

Imprecise continuous-time Markov chains

Efficient computational methods with guaranteed error bounds

Alexander Erreygers Jasper De Bock

Ghent University

ISIPTA'17





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Precise continuous-time Markov chains

Consider a family of random variables $(X_t)_{t \in \mathbb{R}_{\geq 0}}$ where, for all $t \in \mathbb{R}_{\geq 0}$, X_t takes values in a finite and ordered state space \mathcal{X} .

Let $\mathcal{L}(\mathcal{X})$ denote the set of all real-valued functions (vectors) on \mathcal{X} .

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A stochastic process P is a *precise (continuous-time) Markov chain* (pMC) if

$$\begin{aligned} P(X_{t+\Delta} = y | X_{t_1} = x_1, \dots, X_{t_n} = x_n, X_t = x) \\ = P(X_{t+\Delta} = y | X_t = x) =: T_t^{t+\Delta}(x, y). \end{aligned}$$

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The *transition matrix* $T_t^{t+\Delta}$ thus defined determines conditional expectations:

$$\begin{aligned} [T_t^{t+\Delta} f](x) &= E(f(X_{t+\Delta}) | X_t = x) \\ &= E(f(X_{t+\Delta}) | X_{t_1} = x_1, \dots, X_{t_n} = x_n, X_t = x). \end{aligned}$$

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Transition rate matrix

A pMC is called *stationary* if

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In this case, there is a unique *transition rate matrix* Q —a matrix with non-negative off-diagonal elements and rows that sum up to zero—such that,

$$(\forall t \in \mathbb{R}_{\geq 0}) T_t^{t+\delta} = T_\delta \approx (I + \delta Q) \quad \text{for } \delta \text{ suff. small.}$$

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Similarly, for any non-stationary pMC there is a *time-dependent* transition rate matrix Q_t such that

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In practice, a (non-)stationary pMC is characterised by specifying

- (i) a state space \mathcal{X} ,
- (ii) an initial distribution $P(X_0 = x)$, and
- (iii) a (time-dependent) transition rate matrix Q (Q_t).

Precise continuous-time Markov chains

Approximation conditional expectations

Combining some properties of stationary pMCs, we find that

$$\begin{aligned} \mathbb{E}(f(X_t)|X_0 = x) &= [T_t f](x) = [T_{\delta_1} \cdots T_{\delta_n} f](x) \\ &\approx [(I + \delta_1 Q) \cdots (I + \delta_n Q) f](x), \end{aligned}$$

where $\delta_{1:n} := \{\delta_1, \dots, \delta_n\}$ is a sequence of sufficiently small strictly positive time steps such that $\sum_{i=1}^n \delta_i = t$.

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In fact, it is well-known that

$$T_t = e^{tQ} = \lim_{n \rightarrow +\infty} \left(I + \frac{t}{n} Q \right)^n,$$

which is the unique time-dependent matrix that satisfies

$$\frac{d}{dt} T_t = Q T_t \quad \text{with initial condition } T_0 = I.$$

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In general, obtaining an analytical expression for T_t is infeasible!

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In practice, using a stationary pMC is often not warranted, as

- exactly specifying the transition rate matrix Q is often infeasible, and
- assuming stationarity is not always justified.

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Let $\mathbb{P}_{\mathcal{Q}}$ be the set of all Markov chains P consistent with \mathcal{Q} , in the sense that

$$(\forall t \in \mathbb{R}_{\geq 0})(\exists Q_t \in \mathcal{Q}) T_t^{t+\delta} \approx I + \delta Q_t \quad \text{for } \delta \text{ suff. small.}$$

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Krak et al. (2017) use this set $\mathbb{P}_{\mathcal{Q}}$ to characterise an *imprecise (continuous-time) Markov chain*. They define the *lower transition operator* $\underline{T}_t^{t+\Delta}$ as

$$\begin{aligned} [\underline{T}_t^{t+\Delta} f](x) &:= \underline{\mathbb{E}}(f(X_{t+\Delta}) | X_t = x) \\ &= \underline{\mathbb{E}}(f(X_{t+\Delta}) | X_{t_1} = x_1, \dots, X_{t_n} = x_n, X_t = x), \end{aligned}$$

where $\underline{\mathbb{E}}(\cdot)$ is the minimum of the conditional expectations induced by $\mathbb{P}_{\mathcal{Q}}$.

