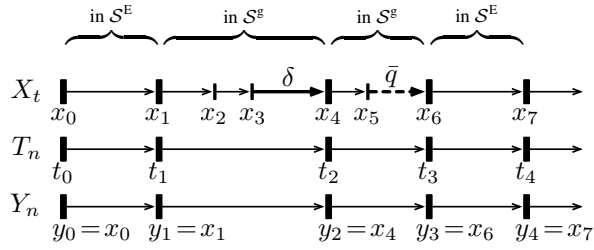


Figure 2. Sample MRP dynamic.

- $\mathbf{Q}(i, j)$ ,  $i \neq j$ : non-preemptive exponential events rate from state  $i$  to state  $j$ ;
- $\bar{\mathbf{Q}}(i, j)$ ,  $i \in \mathcal{S}^g$ : preemptive exponential events rate from state  $i$  to state  $j$  that disables  $g$  enabled in  $i$ ;
- $\mathbf{Q}(i, i)$  is the negative sum of all the rates of exponential events leaving state  $i$ ;
- $\Delta(i, j)$ ,  $i \in \mathcal{S}^g$ : probability that the firing of  $g$  in state  $i$  leads to state  $j$ .

Observe that  $\bar{\mathbf{Q}}(i, i)$  can indeed be non-zero as well (a self-loop with preemption). The diagonal of  $\mathbf{Q}$  accounts for the rates of both  $\mathbf{Q}$  and  $\bar{\mathbf{Q}}$ . Rows of  $\bar{\mathbf{Q}}$  and  $\Delta$  corresponding to exponential states are zero.

MRP formulas are simpler with the help of a *filtering* notation. Let  $\mathcal{S}^U \subseteq \mathcal{S}$  be a subset of  $\mathcal{S}$ , and let  $\mathbf{A}$  be a matrix. With  $\mathbf{A}^U$  we denote the *filtered matrix* where all rows which do not correspond to  $\mathcal{S}^U$  states are zeroed. For instance,  $\mathbf{I}^G$ ,  $\bar{\mathbf{Q}}^g$  and  $\mathbf{Q}^E$  are all filtered matrices w.r.t. the general and the exponential subsets of  $\mathcal{S}$ .

The time evolution of the EMC follows all the regeneration points, and the evolution from one regeneration point  $Y_n$  to the next is given by subordinated CTMCs (one CTMC per regeneration point) of state  $Y_n$ .

Following [12], let  $\Omega^g$  be the *state probability matrix in the instant before  $g$  fires*, defined for a subset  $\mathcal{S}^g$  as:

$$\Omega^g(i, j) \equiv \Pr\{X_{T_1^-} = j \mid Y_0 = i, i \in \mathcal{S}^g\} = \mathbf{I}^g \int_0^\infty e^{\mathbf{Q}^g x} \cdot f^g(x) dx \quad (30)$$

Let  $\Psi^g$  be the *conditional expected sojourn time matrix* in the states of  $X_t$  from the enabling of  $g$  to the firing, defined for a subset  $\mathcal{S}^g$  as:

$$\begin{aligned} \Psi^g(i, j) &\equiv E[\text{sojourn time of } X \text{ in } j, \mid Y_0 = i, i \in \mathcal{S}^g] = \\ &= \int_0^{T_1} \Pr\{X(\tau) = j \mid Y_0 = i, i \in \mathcal{S}^g\} d\tau \\ &= \mathbf{I}^g \int_0^\infty e^{\mathbf{Q}^g x} \cdot (1 - F^g(x)) dx \end{aligned} \quad (31)$$

