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Approximate adaptive uniformization of continuous-time Markov chains

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ABSTRACT

We consider the approximation of transient (time dependent) probability distributions of discrete-state continuous-time Markov chains on large, possibly infinite state spaces. A framework for approximate adaptive uniformization is provided, which generalizes the well-known uniformization technique and many of its variants. Based on a birth process and a discrete-time Markov chain a computationally tractable approximating process/model is constructed. We investigate the theoretical properties of this process and prove that it yields computable lower and upper bounds for the desired transient probabilities. Finally, we discuss different specific ways of performing approximate adaptive uniformization and analyze the corresponding approximation errors. The application is illustrated by an example of a stochastic epidemic model.

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1. Introduction

Continuous-time Markov chains (CTMCs) with large (possibly countably infinite) discrete state spaces are widely used to model real-world systems and processes in many areas such as engineering and environmental processes, computer and communication networks, transportation, logistics, production and manufacturing systems, healthcare systems, epidemic diseases, multiphysics systems, or biochemically reacting systems, amongst many others. Often the interest is in transient (time dependent) system behavior or performance properties, respectively, and the analysis requires the determination of transient probability distributions. For instance, recent real-world applications in which transient probability distributions of CTMCs are highly relevant include such diverse areas as epidemics and the spread of diseases in human and animal populations as well as in computer networks [1–4], upstream inventory information sharing in supply chain networks [5], evacuation route selection of large-scale crowds under emergencies [6], allelopathic interactions between competing phytoplankton species in marine environments [7], or the impact of calcium fluxes on cells in the brain [8].

We consider a regular (conservative and non-explosive) CTMC $X = \{X(t), t \geq 0\}$, that is a discrete-state Markov jump process with only finitely many jumps in any finite time interval and right-continuous sample paths. Without loss of generality we assume that the state space is $S \subseteq \mathbb{N} = \{0, 1, 2, \ldots\}$. The infinitesimal generator of the CTMC is expressed by the matrix $Q = (q_{ij})_{i,j \in S}$, where $q_{ij} < \infty$ for $i \neq j$ are the state transition rates and $q_{ii} := -\sum_{i \neq j} q_{ij}$ such that all row sums of Q are zero, that is the CTMC is conservative. We define $q_i := -q_{ii}$. At any time $t \geq 0$ the transient (time-dependent) distribution is the collection of all state probabilities at that time, represented by the row vector $p(t)$. For any initial distribution $p(0)$ it is given

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by

$$p(t) = p(0)e^{Qt} = p(0)\sum_{k=0}^{\infty}\frac{(Qt)^k}{k!} \tag{1}$$

as the unique solution of the corresponding system of Kolmogorov (backward and forward) differential equations, see [9, pp. 80–81], [10, pp. 251–252].

Since analytical solutions are only possible in special cases, numerical techniques are commonly applied [11,12], but conceptually exact approaches are often computationally intractable due to prohibitively large (possibly infinite) state spaces.

Uniformization, also known as randomization or discrete-time conversion, provides a numerically stable computational scheme to approximate the transient probability distributions of CTMCs with uniformly bounded transition rates. It was originally proposed by Jensen [13], has been used to study computational and theoretical aspects of CTMCs [14–22] and has become one of the most prevalent approaches to the numerical transient analysis of CTMCs.

The underlying principle is to consider a *subordinated discrete-time Markov chain* (DTMC) $Y = \{Y(n), n \in \mathbb{N}\}$ with initial distribution $p(0)$ and transition probability matrix $P = Q/\lambda + I$ where $\sup_i q_i \le \lambda < \infty$. Hence, $Q = \lambda(P - I)$ such that the transient distribution of the CTMC can be written as

$$p(t) = p(0)e^{-\lambda t}e^{\lambda Pt} = p(0)e^{-\lambda t}\sum_{k=0}^{\infty}\frac{(\lambda t)^k P^k}{k!} = \sum_{k=0}^{\infty} p(0)P^k\frac{(\lambda t)^k e^{-\lambda t}}{k!}. \tag{2}$$

