Lumpability for Uncertain Continuous-Time Markov Chains

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Abstract

A continuous-time Markov chain (CTMC) is typically characterized by a number of parameters that describe main activities such as service times in a queuing network and kinetic rates of a reaction. It is widely accepted that the assumption of perfect knowledge of such parameters is undermined when confronted with reality, where they may be uncertain due to lack of knowledge or because of measurement noise. In this paper we consider uncertain CTMCs, where rates are assumed to vary non-deterministically with time from given continuous intervals. This leads to a semantics which associates each state with the reachable set of its probability under all possible choices of the uncertain rates. We develop a notion of lumpability as a partition of the states such that the reachable set of a state in the lumped chain is equal to the reachable set of the sum of the probabilities of the original states belonging to that partition block, essentially lifting the well-known CTMC ordinary lumpability to the uncertain setting. Proceeding with this analogy, we also provide a polynomial time and space algorithm for the minimization of an uncertain CTMC by partition refinement, using the lumping algorithm of CTMCs as an inner step. Finally, we consider a logical characterization similarly to that of Baier *et al.* for CTMCs, showing that uncertain CTMC lumping preserves the validity of a continuous stochastic logic aligned to that of Neuhäusser and Katoen for Markov Decision Processes with finite action spaces.

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1 Introduction

Motivation. Continuous-time Markov chains (CTMCs) are a fundamental tool for describing a wide range of natural and engineered systems and serve as the underlying semantics for several formalisms such as stochastic Petri Nets [16], stochastic process algebra (e.g., [29, 30]), and chemical reaction networks [23]. A CTMC is typically characterized by a number of parameters such as arrival and service rates in a queuing network [44], transmission and infection rates of epidemic processes [42], and the kinetic rates of a chemical reaction. In essentially all practical situations, however, knowing the values of all parameters *precisely* is unlikely. This may be due to measurement noise when parameters are to be estimated from

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observations, as well as to our inability to accurately observe events at certain spatio-temporal scales — a well-known problem notably arising in computational systems biology [14]. In addition, sometimes the modeler wishes to be deliberately imprecise about the value of certain parameters in order to explicitly account for the inevitable disagreement between a model and the real system under consideration.

These motivations have stimulated a vigorous line of research into quantitative modeling frameworks where *uncertainty* is a first-class citizen, with the basic idea to replace known constants with *sets* of values which can be nondeterministically assigned to parameters. A prominent instance is Jonnson and Larsen's interval specification systems [31] (equivalent to interval-valued finite Markov chains [35]), where the probability of making a transition between two states of a discrete-time Markov chain is assumed to be taken from a continuous interval of possible values, later generalized to polynomial constraints [9].

Contributions. In this paper we consider uncertain CTMCs (UCTMCs). They allow time-varying nondeterministic uncertainty in the values of the rate parameters within given bounded intervals. This is essentially the continuous-time analogue of the model of nondeterminism in [21, 41], and can be seen as an over-approximation for a time-invariant interpretation of uncertainty which underlies a family of CTMCs, one for each possible choice of rate parameter values [31]. UCTMCs can also be seen as continuous-time Markov decision processes (MDPs) with uncountable action spaces (representing the values within the uncertainty intervals), see [41] and [24, Section 2.2].

Here we study lumpability for UCTMCs. Similarly to the well-known CTMC counterpart [34, 6], the motivation is to obtain coarser models that preserve quantities of interest for analysis and verification purposes. Our starting point is CTMC ordinary lumpability, which identifies a partition of the state space which induces a lumped CTMC where each macro-state represents a partition block; the probability of being in each macro-state at all time points is equal to the sum of the probabilities of the states of the original CTMC belonging to that block [6]. We proceed by way of analogy with established results for CTMCs, and present three main results:

UCTMC lumping. The semantics of an UCTMC is based on reachable sets that provide the set of all probabilities for each state under all possible values of the uncertain parameter rates. *Mutatis mutandis*, we present a notion of lumpability for UCTMCs such that the lumped UCTMC preserves reachable sets of sums of original UCTMC states for each block. UCTMC lumpability is a conservative extension of CTMC lumpability, in the sense that it collapses to the latter when all UCTMC transition rates are not uncertain. A novel ingredient in our definition of UCTMC lumpability is a structural criterion to be satisfied by an *adjoint equivalence relation* induced on the set of transitions by a candidate partition of UCTMC states.

Minimization algorithm. CTMCs enjoy efficient minimization algorithms based on partition refinement which compute the coarsest ordinarily lumpable partition that refines a given initial partition of states [18, 45]. Here we develop an iterative minimization algorithm that refines a given initial partition of states according to a fixed point, verifying the conditions on the adjoint equivalence of transition at each iteration; the refinement of the UCTMC partition of states can actually be implemented using the already available CTMC lumping algorithm [18, 45]. We prove that our minimization takes $\mathcal{O}(rs\log s)$ steps, where r is the number of transitions and s is the number of states of the UCTMC. Using a prototype implementation, on benchmarks from the literature we experimentally show that our algorithm scales to UCTMCs with millions of states and transitions.

Logical characterization. Finally, we study the logical characterization of UCTMC lumpability. Similarly to the characterization of continuous stochastic logic (CSL) by F-bisimulation [3], a notion closely related to ordinary lumpability, we prove that UCTMC lumpability preserves a conservative extension of CSL to UCTMCs, where a CSL formula is satisfied by a UCTMC if it is true under all possible parameter rates. This aligns our approach to [39], which extends CSL to continuous-time MDPs with finite action spaces.

Further related work. As discussed, a UCTMC can be seen as an MDP with uncountable action space and time-dependent policies. In this respect, here we study a model of uncertainty that is different from a considerable body of literature, which instead typically considers the case where action space is finite and/or policies are time-independent (alternatively, untimed or time-invariant), see for instance, [39, 7, 25, 8, 40]. Apart from the previously mentioned [39, 43] that provide logical characterizations of lumpability in the context of continuous-time MDPs, [27] considers the case of discrete-time MDPs with uncertain transition probabilities and provides a polynomial time reduction algorithm.

Other related models are parametric Markov chains and parametric MDPs [36, 26, 17], formally defined with transition matrices that allow (symbolic) parameters. In particular, the work in [26] is conceptually closely related to ours because it introduces lumpability and efficient reduction algorithms for parametric discrete-time Markov chains and MDPs. Lumpability of parametric Markov chains preserves however sums of reachable probability distributions only when the common lumpability conditions are satisfied under all parameter evaluations. Moreover, parametric Markov chains consider time-constant parameters, while parametric MDPs focus on finite action spaces.

It is well known that ordinary lumpability is sensitive to parameter perturbations. This problem has stimulated two complementary lines of research, namely approximate notions of lumpability (e.g., [22, 20, 13, 40]) and metric-based approaches, e.g. [19, 46, 2]. In this respect, UCTMCs can be seen as abstractions of CTMCs by means of a partitioning of the state space that does not necessarily satisfy the lumpability criterion. Indeed, interval abstractions of uniformized CTMCs were proposed in [33], which focused on relating the verification of the abstraction to the original uniformized CTMC. Our work is complementary because UCTMC lumpability can be seen as a tool that provides a coarsening of the interval abstraction while exactly preserving reachable sets in the sense specified above.

2 Preliminaries

In this section we fix the notation and briefly recall the definitions of CTMCs and lumpability that will be used throughout the paper.

Notation. We use ∂_t to denote derivative with respect to time t, while x^T is the transpose of $x \in \mathbb{R}^{\mathcal{V}}$. For an index i, we denote by e_i the i-th unit vector. Pointwise equivalence of functions is denoted by $\equiv$, while $:=$ signifies a definition. Given two partitions $\mathcal{H}_1$ and $\mathcal{H}_2$ of a given set $\mathcal{V}$, we say that $\mathcal{H}_1$ is a refinement of $\mathcal{H}_2$ if for any $H_1 \in \mathcal{H}_1$ there exists a (unique) $H_2 \in \mathcal{H}_2$ such that $H_1 \subseteq H_2$. We shall not distinguish among an equivalence relation and the partition induced by it.

We start by introducing a time-inhomogeneous (alternatively, time-varying) CTMC. For ease of exposition we consider a definition which uses transitions to single out the non-zero elements of the transition rate matrix.

▶ **Definition 1** (CTMC). A time-varying CTMC is a tuple $(\mathcal{V}, \mathcal{E}, q, \pi[0])$ where

- $(\mathcal{V}, \mathcal{E})$ is a self-loop free directed graph with states $\mathcal{V} = \{1, \ldots, n\}$ and transitions $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$;

- q is a transition rate function, $q = (q_{i,j})_{(i,j)\in\mathcal{E}}$, where $q_{i,j} : \mathbb{R}_{\geq 0} \to \mathbb{R}_{\geq 0}$ denotes the measurable and locally bounded transition rate function from state i into state j;
- $\pi[0] \in \mathbb{R}^{\mathcal{V}}_{\geq 0}$ is the initial probability distribution. ◀

The transition rate function leads to the well-known transition matrix of a CTMC in the following standard way.

▶ **Definition 2** (Transition Matrix)**.** The transition rate matrix $Q = (Q_{i,j})_{1\leq i,j\leq n}$ is given by

$$Q_{i,j} = \begin{cases} q_{i,j} & , \ (i,j) \in \mathcal{E} \\ -\sum_{l:(i,l)\in\mathcal{E}} q_{i,l} & , \ j = i \\ 0 & , \ \text{otherwise} \end{cases}$$

for any admissible transition rate function $q = (q_{i,j})_{(i,j)\in\mathcal{E}}$. ◀

The next well-known result relates the (transient) probability distributions of $(\mathcal{V}, \mathcal{E}, q, \pi[0])$ to the Kolmogorov equations for time-varying transition rates, see [24, Section 2.2].

▶ **Theorem 3.** *Given a CTMC $(\mathcal{V}, \mathcal{E}, q, \pi[0])$, the probability distributions $\pi(t)$ exist and satisfy, for all $t \in \mathbb{R}_{\geq 0}$, the Kolmogorov equation $\partial_t \pi(t) = \pi^T(t) Q(t)$, where $\pi(0) = \pi[0]$.*[1]

Thanks to Theorem 3, ordinary lumpability for time-varying CTMCs is a straightforward generalization of ordinary lumpability for time-homogeneous CTMCs (e.g., [6]).

▶ **Theorem 4** (Ordinary Lumpability)**.** *Given a CTMC $(\mathcal{V}, \mathcal{E}, q, \pi[0])$, a partition $\mathcal{H}$ of the set of states $\mathcal{V}$ is called ordinary lumpability if*

$$\sum_{j\in H':(i_1,j)\in\mathcal{E}} q_{i_1,j} \equiv \sum_{j\in H':(i_2,j)\in\mathcal{E}} q_{i_2,j}, \qquad \text{for all } H, H' \in \mathcal{H} \text{ with } H \neq H' \text{ and } i_1, i_2 \in H.$$

The lumped CTMC $(\hat{\mathcal{V}}, \hat{\mathcal{E}}, \hat{q}, \hat{\pi}[0])$ is given by

- *States $\hat{\mathcal{V}} := \{i_H \mid H \in \mathcal{H}\}$, where $i_H \in H$ is an arbitrary representative of block H.*
- *Transitions $\hat{\mathcal{E}} := \{(i_H, i_{H'}) \mid (i_H, j) \in \mathcal{E}$ for some $j \in H'\}$.*
- *Transition rate function $\hat{q} = (\hat{q}_{i_H,i_{H'}})_{(i_H,i_{H'})\in\hat{\mathcal{E}}}$, where*

$$\hat{q}_{i_H,i_{H'}} := \sum_{j\in H':(i_H,j)\in\mathcal{E}} q_{i_H,j} \qquad \text{for all } H, H' \in \mathcal{H}.$$

- *Initial probabilities $\hat{\pi}[0]_{i_H} := \sum_{i\in H} \pi[0]_i$, where $H \in \mathcal{H}$.*

Probability distributions of $(\hat{\mathcal{V}}, \hat{\mathcal{E}}, \hat{q}, \hat{\pi}[0])$ are given by $\hat{\pi}$ and obey $\hat{\pi}_{i_H} \equiv \sum_{i\in H} \pi_i$ for $H \in \mathcal{H}$.

We remark that this definition of ordinary lumpability imposes condition on transitions $\mathcal{E}$ for pairs of distinct blocks of states. This is equivalent to imposing conditions on the entries of the transition rate matrix for any pair of blocks, see, for instance, [45, Proposition 1].

3 UCTMC Lumpability

In this section we present the main technical results. After introducing UCTMCs in Section 3.1, UCTMC lumpability is discussed in Section 3.2. The UCTMC lumping algorithm, instead, is presented in Section 3.3, while Section 3.4 concludes with the logical characterization of UCTMC lumpability.

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[1] The derivative of $t \mapsto \pi(t)$ actually exits almost everywhere up to a Lebesgue null set. For the benefit of presentation, statements involving time derivatives are to be understood up to a null set.

3.1 Uncertain Continuous Time Markov Chains

UCTMCs allow transition rates to vary non-deterministically with time within bounded continuous intervals.

▶ **Definition 5** (Uncertain CTMC)**.** An uncertain CTMC $(\mathcal{V}, \mathcal{E}, m, M, \pi[0])$ is given by

- a self-loop free directed graph $(\mathcal{V}, \mathcal{E})$ with states $\mathcal{V} = \{1, \ldots, n\}$ and transitions $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$;
- non-negative rational numbers $m = (m_{i,j})_{(i,j) \in \mathcal{E}}$ and $M = (M_{i,j})_{(i,j) \in \mathcal{E}}$, with $m \leq M$, describing the lower and upper bounds of the transition rates, respectively;
- an initial probability distribution $\pi[0]$. ◀

▶ Remark. The assumption of m and M being sequences of rational numbers facilitates later discussion and is a common assumption in practice, see for instance [1]. ◀

Motivated by the fact that probability distributions of a CTMC obey the Kolmogorov equations, the semantics of a UCTMC is given by the set of reachable probability distributions.

▶ **Definition 6** (UCTMC Semantics)**.** The semantics of a UCTMC $(\mathcal{V}, \mathcal{E}, m, M, \pi[0])$ is given by the reachable sets

$$\mathcal{R}\Big(\sum_{i \in H} \pi_i, \tau\Big) = \Big\{ \sum_{i \in H} \pi_i(\tau) \mid \partial_t \pi(t) = \pi^T(t) Q(t) \text{ with } \pi(0) = \pi[0] \text{ and admissible } Q \Big\},$$

where $\tau \geq 0$ and $H \subseteq \mathcal{V}$, while Q is admissible if is induced by an admissible q in the following sense:

- $q_{i,j}(t) \in [m_{i,j}; M_{i,j}]$ for all $t \geq 0$ and $(i,j) \in \mathcal{E}$;
- each $q_{i,j}$ is a finitely piecewise analytic function of time, i.e., a piecewise analytic function with at most finitely many discontinuities on any bounded time interval.[2] ◀

▶ Remark. Note that the common notion of reachable sets is recovered by restricting H to singleton blocks only, i.e., $\{\{i\} \mid i \in \mathcal{V}\}$. We allow for general blocks because our ultimate goal is to relate sums of reachable probability distributions of a UCTMC to the reachable probability distributions of a lumped UCTMC.

Running example. Throughout the remainder of this paper, we will use the UCTMC depicted in Figure 1 as a running example. To favor intuition, it can be interpreted as a symmetric model of two components (e.g., two virtual machines) with a binary state (e.g., down/0 and up/1). Assuming independent events, each UCTMC state tracks the configuration of the two machines. Each transition is labeled with the interval within which the rates can vary; we use distinct symbols α, β, γ to indicate different parameters of an hypothetical system under study, such as start-up, shut-down or machine migration, respectively. When all parameters are precisely known, i.e., $\underline{\alpha} = \overline{\alpha}$, $\underline{\beta} = \overline{\beta}$, and $\underline{\gamma} = \overline{\gamma}$, there is the ordinary lumpability consisting of blocks $\{11\}$, $\{01, 10\}$, and $\{00\}$. In the paper we will develop the theory to capture such symmetry for UCTMCs.

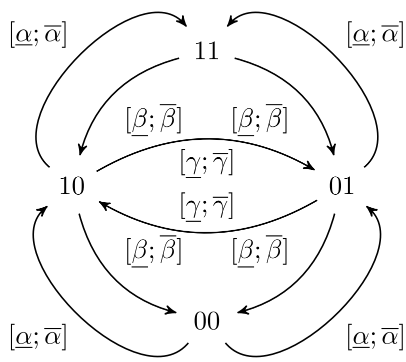

Figure 1 Running example.

[2] With the exception of Section 3.4 in which analyticity and discontinuity points become relevant, finitely piecewise analytic can be replaced with measurable and locally bounded.

3.2 UCTMC Lumpability

As introduced in Section 1, UCTMC lumpability will require criteria to be met on an adjoint partition of transitions. The following definition introduces a number of preliminary concepts that will be used for this.