Imprecise continuous-time Markov chains

Krak et al. (2017) prove that, under certain conditions on \mathcal{Q} ,

$$(\forall t, \Delta \in \mathbb{R}_{\geq 0}) \underline{T}_t^{t+\Delta} = \underline{T}_0^\Delta =: \underline{T}_\Delta.$$

For any stationary precise continuous-time Markov chain,

$$T_t^{t+\Delta} = T_0^\Delta =: T_\Delta.$$

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$$(\forall t, \Delta \in \mathbb{R}_{\geq 0}) \underline{T}_t^{t+\Delta} = \underline{T}_0^\Delta =: \underline{T}_\Delta.$$

Moreover, they show that \underline{T}_t is the unique operator that satisfies

$$\frac{d}{dt} \underline{T}_t = \underline{Q} \underline{T}_t \text{ with } \underline{T}_0 = I,$$

where \underline{Q} is the *lower transition rate operator* associated with \mathcal{Q} , defined as

$$[\underline{Q}f](x) := \min \{[Qf](x) : Q \in \mathcal{Q}\}.$$

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$$\underline{T}_t = \lim_{n \rightarrow +\infty} \left(I + \frac{t}{n} \underline{Q} \right)^n.$$

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For any sequence $\delta_{1:n}$ of *sufficiently small* steps that sum up to t ,

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A convenient framework to compute an approximation g_n of $\underline{T}_t f$ is

