Computational methods for imprecise continuous-time birth-death processes: a preliminary study of flipping times

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The Precise Case

Consider a continuous time and finite-state Markov process with state space $\mathcal{X}$. At any time $t \in [0, +\infty)$, the stochastic matrix of the process P_t is derived from a transition rate matrix Q. For $i, j \in \mathcal{X}$, the element at the i row and j column of Q is denoted by $Q(i,j)$. For the matrix Q, the following properties hold

(P1) $Q(i,j) \geq 0$ for all $i, j \in \mathcal{X}$ such that $i \neq j$
(P2) $\sum_{j \in \mathcal{X}} Q(i,j) = 0, \forall i \in \mathcal{X}$

A matrix Q is said to be bounded if $Q(i,i) > -\infty$ for all $i \in \mathcal{X}$ or, equivalently, if $\|Q\| < \infty$. Our results hold for various types of norm, but the one we consider is the infinite norm defined by $\|Q\| := \|Q\|_\infty = \max\{\sum_{j \in \mathcal{X}} |Q(i,j)| : i \in \mathcal{X}\}$.

When Q is bounded, then P_t satisfies the Kolmogorov backward equation

$$\frac{d}{dt} P_t = Q P_t. \tag{1}$$

If we let $f_t(i) := E_t(f|X_0 = i)$, with f a real-valued function on the finite state space $\mathcal{X}$ and $i \in \mathcal{X}$ an initial state, then we can rewrite Equation (1) as follows

$$\frac{d}{dt} f_t = Q f_t. \tag{2}$$

Combined with the boundary condition $f_0 = f$, the unique solution of Equation (2) is $f_t = e^{tQ} f$. Instead of considering a time-invariant Q, we can also let Q_t be a function of the time t. In that case, Equation (2) can be rewritten as

$$\frac{d}{dt} f_t = Q_t f_t. \tag{3}$$

which, in general, has no analytical solution.

A "messy" case

Consider the state space $\mathcal{X} := \{0, 1, 2, 3\}$, the following set $\mathcal{Q}$ of bounded matrices

$$\left\{ \begin{pmatrix} -p_i & p_i & 0 & 0 \\ q_j & -q_j & 0 & 0 \\ 0 & 0 & -r & r \\ 0 & 0 & s & -s \end{pmatrix} : a_i \in [\underline{a}, \overline{a}] \text{ and } b_j \in [\underline{b}, \overline{b}] \right\}$$

and a function f of the form $[c, c, f_2, f_3]^T$. In this case, we cannot efficiently identify Q_{τ_0}, because for any $Q, Q' \in \mathcal{Q}$, we have that $Q^k f = Q'^k f$, for all $k \in \mathbb{N}$.

Is there a simple way to check when two different matrices Q, Q' yield the same expected value, without calculating Q^k and Q'^k for all k?

Imprecise Birth-Death Process

We focus on the case where every state has an interval-valued birth and/or death rate. The transition rate matrices have the following form

$$\begin{pmatrix} -\lambda_0 & \lambda_0 & 0 & \cdots & \cdots & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & \mu_i & -(\mu_i + \lambda_i) & \lambda_i & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & \cdots & \cdots & 0 & \mu_L & -\mu_L \end{pmatrix}$$

where, for all $i \in \{0, \ldots, L-1\}$ and $j \in \{1, \ldots, L\}$, $\lambda_i \in [\underline{\lambda}, \overline{\lambda}]$ and $\mu_j \in [\underline{\mu}, \overline{\mu}]$ and $L \in \mathbb{N}$. In this way, we have a set of matrices $\mathcal{Q}$ with finite numbers of extreme points, separately specified rows and which avoids the special case above.

