POLITECNICO DI TORINO

Corso di Laurea Magistrale in Ingegneria Matematica

Master Degree Thesis

Foster-Lyapunov criteria with stopping times and applications to Stochastic Reaction Networks



Supervisor prof. Daniele Cappelletti **Candidate** Martina Bonelli

Academic Year 2022-2023

Summary

The main objective in this thesis is to obtain a unified approach to the stability classification of continuous-time Markov chains defined on discrete state space via Foster-Lyapunov criteria. These criteria are tipically stated in terms of the generator of the process.

Aleksandr Lyapunov first introduced these techniques for the study of ordinary differential equations and F. Gordon Foster first adapted them to a stochastic setting.

After an introduction of the preliminaries about the main setting of work, a version of Dynkin's formula and its proof are provided.

Ruling out unstable behaviours of the Markov chains such as explosivity or transience and establishing recurrence and positive recurrence is a complex task. In these regards, the second chapter analyzes the Foster-Lyapunov criteria that imply these properties and the results are proved by the systematic application of Dynkin's formula.

Consider, for istance, the classical Foster-Lyapunov criterion for verifying the positive recurrence: it assumes that the Markov chain tends to drift in unit steps towards some finite subset of the state space, and it does not wander too far when it makes a one-step transition out of this set. The third chapter deals with establishing analogous drift criteria that are defined on random stopping times of the Markov chain.

The first study that addressed such issues was Filonov, who enunciated a sufficient drift condition for a discrete time Markov chain on a countable space to be positive recurrent.

The last chapter is devoted to analyzing some interesting examples of stochastic reaction networks and to studying their limit behaviour by Foster-Lyapunov criteria.

In particular, stochastic reaction networks are a family of continuous time Markov chains used to model biochemical systems and intracellular processes. The idea is quite simple: the species react by a finite number of possible biochemical transformations and the state of the system, which is the count of the available species, changes by the occurrence of a reaction.

Traditionally, the dynamics of the concentration of each species are modelled by means of an ordinary differential equation, however this type of models are inaccurate if the number of constituents of at least one species is extremely low, something common in biological setting. This makes the stochastic descriptions of reaction networks essential.

Contents

1	Intr	oduction	5
	1.1	Operator semigroups	5
	1.2	Stochastic processes and Martingales	7
	1.3	Generators and Markov processes	8
	1.4	Dynkin's formula	10
2	Fost	ter Lyapunov criteria	15
	2.1	Transience	15
	2.2	A condition for non-explosion	17
	2.3	A recurrence criterion	19
	2.4	A positive recurrence criterion	20
3	Gen	eralization to Foster-Lyapunov criteria with stopping times	23
	3.1	Generalization to stopping time based criteria version 1	23
		3.1.1 Transience criterion generalization version 1	24
		3.1.2 Recurrence criterion generalization version 1	26
		3.1.3 Positive recurrence criterion generalization version 1	27
	3.2	Generalization to stopping time based criteria version 2	29
		3.2.1 Transience criterion generalization version 2	29
		3.2.2 Recurrence criterion generalization version 2	31
		3.2.3 Positive recurrence criterion generalization version 2	32
4	Sto	chastic Reaction Networks	34
	4.1	Poisson and general counting process	34
	4.2	The basic model	35
	4.3	Deterministic models of reaction networks	37
	4.4	Networks conditions and complex-balanced equilibra	37
	4.5	Examples	40
5	Con	clusions	53

Bibliography

Chapter 1 Introduction

Along this section we will provide the preliminaries about the main settings where we will work.

1.1 Operator semigroups

Let L denotes a real Banach space.

Definition 1.1. A one parameter $\{T(t), t \ge 0\}$ of bounded linear operators on a Banach space is called **semigroup** if T(0) = I and T(s+t) = T(s)T(t).

Definition 1.2. A semigroup $\{T(t), t \ge 0\}$ on L is said to be strongly continuous if $\lim_{t\to 0} T(t)f = f$, for every $f \in L$.

A (possibly unbounded) *linear operator* A on L is a linear mapping whose domain $\mathcal{D}(A)$ is a subspace of L and whose range $\mathcal{R}(A)$ lies in L. The graph of A is given by

$$\mathcal{R}(A) = \{(f, Af) : f \in \mathcal{D}(A)\} \subset L \times L.$$

Definition 1.3. The *(infinitesimal)* generator of a semigroup $\{T(t)\}$ on L is the linear operator A defined by

$$Af = \lim_{t \to 0} \frac{1}{t} \{ T(t)f - f \}.$$

The domain $\mathcal{D}(A)$ of A is the subspace of all $f \in L$ for which this limit exists in L pointwise.

Let Δ be a closed interval in $(-\infty, +\infty)$, and denote by $C_L(\Delta)$ the space of continuous functions $u : \Delta \to L$. Moreover, let $C_L^1(\Delta)$ be the space of continuously differentiable functions $u : \Delta \to L$. Lemma 1.1. (Fundamental theorem of calculus) If $u \in C_L^1[a, b]$, then

$$\int_{a}^{b} \frac{d}{dt} u(t)dt = u(b) - u(a).$$
(1.1)

Theorem 1.1. Let $\{T(t), t \ge 0\}$ be a strongly continuous semigroup on L with generator A.

- 1. If $f \in \mathcal{D}(A)$ and $t \ge 0$, then $T(t)f \in \mathcal{D}(A)$ and $\frac{d}{dt}T(t)f = AT(t)f = T(t)Af.$ (1.2)
- 2. If $f \in \mathcal{D}(A)$ and $t \ge 0$, then

$$T(t)f - f = \int_0^t AT(s)f \, ds = \int_0^t T(s)Af \, ds.$$
(1.3)

Proof. 1. Using the property that T(t) is a semigroup, T(t+h) - T(t) = T(t)T(h) - T(t):

$$\frac{1}{h}[T(t+h)f - T(t)f] = A_h T(t)f = T(t)A_h f$$

for all h > 0, where $A_h = h^{-1}[T(h) - I]$, it follows that $T(t)f \in \mathcal{D}(A)$, since the limit of A_h for $h \to 0^+$ exists. So $(d/dt)^+T(t)f = AT(t)f = T(t)Af$, for the commutative property of the product operation. Thus, it sufficies to check that $(d/dt)^-T(t)f = AT(t)f = T(t)Af$ (assuming t > 0). But this follows from the identity

$$\frac{1}{-h}[T(t-h)f - T(t)f] - T(t)Af = T(t-h)[A_h - A]f + [T(t-h) - T(t)]Af$$

for $0 < h \leq t$. Clearly we used that for $h \to 0^-$ we have [T(t-h) - T(t)]Af = 0, because the semigroup $\{T(t)\}$ is strongly continuous, and $A_h \to A$.

2.

$$\int_{0}^{t} AT(s)f \, ds = \int_{0}^{t} T(s)Af \, ds = \int_{0}^{t} \frac{d}{ds}T(s)f \, ds = T(t)f - f$$

as a consequence of eq. 1.2 and Lemma 1.1.

1.2 Stochastic processes and Martingales

We consider an abstract set Ω called *probability space*, with the generic element ω called *elementary event*, a Borel field \mathcal{F} of subsets of Ω called *measurable sets* and a countably additive probability measure \mathbb{P} defined on \mathcal{F} .

Definition 1.4. A stochastic process X with index set \mathcal{I} and state space (E, \mathcal{B}) (a measurable space) defined on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ is a function defined on $\mathcal{I} \times \Omega$ with values in E such that for each $t \in \mathcal{I}$, $X(t, \cdot) : \Omega \to E$ is an E-valued random variable, that is $\{\omega : X(t, \omega) \in \Gamma\} \in \mathcal{F}$ for every $\Gamma \in \mathcal{B}$.

In the general case (see Sean P. Meyn [1993]) it is assumed that the state space E is a locally compact and separable metric space and that \mathcal{B} is the Borel field on E.

We denote with B(E) the collection of real-valued Borel measurable functions on E.

We take $\mathcal{I} = (0, \infty)$ (so that the time parameter is taken to be the set of non-negative real numbers, having the continuous parameter case).

We say that X is measurable if $X : [0, \infty) \times \Omega \to E$ is $\mathcal{B}[0, \infty) \times \mathcal{F}$ -measurable. We say that X is (almost surely) continuous (right continuous, left continuous) if for (almost) every $\omega \in \Omega$, $X(\cdot, \omega)$ is continuous (right continuous, left continuous).

The function $X(\cdot, \omega)$ is called the *sample path* of the process at ω .

Definition 1.5. A collection $\{\mathcal{F}_t\} = \{\mathcal{F}_t, t \in [0, \infty)\}$ of σ -algebras of sets in \mathcal{F} is a filtration if $\mathcal{F}_t \subset \mathcal{F}_{t+s}$ for $t, s \in [0, \infty)$.

Intuitively \mathcal{F}_t corresponds to the information known by an observer at time t. In particular, for a process X we define $\{\mathcal{F}_t^X\}$ by $\mathcal{F}_t^X = \sigma(X(s) : s \leq t)$; that is \mathcal{F}_t^X is the information obtained by observing X up to time t.

Definition 1.6. A process X is $\{\mathcal{F}_t\}$ -progressive (or simply $\{\mathcal{F}_t\} = \{\mathcal{F}_t^X\}$) if for each $t \ge 0$ the restriction of X to $[0, t] \times \Omega$ is $\mathcal{B}[0, t] \times \mathcal{F}_t$ -measurable.

Note that every right (left) continuous $\{\mathcal{F}_t\}$ -adapted process is $\{\mathcal{F}_t\}$ -progressive.

Definition 1.7. A process X is **adapted** to a filtration $\{\mathcal{F}_t\}$ (or simply $\{\mathcal{F}_t\}$ adapted) if X(t) is \mathcal{F}_t -measurable for each $t \ge 0$.

Since \mathcal{F}_t is increasing in t, X is $\{\mathcal{F}_t\}$ -adapted if and only if $\mathcal{F}_t^X \subset \mathcal{F}_t$ for each $t \geq 0$.

Definition 1.8. A random variable τ with values in $[0, \infty]$ is an $\{\mathcal{F}_t\}$ -stopping time if $\{\tau \leq t\} \in \mathcal{F}_t$, for every $t \geq 0$.

If $\tau < \infty$ a.s. we say that τ is *finite* a.s.

In some sense a stopping time is a random time that is recognizable by an observer whose information at time t is \mathcal{F}_t .

Definition 1.9. A real-valued process X with $\mathbb{E}[|X(t)|] < \infty$ for all $t \ge 0$ and adapted to a filtration $\{\mathcal{F}_t\}$ is an $\{\mathcal{F}_t\}$ -martingale if

$$\mathbb{E}[X(t+s)|\mathcal{F}_t] = X(t), \quad t, s \ge 0.$$
(1.4)

Definition 1.10. A real-valued process X adapted to the filtration $\{\mathcal{F}_t\}$ is an $\{\mathcal{F}_t\}$ -local martingale if

- The τ_k are almost surely increasing, $\mathbb{P}\{\tau_k < \tau_{k+1}\} = 1$;
- The τ_k diverge almost surely, $\mathbb{P}\{\lim_{k\to\infty}\tau_k=\infty\}=1;$
- The stopped process $X_{t \wedge \tau_k}$ is an $\{\mathcal{F}_t\}$ -martingale $\forall k$.

1.3 Generators and Markov processes

We can say that a Markov process is a special case of a stochastic process, distinguished by a certain Markov property, that is enounced below.

Definition 1.11. X is a Markov process if

$$\mathbb{P}\{X(t+s) \in \Gamma | \mathcal{F}_t^X\} = \mathbb{P}\{X(t+s) \in \Gamma | X(t)\}$$
(1.5)

for all $s, t \ge 0, \Gamma \in \mathcal{B}(E)$.

Definition 1.12. A function $P(t, x, \Gamma)$ defined on $[0, \infty) \times E \times \mathcal{B}(E)$ is a time homogeneous transition function if

$$P(t, x, \cdot) \text{ is a probability measure,} \quad (t, x) \in [0, \infty) \times E,$$

$$P(0, x, \cdot) = \delta_x, \quad x \in E,$$

$$P(\cdot, \cdot, \Gamma) \in B([0, \infty) \times E), \quad \Gamma \in \mathcal{B}(E),$$

$$P(t + s, x, \Gamma) = \int P(s, y, \Gamma) P(t, x, dy), \quad s, t \ge 0, x \in E, \Gamma \in \mathcal{B}(E).$$
(1.6)

The last one property is called the Chapman-Kolmogorov property.