▶ **Definition 7.** Fix UCTMC $(\mathcal{V}, \mathcal{E}, m, M, \pi[0])$ and partitions $\mathcal{H}$, $\mathcal{G}$ of $\mathcal{V}$, $\mathcal{E}$, respectively.

- A transition $(i, j) \in \mathcal{E}$ is called *invariant* (with respect to $\mathcal{H}$) if $i, j \in H$ for some $H \in \mathcal{H}$. Likewise, a block $G \in \mathcal{G}$ is called invariant if all its transitions are invariant.
- A transition $(i, j) \in \mathcal{E}$ is called *deterministic* if $m_{i,j} = M_{i,j}$.
- A block $G \in \mathcal{G}$ consisting of deterministic transitions only is called deterministic.
- We denote by $\mathcal{G}_d$ the set of deterministic blocks of $\mathcal{G}$, while we set $\mathcal{G}_n := \mathcal{G} \setminus \mathcal{G}_d$.
- Given a block $G \in \mathcal{G}$, we let $\chi^G = (\chi^G_{i,j})_{1 \le i,j \le n}$ denote the matrix such that

$$\chi^G_{i,j} = \begin{cases} 1 & \text{if } (i,j) \in G, \\ -|\{(i', j') \in G \mid i' = i\}| & \text{if } i = j, \\ 0 & \text{otherwise.} \end{cases}$$

  That is, χ^G is the negative Laplacian of the adjacency matrix induced by the set of transitions in block G.
- The *deterministic part* of $(\mathcal{V}, \mathcal{E}, m, M, \pi[0])$ is given by

$$Q^d := \sum_{G \in \mathcal{G}_d} m_G \cdot \chi^G.$$

- For $G \in \mathcal{G}$ and $(i_k, j_k), (i_l, j_l) \in G$, we write $(i_k, j_k) \approx_{(\mathcal{H},\mathcal{G})} (i_l, j_l)$ if both transitions have identical origin and target blocks, that is:

$$(i_k, j_k) \approx_{(\mathcal{H},\mathcal{G})} (i_l, j_l) \quad \text{if} \quad \exists H, H' \in \mathcal{H} \text{ such that } i_k, i_l \in H \text{ and } j_k, j_l \in H'.$$

◀

We remark that both the deterministic part of a UCTMC as well as each negative Laplacian χ^G can be seen as transition matrices of time-homogeneous CTMCs. Indeed, in Theorem 12 we will relate the lumpability of UCTMCs to the lumpability of such CTMCs.

With all the above notions in place, we can introduce the adjoint partition.

▶ **Definition 8** (Adjoint Partition)**.** Given a UCTMC $(\mathcal{V}, \mathcal{E}, m, M, \pi[0])$ and a partition $\mathcal{H}$ of $\mathcal{V}$, the *adjoint partition of* $\mathcal{H}$ is the coarsest partition $\mathcal{G}$ of $\mathcal{E}$ satisfying the following:

(i) There are $m_G, M_G \in \mathbb{Q}$ such that $m_G = m_{i,j}$ and $M_G = M_{i,j}$ for all $G \in \mathcal{G}$ and $(i, j) \in G$.
(ii) $(i_k, j_k) \approx_{(\mathcal{H},\mathcal{G})} (i_l, j_l)$ for any $G \in \mathcal{G}_n$ and $(i_k, j_k), (i_l, j_l) \in G$. ◀

Noting that **(i)** and **(ii)** induce equivalence relations on $\mathcal{E}$, we infer the existence and uniqueness of the adjoint partition.

We are now ready to define the main concept of the present paper.

▶ **Definition 9** (UCTMC Lumpability)**.** A partition $\mathcal{H}$ of $\mathcal{V}$ is called UCTMC lumpability of a UCTMC $(\mathcal{V}, \mathcal{E}, m, M, \pi[0])$ if its adjoint partition $\mathcal{G}$ is such that

(iii) for any admissible $(q_{i,j})_{(i,j)\in\mathcal{E}}$ that satisfies the relation $q_{i_k,j_k} \equiv q_{i_l,j_l}$ for all $G \in \mathcal{G}$ and $(i_k, j_k), (i_l, j_l) \in G$, it holds that $\mathcal{H}$ is an ordinary lumpability. ◀

Note that condition **(i)** ensures that $\mathcal{G} = \mathcal{G}_d \dot\cup \mathcal{G}_n$, i.e., a block of $\mathcal{G}$ cannot contain deterministic and non-deterministic transitions at the same time. Instead, condition **(iii)** requires $\mathcal{H}$ to be an ordinary lumpability only for transition rate functions satisfying the symmetry condition $q_{i_k,j_k} \equiv q_{i_l,j_l}$ for all $G \in \mathcal{G}$ and $(i_k, j_k), (i_l, j_l) \in G$. As such, **(iii)** is similar to bisimulation for parametric Markov chains [26], see also discussion after Theorem 13.

▶ **Example**. Let us consider the running example of Figure 1. Then, the partition of states

$$\mathcal{H} = \big\{\{11\}, \{10, 01\}, \{00\}\big\} \tag{1}$$

induces the adjoint partition $\mathcal{G} = \{G_1, G_2, G_3, G_4, G_5\}$, with

$$G_1 := \{(11, 10), (11, 01)\}, \qquad G_2 := \{(10, 11), (01, 11)\}, \qquad G_3 := \{(10, 00), (01, 00)\},$$
$$G_4 := \{(10, 01), (01, 10)\}, \qquad G_5 := \{(00, 10), (00, 01)\}.$$

It is not difficult to see that $\mathcal{H}$ is a UCTMC lumpability. ◀

We recall that the same partition (1) is also an ordinary lumpability in the case of a CTMC, where there is no rate uncertainty. Indeed, we can observe that UCTMC lumpability is a conservative generalization of ordinary lumpability.

▶ **Lemma 10** (Generalization). *Assume that $\mathcal{H}$ is a UCTMC lumpability of a UCTMC $(\mathcal{V}, \mathcal{E}, m, M, \pi[0])$ whose transitions are all deterministic. Then, the set of admissible transition rate functions is a singleton given by m (alternatively, M) and $\mathcal{H}$ is an ordinary lumpability.*

The lumped UCTMC is obtained in a similar way as for ordinary lumpability.

▶ **Definition 11** (Lumped UCTMC). Let $\mathcal{H}$ be a UCTMC lumpability of $(\mathcal{V}, \mathcal{E}, m, M, \pi[0])$ and $\mathcal{G}$ its adjoint partition. For each $H \in \mathcal{H}$, fix some arbitrary representative $i_H \in H$ and define the multiplicity $\mu_G(i_H, i_{H'}) := |\{(i_H, j) \in G \mid j \in H'\}|$ for all $G \in \mathcal{G}_n$. Then, with $Q^d = (q^d_{i,j})_{1\leq i,j,\leq n}$ being the deterministic part, the lumped UCTMC is given by

- States $\hat{\mathcal{V}} := \{i_H \mid H \in \mathcal{H}\}$.
- Transitions $\hat{\mathcal{E}} := \{(i_H, i_{H'}) \mid (i_H, j) \in \mathcal{E}$ for some $j \in H'\}$.
- Lower bounds:
$$\hat{m}_{i_H,i_{H'}} := \sum_{j\in H'} q^d_{i_H,j} + \sum_{G\in\mathcal{G}_n} \mu_G(i_H, i_{H'}) m_{i_H,i_{H'}}.$$
- Upper bounds:
$$\hat{M}_{i_H,i_{H'}} := \sum_{j\in H'} q^d_{i_H,j} + \sum_{G\in\mathcal{G}_n} \mu_G(i_H, i_{H'}) M_{i_H,i_{H'}}.$$
- Initial probabilities $\hat{\pi}[0]_{i_H} := \sum_{i\in H} \pi[0]_i$, for $H \in \mathcal{H}$. ◀

Example. In the case of the UCTMC from Figure 1, the UCTMC lumpability (1) induces the lumped UCTMC in Figure 2. It is interesting to note that the transitions between states 01 and 10 in the original UCTMC correspond to self-loops in the lumped UCTMC. However, since self-loops induce self canceling terms at the level of forward Kolmogorov equations, they do not have an impact on system's dynamics and can be ignored. Note also that this justifies to call the block of transitions $\{(10, 01), (01, 10)\}$ of the adjoint partition invariant.

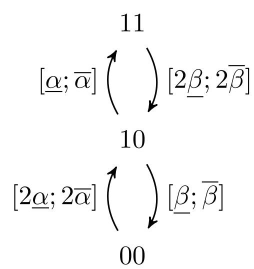

Figure 2 Lumped UCTMC.

The next result ensures that there exists a coarsest UCTMC lumpability. Crucially, it characterizes condition **(iii)** via ordinary lumpability of time-homogeneous CTMCs induced by the deterministic part and the negative Laplacians underlying the adjoint partition.

▶ **Theorem 12.** *Fix UCTMC $(\mathcal{V}, \mathcal{E}, m, M, \pi[0])$ and partitions $\mathcal{H}$, $\mathcal{G}$ of $\mathcal{V}$, $\mathcal{E}$, respectively.*

1) There exists a coarsest refinement $\mathcal{H}'$ of $\mathcal{H}$ such that $\mathcal{H}'$ is a UCTMC lumpability.

2) Let Q^d denote the deterministic part of the UCTMC $(\mathcal{V}, \mathcal{E}, m, M, \pi[0])$. Then, $\mathcal{H}$ and $\mathcal{G}$ satisfy **(i)** *and* **(iii)** *if and only if $\mathcal{G}$ satisfies* **(i)** *and $\mathcal{H}$ is an ordinary lumpability of Q^d and all $(\chi^G)_{G\in\mathcal{G}_n}$.*

Note that Theorem 12 ensures that the multiplicity $\mu_G(i_H, i_{H'})$ in Definition 11, where $G \in \mathcal{G}_n$ and $H, H' \in \mathcal{H}$, does not depend on the choice of representatives.

▶ Remark. In statement 2) of Theorem 12, it is indeed necessary to require **(i)** in order to characterize **(iii)** in terms of ordinary lumpability. This is because **(i)** ensures that the premise of **(iii)**, i.e., $q_{(i_k,j_k)} \equiv q_{(i_l,j_l)}$ for all $(i_k, j_k), (i_l, j_l) \in G$ and $G \in \mathcal{G}$, is satisfiable (note that $M_{i_k,j_k} < m_{i_l,j_l}$ may rule this out). ◀

Our first major result states that sums of reachable probability distributions of a UCTMC coincide with the reachable probability distributions of the corresponding lumped UCTMC.

▶ **Theorem 13** (Preservation of Reachability)**.** *Assume that $\mathcal{H}$ is a UCTMC lumpability of $(\mathcal{V}, \mathcal{E}, m, M, \pi[0])$. Then, for any $\tau \geq 0$ and $H \in \mathcal{H}$, it holds that $\mathcal{R}\big(\sum_{i\in H} \pi_i, \tau\big) = \mathcal{R}\big(\hat{\pi}_{i_H}, \tau\big)$, where $\hat{\pi}$ refers to reachable probability distributions of the lumped UCTMC.*

▶ **Example.** In the case of the running example, Theorem 13 ensures, for instance, that $\mathcal{R}(\pi_{10} + \pi_{01}, t) = \mathcal{R}(\hat{\pi}_{10}, t)$ for all $t \geq 0$. ◀

▶ Remark. Condition **(iii)** is a reminiscent of bisimulation for parametric Markov chains [26]. Note, however, that **(iii)** on its own is not to enough to ensure Theorem 13. This is because admissible transition rate functions do not satisfy the symmetry constraints of **(iii)** in general. However, if combined with **(i)** and **(ii)**, condition **(iii)** implies that sums of reachable probability distributions are preserved, as stated by Theorem 13. In the discussion following Theorem 15, we will argue that conditions **(i)**-**(iii)** are also necessary for the preservation.

We next provide some intuition on the proof Theorem 13 by showing it for the running example (1); we refer to the appendix for the formal proof. The main idea is to prove that we can preserve sums of reachable probabilities in the case when we are restricted to admissible transition rate functions $(q'_{i,j})_{(i,j)\in\mathcal{E}}$ that satisfy $q'_{i_k,j_k} \equiv q'_{i_l,j_l}$ for all $G \in \mathcal{G}$ and $(i_k, j_k), (i_l, j_l) \in G$. This, condition **(iii)** and Theorem 4 yield then the statement.

Let us first fix some arbitrary admissible $(q_{i,j})_{(i,j)\in\mathcal{E}}$ and define (we suppress the explicit dependence on t to increase readability)

$$\begin{aligned}
q_{G_1} &:= q_{11,10}\frac{\pi_{11}}{\pi_{11}+\pi_{11}} + q_{11,01}\frac{\pi_{11}}{\pi_{11}+\pi_{11}}, \quad & q_{G_2} &:= q_{10,11}\frac{\pi_{10}}{\pi_{10}+\pi_{01}} + q_{01,11}\frac{\pi_{01}}{\pi_{10}+\pi_{01}},\\
q_{G_3} &:= q_{10,00}\frac{\pi_{10}}{\pi_{10}+\pi_{01}} + q_{01,00}\frac{\pi_{01}}{\pi_{10}+\pi_{01}}, \quad & q_{G_4} &:= m_{10,01},\\
q_{G_5} &:= q_{11,10}\frac{\pi_{00}}{\pi_{00}+\pi_{00}} + q_{11,01}\frac{\pi_{00}}{\pi_{00}+\pi_{00}}, & & \qquad (2)
\end{aligned}$$

where π denotes the solution of the Kolmogorov equations with respect to q and $\pi[0]$. Thanks to **(i)**, we can set $q_G(t) := m_G$ whenever a denominator in the analytical expression of $q_G(t)$ in (2) is zero. Since $(q_{i,j})_{(i,j)\in\mathcal{E}}$ is admissible, π is finitely piecewise analytic [5], thus ensuring that so is $(q_G)_{G \in \mathcal{G}}$. More importantly, it holds that

$$\begin{aligned}
\partial_t(\pi_{10} + \pi_{01}) &= -q_{10,11}\pi_{10} - q_{10,01}\pi_{10} - q_{10,00}\pi_{10} + q_{11,10}\pi_{11} + q_{01,10}\pi_{01} + q_{00,10}\pi_{00} \\
&\qquad - q_{01,11}\pi_{01} - q_{01,10}\pi_{01} - q_{01,00}\pi_{01} + q_{11,01}\pi_{11} + q_{10,01}\pi_{10} + q_{00,01}\pi_{00} \\
&= -(q_{10,11}\pi_{10} + q_{01,11}\pi_{01}) - (q_{10,00}\pi_{10} + q_{01,00}\pi_{01}) \\
&\qquad + (q_{11,10}\pi_{11} + q_{11,01}\pi_{11}) + (q_{00,10}\pi_{00} + q_{00,01}\pi_{00}) \\
&= -q_{G_2}(\pi_{10} + \pi_{01}) - q_{G_3}(\pi_{10} + \pi_{01}) + 2q_{G_1}\pi_{11} + 2q_{G_5}\pi_{00}, \qquad (3)
\end{aligned}$$

where the cancelations underlying the second identity reflect the invariance of the block $G_4 = \{(10, 01), (01, 10)\}$, while the third identity follows from the choice of $(q_G)_{G \in \mathcal{G}}$. Crucially, similar calculations confirm that $\partial_t \pi_{11}$ and $\partial_t \pi_{00}$ can be expressed in terms of $q_{G_1}, \ldots, q_{G_5}$ and $\pi_{11}, (\pi_{10} + \pi_{01}), \pi_{00}$.

The above discussion shows that replacing $q_{i,j}$ with q_G for all $G \in \mathcal{G}$ and $(i, j) \in G$ does not change $\pi_{11}, (\pi_{10} + \pi_{01}), \pi_{00}$. This motivates to define $(q'_{i,j})_{(i,j) \in \mathcal{E}}$ by $q'_{(i,j)} := q_G$ for all $G \in \mathcal{G}$ and $(i, j) \in G$. Note that $(q'_{i,j})_{(i,j) \in \mathcal{E}}$ is admissible because each q_G is finitely piecewise analytic and satisfies $m_G \leq q_G \leq M_G$. Hence, the lumped CTMC with respect to $(q'_{i,j})_{(i,j) \in \mathcal{E}}$ as given in Theorem 4 is well-defined and

$$\hat{q}'_{i_H, i_{H'}} \equiv \sum_{j \in H' : (i_H, j) \in \mathcal{E}} q'_{i_H, j} \equiv \sum_{j \in H' : (i_H, j) \in \mathcal{E}} q'^{d}_{i_H, j} + \sum_{G \in \mathcal{G}_n} \mu_G(i_H, i_{H'}) \cdot q_G \qquad (4)$$

for all $H, H' \in \mathcal{H}$. This implies that $\hat{q}'_{i_H, i_{H'}} \in [\hat{m}_{i_H, i_{H'}}; \hat{M}_{i_H, i_{H'}}]$. Moreover, Theorem 4 ensures that $\sum_{i \in H} \pi_i \equiv \hat{\pi}'_{i_H}$ because $\sum_{i \in H} \pi_i \equiv \sum_{i \in H} \pi'_i$, where $H \in \mathcal{H}$.

