Lecture 4: Continuous-time Markov Chains

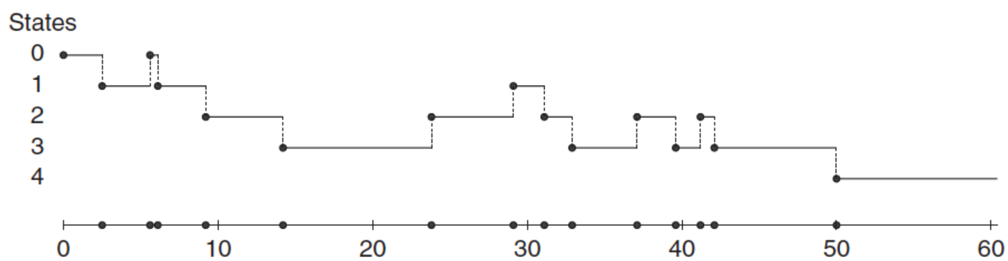
Readings

- Grimmett and Stirzaker (2001) 6.8, 6.9.

Options:

- Grimmett and Stirzaker (2001) 6.10 (a survey of the issues one needs to address to make the discussion below rigorous)
- Norris (1997) Chapter 2,3 (rigorous, though readable; this is the classic text on Markov chains, both discrete and continuous)
- Durrett (2012) Chapter 4 (straightforward introduction with lots of examples)

Many random processes have a discrete state space, but can change their values at any instant of time rather than at fixed time points. Examples of such processes include radioactive atoms decaying, the number of molecules in a chemical reaction, populations with birth/death/immigration/emigration, the number of emails in an inbox, the number of people in the checkout counter at Trader Joe's, etc. Such processes are piecewise constant, with jumps that occur at continuous times, as in this example showing the number of people in a lineup as a function of time (Dobrow (2016)):



We'll look at processes which satisfy a continuous version of the Markov property, and hence are called continuous-time Markov chains (ctMC). This class will introduce tools to describe continuous-time Markov chains, which are variants of the tools we learned in the previous two classes. We'll also point out several links with discrete-time Markov chains.

4.1 Definition and Transition probabilities

Definition. Let $X = (X_t)_{t\geq 0}$ be a stochastic process taking values in a finite or countable state space S, which we can take to be a subset of the integers. X is a *continuous-time Markov chain* (ctMC) if it satisfies the

Markov property:[1]

$$P(X_{t_n} = i_n | X_{t_1} = i_1, \ldots, X_{t_{n-1}} = i_{n-1}) = P(X_{t_n} = i_n | X_{t_{n-1}} = i_{n-1}) \tag{1}$$

for all $i_1, \ldots, i_n \in S$ and any sequence $0 \le t_1 < t_2 < \cdots < t_n$ of times. We assume the process is right-continuous. The process is *time-homogeneous* if the conditional probability does not depend on the current time, so that:

$$P(X_{s+t} = j | X_s = i) = P(X_t = j | X_0 = i), \qquad s \ge 0. \tag{2}$$

We will consider only time-homogeneous processes in this lecture.

The Markov property (1) says that the distribution of the chain at some time in the future, only depends on the current state of the chain, and not its history. The difference from the Markov property that we learned for discrete processes, is that now the set of times t is continuous – the chain can jump between states at any time, not just at integer times.

There is no exact analogue of the transition matrix P, since there is no natural unit of time. Therefore we consider the transition probabilities as a function of time.

Definition. The *transition probability* for a time-homogeneous chain is

$$P_{ij}(t) = P(X_{s+t} = j | X_s = i), \qquad s, t \ge 0. \tag{3}$$

Write $P(t) = (P_{ij}(t))_{i,j \in S}$ for the matrix of transition probabilities at time t. Clearly, $P(t)$ is a stochastic matrix.

Remark. For a time-inhomogeneous chain, the transition probability would be a function of two times, as $P_{ij}(s,t) = P(X_{s+t}) = j | X_s = i)$.

A fundamental relationship from which most other relationships can be derived, is the Chapman-Kolmogorov equation.

Chapman-Kolmogorov Equation. *(time-homogeneous)*

$$P(t+s) = P(t)P(s) \quad \Longleftrightarrow \quad P_{ij}(t+s) = \sum_{k \in S} P_{ik}(t) P_{kj}(s)\ . \tag{4}$$

[1] The Markov property in continuous time can be formulated more rigorously in terms of σ-algebras. Let $(\Omega, \mathscr{F}, P)$ be a probability space and let $\{\mathscr{F}_t\}_{t \ge 0}$ be a filtration: an increasing sequence of σ-algebras such that $\mathscr{F}_t \subseteq \mathscr{F}$ for each t, and $t_1 \le t_2 \Rightarrow \mathscr{F}_{t_1} \subseteq \mathscr{F}_{t_2}$. We suppose the process X_t is *adapted* to the filtration $\{\mathscr{F}_t\}_{t \ge 0}$: each X_t is measurable with respect to $\mathscr{F}_t$. For example, this will be true automatically if we let $\mathscr{F}_t = \sigma(X_t)$, the σ-algebra generated by $(X_s)_{0 \le s \le t}$, i.e. generated by the pre-images $X_s^{-1}(B)$ for Borel sets $B \subset \mathbb{R}$. Then X_t has the Markov property if

$$\mathbb{E}(f(X_t) | \mathscr{F}_s) = \mathbb{E}(f(X_t) | \sigma(X_s))$$

for all $0 \le s \le t$ and bounded, measurable functions f. Another way to say this is $P(X_t \in A | \mathscr{F}_s) = P(X_t \in A | \sigma(X_s))$, where $P(\cdot|\cdot)$ is a *regular conditional probability* (see Koralov and Sinai (2010), p.184).

