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Efficient computation of the bounds of continuous time imprecise Markov chains

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ABSTRACT

When the initial distribution and transition rates for a continuous time Markov chain are not known precisely, robust methods are needed to study the evolution of the process in time to avoid judgements based on unwarranted precision. We follow the ideas successfully applied in the study of discrete time model to build a framework of imprecise Markov chains in continuous time. The imprecision in the distributions over the set of states is modelled with upper and lower expectation functionals, which equivalently represent sets of probability distributions. Uncertainty in transitions is modelled with sets of transition rates compatible with available information. The Kolmogorov's backward equation is then generalised into the form of a generalised differential equation, with generalised derivatives and set valued maps. The upper and lower expectation functionals corresponding to imprecise distributions at given times are determined by the maximal and minimal solutions of these equations. The second part of the paper is devoted to numerical methods for approximating the boundary solutions. The methods are based on discretisation of the time interval. A uniform and adaptive grid discretisations are examined. The latter is computationally much more efficient than the former one, but is not applicable on every interval. Therefore, to achieve maximal efficiency a combination of the methods is used.
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1. Introduction

Modelling with Markov chains requires a large number of parameters to be estimated, which is often impossible to accomplish with without significant degree of uncertainty. Moreover, the assumption of constant transition rates is often unrealistic. To better tackle the implied uncertainties, a robust model for continuous time Markov chains is needed. In this paper we present a model capable of producing probability distributions corresponding to continuous time Markov chains that faithfully reflect the uncertainty in input parameters. Moreover, instead of assuming constant transition rates, we allow them to vary within a given set.

Modelling uncertainty in probability distributions has received a lot of attention in last decades. One of the most widely accepted models of uncertainty in probability distributions is the approach proposed by [18], that is based on subjective Bayesian interpretation of probability. Very briefly, Walley's model introduces non-linear functionals called lower and upper previsions which are generalisations of expectation functionals. A special class of lower or upper previsions that satisfy the condition of coherence is then in a one-to-one correspondence with convex sets of linear expectation functionals. This correspondence then allows a natural interpretation of uncertainty in terms of multiple probabilistic scenarios compatible with

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the available information. Convexity of the sets of expectation functionals may seem restrictive, but in fact sets of possible probabilistic models in most cases imply the same behavioural dispositions as their convex envelopes (see e.g. [13] and references therein).

The models of imprecise probabilities have been successfully applied to the theory of Markov chains in discrete time [4,6,10,15–17]. The questions such as calculating (imprecise) distributions over states after a certain number of steps, (unique) convergence to equilibrium and classification of invariant distributions have been addressed in the listed references.

Concerning continuous time Markov chains modelling under uncertainty, the closest to our problem is the work of [9], who studies the set of solutions of interval matrix differential equations. Its main contribution is the proof of existence and description of the set of solutions; although, it does not provide methods for analytically or numerically estimating the solution bounds. Another related field is the study of dynamical systems via differential inclusions [14], which can be understood as a generalisation of differential equations in the presence of uncertainty. The equations in our model resemble differential inclusions – our equations relate to linear-selectionable differential inclusions in Smirnov's terminology – although we do not stipulate differentiability in the ordinary sense, which would only unnecessarily restrict the dynamics of the transition rates regime. Instead we only use the more general Dini derivatives, which do not require convergence of the difference quotients. Still, it turns out that the boundary solutions are nevertheless differentiable in the ordinary sense. Our approach is also specific in the sense that only maximal and minimal solutions are of interest. This is because convex sets of expectation functionals are completely determined by the values of the corresponding lower and upper expectation functionals. We therefore develop specific numerical methods for evaluation of the boundary solutions.

Another field where Markov chains with multiple transition scenarios are studied are Markov decision processes [1,2,11], where transition rate scenario is selected from a set of scenarios using so-called schedulers, which depend on the process history and rule the transition rates until the next change of state occurs. The main difference between our model and Markov decision process, apart from some technical differences in presentation of the sets of transition scenarios, is that in our model transition rate scenarios depend purely on time and may change during the time before a transition occurs. Compared with our model, this difference results in different bounds for probability distributions and also different methods needed to estimate them.

The aim of the present paper is to propose a framework for continuous time Markov chains under uncertainty and methods for practical calculations of evolution of the distributions over states in time. The model is built on uncertain transition rates that are given in terms of a closed convex set of transition rates. At any time, the only assumption on the transition rates is that they belong to the prescribed set. In this sense our model is very general in comparison with the related models where either continuity or differentiability [9] are required, or that the transition rates only change when transition occurs [1,2,11]. The modelling approach with lower and upper expectation functionals and transition operators, allows us to translate the problem to the form of non-linear matrix differential equations.

In the second part we provide an efficient combined numerical method for solving the non-linear matrix differential equations. We first examine the standard approach with a uniform grid discretisation [7,8], where an approximate solution is obtained by transforming the differential equation into a discrete time difference equation. At each step a set of linear programming problems has to be solved to find the extremal matrix solution. Due to slow convergence the size of the grid must be large to ensure good approximations, resulting in high computational costs.

The improved adaptive grid method is based on the observation (at first empirical), that the extremal solutions of the linear programming problems applied to the uniform grid, remain constant or approximately constant on intervals that are large in comparison with the size of the intervals forming the grid. We therefore develop a method which allows identification of intervals where the solutions remain approximately constant. Consequently we can then apply analytical solutions of ordinary matrix differential equations, which is computationally much cheaper, on large intervals. The uniform grid method is then only needed in a smaller portion of the entire interval of interest. This significantly reduces the computational costs.

The paper has the following structure. In the next section the elements of the theory of imprecise probabilities are described, which form the basis of the model, and the model for continuous time imprecise Markov chains that involves imprecise transition rates and the corresponding imprecise expectation functionals is introduced. In Section 3 we analyse the corresponding differential equations and prove the existence of unique solutions. Methods for numerical solutions are given in Section 4. A discussion on the efficiency of the models and an analysis of computational complexity is given in Section 5.

2. Imprecise continuous time Markov chains

2.1. Coherent lower and upper previsions

First we give a short description of the Walley's model of coherent lower and upper previsions, which is a widely accepted general model for uncertainty in probability distributions. In our case where we only consider finite sets, several aspects will be simplified in comparison with the general theory. Such aspects are for instance boundedness of real valued mappings and compactness of closed sets. There is also no need to make distinction between finite additivity and countable additivity which is a great concern in general theory of imprecise probabilities.

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