MA4546: Introduction to Stochastic Process

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Chapter 4: Continuous-Time Markov Chain

CTMC

Definition (CTMC)

A stochastic process $\{X(t); t \in \mathbb{R}_+\}$ on the state space S [a] is called a CTMC if, for all state i and j in S and $t, s \geq 0$,

$$\Pr(X(s+t) = j | X(s) = i, X(u), 0 \leq u \leq s) = \Pr(X(s+t) = j | X(s) = i).$$

The CTMC $\{X(t); t \geq 0\}$ is said to be time homogeneous[b] if for $t, s \geq 0$,

$$\Pr(X(s+t) = j | X(s) = i) = \Pr(X(t) = j | X(0) = i).$$

[a] We consider finite state space most of time; occasionally we consider the countable infinite state space like $\mathbb{N} = \{0, 1, 2, 3, \cdots\}$

[b] We only study this time-homogeneous case.

The Poisson process and compound Poisson process are both examples of CTMC.

Chapman-Kolmogorov equations

Denote the transition matrix for $X(t)$ by $\mathbf{P}(t) = [P_{ij}(t)]^*$, where the transition probability at time t is defined as

$$P_{ij}(t) := \mathbf{P}(t)_{ij} = \Pr(X(t) = j | X_0 = i).$$

For each t, $\mathbf{P}(t)$ is a stochastic matrix on S for each $t \geq 0$.

We have the following most important result for the family $\{\mathbf{P}(t) : t \geq 0\}$

Theorem (Thm4.1)

If $\{\mathbf{P}(t) : t \in \mathbb{R}_+\}$ is the transient matrix of a CTMC, then it satisfies the following semigroup property: that is

$$\boxed{\mathbf{P}(s+t) = \mathbf{P}(s)\mathbf{P}(t) = \mathbf{P}(t)\mathbf{P}(s)}, \quad \forall s, t \in \mathbb{R}_+$$

$\{\mathbf{P}(t) : t \geq 0\}$ is thus called a transition semigroup.
This is an analogy to the result for DTMC.

*We need save the notation "p''_{ij} for future use.

Two simple Examples of CTMC

A failure model of two-state CTMC

Example (Example 4.1)

Suppose the lifetime of a high-altitude satellite is an Exp(μ) random variable. Once it fails, it stays failed forever since no repair is possible. Let $X(t)$ be 1 if the satellite is operational at time t and 0 otherwise. The transition matrix of this process $\{\mathbf{P}(t)\}$ is

$$\mathbf{P}(t) = \begin{bmatrix} 1 & 0 \\ 1 - e^{-\mu t} & e^{-\mu t} \end{bmatrix}$$

Please verify the semigroup property for this example.

The state space is $\{0, 1\}$. The transition is a jump from "1" to "0", which is triggered by the event of "failure". The waiting time for this event is an $Exp(\mu)$ random variable: $\Pr(X(t) = 0 | X(0) = 1) = 1 - e^{-\mu t}$.

We can understand this example (as well as any CTMC) *intuitively* using what we learnt in Chapter 2 (DTMC) and Chapter 3 (Poisson process):

Wait until, then jump *as if* a DTMC does.

Poisson process with parameter λ

Example

Let $\{N(t)\}$ be a $PP(\lambda)$. How to interpret this process using the above picture ? What is the transition matrix $\{\mathbf{P}(t)\}$ for $\{N(t)\}$?

- The state space $S = \{0, 1, 2, \ldots, \}$ (countable infinite).
- For any value of $N(t)$, say $N(t) = k$, the waiting (sojourn) time (inter-event time interval) at this state is an $Exp(\lambda)$ random variable.
- When the time is up, , N jumps to the state $k+1$.
- Wait the next iid random clock $\sim Exp(\lambda)$ to bomb again , N makes a jump again to $k+2$.
- ..., $\rightarrow$ $\rightarrow$ N jumps.

Transition matrix of Poisson process

$$
\begin{aligned}
P_{ij}(t) &= \Pr(N(t+s)=j)\,|\,N(s)=i) \\
&= \Pr(N(t+s)-N(s)=j-i)(\text{ Poisson r.v with parameter } \lambda t) \\
&= \begin{cases} e^{-\lambda t}\frac{(\lambda t)^{j-i}}{(j-i)!} & \text{if } \ j \ge i, \\ 0 & \text{if } \ j < i. \end{cases}
\end{aligned}
$$

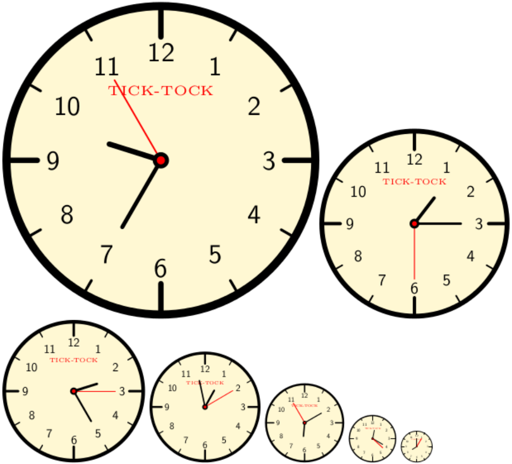
$$
\mathbf{P}(t) = [P_{ij}(t)] = \begin{bmatrix} e^{-\lambda t} & \lambda t e^{-\lambda t} & \frac{\lambda^2 t^2}{2!} e^{-\lambda t} & \frac{\lambda^3 t^3}{3!} e^{-\lambda t} & \cdots \\ 0 & e^{-\lambda t} & \lambda t e^{-\lambda t} & \frac{\lambda^2 t^2}{2!} e^{-\lambda t} & \cdots \\ 0 & 0 & e^{-\lambda t} & \lambda t e^{-\lambda t} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}
$$

Exercise

- *Verify the semigroup property for this example!*
- *If we only count each jump, regardless of the time, we get a DTMC on S. What is the (one-step) transition matrix, written as $[p_{ij}]$, for this DTMC ?*

The clock (Exp r.v.s) can have different rates

The inter-event (waiting) times may have different rates which depend on which state the system is staying.
Some clocks run fast (large λ); some clocks run slow (small λ). See example next page.



Example: Kinematics of chemical reactions

We consider a closed system of two species of molecules, $[A]$ and $[B]$, where the following three chemical reactions occur

1. $[A] \to \emptyset$ (degradation of $[A]$) with rate $\kappa_1 = a/10$
2. $[A] \to [B]$ with rate $\kappa_2 = a$
3. $[B] \to [A]$ with rare $\kappa_3 = 2b$

where the non-negative integers a, b are the number of molecules $[A]$ and $[B]$, respectively. This can be modelled as CTMC. The state space is $S = \{(a,b) \in \mathbb{Z}^2 : a \geq 0, b \geq 0\}$. Each reaction correspond to one event:

1. for Reaction (1): $(a,b) \to (a-1,b)$;
2. for Reaction (2): $(a,b) \to (a-1,b+1)$;
3. for Reaction (3): $(a,b) \to (a+1,b-1)$.