Proof.

$$
\begin{aligned}
P_{ij}(s+t) &= P(X_{s+t}=j|X_0=i) \\
&= \sum_k P(X_{s+t}=j|X_t=k,X_0=i)P(X_t=k|X_0=i) && \text{(LoTP)} \\
&= \sum_k P(X_{s+t}=j|X_t=k)P(X_t=k|X_0=i) && \text{(Markov property)} \\
&= \sum_k P_{ik}(t)P_{kj}(s) && \text{(time-homogeneity.)}
\end{aligned}
$$

□

Remark. A set of operators $(T(t))_{t\geq 0}$ such that $T(t+s)=T(s)T(t)$ and $T(0)=I$ (the identity operator) is a *semigroup*. The transition probabilities $P(t)$ form a semigroup, where $P(t)$ is an operator mapping vectors to vectors. Studying abstract semigroups of operators, sometimes with additional properties like continuity or uniform continuity at $t=0$, is another approach to studying Markov processes. See e.g. Grimmett and Stirzaker (2001), p.256, for more details related to continuous-time MCs, and see Koralov and Sinai (2010); Pavliotis (2014) for a discussion of general Markov processes.

The transition probability characterizes the evolution of probability for a continuous-time Markov chain, but it gives too much information. We don't need to know $P(t)$ for all times t to understand the dynamics of the chain. Rather, we will consider two equivalent ways of characterizing the dynamics of a ctMC:

(i) Through the *generator* Q, which is an infinitesimal version of P.

(ii) By the times at which the chain jumps, and the states that it jumps to.

For the rest of the lecture, we will assume that $|S|=N<\infty$. Most of the results we derive will also be true when $|S|=\infty$, under certain additional, not-very-restrictive assumptions, but they are much harder to prove; see Norris (1997) for a rigorous discussion that includes the case $|S|=\infty$.

4.2 Infinitesimal generator

A fundamental characterization of a ctMC is by its generator, which gives its infinitesimal transition rates. To define the generator, consider the transition probability $P(t)$, and let's make the following assumption:

$$P(t) \textit{ is right-differentiable at } t=0.$$

This assumption will be true in applications and it makes the subsequent theory much easier to derive.[2]

This assumption implies that $P(t)$ is differentiable for all $t>0$, which you can show (as an exercise) from the Chapman-Kolmogorov equations.

[2] The weaker assumption $P(t)\to I$ uniformly as $t\searrow 0$ is sufficient to derive the results in this section; see Grimmett and Stirzaker (2001), Section 6.10 or Norris (1997), Chapter 2. If $P(t)$ is merely continuous at 0, then it is possible that some diagonal elements of the generator, defined via the limit in (5), are $q_{ii}=-\infty$, meaning the process is immediately killed and removed from the system when it hits state i. See Grimmett and Stirzaker (2001), Section 6.10.

Definition. Let $X = (X_t)_{t\geq 0}$ be a ctMC with transition probabilities $P(t)$. The *generator* or *infinitesimal generator* of the Markov Chain is the matrix

$$Q = \lim_{h\to 0^+} \frac{P(h) - I}{h}. \tag{5}$$

Write its entries as $q_{ij} = Q_{ij}$.

In virtually all applications, you are given the *generator* (or you construct it as a model), and not the set of transition probabilities. The generator therefore is the fundamental object of interest; (5) is only used to compute the transition probabilities from the generator, as we will see in Section 4.4.

Some properties of the generator that follow immediately from its definition are:

(i) Its rows sum to 0: $\sum_j q_{ij} = 0$.
(ii) $q_{ij} \geq 0$ for $i \neq j$.
(iii) $q_{ii} \leq 0$.

Proof.

(i) $\sum_j P_{ij}(h) = 1$, since $P(h)$ is a transition matrix, and $\sum_j I_{ij} = 1$. Pass to the limit, using the finiteness of S to interchange limit and sum.
(ii) For $i \neq j$, $P_{ij}(h) \geq 0$, so this is true in the limit.
(iii) Follows from (i) and (ii), since $q_{ii} = -\sum_j q_{ij}$.

□

Remark. We could also construct a ctMC by taking a matrix Q satisfying properties (i–iii) above, and then making the assumption that the transition probabilities satisfy, for all $i, j \in S$,

$$P(X_{t+h} = j | X_t = i) = \delta_{ij} + q_{ij}h + o(h)$$

as $h \downarrow 0$, uniformly in t, together with the Markov property. See Norris (1997), Theorem 2.8.2.

Remark. If $|S| = \infty$, then most of what follows will be true under the assumption that $\sup_i |q_{ii}| < \infty$ (Norris (1997), Chapter 2). This condition ensures the chain cannot blow up to ∞ in finite time. Therefore, we will consider examples with $|S| = \infty$, even though we won't prove here that the theory works in this case.

How should the entries of the generator be interpreted? Each entry q_{ij} with $i \neq j$ is the *rate* of jumping from i to j. The diagonal entries $-q_{ii}$ are the overall rates of leaving each state i. One way to see this is to consider the transition probabilities after a small amount of time h has elapsed:

$$\begin{aligned} P_{ij}(h) &= q_{ij}h + o(h) && (j \neq i) \\ P_{ii}(h) &= 1 + q_{ii}h + o(h) && (j = i) \end{aligned} \tag{6}$$

Then q_{ij} gives the rate at which probability flow from state i to state j, at least over small enough times, and $-q_{ii}$ is the rate at which probability leaves i.