Since $(q_{i,j})_{(i,j) \in \mathcal{E}}$ was chosen arbitrarily, the above yields $\mathcal{R}(\sum_{i \in H} \pi_i, t) \subseteq \mathcal{R}(\hat{\pi}_{i_H}, t)$ for all $H \in \mathcal{H}$ and $t \geq 0$. The converse subset relation, instead, follows from the above discussion and the following auxiliary statement.

▶ **Lemma 14.** *Let $\mathcal{H}$ be a UCTMC lumpability of $(\mathcal{V}, \mathcal{E}, m, M, \pi[0])$, $\mathcal{G}$ its adjoint partition and $(\hat{q}_{i_H, i_{H'}})_{(i_H, i_{H'}) \in \hat{\mathcal{E}}}$ an admissible transition rate of the lumped UCTMC. Then, there is a finitely piecewise analytic $(q_G)_{G \in \mathcal{G}}$ that satisfies, in agreement with (4), the relations*

$$\hat{q}_{i_H, i_{H'}} = \sum_{j \in H'} q^{d}_{i_H, j} + \sum_{G \in \mathcal{G}_n} \mu_G(i_H, i_{H'}) \cdot q_G \qquad \text{and} \qquad q_G \in [m_G; M_G]$$

for all $G \in \mathcal{G}$ and $H, H' \in \mathcal{H}$ if $(q_{i,j})_{(i,j) \in \mathcal{E}}$ is given by $q_{i,j} := q_G$ for all $G \in \mathcal{G}$ and $(i, j) \in G$.

We next present a modification of Theorem 13 that allows one to over-approximate sums of reachable probability distributions when, loosely speaking, partitions $\mathcal{H}$ and $\mathcal{G}$ satisfy **(ii)-(iii)** but violate **(i)**. Since sums of reachable probability distributions are not preserved in general, it resembles [33] which provides over-approximations of uniformized CTMCs.

▶ **Theorem 15** (Over-Approximation)**.** *For a given UCTMC $(\mathcal{V}, \mathcal{E}, m, M, \pi[0])$ and a partition $\mathcal{G}$ of $\mathcal{E}$, define m' and M' by*

$$m'_{i,j} := \min_{(i',j') \in G} m_{i',j'} \qquad \text{and} \qquad M'_{i,j} := \max_{(i',j') \in G} M_{i',j'} \qquad \text{for all } G \in \mathcal{G} \text{ and } (i, j) \in G.$$

Provided that $\mathcal{H}$ is a UCTMC lumpability of $(\mathcal{V}, \mathcal{E}, m', M', \pi[0])$, the following holds true.

1) *The UCTMC $(\mathcal{V}, \mathcal{E}, m, M, \pi[0])$ can be over-approximated by the lumped UCTMC of $(\mathcal{V}, \mathcal{E}, m', M', \pi[0])$. That is, $\mathcal{R}\big(\sum_{i \in H} \pi_i, \tau\big) \subseteq \mathcal{R}\big(\hat{\pi}'_{i_H}, \tau\big)$ for all $H \in \mathcal{H}$ and $\tau \geq 0$.*
2) *In general, the subset relation in 1) is proper, meaning that sums of reachable probability distributions are over-approximated but not preserved.*

Statement 2) of Theorem 15 implies that condition **(i)** is indeed needed to preserve sums of reachable probability distributions. Likewise, given that ordinary lumpability characterizes sums of probability distributions in the case of deterministic CTMCs [6, 10], Lemma 10 readily implies that condition **(iii)** is also needed to preserve sums of reachable probability distributions. The next result ensures that condition **(ii)** cannot be dropped either.

▶ **Theorem 16** (Necessity of **(ii)**). *Assume that partitions $\mathcal{H}$ and $\mathcal{G}$ of $\mathcal{V}$ and $\mathcal{E}$, respectively, satisfy* **(i)**,**(iii)**. *Assume further that it holds that $\mathcal{R}\big(\sum_{i\in H}\pi_i, t\big) \subseteq \mathcal{R}\big(\hat{\pi}_{i_H}, t\big)$ for all $t \geq 0$ and $H \in \mathcal{H}$. At last, require that $m_{i,j} = 0$ for all $(i,j) \in G$ with $G \in \mathcal{G}_n$. Then, for any $G \in \mathcal{G}_n$ and non-invariant $(i_k, j_k), (i_l, j_l) \in G$, it holds that $(i_k, j_k) \approx_{(\mathcal{H},\mathcal{G})} (i_l, j_l)$.*

To show the necessity of **(ii)** in our running example, replace $\mathcal{G}$ in (1) with $\mathcal{G}'$ given by:

$$\Big\{\underbrace{\{(11,10),(11,01),(00,10),(00,01)\}}_{G_1' := G_1 \cup G_5}, \underbrace{\{(10,11),(01,11)\}}_{G_2' := G_2}, \underbrace{\{(10,00),(01,00)\}}_{G_3' := G_3}, \underbrace{\{(10,01),(01,10)\}}_{G_4' := G_4}\Big\}$$

It can be shown that $\mathcal{H}$ and $\mathcal{G}'$ still satisfy **(i)** and **(iii)** if all uncertainty intervals are $[0;1]$. At the same time, however, **(ii)** is violated by the block G_1'. To see that $\mathcal{H}$ and $\mathcal{G}'$ do not allow one to preserve sums of reachable probability distributions, it suffices, thanks to Lemma 14, to note that it is not possible to replace the transition rate functions $\{q_{i,j} \mid (i,j) \in G'\}$ by a common $q_{G'}$ without altering sums of reachable probability distributions. Indeed, let assume towards a contradiction that there exist $q_{G_1'}, \ldots, q_{G_4'}$ achieving this in the case when $0 \equiv q_{10,11} \equiv q_{01,11} \equiv q_{10,00} \equiv q_{01,00}$ and $\pi_{11}(0) = \pi_{00}(0) > 0$. Then, it holds that

$$\partial_t \pi_{11} = -q_{11,10}\pi_{11} - q_{11,01}\pi_{11} + q_{10,11}\pi_{10} + q_{01,11}\pi_{01} = -2q_{G_1'}\pi_{11} + q_{G_2'}(\pi_{10} + \pi_{01}),$$
$$\partial_t \pi_{00} = -q_{00,10}\pi_{00} - q_{00,01}\pi_{00} + q_{10,00}\pi_{10} + q_{01,00}\pi_{01} = -2q_{G_1'}\pi_{00} + q_{G_3'}(\pi_{10} + \pi_{01}).$$

Since this implies that $q_{11,10} + q_{11,01} \equiv q_{00,10} + q_{00,10}$, sums of reachable probability distributions are only preserved under additional constraints on q, thus yielding a contradiction.

3.3 UCTMC Lumping Algorithm

We next present Algorithm 1 for the efficient computation of the coarsest UCTMC lumpability that refines a given partition $\mathcal{H}$. To this end, the algorithm first performs a precomputation step in which the coarsest partition of transitions satisfying **(i)** is computed and stored in $\mathcal{G}$ (line 1). Afterwards, the algorithm adheres to the following recipe:

1) With $\mathcal{H}$ and $\mathcal{G}$ being the current partitions, refine $\mathcal{G}$ with respect to **(ii)** and $\mathcal{H}$, store the result in $\mathcal{G}'$ (line 3);
2) Afterwards, refine $\mathcal{H}$ with respect to **(iii)** and $\mathcal{G}'$, store the result in $\mathcal{H}'$ (line 4);
3) If $\mathcal{H}' = \mathcal{H}$, return $\mathcal{H}'$ and $\mathcal{G}'$; Otherwise, set $\mathcal{H} := \mathcal{H}'$, $\mathcal{G} := \mathcal{G}'$ and go to 1) (line 5).

Thanks to the precomputation step, an application of 1) ensures that $\mathcal{H}$ and $\mathcal{G}'$ satisfy **(i)** and **(ii)**. Hence, if 2) does not refine $\mathcal{H}$, we infer that $\mathcal{H}$ is a UCTMC lumpability with adjoint partition $\mathcal{G}'$. Instead, if $\mathcal{H}$ is refined to $\mathcal{H}'$ with $\mathcal{H}' \neq \mathcal{H}$, the algorithm does not terminate and refines in the next iteration $\mathcal{G}'$ with respect to $\mathcal{H}'$. The process is guaranteed to terminate because $\mathcal{V}$ and $\mathcal{E}$ are finite. Moreover, it can be shown that Algorithm 1 indeed computes the coarsest UCTMC partition because each refinement produces a pair of partitions which, itself, is still refined by the coarsest UCTMC lumpability and its adjoint. The next important result ensures that 2) can be computed by available CTMC lumping algorithms as [18, 45].

Algorithm 1 Partition refinement algorithm for the computation of the coarsest UCTMC lumpability $\mathcal{H}$ and its coarsest adjoint partition $\mathcal{G}$.

Require: Uncertain CTMC $(\mathcal{V}, \mathcal{E}, m, M, \pi[0])$ and initial partition $\mathcal{H}$
$\mathcal{G} \longleftarrow$ coarsest partition of $\mathcal{E}$ satisfying **(i)**
while true do
  $\mathcal{G}' \longleftarrow$ coarsest refinement of $\mathcal{G}$ satisfying **(ii)** w.r.t. $\mathcal{H}$
  $\mathcal{H}' \longleftarrow$ coarsest refinement of $\mathcal{H}$ satisfying **(iii)** w.r.t. $\mathcal{G}'$
  if $\mathcal{H}' = \mathcal{H}$ **then**
    return $\mathcal{H}'$ and $\mathcal{G}'$
  else
    $\mathcal{H} \longleftarrow \mathcal{H}'$ and $\mathcal{G} \longleftarrow \mathcal{G}'$
  end if
end while

▶ **Theorem 17.** *Given a UCTMC $(\mathcal{V}, \mathcal{E}, m, M, \pi[0])$, let $\mathcal{H}$ and $\mathcal{G}$ be partitions of $\mathcal{V}$ and $\mathcal{E}$, respectively. Moreover, let Q^d denote the deterministic part as introduced in Definition 7.*

1) *There exist coarsest partitions $\mathcal{H}'$ and $\mathcal{G}'$ refining $\mathcal{H}$ and $\mathcal{G}$, respectively, that satisfy* **(i)**,**(iii)**. *In particular, $\mathcal{G}'$ is the coarsest refinement of $\mathcal{G}$ satisfying* **(i)**, *while $\mathcal{H}'$ is the coarsest ordinary lumpability of Q^d and all $(\chi^G)_{G \in \mathcal{G}'_n}$.*
2) *The time and space complexity required for the computation of $\mathcal{H}'$ and $\mathcal{G}'$ from above does not exceed $\mathcal{O}(rs \log(s))$, where $r := |\mathcal{E}|$ and $s := |\mathcal{V}|$.*

Armed with Theorem 17, we can show the following.

▶ **Theorem 18** (Computation of UCTMC Lumpability)**.** *For a UCTMC $(\mathcal{V}, \mathcal{E}, m, M, \pi[0])$ and partition $\mathcal{H}$ of $\mathcal{V}$, the following holds true.*

1) *Algorithm 1 computes the coarsest UCTMC lumpability refining $\mathcal{H}$. As a byproduct, it also computes its adjoint partition.*
2) *The time and space complexity required for the computation of one while loop iteration of Algorithm 1 does not exceed $\mathcal{O}(rs \log(s))$, where $r := |\mathcal{E}|$ and $s := |\mathcal{V}|$. The number of while loop iterations, instead, is at most $\min\{r, s\} + 2$.*

The section concludes with the following observation.

▶ **Lemma 19.** *If $(\mathcal{V}, \mathcal{E}, m, M, \pi[0])$ has deterministic transitions only, Algorithm 1 computes the coarsest ordinary lumpability refining $\mathcal{H}$ in at most two while loop iterations.*

3.4 Logical Characterization

In the present section we relate UCTMC lumpability to continuous stochastic logic [3, 4] (CSL). We first present the extension of [3] to time-varying CTMCs from [4, 5]. For the benefit of presentation, we follow [4, 5] by omitting the steady-state operator of [3].

▶ **Definition 20** (CSL)**.** The CSL syntax is given by

$$\phi ::= a \mid \phi \wedge \phi \mid \neg\phi \mid \mathcal{P}_{\bowtie p}\big(\mathbf{X}^{[t_0;t_1]}\phi\big) \mid \mathcal{P}_{\bowtie p}\big(\phi \mathbf{U}^{[t_0;t_1]}\phi\big),$$

where $a \in \mathcal{A}$ and $\mathcal{A}$ is the nonempty finite set of atomic propositions, $p \in [0;1]$ is a probability, $\bowtie \in \{<, \leq, \geq, >\}$ and $0 \leq t_0 \leq t_1 < \infty$. For a time-varying CTMC $(\mathcal{V}, \mathcal{E}, q, \pi[0])$, the satisfiability relation is defined by structural induction over ϕ.

- $i, t \models a$ if and only if $a \in \mathcal{L}(i)$;
- $i, t \models \phi_1 \wedge \phi_2$ if and only if $i, t \models \phi_1$ and $i, t_0 \models \phi_2$;
- $i, t \models \neg\phi$ if and only if not $i, t \models \phi$;
- $i, t \models \mathcal{P}_{\bowtie p}\big(\mathbf{X}^{[t_0;t_1]}\phi\big)$ if and only if $\mathbb{P}\{\sigma \mid \sigma, t \models \mathbf{X}^{[t_0;t_1]}\phi\} \bowtie p$ with $\pi(t) = e_i$;
- $i, t \models \mathcal{P}_{\bowtie p}\big(\phi_1 \mathbf{U}^{[t_0;t_1]}\phi_2\big)$ if and only if $\mathbb{P}\{\sigma \mid \sigma, t \models \phi_1 \mathbf{U}^{[t_0;t_1]}\phi_2\} \bowtie p$ with $\pi(t) = e_i$;
- $\sigma, t \models \mathbf{X}^{[t_0;t_1]}\phi$ if and only if $t_\sigma[1] \in [t + t_0; t + t_1]$ and $\sigma[1], t_\sigma[1] \models \phi$;
- $\sigma, t \models \phi_1 \mathbf{U}^{[t_0;t_1]}\phi_2$ if and only if there exists a $t' \in [t + t_0; t + t_1]$ such that $\sigma@t', t' \models \phi_2$ and $\sigma@t'', t'' \models \phi_1$ for all $t'' \in [t + t_0; t + t')$,

where $\mathbb{P}$ is the probability measure, $\pi(t)$ the probability distribution of the CTMC at time t, σ a path of the CTMC, $\sigma@t$ the state of the CTMC at time point t, $\sigma[1]$ the state at the time of the first jump and $t_\sigma[1]$ the corresponding time point. ◀

The Boolean operators $\wedge$ and $\rightarrow$ are defined as usual; likewise, $\mathrm{tt} := a \vee \neg a$ and $\mathrm{ff} := a \wedge \neg a$ for some $a \in \mathcal{A}$. As in the case of classic model checking [15], $\mathbf{X}$ refers to the next operator, while $\mathbf{U}$ corresponds to the until operator.

We now extend CSL to UCTMCs by defining a formula to be true when it is satisfied by all admissible $q = (q_{i,j})_{(i,j)\in\mathcal{E}}$. This aligns to [39] that considers CSL for CTMDPs with finite action spaces and allows one to study safety properties in presence of uncertainty.

▶ **Definition 21** (CSL for UCTMCs). Given a UCTMC $(\mathcal{V}, \mathcal{E}, m, M, \pi[0])$, the CSL syntax is given by

$$\phi ::= a \mid \phi \wedge \phi \mid \neg\phi \mid \mathcal{P}^{\forall}_{\bowtie p}\big(\mathbf{X}^{[t_0;t_1]}\phi\big) \mid \mathcal{P}^{\forall}_{\bowtie p}\big(\phi \mathbf{U}^{[t_0;t_1]}\phi\big)$$

For an arbitrary small but fixed time step $\Delta > 0$, let $\underline{t}$ denote the smallest grid point in $\{0, \Delta, 2\Delta, \ldots\}$ that minimizes the distance to $t \geq 0$, i.e., $\underline{t} = \Delta \cdot \lfloor t/\Delta \rfloor$, where $\lfloor\cdot\rfloor$ is the floor function. The satisfiability operator is defined by structural induction over ϕ.