If $(a,b) = (10,10)$, then the reaction (2) and (3) between $[A]$ and $[B]$ is fast, but the degradation process of $[A]$ is slow.
If $(a,b) = (100,1)$, then the reaction (1) and (2) are fast, but the $[B] \to [A]$ is slow.
If $(a,b) = (1,100)$, then the reaction (1) and (2) are slow, but the $[B] \to [A]$ is very fast.

Infinitesimal Generator of CTMC

Infinitesimal Generator of Markov Process

- DTMC: n-step transition matrix is determined by one-step transition matrix $\mathbf{P}^{(n)} = \mathbf{P}^n$
- CTMC: transition matrix $\mathbf{P}(t)$ at any time $t > 0$ is also determined by a matrix for an infinitesimal small time step, which is called *Infinitesimal Generator* .
- Here is the idea: For $h \ll 1$, we have the following Taylor expansion

$$\mathbf{P}(h) = \mathbf{I} + hQ + O(h^2)$$

  ($\mathbf{P}(0) = \mathbf{I}$ is the identical matrix.)*
- The matrix Q is the "derivative" of $\mathbf{P}(t)$ at time 0.

*The big O notation means that $f(h) = O(h^2)$ if and only if $\sup_{h>0} |f(h)/h^2| < c$ for some $c < \infty$.

Infinitesimal Generator

Definition

The infinitesimal generator for a semi-group $\{\mathbf{P}(t) : t \geq 0\}$ is defined as [a] [b]

$$Q := \mathbf{P}'(0) = \lim_{h \searrow 0} \frac{\mathbf{P}(h) - \mathbf{P}(0)}{h}$$

[a] sometimes we use dot $\dot{\mathbf{P}}$ to denote the time derivative. Note that the time derivative of a matrix acts on each entry of the matrix.

[b] For CTMC, the analogy of Q is $\mathbf{P} - \mathbf{I}$.

Then, by semigroup property,

$$\begin{aligned}
\mathbf{P}'(t) &= \lim_{h \searrow 0} \frac{\mathbf{P}(t+h) - \mathbf{P}(t)}{h} \\
&= \lim_{h \searrow 0} \frac{\mathbf{P}(t)(\mathbf{P}(h) - \mathbf{P}(0))}{h} = P(t) \lim_{h \searrow 0} \frac{\mathbf{P}(h) - \mathbf{P}(0)}{h} \\
&= \mathbf{P}(t) Q \\
&= \lim_{h \searrow 0} \frac{\mathbf{P}(h) - \mathbf{P}(0)}{h} \mathbf{P}(t) \\
&= Q\mathbf{P}(t)
\end{aligned}$$

Kolmogorov Forward and Backward Equations

Theorem

Kolmogorov forward equation [a]*:* $\boxed{\mathbf{P}'(t) = \mathbf{P}(t)Q}$

Kolmogorov backward equation: $\boxed{\mathbf{P}'(t) = Q\mathbf{P}(t)}$

[a] In the biology literature it is termed the *chemical master equation*

Definition (Review of matrix exponential)

[a] The exponential of a matrix Q is defined as the series sum

$$e^{tQ} \triangleq \mathbf{I} + tQ + \frac{t^2Q^2}{2!} + \frac{t^3Q^3}{3!} + \frac{t^4Q^4}{4!} \dots$$

[a] MATLAB command for eigenvectors of a matrix is : $\mathrm{expm(A)}$

- Using matrix exponentials, the solution $\mathbf{P}(t)$ is given by

$$\mathbf{P}(t) = \mathbf{P}(0)\exp(tQ) = \exp(tQ), t > 0.$$

- scalar case: ODE $\dot{x} = \lambda x \Longrightarrow x(t) = x(0)e^{\lambda t}$

Example (the satellite failure problem)

We first directly verify the Kolmogorov equation. $\mathbf{P}(t) = \begin{bmatrix} 1 & 0 \\ 1-e^{-\mu t} & e^{-\mu t} \end{bmatrix}$,

$\mathbf{P}'(t) = \begin{bmatrix} 0 & 0 \\ \mu e^{-\mu t} & -\mu e^{-\mu t} \end{bmatrix}$. Note that $Q = \mathbf{P}'(0) = \mu \begin{bmatrix} 0 & 0 \\ 1 & -1 \end{bmatrix}$

$$Q\mathbf{P} = \mu \begin{bmatrix} 0 & 0 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 1-e^{-\mu t} & e^{-\mu t} \end{bmatrix} = \mu \begin{bmatrix} 0 & 0 \\ e^{-\mu t} & -ue^{-\mu t} \end{bmatrix} = \mathbf{P}'(t)$$

$$\mathbf{P}Q = \begin{bmatrix} 1 & 0 \\ 1-e^{-\mu t} & e^{-\mu t} \end{bmatrix} \mu \begin{bmatrix} 0 & 0 \\ 1 & -1 \end{bmatrix} = \mu \begin{bmatrix} 0 & 0 \\ e^{-\mu t} & -e^{-\mu t} \end{bmatrix} = \mathbf{P}'(t)$$

The probability that at time t the satellite is still operational is $P_1(t) := \sum_{i\in S} \Pr(X_t = 1 | X_0 = i) a_i^{(0)}$ where $a_i^{(0)} = \Pr(X_0 = i)$. Then using $\mathbf{P}' = \mathbf{P}Q$,

$$\begin{aligned} P_1'(t) &= \sum_{i\in S} P_{i1}'(t) a_i^{(0)} = \sum_{i\in S} \left(P_{i0}(t) Q_{01} + P_{i1}(t) Q_{11}\right) a_i^{(0)} \\ &= \sum_{i\in S} P_{i1}(t)(-\mu) a_i^{(0)} = -\mu P_1(t). \end{aligned}$$