Note that $p(0)P^k =: \pi^{(k)}$ is the probability distribution of the DTMC after k steps and $(\lambda t)^k e^{-\lambda t}/k!$ is the probability that a Poissonian random variable with parameter λt takes the value k, which equals the probability of exactly k events during a time period of length $t \ge 0$ in a Poisson process with rate λ. Hence, the principle of uniformization can be viewed as the construction of a Poisson process $\{N(t),\ t \ge 0\}$ and a DTMC $\{Y(n), n \in \mathbb{N}\}$ such that $Y(N(t))$ has the same distribution as $X(t)$ for every $t \ge 0$.

In numerical computations $\pi^{(k)} = \pi^{(k-1)}P$ can be computed iteratively and the infinite sum in (2) must be truncated, for which a priori truncation error bounds can be set and a corresponding truncation point can be determined based on the cumulated sum of Poisson probabilities, cf. [23], [12, pp. 410–413]. This technique, henceforth referred to as standard uniformization (SU), often works well, but it has several serious drawbacks in case of large and stiff models. In particular, it requires uniformly bounded transition rates and a global *uniformization rate* λ that is a finite upper bound on the maximum outrate of states, which is typically not available in the case of an infinite state space.

Adaptive uniformization (AU) [24] is an approach to cope with large state spaces without assuming uniformly bounded transition rates by adapting the uniformization rate. More precisely, it is shown in [24] that depending on the set of *active states* with nonzero probabilities after a particular number of jumps one can construct a birth process $\{B(t),\ t \ge 0\}$ and a subordinated DTMC $\{Y(n), n \in \mathbb{N}\}$ such that $Y(B(t))$ has the same distribution as $X(t)$ for every $t \ge 0$. The n-th transition rate of the birth process corresponds to the 'fastest' state visited by the DTMC at step n with positive probability. This differs from the (constant) rate λ of the Poisson process in that the birth process jumps at rates smaller than or equal to λ. As a result, the number of vector-matrix multiplications required by AU may be lower than for SU, in particular if the average rate of the birth process is much less than the jump rate λ of the Poisson process in SU. However, in many cases AU is less efficient than SU.

The computation of the probabilities $Pr(B(t) = n)$ required with AU [24] is more difficult than the computation of Poisson probabilities for SU. Furthermore, in general, the rates of the birth process defined by AU converge to the supremum of the transition rates of all non-transient states of the CTMC X. Thus, the potential computational gain that can be achieved by AU as compared to SU is anyway marginal for sufficiently long time horizons. Besides, the initial set of active states can be already large or the adapted set of active states can grow quickly, that is, the number of states with nonzero initial probability is large, or a large number of states have a nonzero probability after only a few steps in the subordinated DTMC. In such cases, even for small and moderate time horizons AU is less efficient than SU.

Another way of applying the uniformization idea to Markov chains with large state spaces is by state space truncation, which effectively reduces the number of nonzero entries in the transition probability matrix of the respective subordinated DTMC Y, thereby reducing the effort required for the vector-matrix multiplications in numerical computations. Such truncation approaches often allow to compute accurate approximations to the transient distributions of infinite-state CTMCs with relatively moderate execution times and memory costs. For instance, approximate uniformization [25] is a truncated version of SU using a fixed state space truncation such that the assumption of uniformly bounded transition rates can be relaxed. Similarly, inexact uniformization [26] proceeds SU while ignoring states with small probabilities below a pre-specified threshold, which in fact corresponds to truncating the state space.

Fast adaptive uniformization [27] combines state space truncation and the use of adaptive uniformization rates. In this approach, the truncation of the state space not only decreases the computational effort of the vector-matrix multiplication, but also allows the use of smaller transition rates for the birth process than with AU. This leads to a further reduction in the number of vector-matrix multiplications required to approximate transient distributions of CTMCs. The method has been applied in [27] to stochastic chemical kinetics by heuristically choosing sets of active states as sets of 'temporarily significant' states with a probability below a certain threshold similarly as in [26] but with adapted uniformization rates

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