On the Formalization of Continuous-Time Markov Chains in HOL

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Technical Report

April 2013

Abstract

Continuous-time Markov chain has been extensively applied to model diverse real-world systems. The analysis of these systems has been conducted using conventional simulation technique and computer algebra systems, more recently, probabilistic model checking. However, these methods either cannot guarantee accurate analysis or are not scalable due to the unacceptable computation consumption. As a complemental technique, theorem proving is proposed to reason about continuous-time Markov chain using HOL theorem proving. To our best knowledge, the formalization of continuous-time Markov chain has not been found in any theorem prover. In this report, we provide the idea on the formal de?nition of continuous-time Markov chain and two of its formally verified properties as the first step to formalize the continuous-time Markov chain theory. Also, we present the next step and the predict the potential challenges in the formalization process. Finally, a certain of applications are listed to be targeted using the formalized continuous-time Markov chain.

1 Introduction

Stochastic processes are mainly used to describe the evolution of numerous real-world systems. Basically, the evolution of a system is a series successive changes. In order to simplify the study of the evolution of a system, a series discrete steps of the evolution process are considered and the system is then abstracted to be a discrete-time stochastic model. However, the behaviors within the small intervals are ignored and not able to be analyzed. In this case, continuous-time stochastic models are usually applied to describe the model so that the gradual changes occurring on many continuous and unpredictable components can be studied. Mathematically, the continuous-time stochastic process is the fundamental concept of constructing such kind of continuous-time models. As one of extensively used continuous-time stochastic processes, continuous-time Markov chains (CTMC) are of interest in numerous science and engineering domains.

A continuous-time Markov chain refers to a random process, in which the random variables remain in the current state for some random (particularly, exponentially distributed) interval of time and then transit to different states. Numerous mathematical theories, such as the embedded Markov chain theory, hidden Markov models theory, Queueing theory, are based on the concept of the CTMC. In the real world, CTMC theory can be applied in constructing reliability models and analyzing system performance. It can also be used to estimate the sojourn time in some diseases, such as breast cancer [10] and diabetes mellitus [6], which are safety critical cases.

Traditionally, engineers have been using paper-and-pencil proof methods to perform probabilistic and statistical analysis of systems. Nowadays, these systems have become considerably complex and the behaviors of some critical subsystems need to be analyzed accurately. Paper-and-pencil proofs can hardly guarantee the analysis of those key components and thus cannot be used to model and analyze the whole system. With the increasing requirements for predicting the reliability of systems, evaluating the performance and dependability of products and verifying systems properties, researchers are investigating all sorts of methods and techniques for providing accurate and reliable results for general systems.

During the last two decades, computer science has developed dramatically fast. Simulation has been the most commonly used computer based analysis technique for Markov chain models. Currently, the most advanced simulation algorithms are Markov chain Monte Carlo (MCMC) methods [25], which are based on constructing a Markov chain that has the desired distribution as that of the random variables. These kind of methods are usually applied to dynamic simulation which is used for modeling the time varying behavior of a system. Whereas, typical use of MCMC sampling can only approximate the desired distribution in terms of the residual effect of the initial position. Although some more sophisticated MCMC-based algorithms are capable of producing exact samples, they introduce additional computation and unbounded running time.

Other state-based approaches to analyze a Markov chain model include some software packages, such as Markov analyzers and reliability or performance evaluation tools, which are all based on numerical methods (for details refer to [23]). The direct methods are only suitable for small models so that most of the models are analyzed by using expanded iterative methods, which often lead to approximations because the computations stop at some convergence point. It is unavoidable that roundoff and truncation errors affect the numerical computations. Hence, the results at convergence point might become unbelievable. Another technique, Stochastic Petri Nets (SPN) [12], has been found as a powerful method for modeling and analyzing Markovian systems because it allows locating modeled states instead of global modeling. The key factor limiting the application of SPN models is the complexity of their complicated analysis. In order to tackle this problem, Generalized Stochastic Petri Net (GSPN) [20] was proposed but the tools based on its principles are seldom. Another major limitation of GSPN is the combinatorial growth of the models' state space.