A transition function $P(t, x, \Gamma)$ is a transition function for a time-homogenous Markov process if

$$\mathbb{P}\{X(t+s) \in \Gamma | \mathcal{F}_t^X\} = P(s, X(t), \Gamma),$$
(1.7)

for all $s, t \geq 0$ and $\Gamma \in \mathcal{B}(E)$, or equivalently, if

$$\mathbb{E}[f(X(t+s))|\mathcal{F}_t^X] = \int f(y)P(s,X(t),dy), \qquad (1.8)$$

for all $s, t \ge 0$ and $f \in B(E)$.

Intuitively, the meaning of $P(t, x, \Gamma)$ is the probability that $X(t) \in \Gamma$ given that the initial state of X was X(0) = x.

We denote the transition semigroup as $\{T(t)\}$, in particular we exploit the fact that

$$T(t)f(x) = \int f(y)P(t, x, dy),$$

so that the Markov property may be expressed

$$\mathbb{E}[f(X(t+s))|\mathcal{F}_s^X] = T(t)f(X(s)), \ s < t < \infty$$

where $\mathcal{F}_s^X = \sigma\{X(u), u : 0 \le u \le s\}.$

We let $\{O_n : n \in \mathbb{Z}_+\}$ be a sequence of precompact sets for which $O_n \to E$ as $n \to \infty$. We let $T^m = \tau_{O_m^c}$ the time of the first entrance to O_m^c .

Definition 1.13. The exit time for the process is defined as $\zeta = \lim_{m \to \infty} T^m$

Definition 1.14. We call the process X non-explosive if $\mathbb{P}_x(\zeta = \infty) = 1$, for all $x \in E$.

1.4 Dynkin's formula

Since the finite-dimensional distributions of a Markov process are determined by a corresponding semigroup $\{T(t)\}$, they are in turn determined by full generator A or by a sufficiently large set contained in A.

One of the best approaches for determining when a set is "sufficiently large" is through the martingale problem of Stroock and Varadhan, which is based on the observation in the following theorem.

Theorem 1.2. (Martingale problem)

Let X be an E-valued, progressive non-explosive Markov process with transition function $P(t, x, \Gamma)$, and $f \in B(E)$ bounded. Moreover, let $\{T(t)\}$ and A be as above. Then

$$M(t) = f(X(t)) - \int_0^t Af(X(s)) \, ds \tag{1.9}$$

is an $\{\mathcal{F}_t^X\}$ -martingale.

Proof. For each $t, u \ge 0$

$$\mathbb{E}\left[M(t+u)|\mathcal{F}_t^X\right] = \int f(y)P(u, X(t), dy) - \int_t^{t+u} \int Af(y)P(s-t, X(t), dy) \, ds$$
$$-\int_0^t Af(X(s)) \, ds$$
$$= T(u)f(X(t)) - \int_0^u T(s)Af(X(t)) \, ds - \int_0^t Af(X(s)) \, ds$$
$$= f(X(t)) - \int_0^t Af(X(s)) \, ds$$
$$= M(t).$$

In the third equation we used Theorem 1.1, 2, while the change in the order of integration in the second line is from Fubini's Theorem, which can be applied since f is a bounded function for hypothesis.

(X(s)) ds], It's useful to note that by means of the Doob's Optional Sampling Theorem we can enounce Theorem 1.2 having instead of an integer time t, a stopping time τ (a.s. finite):

$$\mathbb{E}_x\left[f(X(\tau))\right] = f(X(0)) + \mathbb{E}_x\left[\int_0^\tau Af((X(s))ds\right]$$
(1.10)

Theorem 1.3. (Dynkin's formula)

Let X be an E-valued, progressive Markov process and let $\{T(t)\}$ and A be as above. Moreover suppose that

- L is the Banach space that contains only bounded functions f on compact sets, which means $f \mathbf{1}_K$ is a bounded function $\forall K \subset E$ compact set;
- τ denotes the exit time from the interior of a compact set $K \subset E$, that we denotes by \mathring{K} ;

then

$$\mathbb{E}_x\left[f(X(t\wedge\tau))\right] = f(x) + \mathbb{E}_x\left[\int_0^{\tau\wedge t} Af((X(s))\,ds\right], \ x\in K.$$

Proof.

$$\mathbb{E}_{x}\left[f(x) + \int_{0}^{t\wedge\tau} Af((X(s)) \, ds\right] = f(x) + \mathbb{E}_{x}\left[\int_{0}^{t\wedge\tau} Af((X(s)) \, ds\right]$$
$$= f(x) + \mathbb{E}_{x}\left[\int_{0}^{t} Af((X(s\wedge\tau))\mathbf{1}_{K}(X(s\wedge\tau)) \, ds\right]$$
$$= f(x) + \int_{0}^{t} \int_{E} Af(y)\mathbf{1}_{K}(y) \, dP_{\mathrm{stop}}(s, x, dy) ds$$
$$= f(x) + \int_{0}^{t} \int_{E} A_{\mathrm{stop}}f(y) \, dP_{\mathrm{stop}}(s, x, dy) ds$$
(1.11)

where we denote $P_{\text{stop}}(s, x, dy)$ the transition function associated to the stopped process till time τ and A_{stop} as the generator of the stopped process till time τ . Note also that $Af(y)\mathbf{1}_K(y)$ is equal to the generator of the stopped process. In the last equality we have used Fubini's theorem for change in the order of integration.

Now it's possible to apply Theorem 1.1, 2 to eq. (1.11) and obtain

$$f(x) + \mathbb{E}_x \left[\int_0^{t \wedge \tau} Af(X(s)) \, ds \right] = f(x) + \mathbb{E}_x \left[f(X(t \wedge \tau)) \right] - f(x) = \mathbb{E}_x \left[f(X(t \wedge \tau)) \right]$$

$$(1.12)$$

Supposing the process X is non-explosive and that there exists a sequence of O_n open finite sets s.t. $O_n \to E$ for $n \to \infty$, we can conclude that the previous statement is equivalent to say that $f(t \wedge \tau) - \int_0^{t \wedge \tau} Af(X(s)) ds$ is a local-martingale. It's important to observe that our study will be restricted to the case of continuous time-homogeneous Markov process defined on a discrete state space, that is called Markov chain, mainly to avoid the technical complications of Markov chains with a continuous state space. For this reason now some crucial definitions are given, which are reasonable if we keep in mind this setting.

First of all, we give a result on the generator in the case of a continuous timehomogeneous Markov chain.

$$Af(x) = \sum_{y \neq x} (f(y) - f(x))q(x, y)$$
(1.13)

It's necessary to prove the equation above, first in the case f is bounded, and then assuming f as a non-negative function that is bounded on compact sets.

Proof. 1. Assume f as a bounded function. If $x \nleftrightarrow y$ (which means that, starting from state x, the chain does not reach y in one jump), then

$$p_h(x,y) = \mathbb{P}(2 \text{ or more jumps from } x \text{ in } [0,h]) \le c_2 h^2 \quad \forall y.$$

Consider

$$f(y)p_h(x,y) \leq f(y)\underbrace{\mathbb{P}(x \to y)}_{\frac{q(x,y)}{\lambda(x)}} \mathbb{P}(1 \text{ jump in } [0,h]) + f(y)\mathbb{P}(x \to y)\mathbb{P}(2 \text{ or more jumps from } x \text{ in } [0,h])$$
$$\leq \underbrace{f(y)\frac{q(x,y)}{\lambda(x)}ch + f(y)c_2h^2}_{\text{we call it } \star},$$

where $c = \lambda(x)h + c_1h^2$. Since

$$\sup_{y} \left| f(y)q(x,y) - \frac{\star}{h} \right| \le \sup_{y} \left| f(y)c_1h + f(y)c_2h^2 \right| \xrightarrow{f \text{ bounded}}_{h \to 0} 0.$$

So, we can use the uniform convergence theorem to change the order of limit and summation in the third equality below, concluding the proof for f bounded.

$$Af(x) = \lim_{h \to 0} \frac{\mathbb{E}_{x}[f(X(h))] - f(x)}{h}$$

= $\lim_{h \to 0} \frac{\sum_{y} f(y) p_{h}(x, y) - f(x)}{h}$
= $\lim_{h \to 0} \frac{\sum_{y \neq x} f(y) p_{h}(x, y) + f(x) (p_{h}(x, x) - 1)}{h}$
= $\sum_{y \neq x} \left(f(y) q(x, y) \right) + f(x) q(x, x)$
= $\sum_{y} \left(f(y) q(x, y) \right).$

2. Assume f as non-negative and only bounded on compact sets, we define f_K the function restricted to the compact set K:

$$f_{|_{K}} = \begin{cases} f(x) & \text{if } x \in K \\ 0 & \text{if } x \notin K \end{cases},$$

then $f_{|_K} \leq f$.

It's obvious that $f_{|_K} \to f(f_{|_K}$ converges in a punctual way for size of $K \to +\infty$) and $f_{|_K}$ is bounded. We have

$$\begin{split} \lim_{h \to 0} \frac{\mathbb{E}\left[f(X(h))\right] - f(x)}{h} &= \lim_{h \to 0} \lim_{K \to +\infty} \frac{\mathbb{E}\left[f_{|_{K}}(X(h))\right] - f_{|_{K}}(x)}{h} \\ &= \lim_{K \to +\infty} \lim_{h \to 0} \frac{\mathbb{E}\left[f_{|_{K}}(X(h))\right] - f_{|_{K}}(x)}{h} \\ &= \lim_{K \to +\infty} \lim_{h \to 0} \frac{\sum_{y \neq x} f_{|_{K}}(y) p_{h}(x, y) + f_{|_{K}}(x) (p_{h}(x, x) - 1)}{h} \\ &= \lim_{K \to +\infty} \sum_{y} q(x, y) f_{|_{K}}(y) \\ &= \sum_{y} q(x, y) f(y), \end{split}$$

thanks to the Moore-Os good theorem together with the application of case 1 above to $f_{\cal K}.$

For a measurable set $B \subset E$ we let

 $\tau_B = \inf\{t \ge 0 : X_t \in B \text{ and } X_s \notin B, \ 0 \le s < t\}$

be the hitting time (in the case of $X_0 \in B$, τ_B is also called the return time) of X.

Definition 1.15. Supposing that the Markov chain X is irreducible, for a fixed $B \subset E$ we call:

- X transient, if for some non-empty B, $\mathbb{P}_x(\tau_B < \infty) < 1$ $\forall x \notin B$;
- X recurrent, if for some finite B, $\mathbb{P}_x(\tau_B < \infty) = 1$ $\forall x \in E;$
- X positive recurrent, if for some finite B, $\mathbb{E}_x(\tau_B) < \infty$ $\forall x \in E$.

Chapter 2 Foster Lyapunov criteria

Ruling out unstable behaviours such as explosivity or transience and establishing positive recurrence (or equivalently, the existence of stationary distributions), is a complex task. With this aim we need to introduce the Foster-Lyapunov criteria to test for these properties. These are conditions for these properties that have the purpose to find a function that satisfies various inequalities.

They are named jointly after Aleksandr Lyapunov who first introduced these types of conditions in his study of the solutions of ordinary differential equations and F. Gordon Foster who first adapt them to a stochastic setting.

Before continuing a little reminder is important; throughout the following conditions, in the next sections, we assume that L is the Banach space that contains only bounded functions f on compact sets, $f \in L$ is a positive measurable function, and it has the characteristic of a norm-like function, that is $f(x) \to \infty$ as $x \to \infty$ (i.e. $\{x : V(x) \leq B\}$ is precompact for each $B \geq 0$).

2.1 Transience

Theorem 2.1. If X is a non-explosive, irreducible continous time-homogeneous Markov chain and there exist a norm-like function $f : E \to \mathbb{R}^+$ and a nonempty set $B \subset E$ such that

$$Af(x) \le 0, \ \forall x \notin B \tag{2.1}$$

and

$$f(y) < \inf_{x \in B} f(x), \text{ for some } y \notin B$$
 (2.2)

then X is transient.

Proof. We can use the Dynkin's formula with $x \notin B$, obtaining

$$\mathbb{E}_{x}\left[f\left(X\left((t+h)\wedge T^{m}\wedge\tau_{B}\right)\right)\mid\mathcal{F}_{t}\right] = f(X(t\wedge\tau_{B}\wedge T^{m})) + \mathbb{E}_{x}\left[\int_{t\wedge T^{m}\wedge\tau_{B}}^{(t+h)\wedge T^{m}\wedge\tau_{B}}Af(X(s))\,ds\right]$$
$$\leq f(X(t\wedge\tau_{B}\wedge T^{m}))$$
(2.3)

where we have used the first hypothesis (eq. (2.1)) in the second inequality. From eq. (2.3) we can conclude that $f(X(t \wedge T^m \wedge \tau_B))$ is a non-negative supermartingale.

