Exponential ergodicity of one-dimensional stochastic reaction networks

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Abstract

A stochastically modeled reaction network is a special class of continuous-time Markov chains that describes the stochastic dynamical behavior of biochemical reaction systems. In biology, the system is often approximated as a one-dimensional model to focus on the dynamics of a single species. Previous literature has classified several dynamical properties of one-dimensional stochastic reaction networks but did not address whether non-exponential ergodicity could exist. In this paper, we prove that every ergodic one-dimensional stochastically modeled reaction network with mass-action kinetics is exponentially ergodic. In other words, non-exponential ergodicity cannot exist in this case. Additionally, for the case of Michaelis-Menten kinetics, we classify the dynamical properties and show that non-exponentially ergodic cases may exist.

1 Introduction

Continuous-time Markov chains on a countable state space are widely used to describe various dynamical systems, including genetics, epidemiology, ecology, biochemistry, systems biology, sociophysics, and queueing theory [1, 2, 3, 4, 5, 6]. When the state space of a non-explosive continuous-time Markov chain X is finite and irreducible, the time evolution of the probability distribution of the process converges to a limiting distribution π, a stationary distribution, and in this case, X is ergodic. Furthermore, X on a finite irreducible state space admits exponential ergodicity, which means that the convergence of the probability distribution to π is exponentially fast in time.

While finite state spaces are commonly used, especially for interacting particle systems such as the standard Ising models, countably infinite state spaces often arise in stochastically modeled biochemical systems. For example, certain species can be continually produced in many biochemical systems. In this case, the existence of such a stationary distribution is not always guaranteed, and once it exists, the convergence rate is not necessarily exponential in time. Many studies have examined analytic criteria for the ergodicity and exponential ergodicity of continuous-time Markov chains on a countable state space [7, 8, 9, 10, 11].

In particular, we are interested in one-species reaction networks, where the reactions take the form $nA \to mA$ for two nonnegative integers, $n,\ m$. This kind of reaction network containing only a single species is often considered in biological examples [12, 13, 14, 15, 16]. For example, the biochemical reaction network (1) is known as Schlögl model, which represents various biochemical systems such as the phosphorylation-dephosphorylation cycle and cooperative self-activating genes.

$$
\begin{aligned}
2A &\underset{k_1}{\overset{k_2}{\rightleftharpoons}} 3A \\
0 &\underset{k_3}{\overset{k_4}{\rightleftharpoons}} A.
\end{aligned} \tag{1}
$$

Notably, various dynamical behaviors such as implosivity, explosivity, transience, null recurrence, positive recurrence, the convergence of quasi-stationary distribution, and exponential ergodicity have been almost fully classified for one-dimensional stochastic reaction networks [17]. Those dynamical properties could be classified by using only four parameters which are directly calculated from the network structure and reaction parameters, which is done by the mixture of Foster-Lyapunov-type results. Specifically, by methodically constructing several Lyapunov functions case-by-case and applying the Lyapunov-Foster theory, they found necessary and sufficient conditions for almost every dynamic property using those four parameters. However, only sufficient conditions for exponential ergodicity have been found. This has left the open question about the existence of a non-exponentially ergodic one-dimensional stochastic reaction network. In this paper, we mainly considered the missing piece in [17], by showing that every ergodic one-dimensional stochastic reaction network following mass-action kinetics is always exponentially ergodic. In other words, there does not exist non-exponentially ergodic one-dimensional stochastic reaction networks. In contrast, it is known that there are many non-exponentially ergodic reaction systems that contain more than one species [18, 19].

2 Stochastic reaction networks

2.1 Notations

For $x \in \mathbb{Z}^d$, we denote the ith component of x by $(x)_i$. The set of vectors in $\mathbb{Z}^d$ each of whose component is non-negative is denoted by $\mathbb{Z}^d_{\geq 0} = \{x \in \mathbb{Z}^d \ : \ (x)_i \geq 0 \text{ for each } i\}$. Let $X = \{X(t)\}_{t\geq 0}$ be a continuous-time Markov chain defined on a discrete state space $\mathbb{S} = \mathbb{Z}^d_{\geq 0}$. Throughout this paper, we consider only the case $d = 1$, which represents the dimension of the Markov chain and the number of species in the stochastic reaction networks. We denote the transition rate from state z to w by $q_{z,w}$ such that

$$q_{z,w} = \lim_{h\to 0} \frac{P(X(h) = w|X(0) = z)}{h} \geq 0, \tag{2}$$

and the total transition rate starting from state z is denoted by $q_z := \sum_{w\in\mathbb{S}} q_{z,w}$. We use $P^t(x, \cdot)$ to denote the probability distribution of $X(t)$ starting from state x. That is, for any subset $A \subseteq \mathbb{S}$, $P^t(x, A) = P(X(t) \in A|X(0) = x)$.

2.2 The basic model

Let $X = \{X(t)\}_{t\geq 0}$ be a continuous-time Markov chain defined on a discrete state space $\mathbb{S}$. Let $\mathcal{A}$ be the infinitesimal generator of X that is defined as

$$\mathcal{A}V(z) = \sum_w q_{z,w}(V(w) - V(z)) \ \text{ for a suitable function } \ V \ : \ \mathbb{S} \to \mathbb{R}. \tag{3}$$

Suppose that X admits a stationary distribution π on $\mathbb{S}$ such that

$$\pi(z) \sum_{w\in\mathbb{S}\setminus\{z\}} q_{z,w} = \sum_{w\in\mathbb{S}\setminus\{z\}} \pi(w)q_{w,z} \text{ for each } w \in \mathbb{S}. \tag{4}$$

Throughout this paper, assuming irreducibility of $\mathbb{S}$ and non-explosivity of X, we guarantee that for any initial distribution μ on $\mathbb{S}$, we have $\lim_{t\to\infty} P_\mu(X(t) \in A) = \pi(A)$ for any subset $A \subset \mathbb{S}$ [20]. The convergence rate of $P^t(x, \cdot)$ to π is measured with the total variation norm $||P^t(x, \cdot) - \pi(\cdot)||_{TV}$, where $||\mu - \nu||_{TV} = \sup_{A\subseteq\mathbb{S}} |\mu(A) - \nu(A)| = \frac{1}{2}\sum_{x\in\mathbb{S}} |\mu(x) - \nu(x)|$ for two probability measures $\mu,\ \nu$ on the same discrete measurable space [21]. We now define the ergodicity and exponential ergodicity of X.

Definition 2.1. A continuous-time Markov chain X on a discrete countable state space $\mathbb{S}$ is *ergodic* if $\mathbb{S}$ is irreducible and there exists a probability measure π such that for all $x \in \mathbb{S}$,

$$||P^t(x, \cdot) - \pi(\cdot)||_{TV} \to 0 \ \text{ as } \ t \to \infty. \tag{5}$$

X is *exponentially ergodic* if X is ergodic and there exists $\eta > 0$ such that for all $x \in \mathbb{S}$,

$$||P^t(x, \cdot) - \pi(\cdot)||_{TV} \leq B(x)e^{-\eta t} \ \text{ for all } \ t \geq 0. \tag{6}$$

for some function $B(x) \ : \ \mathbb{S} \to \mathbb{R}_{\geq 0}$. When X is ergodic with a unique stationary distribution π, if there exists $x \in \mathbb{S}$ such that (6) does not hold for any constant $B(x) > 0$ and $\eta > 0$, then X is *non-exponentially ergodic*.

2.3 Stochastic models for reaction networks

In this section, we introduce a stochastic process associated with reaction networks, which is often utilized in biochemistry when the copy numbers of species are small. Assuming the typical spatially well-mixed status of the chemical systems, the stochastic dynamics will be defined as a continuous-time Markov chain on $\mathbb{Z}^d_{\geq 0}$ to model the copy numbers of species in the biochemical systems.