Based on powerful verification techniques, Probabilistic Model Checking Tools (PMCT) combine a range of techniques for calculating the likelihood of the occurrence of certain events during the execution of the system and can establish properties to be considered. Most of the models that they can analyze are Markovian models. However, because of the limitations of the logics that are used to express the properties, some important probabilistic questions are not able to be answered directly. Also, the algorithms integrated in these tools for analysis are based on iterative methods are not able to conduct accurate results. Moreover, these tools suffer from the state-explosion problem even though some advanced data structures, such as Multi-Terminal Binary Disicion Diagram (MTBDD) [36], have been embedded in their algorithms.

Higher-order logic interactive theorem proving provides a conceptually simple formalism with a precise semantics, allowing secure extensions for many mathematical theories, and has been employed to develop probabilistic algorithms [17]. Even probabilistic analysis [13] of many stochastic systems has been available in theorem prover. Later, Coble [7] formalized the measure space as the triple (X, Σ, μ). This allows to define an arbitrary space X and this overcomes the disadvantage of Hurd's work. Coble's probability theory is built upon finitely-valued (standard real numbers) measures and functions. Specifically, the Borel sigma algebra cannot be defined on open sets and this constrains the verification of some applications. More recently, Mhamdi [29] improved the development based on the axiomatic definition of probability proposed by Kolmogorov [21]. Mhamdi's theory provides a mathematical consistent for assigning and deducing probabilities of events. Hölzl [16] has also formalized three chapters of measure theory in Isabelle/HOL. Affeldt [2] simplified the formalization of probability theory in Coq [8]. Among these works, the probability theory formalized by Mhamdi provides a very generic formal reasoning support and thus can be used to analyze wider range of applications.

The main difference between a DTMC and CTMC is the type of random variable: in the DTMC, the random variables are discrete and in CTMC, the random variables are continuous. In [24], the formalization of DTMC in the HOL theorem prover is provided and it is the fundamental of Markov chain theory. Also, the measure and probability theories formalized in [27] offer the flexibility of formally defining continuous ransom processes in HOL4. These fundamentals can facilitate the formalization of continuous-time Markov chains. However, to our best knowledge, continuous-time Markov chains have never been formalized in any theorem prover. This is one of the biggest limitations of this emerging research domain because the probabilistic analysis of a wide variety of real-world systems can only be done using continuous-time Markov chains.

In this report, we present the idea on formalize CTMC using the fundamental concept of DTMC in a higher-order logic. The rest of this report is organized as follows: In Section 2, we give an overview of main definitions of some required notions. Section 3 presents our formalization of the continuous-time Markov chain, which is used in Section 4 to prove two main properties of CTMC. In Section 5, we predict the main challenges in proving the other properties of CTMC. Finally, Section 6 concludes the report and provides hints to future work.

2 Preliminaries

In this section, we present the higher-order-logic theorem proving technique and probability theory, which comprise the foundational material required to understand this thesis.

2.1 Theorem Proving

One of the major methods to formally verify a stochastic system is probabilistic theorem proving, which makes use of higher-order logic [11] to deduct systems with a precise semantics, due to its high expressiveness. The popular theorem proving tools are ACL2 [1], PVS [33], Isabellel/HOL [18], ProofPower [32], HOL-Light [14], HOL4 [15], Coq [8], etc.

In past two decades, some researchers investigated various relevant probabilistic theorems in different tools. Nedzusiak [30] and Bialas [5] were among the first ones who proposed to formalize some probability theory in high-order-logic. Hurd [17] verified probabilistic algorithms in HOL [15]. Then Hasan [13] extended Hurd's work and formalized continuous random variables so that the probabilistic and statistical properties of these random variables are capable of being verified in the HOL system. Based on Hurd's work, Richter [34] and Coble [**?**] devoted to formalize Lebesgue-style integration theory for extending the probability concept of expectation in Isabellel/HOL and HOL4, respectively. Daumas et. al. [9] and Lester [22] presented their work on measure and integration theories in PVS seperately. To overcome the limitations of previous work, Mhamdi et. al. [29] proposed a significant formalization of a measure space to improve in Coble's work and by this formalization, he proved Lesbesgue integral properties and convergence theorems for arbitrary functions. Their work has build upon the foundation for providing the framework to develop formal theories for analyzing stochastic systems.