Another interpretation comes from recalling that a rate measures the average number of events (in the colloquial, not probabilistic, sense), per unit time. In our case an event is a transition from i to j. So we could estimate the rate of transitioning from i to j by starting the chain in state i, letting it run for a small time h, checking whether or not the chain is in j, and repeating many times. The rate can be estimated as

$$\text{rate}(i \to j) \approx \frac{\text{\# of times } X_h = j}{(\text{\# of experiments}) \cdot h} \approx \frac{P(X_{t+h}{=}j|X_t{=}i)}{h} = q_{ij}.$$

Similar reasoning shows the overall rate of leaving is $-q_{ii} = -\sum_j q_{ij}$, because the overall rate of leaving is the rate at which *any* transition happens, so it is the sum of the individual rates.

This argument ignores the possibility of transitioning several times to j in the interval $(0,h]$. A useful fact is that the probability of the process jumping more than once in a time interval of length h is $o(h)$. You can show this from (6) and the Chapman-Kolmogorov equations: the probability of jumping from i to j in two steps in an interval $[0,h]$ is

$$\begin{aligned} P(X_h{=}j, \exists\, s \in (0,h),\, k \neq i,j \text{ s.t. } X_s{=}k|X_0{=}i) &= \sup_s P(X_h = j|X_s{=}k, X_0{=}i)P(X_s{=}k|X_0{=}i) \\ &= \sup_s q_{kj}(h-s)q_{ik}(s) + o((h-s)h) + o(hs) \\ &= \sup_s q_{kj}q_{ik}(h-s)s + o(h^2) \quad = o(h). \end{aligned}$$

Here are some examples of ctMCs and their corresponding generators.

Example 4.1 (Two-state chain) A generic two-state ctMC has generator

$$Q = \begin{pmatrix} -\alpha & \alpha \\ \beta & -\beta \end{pmatrix}$$

where $\alpha, \beta \geq 0$ are parameters. For example, suppose you wish to model a ligand that can bind and unbind to a protein. You might be told that the rate of binding is α binding events per second, and the rate of unbinding is β binding events per second. Your model for the ligand is a continuous-time Markov chain X_t (t is measured in seconds) on the state space $S = \{\text{unbound,bound}\}$, with generator given above.

Example 4.2 (Birth-death process) Suppose you are modeling the population of black bears in the Catskills. You assume that bears are born with rate λ bears per year, and they die with rate μ bears per year. (If there are no more bears, you still assume they are "born" with rate λ; for example this could model immigration from another location.) If X_t is the number of bears at time t (where time is measured in units of years), and $X = (X_t)_{t \geq 0}$ is a Markov process, then the generator for this process is

$$Q = \begin{array}{c c} & \begin{array}{ccccc} 0 & 1 & 2 & 3 & \end{array} \\ \begin{array}{c} 0 \\ 1 \\ 2 \\ 3 \\ \vdots \end{array} & \begin{pmatrix} -\lambda & \lambda & 0 & 0 & \cdots \\ \mu & -(\lambda+\mu) & \lambda & 0 & \cdot \\ 0 & \mu & -(\lambda+\mu) & \lambda & \cdots \\ 0 & 0 & \mu & -(\lambda+\mu) & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \end{array}$$

The generator above is an example of a *birth-death process*, a ctMC on the set of non-negative integers where transitions can only occur to neighbouring states. For a general birth-death process, the birth and death rates can be state-dependent, so that transitions from $i \to i+1$ occur with rate λ_i, and transitions from $i \to i-1$ occur with rate μ_i.

Such a process models a wide range of situations, such as people arriving at and leaving from a lineup, search requests arriving at a Google server, emails arriving in and being deleted from an inbox, the number of individuals in a population infected with a given virus, etc.

Example 4.3 (Poisson process) A *Poisson process with rate* λ is a continuous-time Markov chain $N = (N_t)_{t\geq 0}$ on $S = \{0, 1, 2, \ldots\}$ with generator

$$Q = \begin{pmatrix} -\lambda & \lambda & 0 & 0 & \cdots \\ 0 & -\lambda & \lambda & 0 & \cdots \\ 0 & 0 & -\lambda & \lambda & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

and initial condition $N_0 = 0$.

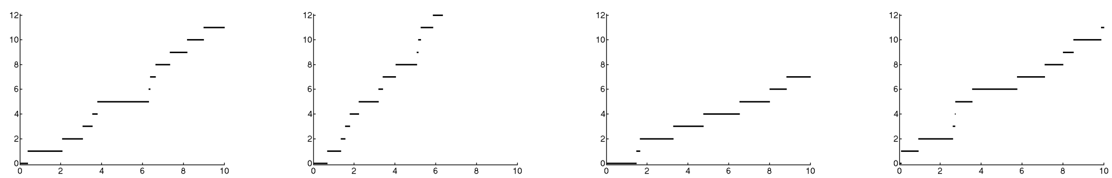


Figure 1: Some realizations of the Poisson process with rate $\lambda = 1$. These were all simulated for 10 time units.