The master equation is (with initial condition $P_i(t=0) = a_i^{(0)}$)

$$\boxed{P_1'(t) = -\mu P_1(t), \quad P_0'(t) = \mu P_1(t)}$$

Example: Poisson process $\mathrm{PP}(\lambda)$

Note that $\frac{d}{dt}\left(\frac{\lambda^n t^n}{n!}e^{-\lambda t}\right)|_{t=0} = 0$ for $n \geq 2$; and $\frac{d}{dt}\left(\lambda t e^{-\lambda t}\right)|_{t=0} = \lambda$; $\frac{d}{dt}\left(e^{-\lambda t}\right)|_{t=0} = -\lambda$. Then

$$
\begin{aligned}
Q = \mathbf{P}'(t)|_{t=0} &= \frac{d}{dt}[P_{ij}(t)]|_{t=0} \\
&= \frac{d}{dt}\begin{bmatrix} e^{-\lambda t} & \lambda t e^{-\lambda t} & \frac{\lambda^2 t^2}{2!}e^{-\lambda t} & \frac{\lambda^3 t^3}{3!}e^{-\lambda t} & \cdots \\ 0 & e^{-\lambda t} & \lambda t e^{-\lambda t} & \frac{\lambda^2 t^2}{2!}e^{-\lambda t} & \cdots \\ 0 & 0 & e^{-\lambda t} & \lambda t e^{-\lambda t} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}|_{t=0} \\
&= \begin{bmatrix} -\lambda & \lambda & 0 & 0 & \cdots \\ 0 & -\lambda & \lambda & 0 & \cdots \\ 0 & 0 & -\lambda & \lambda & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} = \lambda \begin{bmatrix} -1 & 1 & 0 & 0 & \cdots \\ 0 & -1 & 1 & 0 & \cdots \\ 0 & 0 & -1 & 1 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}
\end{aligned}
$$

An equivalent definition of the generator Q

Theorem

Let the state space of CTMC is $S = \{1, 2, \cdots, n\}$. Define the linear mapping (a square matrix) $L : \mathbb{R}^n \to \mathbb{R}^n$ as follows: for any vector $f = (f_1, \cdots, f_n)^T$, the vector Lf is

$$(Lf)_i := \lim_{t\to 0} \frac{\mathrm{E}[f(X_t)|X_0 = i] - f(i)}{t}, \quad i = 1, 2, \cdots, n$$

Show that $L = Q$.

Proof

$$\begin{aligned}
(Lf)_i &= \lim_{t\to 0} \frac{\mathrm{E}[f(X_t)|X_0 = i] - f(i)}{t}, \\
&= \lim_{t\to 0} \frac{\sum_j \left(f(j)P_{ij}(t) - f(j)\delta_{ij} \right)}{t}, \\
&= \sum_j f(j)P'_{ij}(0) \; = \sum_j Q_{ij} f(j) \\
&= (Qf)_i.
\end{aligned}$$

So, the two matrices L and Q are equal.

The master equation for Poisson process PP(λ)

Define

$$P_n(t) := \Pr(N_t = n | N_0 = 0).$$

Then $(P_n(t) : n = 0, 1, 2, \cdots)$ is the first row of $\mathbf{P}(t)$. The master equation for $P_n(t)$ is

$$\begin{aligned} P_n'(t) =& P_{0n}'(t) = \sum_k P_{0k}(t) Q_{kn} \\ =& P_{0n}(t) Q_{nn} + P_{0,n-1}(t) Q_{n-1,n} \\ =& P_n(-\lambda) + P_{n-1}\lambda \end{aligned}$$

So, the master equation is

$$\boxed{P_n'(t) = -\lambda P_n(t) + \lambda P_{n-1}(t), \quad n = 1, 2, \cdots,}$$

together with $P_0'(t) = -\lambda P_0(t)$ and the initial $P_n(t = 0) = \delta_{n,0}$.

- $P_n' + \lambda P_n = \lambda P_{n-1} \implies (e^{\lambda t} P_n)' = e^{\lambda t} \lambda P_{n-1} \implies$
$$P_n(t) = P_n(0) + \int_0^t e^{-\lambda(t-s)} \lambda P_{n-1}(s) ds$$
- $P_0(t) = e^{-\lambda t}$; $\Rightarrow P_1(t) = \int_0^t e^{-\lambda(t-s)} \lambda e^{-\lambda s} ds = \lambda t e^{-\lambda t} \Rightarrow P_2(t)$

Since the master equation for $PP(\lambda)$ is linear, so we multiply the master equation

$$P_n' = -\lambda P_n + \lambda P_{n-1}, \quad n = 1, 2, \cdots,$$

by n on both sides, then

$$\begin{aligned}\sum_{n=1}^{\infty} nP_n' &= -\lambda \sum_{n=1}^{\infty} nP_n + \lambda \sum_{n=1}^{\infty} nP_{n-1} \\ &= -\lambda \sum_{n=1}^{\infty} nP_n + \lambda \sum_{n=1}^{\infty} (n+1)P_n + \lambda P_0 \\ &= \lambda \sum_{n=1}^{\infty} P_n + \lambda P_0 = \lambda(1 - P_0) + \lambda P_0 = \lambda\end{aligned}$$

which means is the derivative $(\mathrm{E}(N_t))' = (\sum nP_n)' = \lambda$. Since $\mathrm{E}(N_0 = 0)$, then $\mathrm{E}(N_t) = \lambda t$. So, we re-derived the first moment from the master equation.

Question: What if we use the Kolmogorov *backward* equation $\mathbf{P}'(t) = Q\mathbf{P}$?

A Probabilistic Understanding of the Q matrix for CTMC

Why the infinitesimal generator Q is useful ?

- *It "generates" the transition matrix* $\mathbf{P}(t)$

$$\mathbf{P}(t) = \mathbf{P}(0)\exp(tQ) = \exp(tQ), t > 0.$$

- It defines the master equation $\mathbf{P}' = \mathbf{P}Q$.
- *It carries the meaning of "rate" and underlying "DTMC" in our previous intuitive picture.*
- Next, we shall see how to directly write the Q matrix from real models by exploring its probabilistic meaning.

Properties and Probabilistic Interpretation of the Q matrix

First we introduce notations. Let the state space $S = \{1, 2, 3, \cdots, N\}$.
From now on, we write $Q = [r_{ij}]$, but the diagonal entries are denoted as $-r_i$ rather than r_{ii} *

$$Q = \begin{bmatrix} -r_1 & r_{12} & \dots & r_{1N} \\ r_{21} & -r_2 & \dots & r_{2N} \\ \dots & \dots & \dots & \dots \\ r_{N1} & r_{N2} & \dots & -r_N \end{bmatrix}$$

*We shall see the reason later. The notation here is a problem. Some references use $Q = [q_{ij}]$, some others use $Q = [\lambda_{ij}]$. Please use my notation or clearly specify the notations you use.