In Table 1, we list some frequently used symbols and functions associated with the description in the following chapters of this thesis.

2.2 Probability Theory

Mathematically, a *measure space* is defined as a triple (Ω, Σ, μ), where Ω is a set, called the *sample space*, Σ represents a σ-algebra of subsets of Ω, where the subsets are usually referred to as *measurable sets*, and μ is a *measure* with domain Σ. A *probability space* is a measure space $(\Omega, \Sigma, \mathcal{P}r)$ such that the measure, referred to as the probability and denoted by $\mathcal{P}r$, of the sample space is 1. Probability theory is developed based on three axioms:

1. $\forall$ A. $0 \leq \mathcal{P}r(A)$
2. $\mathcal{P}r(\Omega) = 1$
3. For any countable collection A_0, A_1, $\cdots$ of mutually exclusive events, $\mathcal{P}r(\bigcap_{i \in \Omega} A_i) = \sum_{i \in \Omega} \mathcal{P}r(A_i)$.

In probability and statistical theory, the probabilistic function called *random variable* is an essential concept. The random variable concept is a function from a probability space to a *measurable space*. A measurable space refers to a pair (S, Σ), where S denotes a set and Σ represents a nonempty collection of subsets of S. Especially, if the set S is a *discrete set*, which contains only isolated elements, then this random variable is called a *discrete random variable*. The probability that a discrete random variable X is exactly equal to some value i is defined as the *probability mass function* (PMF) and it is mathematically expressed as $\mathcal{P}r(X = i)$.

Table 1: HOL Symbols and Functions

HOL Symbol	**Meaning**
$\forall$	Logical *for all*
$\wedge$	Logical *and*
$\vee$	Logical *or*
$(\mathtt{a}, \mathtt{b})$	A pair of two elements
λ`x.fx`	Function that maps x to $f(x)$
$\{\mathtt{x}\vert\mathtt{P}(\mathtt{x})\}$	Set of all x such that $P(x)$
$\emptyset$	Empty Set
$\mathtt{a} \in \mathtt{S}$	a in S
`FINITE S`	S is a finite set
$\bigcap$ `P`	Intersection of all sets in the set P
$\bigcup$ `P`	Union of all sets in the set P
$\mathtt{A} \cap \mathtt{B}$	A intersection B
$\mathtt{A} \cup \mathtt{B}$	A union B
`disjoint A B`	Sets A and B are disjoint
`IMAGE f A`	Set with elements $f(x)$ for all $x \in A$
`SIGMA` $(\lambda$`n. f n`$)$ `s`	$\sum_{n\in s} f(n)$

Mhamdi defined a *probability space* in higher-order logic as a measure space $(\Omega, \Sigma, \mathcal{P}r)$ [29], which is exactly matched with the aforementioned mathematical definition . The probability theory is then developed by giving a probability space `p` and the functions `space` and `subsets` which return the corresponding Ω and Σ, respectively. The above approach has been successfully used to formally verify most basic probability theorems [28], such as:

$$0 \leq \mathcal{P}r(B) \leq 1 \tag{1}$$

$$\sum_{B_i \in \Omega} \mathcal{P}r(B_i) = 1 \tag{2}$$

Another important concept in probability theory is *random process*, which denotes a collection of random variables X_t ($t \in T$). If the indices (t) of random variables X_t are continuous, then this random process is a *continuous-time random process*. In Mhamdi's development, a random variable is formally defined (formalized) as a measurable function `X` between a probability space `p` and a measurable space `s`. It is written as `random_variable X p s` in HOL. The definition of random variables is general enough to formalize both discrete and continuous random variables.