- $i, t \models a$ if and only if $a \in \mathcal{L}(i)$;
- $i, t \models \phi_1 \wedge \phi_2$ if and only if $i, t \models \phi_1$ and $i, t_0 \models \phi_2$;
- $i, t \models \neg\phi$ if and only if not $i, t \models \phi$;
- $i, t \models \mathcal{P}^{\forall}_{\bowtie p}\big(\mathbf{X}^{[t_0;t_1]}\phi_1\big)$ if and only if $i, \underline{t} \models \mathcal{P}_{\bowtie p}\big(\mathbf{X}^{[t_0;t_1]}\phi\big)$ for all admissible q;
- $i, t \models \mathcal{P}^{\forall}_{\bowtie p}\big(\phi_1 \mathbf{U}^{[t_0;t_1]}\phi_2\big)$ if and only if $i, \underline{t} \models \mathcal{P}_{\bowtie p}\big(\phi_1 \mathbf{U}^{[t_0;t_1]}\phi_2\big)$ for all admissible q. ◀

Similarly to [39], existential quantification is given by $\mathcal{P}^{\exists}_{\bowtie p}(\Phi) := \neg\mathcal{P}^{\forall}_{\neg\bowtie p}(\Phi)$, where $\neg\bowtie$ is defined in the obvious manner (e.g., $\neg \leq$ is $>$). Likewise, $\vee$, $\rightarrow$ are defined using $\wedge$, $\neg$. Together with the assumption on transition rate functions (i.e., finitely piecewise analytic), the usage of $\underline{t}$ in Definition 21 ensures that the function $t \mapsto i, t \models \phi$ has finitely many discontinuity points on any bounded time interval. This technical ingredient allows us to establish the next major result, stating that CSL properties given with respect to the original UCTMC can be equally studied in the context of the lumped UCTMC. The proof exploits the sophisticated machinery behind the model checking algorithm of time-varying CTMCs [4] which, in turn, generalizes [3].

▶ **Theorem 22** (Preservation of CSL). *Let $\mathcal{H}$ be a UCTMC lumpability of the UCTMC $(\mathcal{V}, \mathcal{E}, m, M, \pi[0])$. Assume further that $\mathcal{L}$ is invariant with respect to $\mathcal{H}$, i.e., $\mathcal{L}(i) = \mathcal{L}(j)$ for all $H \in \mathcal{H}$ and $i, j \in H$. With this, define $\hat{\mathcal{A}} := \mathcal{A}$ and $\hat{\mathcal{L}}(i_H) := \mathcal{L}(i_H)$ for all $H \in \mathcal{H}$. Then, it holds that*

$$i, t \models_{(\mathcal{V},\mathcal{E})} \phi \Longleftrightarrow i_H, t \models_{(\hat{\mathcal{V}},\hat{\mathcal{E}})} \phi$$

for any $t \geq 0$, $H \in \mathcal{H}$, $i \in H$ and $\boldsymbol{X}$-operator free CSL formula ϕ; the subscripts in $\models_{(\mathcal{V},\mathcal{E})}$ and $\models_{(\hat{\mathcal{V}},\hat{\mathcal{E}})}$ indicate with respect to which UCTMC the formula is being evaluated.

▶ Remark. The assumption of ϕ being $\mathbf{X}$-free in Theorem 22 cannot be dropped in general. Indeed, consider the UCTMC from Figure 1 but assume that $m_{i,j} := M_{i,j} := 1$ for all $(i,j) \in \mathcal{E}$, i.e., all transitions are deterministic. Then, the sojourn time in state (10) is exponentially distributed with rate $3 = q_{10,11} + q_{10,01} + q_{10,00}$. Instead, in the corresponding lumped CTMC, the sojourn time in state 10 is exponentially distributed with rate $4 = q_{10,11} + q_{10,00} + q_{01,11} + q_{01,00}$. Hence, it is possible to find $T, p > 0$ such that the statement of Theorem 22 does not hold true in state $i = (10)$ and $\phi = \mathcal{P}^{\forall}_{\geq p}(\mathbf{X}^{[0;T]}\mathrm{tt})$. ◀

4 Evaluation

In this section we present the results of a numerical assessment of UCTMC lumpability in terms of both its effectiveness and computation time.

Set-up. For our evaluation we used benchmarks from the literature. We considered CTMCs which describe: a protocol for wireless group communication [38]; a dependable cluster of workstations [28]; a peer-to-peer file distribution protocol based on BitTorrent [37]. These models are available in the MRMC format [32], generated from PRISM [36]. Each benchmark represents a family of models of increasing size, as a function of a parameter N that describes the number of components in the system. We considered uncertain variants of these CTMCs by assuming that all transition rates were subject to uncertainty. In particular, we considered equal (but arbitrarily chosen) uncertainty intervals with bounds $m_{i,j} < M_{i,j}$ for all non-zero transitions of the original CTMCs that had equal values.

We remark that, in general, it is not the case that an ordinary lumpability of the original CTMC is a UCTMC lumpability of the so-constructed UCTMC (whereas the converse does indeed hold owing to Lemma 10). To see this, consider the CTMC depicted in Figure 3. Then, condition **(i)** ensures that any UCTMC lumpability of the so-constructed UCTMC has the adjoint partition $\{\{e\} \mid e \in \mathcal{E}\}$. This, however, precludes the ordinary lumpability $\{\{A, B\}, \{C, D\}\}$ from being a UCTMC lumpability. Hence, one can measure the effectiveness of UCTMC lumping by showing how much the coarsest UCTMC lumpability refines the coarsest ordinary lumpability on the original CTMC. Instead, the comparison of the runtimes of the minimization algorithms provides an indication of the increased overhead for the reduction (which is of a factor equal to the number states for the worst case complexity). For our analysis we considered a prototype implementation of the UCTMC minimization algorithm in the tool ERODE [11], which supports CTMC minimization as a special case of lumping algorithms for non-linear ordinary differential equations [10, 12].[3]

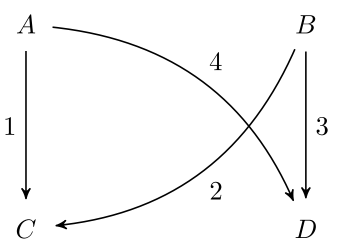

Figure 3 Counterexample.

Results. The results are provided in Table 1. For each benchmark we instantiated different CTMCs with increasing values of the system's size N, and report the number of transitions and states in the second and third column, respectively. The initial input partition of states, denoted by $\mathcal{H}_0$, was induced by the original model specification by creating blocks of states characterized by the same atomic propositions. Runtimes refer to the execution of ERODE on a common desktop machine with 8 GB of RAM.

[3] The tool and the information on how to replicate the experiments is available at `https://sysma.imtlucca.it/tools/erode/UCTMC/`.

Original model (CTMC)				*CTMC Lumpability*		*UCTMC Lumpability*		
N	$\lvert\mathcal{E}\rvert$	$\lvert\mathcal{V}\rvert$	$\lvert\mathcal{H}_0\rvert$	*Red.(s)*	$\lvert\mathcal{H}\rvert$	*Red.(s)*	$\lvert\mathcal{H}\rvert$	$\lvert\mathcal{G}\rvert$
*FDT3E3_PE16E4_S4OD(**N**), from [38]*								
4	5 369	1 125	2	1.30E–2	71	2.67E–1	71	351
16	686 153	103 173	2	4.90E+0	4 846	1.61E+1	4 846	32 947
32	10 954 382	1 329 669	2	5.15E+1	58 906	*Out of memory*		
*WORKSTATION_CLUSTER_(**N**), from [28]*								
8	12 832	2 772	4	1.59E–1	1 413	2.82E–1	1 413	6 443
32	186 400	38 676	4	1.12E+0	19 437	3.20E+0	19 437	93 299
128	2 908 192	597 012	4	2.42E+1	298 893	1.13E+2	298 893	1 454 483
192	6 524 960	1 337 876	4	7.14E+1	669 517	9.31E+2	669 517	3 263 059
256	11 583 520	2 373 652	4	1.75E+2	1 187 597	*Out of memory*		
*TORRENT_(**N**), from [37]*								
2	5 121	1 024	3	7.50E–2	56	2.70E–1	56	141
3	245 761	32 768	3	5.08E–1	252	5.75E+0	252	883
4	10 485 761	1 048 576	3	2.06E+1	792	*Out of memory*		

Table 1 Benchmarks for UCTMC lumpability.

In all our tests UCTMC lumpability gave rise to the same reductions as ordinary lumpability (columns $|\mathcal{H}|$ indicate the size of the coarsest refinement of the initial partition $\mathcal{H}_0$ for both algorithms), demonstrating its potential effectiveness in practice. For completeness, Table 1 also reports the size of the adjoint partitions $|\mathcal{G}|$. As for the runtimes, we registered no more than two while-loop iterations in Algorithm 1 for each model. This enabled reductions of UCTMCs with over 1 million states and 5 million transitions, with runtimes that were about 10 times slower than the CTMC counterpart in the worst case. Larger instance issued out-of-memory errors. However, we do expect improved performance for more mature implementations of the UCTMC lumping algorithm, which is part of future work.

5 Conclusion

Uncertain continuous-time Markov chains (UCTMCs) are a conservative generalization of continuous-time Markov chains (CTMCs) by allowing transition rates to non-deterministically take values within given bounded intervals. We presented UCTMC lumpability as a conservative generalization of ordinary lumpability to UCTMCs. It enjoys a polynomial time and space algorithm for the computation of the largest UCTMC lumpability that refines a given initial partition of the UCTMC states. Similarly to the preservation of sums of probability distributions in CTMC lumping, UCTMC lumping preserves reachable sets of sums of probability distributions. In addition, it is characterized logically in terms of the preservation of continuously stochastic logic, which we appropriately adapted to the continuous-time uncertain setting. We showed the practical applicability of UCTMC lumpability in practice by presenting substantial reductions in a number of benchmark models. The most pressing line of future work is to extend lumpability to other nonlinear uncertain dynamical systems such as ordinary differential equations.

References

1. Adnan Aziz, Kumud Sanwal, Vigyan Singhal, and Robert Brayton. Model-checking continuous-time Markov chains. *ACM Trans. Comput. Logic*, 1(1):162–170, 2000.
2. Giovanni Bacci, Giorgio Bacci, Kim G. Larsen, and Radu Mardare. On the Metric-Based Approximate Minimization of Markov Chains. In *ICALP*, pages 104:1–104:14, 2017.
3. Christel Baier, Boudewijn R. Haverkort, Holger Hermanns, and Joost-Pieter Katoen. Model-Checking Algorithms for Continuous-Time Markov Chains. *IEEE Trans. Software Eng.*, 29(6):524–541, 2003.
4. Luca Bortolussi and Jane Hillston. Fluid Model Checking. In *CONCUR*, pages 333–347, 2012.
5. Luca Bortolussi and Jane Hillston. Model checking single agent behaviours by fluid approximation. *Inf. Comput.*, 242:183–226, 2015.
6. Peter Buchholz. Exact and ordinary lumpability in finite Markov chains. *Journal of Applied Probability*, 31(1):59–75, 1994.
7. Peter Buchholz, Ernst Moritz Hahn, Holger Hermanns, and Lijun Zhang. Model Checking Algorithms for CTMDPs. In *CAV*, pages 225–242, 2011.
8. Yuliya Butkova, Hassan Hatefi, Holger Hermanns, and Jan Krcál. Optimal continuous time Markov decisions. In *ATVA*, pages 166–182, 2015.
9. Benoît Caillaud, Benoît Delahaye, Kim G. Larsen, Axel Legay, Mikkel L. Pedersen, and Andrzej Wasowski. Constraint Markov chains. *Theoretical Computer Science*, 412(34):4373 – 4404, 2011.
10. Luca Cardelli, Mirco Tribastone, Max Tschaikowski, and Andrea Vandin. Symbolic computation of differential equivalences. In *POPL*, pages 137–150, 2016.
11. Luca Cardelli, Mirco Tribastone, Max Tschaikowski, and Andrea Vandin. ERODE: A tool for the evaluation and reduction of ordinary differential equations. In *TACAS*, 2017.
12. Luca Cardelli, Mirco Tribastone, Max Tschaikowski, and Andrea Vandin. Maximal aggregation of polynomial dynamical systems. *Proceedings of the National Academy of Sciences*, 114(38):10029–10034, 2017.
13. Luca Cardelli, Mirco Tribastone, Max Tschaikowski, and Andrea Vandin. Guaranteed error bounds on approximate model abstractions through reachability analysis. In *QEST*, pages 104–121, 2018.
14. Milan Češka, Frits Dannenberg, Nicola Paoletti, Marta Kwiatkowska, and Luboš Brim. Precise parameter synthesis for stochastic biochemical systems. *Acta Informatica*, 54(6):589–623, 2017.
15. Edmund M. Clarke, E. Allen Emerson, and Joseph Sifakis. Model checking: algorithmic verification and debugging. *Commun. ACM*, 52(11):74–84, 2009.
16. René David and Hassane Alla. *Discrete, Continuous, and Hybrid Petri Nets*. Springer, 2005.
17. Christian Dehnert, Sebastian Junges, Nils Jansen, Florian Corzilius, Matthias Volk, Harold Bruintjes, Joost-Pieter Katoen, and Erika Ábrahám. PROPhESY: A PRObabilistic ParamEter SYnthesis Tool. In *CAV*, pages 214–231, 2015.
18. Salem Derisavi, Holger Hermanns, and William H. Sanders. Optimal state-space lumping in markov chains. *Inf. Process. Lett.*, 87(6):309–315, 2003.
19. Josee Desharnais, Vineet Gupta, Radha Jagadeesan, and Prakash Panangaden. Metrics for Labeled Markov Systems. In *CONCUR*, pages 258–273, 1999.
20. Alessandro D'Innocenzo, Alessandro Abate, and Joost-Pieter Katoen. Robust PCTL model checking. In *HSCC*, pages 275–286, 2012.
21. Harald Fecher, Martin Leucker, and Verena Wolf. *Don't Know* in probabilistic systems. In *SPIN*, pages 71–88, 2006.

22 Giuliana Franceschinis and Richard R. Muntz. Bounds for Quasi-Lumpable Markov Chains. *Perform. Eval.*, 20(1-3):223–243, 1994.

23 D.T. Gillespie. Exact stochastic simulation of coupled chemical reactions. *Journal of Physical Chemistry*, 81(25):2340–2361, December 1977.

24 Xianping Guo and Onesimo Hernandez-Lerma. *Continuous-Time Markov Decision Processes*. Springer Verlag, 2009.

25 Ernst Moritz Hahn, Holger Hermanns, Ralf Wimmer, and Bernd Becker. Transient Reward Approximation for Continuous-Time Markov Chains. *IEEE Trans. Reliability*, 64(4):1254–1275, 2015.

26 Ernst Moritz Hahn, Holger Hermanns, and Lijun Zhang. Probabilistic reachability for parametric Markov models. *STTT*, 13(1):3–19, 2011.

27 Vahid Hashemi, Andrea Turrini, Ernst Moritz Hahn, Holger Hermanns, and Khaled M. Elbassioni. Polynomial-Time Alternating Probabilistic Bisimulation for Interval MDPs. In *SETTA*, pages 25–41, 2017.

28 B.R. Haverkort, H. Hermanns, and J.-P. Katoen. On the use of model checking techniques for dependability evaluation. In *SRDS*, pages 228–237, 2000.

29 Holger Hermanns and Michael Rettelbach. Syntax, semantics, equivalences, and axioms for MTIPP. In *Proceedings of Process Algebra and Probabilistic Methods*, pages 71–87, Erlangen, 1994.

30 Jane Hillston. *A Compositional Approach to Performance Modelling*. Cambridge University Press, 1996.

31 Bengt Jonsson and Kim G. Larsen. Specification and refinement of probabilistic processes. In *LICS*, pages 266–277, 1991.

32 J.-P. Katoen, M. Khattri, and I.S. Zapreev. A Markov Reward Model Checker. In *QEST*, pages 243–244, 2005.

33 Joost-Pieter Katoen, Daniel Klink, Martin Leucker, and Verena Wolf. Three-valued abstraction for continuous-time Markov chains. In *CAV*, pages 311–324, 2007.

34 J.G. Kemeny and J.L. Snell. *Finite Markov Chains*. Springer New York, Heidelberg, Berlin, 1976.

35 Igor O. Kozine and Lev V. Utkin. Interval-valued finite Markov chains. *Reliable Computing*, 8(2):97–113, Apr 2002.

36 M. Kwiatkowska, G. Norman, and D. Parker. PRISM 4.0: Verification of Probabilistic Real-time Systems. In *CAV*, pages 585–591, 2011.

37 M. Z. Kwiatkowska, G. Norman, and D. Parker. Symmetry reduction for probabilistic model checking. In *CAV*, pages 234–248, 2006.

38 M. Massink, J.-P. Katoen, and D. Latella. Model checking dependability attributes of wireless group communication. In *DSN*, pages 711–720, 2004.

39 Martin R. Neuhäußer and Joost-Pieter Katoen. Bisimulation and Logical Preservation for Continuous-Time Markov Decision Processes. In *CONCUR*, pages 412–427, 2007.

40 Mahmoud Salamati, Sadegh Soudjani, and Rupak Majumdar. Approximate time bounded reachability for CTMCs and CTMDPs: A Lyapunov approach. In *QEST*, pages 389–406, 2018.