Now we enounce a result that we will use immediately after:

Lemma 2.1. A non-negative super-martingale converges almost surely to a finite limit.

In particular we have that $f(X(t \wedge T^m \wedge \tau_B))$ converges to a finite limit and we can write

$$f(X(t \wedge T^m \wedge \tau_B)) \to f_{\infty}^m \ a.s.$$
 (2.4)

Then, we can proceed as follows

$$f_{\infty}^{m} \geq f_{\infty}^{m} \mathbf{1}_{\{\tau_{B} < \infty\}} \mathbf{1}_{\{T^{m} > \tau_{B}\}}$$

=
$$\lim_{t \to \infty} f(X(t \land \tau_{B} \land T^{m})) \mathbf{1}_{\{\tau_{B} < \infty\}} \mathbf{1}_{\{T^{m} > \tau_{B}\}}$$

=
$$f(X(\tau_{B} \land T^{m})) \mathbf{1}_{\{\tau_{B} < \infty\}} \mathbf{1}_{\{T^{m} > \tau_{B}\}}.$$
 (2.5)

Taking, now, the limit for $m \to \infty$

$$\lim_{m \to \infty} f(X(\tau_B \wedge T^m)) \mathbf{1}_{\{\tau_B < \infty\}} \mathbf{1}_{\{T^m > \tau_B\}} = f(X(\tau_B)) \mathbf{1}_{\{\tau_B < \infty\}}$$
$$\geq \inf_{z \in B} f(z) \mathbf{1}_{\{\tau_B < \infty\}}$$
(2.6)

Using the supermartingale property of $f(X(t \wedge T^m \wedge \tau_B))$ and the monotone convergence theorem:

$$f(x) \geq \lim_{m \to \infty} \mathbb{E}_{x} \left[f_{\infty}^{m} \mathbf{1}_{\{\tau_{B} < \infty\}} \mathbf{1}_{\{T^{m} > \tau_{A}\}} \right]$$

$$\geq \mathbb{E}_{x} \left[\inf_{z \in B} f(z) \mathbf{1}_{\{\tau_{B} < \infty\}} \right]$$

$$= \inf_{z \in B} f(z) \mathbb{P}_{x}(\tau_{B} < \infty).$$

(2.7)

Set now $x_0 \notin B$ such that

$$f(x_0) < \inf_{z \in B} f(z),$$

from eq. (2.2) we can show that

$$\mathbb{P}_{x_0}(\tau_B < \infty) \le \frac{f(x_0)}{\inf_{x \in B} f(x)} < 1$$
(2.8)

which establishes transience.

2.2 A condition for non-explosion

In this section we develop a criterion which ensures that the sample paths of the process X remain bounded on bounded time intervals, in order to have a non-explosive process.

Theorem 2.2. If X is a right continuous time Markov chain and there exists a norm-like function $f: E \to \mathbb{R}^+$ and a constant $c \ge 0$ such that

$$Af(x) \le cf(x) \quad \forall x \in E, \tag{2.9}$$

then $\zeta = \infty$, so that X is non-explosive.

Proof. The proof proceeds by considering the function h(x,t) := f(x)exp(-ct). We obtain, from the product rule, that the generator of the process applied to this new function shows a "negative drift":

$$Ah(x,t) = exp(-ct)[Af(x) - cf(x)] \le 0.$$

The inequality is justified using the hypothesis (eq. 2.9). Consider $t^m = t \wedge T^m$, from Dynkin's formula we have:

$$\mathbb{E}_{x}\left[h\left(X(t^{m}), t^{m}\right)\right] = h(x, 0) + \mathbb{E}_{x}\left[\int_{0}^{t^{m}} Ah\left(X(s), s\right) \, ds\right] \le h(x, 0) = f(x).$$
(2.10)

Let $M_t = exp(-ct)f(X(t))\mathbf{1}_{\{T^m \ge t\}}$. We show that the adapted process (M_t, \mathcal{F}_t^X) is a supermartingale.

Fixed s < t, we take first $\{s > T^m\}$, on this event $M_t = M_s = 0$, because $T^m < s < t$, and in the expression of M_t there is the indicator function $\mathbf{1}_{\{T^m \ge t\}}$. Hence we can write:

$$\mathbb{E}\left[M_t | \mathcal{F}_s^X\right] = M_s \text{ on } \{s > T^m\}.$$

Otherwise considering the event $\{s \leq T^m\}$, we use (2.10) to conclude the desired supermartingale property.

$$\mathbb{E}\left[M_t | \mathcal{F}_s^X\right] = exp(-ct)\mathbb{E}_{X(s)}\left[f\left(X(t-s)\right)\mathbf{1}_{\{T^m \ge t-s\}}\right]$$

$$\leq exp(-cs)\mathbb{E}_{X(s)}\left[h\left(X(t-s)^m, (t-s)^m\right)\right]$$

$$\leq exp(-cs)f(X(s)) = M_s.$$

Now we can use the following Kolmogorov's inequality for supermartingales:

Lemma 2.2. Suppose Z_n , $n \ge 1$ is a nonnegative supermartingale, then for a > 0

$$\mathbb{P}_x(\sup(Z_1,\ldots,Z_n)\geq a)\leq \frac{\mathbb{E}[Z_0]}{a}.$$

In our case we have the following (since $\mathbb{E}[Z_0] = M_0 = f(X(0)) = f(x)$):

$$\mathbb{P}_x\left(\sup_{t\ge 0} M_t \ge a\right) \le \frac{f(x)}{a}, \quad a > 0$$

that can be rewritten as

$$\mathbb{P}_x\left(\sup_{0\le t\le T^m} \left(f\left(X(t)\right)exp(-ct)\right)\ge a\right)\le \frac{f(x)}{a}, \quad a>0$$

Letting $m \to \infty$ and using the monotone convergence theorem, we can write

$$\mathbb{P}_x\left(\sup_{0\le t\le \zeta} \left(f\left(X(t)\right)exp(-ct)\right)\ge a\right)\le \frac{f(x)}{a}, \quad a>0$$

Since f is a norm-like function, technically we have that f(X(t))exp(-ct) is a nonnegative supermartingale $\forall t$.

Before concluding that $\zeta = \infty$ we have to prove it raa (recductio ad absurdum). Suppose that $\zeta < \infty$ and that

$$\sup_{0 \le t \le \zeta} ||X(t)|| = \infty$$

Since f is norm-like we have

$$\sup_{0 \le t \le \zeta} f(X(t)) = \infty$$

Taking t as a finite value, we then have

$$\sup_{0 \le t \le \zeta} (f(X(t))exp(-ct)) = \infty$$

However if we use the Kolmogorov's inequality, we obtain an absurdum, $\forall a > 0$:

$$\mathbb{P}_x \left(\sup_{0 \le t \le \zeta} (f(X(t))exp(-ct) = \infty \right) \le \mathbb{P}_x \left(\sup_{0 \le t \le \zeta} (f(X(t))exp(-ct) \ge a) \right)$$
$$\le \frac{f(x)}{a} \to 0$$

2.3 A recurrence criterion

Theorem 2.3. For X an irreducible continuous time-homogeneous Markov chain, a measurable compact set $C \subset E$ and a norm-like function $f : E \to \mathbb{R}^+$ if

$$Af(x) \le 0, \quad x \notin C \tag{2.11}$$

then X is recurrent.

We might note that if the set C is a finite set and it's recurrent, then at least one state in C is recurrent. If the process X is irreducible, all the states communicate with each others, and so the process itself is recurrent.

Proof. First of all, we observe that since C is a compact set, then we can take

$$K^* = \sup_{x \in C} f(x) < \infty.$$

If we fix $K > K^*$, then

$$f(x) > K \to x \notin C.$$

so we can consider $\{x : f(x) > K\}$ as hypothesis.

Taking $t < \tau_C$, then f(X(t)) > K and on $\{t < \tau_C\}$ we know that $Af(x) \leq 0$ for the hypothesis.

Our goal now is to prove that $f(X(t \wedge \tau_C))$ is a non negative (because f is a norm-like function) supermartingale.

The second equality can be obtained using the Fatou's lemma, which allows us to apply the Dynkin's formula in the third line.

$$\mathbb{E}\left[f(X((t+h)\wedge\tau_{C}))|\mathcal{F}_{t}^{X}\right] = \mathbb{E}\left[\liminf_{m\to\infty}f(X((t+h)\wedge\tau_{C}\wedge T^{m}))|\mathcal{F}_{t}^{X}\right]$$
$$=\liminf_{m\to\infty}\mathbb{E}\left[f(X((t+h)\wedge\tau_{C}\wedge T^{m}))|\mathcal{F}_{t}^{X}\right]$$
$$=f(X(t\wedge\tau_{C}))+\liminf_{m\to\infty}\mathbb{E}\left[\int_{t\wedge\tau_{C}}^{(t+h)\wedge\tau_{C}\wedge T^{m}}Af(X(s))\,ds\right]$$
$$\leq f(X(t\wedge\tau_{C})).$$
(2.12)

Thanks to lemma (2.1) we can conclude that $f(X(t \wedge \tau_C))$ converges almost surely to a finite limit, in particular, \mathbb{P} -a.s. on the event $\{\tau_C = \infty\}$ we have f(X(t)) is converging.

Since we suppose that the Markov chain we are working with is irreducible and

the state space is a discrete set so that $\{x : f(x) < L\}$ is a finite set, then X(t) visits all the sets of the form $\{x : f(x) > L\}$. As a consequence

$$\sup_{t} f(X(t)) = \infty \implies f(x) \to \infty,$$

but this is an absurdum since f(X(t)) is a supermartingale. So it must be $\mathbb{P}_x(\tau_C = \infty) = 0$ and this concludes the proof.

2.4 A positive recurrence criterion

We present the Foster-Lyapunov drift condition that is shown to yield a criterion for positive recurrence.

Theorem 2.4. Consider X an irreducible continuous time-homogeneous Markov chain, a measurable compact set $K \subset E$, for some c, d > 0 and a norm-like function $f : E \to \mathbb{R}^+$ if

$$Af(x) \leq -c + d\mathbf{1}_K(x), \quad x \in E$$

then X is positive recurrent.

Proof. In order to prove that X is positive recurrent, we want:

$$\mathbb{E}_x[\tau_K] < \infty, \ x \in E.$$

We would like to use the Dynkin's formula (eq. (1.10)) but it's necessary that τ is the exit time from a compact set, so we use the trick of writing $\tau_K \wedge T^m$. Now it's possible to use the Dynkin's formula:

$$\mathbb{E}_x\left[f(X(\tau_K \wedge T^m))\right] = f(X(0)) + \mathbb{E}_x\left[\int_0^{\tau_K \wedge T^m} Af((X(s)ds))\right]$$

It's useful to divide the proof into two cases. First, we consider $x \notin K$:

$$\mathbb{E}_{x}\left[f(X(\tau_{K} \wedge T^{m}))\right] \leq f(X(0)) + \mathbb{E}_{x}\left[\int_{0}^{\tau_{K} \wedge T^{m}} -c \, ds\right]$$
$$= f(X(0)) - \mathbb{E}_{x}\left[\int_{0}^{\tau_{K} \wedge T^{m}} c \, ds\right]$$
$$= f(X(0)) - \mathbb{E}_{x}\left[c \left(\tau_{K} \wedge T^{m}\right)\right]$$
$$= f(x) - c\mathbb{E}_{x}\left[\tau_{K} \wedge T^{m}\right],$$
$$(2.13)$$

where we used the hypothesis in the first inequality. So, we have:

$$\mathbb{E}_{x}\left[\tau_{K} \wedge T^{m}\right] \leq \frac{f(x)}{c} - \frac{\mathbb{E}_{x}\left[f(X(\tau_{K} \wedge T^{m}))\right]}{c} \leq \frac{f(x)}{c}$$

$$(2.14)$$

and the second inequality is justified using the fact that f is norm-like.

We can conclude that $\mathbb{E}_x[\tau_K \wedge T^m]$ is a non-decreasing succession w.r.t m, so it admits the limit. Letting $m \to \infty$ and using the monotone convergence theorem:

$$\mathbb{E}_x[\tau_K] = \mathbb{E}_x\left[\lim_{m \to \infty} \tau_K \wedge T^m\right] = \lim_{m \to \infty} \mathbb{E}_x[\tau_K \wedge T^m] \le \frac{f(x)}{c}.$$
 (2.15)

We have proved that $\mathbb{E}_x[\tau_K] < \infty$, for $x \notin K$.

The second case is $x \in K$. It is worth writing the return time τ_K as the sum of two stopping times, that is

$$\tau_K = \tau_1 + \tau_2$$

where τ_1 is the exit time from the set K, while τ_2 is the return time from any point which is not in K to K.