We have the asymptotic expansion for $\mathbf{P}(h) = [P_{ij}(h)]$

$$\mathbf{P}(h) = \mathbf{I} + hQ + O(h^2), \quad 0 < h \ll 1.$$

Consider the transition probability from $X(0)$ to $X(h)$ for a small time step h by using the above notation of Q,

$$\Pr(X(h) = j | X(0) = i) = P_{ij}(h) = \begin{cases} r_{ij}h + O(h^2) & i \neq j, \\ 1 - r_i h + O(h^2) & i = j. \end{cases}$$

Notice that $[P_{ij}(t)]$ is a stochastic matrix for any $t \in \mathbb{R}_+$. So

$$\begin{cases} r_{ij}h \geq 0, \quad i \neq j, \\ (\sum_{j\neq i} r_{ij}h) + (1 - r_i h) + O(h^2) = 1. \end{cases}$$

From the second equation, we know that

$$(\sum_{j\neq i} r_{ij}h) - r_i h = O(h^2)$$

$$(\sum_{j\neq i} r_{ij}) - r_i = O(h)$$

So, as $h \to 0$, we have

$$\boxed{r_i = \sum_{j\neq i} r_{ij}.}$$

Theorem

The infinitesimal generator Q has the following properties

1. *The elements on the main diagonal are all strictly negative.*[a]
2. *The elements off the main diagonal are non-negative.*
3. *The sum of entries at each row of is zero.*

[a] except for the very degenerate case with absorbing state like the satellite failure problem where the rate is zero

remark Q-matrix is not a stochastic matrix. The only requirement for a matrix to be a generator of some CTMC is the above three conditions.

Integration form of backward Kolmogorov equation

Write $\mathbf{P}(t) = [P_{ij}(t)]$ and $Q = [r_{ij}]$ whose diagonals are $-r_i$.
Then the backward Kolmogorov equation $\mathbf{P}'(t) = Q\mathbf{P}(t)$ is

$$P'_{ij}(t) = -r_i P_{ij}(t) + \sum_{k \neq i} r_{ik} P_{kj}(t)$$

Multiply by $e^{r_i t}$, then one gets

$$(e^{r_i t} P_{ij}(t))' = \sum_{k \neq i} r_{ik} e^{r_i t} P_{kj}(t)$$

Integrate both sides and from $P_{ij}(t=0) = \delta_{ij}$, we have

$$\begin{aligned} P_{ij}(t) &= \delta_{ij} e^{-r_i t} + e^{-r_i t} \int_0^t \sum_{k \neq i} r_{ik} e^{-r_i t'} P_{kj}(t') dt', \quad s := t - t' \\ &= \delta_{ij} e^{-r_i t} + \int_0^t e^{-r_i s} \sum_{k \neq i} r_{ik} P_{kj}(t-s) ds. \end{aligned}$$

Resolvent of the semigroup $\{\mathbf{P}(t) : t \geq 0\}$

We know that $\mathbf{P}(t) = e^{Qt}$ where Q is the infinitesimal generator. Now we introduce another new concept for the semigroup.

Definition

The resolvent of the semigroup $\{\mathbf{P}(t)\}$ is the following matrix which is the (componentwise) Laplace transform of the semigroup:

$$R_\lambda := \int_0^\infty e^{-\lambda t}\mathbf{P}(t)dt = \int_0^\infty e^{-(\lambda - Q)t}dt = (\lambda - Q)^{-1}$$

where λ is any positive real number.

- The resolvent is simply the inverse of $\lambda - Q$
- $(\lambda R_\lambda)_{ij} = \int_0^\infty \lambda e^{-\lambda t} P_{ij}(t)dt = \Pr(X_\tau = j | X_0 = i)$ takes value in $[0,1]$, where τ is a r.v. $\sim Exp(\lambda)$ independent of the CTMC $\{X(t)\}$.
- Show that the family of $\{R_\lambda\}$ satisfies the resolvent equation

$$R_\lambda - R_\mu + (\lambda - \mu)R_\lambda R_\mu = 0.$$

In some case, the resolvent R_λ is even more primitive than the generator Q. There is a one-to-one relation between the resolvent $\{R_\lambda\}$ and the semigroup $\{\mathbf{P}(t)\}$. (Hille-Yosida Theorem – advanced topics in functional analysis.)

Probabilistic meaning of (negative) diagonal of Q: $\{r_i\}$

- During a short time $(0,h)$,
$$\Pr(X(h) \neq i \,\big|\, X(0)=i) \simeq \sum_{k\neq i} r_{ik} h = r_i h$$
During the infinitesimal time interval $[0,h]$, the probability of "jump" (leave current state i) is proportional to h with rate r_i.
- The Markovian property implies **exponential** distribution of the sojourn time — time interval between successive "jumps". *Fix a time $t>0$, divide the time interval $[0,t]$ into n equal-length subintervals $[t_k, t_{k+1}]$ where $t_k = k\times h$ and $h = t/n$.*
$$\Pr(\textit{no jump between } [0,t]) = \lim_{n\to\infty} \Pi_{k=0}^{n-1} \Pr(\textit{no jump between } [kh,(k+1)h])$$
$$= \lim_{n\to\infty} \Pi_{i=0}^{n-1} (1-r_i h) = \lim_{n\to\infty} (1-r_i t/n)^n = e^{-r_i t}$$
- If the current state is i, the CTMC waits for exponentially distributed time with rate r_i, then make a jump to one of **other** states than i.

Jump to which state (excluding i) ?

$$\Pr(X(h) \neq i | X(0) = i) \simeq r_i h = \sum_{j \neq i} r_{ij} h.$$

$$\Pr(X(h) = j | X(0) = i) \simeq r_{ij} h, \quad i \neq j$$

- Conditional probability $\Pr(X(h) = j \; | X(h) \neq i, X(0) = i) = \frac{r_{ij}}{r_i}$
- The (conditional) transition probability from i to j is $p_{ij} = \frac{r_{ij}}{r_i}$.
- So, if we ignore all sojourn times and only count the first transition event, the second transition event, ..., we see the process behaves like a DTMC (see below for the embedded DTMC Z_n).
- Figure 4.1 (textbook page 88)

The Discrete-Time Embedded Chain

Consider (T_n) the sequence of jump times of the continuous-time Markov process $\{X(t) : t \in \mathbb{R}_+\}$, defined recursively by $T_0 = 0$, then

$$T_{n+1} = \inf\{t > T_n : X_t \neq X(T_n)\}.$$

The DTMC with transition matrix $[p_{ij}]$ we disccussed above is $\{Z_n\}$ defined by $Z_0 = X(0)$ and

$$Z_n := X(T_n).$$

The DTMC $\{Z_n : n = 0, 1, 2, \ldots\}$ is called the **embedded chain** of $\{X(t) : t \in \mathbb{R}_+\}$.*

- The transition matrix for Z_n is $p_{ij} = \frac{r_{ij}}{r_i}$ if $i \neq j$.
- $p_{ii} = 1 - \sum_{j \neq i} p_{ij} = 0$ because $r_i = \sum_j r_{ij}$

*The graphical representation (transition diagram) of DTMC $\{Z_n\}$ is called rate diagram of CTMC $\{X_t\}$.