The Imprecise Case

Set of matrices Instead of a single transition matrix Q, we consider a set of such matrices, denoted by $\mathcal{Q}$. We assume that each matrix in $\mathcal{Q}$ is bounded and satisfies (P1) and (P2). Let $\mathcal{R}$ be the set of all rate matrices, then for any set $\mathcal{Q} \subseteq \mathcal{R}$ of rate matrices, we let

$$\mathcal{Q}_i := \{Q(i, \cdot) : Q \in \mathcal{Q}\} \text{ for all } i \in \mathcal{X},$$

and we say that $\mathcal{Q}$ has *separately specified rows* if

$$Q \in \mathcal{Q} (\forall i \in \mathcal{X})\ Q(i, \cdot) \in \mathcal{Q}_i.$$

We further assume that $\mathcal{Q}$ is the convex hull of a *finite* number of extreme transition rate matrices.

Our Approach At any time $t \in [0, +\infty)$, the only assumption we make about Q_t is that it is an element of $\mathcal{Q}$. Every such possible choice of non-stationary transition rate matrices will, by (3), result in a—possibly different—solution f_t. Our goal is to calculate exact lower and upper bounds for the set of all these solutions f_t, as denoted by $\underline{f}_t$ and $\overline{f}_t$. In the recent work of Škulj and with respect to the lower bound, $\underline{f}_t$ is the solution to

$$\frac{d}{dt} \underline{f}_t = \min_{Q \in \mathcal{Q}} Q \underline{f}_t, \text{ with boundary condition } \underline{f}_0 = f. \tag{4}$$

Since $\mathcal{Q}$ is the convex hull of a finite number of extreme transition rate matrices and that the solution to (4) is continuous, there must be time points $0 = t_0 < t_1 < \ldots < t_n < t_{n+1} < \ldots$ such that, for all $t \in \tau_n := [t_n, t_{n+1}]$, the minimum in (4) is obtained by the same extreme transition rate matrix $Q_{\tau_n} \in \mathcal{Q}$. We call these time points t_n *flipping times*. Equation (4) is then piecewise linear and has the following solution

$$\underline{f}_t = e^{(t-t_n) Q_{\tau_n}} e^{(t_n - t_{n-1}) Q_{\tau_{n-1}}} \ldots e^{(t_2 - t_1) Q_{\tau_1}} e^{t_1 Q_{\tau_0}} f, \text{ for } t \in [t_n, t_{n+1}]. \tag{5}$$

Calculating Lower Expectations We need to find the flipping times t_n and the corresponding extreme transition rate matrices Q_{τ_n} when calculating the lower expectation of a given f on $\mathcal{X}$. It is known that

$$\frac{\partial}{\partial t} [e^{tQ} f] \Big|_{t=0} = Qf \Rightarrow (\forall \varepsilon > 0)(\exists \delta > 0)(\forall t \in (0, \delta)) \|e^{tQ} f - f - tQf\|_\infty < t\varepsilon \tag{6}$$

and it can be further proved that for any pair of matrices Q, Q' in $\mathcal{Q}$

$$\text{if } Qf < Q'f, \text{ then } (\exists \delta > 0)(\forall t \in (0, \delta))\ e^{tQ} f < e^{tQ'} f,$$

where $Qf < Q'f$ if $Qf(i) \leq Q'f(i)$ for all $i \in \mathcal{X}$ and $Qf \neq Q'f$. In order to find Q_{τ_0} in (5), we need to find a Q such that $Qf < Q'f$, for all $Q' \in \mathcal{Q} \setminus \{Q\}$. Since $\mathcal{Q}$ has separately specified rows, we can identify Q_{τ_0} by minimising Qf at each row separately. Hence, Q_{τ_0} belongs to the set

$$\mathcal{Q}_{\tau_0} := \{Q \in \mathcal{Q} : Qf(i) \leq Q'f(i), \forall i \in \mathcal{X} \text{ and } \forall Q' \in \mathcal{Q} \setminus \{Q\}\}.$$