First analyzing $\mathbb{E}_x[\tau_1]$, $x \in K$ is finite since it represents the exit time from a set K that has only a finite number of points.

Now we consider instead $\mathbb{E}[\tau_2]$.

It is known that $\forall x \in K$,

$$Af(x) = \left[\sum_{y} q(x, y)f(y)\right] \le d$$
(2.16)

If we denote $\sum_{y} q(x, y) f(y)$ as u(x), then obviously

$$\sup_{x \in K} u(x) \le d < \infty. \tag{2.17}$$

Now, we give the definition of the boundary of the set K as follows:

$$\partial K = \{ \hat{x} \in K \text{ s.t. } p(\hat{x}, y) > 0 \text{ for some } y \notin K \}.$$

Denoting

$$\theta = \inf_{\hat{x} \in \partial K} \left(\sum_{\hat{y} \in K} (q(\hat{x}, \hat{y}) > 0) \right)$$
(2.18)

then we can obtain the following inequality on the probability of going from \hat{x} to y, conditioned to the fact that \hat{x} is the last state in K that is visited before X goes out from K:

$$p(\hat{x}, y | \hat{x} \text{ last visited}) = \frac{q(\hat{x}, y)}{\sum_{\hat{y} \notin K} q(\hat{x}, \hat{y})} \le \frac{q(\hat{x}, y)}{\theta}.$$
 (2.19)

Considering that $\mathbb{E}[\tau_2]$ is the mean value of the return time in K from a general state not in K then

$$\mathbb{E}[\tau_2] = \sum_{y \notin K} \mathbb{E}_y[\tau_2] \mathbb{P}(x, y, \tau_1)$$
(2.20)

where $\mathbb{P}(x, y, \tau_1)$ is the probability of going from the state $x \in K$ to the state $y \notin K$ at time τ_1 .

Using what obtained previously in the case $x \notin K$ (see eq. (2.15)), the following inequality can be written

$$\sum_{y \notin K} \mathbb{E}_y[\tau_2] \mathbb{P}(x, y, \tau_1) \le \sum_{y \notin K} \frac{f(y)}{c} \mathbb{P}(x, y, \tau_1)$$
(2.21)

Using now eq. (2.19), we obtain

$$\mathbb{E}[\tau_2] \leq \sum_{y \notin K} \frac{f(y)}{c} \mathbb{P}(x, y, \tau_1)$$

$$= \sum_{y \notin K} \sum_{\hat{x} \in \partial K} p(\hat{x}, y | \hat{x} \text{ last visited}) \mathbb{P}_x(\hat{x} \text{ last visited}) \frac{f(y)}{c}$$

$$\leq \sum_{\hat{x} \in \partial K} \sum_{y \notin K} \frac{q(\hat{x}, y)}{\theta} \frac{f(y)}{c}$$

$$\leq \sum_{\hat{x} \in \partial K} \frac{1}{\theta \cdot c} u(\hat{x})$$

$$\leq \sum_{\hat{x} \in \partial K} \frac{d}{\theta \cdot c}$$

$$< \infty.$$
(2.22)

In the third line it's used the fact that $\mathbb{P}_x(\hat{x} \text{ last visited})$ is less or equal than 1. In the fourth line we have changed the order of summation because the summation on $\hat{x} \in \partial K$ is a finite summation, while the last two inequalities are justified using eq. (2.17).

To conclude we can combine the two cases above, obtaining $\mathbb{E}_x[\tau_K] < \infty, \ \forall x \in E$, which proves the statement. \Box

Chapter 3

Generalization to Foster-Lyapunov criteria with stopping times

3.1 Generalization to stopping time based criteria version 1

The classical Foster criteria that we have explained and proved in the previous pages are well known for testing whether an irreducible Markov chain on a countable state space is transient, recurrent and positive recurrent.

Intuitively, to give an example, the positive recurrence criterion assumes that the chain tends to drift (in unit steps) towards some finite subset of the state space, and the chain does not wander too far when it makes a one-step transition out of this set.

However, now the question is whether is possible to state analogous drift criteria for Markov chains that are defined on steps that may be random steps. In particular are there drift criteria for recurrence, positive recurrence, or transience?

The first study that addressed such issues was Filonov, who gave a sufficient drift condition for a Markov chain on a countable space to be ergodic for steps that are stopping times.

3.1.1 Transience criterion generalization version 1

Theorem 3.1. Consider X an irreducible continuous time-homogeneous Markov chain, for a measurable non-empty set $B \subset E$ and a norm-like function $f : E \to \mathbb{R}^+$ if $\forall x \notin B \exists \tau(x)$ stopping time a.s. finite (indicating the exit time from a compact set containing x) such that

$$\mathbb{E}_x\left[\int_0^{\tau(x)} Af(X(t)) \, dt\right] \le 0, \quad x \notin B \tag{3.1}$$

and

$$f(y) < \inf_{z \in B} f(z), \ y \notin B$$
(3.2)

then X is transient.

Proof. It's useful to define the following DTMC:

• $Y_0 = X(0) = x$

•
$$Y_1 = X(\tau(x))$$

- $Y_2 = X(\tau(X(\tau(x))))$
- ...
- $Y_{n+1} = X(\tau(Y_n))$

The idea is to make a partition into sets of the state space E, where the $\tau(Y_i)$ is the exit time from one of these sets containing Y_i .

Since X is an irreducible CTMC, then $\{Y_n\}$ has an absorbing communication class and $\{Y_n\}$ limited to this class is irreducible.

To make this consideration more intuitive let's consider y_1 the entrance point into a set A_1 and $x_1 \notin A_1$ s.t. there is a non-negative probability of a transition from x_1 to y_1 . Using the irreducibility of X, it returns to visit x_1 , then it's possible to go from x_1 to y_1 . So the entrance points in the sets constitute an irreducible set for Y.

To sum up Y has an irreducible set and it is worth considering the DTMC limited to it to prove transience, choosing B as a non-empty measurable subset of the irreducible set of Y.

Clearly, if we prove that B is a transient set, then we can conclude that Y is transient because Y limited to its absorbing communication class is irreducible. Denoting the hitting time for the DTMC $\{Y_n\}$

$$T_B = \inf \left\{ n \ge 1 : Y_n \in B \right\}$$

we want to show that $\mathbb{P}_x(T_B < \infty) < 1, x \notin B$

We recall that T^m indicates the exit time from the compact set $O_m \in E$. Considering now $\tau(Y_i)$ as the exit times from finite sets that contain Y_i , the idea is to show that $f(Y_{n \wedge T_B \wedge T^m})$ is a non-negative supermartingale, as follows.

$$\mathbb{E}\left[f(Y_{n\wedge T_B\wedge T^m})|\mathcal{F}_0\right] = \mathbb{E}_x\left[f\left(Y_{n\wedge T_B\wedge T^m}\right)\right]$$
$$= \mathbb{E}_x\left[f\left(X\left(\tau\left(Y_{(n\wedge T_B\wedge T^m)-1}\right)\right)\right)\right]$$
$$= f(x) + \mathbb{E}_x\left[\int_0^{\tau(Y_{(n\wedge T_B\wedge T^m)-1})} Af(X(t)) dt\right]$$
$$\leq f(x).$$
(3.3)

In the third equality we suppose that $n \leq T_B$ otherwise we will have finished the proof and we have used the Dynkin's formula, while in the last inequality we use the hypothesis eq. (3.1).

Since we have proved that $f(Y_{n \wedge T_B \wedge T^m})$ is a non-negative supermartingale, it converges almost surely to a finite limit, in particular, on the event $\{T_B = \infty\}$ we have $f(Y_{n \wedge T_B \wedge T^m}) \to f_{\infty}^m$.

Now we can write

$$f_{\infty}^{m} \geq f_{\infty}^{m} \mathbf{1}_{\{T_{B} < \infty\}}$$

=
$$\lim_{n \to \infty} f(Y_{T_{B} \land n \land T^{m}}) \mathbf{1}_{\{T_{B} < \infty\}} \mathbf{1}_{\{T^{m} > T_{B}\}}$$

=
$$f(Y_{T_{B} \land T^{m}}) \mathbf{1}_{\{T_{B} < \infty\}} \mathbf{1}_{\{T^{m} > T_{B}\}}$$

Now, taking the limit with $m \to \infty$

$$f(x) \geq \lim_{m \to \infty} \mathbb{E}_x \left[f(Y_{T_B \wedge T^m}) \mathbf{1}_{\{T_B < \infty\}} \mathbf{1}_{\{T^m > T_B\}} \right]$$

$$\geq \mathbb{E}_x \left[\inf_{z \in B} f(z) \mathbf{1}_{\{T_B < \infty\}} \right]$$

$$= \inf_{z \in B} f(z) \mathbb{P}_x (T_B < \infty).$$

(3.4)

Setting $x_0 \notin B$, using the hypothesis:

$$\mathbb{P}_{x_0}(T_B < \infty) \le \frac{f(x_0)}{\inf_{z \in B} f(z)} < 1.$$

The equation below states that B is a non-empty transient set for the DTMC $\{Y_n\}$, for what has been explained at the beginning of the proof it is sufficient to conclude that Y is transient.

It can be observed that if X is recurrent then also Y is recurrent (using the definition of Y and the irreducibility of X together with the hypothesis of recurrence). Finally, by the contronominal property if Y is transient then X is transient. \Box

3.1.2 Recurrence criterion generalization version 1

Theorem 3.2. Consider X an irreducible continuous time-homogeneous Markov chain, for a measurable compact set $B \subset E$ and a norm-like function $f : E \to \mathbb{R}^+$ if $\forall x \notin B \exists \tau(x)$ stopping time a.s. finite (indicating the exit time from a compact set containing x) such that

$$\mathbb{E}_x\left[\int_0^{\tau(x)} Af(X(t)) \, dt\right] \le 0, \quad x \notin B \tag{3.5}$$

then X is recurrent.

Proof. It's useful to define the following DTMC:

• $Y_0 = X(0) = x$

•
$$Y_1 = X(\tau(x))$$

- $Y_2 = X(\tau(X(\tau(x))))$
- ...

•
$$Y_{n+1} = X(\tau(Y_n))$$

As it has been explained in the introduction of the proof of the transience criterion above, since X is an irreducible CTMC, then $\{Y_n\}$ has an absorbing communication class, and limiting $\{Y_n\}$ to this class it is irreducible.

So, it is worth considering the DTMC limited to this class to prove recurrence and the set K as a subset of the states in this class. Indeed if it is a recurrent finite set, there is a state in the class that has to be recurrent also for X. Using that X is an irreducible chain, X itself is recurrent.

To sum up the idea is to show that $\{Y_n\}$ limited to a closed and irreducible communication class is a recurrence DTMC under the hypothesis of the theorem, the consequence will be that also the CTMC $\{X_t\}$ is a recurrent chain. Denoting the hitting time for the DTMC $\{Y_n\}$

$$T_B = \inf \left\{ n \ge 1 : Y_n \in B \right\}$$

we want to show that $\mathbb{P}_x(T_B < \infty) = 1$. Considering now $\tau(Y_i)$ as the exit times from finite sets that contain Y_i , the idea is to show that $f(Y_{n \wedge T_B})$ is a non-negative supermartingale, as follows.

$$\mathbb{E}\left[f(Y_{n\wedge T_B})|\mathcal{F}_0\right] = \mathbb{E}_x\left[f(Y_{n\wedge T_B})\right]$$

= $\mathbb{E}_x\left[f(X(\tau(Y_{(n\wedge T_B)-1})))\right]$
= $f(x) + \mathbb{E}_x\left[\int_0^{\tau(Y_{(n\wedge T_B)-1})} Af(X(t)) dt\right]$
 $\leq f(x).$ (3.6)

In the third equality we suppose that $n \leq T_B$ otherwise we will have finished the proof and we have used the Dynkin's formula.

Since we have proved that $f(Y_{n \wedge T_B})$ is a non-negative supermartingale, it converges almost surely to a finite limit, in particular, on the event $\{T_B = \infty\}$ we have $f(Y_n)$ is converging.

Since $Y_n \in B \iff f(Y_n) \leq K$ $(K > K^* = \sup_n f(Y_n))$ then Y_n visits all the sets of the form $\{x : f(x) > L\}$.

As a consequence

$$\sup_{t} f(X(t)) = \infty \implies f(x) \to \infty$$

but this is an absurdum since $f(Y_n)$ is a supermartingale. So it must be $\mathbb{P}_x(T_B = \infty) = 0$ with $x \in E$ and this concludes the proof. Indeed we have proven that there exists a finite recurrent set for the DTMC.

