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Irreversibility of biological systems

Relatore

Prof. Marco Baiesi

Laureando

Emanuele Tovazzi

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Abstract

In a context of Markov processes, an ecological model of three interacting species is studied, which dynamics is described by the master equation. It is presented a theoretical method through which to estimate the entropy production of the system along its evolution and its link with the concept of irreversibility of the system state. At each step only two species interact each others through a birth-death or mutation mechanism, bringing an increasing/decreasing by one unit of the number of the specific individuals. All the information about the interactions are encoded in the transition rates of the model which depend by a competition matrix and a mutation matrix. It is also imposed a cyclical competition in these coefficients. Using a van Kampen system's size expansion the deterministic equations at which the model approaches when the total number of individuals tend to infinity are obtained. These assumes the form of antisymmetric Lotka-Volterra differential equations. The Fokker-Planck equations for this model are derived analytically. Numerical simulations of the system evolution at different initial conditions are performed. It is shown that the system present two different type of dynamics. In particular using the Fokker-Planck equations is shown that if the mutation coefficients are above the critical value of 1, any species can cyclically dominates over the others. The entropy production in this case is significantly higher that a condition in which a species prevails. We study the analytic expression of the production of entropy on the plane in which the sum of the three species concentrations is constantly 1. Furthermore it peaks at the point in which all the concentration are equal. In the final plot are shown the two entropy productions regimes for higher/lower values of critical mutation rate.

Contents

Introduction

The study of population dynamics between one or more species has been one of the sectors of ecology, which was profoundly investigated by ecologists, biologists, mathematicians and physicians since the late '20 of the past century [1],[2],[3]. In order to render in the best way the setting upon which our thesis will deal with, we start with the general definition of *Ecosystem*, namely[1]:
"A biological community of interacting organisms and their physical environment."
Beyond the fact that every ecological community can have great different environmental conditions and mechanisms of interaction, some general patterns appear to take place in a wide variety of ecological systems. Of course this suggests that certain properties or dynamical evolutions of multiple systems are not susceptible to the particular details of the interactions, but instead it is possible to make good models that represent in a reliable way the fundamental relations between the constituents elements of an ecosystem. This way to proceed fits perfectly with statistical physics, and the challenge involved is to find those parameters that have major weight for an effective description of the model.
Models defined by Lotka and Volterra were the first to give a qualitative and quantitative description of the dynamics of interacting ecological species in the same environment. Despite the continuous enhancement of the knowledge achieved in this field, there is a diffuse indecision on saying how much populations are influenced by internal density-dependent factors, that are the specific relations of the model that has been taken into account or by external-dependent factors, of which there is less information due to its complexity [4].
During the 70s McArthur and May provided a link between interacting populations with common resources and the Lotka-Volterra equations, besides giving the formulas for the competition matrix (see Chapter 1). We specify that these (deterministic) models are supported by the concept of niche, which must be defined only a posteriori. Furthermore there are many drawbacks that must be taken into account: (1) There are lots of parameters that are not easy to guess from the collection of data. (2) It is hard to extend these models to include space dependence. (3) Ts is not easy to analyze the general patterns of these systems, rather than their time series.
It is of fundamental importance to stress that for a comprehensive study of a particular system, deterministic and stochastic computations of the same model are nec-

[1]From the Oxford dictionary.

essary (in which the only difference is the introduction of random effects)[8]. Indeed, a finite size system sometimes shows effects that can determine a spatio-temporal regular dynamics, revealing degrees of collective behaviors that are absent in the context of the deterministic formulation. Although nature is intimately stochastic, deterministic behaviors can give (not always) a great amount of information about the particular evolution that we are considering and usually they arise as solutions of ordinary differential equations (ODE). We also know that usually, as a system starts to get a little more complex, it immediately becomes mathematically intractable, and only few things can be said by a pure theoretical research. Furthermore, different stochastic realizations of a system can be very different and in some case determine different "end-stage" of one or more specific populations considered (in the case of an exponential growth population with few members fixing the initial condition this can lead to a relative extinction or explosion). However during these past several decades plenty of models that describe very different kind of ecological phenomena have been proposed, of which we present only a summary list: (1) The Malthus exponential growth model, (2) The Verhulst logistic growth model, (3) Competing or colony models, (4) Fluctuating environment models, (5) Spatial and time lag models of population growth, (6) Epidemiological models and so on [5, 6, 7]. Of course all these models and all their variations have been studied in detail with great success, and it is not our goal to study and present them here. The advent of computers brought a huge increase of the complexity and variety of the models just presented. As we will discuss later, in many occasions the intrinsic stochasticity of the simulations permits a more reliable way to study a particular system, with respect to the analytical solutions that can be obtained. For this reason the counterpart of this method is that the numerical results are often of difficult interpretation, since they differ (sometimes quite a lot) from the analytical-based solution of the dynamics at issue. In fact it happens that the stochastic effects change significantly the behavior of non-linear system like the one we will encounter. The context of a Markovian dynamics will be the starting point of our study in this work, where the complete description of system with intrinsic noises will be given by the master equation (ME). In particular we will see a Markovian discrete jump process with continuous time dependence.The master equation contains the deterministic ODE equations of the model dynamics. These are also called Mean-Field equations since the contribution of noise is cancelled out (sometimes this term is used in ecology only if we refer to the non-spatial system). The mean-field equations can be obtained both via Van Kampen's expansion or the Kramers-Moyal's expansions. We present and use the first one for the recovery of the deterministic equations and the second to obtain the Fokker-Planck equation (that describes the Gaussian fluctuations). In this work we study the evolution of a three species population model and how the particular choice and tuning of its parameters gives a more stable/unstable evolution of the system. At last we perform an entropy production estimation for these conditions, which is related to the irreversibility of the system's evolution.