In practice, $\mathcal{Q}_{\tau_0}$ might not be a singleton and in this case, for any two matrices Q, Q' in $\mathcal{Q}_{\tau_0}$, we have that $Qf = Q'f$. Since we know that $\frac{\partial^k}{\partial^k t} [e^{tQ} f] \Big|_{t=0} = Q^k f$, it can be proved that

$$\text{if } Q^k f < Q'^k f \text{ and } Q^{k'} f = Q'^{k'} f \text{ for all } k' \in \{1, \ldots, k-1\}, \text{ then } (\exists \delta > 0)(\forall t \in (0, \delta))\ e^{tQ} f < e^{tQ'} f \tag{7}$$

Therefore, if $\mathcal{Q}_{\tau_0}$ is not a singleton, then Q_{τ_0} is a single matrix Q of $\mathcal{Q}_{\tau_0}$, for which (7) holds.

Having found Q_{τ_0}, then $\underline{f}_{t_1} = e^{t_1 Q_{\tau_0}} f$ and $\tau_0 := [t_1, 0]$ due to (5). In order to find the corresponding, if any, flipping time t_1, we take the derivative of $e^{tQ} \underline{f}_{t_1}$ evaluated at $t = 0$.

$$\frac{\partial}{\partial t} [e^{tQ} \underline{f}_{t_1}] \Big|_{t=0} = Q \underline{f}_{t_1} = Q e^{t_1 Q_{\tau_0}} f$$

and due to continuity, it holds that

$$Q_{\tau_0} e^{t_1 Q_{\tau_0}} f = Q e^{t_1 Q_{\tau_0}} f. \tag{8}$$

We solve (8) for each $i \in \mathcal{X}$ separately, since $\mathcal{Q}$ has separately specified rows and the smallest positive real solution of t_1 is the first flipping time and the corresponding matrix Q is the matrix Q_{τ_1}. We continue the same procedure till we find no more flipping times.

Numerical Results

We calculate the lower expected probability of state 1, $\underline{E}(X_t = 1)$, of an imprecise birth-death chain with state space $\mathcal{X} := \{0, 1, 2, 3\}$ for t approaching infinity. The set of transition rate matrices $\mathcal{Q}$ is derived from the intervals $\lambda_i \in [1, 3]$ and $\mu_j \in [2, 5]$, for all $i \in \{0, \ldots, L-1\}$ and $j \in \{1, \ldots, L\}$ and the input function is $f = [0, 1, 0, 0]^T$.

Following the procedure described before, we start by finding a matrix Q, such that $Qf < Q'f$ for all $Q' \in \mathcal{X} \setminus Q$. Due to the values of f, there are multiple Q, such that Qf is pointwise minimum. These matrices have the following form

$$Q^* = \begin{pmatrix} -1 & 1 & 0 & 0 \\ 5 & -8 & 3 & 0 \\ 0 & 2 & -(2+\lambda_2) & \lambda_2 \\ 0 & 0 & \mu_3 & -\mu_3 \end{pmatrix}$$

where, $\lambda_2 \in \{1, 3\}$ and $\mu_3 \in \{2, 5\}$.

Continuing with the procedure, we check whether there is a matrix Q, such that $Q^2 f < Q'^2 f$ for all $Q' \in \mathcal{X} \setminus Q$. Indeed, there is such a matrix and therefore we have that

$$Q_{\tau_0} = \begin{pmatrix} -1 & 1 & 0 & 0 \\ 5 & -8 & 3 & 0 \\ 0 & 2 & -5 & 3 \\ 0 & 0 & 2 & -2 \end{pmatrix}$$

for which the flipping time is $t_1 = 0.6403991$ and Q_{τ_1} is

$$Q_{\tau_1} = \begin{pmatrix} -3 & 3 & 0 & 0 \\ 2 & -5 & 3 & 0 \\ 0 & 2 & -5 & 3 \\ 0 & 0 & 2 & -2 \end{pmatrix}$$

For the matrix Q_{τ_1} there is no flipping time and by taking $t \to \infty$, we have that $\underline{E}(X = 1) = 0.0937540788$.