# Markov chains

# An introduction

Consider a generic continuous-time stochastic process  $(X_t)_{t \in \mathbb{R}_{>0}}$ , where for all  $t \in \mathbb{R}_{\geq 0}$  the state  $X_t$  is a random variable that takes values x in the finite state space  $\mathscr{X}$ . We provide  $\mathscr{X}$  with some ordering, such that any real-valued function f on  $\mathscr{X}$  can be identified with a row vector. We furthermore let  $\mathscr{L}(\mathscr{X})$  denote the set of all real-valued functions on  $\mathscr{X}$ . Then any linear operator  $T: \mathscr{L}(\mathscr{X}) \to \mathscr{X}$  $\mathscr{L}(\mathscr{X})$  can be identified with a matrix.

#### **Precise Markov chains**

The stochastic process  $(X_t)_{t \in \mathbb{R}_{>0}}$  is a precise (continuous*time) Markov chain* (pMC) if it satisfies the *Markov property*: where  $n \ge 0$  is an integer and  $\{t_1, \ldots, t_n, s, t\}$  is a strictly increasing sequence of non-negative time points. The *transition matrix*  $T_s^t$  thus defined satisfies

 $[T_s^t f](x_s) = \mathbf{E}(f(X_t)|X_s = x_s)$ 

#### (P1)

# Imprecise continuous-time Markov chains

# **Efficient computational methods with guaranteed error bounds**

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#### **Guaranteed approximation methods**

From an application point of view on imprecise (continuoustime) Markov chains (or iMCs, as introduced in Markov chains: **An introduction**), it is essential to have an efficient computational method to numerically approximate  $\underline{T}_t f$  for some  $f \in \mathscr{L}(\mathscr{X})$  and some  $t \in \mathbb{R}_{>0}$ . We are specifically interested in methods that yield an approximation  $\Phi_t f$  of  $\underline{T}_t f$  such that the error  $\|\underline{T}_t f - \Phi_t f\|$  is lower than some desired maximal error  $\varepsilon$ . For ergodic iMCs, it is often also essential to approximate  $\underline{E}_{\infty}(f)$ , see for instance Modelling spectrum assignment in a two-service flexi-grid optical link.

### Adaptive approximation method

We observe that in practice, the a posteriori determined error bound  $\varepsilon'$ is often much smaller than the desired maximal error  $\varepsilon$ . By combining Theorems 1 and 2, we find that one way to get the posterior error bound closer to  $\varepsilon$  is to increase the step size  $\delta$  over time.

In the adaptive approximation method we propose, we achieve this by re-evaluating the step size after every *m* iterations.

**Algorithm 2:** Adaptive approximation  $g_0 \leftarrow f$ ,  $\Delta \leftarrow t$ ,  $i \leftarrow 0$ ,  $\mathcal{E}' \leftarrow 0$ 

#### $= E(f(X_t)|X_{t_1} = x_1, \dots, X_{t_n} = x_n, X_s = x_s).$

A pMC is called *stationary* if it satisfies  $T_t^{t+\Delta} = T_0^{\Delta} \Rightarrow T_{\Delta}$ for all  $t, \Delta \in \mathbb{R}_{>0}$ . 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

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

Furthermore,  $T_t$  then satisfies the differential equation

 $\frac{\mathrm{d}}{\mathrm{d}t}T_t = QT_t, \quad \text{with } T_0 = I.$ (P2)

Similarly, for any non-stationary pMC there is a timedependent transition rate matrix  $Q_t$  such that

 $(\forall t \in \mathbb{R}_{>0}) T_t^{t+\Delta} \approx I + \Delta Q_t$  for  $\Delta$  suff. small.