Notations and Definitions

- $\{\mathbf{P}(t) = [P_{ij}(t)] : t \geq 0\}$: transition matrix of CTMC
- $[p_{ij}]$: transition matrix of the embedded DTMC Z_n (*without self-loops* because $p_{ii} = 0$)
- generator matrix: $Q = [r_{ij}]$ except that the diagonals are $Q_{ii} = -r_i$.
- transition rate * : $r_{ij} = r_i p_{ij}$ $(r_{ii} := 0)$.
- **rate matrix**: $R = [r_{ij}]$ ($r_{ii} := 0$)

  Transition diagram: (the number on the directed edge is the transition rate, not the transition probability as in DTMC).
  example (like chemical reaction formula)

$$① \underset{r_{12}}{\overset{r_{12}}{\rightleftarrows}} ② \underset{r_{32}}{\overset{r_{23}}{\rightleftarrows}} ③$$

*in unit time, the probability that X makes a jump *and* this jump is from i to j

Example:

A molecule transitions between states 0 and 1. The transition rate from 0 to 1 is 3 and the transition from 1 to 0 is 1. Write down the rate matrix R and the generator Q.

The transition matrix of the embedded DTMC is

$$P = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$r_{01} = 3$ and $r_{10} = 1$.

Then the rate matrix is

$$\begin{bmatrix} \square & 3 \\ 1 & \square \end{bmatrix} \to R = \begin{bmatrix} 0 & 3 \\ 1 & 0 \end{bmatrix}$$

So, by filling the diagonal entries, the generator Q is

$$Q = \begin{bmatrix} -3 & 3 \\ 1 & -1 \end{bmatrix}$$

$$⓪ \underset{r_{10}=1}{\overset{r_{01}=3}{\rightleftarrows}} ①$$

Example: lifetime of a high-altitude satellite (Example 4.1)

The transition rate from 0 to 1 is 0. The transition rate from 0 to 1 is μ.

The transition matrix of the embedded DTMC is $P = \begin{bmatrix} n.a. & n.a. \\ 1 & 0 \end{bmatrix}$ (the first row has not definition)

The rate matrix is

$$R = \begin{bmatrix} 0 & 0 \\ \mu & 0 \end{bmatrix}$$

So, the generator $Q = [r_{ij}]$ is

$$Q = \begin{bmatrix} 0 & 0 \\ \mu & -\mu \end{bmatrix}$$

The transition matrix of the CTMC is

$$\mathbf{P}(t) = e^{tQ} = \begin{bmatrix} 1 & 0 \\ 1 - e^{-\mu t} & e^{-\mu t} \end{bmatrix}$$

$$⓪ \underset{\mu}{\leftarrow} ①$$

Example: Poisson process with parameter λ

generator matrix Q

- The transition matrix for the DTMC embedded in Poisson process

$$[p_{ij}] = \begin{bmatrix} 0 & 1 & 0 & 0 & \cdots \\ 0 & 0 & 1 & 0 & \cdots \\ 0 & 0 & 0 & 1 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

- How long to make a jump ? The sojourn time is Exp(λ). So $r_i \equiv \lambda$
- Calculate transition rate $r_{ij} = r_i p_{ij} = \lambda p_{ij}$
-

$$Q = \begin{bmatrix} -\lambda & \lambda & 0 & 0 & \cdots \\ 0 & -\lambda & \lambda & 0 & \cdots \\ 0 & 0 & -\lambda & \lambda & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} = \lambda \begin{bmatrix} -1 & 1 & 0 & 0 & \cdots \\ 0 & -1 & 1 & 0 & \cdots \\ 0 & 0 & -1 & 1 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

$$⓪ \xrightarrow{\lambda} ① \xrightarrow{\lambda} ② \xrightarrow{\lambda} ③ \ldots$$

Example: Poisson process with parameter λ

The transition semigroup $\mathbf{P}(t)$

$$\mathbf{P}(t) = \begin{bmatrix} e^{-\lambda t} & \lambda t e^{-\lambda t} & \frac{\lambda^2 t^2}{2!} e^{-\lambda t} & \frac{\lambda^3 t^3}{3!} e^{-\lambda t} & \cdots \\ 0 & e^{-\lambda t} & \lambda t e^{-\lambda t} & \frac{\lambda^2 t^2}{2!} e^{-\lambda t} & \cdots \\ 0 & 0 & e^{-\lambda t} & \lambda t e^{-\lambda t} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

We can verify (<u>`Homework`</u>) that the above Q and $\mathbf{P}(t)$ satisfy the Kolmogorov equation or verify directly $\mathbf{P}(t) = e^{tQ}$.

Example: chemical reaction

1. $[A] \to \emptyset$ (degradation of $[A]$) with rate $\kappa_2 = a/10$
2. $[A] \to [B]$ with rate $\kappa_1 = a$
3. $[B] \to [A]$ with rare $\kappa_3 = 2b$

Define $P_m^A(t) = \Pr(a(t) = m)$ and $P_n^B(t) = \Pr(b(t) = n)$, where $a(t), b(t)$ are the numbers of molecule [A] and [B], respectively, at time t. then the master equation is the following system of ODEs

$$\begin{cases} \dot{P}_m^A(t) = -\dfrac{m}{10} P_m^A(t) - mP_m^A(t) + 2nP_n^B(t) \\ \dot{P}_n^B(t) = -2nP_n^B(t) + mP_m^A(t) \end{cases}$$

with certain boundary and initial conditions.

? If without the first reaction, what is the master equation ? And show that in this case the total number of $[A]$ and $[B]$ is conserved: $\frac{d}{dt}(P_m^A(t) + P_n^B(t)) \equiv 0$

Write Q matrix from master equation

Exercise

Assume a CTMC X_t has the state space $S = \{0, 1, \ldots\}$. $P_n(t) := \Pr(X_t = n | N_0 = 0)$ satisfies

$$P'_n(t) = -\alpha_n P_n + \lambda(n-1) P_{n-1} + \lambda P_{n+1}, \quad n = 1, 2, \cdots,$$

and $P'_0(t) = \lambda P_1$ and $P'_1(t) = -2\lambda P_1 + \lambda P_2$. What is the value of α_n? What is the Q-matrix and transition diagram of this CTMC?