3.1.3 Positive recurrence criterion generalization version 1

Theorem 3.3. Consider X an irreducible continuous time-homogeneous Markov chain, c, d > 0, a measurable finite set K and $f : E \to \mathbb{R}^+$ norm-like function. If for all $x \in E \exists \tau(x)$ stopping time a.s. finite (indicating the exit time from a compact set containing x) such that

$$\mathbb{E}_x\left[\int_0^{\tau(x)} Af(X(t)) dt\right] < -c\mathbb{E}_x\left[\tau(x)\right] + d\mathbf{1}_K(x), \quad x \in E$$

then X is positive recurrent.

Proof. We proceed in a similar way as in the proof of Theorem (2.4). We must show that $\mathbb{E}_x[\tau_K] < \infty \ \forall x \in E$.

We define $\tau(x_i)$ as the exit time of the process from a compact set that contains the state x_i .

Let $T_0 = 0$ and for $m \ge 1$ denote

$$T_m = \tau(x_1) + \tau(x_2) + \dots + \tau(x_m)$$

Now it's possible to use Theorem (1.10):

$$\mathbb{E}_{x}\left[f(X(\tau_{K} \wedge T_{m}))\right] = f(x) + \mathbb{E}_{x}\left[\int_{0}^{\tau_{K} \wedge T_{m}} Af(X(t)) dt\right]$$

$$= f(x) + \sum_{i=0}^{m-1} \mathbb{E}_{x}\left[\int_{\tau_{K} \wedge T_{i}}^{\tau_{K} \wedge T_{i+1}} Af(X(t)) dt\right]$$

$$< f(x) + \sum_{i=0}^{m-1} \mathbb{E}_{x}\left[\left(-c\mathbb{E}_{x_{i}}\left[\tau(x_{i})\right] + d\mathbf{1}_{K}(x_{i})\right)\mathbf{1}_{\{x_{i+1}\notin K\}}\right]$$

$$= f(x) + \sum_{i=0}^{m-1} \mathbb{E}_{x}\left[\left(-c\mathbb{E}_{x}\left[\tau(x_{i})|X(T_{i})\right] + d\mathbf{1}_{K}(x_{i})\right)\mathbf{1}_{\{x_{i+1}\notin K\}}\right]$$

$$= f(x) + \sum_{i=0}^{m-1} \mathbb{E}_{x}\left[\left(-c\tau(x_{i}) + d\mathbf{1}_{K}(x_{i})\right)\mathbf{1}_{\{x_{i+1}\notin K\}}\right]$$

$$(3.7)$$

where we used the hypothesis in the third inequality, since the stopping times $\tau(x_i), i = 1, \ldots, m$ are a.s. finite, and we suppose $x_i \notin K$, otherwise we will have finished the proof because we have the thesis.

So, having that $\{X(T_{i+1}) \notin K\} = \{T_{i+1} < \tau_K\}$, we can combine the summations, obtaining:

$$\mathbb{E}_{x}\left[f(X(\tau_{K} \wedge T_{m}))\right] = f(x) + \mathbb{E}_{x}\left[\int_{0}^{\tau_{K} \wedge T_{m}} Af(X(t)) dt\right]$$

$$< f(x) + \sum_{i=0}^{m-1} \mathbb{E}_{x}\left[(-c\tau(x_{i}) + d\mathbf{1}_{K}(x_{i}))\mathbf{1}_{\{x_{i+1}\notin K\}}\right] \quad (3.8)$$

$$= f(x) - c\mathbb{E}_{x}\left[\tau_{K} \wedge T_{m}\right] + d\mathbb{E}_{x}\left[\mathbf{1}_{K}(x)\right]$$

$$= f(x) - c\mathbb{E}_{x}\left[\tau_{K} \wedge T_{m}\right] + d\mathbf{1}_{K}(x).$$

We have

$$\mathbb{E}_x[\tau_K \wedge T_m] < \frac{f(x) + d\mathbf{1}_K(x)}{c}$$

because f is norm-like.

We can conclude as before letting $m \to \infty$ and using the monotone convergence theorem:

$$\mathbb{E}_{x}\left[\tau_{K}\right] = \mathbb{E}_{x}\left[\lim_{m \to \infty} \tau_{K} \wedge T_{m}\right] = \lim_{m \to \infty} \mathbb{E}\left[\tau_{K} \wedge T_{m}\right] < \frac{f(x) + d\mathbf{1}_{K}(x)}{c} \qquad (3.9)$$

which finishes the proof since we have proved that $\mathbb{E}_x[\tau_K] < \infty$, for $x \in E$. \Box

3.2 Generalization to stopping time based criteria version 2

In the criteria above we used τ as the stopping time representing the exit time from a finite set containing x. Using the formulation above we cannot extend the criteria with τ indicating the exit time from a general non-empty set containing x (as the Dynkin's formula is no longer available to be used). To overcome this problem we formulate now a second version of these criteria. Before enouncing the criteria it's necessary to give some definitions.

It is assumed that on the probability space, there is a semi-group of shiftoperators (θ_t) so that the relation $X(t+s) = X(t) \circ \theta_s$ holds almost surely for all $t, s \ge 0$.

Let

$$t_1 = \inf\{s > t_n : X(s) \neq X(s-)\},\tag{3.10}$$

the first instant of jump of (X(t)) and for $n \ge 1$,

$$t_{n+1} = \inf\{s > t_n : X(s) \neq X(s-)\} = t_n + t_1 \circ \theta_{t_n}, \tag{3.11}$$

the sequence of the instants of successive jumps of the process.

3.2.1 Transience criterion generalization version 2

Theorem 3.4. Consider X an irreducible continuous time-homogeneous Markov chain, c > 0, a non-empty measurable set B and $f : E \to \mathbb{R}^+$ norm-like function. If there exists τ an integrable stopping time such that $\tau \ge \eta \wedge t_1$, for a constant $\eta > 0$ and t_1 indicates the first instant of jump of X(t), and

$$\mathbb{E}_x[f(X(\tau))] - f(x) \le 0, \quad x \notin B, \tag{3.12}$$

$$f(y) < \inf_{z \in B} f(z), \quad y \notin B$$
(3.13)

then X is transient.

Proof. We define a sequence of induced stopping times (s_n) by induction, by $s_1 = \tau$ and

$$s_{n+1} = s_n + \tau \circ \theta_{s_n} \tag{3.14}$$

Using the hypothesis on τ , it follows that (s_n) is almost surely an increasing sequence, i.e. $s_n < s_{n+1}, \forall n \ge 1$. We then define

$$\tau_B = \inf\{s \ge 1 : X(s) \in B\}$$
(3.15)

and

$$\nu = \inf\{n \ge 1 : X(s_n) \in B\}$$
(3.16)

and clearly $\tau_B \leq s_{\nu}$. Define for $n \geq 1$

$$U_n = f(X(s_n)) \tag{3.17}$$

then, with eq. (3.12) and the strong Markov property of X(t) for the stopping time s_n , we obtain the relation

$$\mathbb{E}[U_{n+1}|\mathcal{F}_{s_n}] = \mathbb{E}_{X(s_n)}[f(X(\tau))] = \mathbb{E}_{X(s_n)}[f(X(\tau)) - f(x)] + U_n \le U_n \quad (3.18)$$

on the event $\{\nu > n\}$.

The process $U_{\nu \wedge n}$ is therefore a non-negative supermartingale, in particular it is converging almost surely to a finite limit, that is called U_{∞} . Then, we can proceed as follows.

$$U_{\infty} \geq U_{\infty} \mathbf{1}_{\{\tau_B < \infty\}}$$

= $\lim_{n \to \infty} U_{n \wedge \nu} \mathbf{1}_{\{\tau_B < \infty\}}$
= $U_{\nu} \mathbf{1}_{\{\tau_B < \infty\}}$
 $\geq \inf_{z \in B} f(z) \mathbf{1}_{\{\tau_B < \infty\}}.$ (3.19)

Using now the supermartingale property of $U_{\nu \wedge n}$:

$$U_{0} = f(X(s_{0}))$$

$$= f(X(0))$$

$$= f(x)$$

$$\geq \mathbb{E}_{x}[U_{\infty}]$$

$$\geq \mathbb{E}_{x}\left[U_{\infty}\mathbf{1}_{\{\tau_{B}<\infty\}}\right]$$

$$\geq \inf_{z\in B} f(z)\mathbb{P}_{x}(\tau_{B}<\infty).$$
(3.20)

Set now $x_0 \notin B$ such that

$$f(x_0) < \inf_{z \in B} f(z),$$

from the second hypothesis, which is eq. (3.13), it is shown that

$$\mathbb{P}_{x_0}(\tau_B < \infty) \le \frac{f(x_0)}{\inf_{z \in B} f(z)} < 1.$$
 (3.21)

which establishes transience.

3.2.2 Recurrence criterion generalization version 2

Theorem 3.5. Consider X an irreducible continuous time-homogeneous Markov chain, a measurable finite set K and $f: E \to \mathbb{R}^+$ norm-like function. If there exists τ an integrable stopping time such that $\tau \ge \eta \land t_1$ (for a constant $\eta > 0$ and t_1 indicating the first instant of jump of X(t)), and

$$\mathbb{E}_x[f(X(\tau))] - f(x) \le 0, \quad x \notin K$$
(3.22)

then X is recurrent.

Proof. We define a sequence of induced stopping times (s_n) by induction, by $s_1 = \tau$ and

$$s_{n+1} = s_n + \tau \circ \theta_{s_n}. \tag{3.23}$$

Using the hypothesis on τ , it follows that (s_n) is almost surely an increasing sequence, i.e. $s_n < s_{n+1}, \forall n \ge 1$.

We then define

$$\tau_K = \inf\{s \ge 0 : f(X(s)) \le C\}$$
(3.24)

and

$$\nu = \inf\{n \ge 0 : f(X(s_n)) \le C\}$$
(3.25)

and clearly $\tau_K \leq s_{\nu}$. Define for $n \geq 1$

$$U_n = f(X(s_n)) \tag{3.26}$$

then, with eq. (3.22) and the strong Markov property of X(t) for the stopping time s_n , we obtain the relation

$$\mathbb{E}[U_{n+1}|\mathcal{F}_{s_n}] = \mathbb{E}_{X(s_n)}[f(X(\tau))] = \mathbb{E}_{X(s_n)}[f(X(\tau)) - f(x)] + U_n \le U_n \quad (3.27)$$

on the event $\{\nu > n\}$.

The process $U_{\nu \wedge n}$ is therefore a non-negative supermartingale, in particular it is converging almost surely to a finite limit.

Let's prove using reductio ad absurdum that $\tau_K < \infty$, supposing $\tau_K = \infty$. Then, $U_n = f(X(s_n))$ converges almost surely to U_∞ .

Assume that $f(X(s_n))$ is transient, then $f(X(s_n))$ leaves any compact set, so that

$$\limsup_{n \to \infty} f(X(s_n)) = \infty$$

obtaining a first absurdum, since $f(X(s_n))$ should converge almost surely to a finite limit U_{∞} .

As a consequence, on the event $\{\tau_K = \infty\}$, $f(X(s_n))$ is recurrent, which implies

that X(t) visits infinitely many times a state x. Using the irreducibility of the process, X will visit infinitely many times the set $\{x : f(x) \leq K\}$. This fact leads to the second absurdum, implying $\tau_K < \infty$, that concludes the proof. \Box

3.2.3 Positive recurrence criterion generalization version 2

Theorem 3.6. Consider X an irreducible continuous time-homogeneous Markov chain, c > 0, a measurable finite set K and $f : E \to \mathbb{R}^+$ norm-like function. If there exists an integrable stopping time τ such that $\tau \ge \eta \land t_1$ (for a constant $\eta > 0$ and t_1 indicates the first instant of jump of X(t)) and

$$\mathbb{E}_x[f(X(\tau))] - f(x) \le -c\mathbb{E}_x[\tau] + d\mathbf{1}_K(x), \quad x \in E;$$
(3.28)

then X is positive recurrent.

Proof. We define $\tau(x_i)$ as the exit time of the process from a non-empty set that contains the state x_i .