The Poisson process is often used to count the number of events that have happened at time t, if the events occur completely independently of each other with rate λ. For example, it could count the number of busses that pass a bus stop in a certain time t, if the drivers have absolutely no idea where the other drivers are, and are so delayed by bad traffic that their arrival times are completely random. Other examples include the number of radioactive atoms that have decayed, or the number of telephone calls that arrive at a call center, or the number of search requests received by Google's servers, or the number of large waves that arrive at an oil platform.

Remark. Another definition of the Poisson process, which is sometimes more useful in practical calculations and doesn't require the theory of continuous-time Markov chains, is as a process $N = (N_t)_{t\geq 0}$ taking values in $S = \{0, 1, 2, \ldots\}$ such that:

(i) $N_0 = 0$;

(ii) N_t has *stationary and independent increments*: for any $0 \leq t_1 < t_2 < \cdots < t_n$, the random variables

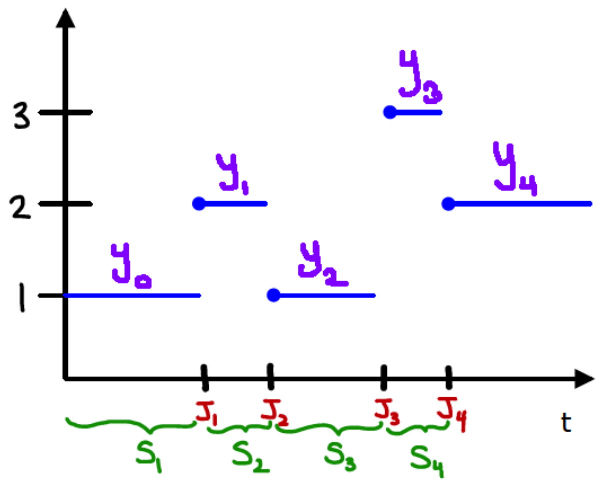
$$N_{t_2} - N_{t_1},\ N_{t_3} - N_{t_2},\ \ldots, N_{t_n} - N_{t_{n-1}}$$

are independent, and for any $t \geq 0$, $s \geq 0$, the distribution of $N_{t+s} - N_t$ is independent of t;

(iii) $N_t \sim \text{Poisson}(\lambda t)$.

4.3 Transition times and jumps

A continuous-time Markov chain stays in one state for a certain amount of time, then jumps immediately to another state where it stays for another amount of time, etc. A natural way to characterize this process by the the times at which it jumps, and the distributions of the states it jumps to. Such a characterization will also lead to a method to simulate exact realizations of the process.



Definition. Let us define the following:

- The *jump time* J_m is the time of mth jump. It is defined recursively by

$$J_{m+1} = \inf\{t > J_m : X_t \neq X_{J_m}\}, \qquad J_0 = 0.$$

- The *holding time* S_m is the length of time a ctMC stays in its state, before jumping for the mth time. It is calculated from the jump times as $S_m = J_m - J_{m-1}$.
- The discrete-time process $(Y_n)_{n=0}^{\infty}$ given by $Y_n = X_{J_n}$ is called the *jump process*, *jump chain*, or *embedded chain*.

We will determine the probability distributions of $(J_m)_{m\geq 0}$ and $(Y_m)_{m\geq 0}$. First, we need a couple of technical results.

Definition. A random variable T with values in $[0,\infty]$ is a *stopping time* for a continuous-time process X, if, for each $t \in [0,\infty)$, the event $\{T \leq t\}$ depends only on $(X_s : s \leq t)$.

Theorem. *The jump time J_m is a stopping time of $(X_t)_{t\geq 0}$ for all m.*

For a proof, see Norris (1997), Lemma 6.5.2 p. 226.

Theorem (Strong Markov property)**.** *Let $X = (X_t)_{t\geq 0}$ be a ctMC with generator Q and let T be a stopping time. Assume that $P(T < \infty) = 1$. Then $(X_{T+t})_{t\geq 0}$ is a continuous-time Markov chain with generator Q, and initial distribution equal to the distribution of X_T.*

Remark. Proving this theorem (and even properly making sense of a stopping time in the continuous-time case) requires measure theory, so we won't do this. See Norris (1997) Section 6.5, Theorem 6.5.4, p.227.

The Strong Markov Property says that if we stop X at a stopping time, and then consider the subsequent process, then it has exactly the same transition probabilities as the original process. In other words,

$$P(X_{T+t} = j | X_T = i, X_s = x_s, 0 \le s \le T) = P(X_t = j | X_0 = i)\,. \tag{7}$$

Now let's use these results to compute the jump times and jump probabilities. We start with the jump times. Suppose we are in state i after the $m-1$th jump, and we wish to know the distribution of S_m, the time we wait until we jump again.

Theorem. *Suppose $X_{J_{m-1}} = i$. The holding time S_m is an exponentially distributed random variable with parameter $-q_{ii}$.*

Remark. Recall that a random variable Y is exponentially distributed with parameter $\lambda > 0$, if it has probability density function $p(y) = \lambda^{-1} e^{-\lambda y}$, or equivalently if (one minus) its cumulative distribution function satisfies $P(Y > y) = e^{-\lambda y}$. Exponential random variables have the "lack-of-memory" property: $P(Y > y + x | Y > y) = P(Y > x)$, and in fact, one can show they are the only continuous random variables with this property (Grimmett and Stirzaker, 2001, p. 259, 140).

