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An Imprecise Probabilistic Estimator for the Transition Rate Matrix of a Continuous-Time Markov Chain

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ABSTRACT

Continuous-time Markov chains (CTMCs) are mathematical models that describe the evolution of dynamical systems under uncertainty [Norris, 1998]. They are pervasive throughout science and engineering, finding applications in areas as disparate as medicine, mathematical finance, epidemiology, queueing theory, and others. We here consider time-homogeneous CTMCs that can only be in a finite number of states.

The dynamics of these models are uniquely characterised by a single *transition rate matrix* Q. This Q describes the (locally) linearised dynamics of the model, and is the generator of the semi-group of transition matrices $T_t = \exp(Qt)$ that determines the conditional probabilities $P(X_t = y \mid X_0 = x) = T_t(x, y)$. In this expression, X_t denotes the uncertain state of the system at time t, and so, for all x, y, the element $T_t(x, y)$ is the probability for the system to move from state x at time zero, to state y at time t.

In this work, we consider the problem of estimating the matrix Q from a single realisation of the system up to some finite point in time. This problem is easily solved in both the classical frequentist and Bayesian frameworks, due to the likelihood of the corresponding CTMC belonging to an exponential family; see e.g. the introductions of [Inamura, 2006, Bladt and Sørensen, 2005]. The novelty of the present work is that we instead consider the estimation of Q in an *imprecise probabilistic* context [Walley, 1991, Augustin *et al.*, 2014].

Specifically, we approach this problem by considering an entire *set* of Bayesian priors on Q, leading to a *set-valued* estimator for this parameter. In order to obtain well-founded hyperparameter settings for this set of priors, we recast the problem by interpreting a continuous-time Markov chain as a limit of *discrete*-time Markov chains. This allows us to consider the imprecise-probabilistic estimators of these discrete-time Markov chains, which are described by the popular Imprecise Dirichlet Model (IDM) [Quaeghebeur, 2009]. The upshot of this approach is that the IDM has well-known prior hyperparameter settings which can be motivated from first principles [Walley, 1996, De Cooman *et al.*, 2015].

This leads us to the two main results of this work. First of all, we show that the limit of these IDM estimators is a set $\mathcal{Q}_s$ of transition rate matrices that can be described in closed-form using a very simple formula. Secondly, we identify the hyperparameters of our imprecise CTMC prior such that the resulting estimator is equivalent to the estimator obtained from this discrete-time limit. The only parameter of the estimator is a scalar $s \in \mathbb{R}_{\geq 0}$ that controls the degree of imprecision. In the special case where $s = 0$ there is no imprecision, and then $\mathcal{Q}_0 = \{Q^{\mathrm{ML}}\}$, where Q^{ML} is the standard maximum likelihood estimate of Q.

The immediate usefulness of our results is two-fold. From a domain-analysis point of view, where we are interested in the parameter values of the process dynamics, our imprecise estimator provides prior-insensitive information about these values based on the data. If we are instead interested in robust inference about the future behaviour of the system, our imprecise estimator can be used as the main parameter of an *imprecise continuous-time Markov chain* [Škulj, 2015, De Bock, 2016, Krak *et al.*, 2017].

The results that we present here have previously been published in [Krak *et al.*, 2018].

References

[Augustin *et al.*, 2014] Augustin, T., Coolen, F.P.A., De Cooman, G., Troffaes, M.C.M. (eds.): *Introduction to Imprecise Probabilities*. John Wiley & Sons (2014)

[Bladt and Sørensen, 2005] Bladt, M., Sørensen, M.: Statistical inference for discretely observed Markov jump processes. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* 67(3), 395–410 (2005)

[De Cooman *et al.*, 2015] De Cooman, G., De Bock, J., Diniz, M.A.: Coherent predictive inference under exchangeability with imprecise probabilities. *Journal of Artificial Intelligence Research* 52, 1–95 (2015)

[De Bock, 2016] De Bock, J.: The limit behaviour of imprecise continuous-time markov chains. *Journal of Nonlinear Science* 27(1), 159–196 (2017)

[Inamura, 2006] Inamura, Y.: Estimating continuous time transition matrices from discretely observed data. Bank of Japan (2006)

[Krak *et al.*, 2017] Krak, T., De Bock, J., Siebes, A.: Imprecise continuous-time Markov chains. *International Journal of Approximate Reasoning* 88, 452–528 (2017)

[Krak *et al.*, 2018] Krak, T., Errerygers, A., De Bock, J.: An Imprecise Probabilistic Estimator for the Transition Rate Matrix of a Continuous-Time Markov Chain. *Proceedings of SMPS 2018*, 124–132 (2018)

[Norris, 1998] Norris, J.R.: *Markov chains*. Cambridge university press (1998)

[Quaeghebeur, 2009] Quaeghebeur, E.: *Learning from samples using coherent lower previsions*. Ph.D. thesis

[Škulj, 2015] Škulj, D.: Efficient computation of the bounds of continuous time imprecise Markov chains. *Applied Mathematics and Computation* 250(C), 165–180 (2015)

[Walley, 1991] Walley, P.: *Statistical reasoning with imprecise probabilities*. Chapman and Hall, London (1991)

[Walley, 1996] Walley, P.: Inferences from multinomial data: learning about a bag of marbles. *Journal of the Royal Statistical Society, Series B* 58, 3–57 (1996)