Let $\tilde{T}_0 = 0$ and for $m \ge 1$ denote

$$\tilde{T}_m = \tau(x_1) + \tau(x_2) + \dots + \tau(x_m)$$

We cannot use the Dynkin's formula, however the first equality can be obtained adding pairs of consecutive terms that cancel each others (as a sort of telescopic sum):

$$\mathbb{E}_{x}\left[f(X(\tau_{K} \wedge \tilde{T}_{m}))\right] = f(x) + \sum_{i=0}^{m-1} \mathbb{E}_{x}\left[f(X(\tau_{K} \wedge \tilde{T}_{i+1})) - f(X(\tau_{K} \wedge \tilde{T}_{i}))\right] < f(x) + \sum_{i=0}^{m-1} \mathbb{E}_{x}\left[(-c\mathbb{E}_{x_{i}}\left[\tau(x_{i})\right] + d\mathbf{1}_{K}(x_{i}))\mathbf{1}_{\{x_{i+1}\notin K\}}\right] = f(x) + \sum_{i=0}^{m-1} \mathbb{E}_{x}\left[(-c\mathbb{E}_{x}\left[\tau(x_{i})|X(\tilde{T}_{i})\right] + d\mathbf{1}_{K}(x_{i}))\mathbf{1}_{\{x_{i+1}\notin K\}}\right] = f(x) + \sum_{i=0}^{m-1} \mathbb{E}_{x}\left[(-c\tau(x_{i}) + d\mathbf{1}_{K}(x_{i}))\mathbf{1}_{\{x_{i+1}\notin K\}}\right] (3.29)$$

where we used the hypothesis in the third inequality, since the stopping times $\tau(x_i), i = 1, \ldots, m$ are a.s. finite, and we suppose $x_i \notin K$, otherwise we will have finished the proof because we have the thesis.

So, having that $\{X(\tilde{T}_{i+1}) \notin K\} = \{\tilde{T}_{i+1} < \tau_K\}$, we can combine the summations, obtaining:

$$\mathbb{E}_{x}\left[f(X(\tau_{K}\wedge\tilde{T}_{m}))\right] = f(x) - c\mathbb{E}_{x}\left[\tau_{K}\wedge\tilde{T}_{m}\right] + d\mathbb{E}_{x}\left[\mathbf{1}_{K}(x)\right]$$

= $f(x) - c\mathbb{E}_{x}\left[\tau_{K}\wedge\tilde{T}_{m}\right] + d\mathbf{1}_{K}(x).$ (3.30)

We have

$$\mathbb{E}_x[\tau_K \wedge \tilde{T}_m] < \frac{f(x) + d\mathbf{1}_K(x)}{c}$$

because f is norm-like.

We can conclude as before letting $m \to \infty$ and using the monotone convergence theorem:

$$\mathbb{E}_{x}\left[\tau_{K}\right] = \mathbb{E}_{x}\left[\lim_{m \to \infty} \tau_{K} \wedge \tilde{T}_{m}\right] = \lim_{m \to \infty} \mathbb{E}\left[\tau_{K} \wedge \tilde{T}_{m}\right] < \frac{f(x) + d\mathbf{1}_{K}(x)}{c} \quad (3.31)$$

which finishes the proof since we have proved that $\mathbb{E}_x[\tau_K] < \infty$, for $x \in E$. \Box

Chapter 4 Stochastic Reaction Networks

4.1 Poisson and general counting process

The basic building block of the models that we will consider are counting processes, which are processes N such that N(t) is the number of times that a particular phenomenon has been observed by time t. We assume that these observations occur one at a time, so we have the following definitions:

Definition 4.1. N is a counting process if N(0) = 0 and N is constant except for jumps of +1.

If we have that N is a counting process, and t < s, then N(t) - N(s) is the number of observations in the interval (t, s]. The simplest counting process is a Poisson process.

Definition 4.2. A counting process is a **Poisson process** if these conditions are satisfied:

- In disjoint time intervals the number of observations are independent random variables, that is if $t_0 < t_1 < \cdots < t_n$, then $N(t_k) - N(t_{k-1})$, $k = 1, \ldots, n$ are independent random variables.
- The distribution on N(t+s) N(t) is not dependent from t.

Theorem 4.1. If N is a Poisson process, then there exists a constant $\lambda > 0$ such that N(s) - N(t) is Poisson distributed with parameter $\lambda(s-t)$ or, rather,

$$\mathbb{P}((N(s) - N(t)) = k) = \frac{(\lambda(s-t))^k}{k!} e^{-\lambda(s-t)}$$

$$\tag{4.1}$$

In general the intensity for a counting process at time t may depend on the behaviour of the counting process prior to time t, but also on other stochastic inputs.

Definition 4.3. A Cox process is a point process which is a generalization of a Poisson process where the intensity that varies across the underlying mathematical space (often space or time) is itself a stochastic process.

Indeed a Cox process can be interpreted as the result of a doubly stochastic procedure, which generates first a random measure ξ and then a Poisson process with intensity measure ξ .

4.2 The basic model

We can think about a reaction network as a collection of objects that dynamically interfere with each other, with some rules. A biochemical system consists of two parts: a reaction *network*, and a choice of *dynamics*. The network is a static objects consisting of:

- Species S, that are the chemical components.
- Complexes C, which are nonnegative linear combinations of the species. They describe how species interact.
- Reactions \mathcal{R} , which describe how to convert one such complex to another.

Definition 4.4. A chemical reaction network consists of a triple $\{S, C, R\}$ where:

- 1. $S = \{S_1, \ldots, S_n\}$ is the set of species, with cardinality n where n is finite;
- 2. C is the set of complexes, consisting of nonnegative integer linear combinations of the species;
- 3. $\mathcal{R} = \{y_k \longrightarrow y'_k : y_k, y'_k \in \mathcal{C}\}$ is the set of reactions, that is a finite set of ordered couples of complexes.

The notation that we use to write the k-th reaction is the stoichiometric equation:

$$\sum_{i} y_{ki} S_i \longrightarrow \sum_{i} y'_{ki} S_i$$

where the vectors $y_k, y'_k \in \mathbb{Z}^n_{\geq 0}$ are associated with the source and the product complex, respectively.

We then define the *reaction vectors* of the network as $\zeta_k = y'_k - y_k \in \mathbb{Z}^n_{\geq 0}$.

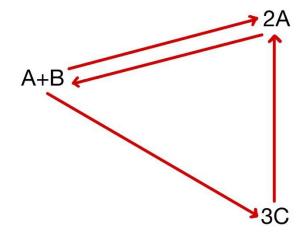


Figure 4.1. Example of a reaction network, where: Species $X = \{A, B, C\}$, Complexes $C = \{A + B, 2A, 3C\} \in \mathcal{Z}_{\geq 0}^{|X|}$, Reactions $\mathcal{R} \in C \times C$.

Having a notion of a reaction system in hand, now the question is how to model the dynamical behavior of the counts of the different species. The stochastic model is a continuous time Markov chain $\{X(t), t \ge 0\}$, where X(t) counts the number of molecules of the different species at time t. For each reaction $y_k \longrightarrow y'_k \in \mathcal{R}$ we specify an intensity function $\lambda_k : \mathbb{Z}^n_{\ge 0} \to \mathbb{R}_{\ge 0}$. The number of times that the k-th reaction occurs by time t is described by the counting process

$$R_k(t) = Y_k\left(\int_0^t \lambda_k(X(s))ds\right),\tag{4.2}$$

where the Y_k are independent unit Poisson process. The state of the system then satisfies the equation $X(t) = X(0) + \sum_k R_k(t)\zeta_k$, or

$$X(t) = X(0) + \sum_{k} Y_k \left(\int_0^t \lambda_k(X(s)) ds \right) \zeta_k, \tag{4.3}$$

where the sum is over the reaction channels.

Now we need to specify the intensity functions or the *kinetics*. The minimal hypothesis that we can make on the kinetics is that it is *stochiometrically* admissible, which means that $\lambda_k(x) = 0$ if $x_i < y_{ki}, \forall i \in \{1, \ldots n\}$. The definition suggests that a reaction can take place only if the number of molecules is sufficient to produce the source complex and ensure the process remains within $\mathcal{Z}_{>0}^n$ for all time.

One of the most common type of kinetics is the mass-action kinetics. The stochastic form of the law of mass action says that for some constant κ_k , termed the reaction rate constant, the rate of the k-th reaction should be

$$\lambda_k(x) = \kappa_k \prod_{i=1}^n y_{ki}! \binom{x}{y_k} = \kappa_k \prod_{i=1}^n \frac{x_i!}{(x_i - y_{ki})!}$$
(4.4)

that corresponds to the hypothesis that the system is well stirred. The rate function is proportional to the number of possible combinations of molecules present in the system that can give rise to the reaction.

4.3 Deterministic models of reaction networks

In this section we consider a chemical reaction network where the number of constituents is extremely high, so that the dynamics of the concentrations is described accurately by a deterministic model.

Set $x(t) \in \mathbb{R}^n_{\geq 0}$ as the vector whose components $x_i(t)$ contains the concentration of species S_i at t.

The most common choice for the deterministically modeled system is

$$\dot{x}(t) = \sum_{k} \kappa_k x(t)^{y_k} \zeta_k, \qquad (4.5)$$

where for two vectors $a, b \in \mathbb{R}^m_{\geq 0}$ we write $a^b = \prod_{j=1}^m a_j^{b_j}$. The option of $\kappa_k x^{y_k}$ is called deterministic mass-action kinetics.

4.4 Networks conditions and complex-balanced equilibra

The definitions that follow allow us to relate the network architecture to its associated dynamical systems.

Definition 4.5. A chemical reaction network, $\{S, C, \mathcal{R}\}$ is called **weaklyreversible** if for any reaction $y_k \to y'_k \in \mathcal{R}$, there is a sequence of directed reactions beginning with y'_k as a source complex and ending with y_k as a product complex. This means that $y'_k \to y_1, y_1 \to y_2, \ldots, y_r \to y_k \in \mathcal{R}$.

Definition 4.6. A network is called **reversible** if $y'_k \to y_k \in \mathcal{R}$, whenever $y_k \to y'_k$.

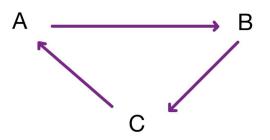


Figure 4.2. Example of a reaction network that is weakly reversible but not reversible.

The connected components of the graph form a partition of the complexes into different linkage classes.

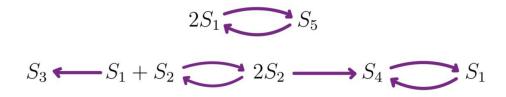


Figure 4.3. The graph above has two connected components and each component is partitioned into the following linkage classes $\{2S_1, S_5\}$ and $\{S_3, S_1 + S_2, 2S_2, S_4, S_1\}$.

Definition 4.7. The stoichiometric subspace of the network is $S = span_{\{y_k \to y'_k \in \mathcal{R}\}} \{y'_k - y_k\}.$

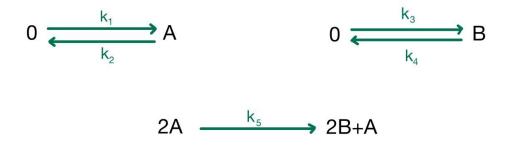
Definition 4.8. Given $c \in \mathbb{R}^n$, we call c + S the stoichiometric compatibility classes, while $(c + S) \cap \mathbb{R}^n_{\geq 0}$ are the non-negative stoichiometric compatibility classes of the network.

4.5 Examples

We give now some cases of study and try to apply the Foster-Lyapunov criteria in order to establish transience, recurrence and positive recurrence.

Example 4.1. Consider the following chemical reaction network, characterized by:

- species $X = \{A, B\};$
- complexes $C = \{0, A, B, 2A, A + 2B\} \in \mathcal{Z}_{\geq 0}^{|X|};$
- reactions $\mathcal{R} \in C \times C$.



The CRN has 3 linkage classes, the first two are reversible, while the last one is not reversible nor weakly reversible.

Denote with $X(t) = [X_1(t), X_2(t)] \in \mathbb{Z}_{\geq 0}^2$ respectively the number of species of type A and type B.