First, each reaction $y \to y'$ is associated with an intensity function $\lambda_{y\to y'} : \mathbb{Z}^d \to \mathbb{R}_{\geq 0}$, which quantifies the expected time for the reaction to occur. It is natural to assume that $\lambda_{y\to y'}(x) > 0$ only if $x_i \geq y_i$ for all $i \in \mathbb{S}$. This means that $y \to y'$ can take place only if enough reacting species exist. Mass-action kinetics is the most common kinetics for defining $\lambda_{y\to y'}$, where the intensity of a reaction is proportional to the number of combinations of the present species engaged in the reaction. Specifically, $\lambda_{y\to y'}$ is defined under mass-action kinetic as

$$\lambda_{y\to y'}(x) = \kappa_{y\to y'}\lambda_y(x) \text{ where } \lambda_y(x) = \prod_{i=1}^{d} \frac{x_i!}{(x_i - y_i)!}\mathbf{1}_{x_i \geq y_i}, \tag{7}$$

for some positive parameter $\kappa_{y\to y'}$. A reaction network together with a choice of a set of parameters $\kappa = \{\kappa_{y\to y'} :$ there exists a reaction $y \to y'\}$ is called a *reaction system*.

For a reaction system, let $X = \{X(t)\}_{t\geq 0}$ be the associated continuous-time Markov chain. Then the transition rate from state z to state w is given by

$$q_{z,w} = \sum_{y\to y' : y'-y = w-z} \lambda_{y\to y'}(z). \tag{8}$$

Then, the infinitesimal generator $\mathcal{A}$ of X is given by

$$\mathcal{A}V(z) = \sum_z q_{z,w}(V(w) - V(z)) = \sum_{y\to y'} \lambda_{y\to y'}(z)(V(z + y' - y) - V(z)), \tag{9}$$

where $V : \mathbb{Z}^d_{\geq 0} \to \mathbb{R}$ [22]. Note that $q_{z,w} > 0$ for $z, w \in \mathbb{Z}^d_{\geq 0}$ if and only if there exists a reaction $y \to y'$ such that $w - z = y \to y'$ and $\lambda_{y\to y'}(z) = \kappa_{y\to y'}\lambda_y(z) > 0$

3 One-dimensional stochastic reaction networks

3.1 Notations

As in [17], we use four parameters α, β, γ, and R to fully classify the exponential ergodicity of stochastic reaction systems with a single species. These four parameters are defined by the structure of the reaction network and its reaction rates. More precisely, given $(\mathcal{S}, \mathcal{C}, \mathcal{R}, \kappa)$ a reaction system with $\mathcal{S} = \{A\}$, parameters are defined as follows:

- $R := \max_{r\in\mathcal{R}} m_r$.
- $\alpha := \sum_{m_r = R} \kappa_r(n_r - m_r)$.
- $\gamma := \sum_{m_r = R-1} \kappa_r(n_r - m_r)$.
- $\beta := \gamma - \frac{1}{2}\sum_{m_r = R} \kappa_r(n_r - m_r)^2$.

Here, R is the largest order of source complexes, which signifies the highest order among reactions. α is the weighted average of reaction vectors for reactions of order R, determining the mean drift of the associated Markov chain. And γ is the weighted average of reaction vectors for reactions of order $R-1$, determining the mean drift when $\alpha = 0$. When $\alpha = 0$, variance generated by reactions of order R also determines the qualitative dynamical properties together with γ. For this reason, we also consider β, which represents γ minus half of the variance of the drift.

3.2 Theorems

More generalized parameters were used in [17] to fully classify many qualitative properties of one-dimensional continuous-time Markov chains with polynomial reaction rates, including transience, recurrence, null recurrence, positive recurrence, and so on. In particular, for the ergodicity of one-dimensional stochastic reaction networks, [17] proved the following criteria.

Theorem 3.1 ([17]). *Let $(\mathcal{S}, \mathcal{C}, \mathcal{R}, \kappa)$ be a mass-action reaction system with $\mathcal{S} = \{A\}$, and X_t be the associated continuous-time Markov chain which is irreducible on an infinite state space $\mathbb{S} \in \mathbb{Z}_{\geq 0}$. X_t is positive recurrent if and only if one of the following holds:*

- $\alpha < 0$.
- $\alpha = 0$, $\beta < 0$, $R > 1$.
- $\alpha = \beta = 0$, $R > 2$.

However, for exponential ergodicity, they only suggested the following sufficient condition.

Theorem 3.2 ([17]). *Let $(\mathcal{S}, \mathcal{C}, \mathcal{R}, \kappa)$ be a mass-action reaction system with $\mathcal{S} = \{S\}$, and X_t be the associated continuous-time Markov chain which is irreducible on an infinite state space $\mathbb{S} \in \mathbb{Z}_{\geq 0}$. X_t is exponentially ergodic if one of the following holds:*

- $\alpha < 0$, $R \geq 1$.
- $\alpha = 0$, $\beta \leq 0$, $R > 2$.

Thus, to prove the exponential ergodicity of all ergodic one-dimensional reaction networks, it is necessary to address the following case: $\alpha = 0$, $\beta < 0$, and $R = 2$. This case is tricky because for $R \geq 3$, it must have strong inward drifts (that are more than quadratic) if it is ergodic, and for $R = 1$, only a few options for reaction networks so that it is easy to prove exponential ergodicity if it is ergodic. To deal with the case, we will introduce a critical chemical reaction with a single species, (10). Loosely speaking, (10) can be viewed as a simplification of all chemical reaction networks that belong to the class defined in Theorem 3.2.

$$A \underset{\kappa_2}{\overset{\kappa_1}{\rightleftharpoons}} 2A \underset{\kappa_1}{\longrightarrow} 3A. \tag{10}$$

Here, we assume $\kappa_1 > \kappa_2$ in order to provide that $\beta < 0$. The associated Markov chain is the birth and death process, so we can use the following criteria to show that it is exponentially ergodic.

Proposition 3.3 ([23]). *Let X_t be a non-explosive birth and death process. Then, X_t is exponentially ergodic if and only if*

$$q := \inf_{i \geq 0} q_i > 0 \quad \textit{and} \quad \delta := \sup_{i > 0} \sum_{j=0}^{i-1} \frac{1}{\mu_j b_j} \sum_{j=i}^{\infty} \mu_j < \infty.$$

where a_i, b_i are death rate and birth rate at state $i \in \mathbb{Z}_{\geq 0}$, respectively, and $\mu_i = b_0 b_1 \cdots b_{i-1}/a_1 a_2 \cdots a_i$ for $i \geq 1$.

Lemma 3.4. *Continuous-time Markov chains associated with (10) are exponentially ergodic.*

Finally, we will consider general one-dimensional stochastic reaction networks with $\alpha = 0$, $\beta < 0$, and $R = 2$. The following theorem is a classical criterion for exponential ergodicity.

Proposition 3.5 ([10]). *Let X_t be an irreducible non-explosive continuous-time Markov chain on countable state space $\mathbb{S}$, and H be an arbitrary nonempty finite subset of $\mathbb{S}$. Then the following statement holds:*

X_t is exponentially ergodic if and only if for some $\lambda > 0$ with $\lambda < q_i$ for all $i \in \mathbb{S}$, the system of inequalities

$$\begin{cases} y_i \geq 1, \quad i \in \mathbb{S}, \\ \sum q_{ij} y_j \leq -\lambda y_i, \quad i \notin H, \\ \sum_{i \in H} \sum_{j \neq i} q_{ij} y_j < \infty, \end{cases} \tag{11}$$

has a finite solution (y_i).

Note that Prop. 3.5 is exactly the condition of the existence of the Lyapunov function, where $V(i) = y_i$ for all $i \in \mathbb{S}$ in the above proposition. According to the above proposition, it remains to prove the existence of (y_i) and λ satisfying (11) for every reaction system with $\alpha = 0$, $\beta < 0$, and $R = 2$.

First of all, the third condition holds for every stochastic reaction network. Secondly, for every reaction system with the form of (10), there exists some (y_i) and λ satisfying (11). Moreover, for some $\lambda > 0$, $(E_i(e^{\lambda\tau_1}))$ is a finite solution to (11) with λ, where $\tau_1 := \inf\{t > 0 | X_t = 1\}$. Indeed, for each reaction system with $\alpha = 0$, $\beta < 0$, and $R = 2$, we can find suitable reaction system of the form of (10), so that $(E_i(e^{\lambda\tau_1}))$ is also a finite solution to (11) for the former reaction system. Thus we have our main theorem.