41 Koushik Sen, Mahesh Viswanathan, and Gul Agha. Model-checking Markov chains in the presence of uncertainties. In *TACAS*, pages 394–410, 2006.

42 Péter L. Simon, Michael Taylor, and Istvan Z. Kiss. Exact epidemic models on graphs using graph-automorphism driven lumping. *Journal of Mathematical Biology*, 62(4):479–508, 2010.

43 Lei Song, Lijun Zhang, and Jens Chr. Godskesen. Bisimulations and Logical Characterizations on Continuous-Time Markov Decision Processes. In *VMCAI*, pages 98–117, 2014.

44 William J. Stewart. *Probability, Markov Chains, Queues, and Simulation*. Princeton University Press, 2009.

45 Antti Valmari and Giuliana Franceschinis. Simple $O(m \log n)$ time Markov chain lumping. In *TACAS*, pages 38–52, 2010.

46 Franck van Breugel and James Worrell. Towards quantitative verification of probabilistic transition systems. In *ICALP*, pages 421–432, 2001.

Proofs

To allow for a concise presentation, $(\mathcal{H}, \mathcal{G})$ denotes in the following a partition of $(\mathcal{V}, \mathcal{E})$ that is not necessarily a UCTMC lumpability and its adjoint.

Proof of Theorem 4. It suffices to observe that standard lumpability conditions [10, 6] carry over in a straightforward manner to the case when transition rates are time-varying. ◀

Lemma 10. Since $\mathcal{G} = \mathcal{G}_d$, property **(i)** ensures that $m_G = m_{i,j} = M_{i,j} = M_G$ for all $G \in \mathcal{G}$ and $(i, j) \in G$. With this, property **(iii)** yields the claim. ◀

Proof of Theorem 12. Let us first prove statement 2). Since the only-if direction is trivial, let us assume that **(i)**,**(iii)** hold true. If $\mathcal{G}_n = \emptyset$, it trivially holds true that $Q = Q^d$ and the claim is trivial. If $\mathcal{G}_n \neq \emptyset$, instead, fix some arbitrary $G_0 \in \mathcal{G}_n$, pick some *irrational* number $q_{G_0} \in (m_{G_0}; M_{G_0})$ and set $q_{i,j} := q_{G_0}$ for all $(i, j) \in G_0$. Instead, for all $G \in \mathcal{G}_n$ with $G \neq G_0$, pick some *rational* number $q_G \in [m_G; M_G]$ and set $q_{i,j} := q_G$ for all $(i, j) \in G$. Since $\mathcal{H}$ is an ordinary lumpability of $Q = Q^d + \sum_{G \in \mathcal{G}_n} q_G \chi^G$ for this particular choice of (time constant) transition rate functions, it is easy to see that $\mathcal{H}$ has to be an ordinary lumpability of χ^{G_0}. This is because

- entries of Q^d are rational numbers because $q_G \in \mathbb{Q}$ for all $G \in \mathcal{G}_d$;
- entries of $q_G \chi^G$ are rational numbers if $G \in \mathcal{G}_n \setminus \{G_0\}$;
- entries of $q_{G_0} \chi^{G_0}$ are irrational numbers;
- integer multiples of rational numbers are rational numbers;
- integer multiples of irrational numbers are irrational numbers.

This shows that $\mathcal{H}$ is an ordinary lumpability of each χ^G with $G \in \mathcal{G}_n$. To see that $\mathcal{H}$ is also an ordinary lumpability Q^d, assume that we are given some admissible $(q_{i,j})_{(i,j) \in \mathcal{E}}$ such that $q_G = q_{i,j}$ for all $G \in \mathcal{G}$ and $(i, j) \in G$. Then, thanks to above discussion, $\mathcal{H}$ is an ordinary lumpability of Q and each $q_G \chi^G$ with $G \in \mathcal{G}_n$. Hence, $\mathcal{H}$ is an ordinary lumpability of $Q^d = Q - \sum_{G \in \mathcal{G}_n} q_G \chi^G$.

We next prove statement 1). Let us assume that we are given two UCTMC lumpability partitions $(\mathcal{H}_1, \mathcal{G}_1)$, $(\mathcal{H}_2, \mathcal{G}_2)$. We next show that $(\mathcal{H}, \mathcal{G})$ satisfies **(i)**-**(iii)**, where, by denoting the transitive closure of equivalence relations by an asterisk, we define

- $\mathcal{H} := \mathcal{V}/(\sim_{\mathcal{H}_1} \cup \sim_{\mathcal{H}_2})^*$ with $i \sim_{\mathcal{H}_\nu} j$ when $i, j \in H$ for some $H \in \mathcal{H}_\nu$ and;
- $\mathcal{G} := \mathcal{E}/(\sim_{\mathcal{G}_1} \cup \sim_{\mathcal{G}_2})^*$ if $(i_k, j_k) \sim_{\mathcal{G}_\nu} (i_l, j_l)$ when $(i_k, j_k), (i_l, j_l) \in G$ for some $G \in \mathcal{G}_\nu$.

Since $\mathcal{G}$ satisfies **(i)**, statement 2) ensures that $(\mathcal{H}, \mathcal{G})$ satisfies **(i)**,**(iii)**. Assume that we are given arbitrary $G_1 \in \mathcal{G}_1$ and $G_2 \in \mathcal{G}_2$ such that $(i_l, j_l) \in G_1 \cap G_2$. Fix arbitrary $(i_k, j_k) \in G_1$ and $(i_m, j_m) \in G_2$. If (i_l, j_l) is deterministic, then (i_k, j_k) and (i_m, j_m) must be deterministic as well. Instead, if (i_l, j_l) is not deterministic, it suffices to prove that $(i_k, j_k) \approx_{(\mathcal{H}_1, \mathcal{G}_1)} (i_l, j_l)$ and $(i_l, j_l) \approx_{(\mathcal{H}_2, \mathcal{G}_2)} (i_m, j_m)$ implies $(i_k, j_k) \approx_{(\mathcal{H}, \mathcal{G})} (i_m, j_m)$. To this end, we first observe that the assumption yields the existence of $H_1, H_1' \in \mathcal{H}_1$ and $H_2, H_2' \in \mathcal{H}_2$ such that

- $(i_k, j_k) \in \mathcal{E}$ with $i_k \in H_1$ and $j_k \in H'_1$;
- $(i_l, j_l) \in \mathcal{E}$ with $i_l \in H_1$ and $j_l \in H'_1$;
- $(i_l, j_l) \in \mathcal{E}$ with $i_l \in H_2$ and $j_l \in H'_2$;
- $(i_m, j_m) \in \mathcal{E}$ with $i_m \in H_2$ and $j_m \in H'_2$.

Since $i_l \in H_1 \cap H_2$ and $j_l \in H'_1 \cap H'_2$, the definition of $\mathcal{H}$ ensures the existence of $H, H' \in \mathcal{H}$ such that $H_1, H_2 \subseteq H$ and $H'_1, H'_2 \subseteq H'$. With this, we infer that

- $(i_k, j_k) \in \mathcal{E}$ with $i_k \in H$ and $j_k \in H'$;
- $(i_m, j_m) \in \mathcal{E}$ with $i_m \in H$ and $j_m \in H'$,

which readily implies that $(i_k, j_k) \approx_{(\mathcal{H},\mathcal{G})} (i_m, j_m)$. Overall, we infer that $(\mathcal{H}, \mathcal{G})$ satisfies **(i)**-**(iii)**. Let $\mathcal{G}'$ denote the partition of $\mathcal{E}$ that is induced by $\mathcal{H}$ via **(i)** and **(ii)**. By construction, $\mathcal{G}$ is a refinement of $\mathcal{G}'$. If $\mathcal{G} = \mathcal{G}'$, it trivially holds true that $\mathcal{H}$ is a UCTMC lumpability with adjoint $\mathcal{G}$. Instead, if $\mathcal{G}$ is a proper refinement of $\mathcal{G}'$, it can be easily seen that **(iii)** remains true when $\mathcal{G}$ is replaced with $\mathcal{G}'$ (because $\mathcal{G}$ refines $\mathcal{G}'$). This, in turn, implies that $\mathcal{H}$ is a UCTMC lumpability with adjoint $\mathcal{G}'$, thus yielding the claim. ◀

Proof of Theorem 13. Let $(\mathcal{H}, \mathcal{G})$ be the UCTMC lumpability in question. For arbitrary $G \in \mathcal{G}$ and $(i_k, j_k) \in G$, let $f_i^{i_k,j_k}$ denote the change in π_i due to q_{i_k,j_k}. More formally, if $f(\pi) := \pi^T Q$ for all $\pi \in \mathbb{R}^{\mathcal{V}}$, then $f_i^{i_k,j_k} := \partial_{q_{i_k,j_k}} f_i$. It is not hard to see that

$$f_i^{i_k,j_k} = \begin{cases} -\pi_{i_k} & , \ i = i_k \\ \pi_{i_k} & , \ i = j_k \end{cases}$$

For an arbitrary $H \in \mathcal{H}$, we note that

$$\begin{aligned} \partial_t\Big(\sum_{i\in H} \pi_i(t)\Big) &= \sum_{i\in H} \sum_{G\in\mathcal{G}} \sum_{(i_k,j_k)\in G} q_{i_k,j_k}(t) f_i^{i_k,j_k}(\pi(t)) \\ &= \sum_{G\in\mathcal{G}} \sum_{(i_k,j_k)\in G} q_{i_k,j_k}(t) \sum_{i\in H} f_i^{i_k,j_k}(\pi(t)) \\ &= \sum_{G\in\mathcal{G}} q_{G,H}(t) \sum_{(i_l,j_l)\in G} \sum_{i\in H} f_i^{i_l,j_l}(\pi(t)), \end{aligned}$$

provided that $q_{G,H}$ satisfies

$$q_{G,H}(t) \sum_{(i_l,j_l)\in G} \sum_{i\in H} f_i^{i_l,j_l}(\pi(t)) = \sum_{(i_k,j_k)\in G} q_{i_k,j_k}(t) \sum_{i\in H} f_i^{i_k,j_k}(\pi(t))$$

When $\sum_{(i_l,j_l)\in G} \sum_{i\in H} f_i^{i_l,j_l}(\pi(t)) \neq 0$, it must obviously hold true that

$$q_{G,H}(t) = \sum_{(i_k,j_k)\in G} q_{i_k,j_k}(t) \Big(\frac{\sum_{i\in H} f_i^{i_k,j_k}(\pi(t))}{\sum_{(i_l,j_l)\in G} \sum_{i\in H} f_i^{i_l,j_l}(\pi(t))} \Big) \tag{5}$$

If the denominator is zero, instead, the value $q_{G,H}(t)$ can be chosen arbitrarily. We next show that setting $q_{G,H} := q_G$ does the job if

$$q_G(t) = \begin{cases} \text{admissible value} & , \ G \in \mathcal{G}_d \cup \mathcal{G}_i \text{ or } \sum_{(i_l,j_l)\in G} \pi_{i_l}(t) = 0 \\ \sum_{(i_k,j_k)\in G} q_{i_k,j_k}(t) \Big(\frac{\pi_{i_k}(t)}{\sum_{(i_l,j_l)\in G} \pi_{i_l}(t)} \Big) & , \ \text{otherwise} \end{cases}$$

for all $G \in \mathcal{G}$ and $t \geq 0$, provided that $\mathcal{G}_i$ denotes the set of invariant blocks in $\mathcal{G}$. Key to this is to prove that the value of the fraction term in (5) is, whenever defined, invariant with respect to $H \in \mathcal{H}$. To see this, fix an arbitrary non-deterministic $G \in \mathcal{G}$, $(i_k, j_k) \in G$ and $H, H' \in \mathcal{H}$ such that $H \neq H'$. We consider the following case distinction.

- $i_k \in H \wedge j_k \in H'$: Since $(\mathcal{H}, \mathcal{G})$ is a UCTMC lumpability, it holds that $i_l \in H \wedge j_l \in H'$ for all $(i_l, j_l) \in G$. Hence

  $$\frac{\sum_{i \in H} f_i^{i_k, j_k}(\pi(t))}{\sum_{(i_l, j_l) \in G} \sum_{i \in H} f_i^{i_l, j_l}(\pi(t))} = \frac{-\pi_{i_k}(t)}{-\sum_{(i_l, j_l) \in G} \pi_{i_l}(t)}$$

  and

  $$\frac{\sum_{i \in H'} f_i^{i_k, j_k}(\pi(t))}{\sum_{(i_l, j_l) \in G} \sum_{i \in H'} f_i^{i_l, j_l}(\pi(t))} = \frac{\pi_{i_k}(t)}{\sum_{(i_l, j_l) \in G} \pi_{i_l}(t)},$$

  meaning that both fraction terms are either identical or undefined. In the latter case, neither H nor H' constrain the value of q_G.
- $i_k \in H \wedge j_k \in H$: Since $(\mathcal{H}, \mathcal{G})$ is a UCTMC lumpability, it holds that $i_l \in H \wedge j_l \in H$ for all $(i_l, j_l) \in G$. Hence

  $$\sum_{(i_l, j_l) \in G} \sum_{i \in H} f_i^{i_l, j_l}(\pi(t)) = \sum_{(i_l, j_l) \in G} (\pi_{i_l}(t) - \pi_{i_l}(t)) = 0$$

  for all $t \geq 0$, meaning that H does not constrain the value of q_G (note that in this case G is invariant).
- $i_k \notin H \wedge j_k \notin H$: Let $H_1, H_2 \in \mathcal{H}$ be such that $i_k \in H_1$ and $j_k \in H_2$. Since $(\mathcal{H}, \mathcal{G})$ is a UCTMC lumpability, it holds that $i_l \in H_1 \wedge j_l \in H_2$ for all $(i_l, j_l) \in G$. Hence $\sum_{(i_l, j_l) \in G} \sum_{i \in H} f_i^{i_l, j_l}(\pi(t)) = 0$ for all $t \geq 0$, meaning that H does not constrain the value of q_G.

Since the above discussion shows that $q_{G,H} = q_G$ for all non-deterministic $G \in \mathcal{G}$ and $H \in \mathcal{H}$ whenever $q_{G,H}$ is defined, we infer that

$$\begin{aligned} \partial_t \Big(\sum_{i \in H} \pi_i(t) \Big) &= \sum_{i \in H} \sum_{G \in \mathcal{G}} \sum_{(i_k, j_k) \in G} q_{i_k, j_k}(t) f_i^{i_k, j_k}(\pi(t)) \\ &= \sum_{i \in H} \sum_{G \in \mathcal{G}} \sum_{(i_k, j_k) \in G} q_G(t) f_i^{i_l, j_l}(\pi(t)) \end{aligned} \tag{6}$$

for all $H \in \mathcal{H}$. That is, if we replace, for all $G \in \mathcal{G}$ and $(i_k, j_k) \in G$, the transition rate $q_{i_k, j_k}(t)$ with $q_G(t)$, the solution of the forward Kolmogorov equation will not be affected as far as sums $\sum_{i \in H} \pi_i$, where $H \in \mathcal{H}$, are considered. This and the fact that $(\mathcal{H}, \mathcal{G})$ is a UCTMC lumpability yields, together with Theorem 4, the statement

$$\mathcal{R}\Big(\sum_{i \in H} \pi_i, t \Big) \subseteq \mathcal{R}\Big(\hat{\pi}_{i_H}, t \Big), \qquad \text{for all} \quad H \in \mathcal{H}, \ t \geq 0.$$

To see the second part of the theorem, set $q_{i,j}(t) := q_G(t)$ for all $G \in \mathcal{G}$, $(i, j) \in G$ and $t \geq 0$, where q_G is as above. With this, the foregoing discussion remains valid, allowing us to conclude the claim thanks to Lemma 14. ◀

Theorem 15. Since $m' \leq m$ and $M \leq M'$, statement 1) follows as a direct application of Theorem 13 to $(\mathcal{V}, \mathcal{E}, m', M', \pi[0])$. To see statement 2), consider the running example from Figure 1 in the case when $\pi[0]$ is a uniform probability distribution and

$$m_{11,10} = M_{11,10} = m_{11,01} = M_{11,01} = 0$$
$$m_{00,10} = M_{00,10} = m_{00,01} = M_{00,01} = 0$$
$$m_{10,11} = M_{10,11} = m_{10,00} = M_{10,00} = m_{10,01} = M_{10,01} = 1$$
$$m_{01,11} = M_{01,11} = m_{01,00} = M_{01,00} = m_{01,10} = M_{01,10} = 2$$

Note that in this case the UCTMC from Figure 1 degenerates to a deterministic CTMC. Moreover

$$\partial_t \pi_{10} = -q_{10,11}\pi_{10} - q_{10,01}\pi_{10} - q_{10,00}\pi_{10} + q_{11,10}\pi_{11} + q_{01,10}\pi_{01} + q_{00,10}\pi_{00}$$
$$\partial_t \pi_{01} = -q_{01,11}\pi_{01} - q_{01,10}\pi_{01} - q_{01,00}\pi_{01} + q_{11,01}\pi_{11} + q_{10,01}\pi_{10} + q_{00,01}\pi_{00}$$

yield $\partial_t \pi_{10}(0) = -1/4$ and $\partial_t \pi_{01}(0) = -5/4$.