The five reaction channels have reaction vectors

1.
$$\zeta_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix},$$

2. $\zeta_2 = \begin{bmatrix} -1 \\ 0 \end{bmatrix},$
3. $\zeta_3 = \begin{bmatrix} 0 \\ 1 \end{bmatrix},$

4. $\zeta_4 = \begin{bmatrix} 0 \\ -1 \end{bmatrix}$, 5. $\zeta_5 = \begin{bmatrix} -1 \\ 2 \end{bmatrix}$;

and respective intensities (using the law of mass action)

- 1. $\lambda_1(x) = \kappa_1$,
- 2. $\lambda_2(x) = \kappa_2 x_1$,
- 3. $\lambda_3(x) = \kappa_3$,
- 4. $\lambda_4(x) = \kappa_1 x_2$,
- 5. $\lambda_5(x) = \kappa_5 x_1(x_1 1).$

Recall that the generator A can be written as

$$Af(x) = \sum_{k} \lambda_k(x) \left(f(x + \zeta_k) - f(x) \right).$$
(4.6)

Choosing a linear Lyapunov function f of the form $f(x) = \alpha x_1 + \beta x_2$, then:

$$\begin{aligned} Af(x) &= \lambda_1(x)[f(x+\zeta_1) - f(x)] + \lambda_2(x)[f(x+\zeta_2) - f(x)] + \lambda_3(x)[f(x+\zeta_3) - f(x)] \\ &+ \lambda_4(x)[f(x+\zeta_4) - f(x)] + \lambda_5(x)[f(x+\zeta_5) - f(x)] \\ &= \kappa_1[f(x_1+1, x_2) - f(x_1, x_2)] + \kappa_2 x_1[f(x_1 - 1, x_2) - f(x_1, x_2)] \\ &+ \kappa_3[f(x_1, x_2 + 1) - f(x_1, x_2)] + \kappa_4 x_2[f(x_1, x_2 - 1)] \\ &+ \kappa_5 x_1(x_1 - 1)[f(x_1 - 1, x_2 + 2)] \\ &= \kappa_1[\alpha(x_1 + 1) + \beta x_2 - \alpha x_1 - \beta x_2] + \kappa_2 x_1[\alpha(x_1 - 1) + \beta x_2 - \alpha x_1 - \beta x_2] \\ &+ \kappa_3[\alpha x_1 + \beta(x_2 + 1) - \alpha x_1 - \beta x_2] + \kappa_4 x_2[\alpha x_1 + \beta(x_2 - 1)] \\ &+ \kappa_5 x_1(x_1 - 1)[\alpha x_1(x_1 - 1) + \beta(x_2 + 2) - \alpha x_1 - \beta x_2] \\ &= \alpha \kappa_1 - \alpha \kappa_2 x_1 + \beta \kappa_3 - \beta \kappa_4 x_2 + (-\alpha + 2\beta) \kappa_5 x_1(x_1 - 1) \end{aligned}$$

$$(4.7)$$

Using $\alpha = 2$ and $\beta = 1$, then in order to use Theorem 2.4 it's necessary that

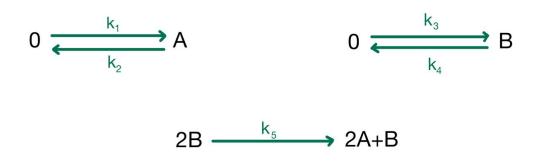
$$Af(x) = 2\kappa_1 - 2\kappa_2 x_1 + \kappa_3 - \kappa_4 x_2 \le -c \tag{4.8}$$

for c > 0 and $x \notin K$, where K is a compact set. Since $\kappa_1 > 0$ and $\kappa_3 > 0$ if we call $M = c + 2\kappa_1 + \kappa_3$, then M > 0 and the condition of Theorem 2.4 can be written as

$$2\kappa_2 x_1 + \kappa_4 x_2 > M. \tag{4.9}$$

Since $2\kappa_2 x_1 + \kappa_4 x_2 = M$ is the equation of a straight line, Af(x) > 0 is valid out from a compact set, thanks to this it can be concluded that the CRN is positive recurrent.

Example 4.2. It can be seen that, for symmetry, this second example is almost similar to the one above.



The five reaction channels have reaction vectors

1. $\zeta_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix},$ 2. $\zeta_2 = \begin{bmatrix} -1 \\ 0 \end{bmatrix},$ 3. $\zeta_3 = \begin{bmatrix} 0 \\ 1 \end{bmatrix},$ 4. $\zeta_4 = \begin{bmatrix} 0 \\ -1 \end{bmatrix},$ 5. $\zeta_5 = \begin{bmatrix} 2 \\ -1 \end{bmatrix};$

and respective intensities (using the law of mass action)

- 1. $\lambda_1(x) = \kappa_1$,
- 2. $\lambda_2(x) = \kappa_2 x_1$,
- 3. $\lambda_3(x) = \kappa_3$,

- 4. $\lambda_4(x) = \kappa_1 x_2$,
- 5. $\lambda_5(x) = \kappa_5 x_2(x_2 1).$

Using, as in the first example, a linear Lyapunov function $f(x) = \alpha x_1 + \beta x_2$, we obtain

$$\begin{aligned} Af(x) &= \lambda_1(x)[f(x+\zeta_1) - f(x)] + \lambda_2(x)[f(x+\zeta_2) - f(x)] + \lambda_3(x)[f(x+\zeta_3) - f(x)] \\ &+ \lambda_4(x)[f(x+\zeta_4) - f(x)] + \lambda_5(x)[f(x+\zeta_5) - f(x)] \\ &= \kappa_1[f(x_1+1, x_2) - f(x_1, x_2)] + \kappa_2 x_1[f(x_1-1, x_2) - f(x_1, x_2)] \\ &+ \kappa_3[f(x_1, x_2+1) - f(x_1, x_2)] + \kappa_4 x_2[f(x_1, x_2-1)] \\ &+ \kappa_5 x_2(x_2-1)[f(x_1+2, x_2-1)] \\ &= \kappa_1[\alpha(x_1+1) + \beta x_2 - \alpha x_1 - \beta x_2] + \kappa_2 x_1[\alpha(x_1-1) + \beta x_2 - \alpha x_1 - \beta x_2] \\ &+ \kappa_3[\alpha x_1 + \beta(x_2+1) - \alpha x_1 - \beta x_2] + \kappa_4 x_2[\alpha x_1 + \beta(x_2-1)] \\ &+ \kappa_5 x_2(x_2-1)[\alpha x_1(x_1+2) + \beta(x_2-1) - \alpha x_1 - \beta x_2] \\ &= \alpha \kappa_1 - \alpha \kappa_2 x_1 + \beta \kappa_3 - \beta \kappa_4 x_2 + (2\alpha - \beta) \kappa_5 x_2(x_2 - 1). \end{aligned}$$

$$(4.10)$$

For symmetry we choose $\alpha = 1$ and $\beta = 2$ and in order to use Theorem 2.4 it's necessary that

$$Af(x) = \kappa_1 - \kappa_2 x_1 + 2\kappa_3 - 2\kappa_4 x_2 \le -c \tag{4.11}$$

for c > 0 and $x \notin K$, where K is a compact set.

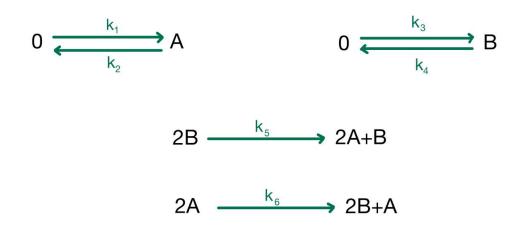
Since $\kappa_1 > 0$ and $\kappa_3 > 0$ if we call $M = c + 2\kappa_1 + \kappa_3$, then M > 0 and the condition of Theorem 2.4 can be written as

$$\kappa_2 x_1 + 2\kappa_4 x_2 > M. \tag{4.12}$$

Since $\kappa_2 x_1 + 2\kappa_4 x_2 = M$ is the equation of a straight line, Af(x) > 0 is valid out from a compact set, thanks to this it can be concluded that the CRN is positive recurrent.

Example 4.3. Consider now a CRN that is a union of the two models described above.

It's interesting to observe that, although the two single models are positive recurrent as shown in the previous two examples, their combination is recurrent, as we prove in the following.



The six reaction channels have reacton vectors

1.
$$\zeta_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$
,
2. $\zeta_2 = \begin{bmatrix} -1 \\ 0 \end{bmatrix}$,
3. $\zeta_3 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$,
4. $\zeta_4 = \begin{bmatrix} 0 \\ -1 \end{bmatrix}$,
5. $\zeta_5 = \begin{bmatrix} -1 \\ 2 \end{bmatrix}$,
6. $\zeta_6 = \begin{bmatrix} 2 \\ -1 \end{bmatrix}$;

and respective intensities (using the law of mass action)

1.
$$\lambda_1(x) = \kappa_1$$
,

2.
$$\lambda_2(x) = \kappa_2 x_1$$
,

3.
$$\lambda_3(x) = \kappa_3$$
,

4.
$$\lambda_4(x) = \kappa_1 x_2$$
,

- 5. $\lambda_5(x) = \kappa_5 x_1(x_1 1),$
- 6. $\lambda_6(x) = \kappa_6 x_2(x_2 1).$

Choosing a Lypaunov function f of the form $f(x) = \frac{1}{x_1+x_2}$, then

$$\begin{aligned} Af(x) &= \lambda_{1}(x)[f(x+\zeta_{1})-f(x)] + \lambda_{2}(x)[f(x+\zeta_{2})-f(x)] + \lambda_{3}(x)[f(x+\zeta_{3})-f(x)] \\ &+ \lambda_{4}(x)[f(x+\zeta_{4})-f(x)] + \lambda_{5}(x)[f(x+\zeta_{5})-f(x)] + \lambda_{6}(x)[f(x+\zeta_{6})-f(x)] \\ &= \kappa_{1}[f(x_{1}+1,x_{2})-f(x_{1},x_{2})] + \kappa_{2}x_{1}[f(x_{1}-1,x_{2})-f(x_{1},x_{2})] \\ &+ \kappa_{3}[f(x_{1},x_{2}+1)-f(x_{1},x_{2})] + \kappa_{4}x_{2}[f(x_{1},x_{2}-1)] \\ &+ \kappa_{5}x_{1}(x_{1}-1)[f(x_{1}-1,x_{2}+2)] + \kappa_{6}x_{2}(x_{2}-1)[f(x_{1}+2,x_{2}-1)] \\ &= \kappa_{1}[\frac{1}{(x_{1}+1)+x_{2}} - \frac{1}{x_{1}+x_{2}}] + \kappa_{2}x_{1}[\frac{1}{(x_{1}-1)+x_{2}} - \frac{1}{x_{1}+x_{2}}] \\ &+ \kappa_{5}x_{1}(x_{1}-1)[\frac{1}{(x_{1}-1)+(x_{2}+2)} - \frac{1}{x_{1}+x_{2}}] \\ &+ \kappa_{5}x_{1}(x_{1}-1)[\frac{1}{(x_{1}-1)+(x_{2}+2)} - \frac{1}{x_{1}+x_{2}}] \\ &+ \kappa_{6}x_{2}(x_{2}-1)[\frac{1}{(x_{1}+x_{2}+1)(x_{1}+x_{2})}] \\ &+ \kappa_{5}x_{1}(x_{1}-1)[-\frac{1}{(x_{1}+x_{2}+1)(x_{1}+x_{2})}] \\ &+ \kappa_{5}x_{1}(x_{1}-1)[-\frac{1}{(x_{1}+x_{2}+1)(x_{1}+x_{2})}] \\ &+ \kappa_{6}x_{2}(x_{2}-1)[-\frac{1}{(x_{1}+x_{2}+1)(x_{1}+x_{2})}] \\ &+ \kappa_{6}x_{2}(x_{2}-1)[-\frac{1}{(x_{1}+x_{2}+1)(x_{1}+x_{2})}] \\ &+ \kappa_{6}x_{2}(x_{2}-1)[-\frac{1}{(x_{1}+x_{2}+1)(x_{1}+x_{2})}] \\ &+ (\kappa_{2}x_{1}+\kappa_{4}x_{5})(\frac{1}{(x_{1}+x_{2}-1)(x_{1}+x_{2})}) \\ &+ (\kappa_{2}x_{1}+\kappa_{4}x_{2})(\frac{1}{(x_{1}+x_{2}-1)(x_{1}+x_{2})}) \end{aligned}$$

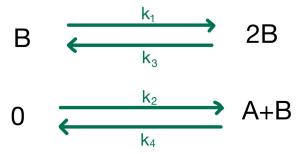
Since the set $\{x : Af(x) \leq 0\}$ is the region outside a non-empty set (in particular an ellipse since det $(A_{3,3}) > 0$ where $A_{3,3} = \begin{bmatrix} k_5 & 0 \\ 0 & k_6 \end{bmatrix}$), the first condition of Theorem 2.1 is satisfied.

Finally, it remains to prove the second condition of the transience criterion (eq. 2.2) which is:

$$f(y) < \inf_{x \in B} f(x), \text{ for some } y \notin B$$
 (4.14)

Since the chosen Lyapunov function f is positive in the ellips and it decreases, converging to 0 as $x_1 \to \infty$ and $x_2 \to \infty$, we have the conclusion, and the reaction model in this example is transient.