Theorem 3.6. *Let $(\mathcal{S}, \mathcal{C}, \mathcal{R}, \kappa)$ be a reaction system with $\mathcal{S} = \{A\}$, and X_t be the associated continuous-time Markov chain which is irreducible on an infinite state space $\mathbb{S} \in \mathbb{Z}_{\geq 0}$. If $\alpha = 0$, $\beta < 0$, and $R = 2$, then X_t is exponentially ergodic. In other words, every one-dimensional ergodic stochastic reaction network following mass-action kinetics is always exponentially ergodic.*

Remark 3.1. Foster-Lyapunov criteria are one of the most common approaches to showing ergodicity and exponential ergodicity of continuous-time Markov chains. The Foster-Lyapunov criteria is stated as follows:

Proposition 3.7. *[8, 24] Consider an irreducible Markov process on a countable state space. Then*

- *It is positive recurrent if and only if there exists a function $V : \mathbb{Z}^d_{\geq 0} \to \mathbb{R}_{\geq 0}$ such that $\mathcal{L}V(x) \leq -1$ for all but finitely many values of x.*
- *It is exponentially ergodic if and only if there exists a function $V : \mathbb{Z}^d_{\geq 0} \to \mathbb{R}_{\geq 0}$ with $V(x) \to \infty$ as $|x| \to \infty$, $c > 0$, $d < \infty$ such that $\mathcal{L}V(x) \leq -cV(x) + d$ for all x outside some compact set.*

While [17] has left the exponential ergodicity of a one-dimensional stochastic mass-action system unsolved, it provided a candidate for Lyapunov functions. We found that the exponential ergodicity of a one-dimensional mass-action system with $\alpha = 0$, $\beta < 0$, and $R = 2$ holds with one of the Lyapunov functions suggested by [17]. Specifically, if $V(x) = x^\delta$ for some $0 < \delta$, $\mathcal{L}V(x) \approx \delta x^\delta\{(\beta + \delta\theta) + O(x^{-1})\}$ for large x with some $\theta > 0$. Therefore, if we choose $\delta > 0$ small enough such that $\beta + \delta\theta < 0$, then $\mathcal{L}V(x) \approx \delta(\beta + \delta\theta)V(x) \leq -cV(x)$ for all large x with some $c > 0$. However, as we still believe the methodology we provided is meaningful, we provided an alternative proof. Indeed, our method can be used to study the exponential ergodicity of general Markov chains with non-polynomial transition rates (See Section 6).

4 Main Examples

In this section, we will show how to extend 3.4 to the general cases.

Example 4.1. Consider the following reaction system:

$$\begin{gathered} A \underset{1}{\overset{1/2}{\rightleftharpoons}} 2A \\ 3A \underset{1/3}{\longleftarrow} 2A \underset{1/3}{\longrightarrow} 4A. \end{gathered} \tag{12}$$

For this reaction system, $\alpha = 0$, $\beta = -\frac{5}{6}$, and $R = 2$. Let X_t be the associated Markov chain on $\mathbb{Z}_{\geq 1}$. Then X_t is irreducible. However, unlike the previous example, it is not a birth and death process. Thus, we cannot directly apply Prop. 3.3. Hence we need another approach, Prop. 3.5.

Let $H = \{1\}$. Since stochastic reaction networks have finitely many possible jumps, the third inequalities of (11) hold. So we need to find suitable $\lambda > 0$ and (y_i) with $y_i \geq 1$ satisfying the first and second inequalities of (11). For this purpose, let's consider the following reaction system:

$$A \underset{1}{\overset{1/2}{\rightleftharpoons}} 2A \underset{1}{\rightarrow} 3A. \tag{13}$$

(13) has the same mean drift as (12), but smaller variance. We can intuitively think that (13) has faster mixing than (12) so that exponential ergodicity of (13) implies exponential ergodicity of (12). We already proved that the associated

continuous-time Markov chain X_t on $\mathbb{Z}_{\geq 1}$ is exponentially ergodic. Hence $\mathbb{E}_i(e^{\lambda\tau_1}) < \infty$ for all $i \in \mathbb{Z}_{\geq 1}$ for some $\lambda > 0$, where τ_i is the first entrance time of i, that is, $\tau_i := \inf\{t \geq 0 : X_t = i\}$. Denote $y_i = \mathbb{E}_i(e^{\lambda\tau_1})$. Then for λ, (y_i) is a solution of (11). (Indeed, for the second condition, the equalities hold)

Returning to (12), we will show that (y_i) for (13) is also a solution of (11) for λ of (12) with some $\lambda > 0$. It suffices to show that for $i \geq 2$, $\sum_j q_{ij}y_j$ is smaller for (12) than (13). For (12),

$$\sum_j q_{ij}y_j = i(i-1)(y_{i-1}-y_i) + \left\{\frac{1}{3}i(i-1) + \frac{1}{2}i\right\}(y_{i+1}-y_i) + \frac{1}{3}i(i-1)(y_{i+2}-y_i) \quad \text{for} \quad i \geq 2. \tag{14}$$

For (13),

$$\sum_j q_{ij}y_j = i(i-1)(y_{i-1}-y_i) + \left\{i(i-1) + \frac{1}{2}i\right\}(y_{i+1}-y_i) \quad \text{for} \quad i \geq 2. \tag{15}$$

Consequently, for $i \geq 2$, we have

$$\begin{aligned}(15) - (14) &= \frac{2}{3}i(i-1)(y_{i+1}-y_i) - \frac{1}{3}i(i-1)(y_{i+2}-y_i) \\ &= \frac{2}{3}i(i-1)\left\{y_{i+1} - \frac{1}{2}(y_i + y_{i+2})\right\}.\end{aligned}$$

It remains to show that (15) − (14) ≥ 0 for large i, that is, (y_i) is concave for large i. By one-step analysis of (13), we have the following equalities:

$$\left\{2i(i+1) + \frac{1}{2}(i+1)\right\}y_{i+1} - i(i+1)y_i - \left\{i(i+1) + \frac{1}{2}(i+1)\right\}y_{i+2} = \lambda y_{i+1} \quad \text{for} \quad i \geq 2. \tag{16}$$

Since (y_i) is increasing,

$$\begin{aligned}&\left\{2i(i+1) + \frac{1}{2}(i+1)\right\}y_{i+1} - \left\{i(i+1) + \frac{1}{4}(i+1)\right\}y_i - \left\{i(i+1) + \frac{1}{4}(i+1)\right\}y_{i+2} \\ \geq &\left\{2i(i+1) + \frac{1}{2}(i+1)\right\}y_{i+1} - i(i+1)y_i - \left\{i(i+1) + \frac{1}{2}(i+1)\right\}y_{i+2} > 0 \quad \text{for} \quad i \geq 2.\end{aligned}$$

Thus, we have $y_{i+1} - \frac{1}{2}(y_i + y_{i+2}) > 0$ for $i \geq 2$.