We use the shorthand notations  $\Omega = \sum_{g \in G} \Omega^g$  and  $\Psi = \sum_{g \in G} \Psi^g$  to denote the summations for each general event (30) and (31). Let  $\text{diag}^{-1}(\mathbf{Q}^E)$  be the diagonal matrix where the diagonal entry of each exponential state  $i \in \mathcal{S}^E$  is  $\mathbf{Q}(i, i)^{-1}$ , and 0 in every other entry. The stochastic matrix  $\mathbf{P}$  of the EMC is then [12]:

$$\mathbf{P} = \mathbf{I}^E - \text{diag}^{-1}(\mathbf{Q}^E) \mathbf{Q}^E + \Omega \Delta + \Psi \bar{\mathbf{Q}} \quad (32)$$

along with its conversion factors matrix  $\mathbf{C}$ :

$$\mathbf{C} = -\text{diag}^{-1}(\mathbf{Q}^E) + \Psi \quad (33)$$

such that  $\mathbf{C}(i, j) = E[\text{sojourn time of } X \text{ in state } j \mid Y_0 = i]$ . The conversion factors matrix is used to convert a state probability vector from discrete-time to continuous-time. Therefore if  $\boldsymbol{\pi}^{\mathcal{D}}(\boldsymbol{\alpha})$  and  $\boldsymbol{\xi}^{\mathcal{D}}(\boldsymbol{\rho})$  are the forward and backward stationary solution of the EMC, then the stationary solutions of the MRP process  $\mathcal{R}$  at any time instant ( $\boldsymbol{\pi}^{\mathcal{R}}(\boldsymbol{\alpha})$  and  $\boldsymbol{\xi}^{\mathcal{R}}(\boldsymbol{\rho})$ ) can be obtained by multiplying  $\boldsymbol{\pi}^{\mathcal{D}}(\boldsymbol{\alpha})$  and  $\boldsymbol{\xi}^{\mathcal{D}}(\boldsymbol{\rho})$  with the conversion factors matrix  $\mathbf{C}$  (with a proper normalization).

## 6 Forward and backward MRP iterative solutions with matrix-free products

Using  $\mathbf{P}$  explicitly may not be feasible since the matrices defined by equations (32) and (33) tend to have dense portions, that make its storage impractical for large systems even when  $\mathbf{Q}$ ,  $\bar{\mathbf{Q}}$  and  $\Delta$  are sparse matrices. This happens because  $\Omega$  and  $\Psi$  contain a matrix exponential, which generates the transitive closure of  $\mathbf{Q}^G$ . This is the well-known problem of *fill-in*, which has been studied in [20] and [13]. The solution in [13] consists in avoiding entirely the computation and the storage of  $\mathbf{P}$  and  $\mathbf{C}$ : every time a vector-matrix product is needed with these two matrices, it can be computed by expanding the expressions of (32) and (33).

Given the product:  $\mathbf{y} = \mathbf{xP}$ , it can be rewritten as:

$$\begin{aligned} \mathbf{y} &= \mathbf{x}(\mathbf{I}^E - \text{diag}^{-1}(\mathbf{Q}^E)\mathbf{Q}^E + \Omega\Delta + \Psi\bar{\mathbf{Q}}) = \\ &= \mathbf{x}(\mathbf{I}^E - \text{diag}^{-1}(\mathbf{Q}^E)\mathbf{Q}^E) + (\mathbf{x}\Omega)\Delta + (\mathbf{x}\Psi)\bar{\mathbf{Q}} \end{aligned} \quad (34)$$

A product:  $\mathbf{y} = \mathbf{Px}$ , can instead be written as:

$$\begin{aligned} \mathbf{y} &= (\mathbf{I}^E - \text{diag}^{-1}(\mathbf{Q}^E)\mathbf{Q}^E + \Omega\Delta + \Psi\bar{\mathbf{Q}})\mathbf{x} = \\ &= (\mathbf{I}^E - \text{diag}^{-1}(\mathbf{Q}^E)\mathbf{Q}^E)\mathbf{x} + \Omega(\Delta\mathbf{x}) + \Psi(\bar{\mathbf{Q}}\mathbf{x}) \end{aligned} \quad (35)$$

The four terms  $(\mathbf{x}\Omega)$ ,  $(\mathbf{x}\Psi)$ ,  $(\Omega\mathbf{x})$  and  $(\Psi\mathbf{x})$  of (34) and (35) are vector by matrix products that can be rewritten by expanding the matrix exponentials  $\Omega$  and  $\Psi$  with their Taylor series expansions, resulting in the *Jensen's formulas* [24] for transient and cumulative transient probabilities under the time distribution of  $g$ . Jensen's formulas require only left and right vector multiplications with  $\mathbf{Q}^g$ .