Example 4.4. Consider the following chemical reaction network The reaction vectors are:



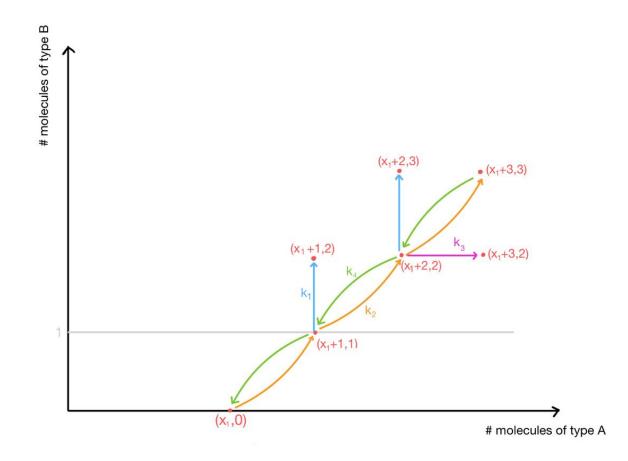
1. $\zeta_1 = \begin{bmatrix} 0 \\ -1 \end{bmatrix}$, 2. $\zeta_2 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$, 3. $\zeta_3 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$, 4. $\zeta_4 = \begin{bmatrix} -1 \\ -1 \end{bmatrix}$;

and the respective intensities are

- 1. $\lambda_1(x) = \kappa_1 x_2$,
- 2. $\lambda_2(x) = \kappa_2$,
- 3. $\lambda_3(x) = \kappa_3 x_2(x_2 1),$
- 4. $\lambda_4(x) = \kappa_4 x_1 x_2$.

This example is significant because it shows that it is not possible to prove positive recurrence using the classicl Foster-Lyapunov criterion as in the models above. Indeed if we choose as Lyapunov function $f(x) = x_1 + x_2$, taking a point of type $(x_1,0)$, the only possible reaction is $0 \rightarrow A + B$. However along this path the Lyapunov function does not decrease.

Another problem is that from the state $(x_1,0)$, we can go to $(x_1+1,1)$. Assuming x_1 very big, the dominant reaction is $A + B \rightarrow 0$, so that from $(x_1 + 1,1)$ we return back to $(x_1,0)$ and we remain "trapped" in a sort of cycle as indicated in the figure below. Clearly if the Lyapunov function is chosen in order to decrease in one direction of the cycle, it cannot decrease also in the other direction.



All these observations lead to the conclusion that it is necessary, in this case,

to use the Foster-Lyapunov criterion with stopping times. The main technical difficulty is of gluing different functions in order to have a global Foster-Lyapunov function. In particular the goal is to prove the positive recurrence of the model using Theorem 3.6 with the following Lyapunov function:

$$f(x) = \begin{cases} e^{x_1 + x_2} & \text{if } x_2 \ge 2\\ e^{x_1 + 4} & \text{if } x = (x_1 + 1, 1) \text{ or } x = (x_1, 0) \end{cases}$$
(4.15)

We define the stopping time τ as

$$\tau = \begin{cases} t_1 & \text{if } X_2(0) \ge 3\\ \inf\{t : X(t) \notin \{(x_1, 0), (x_1 + 1, 1), (x_1 + 2, 2)\} & \text{if } X(0) \in \{(x_1, 0), (x_1 + 1, 1), (x_1 + 2, 2)\} \end{cases}$$
(4.16)

• Set $X_2(0) = x_2 \ge 3$. Thanks to Dynkin's formula:

$$\mathbb{E}_{x}\left[f(X(\tau))\right] - f(x) = \mathbb{E}_{x}\left[f(X(t_{1})) - f(x)\right]$$
$$= \mathbb{E}_{x}\left[\int_{0}^{t_{1}} Af(X(s))ds\right]$$
$$= Af(x)\mathbb{E}_{x}\left[t_{1}\right]$$
$$\leq -c\mathbb{E}_{x}\left[t_{1}\right]$$
(4.17)

So, it is sufficient to prove $Af(x) \leq -c, \forall x \notin K$ where K is a compact set.

$$A(f(x)) = \lambda_1(x) \left(f(x+\zeta_1) - f(x) \right) + \lambda_2(x) \left(f(x+\zeta_2) - f(x) \right) + \\ + \lambda_3(x) \left(f(x+\zeta_3) - f(x) \right) + \lambda_4(x) \left(f(x+\zeta_4) - f(x) \right) \\ = e^{x_1+x_2} \left(\left[\frac{1}{e} - 1 \right] k_1 x_2 + \left[e^2 - 1 \right] k_2 + \left[e - 1 \right] k_3 x_2 \left(x_2 - 1 \right) - \left[\frac{1}{e^2} - 1 \right] k_4 x_1 x_2 \right) \\ \leq -\gamma$$

$$(4.18)$$

 $\begin{aligned} \forall x \text{ not in } K \text{ and } \gamma > 0. \\ \text{We call } M &= [e^2 - 1]k_2 + [e - 1]k_3 x_2^2 > 0, \, M + \gamma = c \text{ and } a = -k_4 [\frac{1}{e^2} - 1] > 0, \\ b &= k_1 [-e^{-1} + 1] + k_3 [-1 + e] > 0. \\ \text{Then eq. (3.28) can be rewritten as} \end{aligned}$

$$-ax_2 - bx_1x_2 \le -c \qquad \forall x \notin B. \tag{4.19}$$

Let us fix $x_1 \ge \frac{c}{bx_2}$,

 $ax_2 + bx_1x_2 \ge ax_2 + c \ge c.$

Since $x_2 \ge 3$ eq. (4.19) is satisfied $\forall x$ not in a rectangle (that is a compact set).

Set X(0) ∈ T = {(x₁,0), (x₁+1,1), (x₁+2,2)}. The possible states out from this set of three points that the model can visit after one single reaction are R = {(x₁+1,2), (x₁+2,3), (x₁+3,3), (x₁+3,2)}. It's worth to consider the continuous time Markov chain with the set of seven possible states T ∪ R. In particular we consider the set T as transient states and R as recurrence states.

The intuition is that the event with the greatest probability that allow us to exit from T is the reaction $B \to 2B$ in the state $(x_1 + 1, 1)$. To understand this, we compute the exit probabilities from each of the three states in T and show that the limit for $x_1 \to \infty$ of the exit probability goes to 0 from $(x_1, 0), (x_1 + 2, 2)$ and to 1 from $(x_1 + 1, 1)$. In order to compute the exit probabilities from each of the three states in T, we use the following formula

$$-Q_{T,T}^{-1}Q_{T,R}, (4.20)$$

clearly the $Q_{T,T}^{-1}$ is the inverse of the matrix $Q_{T,T}$. Notice that, using the values of the reaction intensities we can write the transition rate matrix Q and especially $Q_{T,T}$ that contains only the transitions among the transient states as

$$Q_{T,T} = \begin{bmatrix} -k_2 & k_2 & 0\\ k_4(x_1+1) & -k_4(x_1+1) - k_2 - k_1 & k_2\\ 0 & k_4(2x_1+4) & -k_4(2x_1+4) - k_2 - 2k_1 - 2k_3 \end{bmatrix}$$

We use the math solver Symbolab (any math solver is sufficient) to compute the inverse of this matrix and we paste in Fig. 4.4 the result of the inverse operation. Then, we write the matrix $Q_{T,R}$ as

$$Q_{T,R} = \begin{bmatrix} 0 & 0 & 0 & 0\\ k_1 & 0 & 0 & 0\\ 0 & 2k_1 & k_2 & 2k_3 \end{bmatrix}$$

Using eq.(4.20), we obtain the matrix of the exit distributions from the states in T, calling $-Q_{T,T}^{-1} = A$ and $Q_{T,R} = B$. It's interesting to notice that, because of the structure of the matrix $Q_{T,R}$, we are only interested in the elements of the second and third columns of matrix Q_{TT}^{-1} .

$$-Q_{T,T}^{-1}Q_{T,R} = \begin{bmatrix} A_{1,2}B_{2,1} & A_{1,3}B_{3,2} & A_{1,3}B_{3,3} & A_{1,3}B_{3,4} \\ A_{2,2}B_{2,1} & A_{2,3}B_{3,2} & A_{2,3}B_{3,3} & A_{2,3}B_{3,4} \\ A_{3,2}B_{2,1} & A_{3,3}B_{3,2} & A_{3,3}B_{3,3} & A_{3,3}B_{3,4} \end{bmatrix}$$

Consider again the matrix $Q_{T,T}^{-1}$ depicted in the figure above, it's clear that the elements in the second column tend to a constant as $x_1 \to \infty$, while those of the third column go to 0 as $x_1 \to \infty$.

This is particular useful, since taking $x_1 \to \infty$, the only elements that do not tend to 0 in the matrix $-Q_{T,T}^{-1}Q_{T,R}$ of exit distribution are those of the first column. This is to say that the only probabilities that do not vanish as $x_1 \to \infty$ are the exit probabilities from each transient state to the state $(x_1 + 1, 2)$.

Now, we are able to apply Theorem 3.6.

$$\mathbb{E}_{x} [f(X(\tau))] - f(x) = [f(x_{1} + 1, 2) - f(x_{1}, x_{2})]\mathbb{P}_{x}(X(\tau) = (x_{1} + 1, 2)) + [f(x_{1} + 2, 3) - f(x_{1}, x_{2})]\mathbb{P}_{x}(X(\tau) = (x_{1} + 2, 3) + [f(x_{1} + 3, 2) - f(x_{1}, x_{2})]\mathbb{P}_{x}(X(\tau) = (x_{1} + 3, 2)) + [f(x_{1} + 3, 3)) - f(x_{1}, x_{2})]\mathbb{P}_{x}(X(\tau) = (x_{1} + 3, 3).$$

$$(4.21)$$

Consider to take x_1 very large, so that the only probability that survives is $\mathbb{P}_x(X(\tau) = (x_1 + 1, 2))$.

Notice that the sum along the rows of the matrix $Q_{T,T}^{-1}$ represents the mean time spent in each one of the three states in T and it is a polynomial w.r.t. x_1 .

Then,

$$\mathbb{E}_{x} [f(X(\tau))] - f(x) = e^{x_{1}+3} - e^{x_{1}+4}$$

= $e^{x_{1}}(e^{3} - e^{4})$
 $\leq -\gamma(r + q_{n}(x_{1}))$ (4.22)

so we have the conclusion.

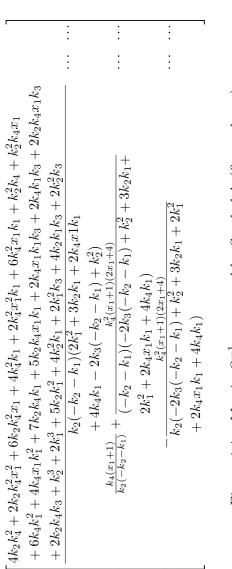
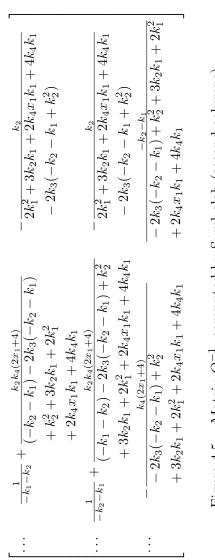
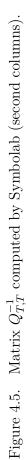


Figure 4.4. Matrix $Q_{T,T}^{-1}$ computed by Symbolab (first column).





Chapter 5 Conclusions

In this thesis we analyzed the Foster-Lyapunov criteria to study the stability of continuous-time Markov chains defined on countable state space and we presented some interesting applications to Stochastic Reaction Networks.

We proposed and proved a more general version of the Dynkin's formula, extending it to functions only bounded on compact sets and to stopping times that are exit times from compact sets. This approach has been crucial since the classical Foster-Lyapunov criteria are proved by a systematic application of the Dynkin's formula.

The main goal of the work has been to enunciate the Foster-Lyapunow criteria with stopping times, which are a generalization of the classical criteria. Considering, for instance, the positive recurrence criterion, the idea is that starting from an initial state x of high energy this does not lead quickly to a lower energy level, so that $Af(x) \leq -c, c > 0$. Indeed there could be the possibility of having to wait for some amount of time, the stopping time τ , before the generator applied to f can significantly decrease.

Moreover, the stopping time τ may be chosen in a way that $X(\tau)$ is in some convenient subspace.

As shown in the last example, the criteria with the stopping times are, in some cases, essential to study the limit behaviour of the Stochastic Reaction Networks. In this particular example, it is too much difficult to find a global Lyapunov function that satisfies the classical drift criterion, making the generalized version of it needful.

Bibliography

- Thomas G. Kurtz David F. Anderson. Stochastic Analysis of Biochemical Systems. Springer, 2015.
- Y.P. Filonov. Criterion for ergodicity of homogeneous discrete markov chains. Ukr Math J, 41:1223–1225, 1989.

Philippe Robert. Stochastic Networks and Queues. Springer, 2003.

- R. L. Tweedie Sean P. Meyn. Stability of markovian processes iii: Fosterlyapunov criteria for continuous-time processes. Adv. Appl. Prob, 25:518–548, 1993.
- Thomas G. Kurtz Stewart N. Either. Markov Processes Characterization and Convergence. John Wiley & Sons, 1986.