Example 4.2. Lastly, consider the following reaction system:

$$\begin{aligned}&A \underset{1}{\overset{7/6}{\rightleftarrows}} 2A \\ &3A \underset{1/3}{\longleftarrow} 2A \underset{1/3}{\longrightarrow} 4A.\end{aligned} \tag{17}$$

For this reaction system, $\alpha = 0$, $\beta = -\frac{1}{6}$, and $R = 2$. Similarly to the previous example, let us also consider the following reaction system:

$$A \underset{1}{\overset{7/6}{\rightleftarrows}} 2A \underset{1}{\rightarrow} 3A. \tag{18}$$

For this reaction system, $\kappa_1 = 1 \leq \frac{7}{6} = \kappa_2$. Indeed, the associated continuous-time Markov chain on $\mathbb{Z}_{\geq 1}$ is not exponentially ergodic, moreover, not positive recurrent. Thus, the comparison method above cannot be directly applied. Instead of (18), let's consider the following reaction system:

$$A \underset{1}{\overset{7/6-\kappa}{\rightleftarrows}} 2A \underset{1}{\rightarrow} 3A, \tag{19}$$

where $\kappa > \frac{1}{6}$ to be determined. Then $y_i = \mathbb{E}_i(e^{\lambda\tau_1}) < \infty$ for some $\lambda > 0$ and for all $i \geq 1$. We will show that there exists such $\kappa > \frac{1}{6}$ such that $\sum_j q_{ij} y_j$ is smaller for (19) than (17) for large i. For (17),

$$\sum_j q_{ij} y_j = i(i-1)(y_{i-1} - y_i) + \left\{\frac{1}{3}i(i-1) + \frac{7}{6}i\right\}(y_{i+1} - y_i) + \frac{1}{3}i(i-1)(y_{i+2} - y_i) \quad \text{for} \quad i \geq 2. \tag{20}$$

For (19),

$$\sum_j q_{ij} y_j = i(i-1)(y_{i-1} - y_i) + \left\{i(i-1) + \left(\frac{7}{6} - \kappa\right)i\right\}(y_{i+1} - y_i) \quad \text{for} \quad i \geq 2. \tag{21}$$

Consequently, for $i \geq 2$, we have

$$\begin{aligned}
(21) - (20) &= \frac{2}{3}i(i-1)(y_{i+1} - y_i) - \frac{1}{3}i(i-1)(y_{i+2} - y_i) - \kappa i(y_{i+1} - y_i) \\
&= \frac{2}{3}i\left(i - 1 - \frac{3}{2}\kappa\right)(y_{i+1} - y_i) - \frac{1}{3}i(i-1)(y_{i+2} - y_i) \\
&= \frac{2}{3}i\left(i - 1 - \frac{3}{2}\kappa\right)(y_{i+1} - y_i) - \frac{1}{3}i(i-1)(y_{i+2} - y_{i+1} + y_{i+1} - y_i) \\
&= \frac{1}{3}i(i - 1 - 3\kappa)(y_{i+1} - y_i) - \frac{1}{3}i(i-1)(y_{i+2} - y_{i+1}) \\
&= \frac{1}{3}i\{(i - 1 - 3\kappa)(y_{i+1} - y_i) - (i-1)(y_{i+2} - y_{i+1})\}.
\end{aligned} \tag{22}$$

By one-step analysis of (19), we have the following inequalities:

$$\begin{aligned}
&\left\{2i(i+1) + (\frac{7}{6} - \kappa)(i+1)\right\} y_{i+1} - i(i+1)y_i - \left\{i(i+1) + \left(\frac{7}{6} - \kappa\right)(i+1)\right\} y_{i+2} \\
&= (i+1)\{i(y_{i+1} - y_i) - \{(i + \frac{7}{6} - \kappa)\}(y_{i+2} - y_{i+1})\} = \lambda y_{i+1} > 0 \quad \text{for} \quad i \geq 2.
\end{aligned}$$

Hence we have

$$i(y_{i+1} - y_i) - \{(i + \frac{7}{6} - \kappa)\}(y_{i+2} - y_{i+1}) > 0. \tag{23}$$

By plugging (23) into (22), it is straightforward that for $\frac{1}{6} < \kappa < \frac{7}{24}$, (22) ≥ 0 for large i.

5 Proof of Theorems

Proof of Lemma 3.4. Let X_t be the associated Markov chain on $\mathbb{Z}_{\geq 1}$. Then X_t is a birth and death process. Moreover, since ergodicity implies non-explosivity, we can apply Prop. 3.3 to prove exponential ergodicity of X_t. It is sufficient to prove the exponential ergodicity of $Y_t := X_t - 1$. We denote the transition rates of Y_t from i to j by q_{ij} for $i, j \in \mathbb{Z}_{\geq 0}$. Then $a_i := q_{i,i-1} = \kappa_1 i(i+1)$, and $b_i := q_{i,i+1} = (\kappa_1 i + \kappa_2)(i+1)$ for $i \in \mathbb{Z}_{\geq 0}$.

$q := \inf_{i \geq 0} q_i$ is positive since $q \geq \min(\kappa_1, \kappa_2) > 0$. Now, it remains to show that $\delta < \infty$. We have $\mu_i = \dfrac{(i - 1 + (\kappa_2/\kappa_1))!}{\kappa_1 (i+1)!}$. Hence we have

$$\delta = \sup_{i>0} \sum_{j=0}^{i-1} \frac{j!}{(j + (\kappa_2/\kappa_1))!} \sum_{j=i}^{\infty} \frac{(j - 1 + (\kappa_2/\kappa_1))!}{\kappa_1 (j+1)!} \tag{24}$$

$$= \frac{1}{\kappa_1} \sup_{i>0} \sum_{j=0}^{i-1} \frac{\Gamma(j+1)}{\Gamma(j + 1 + (\kappa_2/\kappa_1))} \sum_{j=i}^{\infty} \frac{\Gamma(j + (\kappa_2/\kappa_1))}{\Gamma(j+2)}. \tag{25}$$

It is straightforward to verify that for each finite $i \in \mathbb{Z}_{\geq 0}$,

$$\sum_{j=0}^{i-1} \frac{\Gamma(j+1)}{\Gamma(j+1+(\kappa_2/\kappa_1))} \sum_{j=i}^{\infty} \frac{\Gamma(j+(\kappa_2/\kappa_1))}{\Gamma(j+2)} < \infty.$$

Hence it suffices to show that

$$\lim_{i\to\infty} \sum_{j=0}^{i-1} \frac{\Gamma(j+1)}{\Gamma(j+1+(\kappa_2/\kappa_1))} \sum_{j=i}^{\infty} \frac{\Gamma(j+(\kappa_2/\kappa_1))}{\Gamma(j+2)} < \infty.$$

By Stirling's formula, we have the following approximations:

$$\sum_{j=0}^{i-1} \frac{\Gamma(j+1)}{\Gamma(j+1+(\kappa_2/\kappa_1))} \approx i^{1-(\kappa_2/\kappa_1)}, \quad \text{and} \quad \sum_{j=i}^{\infty} \frac{\Gamma(j+(\kappa_2/\kappa_1))}{\Gamma(j+2)} \approx i^{(\kappa_2/\kappa_1)-1} \quad \text{as} \quad i \to \infty.$$

Thus,

$$\sum_{j=0}^{i-1} \frac{\Gamma(j+1)}{\Gamma(j+1+(\kappa_2/\kappa_1))} \sum_{j=i}^{\infty} \frac{\Gamma(j+(\kappa_2/\kappa_1))}{\Gamma(j+2)} = O(1) \quad \text{as } i \to \infty.$$

□

Proof of Thm. 3.6. Since $R = 2$, $\mathcal{R}$ can be written as follows:

$$\begin{aligned}
\mathcal{R} =&\{2A \xrightarrow{\kappa^+_{2j}} (2+m^+_{2j})A : j = 1,2,\dots,M^+_2\} \\
&\cup\{2A \xrightarrow{\kappa^-_{2j}} (2-m^-_{2j})A : j = 1,2,\dots,M^-_2\} \\
&\cup\{A \xrightarrow{\kappa^+_{1j}} (1+m^+_{1j})A : j = 1,2,\dots,M^+_1\} \\
&\cup\{A \xrightarrow{\kappa^-_{1j}} (1-m^-_{1j})A : j = 1,2,\dots,M^-_1\} \\
&\cup\{0 \xrightarrow{\kappa^+_{0j}} (m^+_{0j})A : j = 1,2,\dots,M^+_0\},
\end{aligned} \tag{26}$$

where $m^\pm_{l1} < m^\pm_{l2} < \cdots < m^\pm_{lM^\pm_l}$ for $l = 0,1,2$. Here, $\alpha = 0$ implies that $\sum_j \kappa^+_{2j} m^+_{2j} = \sum_j \kappa^-_{2j} m^-_{2j}$. For simplicity, we will assume that $\sum_j \kappa^+_{2j} m^+_{2j} = \sum_j \kappa^-_{2j} m^-_{2j} = 1$.