In general: $P'_n(t) = -r_n P'_n(t) + \sum_{k \neq n} P_k r_{kn}$. Compare this to the given master equation, then $r_0 = 0$ (which implies that $r_{0k} = 0, \quad \forall k$) and $r_{n,n+1} = n\lambda$ and $r_{n,n-1} = \lambda$ for all $n \geq 1$. So, the (negative) diagonal is

$$\alpha_n = r_n = r_{n,n+1} + r_{n,n-1} = -\lambda(n+1). \quad Q = \lambda \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \cdots \\ 1 & -2 & 1 & 0 & 0 \cdots \\ 0 & 1 & -3 & 2 & 0 \cdots \\ 0 & 0 & 1 & -4 & 3 \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}.$$

$$⓪ \underset{\lambda}{\leftarrow} ① \underset{\lambda}{\overset{\lambda}{\rightleftarrows}} ② \underset{\lambda}{\overset{2\lambda}{\rightleftarrows}} ③ \underset{\lambda}{\overset{3\lambda}{\rightleftarrows}} ④ \ldots$$

Example: pure birth process

We have a finite number of organisms which independently and randomly split into two. We let $X(t)$ denote the number of organisms at time t and assume that $X(0) = 1$. The law for splitting of a single organism is given by $\Pr[\text{ splitting in } h \text{ units of time}] \simeq \lambda h$. So the law for splitting of n organism is

$$\Pr[\text{ splitting in } (t, t+h] \text{ time interval } |X(t) = n] \simeq n\lambda h.$$

Exercise

What is the generator of the pure birth process on state space $S = \{1, 2, 3, \dots\}$

$$Q = \begin{bmatrix} -\lambda & \lambda & 0 & 0 & \cdots \\ 0 & -2\lambda & 2\lambda & 0 & \cdots \\ 0 & 0 & -3\lambda & 3\lambda & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

What is the transition semigroup $\mathbf{P}(t)$? Challenging !! But we can write down the Kolmogorov equation (a first order linear PDE),

Example: Birth and Death Process

The generator of the birth and death process on $\{0,1,...,N\}$ is

$$Q=\begin{bmatrix} -\lambda_0 & \lambda_0 & 0 & 0 & \cdots & \cdots & \cdots & 0 & 0 \\ \mu_1 & -\lambda_1-\mu_1 & \lambda_1 & 0 & \cdots & \cdots & \cdots & 0 & 0 \\ 0 & \mu_2 & -\lambda_2-\mu_2 & \lambda_2 & \cdots & \cdots & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \vdots & \ddots & \ddots & \mu_{N-1} & -\lambda_{N-1}-\mu_{N-1} & \lambda_{N-1} \\ 0 & 0 & 0 & 0 & \ddots & \ddots & \ddots & \mu_N & -\mu_N \end{bmatrix}$$

with $\mu_0=\lambda_N=0$. The master equation for $P_n(t)=\Pr(X_t=n|X_0=0)$ is

$$P_n'=\lambda_{n-1}P_{n-1}-(\lambda_n+\mu_n)P_n+\mu_{n+1}P_{n+1}$$

and $P_0'=-\lambda_0P_0+\mu_1P_1$. Here λ_i means the birth rate and μ_i means the death rate.

$$\text{n-1} \underset{\mu_n}{\overset{\lambda_{n-1}}{\rightleftarrows}} \text{n} \underset{\mu_{n+1}}{\overset{\lambda_n}{\rightleftarrows}} \text{n+1}.$$

Tricks to write the master equation directly

We can write explicitly the generator Q from the rate matrix R by reading the transition diagram. Then use $\mathbf{P}' = \mathbf{P}Q$ to find the master equation. We actually can write the master equation for $P_n(t) = \Pr(X_t = n)$ directly by noting that

$$P_n'(t) = \sum_{i \in S} P_i Q_{in} = -r_n P_n + \sum_{i \neq n} r_{in} P_i = -(\sum_{k \neq n} r_{nk}) P_n + \sum_{i \neq n} r_{in} P_i$$

So

- the coefficient for P_i is r_{in}, which is the rate for $i \to n$ (point into the current state n). This looks like all incoming flux from all other states than the state n.
- the coefficient for P_n is always negative and the absolute value is $\sum_{k \neq n} r_{nk}$, which the sum of rates for n to all other states. This is all flux flows leaving the state n.

Exercise (Example 4.18): Solve the transition semi-group for the two-State CTMC

Exercise

Consider a two-state CTMC with the infinitesimal generator

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

with $\alpha, \beta \geq 0$. Find $\mathbf{P}(t)$.

The forward Kolmogorov equation reads

$$\begin{cases} P'_{0,0}(t) = -\alpha P_{0,0}(t) + \beta P_{0,1}(t), \quad P'_{0,1}(t) = \alpha P_{0,0}(t) - \beta P_{0,1}(t), \\ P'_{1,0}(t) = -\alpha P_{1,0}(t) + \beta P_{1,1}(t), \quad P'_{1,1}(t) = \alpha P_{1,0}(t) - \beta P_{1,1}(t), \end{cases}$$

with initial condition $P_{0,0}(0) = P_{1,1}(0) = 1$, $P_{0,1}(0) = P_{1,0}(0) = 0$.
We may solve this ODE system by making a change of variables. Let

$$u(t) = P_{0,0}(t) + P_{0,1}(t), \quad v(t) = \alpha P_{0,0}(t) - \beta P_{0,1}(t).$$

Then the first two equations become simply

$$u'(t) = 0, \quad v'(t) = -(\alpha + \beta)v(t),$$

with initial condition $u(0) = 1$, $v(0) = \alpha$.

Solving Kolmogorov Equation

It is easy to solve

$$u(t) = 1, \quad v(t) = \alpha \mathrm{e}^{-(\alpha+\beta)t}.$$

Then we get

$$P_{0,0}(t) = \frac{\beta}{\alpha+\beta} + \frac{\alpha}{\alpha+\beta}\mathrm{e}^{-(\alpha+\beta)t}, \quad P_{0,1}(t) = \frac{\alpha}{\alpha+\beta} - \frac{\alpha}{\alpha+\beta}\mathrm{e}^{-(\alpha+\beta)t}.$$

The last two equations can be solved similarly as

$$P_{1,0}(t) = \frac{\beta}{\alpha+\beta} - \frac{\beta}{\alpha+\beta}\mathrm{e}^{-(\alpha+\beta)t}, \quad P_{1,1}(t) = \frac{\alpha}{\alpha+\beta} + \frac{\beta}{\alpha+\beta}\mathrm{e}^{-(\alpha+\beta)t}.$$

What is the limit of $\lim_{t\to\infty} \mathbf{P}(t)$?

The above method of solving the Kolmogorov equation actually amounts to computing the matrix exponential e^{tQ} by the diagonalization technique.