Now, utilizing the formalization of random variables, the random process $\{X_t\}_{t\geq 0}$ can be easily written as $\forall$ `t. random_variable (X t) p s` in higher-order logic. The distribution and conditional probability are defined in [27]:

```
|- !p X. distribution p X = (\s. prob p (PREIMAGE X s INTER p_space p))
|- !p X Y.
        joint_pmf p X Y =
```

```
        (\(A,B). prob p (PREIMAGE X A INTER PREIMAGE Y B INTER p_space p))
|- !p X Y.
        cond_pmf p X Y =
        (\(A,B). joint_pmf p X Y (A,B) / distribution p Y B)
```

We can prove that `cond_pmf` is equivalent to the following *conditional probability*:

Definition 1. *(Conditional Probability)*
The conditional probability of the event A given the occurrence of the event B is

$$\mathcal{P}r(A|B) = \mathcal{P}r(A \cap B)/\mathcal{P}r(B)$$

```
⊢ ∀ A B. cond_prob p A B = prob p (A ∩ B) / prob p B
```

In order to facilitate the formalization of Markov chains, we verified various classical properties of conditional probability based on Definition 2.1. Some of the prominent ones are listed below:

$$\mathcal{P}r(A \cap B) = \mathcal{P}r(A|B)\mathcal{P}r(B) \tag{3a}$$

$$\mathcal{P}r(A) = \sum_{i \in \Omega} \mathcal{P}r(B_i)\mathcal{P}(A|B_i) \tag{3b}$$

$$\sum_{i \in \Omega} \mathcal{P}r(B_i|A) = 1 \tag{3c}$$

where A, B and C are events in the event space, and the finite events set $\{B_i\}_{i \in \Omega}$ contains mutually exclusive and exhaustive events. The first two theorems are obviously based on Definition 1. The third one is the Total Probability Theorem and the fourth one is a lemma of the Total Probability Theorem. The last theorem is the Additivity Theorem.

3 Formalization of Continuous-time Markov Chain

Given a probability space, a stochastic process $\{X_t : \Omega \to S\}$ represents a sequence of random variables X, where t represents the time that can be discrete (represented by non-negative integers) or continuous (represented by real numbers) [4]. The set of values taken by each X_t, commonly called states, is referred to as the *state space*. The *sample space* Ω of the process consists of all the possible state sequences based on a given state space S. Now, based on these definitions, a *Markov process* can be defined as a stochastic process with Markov property. If a Markov process has finite or countably infinite state space, then it is called a *Markov chain* and satisfies the following Markov property: $0 \leq t_0 \leq \cdots \leq t_n$ and $f_0, \cdots, f_{n+1}$ in the state space, then:

$$\mathcal{P}r\{X_{t_{n+1}} = f_{n+1}|X_{t_n} = f_n, \ldots, X_{t_0} = f_0\} = \mathcal{P}r\{X_{t_{n+1}} = f_{n+1}|X_{t_n} = f_n\} \tag{4}$$

This mathematical equation expresses that the future state X_{t+1} only depends on the current state $X_{\mathtt{t_n}}$ and is independent of the passed state $X_{\mathtt{t_i}}$. This feature can be formally expressed in higher-order logic as Definition 2.

Definition 2. *(Markov Property)*

```
  |- !X p s.
       mc_property X p s <=>
```

```
(!t. random_variable (X t) p s) /\
!f t n.
  increasing_seq t /\
  prob p
    (BIGINTER
       (IMAGE (\k. PREIMAGE (X (t k)) {f k} INTER p_space p)
          (count n))) <> 0 ==>
  (cond_pmf p (X (t (n + 1))) (X (t n)) ({f (n + 1)},{f n}) =
   cond_prob p
     (PREIMAGE (X (t (n + 1))) {f (n + 1)} INTER p_space p)
     (PREIMAGE (X (t n)) {f n} INTER p_space p INTER
      BIGINTER
        (IMAGE (\k. PREIMAGE (X (t k)) {f k} INTER p_space p)
           (count n))))
```

where the type of variable `t` is *real* and the index sequence `increasing_seq` is defined as:

Definition 3. *(Increasing Sequence)*

```
|- !t. increasing_seq t <=> !i j. i < j ==> t i < t j
```

In our work, we mainly focus on the continuous-time Markov chain (CTMC), in which the states are discrete in a finite space and for readability reasons, we abbreviate it as *CTMC*.