Let $(\mathcal{S}, \mathcal{C}', \mathcal{R}', \kappa')$ be the following reaction network:

$$A \underset{\kappa^*}{\overset{1}{\rightleftarrows}} 2A \xrightarrow{1} 3A, \tag{27}$$

where $0 < \kappa^* < 1$ to be determined. Lemma 3.4 implies that there exists $\lambda > 0$ such that $y_i := \mathbb{E}_i(e^{\lambda\tau_1}) < \infty$ for all $i \in \mathbb{Z}_{\geq 1}$(see [25, Proposition 12]).

Indeed, (y_i) with λ solves (11) with equality for the second line. (If the state space of X_t contains 0, define $y_0 := 1$.) Clearly, $y_i \geq 1$ for all $i \in \mathbb{Z}_{\geq 1}$. Actually, the equality of second line of (11) is equivalent to one-step analysis for $y_i := \mathbb{E}_i(e^{\lambda\tau_1})$ for $i \geq 2$. More precisely,

$$i(i-1)(y_i - y_{i-1}) - \lambda y_i = i(i-1+\kappa^*)(y_{i+1} - y_i) \quad \text{for} \quad i \geq 2. \tag{28}$$

Denote transition rates for $(\mathcal{S}, \mathcal{C}, \mathcal{R}, \kappa)$ and $(\mathcal{S}, \mathcal{C}', \mathcal{R}', \kappa')$ by (q_{ij}) and (q'_{ij}) respectively. Our goal is to show that

$$\sum q_{ij} y_j \leq \sum q'_{ij} y_j = -\lambda y_i, \tag{29}$$

for sufficiently large $i \in \mathbb{Z}_{\geq 0}$. Hence it suffices to show that

$$\sum q'_{ij} y_j - \sum q_{ij} y_j \geq 0, \tag{30}$$

for sufficiently large $i \in \mathbb{Z}_{\geq 0}$. For $i \geq 2$, we have

$$\begin{aligned}\sum q'_{ij}y_j - \sum q_{ij}y_j &= i(i-1)(y_{i+1}-y_i) + i(i-1)(y_{i-1}-y_i) + \kappa^* i(y_{i+1}-y_i)\\ &- \{\sum_j \kappa_{2j}^+ i(i-1)(y_{i+m_{2j}^+}-y_i) + \sum_j \kappa_{2j}^- i(i-1)(y_{i-m_{2j}^-}-y_i) + \sum_j \kappa_{1j}^+ i(y_{i+m_{1j}^+}-y_i)\\ &+ \sum_j \kappa_{1j}^- i(y_{i+m_{1j}^-}-y_i) + \sum_j \kappa_{0j}^+ (y_{i+m_{0j}^+}-y_i)\}.\end{aligned}$$

By rearranging the terms, we derive the following:

$$\begin{aligned}\sum q'_{ij}y_j - \sum q_{ij}y_j &= i(i-1)\{(y_{i+1}-y_i) - \sum_j \kappa_{2j}^+ (\sum_{k=1}^{m_{2j}^+}(y_{i+k}-y_{i+k-1}))\}\\ &+ i(i-1)\{(y_{i-1}-y_i) - \sum_j \kappa_{2j}^- (\sum_{k=1}^{m_{2j}^-}(y_{i-k}-y_{i-k+1}))\}\\ &+ i\{\kappa^*(y_{i+1}-y_i) - \sum_j \kappa_{1j}^+ (\sum_{k=1}^{m_{1j}^+}(y_{i+k}-y_{i+k-1})) - \sum_j \kappa_{1j}^- (\sum_{k=1}^{m_{1j}^-}(y_{i-k}-y_{i-k+1}))\}\\ &- \sum_j \kappa_{0j}^+ (\sum_{k=1}^{m_{0j}^+}(y_{i+k}-y_{i+k-1})).\end{aligned}$$

And then by using $\sum_j \kappa_{2j}^+ m_{2j}^+ = \sum_j \kappa_{2j}^- m_{2j}^- = 1$,

$$\begin{aligned}\sum q'_{ij}y_j - \sum q_{ij}y_j &= \{\sum_{j=1}^{M_2^+} \sum_{m_{2(j-1)}^+ < m \leq m_{2j}^+} (\sum_{n=j}^{M_2^+} \kappa_{2n}^+) i(i-1)\{(y_{i+1}-y_i) - (y_{i+m}-y_{i+m-1})\}\\ &+ \{\sum_{j=1}^{M_2^-} \sum_{m_{2(j-1)}^- < m \leq m_{2j}^-} (\sum_{n=j}^{M_2^-} \kappa_{2n}^-) i(i-1)\{(y_{i-1}-y_i) - (y_{i-m}-y_{i-m+1})\}\}\\ &+ i\{\kappa^*(y_{i+1}-y_i) - \sum_j \kappa_{1j}^+ (\sum_{k=1}^{m_{1j}^+}(y_{i+k}-y_{i+k-1})) - \sum_j \kappa_{1j}^- (\sum_{k=1}^{m_{1j}^-}(y_{i-k}-y_{i-k+1}))\}\\ &- \sum_j \kappa_{0j}^+ (\sum_{k=1}^{m_{0j}^+}(y_{i+k}-y_{i+k-1})).\end{aligned} \tag{31}$$

Here, we will use two inequalities derived from (28).

$$y_{i+1} - y_i > y_{i+2} - y_{i+1}, \tag{32}$$

$$i(i+1)(y_{i+1}-y_i) > (i+\kappa^*)(i+1)(y_{i+2}-y_{i+1}). \tag{33}$$

By plugging (32) into last two lines of (31),

$$\begin{aligned}\sum q'_{ij}y_j - \sum q_{ij}y_j &> \{\sum_{j=1}^{M_2^+} \sum_{m_{2(j-1)}^+ < m \leq m_{2j}^+} (\sum_{n=j}^{M_2^+} \kappa_{2n}^+) i(i-1)\{(y_{i+1}-y_i) - (y_{i+m}-y_{i+m-1})\}\\ &+ \{\sum_{j=1}^{M_2^-} \sum_{m_{2(j-1)}^- < m \leq m_{2j}^-} (\sum_{n=j}^{M_2^-} \kappa_{2n}^-) i(i-1)\{(y_{i-1}-y_i) - (y_{i-m}-y_{i-m+1})\}\}\\ &+ i\{\kappa^* - \sum_j \kappa_{1j}^+ m_{1j}^+ + \sum_j \kappa_{1j}^- m_{1j}^-\}(y_{i+1}-y_i) - \sum_j \kappa_{0j}^+ m_{0j}^+ (y_{i+1}-y_i).\end{aligned} \tag{34}$$

From (33), we can easily induce that for each $0 < \kappa^{**} < \kappa^*$ and $m \geq 1$,

$$\begin{aligned} i\{i-1-(m-1)\kappa^{**}\}(y_{i+1}-y_i) &> i(i-1)(y_{i+m}-y_{i+m-1}) \\ i\{i-1-(m-1)\kappa^{**}\}(y_{i-1}-y_i) &> i(i-1)(y_{i-m}-y_{i-m+1}), \end{aligned} \tag{35}$$

for large i. Take arbitrary $0 < \kappa^{**} < \kappa^*$ to be determined, and modify (34) as follows:

$$\begin{aligned} \sum q'_{ij}y_j - \sum q_{ij}y_j > &\{\sum_{j=1}^{M_2^+} \sum_{m^+_{2(j-1)} < m \leq m^+_{2j}} (\sum_{n=j}^{M_2^+} \kappa^+_{2n})\{i\{i-1-(m-1)\kappa^{**}\}(y_{i+1}-y_i) - i(i-1)(y_{i+m}-y_{i+m-1})\} \\ &+ \{\sum_{j=1}^{M_2^-} \sum_{m^-_{2(j-1)} < m \leq m^-_{2j}} (\sum_{n=j}^{M_2^-} \kappa^-_{2n})\{i\{i-1-(m-1)\kappa^{**}\}(y_{i-1}-y_i) - i(i-1)(y_{i-m}-y_{i-m+1})\}\} \\ &- (1-\frac{1}{2}\{\sum_j \kappa^+_{2j}(m^+_{2j})^2 + \sum_j \kappa^-_{2j}(m^-_{2j})^2\})i\kappa^{**}(y_{i+1}-y_i) \\ &+ i\{\kappa^* - \sum_j \kappa^+_{1j}m^+_{1j} + \sum_j \kappa^-_{1j}m^-_{1j}\}(y_{i+1}-y_i) - \sum_j \kappa^+_{0j}m^+_{0j}(y_{i+1}-y_i). \end{aligned} \tag{36}$$