## **Imprecise Markov chains**

It is often infeasible to precisely specify the transition rate matrix Q of a stationary pMC. Furthermore, assuming stationarity is not always justified. Therefore, we here consider the case where the (time-dependent) transition rate matrix  $Q_t$  of a (non-stationary) pMC is only known to be contained in some (non-empty and bounded) set  $\mathcal{Q}$ . In other words, we consider the set  $\mathbb{P}_{\mathscr{Q}}$  of all pMCs that are consistent with  $\mathcal{Q}$ , in the sense that

#### **Some theoretical results**

Throughout this poster, we let  $\mathscr{X}$  be a finite and ordered state space, and  $Q: \mathscr{L}(\mathscr{X}) \to \mathscr{L}(\mathscr{X})$  a generic lower transition rate operator. For any  $f \in \mathscr{L}(\mathscr{X})$ , we define

 $||f|| \coloneqq \max\{|f(x)| : x \in \mathscr{X}\}$  and  $||f||_c \coloneqq (\max f - \min f)/2.$ 

A first—although minor—result we prove is that

 $||Q|| \coloneqq \sup\{||Qf|| : f \in \mathscr{L}(\mathscr{X}), ||f|| = 1\} = 2\max\{|[Q\mathbb{I}_x](x)| : x \in \mathscr{X}\}.$ 

The two computational methods with guaranteed error bounds we consider are based on the following theorem.

**Theorem 1.** Fix some  $f \in \mathscr{L}(\mathscr{X})$  and  $t \in \mathbb{R}_{>0}$ . Let  $\Phi_t f$  be an approximation of  $\underline{T}_t f$ . Then for any  $\delta \in \mathbb{R}_{>0}$  such that  $\delta \|Q\| \leq 2$  and any  $m \in \mathbb{N}$ ,

 $\left\|\underline{T}_{t+m\delta}f - (I+\delta Q)^m \Phi_t f\right\| \leq \left\|\underline{T}_t f - \Phi_t f\right\| + m\delta^2 \left\|Q\right\|^2 \left\|\Phi_t f\right\|_c.$ 

For any *lower transition operator* <u>T</u> (a super-additive, positively homogeneous operator that dominates the minimum), Skulj and Hable (2013) define the *coefficient of ergodicity* 

> $\rho(\underline{T}) \coloneqq \max\{2 \| \underline{T}f \|_{c} \colon f \in \mathscr{L}(\mathscr{X}), 0 \le f \le 1\}.$ (1)

Obtaining the solution of the optimisation problem in (1) is, in general,

while  $\Delta > 0$  and  $\|g_i\|_c > 0$  do  $i \leftarrow i + 1$  $\delta_i \leftarrow \min\{\Delta, 2/\|\underline{Q}\|, \varepsilon/(t\|\underline{Q}\|^2 \|g_{i-1}\|_c)\}$ if  $m\delta_i > \Delta$  then  $m_i \leftarrow \left\lceil \Delta / \delta_i \right\rceil$  $\delta_i \leftarrow \Delta/m_i$ else  $m_i \leftarrow m$  $g_i \leftarrow g_{i-1}$ repeat  $m_i$  times  $\boldsymbol{\varepsilon}' \leftarrow \boldsymbol{\varepsilon}' + \delta_i^2 \left\| Q \right\|^2 \left\| g_i \right\|_c$ ▷ If interested in a tighter error bound  $g_i \leftarrow g_i + \delta_i Q g_i$  $\Delta \leftarrow \Delta - m_i \delta$ return  $\underline{T}_t f = g_i \pm \varepsilon$  (or  $\underline{T}_t f = g_i \pm \varepsilon'$ )

#### **Computational comparison**

We compare the uniform and adaptive approximation methods using the Healthy-Sick model introduced in (Krak et al., 2017). The obtained results are collected in the table below, where *n* is the number of iterations and D(D') is the duration in seconds of the computations without (with) keeping track of  $\varepsilon'$ . We chose  $\varepsilon = 10^{-4}$ .

	n	D	D'	$\mathcal{E}'$
Uniform	80000	0.414	1.19	$4.29 imes10^{-5}$
Adaptive $(m = 1)$	34360	0.593	0.856	$1.00 imes10^{-4}$

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

This set  $\mathbb{P}_{\mathscr{Q}}$  characterises an *imprecise (continuous-time) Markov chain* (iMC) as follows. Analogous to (P1), we define a lower transition operator  $\underline{T}_{s}^{t}$  as

 $[\underline{T}_{s}^{t}f](x_{s}) := \underline{\mathrm{E}}(f(X_{t})|X_{s} = x_{s})$ (l1)  $= \underline{\mathrm{E}}(f(X_t)|X_{t_1}=x_1,\ldots,X_{t_n}=x_n,X_s=x_s),$ 

where  $\underline{E}(\cdot|\cdot)$  is the minimum of the conditional expectations that are induced by the set of consistent processes.