A *DTMC with finite state space* is usually expressed by specifying: an initial distribution p_0 which gives the probability of initial occurrence $\mathcal{P}r(X_0 = s) = p_0(s)$ for every state; and transition probabilities $p_{ij}(t)$ which give the probability of going from i to j for every pair of states i, j in the state space [31]. For states i, j and a time t, the *transition probability* $p_{ij}(t)$ is defined as $\mathcal{P}r\{X_{t+1} = j | X_t = i\}$, which can be easily generalized to *n-step transition probability.*

$$p_{ij}^{(n)}(t) = \begin{cases} \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i = j \end{cases} & n = 0 \\ \mathcal{P}r\{X_{t+n} = j | X_t = i\} & n > 0 \end{cases} \tag{5}$$

This is formalized in HOL as follows:

Definition 4. *(Transition Probability)*

```
|- !X p s t n i j.
     Trans X p s t n i j =
     if i IN space s /\ j IN space s then
       if n = 0 then
         if i = j then 1 else 0
       else
         cond_prob p (PREIMAGE (X (t + n)) {j} INTER p_space p)
           (PREIMAGE (X t) {i} INTER p_space p)
     else 0
```

where the type of variable `t` is *real*.

It is easy to understand that the probability of an event is zero, when this event is not in the event space. For instance, i is not in the state space implies that event $\{X_t = i\} = \emptyset$. In this case, the conditional probability related to an empty set is zero.

Now, the continuous-time Markov chain (CTMC) can be formalized as follows:

Definition 5. *(Continuous-Time Markov Chain)*

```
|- !X p s Linit Ltrans.
        ctmc X p s Linit Ltrans <=>
        mc_property X p s /\ (!x. x IN space s ==> {x} IN subsets s) /\
        (!i. i IN space s ==> (Linit i = distribution p (X 0) {i})) /\
        !i j t.
          distribution p (X t) {i} <> 0 ==>
          (Ltrans t i j = Trans X p s t 1 i j)
```

where the first three variables are inherited from Definition 2, p_0 and p_{ij} refer to the functions expressing the given initial status and transition matrix associated with this random process, respectively. The first condition in this definition describes Markov property presented in Definition 2 and the second one ensures the events associated with the state space (`space s`) are discrete in the event space (`subsets s`), which is a *discrete space*. The last two conditions assign the functions `p0` and `pij` to initial distributions and transition probabilities.

It is important to note that `X` is polymorphic, i.e., it is not constrained to a particular type, which is a very useful feature of our definition.

Most of the applications actually make use of *time-homogenous CTMCs*, i.e., CTMCs with finite state-space and time-independent transition probabilities [3]. The time-homogenous property refers to the time invariant feature of a random process. Thus, the transition probability of the random process in a fixed interval, say [0, t - n], is independent of the start time. This can be simplified as $p_{ij} = \mathcal{P}r\{X_t = j|X_n = i\} = p_{ij}(t-n)$, based on Equation (5). Then, the time-homogenous DTMC with finite state-space can be formalized as follows:

Definition 6. *(Time homogeneous DTMC)*

```
|- !X p s Linit Ltrans.
        th_ctmc X p s Linit Ltrans <=>
        ctmc X p s Linit Ltrans /\ FINITE (space s) /\
        !t n i j.
          n < t ==> (Trans X p s t n i j = Trans X p s 0 (t - n) i j)
```

4 Verification of Two Properties

Using the formalized CTMC in previous section, we formally verified two of its properties in this section.

4.1 Unconditional Probability

The unconditional probabilities associated with a Markov chain are called *absolute probabilities*, which can be computed by applying the initial distributions and n-step transition probabilities. This shows that, given a distributions at the start time v and the transition probabilities in time interval , the absolute probability in the state j after n steps from the start time 0 can be obtained by using this equation.