The first two lines are positive for sufficiently large i by (35). Furthermore, by definitions, the last two lines are equal to

$$[i\{\kappa^* - \gamma - \kappa^{**} + \frac{1}{2}\{\sum_j \kappa^+_{2j}(m^+_{2j})^2 + \sum_j \kappa^-_{2j}(m^-_{2j})^2\}\kappa^{**}\} - \sum_j \kappa^+_{0j}m^+_{0j}](y_{i+1}-y_i). \tag{37}$$

For the formula to be positive for large i, it suffices to determine suitable κ^* and κ^{**} satisfying

$$\kappa^* - \gamma - \kappa^{**} + \frac{1}{2}\{\sum_j \kappa^+_{2j}(m^+_{2j})^2 + \sum_j \kappa^-_{2j}(m^-_{2j})^2\}\kappa^{**} > 0. \tag{38}$$

Since $\beta = \gamma - \frac{1}{2}\{\sum_j \kappa^+_{2j}(m^+_{2j})^2 + \sum_j \kappa^-_{2j}(m^-_{2j})^2\} < 0$, we can choose positive constants κ^* and κ^{**} such that

$$\gamma < \kappa^{**}\frac{1}{2}\{\sum_j \kappa^+_{2j}(m^+_{2j})^2 + \sum_j \kappa^-_{2j}(m^-_{2j})^2\}, \tag{39}$$

and $\kappa^{**} < \kappa^* < 1$. □

By the proof of Thm. 3.6, we conclude that a one-dimensional stochastic mass-action reaction network with $\alpha = 0$, $\beta < 0$, and $R = 2$ is exponentially ergodic. Since $\alpha = 0$, $\beta < 0$, and $R = 2$ is the only remaining piece for the existence of non-exponential ergodicity, we conclude that every one-dimensional ergodic stochastic mass-action reaction network is always exponentially ergodic. However, mass-action kinetics is not the only choice, especially if we consider whether it is biologically meaningful. Therefore, in the following section, we will consider the Michaelis-Menten kinetics, the other kinetic law which is more biologically meaningful.

6 Exponential ergodicity of one-dimensional Michaelis-Menten kinetics

We now consider stochastic reaction networks following Michaelis-Menten kinetics without cooperativity, which is commonly used in many biochemical systems. Under this kinetic law, $\lambda_{cA\to dA}$ is defined as

$$\lambda_{cA\to dA}(x) = \frac{V_{max}x^c}{(K_m+x)^c}. \tag{40}$$

Notably, $\lim_{x\to\infty}\lambda_{cA\to dA}(x) = V_{max}$, meaning that it could be considered as a zero-order reaction. As a toy example, let us consider the following stochastic reaction network, which is a birth-death process.

$$\begin{aligned} c_1 A &\xrightarrow{V_1} (c_1-1)A \\ c_2 A &\xrightarrow{V_2} (c_2+1)A. \end{aligned} \tag{41}$$

First, let us assume $V_1 > V_2$. Then, by denoting i as a state with $i+1$ copy number of A, we get

$$\begin{aligned} a_i &= \frac{V_1(i+1)^{c_1}}{(K_1+i+1)^{c_1}} \ \text{ for } \ i \geq 1, \\ a_0 &= 0, \\ b_i &= \frac{V_2(i+1)^{c_2}}{(K_2+i+1)^{c_2}} \ \text{ for } \ i \geq 0, \\ \mu_i &= (\frac{V_2}{V_1})^i \prod_{j=0}^{i-1}(1+\frac{K_1}{j+2})^{c_1}(1+\frac{K_2}{j+1})^{-c_2} \\ &= (\frac{V_2}{V_1})^i \frac{(K_1+2)^{c_1}}{(K_2+1)^{c_2}}(\frac{\Gamma(K_1+i+2)}{\Gamma(K_1+3)\Gamma(i+2)})^{c_1}(\frac{\Gamma(K_2+2)\Gamma(i+1)}{\Gamma(K_2+i+1)})^{c_2}. \end{aligned} \tag{42}$$

It is obvious that $q := \inf_{i\geq 0}(a_i+b_i) > 0$. Therefore, in order to check exponential ergodicity using Prop. 3.3, it suffices to check whether $\delta := \sup_{i>0}\sum_{j=0}^{i-1}\frac{1}{\mu_j b_j}\sum_{j=i}^{\infty}\mu_j < \infty$. We could easily check that if i is finite, then $\sum_{j=0}^{i-1}\frac{1}{\mu_j b_j}\sum_{j=i}^{\infty}\mu_j$ is also finite. If $i\to\infty$,

$$\begin{aligned} \sum_{j=i}^{\infty}\mu_j &= \frac{(K_1+2)^{c_1}}{(K_2+1)^{c_2}}\frac{(\Gamma(K_2+2))^{c_2}}{(\Gamma(K_1+3))^{c_1}}\sum_{j=i}^{\infty}(\frac{V_2}{V_1})^j(\frac{\Gamma(j+2+K_1)}{\Gamma(j+2)})^{c_1}(\frac{\Gamma(j+1)}{\Gamma(j+1+K+2)})^{c_2} \\ &\approx \frac{(K_1+2)^{c_1}}{(K_2+1)^{c_2}}\frac{(\Gamma(K_2+2))^{c_2}}{(\Gamma(K_1+3))^{c_1}}\sum_{j=i}^{\infty}(\frac{V_2}{V_1})^j(j+2)^{K_1c_1}(j+1)^{-K_2c_2} \\ &\approx (\frac{V_2}{V_1})^i i^{K_1c_1-K_2c_2}, \end{aligned} \tag{43}$$

and

$$\begin{aligned} \sum_{j=0}^{i-1}\frac{1}{\mu_j b_j} &= \frac{1}{V_2}\frac{(K_2+1)^{c_2}}{(K_1+2)^{c_1}}\frac{(\Gamma(K_1+3))^{c_1}}{(\Gamma(K_2+2))^{c_2}}\sum_{j=0}^{i-1}(\frac{V_1}{V_2})^j(1+\frac{K_2}{j+1})^{c_2}(\frac{\Gamma(j+2)}{\Gamma(K_1+j+2)})^{c_1}(\frac{\Gamma(K_2+j+1)}{\Gamma(j+1)})^{c_2} \\ &\approx \sum_{j=0}^{i-1}(1+K_2)^{c_2}(\frac{V_1}{V_2})^j(j+2)^{-K_1c_1}(j+1)^{K_2c_2} \\ &\approx (\frac{V_1}{V_2})^i i^{K_2c_2-K_1c_1}, \end{aligned} \tag{44}$$

so we get,

$$\sum_{j=0}^{i-1}\frac{1}{\mu_j b_j}\sum_{j=i}^{\infty}\mu_j = O(1) \ \text{ as } \ i\to\infty. \tag{45}$$

Therefore, by Prop. 3.3, (41) is exponentially ergodic if $V_1 > V_2$.

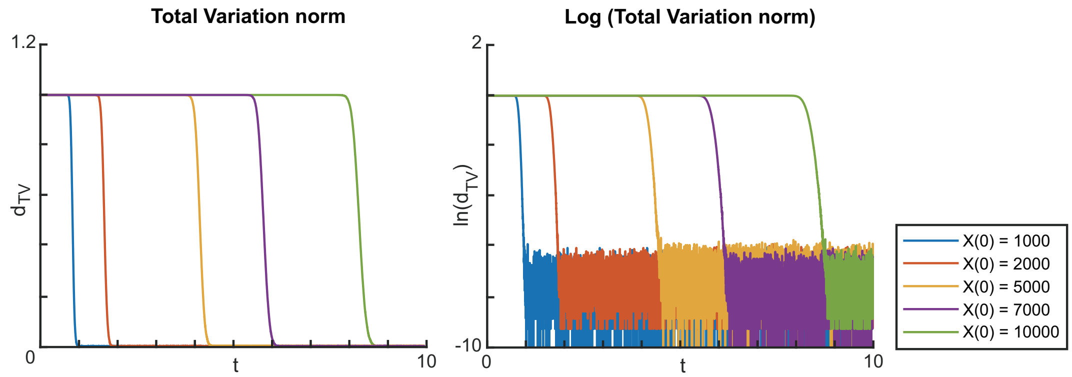

Figure 1: $||P^t, \pi||_{TV}$ (left) and $log(||P^t, \pi||_{TV})$ (right) of (41) with $V_1 = 1.2$, $V_2 = 2.4$, $K_1 = K_2 = 2$, $c_1 = c_2 = 3$ by changing the initial value $X(0)$. The left plot exhibits the cutoff phenomena. In the right plot, every line has the same slope, even though changing the initial copy number of A. Simulated 50,000 times each to numerically generate the probability distribution.