Compute the Matrix Exponential by Diagonalization

We want to compute

$$P(t) = \exp(tQ) = \exp\left(t\begin{bmatrix} -\alpha & \alpha \\ \beta & -\beta \end{bmatrix}\right).$$

Observe that the matrix Q can be put in the diagonal form

$$Q = PDP^{-1} = \begin{bmatrix} 1 & -\alpha \\ 1 & \beta \end{bmatrix}\begin{bmatrix} 0 & 0 \\ 0 & -\alpha-\beta \end{bmatrix}\begin{bmatrix} \frac{\beta}{\alpha+\beta} & \frac{\alpha}{\alpha+\beta} \\ -\frac{1}{\alpha+\beta} & \frac{1}{\alpha+\beta} \end{bmatrix}.$$

Consequently,

$$\begin{aligned}
\exp(tQ) &= \sum_{n=0}^{\infty} \frac{t^n}{n!} Q^n = \sum_{n=0}^{\infty} \frac{t^n}{n!} \left(PDP^{-1}\right)^n = \sum_{n=0}^{\infty} \frac{t^n}{n!} PD^nP^{-1} = P\left(\sum_{n=0}^{\infty} \frac{t^n}{n!} D^n\right)P^{-1} \\
&= P\begin{bmatrix} 1 & 0 \\ 0 & \sum_{n=0}^{\infty} \frac{t^n(-\alpha-\beta)^n}{n!} \end{bmatrix} P^{-1} = \begin{bmatrix} 1 & -\alpha \\ 1 & \beta \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & \mathrm{e}^{-(\alpha+\beta)t} \end{bmatrix}\begin{bmatrix} \frac{\beta}{\alpha+\beta} & \frac{\alpha}{\alpha+\beta} \\ -\frac{1}{\alpha+\beta} & \frac{1}{\alpha+\beta} \end{bmatrix} \\
&= \frac{1}{\alpha+\beta}\begin{bmatrix} \beta & \alpha \\ \beta & \alpha \end{bmatrix} + \frac{\mathrm{e}^{-(\alpha+\beta)t}}{\alpha+\beta}\begin{bmatrix} \alpha & -\alpha \\ -\beta & \beta \end{bmatrix}.
\end{aligned}$$

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Uniformization Method of Computing Transition Matrix (*optional*)

Take $r \geq \max_{1 \leq i \leq N} \{r_i\}$. Define $\hat{P}$ as

$$[\hat{P}_{i,j}] = \begin{cases} 1 - \frac{r_i}{r} & \text{if} \quad i = j, \\ \frac{r_{i,j}}{r} & \text{if} \quad i \neq j. \end{cases}$$

Note that $\hat{P}$ is a stochastic matrix (all entries $\in [0,1]$) and

$$Q = r(\hat{P} - I_d) = r\hat{P} - rI_d.$$

Hence

$$P(t) = e^{tQ} = e^{-rtI_d} e^{rt\hat{P}} \; * = e^{-rt} e^{rt\hat{P}} = \sum_{k=0}^{\infty} e^{-rt} \frac{(rt)^k}{k!} \hat{P}^k.$$

Theorem (Thm 4.3)

$$P(t) = \sum_{k=0}^{\infty} e^{-rt} \frac{(rt)^k}{k!} \hat{P}^k.$$

$^*e^{A+B} = e^A e^B$ does not hold in general unless $AB = BA$.

Example(Example 4.18): Two-State CTMC

Consider a two-state CTMC with the infinitesimal generator

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

with $\alpha, \beta \geq 0$. Find $P(t)$.
Here the trick is to take $r = \alpha + \beta$. Then

$$\hat{P} = \frac{1}{r} \begin{bmatrix} \beta & \alpha \\ \beta & \alpha \end{bmatrix} = \frac{1}{r} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \begin{bmatrix} \beta & \alpha \end{bmatrix}.$$

$$\hat{P}^k = \hat{P} = \frac{1}{r} \begin{bmatrix} \beta & \alpha \\ \beta & \alpha \end{bmatrix}, \quad k \geq 1.$$

Then by Thm 4.3,

$$P(t) = \sum_{k=0}^{\infty} \mathrm{e}^{-rt} \frac{(rt)^k}{k!} \hat{P}^k = \mathrm{e}^{-rt} \left(I_2 + \hat{P} \sum_{k=1}^{\infty} \frac{(rt)^k}{k!} \right) = \mathrm{e}^{-rt} \left(I_2 + (\mathrm{e}^{rt} - 1) \hat{P} \right)$$

$$= \frac{1}{\alpha + \beta} \begin{bmatrix} \beta & \alpha \\ \beta & \alpha \end{bmatrix} + \frac{1}{\alpha + \beta} \begin{bmatrix} \alpha & -\alpha \\ -\beta & \beta \end{bmatrix} \mathrm{e}^{-(\alpha+\beta)t}.$$

Review of this chaper

- The transition semi-group and its infinitesimal generator Q.
- The property of the generator Q.
- The master equation and the generator. Matrix Exponential.
- The embedded DTMC, transition diagram, rate matrix and the Q matrix: they are closely related.
- Derive the master equation for models from application.
- Solve the master equation for the two-state model.

Homework

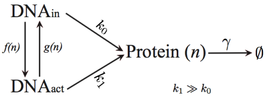
- What is the transition semigroup $\mathbf{P}(t)$ and the generator Q of a Poisson process with rate λ. Verify they do satisfy forward Kolmogorov equation and $\mathbf{P}(t) = e^{tQ}$ by the definition of matrix exponential.
- Consider the following time-homogeneous compound Poisson process with rate λ: $X_t = \sum_{i=0}^{N(t)} Z_i$ where Z_0=0 and for $i \geq 1$, $Z_i = \pm a$ with the equal probability $1/2$. $N(t)$ is the $PP(\lambda)$. $a > 0$ is a constant. This process X_t has independent and stationary increment. What is the master equation and the generator Q of this process? What is $\mathrm{E}(X_t)$? For what condition on a and λ, the variance of X_t is equal to t? Under this condition, find $\mathrm{cov}(X_s, X_t)$.
- A professor wanders between three coffee shops with the rate diagram

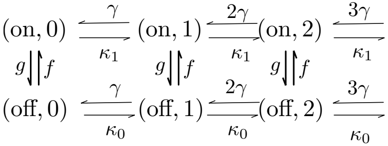
$$\text{Ⓐ} \underset{\lambda_1}{\overset{\mu_1}{\rightleftarrows}} \text{Ⓑ} \underset{\lambda_2}{\overset{\mu_2}{\rightleftarrows}} \text{Ⓒ}.$$

  1. What is the generator Q matrix ?
  2. What is the transition matrix for the embedded DTMC?
  3. Given that the professor is at coffee shop B right now, what is the probability that he will next head to shop A, rather than C ?
- TEXTBOOK. Page 138: Exercise 4.1, 4.6 and Page 141: Exercise 4.1, 4.4

Exercise: genetic switching model

We consider the following genetic switching model in system biology.