The terms  $(\mathbf{x}\Omega)$  and  $(\mathbf{x}\Psi)$  can be expanded as:

$$\mathbf{x}\Omega = \sum_{g \in G} \mathbf{I}^g \int_0^\infty \mathbf{x} \cdot e^{\mathbf{Q}^g x} \cdot f^g(x) dx \quad (36)$$

$$\mathbf{x}\Psi = \sum_{g \in G} \mathbf{I}^g \int_0^\infty \mathbf{x} \cdot e^{\mathbf{Q}^g x} \cdot (1 - F^g(x)) dx \quad (37)$$

A complete expansion of these equations can be found in [13]. The other two products  $(\Omega\mathbf{x})$  and  $(\Psi\mathbf{x})$  needed for backward formulas are as (36) and (37), with  $\mathbf{x}$  on the right side of the exponential.

Forward stationary behavior of an irreducible EMC requires the fixed point solution of the linear equation system  $\boldsymbol{\pi}^{\mathcal{R}}(\boldsymbol{\alpha}) = \boldsymbol{\pi}^{\mathcal{D}}(\boldsymbol{\alpha}) \cdot \mathbf{P}$ . For instance, the iterative *power method* [22] algorithm uses only vector-matrix products with  $\mathbf{P}$ , so



the steady-state solution can be computed with (34) or (35), avoiding the *fill-in* of  $\mathbf{P}$ . Also Krylov-subspace methods uses only vector-matrix products, so they are suitable for a *matrix-free* solution of MRPs (as in [7]).

### Reducible MRPs.

When the MRP is reducible, the EMC matrix  $\mathbf{P}$  can be written in reducible normal form, derivable from a structural analysis of  $\mathbf{Q} + \bar{\mathbf{Q}} + \Delta$  (as shown in [12, p. 237]). Also in this case it is very important to avoid the explicit construction of  $\mathbf{P}$ . In [7] the matrix-free products with the sub-matrices  $\mathbf{T}$ ,  $\mathbf{F}_i$  and  $\mathbf{R}_i$  of  $\mathbf{P}$  were derived, as required by the equations in (12). In short, the products  $(\mathbf{x}_T \mathbf{T})$  and  $(\mathbf{T} \mathbf{x}_T)$  are easily done by restricting the MRP to the  $\mathcal{S}_T$  states, i.e. by using  $\mathbf{Q}_T$ ,  $\bar{\mathbf{Q}}_T$  and  $\Delta_T$ . The same applies for  $(\mathbf{x}_{R_i} \mathbf{R}_i)$  and  $(\mathbf{R}_i \mathbf{x}_{R_i})$  using  $\mathbf{Q}_{R_i}$ ,  $\bar{\mathbf{Q}}_{R_i}$  and  $\Delta_{R_i}$ . It has been shown [7, sec. 5] that the product  $\mathbf{x}_T \mathbf{F}_i$  can be computed from:

$$\begin{bmatrix} \mathbf{x}_T & 0 \end{bmatrix} \cdot \begin{bmatrix} \mathbf{T} & \mathbf{F}_i \\ 0 & \mathbf{R}_i \end{bmatrix} = \begin{bmatrix} \mathbf{x}_T \mathbf{T} \\ \mathbf{x}_T \mathbf{F}_i \end{bmatrix}$$

using the subset  $\mathcal{S}_T \cup \mathcal{S}_{R_i}$ . A similar schema can be derived for the transposed product  $(\mathbf{F}_i \mathbf{x}_T)$ . Since these products with the sub-matrices of an MRP can be done just by isolating the corresponding blocks in the generator matrices  $\mathbf{Q}$ ,  $\bar{\mathbf{Q}}$  and  $\Delta$ , then forward and backward solutions can be computed avoiding the *fill-in* even when the EMC is reducible.