If $V_1 = V_2$, we need to consider two cases

- $K_1c_1 - K_2c_2 \geq -1$: $\sum_{j=i}^{\infty} \mu_j = \infty$ for finite i, therefore $\delta = \infty$ and not exponentially ergodic.
- $K_1c_1 - K_2c_2 < -1$: $\sum_{j=i}^{\infty} \mu_j < \infty$ for finite i. If $i \to \infty$,

$$\begin{aligned}\sum_{j=i}^{\infty} \mu_j &\approx i^{K_1c_1 - K_2c_2 + 1}, \\ \sum_{j=0}^{i-1} \frac{1}{\mu_j b_j} &\approx i^{-K_1c_1 + K_2c_2 + 1},\end{aligned} \tag{46}$$

therefore, $\sum_{j=0}^{i-1} \frac{1}{\mu_j b_j} \sum_{j=i}^{\infty} \mu_j = O(i^2)$ as $i \to \infty$, so $\delta = \infty$ and not exponentially ergodic.

If $V_1 < V_2$, then it is obviously transient and not exponentially ergodic.

Proposition 6.1 ([26, 20]). *A birth-death process is*

- ***Ergodic*** *if and only if*

$$\sum_{i=1}^{\infty} \prod_{n=1}^{i} \frac{a_n}{b_n} = \infty \;\; \textit{and} \;\; \sum_{i=1}^{\infty} \prod_{n=1}^{i} \frac{b_{n-1}}{a_n} < \infty. \tag{47}$$

- ***Null-recurrent*** *if and only if*

$$\sum_{i=1}^{\infty} \prod_{n=1}^{i} \frac{a_n}{b_n} = \infty \;\; \textit{and} \;\; \sum_{i=1}^{\infty} \prod_{n=1}^{i} \frac{b_{n-1}}{a_n} = \infty. \tag{48}$$

- ***Transient*** *if and only if*

$$\sum_{i=1}^{\infty} \prod_{n=1}^{i} \frac{a_n}{b_n} < \infty. \tag{49}$$

To check ergodicity of (41) when $V_1 = V_2$,

$$\begin{aligned}\sum_{i=1}^{\infty} \prod_{n=1}^{i} \frac{a_n}{b_n} &= \sum_{i=1}^{\infty} \prod_{n=1}^{i} \frac{(n+1)^{c_1}}{(K_1+n+1)^{c_1}} \frac{(K_2+n+1)^{c_2}}{(n+1)^{c_2}} \approx \sum_{i=1}^{\infty} (i+2)^{-K_1c_1+K_2c_2}, \\ \sum_{i=1}^{\infty} \prod_{n=1}^{i} \frac{b_{n-1}}{a_n} &= \sum_{i=1}^{\infty} \prod_{n=1}^{i} \frac{(K_1+n+1)^{c_1}}{(n+1)^{c_1}} \frac{n^{c_2}}{(K_2+n)^{c_2}} \approx \sum_{i=1}^{\infty} (i+2)^{c_1K_1} (i+1)^{-c_2K_2}.\end{aligned} \tag{50}$$

Using 6.1, we split into three cases.

- $1 < -K_1c_1 + K_2c_2 : \sum_{i=1}^{\infty} \prod_{n=1}^{i} \frac{a_n}{b_n} = \infty$ and $\sum_{i=1}^{\infty} \prod_{n=1}^{i} \frac{b_{n-1}}{a_n} < \infty$, therefore positive recurrent.
- $-1 \leq -K_1c_1 + K_2c_2 \leq 1 : \sum_{i=1}^{\infty} \prod_{n=1}^{i} \frac{a_n}{b_n} = \infty$ and $\sum_{i=1}^{\infty} \prod_{n=1}^{i} \frac{b_{n-1}}{a_n} = \infty$, therefore null recurrent.
- $-K_1c_1 + K_2c_2 < -1 : \sum_{i=1}^{\infty} \prod_{n=1}^{i} \frac{a_n}{b_n} < \infty$, therefore transient.

The classification of dynamical properties is summarized in Table 1.

$V_1 < V_2$	$V_1 = V_2$			$V_1 > V_2$
	$-K_1c_1 + K_2c_2 < -1$	$-1 \leq -K_1c_1 + K_2c_2 \leq 1$	$1 < -K_1c_1 + K_2c_2$	
Transient	Transient	Null recurrent	Non-exponentially ergodic	Exponentially ergodic

Table 1: Classification of dynamics of birth-death process with Michaelis-Menten kinetics (41)

7 Discussion

In this paper, we showed that for one-dimensional stochastic reaction networks following mass-action kinetics, ergodic reaction networks are always exponentially ergodic. From the definition of exponential ergodicity, we observed that

$$log(||P^t(x,\cdot) - \pi(\cdot)||_{TV}) \leq -\eta t + log(B(x)) \text{ for all } t \geq 0. \tag{51}$$

In other words, $log(||P^t, \pi)||_{TV})$ decreases linearly with the slope η, where the initial distribution x determines the y-intercept. Therefore, if we simulate the stochastic reaction network by changing the initial distribution, every $log(||P^t, \pi)||_{TV})$ can be bounded by a linear function with the same slope η for each initial condition. This can be easily validated through numerical simulation via Gillespie's algorithm [27]. For example, Fig. 2 shows the plot of $log(||P^t, \pi)||_{TV})$ by varying initial values of the example (1) with mass-action kinetics. We could observe that the slope is independent of the initial copy number.

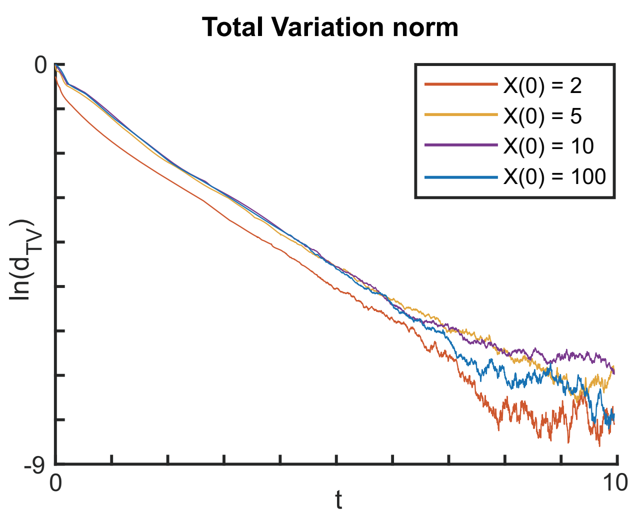

Figure 2: $log(||P^t, \pi||_{TV})$ of (1) by changing the initial value $X(0)$. Every plot has the same slope, even though changing the initial copy number of A. Simulated 50,000 times each to numerically generate the probability distribution.

As another example, consider the following stochastic reaction network associated with mass-action kinetics

$$A \xrightarrow{\kappa_1} 2A \xrightarrow{\kappa_2} 3A \xrightarrow{\kappa_3} A. \tag{52}$$

Example (52) is ergodic by Thm 3.1. Therefore, by Thm 3.6, (52) is exponentially ergodic. The plot of $log(||P^t, \pi)||_{TV})$ for this example is in Fig. 3.