In case  $\mathscr{Q}$  has separately specified rows, Krak et al. (2017) show that  $\underline{T}_{t}^{t+\Delta} = \underline{T}_{0}^{\Delta} \eqqcolon \underline{T}_{\Lambda}$  for all  $t, \Delta \in \mathbb{R}_{\geq 0}$ . Moreover, they show that  $\underline{T}_{\Lambda}$  is the unique operator that satisfies

> $\frac{\mathrm{d}}{\mathrm{d}t} \underline{T}_t = \underline{Q} \underline{T}_t, \quad \text{with } \underline{T}_0 = I.$ (|2)

In (I2), *Q* is the so-called *lower transition rate operator* of  $\mathscr{Q}$ , which, for any  $f \in \mathscr{L}(\mathscr{X})$  and  $x \in \mathscr{X}$ , is defined as

infeasible. However, we prove that a computable upper bound is

 $\rho(\underline{T}) \leq \overline{\rho}(\underline{T}) \coloneqq \max\left\{\max_{\substack{x, y \in \mathscr{X}}} \left([\overline{T}\mathbb{I}_A](x) - [\underline{T}\mathbb{I}_A](y)\right) : \emptyset \neq A \subset \mathscr{X}\right\}, \quad (2)$ 

where  $\overline{T}\mathbb{I}_A := -\underline{T}(-\mathbb{I}_A)$ . The following novel theorem is useful because, for all  $f \in \mathscr{L}(\mathscr{X})$ ,  $m \in \mathbb{N}$  and  $\delta \in \mathbb{R}_{>0}$  such that  $\delta ||Q|| \leq 2$ ,

> $\left\| (I + \delta \underline{Q})^m f \right\|_c \leq \rho \left( (I + \delta \underline{Q})^m \right) \|f\|_c \leq \overline{\rho} \left( (I + \delta \underline{Q})^m \right) \|f\|_c.$ (3)

**Theorem 2.** If  $\underline{Q}$  is ergodic (De Bock, 2017), then there is some  $n < |\mathcal{X}|$ such that, for any  $m \ge n$  and any  $\delta \in \mathbb{R}_{>0}$  that satisfies  $\delta ||Q|| < 2$ ,

 $\rho((I+\delta Q)^m) \leq \overline{\rho}((I+\delta Q)^m) < 1.$ 

#### **Uniform approximation method**

The uniform approximation method was introduced by (Krak et al., 2017). They suggest to approximate  $\underline{T}_t f$  with  $\Psi(\delta, n) f$ , where

 $\Psi(\delta,n) \coloneqq \left(I + \delta Q\right)^n$ 

and  $t = n\delta$ . Given some desired maximal error  $\varepsilon \in \mathbb{R}_{>0}$ , they propose a way to select the required number of grid steps n—or equivalently, the step size  $\delta = t/n$ —which a priori guarantees that  $\|\underline{T}_t f - \Psi(\delta, n) f\| \leq \varepsilon$ . We modify their method in two ways:

(i) we use a less conservative lower bound for *n*; and

Adaptive (m = 10) 34369 0.224 0.529  $1.00 \times 10^{-4}$ 

## Approximating $\underline{E}_{\infty}(f)$

Let Q be the transition rate matrix of a stationary and ergodic precise Markov chain. Then

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

It is well known that  $E_{\infty}$  is the unique expectation operator that satisfies

 $\mathrm{E}_{\infty}(Qf) = 0$  for all  $f \in \mathscr{L}(\mathscr{X})$ .

Consequently, it is also the unique expectation operator that, for all  $\delta \in \mathbb{R}_{>0}$  such that  $\delta \|Q\| < 2$ , satisfies

 $\mathrm{E}_{\infty}((I+\delta Q)f) = \mathrm{E}_{\infty}(f)$  for all  $f \in \mathscr{L}(\mathscr{X})$ .