## 7 Application to CSL<sup>TA</sup> model checking

CSL<sup>TA</sup> [11] is a stochastic logic which extends CSL by allowing a richer definition of paths, described as the accepted and rejected paths of a (timed) automaton that reads the language of CTMC paths. The CSL<sup>TA</sup> probabilistic path formula is written as  $\mathcal{P}_{\bowtie \lambda}(\mathcal{A})$ , where  $\mathcal{A}$  is a *single-clock Deterministic Timed Automaton* (DTA). A state  $s$  of a CTMC satisfies a formula  $\mathcal{P}_{\bowtie \lambda}(\mathcal{A})$  if the probability of the set of paths accepted by the DTA  $\mathcal{A}$  is  $\bowtie \lambda$ .

CSL<sup>TA</sup> is a superset of CSL, since it is possible to express the neXt and the Until with two appropriate DTAs. The model checking of  $\varphi = \mathcal{P}_{\bowtie \lambda}(\mathcal{A})$  over a CTMC  $\mathcal{M}$  is done as follows ([11, sec. III]). A new process  $\mathcal{M} \times \mathcal{A}$  is constructed as the “synchronized product” of the CTMC  $\mathcal{M}$  with the DTA  $\mathcal{A}$ . This process  $\mathcal{M} \times \mathcal{A}$  is an MRP that has a large initial transient and  $m \geq 2$  recurrent classes, of which two special absorbing classes  $\mathcal{S}_\top$  and  $\mathcal{S}_\perp$  are identified. The reducible normal form of the EMC  $\mathbf{P}$  is therefore:

$$\mathbf{P} = \left[ \begin{array}{c|cc} \overbrace{\mathbf{T}}^{\mathcal{S}_T} & \overbrace{\mathbf{F}_1}^{\mathcal{S}_{R_1}} & \dots & \overbrace{\mathbf{F}_{m-2}}^{\mathcal{S}_{R(m-2)}} & \overbrace{\mathbf{F}_\top}^{\mathcal{S}_\top} & \overbrace{\mathbf{F}_\perp}^{\mathcal{S}_\perp} \\ & \mathbf{R}_1 & & & & \\ & & \ddots & & & \\ & & & \mathbf{R}_{m-2} & & \\ \hline & & & & 1 & \\ & & & & & 1 \end{array} \right]$$

The absorbing state in  $\mathcal{S}_\top$  is the  $\top$ -state, i.e. the state that is reached by  $\mathcal{A}$  when the CTMC path is accepted. The computation of the *Sat* set of the CSL<sup>TA</sup> formula  $\varphi = \mathcal{P}_{\bowtie\lambda}(\mathcal{A})$  for an initial state  $s$  is equivalent to the problem of finding the steady state probability of being in the  $\top$  state of the EMC of the process  $\mathcal{M} \times \mathcal{A}$ , starting with  $\alpha = \mathbf{i}_s$ . Observe that  $\top$  is a *regeneration point* of the  $\mathcal{M} \times \mathcal{A}$  MRP, so it appears in the renewal sequence  $Y_n$ , and therefore is an EMC state.