Note that partition (1) is not a UCTMC lumpability for the above choice of m, M. However, if we define m' and M' by using the partition $\mathcal{G}$ from (1), we get

$$m'_{11,10} = m'_{11,01} = 0 \qquad m'_{10,11} = m'_{10,00} = m'_{10,01} = 1$$
$$M'_{11,10} = M'_{11,01} = 0 \qquad M'_{10,11} = M'_{10,00} = M'_{10,01} = 2$$
$$m'_{00,10} = m'_{00,01} = 0 \qquad m'_{01,11} = m'_{01,00} = m'_{01,01} = 1$$
$$M'_{00,10} = M'_{00,01} = 0 \qquad M'_{01,11} = M'_{01,00} = M'_{01,01} = 2$$

With this, partition $\mathcal{H}$ from (1) is a UCTMC lumpability of the UCTMC $(\mathcal{V}, \mathcal{E}, m', M', \pi[0])$. Moreover, the bounds m' and M' allow us to chose

$$q_{10,11} \equiv q_{10,01} \equiv q_{10,00} = 2 \qquad q_{01,11} \equiv q_{01,10} \equiv q_{01,00} = 1$$

which give rise to $\partial_t \pi_{10}(0) = -5/4$ and $\partial_t \pi_{01}(0) = -1/4$. Noting that this does not coincide with the derivatives of the deterministic CTMC from above, we infer statement 2). ◀

Lemma 14. For any $G_0 \in \mathcal{G}_d$, we set $q_{G_0} := m_{G_0}$ (note that $M_{G_0} = m_{G_0}$). Instead, for any $G_0 \in \mathcal{G}_n$, we first observe that there exist unique $H, H' \in \mathcal{H}$ such that $i_k, i_l \in H$ and $j_k, j_l \in H'$ for all $(i_k, j_k), (i_l, j_l) \in G_0$. Let $\mathcal{G}_0 \subseteq \mathcal{G}_n$ denote all blocks whose transitions originate in H and go to H' (note, in particular, that $G_0 \in \mathcal{G}_0$). Since Q^d is known because it is induced by $(q_G)_{G \in \mathcal{G}_d}$, it suffices to find $(q_G)_{G \in \mathcal{G}_0}$ satisfying

$$\xi := \hat{q}_{i_H, i_{H'}} - \sum_{j \in H'} q^d_{i_H, j} \equiv \sum_{G \in \mathcal{G}_0} \mu_G(i_H, i_{H'}) q_G$$

To this end, define $\theta(s) := \sum_{G \in \mathcal{G}_0} \mu_G(i_H, i_{H'}) \big(m_G + (M_G - m_G)s\big)$ and observe that, for any $z \in [\theta(0); \theta(1)]$, it holds that $\theta(s(z)) = z$ when

$$s(z) := \Big(z - \sum_{G \in \mathcal{G}_0} \mu_G(i_H, i_{H'}) m_G\Big) / \Big(\sum_{G \in \mathcal{G}_0} \mu_G(i_H, i_{H'})(M_G - m_G)\Big)$$

Since $t \mapsto s(\xi(t))$ is finitely piecewise analytic, so is $q_G(t) := \big(m_G + (M_G - m_G)s(\xi(t))\big)$ for every $G \in \mathcal{G}_0$. This yields the claim. ◀

Proof of Theorem 16. Let us assume towards a contradiction that there exist $G \in \mathcal{G}_n$, $(i_k, j_k), (i_l, j_l) \in G$ and $H_{i_k}, H_{j_k}, H_{i_l}, H_{j_l} \in \mathcal{H}$ satisfying the following three conditions:

- $i_k \in H_{i_k}, j_k \in H_{j_k}$ and $i_l \in H_{i_l}, j_l \in H_{j_l}$;
- $H_{i_k} \neq H_{j_k}$ and $H_{i_l} \neq H_{j_l}$;
- $H_{i_k} \neq H_{i_l}$ or $H_{j_k} \neq H_{j_l}$.

We consider the following case distinction.

- $H_{j_k} \neq H_{j_l}$: By setting $H := H_{j_k}$, $H' := H_{j_l}$ and $\pi_\nu(0) := 0$ for all $\nu \notin \{i_k, i_l\}$, we infer that

$$\frac{\sum_{i \in H} f_i^{i_k,j_k}(\pi(0))}{\sum_{(i_\nu,j_\nu)\in G} \sum_{i\in H} f_i^{i_\nu,j_\nu}(\pi(0))} = \begin{cases} \frac{\pi_{i_k}(0)}{\pi_{i_k}(0)} & , H_{j_k} \neq H_{i_l} \\ \frac{\pi_{i_k}(0)}{\pi_{i_k}(0)-\pi_{i_l}(0)} & , H_{j_k} = H_{i_l} \end{cases}$$

and

$$\frac{\sum_{i \in H'} f_i^{i_k,j_k}(\pi(0))}{\sum_{(i_\nu,j_\nu)\in G} \sum_{i\in H'} f_i^{i_\nu,j_\nu}(\pi(0))} = \begin{cases} \frac{0}{\pi_{i_l}(0)} & , H_{j_l} \neq H_{i_k} \\ \frac{-\pi_{i_k}(0)}{\pi_{i_l}(0)-\pi_{i_k}(0)} & , H_{j_l} = H_{i_k} \end{cases}$$

Let $q_{i_k,j_k}(0) > 0$ while $q_{i_\nu,j_\nu}(0) = 0$ for all $(i_\nu, j_\nu) \neq (i_k, j_k)$. Moreover, let us pick $\pi_{i_k}(0) = 1/3$ and $\pi_{i_l}(0) = 2/3$. Thanks to the proof of Theorem 13, it has to hold that $q_{G,H}(0) = q_{G,H'}(0)$. At the same time, the only way to ensure that $q_{G,H}(0) = q_{G,H'}(0)$ is to require $H_{j_k} = H_{i_l}$ and $H_{j_l} = H_{i_k}$. This, however, yields the non-admissible transition rate value $q_{G,H}(0) = q_{G,H'}(0) = -1$.
- $H_{i_k} \neq H_{i_l}$: By setting $H := H_{i_k}$, $H' := H_{i_l}$ and $\pi_\nu(0) := 0$ for all $\nu \notin \{i_k, i_l\}$, we infer that

$$\frac{\sum_{i \in H} f_i^{i_k,j_k}(\pi(0))}{\sum_{(i_\nu,j_\nu)\in G} \sum_{i\in H} f_i^{i_\nu,j_\nu}(\pi(0))} = \begin{cases} \frac{-\pi_{i_k}(0)}{-\pi_{i_k}(0)} & , H_{j_l} \neq H_{i_k} \\ \frac{-\pi_{i_k}(0)}{-\pi_{i_k}(0)+\pi_{i_l}(0)} & , H_{j_l} = H_{i_k} \end{cases}$$

and

$$\frac{\sum_{i \in H'} f_i^{i_k,j_k}(\pi(0))}{\sum_{(i_\nu,j_\nu)\in G} \sum_{i\in H'} f_i^{i_\nu,j_\nu}(\pi(0))} = \begin{cases} \frac{0}{-\pi_{i_l}(0)} & , H_{j_k} \neq H_{i_l} \\ \frac{\pi_{i_k}(0)}{\pi_{i_k}(0)-\pi_{i_l}(0)} & , H_{j_k} = H_{i_l} \end{cases}$$

Let $q_{i_k,j_k}(0) > 0$ while $q_{i_\nu,j_\nu}(0) = 0$ for all $(i_\nu, j_\nu) \neq (i_k, j_k)$. Moreover, let us pick $\pi_{i_k}(0) = 1/3$ and $\pi_{i_l}(0) = 2/3$. Thanks to the proof of Theorem 13, it has to hold that $q_{G,H}(0) = q_{G,H'}(0)$. At the same time, the only way to ensure that $q_{G,H}(0) = q_{G,H'}(0)$ is to require $H_{j_k} = H_{i_l}$ and $H_{j_l} = H_{i_k}$. This, however, yields the non-admissible transition rate $q_{G,H}(0) = q_{G,H'}(0) = -1$.

Hence, it must hold that $H_{i_k} = H_{i_l}$ and $H_{j_k} = H_{j_l}$, thus showing the claim. ◀

Proof of Theorem 17. Since the first statement is a direct consequence of Theorem 12, let us consider the second statement. The computation of $\mathcal{G}'$ can be accomplished by sorting with respect to the lower and upper bounds which can be done in $\mathcal{O}(r \cdot \log(r))$ time and space. Since $r \leq s^2$, it holds that $\mathcal{O}(r \cdot \log(r)) = \mathcal{O}(r \cdot \log(s))$ and we can assume without loss of generality that $\mathcal{G}$ satisfies **(i)**. Write $\mathcal{G} \setminus \mathcal{G}_d = \{G_1, \ldots, G_\nu\}$. Then, $\mathcal{H}'$ can be obtained as follows. First, compute the coarsest ordinary lumpability of Q^d that refines $\mathcal{H}$ and store it as $\mathcal{H}_0$. Afterwards, compute $\mathcal{H}_1, \ldots, \mathcal{H}_\nu$, where $\mathcal{H}_{\nu'}$ is the coarsest lumpability of $\chi^{G_{\nu'}}$ that refines $\mathcal{H}_{\nu'-1}$ for $1 \leq \nu' \leq \nu$. By construction, it then holds that $\mathcal{H}_\nu = \mathcal{H}'$. The complexity statement, instead, follows by noting that the computation of $\mathcal{H}_{\nu'}$ and $\mathcal{H}_0$ requires at most $\mathcal{O}(|G_{\nu'}| \cdot s \cdot \log(s))$ and $\mathcal{O}(|\dot{\bigcup}_{G\in\mathcal{G}_d} G| \cdot s \cdot \log(s))$ time and space, respectively, see [18, 45]. ◀

Proof of Theorem 18. To see the correctness of Algorithm 18, let us assume that $(\mathcal{H}_*, \mathcal{G}_*)$ denotes the coarsest UCTMC lumpability that refines $\mathcal{H}$. Further, let $(\mathcal{H}_0, \mathcal{G}_0)$ be such that $\mathcal{H}_0 = \mathcal{H}$ and $\mathcal{G}_0$ is the coarsest refinement of $\mathcal{E}$ satisfying **(i)**. With this, define

$$\begin{aligned}\mathcal{G}_{\nu+1} &:= \text{coarsest refinement of } \mathcal{G}_\nu \text{ satisfying } \textbf{(ii)} \text{ w.r.t. } \mathcal{H}_\nu \\ \mathcal{H}_{\nu+1} &:= \text{coarsest refinement of } \mathcal{H}_\nu \text{ satisfying } \textbf{(iii)} \text{ w.r.t. } \mathcal{G}_{\nu+1}\end{aligned}$$

Then, the sequence $(\mathcal{H}_0, \mathcal{G}_0), (\mathcal{H}_1, \mathcal{G}_1), (\mathcal{H}_2, \mathcal{G}_2), \ldots$ is such that

a) $(\mathcal{H}_*, \mathcal{G}_*)$ is a refinement of $(\mathcal{H}_\nu, \mathcal{G}_\nu)$
b) $(\mathcal{H}_\nu, \mathcal{G}_\nu)$ is a refinement of $(\mathcal{H}_{\nu-1}, \mathcal{G}_{\nu-1})$

for all $\nu \geq 1$. The second claim is trivial. Instead, the first claim is shown by induction on ν.

- $\nu = 1$: Since $(\mathcal{H}_*, \mathcal{G}_*)$ is a refinement of $(\mathcal{H}_0, \mathcal{G}_0)$, it holds true that $(\mathcal{H}_*, \mathcal{G}_*)$ refines $(\mathcal{H}_0, \mathcal{G}_1)$. This and Theorem 12, in turn, implies that $(\mathcal{H}_*, \mathcal{G}_*)$ refines $(\mathcal{H}_1, \mathcal{G}_1)$.
- $\nu \to \nu + 1$: Since $(\mathcal{H}_*, \mathcal{G}_*)$ is a refinement of $(\mathcal{H}_\nu, \mathcal{G}_\nu)$ by induction hypothesis, it holds true that $(\mathcal{H}_*, \mathcal{G}_*)$ refines $(\mathcal{H}_\nu, \mathcal{G}_{\nu+1})$. This and Theorem 12, in turn, implies that $(\mathcal{H}_*, \mathcal{G}_*)$ refines $(\mathcal{H}_{\nu+1}, \mathcal{G}_{\nu+1})$.

We proceed by exploiting *a)* and *b)*. In particular, since $(\mathcal{H}_*, \mathcal{G}_*)$ is a refinement of any $(\mathcal{H}_\nu, \mathcal{G}_\nu)$, it holds that $(\mathcal{H}_*, \mathcal{G}_*) = (\mathcal{H}_\nu, \mathcal{G}_\nu)$ whenever $(\mathcal{H}_\nu, \mathcal{G}_\nu)$ is a UCTMC lumpability. Thanks to the fact that $(\mathcal{H}_\nu, \mathcal{G}_\nu)$ is a refinement of $(\mathcal{H}_{\nu-1}, \mathcal{G}_{\nu-1})$ for all $\nu \geq 1$ and since $\mathcal{V}$, $\mathcal{E}$ are finite, we can fix the smallest $\nu \geq 1$ such that $(\mathcal{H}_\nu, \mathcal{G}_\nu) = (\mathcal{H}_{\nu-1}, \mathcal{G}_{\nu-1})$. This yields

$$\begin{aligned}\mathcal{G}_\nu &= \text{satisfies } \textbf{(ii)} \text{ w.r.t. } \mathcal{H}_\nu \\ \mathcal{H}_\nu &= \text{satisfies } \textbf{(iii)} \text{ w.r.t. } \mathcal{G}_\nu,\end{aligned}$$

thus ensuring that $(\mathcal{H}_\nu, \mathcal{G}_\nu)$ is a UCTMC lumpability.

We are left with proving the statement concerning the complexity of the algorithm. Thanks to Theorem 17, line 4 requires at most $\mathcal{O}(r \cdot s \cdot \log(s))$ time and space. To see that this holds true also for line 3, we first note that sorting the transitions in a block $G \in \mathcal{G}_n$ with respect to origin and target blocks can be done in $\mathcal{O}(|G| \cdot \log(|G|))$ time and $\mathcal{O}(|G|)$ space. Hence, sorting all transitions in all blocks can be done in $\mathcal{O}(r \cdot \log(r))$ time and $\mathcal{O}(r)$ space. Since $r \leq s^2$, it holds that $\log(r) \leq 2\log(s)$, thus showing that line 3 requires at most $\mathcal{O}(r \cdot \log(s))$ time and $\mathcal{O}(r)$ space. The number of while loop iterations, instead, can be bounded as follows. Assume that we are at the beginning of the ν-th while loop iteration with $\nu \geq 2$. Then, if there is no refinement in line 3 during the ν-th iteration, there will be no refinement in line 4 during the ν-th iteration either. This is because line 4 in the $(\nu - 1)$-th iteration has been computed using the current value of $\mathcal{G}$. Instead, if during the ν-th iteration there is no refinement in line 4, there will be no refinement in line 3 in the $(\nu + 1)$-th iteration. This, in turn, implies that during the $(\nu + 1)$-th iteration there will be no refinement in line 4 either. ◀

Lemma 19. Thanks to the fact that all transitions of the UCTMC $(\mathcal{V}, \mathcal{E}, m, M, \pi[0])$ are deterministic, line 3 does not refine $\mathcal{G}$, while line 4 computes the coarsest ordinary lumpability thanks to Theorem 12. Observing that the second iteration of the while loop of Algorithm 1 does not lead to further refinements, we obtain the claim. ◀

Proof of Theorem 22

We prove Theorem 22 by exploiting the fact that the validity of an until formula can be expressed in terms of a reachability probability [3, 4, 5]. We begin by introducing a version of the auxiliary CTMC from [5] that is tailored to our needs.