Proof. We will show that S_m is memoryless. First, notice that

$$\{S_m > r\} = \{X_{J_{m-1}+u} = i \text{ for all } 0 \le u \le r\}\,.$$

Therefore

$$\begin{aligned}
P(S_m > r+t \,|\, S_m > r, X_{J_{m-1}}{=}i) &= P(S_m > r+t \,|\, X_{J_{m-1}+u}{=}i,\ 0 \le u \le r) && \text{conditioning on same event}\\
&= P(S_m > t+r \,|\, X_{J_{m-1}+r}{=}i) && \text{Strong Markov property}\\
&= P(S_m > t \,|\, X_{J_{m-1}}{=}i) && \text{time-homogeneity}
\end{aligned}$$

We can use the Strong Markov property, since $\{S_m > r\}$ is an event that depends only on the values of X at times J_{m-1} and later, as shown above. Therefore, S_m is memoryless, and since it is continuous it must have an exponential distribution: $P(S_m > t \,|\, X_{J_{m-1}}{=}i) = e^{-\lambda_i t}$ for some parameter λ_i.

What is λ_i? Let's calculate:

$$\begin{aligned}
\lambda_i &= -\frac{d}{dt}\Big|_{t=0} P(S_m > t \,|\, X_{J_{m-1}}{=}i)\\
&= \lim_{h\to 0} \frac{1 - P(S_m > h | X_{J_{m-1}}{=}i)}{h} = \lim_{h\to 0} \frac{1 - P(X_h{=}i | X_0{=}i) + o(h)}{h} = \lim_{h\to 0} \frac{-q_{ii}h + o(h)}{h} = -q_{ii}.
\end{aligned}$$

Therefore $\lambda_i = -q_{ii}$. The $o(h)$ term above represents the possibility that there were two or more jumps in the interval $(0,h]$, that brought the process back to i. □

Remark. The same proof can be straightforwardly adapted to show that, if $X_s = i$ for some *deterministic* time s, then the waiting time until the next jump is Exponential$(-q_{ii})$. Just replace J_{m-1} with s in the proof above, and use the (regular) Markov property. In words, because the exponential distribution is memoryless, the waiting time distribution does not depend on the time at which we start counting.

Now we consider the jump process $Y_0, Y_1, \ldots$. By the Strong Markov property and the fact that J_m is a stopping time, this process is a discrete-time Markov chain. It is time-homogeneous because X is time-homogeneous. Therefore we can characterize the jump chain by its transition matrix, which we will call $\tilde{P}$. It has elements

$$\tilde{P}_{ij} = P(Y_m = j | Y_{m-1} = i) = P(X_{J_m} = j \,|\, X_{J_{m-1}} = i)\,. \tag{8}$$

By definition, the diagonal elements are $\tilde{P}_{ii} = 0$ if $q_{ii} \neq 0$, and $\tilde{P}_{ii} = 1$ if $q_{ii} = 0$.

Proposition. *The transition matrix of the embedded chain has elements $\tilde{P}_{ij} = -q_{ij}/q_{ii}$ for $i \neq j$. Furthermore, Y_m is independent of S_m.*

Here is a rough sketch of the proof below. Suppose that $X_{J_{m-1}} = i$, and that $t < S_m \leq t+h$, and suppose that h is small enough that the chain jumps only once in $(t, t+h]$. Then

$$\begin{aligned} P(\text{it jumps to } j | \text{it first jumps in } (t,t+h], X_{J_{m-1}}{=}i) &= P(\text{it jumps to } j | \text{it first jumps in } (t,t+h], X_t{=}i) \\ &= \frac{P(\text{it jumps to } j \cap \text{it first jumps in } (t,t+h] | X_t{=}i)}{P(\text{it first jumps in } (t,t+h] | X_t{=}i)} \\ &\approx \frac{P(X_{t+h} = j || X_t{=}i)}{1 - p_{ii}(h)} \approx \frac{p_{ij}(h)}{1-p_{ii}(h)} \to -\frac{q_{ij}}{q_{ii}} \quad \text{as} \quad h \searrow 0. \end{aligned}$$

Proof. To show this statement in more detail, we need to condition on each possible value of S_m, and work out the embedded chain's transition probability using known behaviour of $P(t)$. We then additionally want to show this transition probability doesn't depend on the value of S_m. However, a conditional probability such as $P(Y_m = j | Y_{m-1} - i, S_m = t)$ doesn't make sense, since we can't condition on an event of measure zero, so instead we condition on the jump occurring in a small interval $(t, t+h]$, and then let $h \to 0$.

That is, let's define

$$\tilde{P}^t_{ij} = \lim_{h \to 0+} P(X_{J_{m-1}+t+h}{=}j | X_{J_{m-1}}{=}i, t < S_m \leq t+h)$$

to be the probability that the next state is j, given the holding time is $S_m = t$. By the Strong Markov Property and the definition of S_m, we can replace $\{X_{J_{m-1}}{=}i\}$ with $\{X_{J_{m-1}+t}{=}i\}$, to obtain

$$\tilde{P}^t_{ij} = \lim_{h \to 0+} P(X_{J_{m-1}+t+h}{=}j | X_{J_{m-1}+t}{=}i, t < S_m \leq t+h).$$

Now we want to shift time by J_{m-1}. To handle S_m, we define $U = \inf\{s > t : X_s \neq i\}$ to be the first time after time t that the process is not in state i, and calculate, by time-homogeneity, and then by the definition of conditional probability,

$$\tilde{P}^t_{ij} = \lim_{h \to 0+} P(X_{t+h}{=}j | X_t{=}i, t < U \leq t+h) = \lim_{h \to 0+} \frac{P(X_{t+h}{=}j, t < U \leq t+h | X_t{=}i)}{P(t < U \leq t+h | X_t{=}i)}\,.$$

Now we use two facts:

- $P(X_{t+h}{=}j, t < U \leq t+h | X_t{=}i) = P(X_{t+h}{=}j | X_t{=}i) + o(h)$, since the probability of two or more jumps in an interval of length h is $o(h)$,
- $P(t < U \leq t+h | X_t{=}i) = -q_{ii}h + o(h)$, since $U \sim \text{Exp}(-q_{ii})$.