The DNA switches between the active state ("on") and the inactive state ("off"), with rate $f(n)$ and $g(n)$, respectively, as shown in the figure, where n is the number of the proteins. When the DNA is on, one protein will be produced with rate k_1 while the rate is k_0 when the DNA is off. $k_1 > k_0$. For each protein, the degradation rate is γ. For this model, the state space consists of the following pair (DNA_state, # of proteins), i.e., S is the following product space $S = \{\text{on}, \text{off}\} \times \{0, 1, 2, \cdots\}$. The transition diagram is shown above on the right figure (note the dependence of the functions f and g on n is dropped off for better visualization in this figure). Write down the master equations for $P_{\text{on}}(n,t)$ and $P_{\text{off}}(n,t)$ which are the probability of n proteins when the DNA is on or off, respectively. You may start from the special case $f = g = 0$.

$f = g = 0$

In this case, $P_{\text{on}}(n,t)$ and $P_{\text{off}}(n,t)$ correspond to two independent birth-death processes with state space $\{0,1,2,\cdots\}$ We only need consider $P_{\text{on}}(n,t)$ as follows. The rate matrix is

$$R = \begin{bmatrix} 0 & \kappa_1 & 0 & 0 & 0 & \cdots \\ \gamma & 0 & \kappa_1 & 0 & 0 & \cdots \\ 0 & 2\gamma & 0 & \kappa_1 & 0 & \cdots \\ 0 & 0 & 3\gamma & 0 & \kappa_1 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \cdots \end{bmatrix}$$

So, the Q matrix is

$$Q = \begin{bmatrix} -\kappa_1 & \kappa_1 & 0 & 0 & 0 & \cdots \\ \gamma & -\kappa_1-\gamma & \kappa_1 & 0 & 0 & \cdots \\ 0 & 2\gamma & -\kappa_1-2\gamma & \kappa_1 & 0 & \cdots \\ 0 & 0 & 3\gamma & -\kappa_1-3\gamma & \kappa_1 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \cdots \end{bmatrix}.$$

The master equation is

$P'_{\text{on}}(n,t) = \kappa_1 P_{\text{on}}(n-1,t) + (n+1)\gamma P_{\text{on}}(n+1,t) - (\kappa_1 + n\gamma)P_{\text{on}}(n,t), \ \forall n \geq 1$ and
$P'_{\text{on}}(0,t) = -\kappa_1 P_{\text{on}}(0,t) + \gamma P_{\text{on}}(1,t)$.

general case

We label the state space S by mapping S to $\{0,1,2,3,4,\cdots\}$ as follows: new state 2i $\leftrightarrow$ (on, i) state 2i+1 $\leftrightarrow$ (off, i) for $i = 0,1,2,3\cdots$. The rate matrix can be written in block form $R = \begin{bmatrix} R_{\text{on,on}} & R_{\text{on,off}} \\ R_{\text{off,on}} & R_{\text{off,off}} \end{bmatrix}$

$$R_{\text{on,on}} = \begin{bmatrix} 0 & \kappa_1 & 0 & 0 & 0 & \cdots \\ \gamma & 0 & \kappa_1 & 0 & 0 & \cdots \\ 0 & 2\gamma & 0 & \kappa_1 & 0 & \cdots \\ 0 & 0 & 3\gamma & 0 & \kappa_1 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \cdots \end{bmatrix}, R_{\text{on,off}} = \begin{bmatrix} g(0) & 0 & 0 & 0 & \cdots \\ 0 & g(1) & 0 & 0 & \cdots \\ 0 & 0 & g(3) & 0 & \cdots \\ 0 & 0 & 0 & g(4) & \cdots \\ \vdots & \vdots & \vdots & \ddots & \cdots \end{bmatrix}$$

$$R_{\text{off,on}} = \begin{bmatrix} f(0) & 0 & 0 & 0 & \cdots \\ 0 & f(1) & 0 & 0 & \cdots \\ 0 & 0 & f(3) & 0 & \cdots \\ 0 & 0 & 0 & f(4) & \cdots \\ \vdots & \vdots & \vdots & \ddots & \cdots \end{bmatrix}, R_{\text{off,off}} = \begin{bmatrix} 0 & \kappa_0 & 0 & 0 & 0 & \cdots \\ \gamma & 0 & \kappa_0 & 0 & 0 & \cdots \\ 0 & 2\gamma & 0 & \kappa_0 & 0 & \cdots \\ 0 & 0 & 3\gamma & 0 & \kappa_0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \cdots \end{bmatrix}$$

The Q matrix can written accordingly (skipped due to no space here) by filling in the main diagonal elements to make sure the sum of each row is zero.

The master equation for the vector
$(P_{\mathsf{on}}(0,t), P_{\mathsf{on}}(1,t), P_{\mathsf{on}}(2,t), \cdots, P_{\mathsf{off}}(0,t), P_{\mathsf{off}}(1,t), P_{\mathsf{off}}(2,t), \cdots)$ is

$$\begin{cases} P'_{\mathsf{on}}(n,t) = \kappa_1 P_{\mathsf{on}}(n-1,t) + (n+1)\gamma P_{\mathsf{on}}(n+1,t) + f(n) P_{\mathsf{off}}(n,t) \\ \qquad\qquad - (n\gamma + \kappa_1 + g(n)) P_{\mathsf{on}}(n,t) \\ P'_{\mathsf{off}}(n,t) = \kappa_0 P_{\mathsf{off}}(n-1,t) + (n+1)\gamma P_{\mathsf{off}}(n+1,t) + g(n) P_{\mathsf{on}}(n,t) \\ \qquad\qquad - (n\gamma + \kappa_0 + f(n)) P_{\mathsf{off}}(n,t) \end{cases}$$

and

$$\begin{cases} P'_{\mathsf{on}}(0,t) = \gamma P_{\mathsf{on}}(1,t) + f(0) P_{\mathsf{off}}(0,t) - (\kappa_1 + g(0)) P_{\mathsf{on}}(0,t) \\ P'_{\mathsf{off}}(0,t) = \gamma P_{\mathsf{off}}(1,t) + f(0) P_{\mathsf{on}}(n,t) - (\kappa_0 + g(0)) P_{\mathsf{off}}(0,t) \end{cases}$$

Compared with the case of $f = g = 0$, the extra terms are

$$\begin{bmatrix} P'_{\mathsf{on}}(n,t) \\ P'_{\mathsf{off}}(n,t) \end{bmatrix} = \cdots + \begin{bmatrix} -g(n) & f(n) \\ g(n) & -f(n) \end{bmatrix} \begin{bmatrix} P_{\mathsf{on}}(n,t) \\ P_{\mathsf{off}}(n,t) \end{bmatrix}$$