This property is formally verified as the following theorem: In a finite time homogeneous DTMC, the absolute probabilities $p_j^{(t)}$ satisfy

$$p_j^{(t)} = \mathcal{P}r(X_t = j) = \sum_{k \in \Omega} \mathcal{P}r(X_0 = k)\mathcal{P}r(X_t = j|X_0 = k)$$

Theorem 1. *(Unconditional Probability)*

```
|- !X p s Linit Ltrans t j.
         ctmc X p s Linit Ltrans /\ FINITE (space s) ==>
         (prob p (PREIMAGE (X t) {j} INTER p_space p) =
          SIGMA (\i. cond_prob p (PREIMAGE (X t) {j} INTER p_space p)
                 (PREIMAGE (X 0) {i} INTER p_space p) *
              prob p (PREIMAGE (X 0) {i} INTER p_space p)) (space s)) :
```

The proof of Theorem 1 is based on the Total Probability theorem (3b) along with some basic arithmetic and probability theoretic reasoning.

4.2 Chapman-Kolmogorov Equation

The *Chapman-Kolmogorov equation* [4] is a widely used property of time homogeneous DTMCs. It gives the probability of going from state i to j in $m+n$ steps. Assuming the first m steps take the system from state i to some intermediate state k and the remaining n steps then take the system from state k to j, we can obtain the desired probability by adding the probabilities associated with all the intermediate steps.

For a finite time homogeneous DTMC $\{X_t\}_{t\geq 0}$, its transition probabilities satisfy the Chapman-Kolmogorov Equation

$$p_{ij}(v,t) = \sum_{k\in\Omega} p_{ik}(v,u)pkj(u,t)\ for 0 \leq v < u < t$$

Theorem 2. *(Chapman-Kolmogorov Equation)*

```
    |- !X p s Linit Ltrans t v i j.
         ctmc X p s Linit Ltrans /\ u < t /\ 0 <= v /\ v < u /\
         FINITE (space s) ==>
         (cond_prob p (PREIMAGE (X t) {j} INTER p_space p)
            (PREIMAGE (X v) {i} INTER p_space p) =
          SIGMA (\k. Trans X p s u (t - u) k j * Trans X p s v (u - v) i k)
            (space s))
```

Proof. Theorem 2 is again verified using induction on the variables t and v.

5 Potential Challenges

The verified two properties are the basic theorems, which might be required in diverse other CTMC theorems. In fact, the most important concept in CTMC theory is the *transition rate*, which is a nonnegative continuous function $q_{ij}(t)$. Usually, in a CTMC model, the transition rates are given instead of transition probabilities. The mathematic expression of a transition rate is shown as follows:

$$\frac{\partial p_{ij}(v,t)}{\partial t} = [\sum_{k\neq i} p_{kj}(v,t)q_{ik}(t)] - p_{ij}(v,t)q_i(t). \tag{6}$$

where it requires the limit theory to define the transition rate and the verification of the related theorems will associated with the limit, derivative and integral theories. For example, the *Kolmogorov's forward equation*

$$\frac{\partial p_{ij}(v,t)}{\partial t} = [\sum_{k \neq i} p_{kj}(v,t) q_{ik}(t)] - p_{ij}(v,t) q_i(t); \tag{7}$$

and *Kolmogorov's backward equation*

$$\frac{\partial p_{ij}(v,t)}{\partial v} = [\sum_{k \neq i} p_{kj}(v,t) q_{ik}(v)] - p_{ij}(v,t) q_i(v). \tag{8}$$

Equations (7) and (8) can be used to derive the unconditional probability by the following differential equation:

it is able to formally derive the *Kolmogorov's backward equation* [35] as well as variety of its other properties in HOL4.

6 Conclusions & Future Work

In this report, we explored the formalization of continuous-time Markov chain (CTMC) based on the development of discrete-time Markov chain (DTMC) in [24]. Using the formal definition of the continuous-time Markov chain and two of its verified properties presented in this report, diverse systems described as CTMCs can be formally analyzed. This report provides a simply definition as a prototype and offers the necessary information on the formalization of CTMC.

The formalization of CTMC lead to many new directions of research in the domain of formal verification. For example, continuous-time HMMs, which are used for formally assessing the diseases in medical and biological domains, as well as estimating the electronic system reliability; and continuous-time semi-Markov process [19] and Markov jump process [26] can be formalized using the CTMC formalization.

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