By the theory of discrete-time Markov chains, the above equality actually implies that, for **all**  $\delta \in \mathbb{R}_{>0}$  such that  $\delta ||Q|| < 2$ ,

 $\mathrm{E}_{\infty}(f) = \lim_{n \to +\infty} (I + \delta Q)^n f \quad \text{for all } f \in \mathscr{L}(\mathscr{X}).$ 

In the imprecise case, all these nice connections do not necessarily hold. Let Q be the lower transition rate operator of an ergodic iMC.

 $[Qf](x) \coloneqq \min\{[Qf](x) \colon Q \in \mathcal{Q}\}.$ (I3)

### Ergodicity

We are often interested in the long-term limit behaviour of stationary pMCs and iMCs. For iMCs, a special case is when

 $\lim_{t \to +\infty} [\underline{T}_t f](x) = \underline{E}_{\infty}(f) \quad \text{for all } f \in \mathscr{L}(\mathscr{X}) \text{ and } x \in \mathscr{X}.$ 

If this is the case, then the iMC is said to be *ergodic* and  $\underline{E}_{\infty}(f)$  is called the *limit lower expectation*. Similarly, a stationary pMC is ergodic if

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

where  $E_{\infty}$  is now called the limit expectation.

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(ii) we a posteriori compute a tighter guaranteed error bound \varepsilon'.
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Algorithm 1: Uniform approximation	on
$\overline{g_0 \leftarrow f}$ , $oldsymbol{arepsilon'} \leftarrow 0$	
$n \leftarrow \left[ \max\{ t \ \underline{Q}\ /2, t^2 \ \underline{Q}\ ^2 \ f\ _c / \varepsilon \right]$	}]
$\delta \leftarrow t/n$	
for $i = 0,, n - 1$ do	
$\varepsilon' \leftarrow \varepsilon' + \delta^2 \left\  \underline{Q} \right\ ^2 \left\  g_i \right\ _c$ $\triangleright$	If interested in a tighter error bound
$g_{i+1} \leftarrow g_i + \delta \underline{Q} g_i$	
return $\underline{T}_t f = g_n \pm \varepsilon$ (or $\underline{T}_t f = g_n \pm \varepsilon$ )	<b>'</b> )

As a consequence of Theorems 1 and 2 and Eqn. (3), in case Q is ergodic, an alternative a priori guaranteed upper bound for the error is

$$\left\|\underline{T}_{t}f - \Psi(\delta, n)f\right\| \leq \delta^{2} \left\|\underline{Q}\right\|^{2} \left\|f\right\|_{c} \frac{1 - \alpha^{k}}{1 - \alpha} \leq \delta^{2} \left\|\underline{Q}\right\|^{2} \left\|f\right\|_{c} \frac{1 - \beta^{k}}{1 - \beta}, \quad (4)$$

where  $k := \lceil n/m \rceil$ ,  $\alpha := \rho((I + \delta Q)^m)$  and  $\beta := \overline{\rho}((I + \delta Q)^m)$ .

Then

 $\lim_{t \to +\infty} [\underline{T}_t f](x) = \underline{E}_{\infty}(f) \quad \text{for all } f \in \mathscr{L}(\mathscr{X}) \text{ and all } x \in \mathscr{X},$ 

where  $\underline{E}_{\infty}$  is a lower expectation operator. Unfortunately, it does not hold in general that

 $\underline{\mathbf{E}}_{\infty}(Qf) = 0$  for all  $f \in \mathscr{L}(\mathscr{X})$ , or that, for all  $\delta \in \mathbb{R}_{>0}$  such that  $\delta \|Q\| < 2$ ,  $\underline{\mathbf{E}}_{\infty}((I+\delta Q)f) = \underline{\mathbf{E}}_{\infty}(f) \text{ for all } f \in \mathscr{L}(\mathscr{X}).$ 

Therefore, to the best of our knowledge, the only way to approximate  $\underline{\mathbf{E}}_{\infty}(f) = \lim_{t \to +\infty} [\underline{T}_t f](x)$  is to use an approximation  $\Phi_t f$  of  $\underline{T}_t f$ . If  $\|\underline{T}_t f - \Phi_t f\| \leq \varepsilon/2$  and  $\|\Phi_t f\|_c \leq \varepsilon/2$ , then