The forward probability measure is given by:

$$Prob^{\mathcal{M} \times \mathcal{A}}(s) = \mathbf{i}_\top \cdot \boldsymbol{\pi}^{\mathcal{M} \times \mathcal{A}}(\mathbf{i}_s) \quad (38)$$

where  $\mathbf{i}_\top$  is 1 in  $\top$ , and 0 otherwise. Since the only interesting value is the  $\top$  probability, we can rewrite (38) by expanding (12) with the matrix structure of  $\mathbf{P}$ :

$$Prob^{\mathcal{M} \times \mathcal{A}}(s) = \mathbf{i}_s \cdot (\mathbf{I} - \mathbf{T})^{-1} \cdot \mathbf{F}_\top \cdot \mathbf{1} \quad (39)$$

where  $\mathbf{1}$  is a single element vector with value 1, and  $\mathbf{F}_\top$  is the single-step transition to  $\top$ . The backward case for CSL<sup>TA</sup> is more interesting: the backward probability vector is defined as:

$$\underline{Prob}^{\mathcal{M} \times \mathcal{A}} = \boldsymbol{\xi}^{\mathcal{M} \times \mathcal{A}}(\mathbf{i}_\top) \quad (40)$$

with  $\boldsymbol{\rho} = \mathbf{i}_\top$ . Therefore the backward probability  $\boldsymbol{\xi}_{\text{Ri}}^{\mathcal{M} \times \mathcal{A}}(\boldsymbol{\rho})$  is 1 in  $\mathcal{S}_\top$  and 0 in every other recurrent class. The values of  $\boldsymbol{\xi}_\top^{\mathcal{M} \times \mathcal{A}}(\boldsymbol{\rho})$  are less trivial: we can simplify (40) by expanding (12) with the DTMC structure of  $\mathcal{M} \times \mathcal{A}$  and obtain:

$$\underline{Prob}_\top^{\mathcal{M} \times \mathcal{A}} = (\mathbf{I} - \mathbf{T})^{-1} \cdot \mathbf{F}_\top \cdot \mathbf{1} \quad (41)$$

which is simply the solution of the linear equations system:

$$(\mathbf{I} - \mathbf{T}) \cdot \underline{Prob}_\top^{\mathcal{M} \times \mathcal{A}} = \mathbf{b} \quad (42)$$

with  $\mathbf{b} = \mathbf{F}_\top \cdot \mathbf{1}$ . Hence, the backward computation of the CSL<sup>TA</sup> formula  $\varphi$  reduces to the solution of (42). The two equations (38) and (40) are easily proven to be equivalent, since:  $\mathbf{i}_\top \cdot \boldsymbol{\pi}^{\mathcal{M} \times \mathcal{A}}(\mathbf{i}_s) = \boldsymbol{\xi}^{\mathcal{M} \times \mathcal{A}}(\mathbf{i}_\top) \cdot \mathbf{i}_s$  by relation (22), which is similar to theorem 4.1 for CSL. Observe also that (39), (41) and (42) are computable with a *fill-in* avoidance strategy for reducible MRPs.

## 8 Conclusions

In this paper we have discussed the computation and the possible applications of backward probabilities of Markov chains and Markov regenerative processes. All the equations and the outlined solution methods presented in this paper are available as concrete implementations, with accessible source code, at <http://www.di.unito.it/~amparore/DSPN.tgz>, and are currently under integration in the existing (forward) CSL<sup>TA</sup> model checker MC4CSL<sup>TA</sup> [6], and in the DSPN solver DSPN-tool[5].

For CSL model checking the definition of backward probability provides a probabilistic formalization of the CSL model-checking algorithm given in [15], which is the basis for current CSL tools. It is known to be  $|\mathcal{S}|$  times faster than a classical forward approach when nested formulas have to be evaluated, or when the whole *Sat* set is the goal. The probabilistic formalization also allows a clear understanding

of the dualism between forward and backward solutions of reducible CTMCs, which explain why a two-steps procedure it is not required by CSL model checkers, even if typically they need to solve non-ergodic CTMCs.

For MRPs we have shown that they can be solved backward with a matrix-free approach, and we are currently investigating whether the backward approach can be applied together with the decomposition-based solution of reducible MRPs proposed in [4]. This will pave the way for an efficient model-checking of  $CSL^{TA}$ .

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