▶ **Definition 23** (Auxiliary UCTMC)**.** Assume that $(\mathcal{H}, \mathcal{G})$ is a UCTMC lumpability of the UCTMC $(\mathcal{V}, \mathcal{E}, m, M, \pi[0])$. Moreover, let $\mathcal{U}, \mathcal{T} \subseteq \mathcal{V}$ be such that both $\mathcal{U}$ and $\mathcal{T}$ can be written as unions of blocks from $\mathcal{H}$. With this, $(\tilde{\mathcal{V}}, \tilde{\mathcal{E}}, \tilde{m}, \tilde{M}, \tilde{\pi}[0])$ is given by $\tilde{\mathcal{V}} = \mathcal{V} \cup \bar{\mathcal{V}}$, where $\bar{\mathcal{V}} = \{\bar{i} \mid i \in \mathcal{V}\}$, and

- $(i, j) \in \mathcal{E} \wedge i \notin \mathcal{U} \cup \mathcal{T} \wedge j \notin \mathcal{T}$ iff $(i, j) \in \mathcal{V} \times \mathcal{V}$;
- $(i, j) \in \mathcal{E} \wedge i \notin \mathcal{U} \cup \mathcal{T} \wedge j \in \mathcal{T}$ iff $(i, \bar{j}) \in \mathcal{V} \times \bar{\mathcal{V}}$;
- $\tilde{\mathcal{E}} \setminus \big((\mathcal{V} \times \mathcal{V}) \cup (\mathcal{V} \times \bar{\mathcal{V}})\big) = \emptyset$.

Moreover, $\tilde{\pi}[0]_i := \pi[0]_i$ and $\tilde{\pi}[0]_{\bar{i}} := 0$ for all $i \in \mathcal{V}$ and

- $\tilde{m}_{i,j} := m_{i,j}$ and $\tilde{M}_{i,j} := M_{i,j}$ for every $(i, j) \in \tilde{\mathcal{E}} \cap (\mathcal{V} \times \mathcal{V})$;
- $\tilde{m}_{i,\bar{j}} := m_{i,j}$ and $\tilde{M}_{i,\bar{j}} := M_{i,j}$ for every $(i, \bar{j}) \in \tilde{\mathcal{E}} \cap (\mathcal{V} \times \bar{\mathcal{V}})$.

Likewise, an admissible $(q_{i,j})_{(i,j)\in\mathcal{E}}$ induces the admissible $(\tilde{q}_{\iota,\iota'})_{(\iota,\iota')\in\tilde{\mathcal{E}}}$ via

- $\tilde{q}_{i,j} := q_{i,j}$ for every $(i, j) \in \tilde{\mathcal{E}} \cap (\mathcal{V} \times \mathcal{V})$;
- $\tilde{q}_{i,\bar{j}} := q_{i,j}$ for every $(i, \bar{j}) \in \tilde{\mathcal{E}} \cap (\mathcal{V} \times \bar{\mathcal{V}})$. ◀

For the benefit of presentation, let us assume without loss of generality that $\mathcal{V} = \{1, \ldots, n\}$, meaning that we have $\bar{\mathcal{V}} = \{\bar{1}, \ldots, \bar{n}\}$. As shown next, a UCTMC lumpability of $(\mathcal{V}, \mathcal{E}, m, M, \pi[0])$ induces a UCTMC lumpability of $(\tilde{\mathcal{V}}, \tilde{\mathcal{E}}, \tilde{m}, \tilde{M}, \tilde{\pi}[0])$.

▶ **Proposition** 24. Assume that $(\mathcal{H}, \mathcal{G})$ is a UCTMC lumpability of the UCTMC $(\mathcal{V}, \mathcal{E}, m, M, \pi[0])$. Moreover, let $\mathcal{U}, \mathcal{T} \subseteq \mathcal{V}$ be such that both $\mathcal{U}$ and $\mathcal{T}$ can be written as unions of blocks from $\mathcal{H}$. Then

$$\tilde{G} := \begin{cases} G & , \exists (i,j) \in G \text{ such that } i \notin \mathcal{U} \cup \mathcal{T} \wedge j \notin \mathcal{T} \\ \{(i, \bar{j}) \mid (i,j) \in G\} & , \exists (i,j) \in G \text{ such that } i \notin \mathcal{U} \cup \mathcal{T} \wedge j \in \mathcal{T} \\ \emptyset & , \text{otherwise} \end{cases}$$

is well-defined for all $G \in \mathcal{G}$ and $(\tilde{\mathcal{H}}, \tilde{\mathcal{G}})$ is a UCTMC lumpability of $(\tilde{\mathcal{V}}, \tilde{\mathcal{E}}, \tilde{m}, \tilde{M}, \tilde{\pi}[0])$, where $\tilde{\mathcal{H}} = \mathcal{H} \cup \bar{\mathcal{H}}$ and $\tilde{\mathcal{G}} = \{\tilde{G} \mid G \in \mathcal{G} \text{ and } \tilde{G} \neq \emptyset\}$.

Proof. Similarly to the definition of χ^G from the main text, let $\tilde{\chi}^G$ be the matrix encoding of the transitions in $\tilde{G}$, that is:

- $e_i^T \tilde{\chi}^G e_j = 1$ if $(i, j) \in G \wedge i \notin \mathcal{U} \cup \mathcal{T} \wedge j \notin \mathcal{T}$;
- $e_i^T \tilde{\chi}^G e_{\bar{j}} = 1$ if $(i, j) \in G \wedge i \notin \mathcal{U} \cup \mathcal{T} \wedge j \in \mathcal{T}$;
- $e_i^T \tilde{\chi}^G e_i = \sum_{j:j\neq i} e_i^T \tilde{\chi}^G (e_j + e_{\bar{j}})$ for all $i \in \mathcal{V}$;
- $e_\iota^T \tilde{\chi}^G e_{\iota'} = 0$ for any other $(\iota, \iota') \in \tilde{\mathcal{V}} \times \tilde{\mathcal{V}}$.

Pick arbitrary $G \in \mathcal{G}_n$, $(i_k, j_k) \in G$ and let $H_0, H_1 \in \mathcal{H}$ be such that $i_k \in H_0$ and $j_k \in H_1$. By exploiting that

- $i_l \in H_0$ and $j_l \in H_1$ for all $(i_l, j_l) \in G$ and;
- $\mathcal{U}$, $\mathcal{T}$ can be written as a unions of blocks from $\mathcal{H}$,

we make the following observations:

- If $i_k \notin \mathcal{U} \cup \mathcal{T} \wedge j_k \notin \mathcal{T}$: Then $i_l \notin \mathcal{U} \cup \mathcal{T} \wedge j_l \notin \mathcal{T}$ for all $(i_l, j_l) \in G$. Since this implies that $\tilde{\chi}^G = \begin{pmatrix} \chi^G & 0 \\ 0 & 0 \end{pmatrix}$ and $\mathcal{H}$ is an ordinary lumpability of χ^G by Theorem 12, it holds that $\mathcal{H} \cup \bar{\mathcal{H}}$ is an ordinary lumpability of $\tilde{\chi}^G$. Moreover, $i_l \in H_0$ and $j_l \in H_1$ for all $(i_l, j_l) \in G$, justifying that $\tilde{G} = G$.
- If $i_k \notin \mathcal{U} \cup \mathcal{T} \wedge j_k \in \mathcal{T}$: Then $i_l \notin \mathcal{U} \cup \mathcal{T} \wedge j_l \in \mathcal{T}$ for all $(i_l, j_l) \in G$. Since this implies that $\tilde{\chi}^G = \begin{pmatrix} \mathrm{diag}(\chi^G) & \chi^G - \mathrm{diag}(\chi^G) \\ 0 & 0 \end{pmatrix}$ and $\mathcal{H}$ is an ordinary lumpability of χ^G by Theorem 12, it holds that $\mathcal{H} \cup \bar{\mathcal{H}}$ is an ordinary lumpability of $\tilde{\chi}^G$. Moreover, $i_l \in H_0$ and $\bar{j}_l \in \bar{H}_1$ for all $(i_l, j_l) \in G$, justifying that $\tilde{G} = \{(i_l, \bar{j}_l) \mid (i_l, j_l) \in G\}$.
- If (i_k, j_k) does not satisfy either of the two conditions from above: Then none of the transitions in G induces a transition, meaning that $\tilde{\chi}^G = 0$. This justifies $\tilde{G} = \emptyset$ and trivially implies that $\mathcal{H} \cup \bar{\mathcal{H}}$ is an ordinary lumpability of $\tilde{\chi}^G$.

Define $\chi^{\tilde{G}} := \tilde{\chi}^G$ for all $G \in \mathcal{G}$ with $\tilde{G} \neq \emptyset$. The above discussion shows that $\tilde{\mathcal{H}}$ is an ordinary lumpability of $\chi^{\tilde{G}}$ for every $G \in \mathcal{G}_n$. Hence, provided that $\tilde{\mathcal{H}}$ is also an ordinary lumpability of $\tilde{Q}^d$, Theorem 12 and the definition of $\tilde{\mathcal{G}}$ imply that $(\tilde{\mathcal{H}}, \tilde{\mathcal{G}})$ is a UCTMC lumpability of $(\tilde{\mathcal{V}}, \tilde{\mathcal{E}}, \tilde{m}, \tilde{M}, \tilde{\pi}[0])$. This, however, can be seen by noting that $\tilde{Q}$ is obtained from Q by redirecting and eliminating the transitions of Q blockwise because

- $\tilde{q}^d_{i,j} = q^d_{i,j}$ if $(i,j) \in \bigcup_{G \in \mathcal{G}_d} G \wedge i \notin \mathcal{U}_\nu \cup \mathcal{T}_\nu \wedge j \notin \mathcal{T}_\nu$;
- $\tilde{q}^d_{i,\bar{j}} = q^d_{i,j}$ if $(i,j) \in \bigcup_{G \in \mathcal{G}_d} G \wedge i \notin \mathcal{U}_\nu \cup \mathcal{T}_\nu \wedge j \in \mathcal{T}_\nu$;
- $\mathcal{U}_\nu$, $\mathcal{T}_\nu$ can be written as a unions of blocks.

◀

The model checking of until formulae is ultimately related to the probability that a time-varying target set can be reached by avoiding a time-varying set of unsafe states [4, 5]. The next definition formalizes this in our context.

▶ **Definition 25.** Assume that $(\mathcal{H}, \mathcal{G})$ is a UCTMC lumpability of $(\mathcal{V}, \mathcal{E}, m, M, \pi[0])$ and fix some admissible $(q_{i,j})_{(i,j) \in \mathcal{E}}$. Further, let $\mathcal{U}, \mathcal{T} : [0; \infty) \to \mathrm{Powerset}(\mathcal{V})$ be such that

- $\mathcal{U}, \mathcal{T}$ have, on any bounded time interval at most finitely many discontinuity points with respect to the discrete topology;
- both $\mathcal{U}(t)$ and $\mathcal{T}(t)$ can be written, for any $t \geq 0$, as unions of blocks from $\mathcal{H}$.

Then, $\mathcal{P}_{\mathrm{reach}}(Q, t, T, \mathcal{T}, \mathcal{U})[i]$ is the probability of the set of paths underlying Q reaching a (target) state in $\mathcal{T}(\tau)$ at time $\tau \in [t; t+T]$ without passing through a (unsafe) state in $\mathcal{U}(\tau')$ for any $\tau' \in [t; \tau]$, when starting in state $i \in \mathcal{V}$ at time t. ◀

The following result is key for the proof of Theorem 22.

▶ **Proposition** 26. Assume that $(\mathcal{H}, \mathcal{G})$ is a UCTMC lumpability of $(\mathcal{V}, \mathcal{E}, m, M, \pi[0])$. Let $(\mathcal{H}, \mathcal{G})$ induce $(\tilde{\mathcal{V}}, \tilde{\mathcal{E}}, \tilde{m}, \tilde{M}, \tilde{\pi}[0])$ as in Theorem 17 and $\mathcal{U}, \mathcal{T} : [0; \infty) \to \mathrm{Powerset}(\mathcal{V})$ be such that

- $\mathcal{U}, \mathcal{T}$ have, on any bounded time interval at most finitely many discontinuity points with respect to the discrete topology;
- both $\mathcal{U}(\tau)$ and $\mathcal{T}(\tau)$ can be written, for any $\tau \geq 0$, as unions of blocks from $\mathcal{H}$.

With this, set $\hat{\mathcal{U}}(\tau) := \{i_H \mid H \in \mathcal{H} \wedge H \subseteq \mathcal{U}(\tau)\}$ and $\hat{\mathcal{T}}(\tau) := \{i_H \mid H \in \mathcal{H} \wedge H \subseteq \mathcal{T}(\tau)\}$. Then, for given $T > 0$, $t \geq 0$, $H \in \mathcal{H}$ and $i \in H$:

- if provided with admissible $(q_{i,j})_{(i,j)\in\mathcal{E}}$, we construct admissible $(\hat{q}_{i_H,i_{H'}})_{(i_H,i_{H'})\in\hat{\mathcal{E}}}$;
- instead, if given admissible $(\hat{q}_{i_H,i_{H'}})_{(i_H,i_{H'})\in\hat{\mathcal{E}}}$, we construct admissible $(q_{i,j})_{(i,j)\in\mathcal{E}}$,

such that $\mathcal{P}_{\text{reach}}(Q,t,T,\mathcal{U},\mathcal{T})[i] = \mathcal{P}_{\text{reach}}(\hat{Q},t,T,\hat{\mathcal{U}},\hat{\mathcal{T}})[i_H]$.

Proof. Let $t = T_0 < T_1 < \ldots < T_{\kappa+1} = t+T$ be the time points in $[t;t+T]$ at which discontinuities of $\mathcal{U}$ or $\mathcal{T}$ may arise. Following [5], we set $W(s) = \mathcal{V} \setminus (\mathcal{U}(s) \cup \mathcal{T}(s))$ and let $\zeta_W(T_\nu)$ be the $n \times n$ matrix equal to 1 only on the diagonal elements corresponding to states ι belonging to both $W(T_\nu^-)$ and $W(T_\nu^+)$ (i.e., states that are safe and not a target both before and after T_ν), and equal to 0 elsewhere. Furthermore, let $\zeta_{\mathcal{T}}(T_\nu)$ be the $n \times n$ matrix equal to 1 in the diagonal elements corresponding to states ι belonging to $W(T_\nu^-) \cap \mathcal{T}(T_\nu^+)$ and zero elsewhere. Finally, let $\zeta(T_\nu)$ be the $2n \times 2n$ matrix defined by

$$\zeta(T_\nu) := \begin{pmatrix} \zeta_W(T_\nu) & \zeta_{\mathcal{T}}(T_\nu) \\ 0 & I_{n\times n} \end{pmatrix}$$

Let us assume that we are given an admissible $(q_{i,j})_{(i,j)\in\mathcal{E}}$. Thanks to the fact that $(q_{i,j})_{(i,j)\in\mathcal{E}}$ is piecewise analytic with finitely many discontinuity points on any bounded time interval, the discussion in [5] ensures that

$$\mathcal{P}_{\text{reach}}(Q,t,T,\mathcal{U},\mathcal{T})[i] = \sum_{\bar{j}\in\bar{\mathcal{V}}} \Upsilon(t,t+T)_{i,\bar{j}} + \mathbb{1}\{i \in \mathcal{T}(t)\},$$

where $\mathbb{1}$ denotes the characteristic function, while

$$\Upsilon(t,t+T) = \tilde{\Pi}(t,T_1)\zeta(T_1)\tilde{\Pi}(T_1,T_2)\zeta(T_2)\cdot\ldots\cdot\zeta(T_\kappa)\tilde{\Pi}(T_\kappa,t+T)$$

is such that $\tilde{\Pi}(t_1,t_2)$ is the $2n \times 2n$ matrix where $e_\iota^T\tilde{\Pi}(t_1,t_2)e_{\iota'}$ is the probability that the auxiliary CTMC is in state $\iota' \in \tilde{\mathcal{V}}$ at time t_2, provided that it was initialized with state $\iota \in \tilde{\mathcal{V}}$ at time t_1. The auxiliary CTMC in turn is given by Definition 23 and

- $\mathcal{U}_\nu := \mathcal{U}(\frac{T_{\nu-1}+T_\nu}{2})$ and $\mathcal{T}_\nu := \mathcal{T}(\frac{T_{\nu-1}+T_\nu}{2})$;
- $\tilde{\pi}[T_\nu] := \tilde{\pi}[T_{\nu-1}]^T \cdot \tilde{\Pi}_{|\mathcal{V}\times\mathcal{V}}(T_{\nu-1},T_\nu)$ with $\tilde{\pi}[T_0] := e_i^T$;
- $(\tilde{q}_{i,j})_{(i,j)\in\tilde{\mathcal{E}}}$ on $[T_{\nu-1};T_\nu]$ is induced by $\mathcal{U}_\nu$, $\mathcal{T}_\nu$, $\tilde{\pi}[T_{\nu-1}]$ and $(q_{i,j})_{(i,j)\in\mathcal{E}}$.

