An Efficient Lower Transition Rate Operator for the Sensitivity Analysis of Continuous-Time Markov Chains*

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Continuous-time Markov chains (CTMCs) are popular probabilistic models that describe the uncertain evolution of a dynamical system whose time domain is the non-negative reals $\mathbb{R}_{\geq 0}$. We assume that this system takes values in a non-empty and finite *state space* $\mathscr{X}$, with size $n := |\mathscr{X}|$. When a CTMC is *time-homogeneous*, it can be characterised—up to its initial distribution—by a single *rate matrix* Q. This is a $n \times n$ matrix with entries $Q(x,y) \in \mathbb{R}$, such that for all $x \in \mathscr{X}$, $\sum_{y \in \mathscr{X}} Q(x,y) = 0$ and $Q(x,y) \geq 0$ for all $y \in \mathscr{X}$ with $x \neq y$. We use $\mathscr{R}$ to denote the set of all rate matrices.

When faced with uncertainty about the specification of a CTMC—be it with respect to the numerical parameters, or structural assertions like Markovianity or time-homogeneity—a sensitivity analysis may be performed using a continuous-time *imprecise*-Markov chain (CTIMC). This model can be seen as a *set* $\mathbb{P}_{\mathscr{Q}}$ of stochastic processes that are *consistent* with a non-empty bounded *set* $\mathscr{Q} \subset \mathscr{R}$ of rate matrices. One may consider different types of CTIMCs by including different types of models in $\mathbb{P}_{\mathscr{Q}}$. For example, one may include all time-homogeneous CTMCs characterised by the elements $Q \in \mathscr{Q}$. However, one could additionally include non-homogeneous CTMCs, or even more general—non-Markovian—processes; see Krak [1] for an analysis of these different types. Given a CTIMC $\mathbb{P}_{\mathscr{Q}}$, the associated (conditional) lower- and upper expectations $\underline{\mathbb{E}}_{\mathscr{Q}}[\cdot\,|\,\cdot]$ and $\overline{\mathbb{E}}_{\mathscr{Q}}[\cdot\,|\,\cdot]$ provide tight lower- and upper bounds, for any inference of interest, with respect to every model included in $\mathbb{P}_{\mathscr{Q}}$. To make this practicable, we need efficient methods to compute these lower- and upper expectations; by the well-known *conjugacy* property $\overline{\mathbb{E}}_{\mathscr{Q}}[\cdot\,|\,\cdot] = -\underline{\mathbb{E}}_{\mathscr{Q}}[-\cdot\,|\,\cdot]$, it suffices to focus on only the lower expectations.

Following Škulj [2], we associate with $\mathscr{Q}$ its corresponding *lower transition rate operator* $\underline{Q}$, which is a map $\underline{Q} : f \mapsto \underline{Q}f$ from $\mathbb{R}^{\mathscr{X}}$ to $\mathbb{R}^{\mathscr{X}}$, where for all $f \in \mathbb{R}^{\mathscr{X}}$ and $x \in \mathscr{X}$, we let $\underline{Q}f(x) := \inf_{Q \in \mathscr{Q}} Qf(x)$. Then for any $f \in \mathbb{R}^{\mathscr{X}}$ and $t \in \mathbb{R}_{\geq 0}$, the quantity $\underline{\mathbb{E}}_{\mathscr{Q}}[f(X_t)\,|\,X_0]$ can be conservatively bounded by the solution $\underline{f}_t \in \mathbb{R}^{\mathscr{X}}$ to the initial value problem

$$\frac{\mathrm{d}\underline{f}_t}{\mathrm{d}t} = \underline{Q}\,\underline{f}_t \quad \text{for all } t \in \mathbb{R}_{\geq 0}, \text{ with } \underline{f}_0 = f. \tag{1}$$

That is, it holds that $\underline{f}_t(x) \leq \underline{\mathbb{E}}_{\mathscr{Q}}[f(X_t)\,|\,X_0 = x]$ for all $t \in \mathbb{R}_{\geq 0}$ and $x \in \mathscr{X}$; crucially however, this bound is satisfied with equality under some relatively mild assumptions on $\mathbb{P}_{\mathscr{Q}}$ and $\mathscr{Q}$ [2, 1]. Hence in those cases, solving (1) amounts to computing the lower expectation of interest exactly. The differential equation (1) may be solved e.g. by iterative methods described by Škulj [2], Krak [1]. To apply these methods, we need an (ideally efficient) way to evaluate $\underline{Q}f$ for any $f \in \mathbb{R}^{\mathscr{X}}$.

We here consider a special case that we feel is important for sensitivity analysis, where we construct a simple perturbation model for a given rate matrix Q; we let $\mathscr{Q} := \mathscr{B}(Q,r) := \{Q' \in \mathscr{R} : \|Q - Q'\|_\infty \leq r\}$ be the closed ball in $\mathscr{R}$ of radius $r \in \mathbb{R}_{\geq 0}$ around Q. This $\mathscr{Q}$ satisfies the required properties to make the solution of (1) coincide with the lower expectation of interest [1, Prop. 6.20 and Cor. 6.25]. Our main current contribution is Algorithm 1, which enables the efficient computation of $\underline{Q}f$ in this case; for a proof of correctness, see Krak [1, Prop. 6.21]. It is easily seen that the runtime complexity of this algorithm is $O(n^2)$. This enables the exceptionally efficient computation of exact bounds on inferences under this perturbation model.

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input: Rate matrix Q ∈ ℛ, radius r ∈ ℝ_{≥0}, function f ∈ ℝ^𝒳
output: Function Q̲f ∈ ℝ^𝒳, where Q̲ corresponds to 𝒬 = ℬ(Q,r) ⊂ ℛ
(x_1,...,x_n) := SortDecreasing(𝒳, f); // sort 𝒳 such that f(x_i) ≥ f(x_{i+1}) for all i ∈ {1,...,n−1}
for x ∈ 𝒳 do
    r_0 := r/2
    for i ∈ {1,...,n} do
        if x_i = x then Δ_i := r_{i−1} else Δ_i := min{r_{i−1}, Q(x,x_i)}
        r_i := r_{i−1} − Δ_i
    Q̲f(x) := Qf(x) − Σ_{i=1}^{n} Δ_i (f(x_i) − f(x_n))
return Q̲f
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Algorithm 1: Efficiently evaluate $\underline{Q}f$.

References

[1] Thomas Krak. *Continuous-Time Imprecise-Markov Chains: Theory and Algorithms*. PhD thesis, 2021.

[2] Damjan Škulj. Efficient computation of the bounds of continuous time imprecise Markov chains. *Appl. Math. Comput.*, 250:165–180, 2015.

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