Putting these together with the known expansion of $P(h)$ near zero gives

$$\tilde{P}^t_{ij} = \lim_{h\to 0+} \frac{q_{ij}h + o(h)}{-q_{ii}h + o(h)} = -\frac{q_{ij}}{q_{ii}}\,.$$

Since $\tilde{P}^t_{ij}$ is independent of t, we have that Y_m, S_m are independent, and $\tilde{P}_{ij} = \tilde{P}^t_{ij}$. □

Putting these results together shows that if we are given Q, we can calculate the holding time distributions and $\tilde{P}$, and conversely if we are given the holding time distributions and $\tilde{P}$, we can recover Q.

***Exercise* 4.1.** Work out the transition probabilities for the embedded chains in Examples 4.1, 4.2, 4.3.

From the jump chain and holding times we obtain a method to simulate exact realizations of X.

Gillespie algorithm. Also known as the *stochastic simulation algorithm* (SSA), or the *Kinetic Monte Carlo algorithm (KMC)*. This is an algorithm to simulate exact realizations of X. Suppose $X_t = i$. Update the process as follows.

- Generate a random variable τ from an exponential distribution with parameter $-q_{ii}$;
- Choose a state j to jump to from the probability distribution given by the ith row of $\tilde{P}$;
- Jump to j at time $t+\tau$, i.e. set $X_s = i$ for $t \le s < t+\tau$, and $X_{t+\tau} = j$.
- Repeat, starting at state j at time $t+\tau$.

This algorithm is used to simulate a wide range of problems, such as crystal growth, evolution of genetic mutations, virus spreading in a population, molecular motors moving along a microtubule, RNA folding, chemical reactions with a small number of molecules such an in the interior of a cell, and many more.

4.4 Forward and backward equations

We defined the generator from the full time-dependent transition probabilities. The next question we want to know is: can we recover $P(t)$ from Q? The answer is yes. Let's show this, by deriving an evolution equation for $P(t)$, and then solving it.

We calculate:

$$\begin{aligned} \frac{d}{dt}\Big|_{t=0+} P(t) &= \lim_{h\to 0^+} \frac{P(t+h)-P(t)}{h} = \lim_{h\to 0^+} \frac{P(t)P(h)-P(t)I}{h} = P(t)\left(\lim_{h\to 0^+}\frac{P(h)-I}{h}\right) \\ &= P(t)Q. \end{aligned}$$

We factored $P(t+h) = P(t)P(h)$, using the Chapman-Kolmogorov equations, and interchanged the limit and sum since $|S| < \infty$ (the equation is true for the case $|S| = \infty$ too, but is much harder to prove). The result is an evolution equation for $P(t)$.

We may also consider the evolution of a probability distribution $\mu(t)$, which is a row vector with components

$$\mu_i(t) = P(X_t = i).$$

Since $\mu(t) = \mu(0)P(t)$ and therefore $\mu'(t) = \mu(0)P'(t)$, we can multiply the above equation on the left by $\mu(0)$ to obtain an evolution equation for $\mu(t)$. We obtain two versions of the forward equation:

Forward Kolmogorov Equation. *Given a time-homogeneous ctMC with generator Q, the transition probabilities $P(t)$ evolves as*

$$\frac{dP}{dt} = PQ\,, \qquad P(0) = I\,. \tag{9}$$

Given initial probability distribution $\mu^{(0)}$, the probability distribution $\mu(t)$ evolves as

$$\frac{d\mu}{dt} = \mu Q\,, \qquad \mu(0) = \mu^{(0)}\,. \tag{10}$$

Now we look for the backward equation. Going back to our initial calculation, we can factor out $P(t)$ on the right instead, to get

$$\begin{aligned}\frac{d}{dt}\Big|_{t=0+} P(t) &= \lim_{h\to 0^+} \frac{P(t+h)-P(t)}{h} = \lim_{h\to 0^+} \frac{P(h)P(t)-IP(t)}{h} = \left(\lim_{h\to 0^+} \frac{P(h)-I}{h}\right)P(t)\\ &= QP(t).\end{aligned}$$

From this equation we may consider expectations of functions of the Markov chain. Let $u(t)$ be a column vector with components

$$u_k(t) = \mathbb{E}_k f(X_t) = \mathbb{E}(f(X_t)|X_0 = k).$$

Write $f = (f(1), f(2), \dots, f(N))^T$, so that $u(0) = f$. Then $u(t) = P(t)f$, and $u'(t) = P'(t)f$, so multiplying the equation above by f on the right gives an evolution equation for $u(t)$. We obtain two versions of the backward equation:

Backward Kolmogorov Equation. *Given a time-homogeneous ctMC with generator Q, the transition probabilities $P(t)$ evolve as*

$$\frac{dP}{dt} = QP\,, \qquad P(0) = I\,, \tag{11}$$

and the statistic $u(t)$ evolves as

$$\frac{du}{dt} = Qu\,, \qquad u(0) = f\,. \tag{12}$$

From the forward and backward equations we may make several observations. First, putting (9), (11) together, shows that

$$QP(t) = P(t)Q,$$

i.e. the transition probability matrix commutes with the generator. We can also solve explicitly for $P(t)$, to obtain

$$P(t) = e^{Qt}P(0) = e^{Qt}\,.$$

Recall that $e^{Qt} \equiv \sum_{n=0}^{\infty} \frac{1}{n!} Q^n t^n$ for any square matrix Q.[3] Therefore, if we know the infinitesimal generator Q, then we can determine the transition probabilities $P(t)$ for $t > 0$.