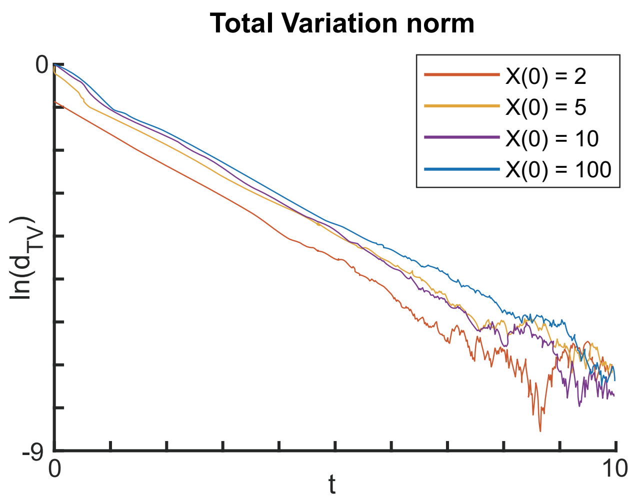

Figure 3: $log(||P^t, \pi||_{TV})$ of (52) by changing the initial value $X(0)$. Every plot has the same slope, even though changing the initial copy number of A. Simulated 50,000 times each to numerically generate the probability distribution.

For two-dimensional stochastic reaction networks, there exists both exponential and non-exponential ergodic stochastic reaction networks [18, 11].

$$\begin{aligned} 0 &\underset{1}{\overset{1}{\rightleftharpoons}} A + B \\ B &\underset{1}{\overset{1}{\rightleftharpoons}} 2B. \end{aligned} \tag{53}$$

Example (53) is known to exhibit non-exponential ergodicity. On the other hand, the following example (54) is known to exhibit exponential ergodicity.

$$\begin{gathered} 0 \underset{1}{\overset{1}{\rightleftharpoons}} A \\ 0 \underset{1}{\overset{1}{\rightleftharpoons}} B \\ 0 \xrightarrow{1} 2A + B \xrightarrow{1} 3A + 2B \xrightarrow{1} 0. \end{gathered} \tag{54}$$

Unlike a one-dimensional stochastic mass-action system, a two-dimensional stochastic mass-action system could exhibit either exponential or non-exponential ergodicity. This shows that there could be some bifurcation structure for the exponential and non-exponential ergodicity. It would be interesting to further analyze the bifurcation structure of exponential and non-exponential ergodicity.

Another interesting part is the cutoff phenomena, the phenomenon that the total variation norm suddenly decreases at some time point, described in Fig. 1. While the cutoff phenomena have been analyzed in various works [28, 29, 30], it has not been investigated in stochastic reaction networks. It would be another challenge to analyze the cutoff phenomena in stochastic reaction networks and determine how it is related to the parameters and orders of Michaelis-Menten kinetics. Additionally, the phase transition between exponential ergodicity and non-exponential ergodicity in Michaelis-Menten kinetics would be another interesting aspect to investigate.

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References

[1] Warren John Ewens. *Mathematical population genetics: theoretical introduction*, volume 27. Springer, 2004.

[2] Romualdo Pastor-Satorras, Claudio Castellano, Piet Van Mieghem, and Alessandro Vespignani. Epidemic processes in complex networks. *Reviews of modern physics*, 87(3):925–979, 2015.

[3] CW Gardiner. Handbook of stochastic methods for physics, chemistry, and the natural sciences springer. *Berlin (4th Ed)*, 2009.

[4] Darren J Wilkinson. *Stochastic modelling for systems biology*. Chapman and Hall/CRC, 2018.

[5] Wolfgang Weidlich and Günter Haag. *Concepts and models of a quantitative sociology: The dynamics of interacting populations*, volume 14. Springer Science & Business Media, 2012.

[6] John F Shortle, James M Thompson, Donald Gross, and Carl M Harris. *Fundamentals of queueing theory*, volume 399. John Wiley & Sons, 2018.

[7] Persi Diaconis. The mathematics of mixing things up. *Journal of Statistical Physics*, 144(3):445–458, 2011.

[8] Sean P Meyn and Richard L Tweedie. Stability of markovian processes iii: Foster–lyapunov criteria for continuous-time processes. *Advances in Applied Probability*, 25(3):518–548, 1993.

[9] Chen Mufa. Exponential l 2-convergence and l 2-spectral gap for markov processes. *Acta Mathematica Sinica*, 7(1):19–37, 1991.

[10] Richard L Tweedie. Criteria for ergodicity, exponential ergodicity and strong ergodicity of markov processes. *Journal of Applied Probability*, 18(1):122–130, 1981.

[11] David F Anderson, Daniele Cappelletti, Wai-Tong Louis Fan, and Jinsu Kim. A new path method for exponential ergodicity of markov processes on z d, with applications to stochastic reaction networks. *arXiv Preprint*, 2023.

[12] Melissa Vellela and Hong Qian. Stochastic dynamics and non-equilibrium thermodynamics of a bistable chemical system: the schlögl model revisited. *Journal of The Royal Society Interface*, 6(39):925–940, 2009.

[13] Shay Be'er and Michael Assaf. Rare events in stochastic populations under bursty reproduction. *Journal of Statistical Mechanics: Theory and Experiment*, 2016(11):113501, 2016.

[14] Xian Chen and Chen Jia. Limit theorems for generalized density-dependent markov chains and bursty stochastic gene regulatory networks. *Journal of Mathematical Biology*, 80(4):959–994, 2020.

[15] Michael C Mackey, Marta Tyran-Kaminska, and Romain Yvinec. Dynamic behavior of stochastic gene expression models in the presence of bursting. *SIAM Journal on Applied Mathematics*, 73(5):1830–1852, 2013.

[16] Vahid Shahrezaei and Peter S Swain. Analytical distributions for stochastic gene expression. *Proceedings of the National Academy of Sciences*, 105(45):17256–17261, 2008.

[17] Chuang Xu, Mads Christian Hansen, and Carsten Wiuf. Full classification of dynamics for one-dimensional continuous-time markov chains with polynomial transition rates. *Advances in Applied Probability*, pages 1–35, 2022.

[18] Minjoon Kim and Jinsu Kim. A path method for non-exponential ergodicity of markov chains and its application for chemical reaction systems, 2024.

[19] Wai-Tong Louis Fan, Jinsu Kim, and Chaojie Yuan. Boundary-induced slow mixing for markov chains and its application to stochastic reaction networks, 2024.

[20] S Norris. Markov chains, 1997.

[21] DA Levin and Y Peres. Markov chains and mixing times american mathematical society, providence, ri. of [mr2466937], with contributions by elizabeth l. *Wilmer, With a chapter on "Coupling from the past" by James G. Propp and David B. Wilson*, 2009.

[22] Stewart N Ethier and Thomas G Kurtz. *Markov processes: characterization and convergence*. John Wiley & Sons, 2009.

[23] Yong-Hua Mao and Yu-Hui Zhang. Exponential ergodicity for single-birth processes. *Journal of Applied Probability*, 41(4):1022–1032, 1981.

[24] Martin Hairer. Convergence of markov processes. *Lecture notes*, 18(26):13, 2010.

[25] J.F.C. Kingman. The stochastic theory of regenerative events. *Zeitschrift für Wahrscheinlichkeitstheorie und Verwandte Gebiete*, 2(3):180–224, 1964.

[26] Samuel Karlin and James McGregor. The classification of birth and death processes. *Transactions of the American Mathematical Society*, 86(2):366–400, 1957.

[27] Daniel T Gillespie. Stochastic simulation of chemical kinetics. *Annu. Rev. Phys. Chem.*, 58(1):35–55, 2007.

[28] Persi Diaconis. The cutoff phenomenon in finite markov chains. *Proceedings of the National Academy of Sciences*, 93(4):1659–1664, 1996.

[29] Riddhipratim Basu, Jonathan Hermon, and Yuval Peres. Characterization of cutoff for reversible markov chains. In *Proceedings of the twenty-sixth annual ACM-SIAM symposium on Discrete algorithms*, pages 1774–1791. SIAM, 2014.

[30] Bernard Ycart. Cutoff for markov chains: some examples and applications. In *Complex Systems*, pages 261–300. Springer, 2001.