Since $\tilde{\Pi}(T_{\nu-1},T_{\nu-1}) = I_{2n\times 2n}$, matrix $\tilde{\Pi}(T_{\nu-1},T_\nu)$ can be obtained by solving the forward Kolmogorov equation $\partial_\tau\tilde{\Pi}(T_{\nu-1},\tau) = \tilde{\Pi}(T_{\nu-1},\tau)\cdot\tilde{Q}(\tau)$ on the interval $\tau \in [T_{\nu-1};T_\nu]$. In particular, $e_\iota^T \cdot \tilde{\Pi}(T_{\nu-1},T_\nu)$ is given by $\tilde{\pi}(T_\nu)$ when $\tilde{\pi}(T_{\nu-1}) = e_\iota$ and $\partial_\tau\tilde{\pi}(\tau) = \tilde{\pi}^T(\tau)\cdot\tilde{Q}(\tau)$ for all $\tau \in [T_{\nu-1};T_\nu]$. The composite term $\tilde{\Pi}(T_{\nu-1},T_\nu)\zeta(T_\nu)$ writes as (for the benefit of presentation, we suppress the explicit time dependence in the following equation):

$$\tilde{\Pi}\cdot\zeta = \begin{pmatrix} \tilde{\Pi}_{|\mathcal{V}\times\mathcal{V}} & \tilde{\Pi}_{|\mathcal{V}\times\bar{\mathcal{V}}} \\ 0 & I_{n\times n} \end{pmatrix} \cdot \begin{pmatrix} \zeta_W & \zeta_{\mathcal{T}} \\ 0 & I_{n\times n} \end{pmatrix} = \begin{pmatrix} \tilde{\Pi}_{|\mathcal{V}\times\mathcal{V}}\cdot\zeta_W & \tilde{\Pi}_{|\mathcal{V}\times\mathcal{V}}\cdot\zeta_{\mathcal{T}} + \tilde{\Pi}_{|\mathcal{V}\times\bar{\mathcal{V}}} \\ 0 & I_{n\times n} \end{pmatrix}$$

Note that, for all $H \in \mathcal{H}$ and $\iota,\iota' \in H$, it holds that $e_\iota^T\zeta_W e_\iota = e_{\iota'}^T\zeta_W e_{\iota'}$ and $e_\iota^T\zeta_{\mathcal{T}} e_\iota = e_{\iota'}^T\zeta_{\mathcal{T}} e_{\iota'}$ because $\mathcal{U}_\nu$ and $\mathcal{T}_\nu$ are unions of blocks from $\mathcal{H}$. Hence, ζ_W and $\zeta_{\mathcal{T}}$ are cutoff functions that are operating blockwise.

The above discussion and Proposition 24 ensure that a given probability distribution $\tilde{\pi}[T_{\nu-1}]$ induces (piecewise analytic) functions $(\tilde{q}_{\tilde{G}})_{\tilde{G}\in\tilde{\mathcal{G}}}$ on $[T_{\nu-1};T_\nu]$ such that

$$\sum_{\iota\in X} \tilde{\pi}_\iota(\tau) = \hat{\tilde{\pi}}_{\iota_X}(\tau) \text{ for all } X \in \mathcal{H}\cup\bar{\mathcal{H}} \text{ and } \tau \in [T_{\nu-1};T_\nu],$$

where $\hat{\tilde{\pi}}$ is the transient probability of the lumped auxiliary CTMC underlying $(\tilde{q}_{\tilde{G}})_{\tilde{G}\in\tilde{\mathcal{G}}}$ (see Lemma 14 and Theorem 4), while $(\tilde{q}_{\tilde{G}})_{\tilde{G}\in\tilde{\mathcal{G}}}$ is induced by $(\tilde{q}_{\iota,\iota'})_{(\iota,\iota')\in\tilde{\mathcal{E}}}$ and $\tilde{\pi}[T_{\nu-1}]$ (see Proposition 24, Lemma 14 and proof of Theorem 13). Hence, for all $H'\in\mathcal{H}$, it holds that

$$\tilde{\pi}[T_{\nu-1}]^T\cdot\tilde{\Pi}_{|\mathcal{V}\times\mathcal{V}}(T_{\nu-1},T_\nu)\cdot\Big(\sum_{\iota\in H'}e_\iota\Big)=\hat{\tilde{\pi}}[T_{\nu-1}]^T\cdot\hat{\tilde{\Pi}}_{|\hat{\mathcal{V}}\times\hat{\mathcal{V}}}(T_{\nu-1},T_\nu)\cdot e_{i_{H'}}$$
$$\tilde{\pi}[T_{\nu-1}]^T\cdot\tilde{\Pi}_{|\mathcal{V}\times\bar{\mathcal{V}}}(T_{\nu-1},T_\nu)\cdot\Big(\sum_{\iota\in\bar{H}'}e_\iota\Big)=\hat{\tilde{\pi}}[T_{\nu-1}]^T\cdot\hat{\tilde{\Pi}}_{|\hat{\mathcal{V}}\times\hat{\mathcal{V}}}(T_{\nu-1},T_\nu)\cdot e_{i_{\bar{H}'}},$$

where $\hat{\tilde{\Pi}}$ is the matrix of transient probabilities of the lumped CTMC induced by $(\tilde{q}_{\tilde{G}})_{\tilde{G}\in\tilde{\mathcal{G}}}$. The above discussion ensures that

$$\begin{aligned}e_i^T\Upsilon(t,t+T)&=e_i^T\tilde{\Pi}(t,T_1)\zeta(T_1)\tilde{\Pi}(T_1,T_2)\zeta(T_2)\cdot\ldots\cdot\zeta(T_\kappa)\tilde{\Pi}(T_\kappa,t+T)\\&=e_{i_H}^T\hat{\tilde{\Pi}}(t,T_1)\hat{\zeta}(T_1)\hat{\tilde{\Pi}}(T_1,T_2)\hat{\zeta}(T_2)\cdot\ldots\cdot\hat{\zeta}(T_\kappa)\hat{\tilde{\Pi}}(T_\kappa,t+T)\end{aligned}$$

for all $H\in\mathcal{H}$ and $i\in H$, where $\hat{\zeta}$ is defined in the obvious manner. This implies the statement if we can find an admissible $(\hat{q}_{i_H,i_{H'}})_{(i_H,i_{H'})\in\hat{\mathcal{E}}}$ such that $\hat{\tilde{Q}}=\tilde{\hat{Q}}$.

To this end, write $Q=\sum_{G\in\mathcal{G}}Q_G$, where Q_G is the time-varying transition rate matrix satisfying $e_i^TQ_Ge_j=q_{i,j}$ if $(i,j)\in G$ and zero if $(i,j)\in\mathcal{E}\setminus G$. With this, $Q^d=\sum_{G\in\mathcal{G}_d}Q_G$ and $\hat{\tilde{Q}}^d=\tilde{\hat{Q}}^d$ follows by noting that

- $\tilde{q}^d_{i,j}=q^d_{i,j}$ if $(i,j)\in\bigcup_{G\in\mathcal{G}_d}G\wedge i\notin\mathcal{U}_\nu\cup\mathcal{T}_\nu\wedge j\notin\mathcal{T}_\nu$ and;
- $\tilde{q}^d_{i,\bar{j}}=q^d_{i,j}$ if $(i,j)\in\bigcup_{G\in\mathcal{G}_d}G\wedge i\notin\mathcal{U}_\nu\cup\mathcal{T}_\nu\wedge j\in\mathcal{T}_\nu$ and;
- by recalling that $\mathcal{U}_\nu$, $\mathcal{T}_\nu$ can be written as a unions of blocks.

We next construct a $\hat{Q}_G$ such that $\tilde{\hat{Q}}_G=\hat{\tilde{Q}}_G$ for all $G\in\mathcal{G}_n$.

- With $\hat{\mathcal{E}}_G:=\{(i_H,i_{H'})\mid(i_H,j)\in G$ for some $j\in H'$ with $H\neq H'\}$, where $G\in\mathcal{G}_n$, we note that $\hat{\mathcal{E}}_G$ contains exactly one transition if G is non-invariant and no transitions if G is invariant. To see this, recall that $(\mathcal{H},\mathcal{G})$ is a UCTMC lumpability; hence, there exist unique $H,H'\in\mathcal{H}$ such that $i_k,i_l\in H$ and $j_l,j_l\in H'$ for all $(i_k,j_k),(j_l,j_l)\in G$.
- Define $\tilde{\mathcal{E}}_G:=\{(\iota,\iota')\in\tilde{\mathcal{E}}\mid(\iota,\iota')$ is induced by $G\}$ for $G\in\mathcal{G}_n$. In the proof of Proposition 24, it has been shown that

$$\tilde{\mathcal{E}}_G=\begin{cases}G&,\ H\cap(\mathcal{U}_\nu\cup\mathcal{T}_\nu)=\emptyset\wedge H'\cap\mathcal{T}_\nu=\emptyset\\\{(i,\bar{j})\mid(i,j)\in G\}&,\ H\cap(\mathcal{U}_\nu\cup\mathcal{T}_\nu)=\emptyset\wedge H'\subseteq\mathcal{T}_\nu\\\emptyset&,\ H\subseteq(\mathcal{U}_\nu\cup\mathcal{T}_\nu)\end{cases}$$

  where $H,H'\in\mathcal{H}$ are such that $i\in H$ and $j\in H'$ for all $(i,j)\in G$.

Fix an arbitrary non-invariant $G\in\mathcal{G}_n$. The above discussion ensures that there exist unique $H,H'\in\mathcal{H}$ that satisfy $H\neq H'$ and $i\in H$, $j\in H'$ for all $(i,j)\in G$. Together with the multiplicity $\mu_G:=\mu_G(i_H,i_{H'})=\{(i_H,j)\in G\mid j\in H'\}$, we next study $\hat{\tilde{Q}}_G$ via the following case distinction (since $\mathcal{U}_\nu,\mathcal{T}_\nu$ are unions of blocks from $\mathcal{H}$, it suffices to consider the following three cases for $H,H'\in\mathcal{H}$):

- If $H\cap(\mathcal{U}_\nu\cup\mathcal{T}_\nu)=\emptyset\wedge H'\cap\mathcal{T}_\nu=\emptyset$: Then $\tilde{\mathcal{E}}_G=G$, hence we have $\hat{\tilde{\mathcal{E}}}_G=\{(i_H,i_{H'})\}$ and

$$(\hat{\tilde{Q}}_G(t))_{i_H,i_{H'}}=\mu_G\sum_{(i_k,j_k)\in G}q_{i_k,j_k}(t)\Big(\frac{\tilde{\pi}_{i_k}(t)}{\sum_{(i_l,j_l)\in G}\tilde{\pi}_{i_l}(t)}\Big).$$

- If $H \cap (\mathcal{U}_\nu \cup \mathcal{T}_\nu) = \emptyset \wedge H' \subseteq \mathcal{T}_\nu$: Then $\tilde{\mathcal{E}}_G = \{(i, \bar{j}) \mid (i,j) \in G\}$, which implies that $\hat{\tilde{\mathcal{E}}}_G = \{(i_H, i_{\bar{H}'})\}$ and

$$(\hat{\tilde{Q}}_G(t))_{i_H, i_{\bar{H}'}} = \mu_G \sum_{(i_k,j_k)\in G} q_{i_k,j_k}(t)\Big(\frac{\tilde{\pi}_{i_k}(t)}{\sum_{(i_l,j_l)\in G}\tilde{\pi}_{i_l}(t)}\Big)$$

- If $H \subseteq (\mathcal{U}_\nu \cup \mathcal{T}_\nu)$: Then $\tilde{\mathcal{E}}_G = \emptyset$, hence $\hat{\tilde{Q}}_G = 0$.

The above case distinction suggests to pick

$$q_G(t) := \mu_G \sum_{(i_k,j_k)\in G} q_{i_k,j_k}(t)\Big(\frac{\tilde{\pi}_{i_k}(t)}{\sum_{(i_l,j_l)\in G}\tilde{\pi}_{i_l}(t)}\Big)$$

We next show that q_G induces a $\hat{Q}$ which, in turn, induces a $\tilde{\hat{Q}}_G$ such that $\tilde{\hat{Q}}_G = \hat{\tilde{Q}}_G$. We proceed by the following case distinction.

- If $H \cap (\mathcal{U}_\nu \cup \mathcal{T}_\nu) = \emptyset \wedge H' \cap \mathcal{T}_\nu = \emptyset$: Since $\hat{\mathcal{E}}_G = \{(i_H, i_{H'})\}$, the definition of $\hat{\mathcal{U}}_\nu$ and $\hat{\mathcal{T}}_\nu$ ensures that $\tilde{\hat{\mathcal{E}}}_G = \{(i_H, i_{H'})\}$. Hence, $(\tilde{\hat{Q}}_G(t))_{i_H,i_{H'}} = \mu_G \cdot q_G(t)$ ensures $\tilde{\hat{Q}}_G(t) = \hat{\tilde{Q}}_G(t)$.
- If $H \cap (\mathcal{U}_\nu \cup \mathcal{T}_\nu) = \emptyset \wedge H' \subseteq \mathcal{T}_\nu$: Since $\hat{\mathcal{E}}_G = \{(i_H, i_{H'})\}$, the definition of $\hat{\mathcal{U}}_\nu$ and $\hat{\mathcal{T}}_\nu$ ensures that $\tilde{\hat{\mathcal{E}}}_G = \{(i_H, i_{\bar{H}'})\}$. Hence, $(\tilde{\hat{Q}}_G(t))_{i_H,i_{\bar{H}'}} = \mu_G \cdot q_G(t)$ ensures $\tilde{\hat{Q}}_G(t) = \hat{\tilde{Q}}_G(t)$.
- If $H \subseteq (\mathcal{U}_\nu \cup \mathcal{T}_\nu)$: Then $\tilde{\hat{\mathcal{E}}}_G = \emptyset$ and $\tilde{\hat{Q}}_G = 0$, implying in particular that $\tilde{\hat{Q}}_G = \hat{\tilde{Q}}_G$.

The above discussion establishes $\tilde{\hat{Q}}_G = \hat{\tilde{Q}}_G$ for all $G \in \mathcal{G}_n$ (the case where G is invariant is trivial because this yields $\tilde{\hat{\mathcal{E}}}_G = \emptyset$ and $\hat{\tilde{\mathcal{E}}}_G = \emptyset$). Hence, Lemma 14 completes the proof in the case where we are given an admissible $(q_{i,j})_{(i,j)\in\mathcal{E}}$ and have to find an admissible $(\hat{q}_{i_H,i_{H'}})_{(i_H,i_{H'})\in\hat{\mathcal{E}}}$ such that

$$\mathcal{P}_{\text{reach}}(Q,t,T,\mathcal{U},\mathcal{T})[i] = \mathcal{P}_{\text{reach}}(\hat{Q},t,T,\hat{\mathcal{U}},\hat{\mathcal{T}})[i_H] \tag{7}$$

The other direction where one is given some admissible $(\hat{q}_{i_H,i_{H'}})_{(i_H,i_{H'})\in\hat{\mathcal{E}}}$ and has to find an admissible $(q_{i,j})_{(i,j)\in\mathcal{E}}$ such that (7) holds true follows from the above discussion and Lemma 14. ◀

Armed with Proposition 26, we are in a position to prove Theorem 22.

Proof of Theorem 22. The proof proceeds by structural induction over ϕ.

- $\phi = a$: Follows from the fact that $\hat{\mathcal{L}}(i_H) = \mathcal{L}(i)$ for all $H \in \mathcal{H}$ and $i \in H$.
- $\phi = \phi_1 \wedge \phi_2$: Follows by induction hypothesis.
- $\phi = \neg\phi_1$: Follows by induction hypothesis.
- $\phi = \mathcal{P}^{\forall}_{\bowtie p}(\phi_1 \mathbf{U}^{[t_0;t_1]} \phi_2)$: Let us define

  $$\mathcal{U}(t) := \{j \in \mathcal{V} \mid j,t \models \neg\phi_1\} \qquad \text{and} \qquad \mathcal{T}(t) := \{j \in \mathcal{V} \mid j,t \models \phi_2\}$$

  By induction hypothesis, it holds that both $\mathcal{U}(\tau)$ and $\mathcal{T}(\tau)$ can be written, for any $\tau \geq 0$, as unions of blocks from $\mathcal{H}$. The definition of the semantics, instead, ensures that $\mathcal{U}$ and $\mathcal{T}$ have finitely many discontinuity points on any bounded time interval. Together with $\hat{\mathcal{U}}(t) := \{i_H \mid H \in \mathcal{H} \wedge H \subseteq \mathcal{U}(t)\}$ and $\hat{\mathcal{T}}(t) := \{i_H \mid H \in \mathcal{H} \wedge H \subseteq \mathcal{T}(t)\}$, the discussion in [5] implies that

  - For any admissible q: $i,t \models \mathcal{P}_{\bowtie p}(\phi_1 \mathbf{U}^{[t_0;t_1]}\phi_2)$ iff $\mathcal{P}_{\text{reach}}(Q,t,t_1-t_0,\mathcal{U},\mathcal{T})[i] \bowtie p$;
  - For any admissible $\hat{q}$: $i_H,t \models \mathcal{P}_{\bowtie p}(\phi_1 \mathbf{U}^{[t_0;t_1]}\phi_2)$ iff $\mathcal{P}_{\text{reach}}(\hat{Q},t,t_1-t_0,\hat{\mathcal{U}},\hat{\mathcal{T}})[i_H] \bowtie p$.

  With this, Proposition 26 yields the claim.

◀