[3] That this power series converges for a finite generator Q is shown in Norris (1997), Section 2.10.

Example 4.4 (Poisson process) Let's calculate the probability distribution of the Poisson process at each point in time. Let $\mu_j(t) = P(N_t = j)$, $j = 0, 1, 2, \ldots$. We solve for $\mu_j(t)$ using the forward Kolmogorov equations (10), recalling that $\mu(0) = (1, 0, \ldots)$. When $j = 0$ we have

$$\frac{d\mu_0}{dt} = -\lambda \mu_0, \qquad \mu_0(0) = 1.$$

The solution is $\mu_0(t) = e^{-\lambda t}$. The next equation is

$$\frac{d\mu_1}{dt} = \lambda \mu_0 - \lambda \mu_1, \qquad \mu_1(0) = 0.$$

Substituting for $\mu_0(t)$ and solving gives $\mu_1(t) = \lambda t e^{-\lambda t}$. In general, we have

$$\frac{d\mu_j}{dt} = -\lambda \mu_j + \lambda \mu_{j-1}, \qquad \mu_j(0) = 0 \quad (j > 0).$$

We can solve these by induction to find that

$$\mu_j(t) = \frac{\lambda^j t^j}{j!} e^{-\lambda t}.$$

This shows that at fixed time t, N_t is a Poisson random variable with parameter λt.

4.5 Long-time behaviour

The long-time behaviour of a continuous-time Markov chain is similar to the discrete case.

Definition. A probability distribution λ is a *limiting distribution* of a continuous-time Markov chain if, for all i, j, $\lim_{t\to\infty} P_{ij}(t) = \lambda_j$.

Definition. A probability distribution π is a *stationary distribution* of a continuous-time Markov chain if

$$\pi = \pi P(t) \qquad \forall\, t \geq 0. \tag{13}$$

A stationary distribution is, as in the discrete-time case, a probability distribution such that if the Markov chain starts with this distribution, then the distribution never changes. As for a discrete-time Markov chain, a limiting distribution is a stationary distribution, but the converse is not true in general.

How do we find the stationary distribution? We can find it directly from the generator.

Theorem. *Let $P(t)$ be the transition function for a ctMC. Then a probability distribution π is a stationary distribution if and only if*

$$\pi Q = 0\,. \tag{14}$$

Proof. Take d/dt of (13) to get $\pi P'(t) = 0$. From the forward equation (9) this implies $\pi P(t) Q = 0$. But $\pi P(t) = \pi$, so the result follows. □

Equation (14) says that π is a left eigenvector of Q corresponding to eigenvalue 0. Therefore, we can find it by linear algebra.

There is a formal link to the formula for a discrete-time Markov chain – recall that if Y_n is a discrete-time Markov chain with transition matrix P, then the stationary distribution solves $(P-I)\pi = 0$. But $(P-I)$ is like a forward-difference approximation to $\frac{dP}{dt}|_t = 0$ using a time step of $\Delta t = 1$.

Detailed balance is also quite similar to the discrete-time case.

Definition. A ctMC with generator Q and stationary distribution π satisfies *detailed balance with respect to* π, or is *reversible with respect to* π, if it satisfies the *detailed balance equations*

$$\pi_i q_{ij} = \pi_j q_{ji} \,. \tag{15}$$

***Exercise* 4.2.** Find the stationary distribution for the birth-death chain, and give the conditions under which it exists. Is the chain reversible?

When will a stationary distribution be a limiting distribution? Recall the following definition, which is only very slightly modified from the discrete-time case.

Definition. A continuous-time Markov chain is *irreducible* if, for all i, j, there exists $t > 0$ s.t. $P_{ij}(t) > 0$.

Theorem. *The following are equivalent: for all i, j,*

(i) $P_{ij}(t) > 0$ for some $t > 0$ (the chain is irreducible);

(ii) $P_{ij}(t) > 0$ for all $t > 0$;

(iii) There exists a $n > 0$ s.t. $(\tilde{P}^n)_{ij} > 0$ (the embedded chain is irreducible).

Note that this means is no notion of periodicity for a continuous-time chain: if it can travel from i to j in some time t, it can travel from i to j in any time t.

In words, the reason this is true is as follows: if $P_{ij}(t) > 0$ for some t, then there exists a path in state space from $i \to j$, so the embedded chain is irreducible. Furthermore, there is a positive probability density of performing each step of the path in any positive time, and therefore there is a positive probability of reaching j from i in any amount of time s.