$g_0 \leftarrow f, \Delta_r \leftarrow \Delta, i \leftarrow 0$

while $\Delta_r > 0$ **do**

$i \leftarrow i + 1$

select some sufficiently small $0 < \delta_i \leq \Delta_r$

$g_i \leftarrow g_{i-1} + \delta_i \underline{Q} g_{i-1}$

$\Delta_r \leftarrow \Delta_r - \delta_i$

return g_n

numerical integration
of a non-linear vector
differential equation

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g0 ← f, Δr ← Δ, i ← 0
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  select some sufficiently small 0 < δi ≤ Δr
  gi ← gi-1 + δi Q gi-1
  Δr ← Δr - δi
return gn
```

numerical integration
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We are interested in approximation methods (i.e., methods that **select** $\delta_{1:n}$) that *a priori and theoretically* guarantee that the error

$$\|\underline{T}_t f - g_n\| := \max\{|\underline{T}_t f(x) - g_n(x)| : x \in \mathcal{X}\}$$

is **lower than the desired maximal error** ϵ .

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return $g_n \pm \epsilon$

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Uniform approximation method

Krak et al. (2017) propose to use the *same* step size $\delta := t/n$ for every step.

They show that if n is greater than two lower bounds, one is guaranteed that

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We modify their method slightly on two fronts:

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- we show that one of the two lower bounds can be less conservative, and we provide a method to compute a *posterior error bound* that is lower than—or at worst equal to— ϵ .

In practice, the posterior error bound is often **significantly smaller** than ϵ .

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Adaptive approximation method

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The adaptive method is *more efficient* than the uniform method, in the sense that

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- + it requires (considerably) fewer iteration steps than the uniform approximation method.

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However,

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Want to know how this method actually works?

Come see our poster on friday!

Numerical comparison

We consider the Healthy-Sick imprecise Markov chain introduced in (Kraak et al., 2017), and determine $\underline{T}_t f$ up to the desired maximal error $\epsilon = 10^{-4}$ for some t and some f .

method	# iter.	duration of comp.		p. e. b.
		no p.e.b.	with p.e.b.	
uniform	80 000	0.414	1.19	4.29×10^{-5}
adaptive ($m = 1$)	34 360	0.593	0.856	1.00×10^{-4}
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- takes **less** computational time than, and

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The adaptive method indeed

- needs fewer iterations than,
- takes less computational time than, and
- results in a posterior error bound that is closer to ϵ compared to

the uniform method.

Ergodicity

Definition (De Bock, 2017)

An imprecise Markov chain is **ergodic** if

$$\lim_{t \rightarrow +\infty} [T_t f](x) = \underline{E}_\infty(f) \quad \text{for all } x \in \mathcal{X} \text{ and all } f \in \mathcal{L}(\mathcal{X}).$$

If this is the case, then \underline{E}_∞ is called the *limit lower expectation*.

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Stationary precise Markov chains are a degenerate case of this definition. Indeed, a stationary precise Markov chain is ergodic if

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How do we approximate $\underline{E}_\infty(f)$?

Precise & stationary

ergodic CTMC with
TRM Q



$$\forall \delta > 0, \\ \delta \|Q\| < 2$$

ergodic DTMC with
TM $(I + \delta Q)$

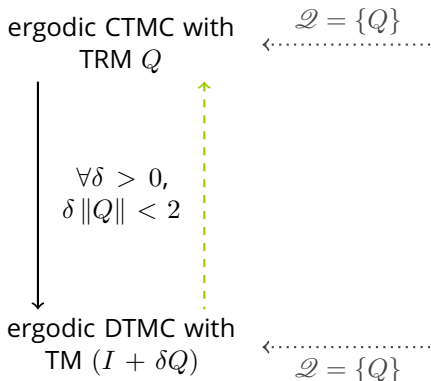


Imprecise

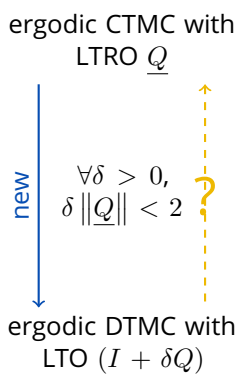
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The limit lower expectation \underline{E}_∞

Precise & stationary



Imprecise

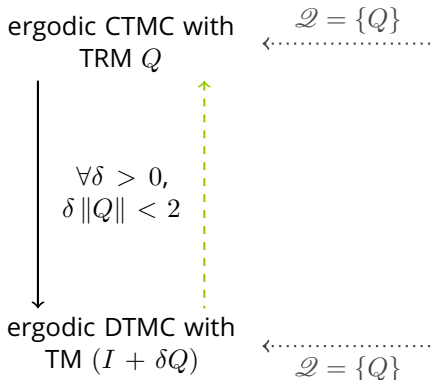


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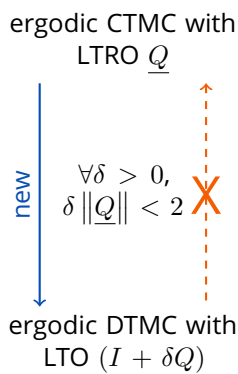
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Imprecise



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~~$$\underline{E}_\infty(f) = \lim_{n \rightarrow +\infty} [(I + \delta \underline{Q})^n f](x)$$~~

at least not for all δ such that $\delta \|\underline{Q}\| < 2!$

Interested in a more detailed explanation?

Did not understand a word of what I was saying?

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Alexander Erreygers
MSc Research Student, University of Bath

Jasper De Boek
MSc Student, University of Bath

Guaranteed approximation methods

From an approximation point of view, an **imprecise continuous-time Markov chain (ICTMC)** is introduced as a Markov chain with **Markovian (CTMC)** transitions but with an **imprecise generator**. An **approximation** is an explicit CTMC for which $\mathbb{E}[X(t)] = \mathbb{E}[Y(t)]$ and $\text{Var}[X(t)] \leq \text{Var}[Y(t)]$. We are interested in the error $\mathbb{E}[|X(t) - Y(t)|]$ between an approximation $Y(t)$ and the ICTMC $X(t)$. We obtain some closed-form error bounds for the expected value and also extend to approximate $\text{Var}[X(t)]$ via the **Lyapunov operator**.

Some theoretical results

Throughout this section, we let \mathbb{P} be a finite and ordered state space and $\mathbb{Q} = (\mathbb{Q}(i, j))_{i, j \in \mathbb{P}}$ a generator matrix. **Transition rate operators** for \mathbb{P} are $(\mathbb{Q}(i, j))_{i, j \in \mathbb{P}}$ and $(\mathbb{Q}(i, j))_{i, j \in \mathbb{P}}$.

A **CTMC** with generator matrix \mathbb{Q} is said to be **positive** if $\mathbb{Q}(i, j) \geq 0$ for all $i, j \in \mathbb{P}$. The **non-negativity** of the transition rates is essential for the CTMC to be a Markov chain. The **non-negativity** of the transition rates is essential for the CTMC to be a Markov chain. The **non-negativity** of the transition rates is essential for the CTMC to be a Markov chain.

Computational comparison

We compare the various approximation methods using the **relative error** introduced in [10]. The **relative error** is defined as the ratio of the absolute error and the expected value of the approximation. The **relative error** is defined as the ratio of the absolute error and the expected value of the approximation.

Uniform approximation method






The uniform approximation method was introduced by [10] and [11]. It is based on the **Lyapunov operator** and the **Lyapunov operator**. The **Lyapunov operator** is defined as $\mathbb{L}f = \mathbb{Q}f - \lambda f$ for some $\lambda > 0$. The **Lyapunov operator** is defined as $\mathbb{L}f = \mathbb{Q}f - \lambda f$ for some $\lambda > 0$.

Adaptive approximation method

An adaptive approximation method is a procedure that adapts the approximation to the problem at hand. The **adaptive approximation method** is a procedure that adapts the approximation to the problem at hand.

See you at the poster session on Friday!

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