Proof. (From Norris (1997), Theorem 3.2.1 p.111.) Clearly (ii)⇒(i). For (i)⇒(iii), notice that if a ctMC is irreducible, then for each i, j there are states $i_0, i_1, \ldots i_n$ with $i_0 = i$, $i_n = j$, and $\tilde{P}_{i_0 i_i}\tilde{P}_{i_1 i_2}\ldots\tilde{P}_{i_{n-1} i_n} > 0$, where $\tilde{P}$ is the transition matrix for the embedded chain. For (iii)⇒(ii), further observe that $\tilde{P}_{i_0 i_i}\tilde{P}_{i_1 i_2}\ldots\tilde{P}_{i_{n-1} i_n} > 0$ implies $q_{i_0 i_i} q_{i_1 i_2}\ldots q_{i_{n-1} i_n} > 0$. If $q_{i' j'} > 0$ then (writing $\lambda_i = -q_{ii}$)

$$P_{i'j'}(t) \geq P(J_1 \leq t, Y_1 = j', S_2 > t) = (1 - e^{-\lambda_{i'} t})\tilde{P}_{i'j'} e^{-\lambda_{i'} t} > 0$$

for all t. Therefore, since one way to travel from i to j in some time t is by jumping at intervals of t/n,

$$P_{ij}(t) \geq P_{i_0 i_1}(t/n)\ldots P_{i_{n-1} i_n}(t/n) > 0$$

for all $t > 0$. □

Theorem. *Let X be an irreducible continuous-time Markov chain with transition function $P(t)$ which is continuous at $t = 0$. Then*

(a) If there exists a stationary distribution π then it is unique, and it is a limiting distribution: $P_{ij}(t) \to \pi_j$ as $t \to \infty$, for all i and j;

(b) If there is no stationary distribution then $P_{ij}(t) \to 0$ as $t \to \infty$, for all i and j.

This theorem holds when $|S| = \infty$, with no other conditions. For a sketch of a proof, see Grimmett and Stirzaker (2001, Theorem (21), Section 6.9, p.261). Clearly, the second condition can only hold if $|S| = \infty$. Therefore, *for a finite irreducible ctMC, there is always a unique stationary distribution, which is the limiting distribution.*

Example 4.5 A Poisson process is an example of a ctMC with no stationary distribution. It is not even irreducible, since since the process can only increase.

4.6 Mean first-passage time

Recall that given a set $A \subset S$, the first-passage time to A is the random variable T_A defined by

$$T_A = \inf\{t \geq 0 : X_t \in A\} .$$

The mean first passage time (mfpt) to A, starting at $i \in S$, is $\tau_i = \mathbb{E}_i T_A$. We can solve for the mfpt by solving a system of linear equations.

Mean first-passage time. The mfpt solves the system of equations

$$\begin{cases} \tau_i = 0 & j \in A \\ 1 + \sum_j Q_{ij}\tau_j = 0 & i \notin A \end{cases} \tag{16}$$

Remark. System (16) is sometimes written (heuristically) as

$$Q'\tau = -1, \qquad \tau(A) = 0$$

where Q' is the matrix formed from Q by removing the rows and columns corresponding to states in A. Therefore the mfpt solves the non-homogeneous backward equation with a particular boundary condition.

Remark. Recall that for the discrete-time case, we had $(P-I)\tau = -1$, $\tau(A) = 0$. Again, $(P-I)$ is like a forward-difference approximation to $\frac{dP}{dt}|_t = 0$ using a time step of $\Delta t = 1$.

The proof is slightly less straightforward that in the discrete case, since we need to account for the time spent in each state, not just where it transitions to next. It will use the notation of *conditional expectation*. Given two random variables A, B with some joint distribution, the conditional expectation is defined by

$$\mathbb{E}[A|B=b] \quad = \begin{cases} \sum_a aP(A=a|B=b) & \text{if } A,B \text{ are discrete,} \\ \int_a aP(A=a|B=b)da & \text{if } A \text{ is continuous, } B \text{ is discrete.} \end{cases}$$

Proof. Clearly $\tau_i = 0$ for $i \in A$. Suppose $X_0 = i \notin A$. Let

$$\begin{aligned} J_1 &= \text{next jump time, given } X_0 = i \\ Y_1 &= \text{next state jump to, given } X_0 = i \end{aligned}$$

Let's calculate the mfpt, by conditioning on the first jump, and then subtracting the time of the first jump. We have

$$\begin{aligned}\tau_i = \mathbb{E}[T_A|X_0{=}i] &= \mathbb{E}[J_1|X_0{=}i] + \mathbb{E}[T_A - J_1|X_0{=}i] \\ &= \mathbb{E}[J_1|X_0{=}i] + \sum_{j\neq i} \mathbb{E}[T_A - J_1, Y_1 = j|X_0{=}i] \\ &= \mathbb{E}[J_1|X_0{=}i] + \sum_{j\neq i} \mathbb{E}[T_A - J_1|Y_1{=}j, X_0{=}i] P(Y_1{=}j|X_0{=}i)\end{aligned}$$

Now, we will use three short calculations:

- $\mathbb{E}[T_A - J_1|Y_1{=}j, X_0{=}i] = \mathbb{E}[T_A|X_0{=}j]$, by the Strong Markov property.
- $P(Y_1{=}j|X_0{=}i) = \tilde{P}_{ij} = \frac{q_{ij}}{-q_{ii}}$.
- $\mathbb{E}[J_1|X_0{=}i] = -1/q_{ii}$, since this is the mean of an exponential random variable with parameter $-q_{ii}$.

Substituting these calculations gives

$$\tau_i = \frac{1}{-q_{ii}} + \sum_{j\neq i} \tau_j \frac{q_{ij}}{-q_{ii}}$$

Rearranging gives the desired equations. $\square$

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