Most of the physical processes in nature deal with their apparent irreversibility and

with the growth of uncertainty in our predictions about them. This refers first to our approximate description of the model and second to our inability to drive a system exactly backward by reversing the external forces that guide its evolution. In classical statistical mechanics this is linked with the entropy production and to the dissipation of energy towards the environment. The difference of the effects depending on the couplings of the system with the environment is the reason behind this "arrow" of the flow of energy [9, 35]. This privileged direction of the evolution of the processes is nothing else than the manifestation of the irreversibility of the dynamics of the system itself. A measure of this irreversibility can be given immediately by taking the ratio of the probabilities P of the system to evolve along an allowed trajectory ω, i.e. $P[\omega]$, and the reversed one, i.e. $P[\omega^R]$ [10]. This ratio is connected with the entropy production of the system and is equal to one only if the process is perfectly reversible, which implies equilibrium (see Chapter 3). Out of equilibrium, $P[\omega] \neq P\left[\omega^R\right]$ and the time-reversibility is broken. So the computation of the entropy production along the temporal evolution of the system, is a reliable way to study how much the system itself departs from an equilibrium configuration. This is the fundamental aim of this thesis: to examine the entropy production of a system of mutating/competing species and see if this quantity has a particular growth for certain types of dynamics (in particular, we impose a cyclicity underlying the interaction between these species).
Usually the natural processes are out of equilibrium and the notion of being out of equilibrium will be presented in Chapter 2. A central tool in this thesis is Stochastic Thermodynamics (which deals with quantities such as entropy, energy, heat, and work, that are defined on the stochastic trajectory-level of the system). That, together with Markovian jumps, provides the right conceptual framework for the description of complex systems that are fairly out of equilibrium.
Classical thermodynamics plays an important role in equilibrium dynamics, with systems with a very large number of particles ($N \sim 10^{23}$) but if we consider systems that are completely irreversible or simply out of equilibrium, then the classical thermodynamics can not be used anymore as a good tool in order to give a description of their main properties. As we will see, it is possible to have a well-defined expression of the entropy production along a Markovian trajectory, i.e. the framework underlaying our model. Indeed, we know that in most physical situations the system under consideration is not isolated, but it interacts with the environment.

We now present the plan of the thesis:

Chapter 1: We discuss the notion of Ecology, its stability and we present the main results of nonlinear dynamical systems. After that we introduce a particular type of nonlinear differential equations named Lotka-Volterra (LV) and sketch some theoretical properties of these equations, taking into account the important case of antisymmetric coefficients of the mentioned *community matrix*.

Chapter 2: We introduce the definition of a Markov process and derived the fundamental object for the description of stochastic systems like ours: the master equa-

tion. Then, the Fokker-Planck equation is introduced and the existing bridge between these two objects. Furthermore, we discuss the concept of detailed balance and its connection to thermodynamics and the consequences on it dealing with a non-equilibrium state. Since it will be performed in Chapter 4, it is presented the systematic procedure of the Van Kampen's expansion that bring us to the deterministic equations of our model.

Chapter 3: A chapter dedicated to the main concept of non equilibrium and to Stochastic Thermodynamics and is illustrated how a well defined quantity of entropy production can be assigned to a single path of our system. It is also shown how the entropy production can be splitted in two subterms, one relative to the internal entropy production of the system and the other one about the external entropy production in the environment.

Chapter 4: Here is presented and analytically described the specific system of three interacting species, then is shown the stochastic simulation in various cases with different parameters, demonstrating how the performance and stability of the system is affected by different values of the matrices entries of the transition rates that rule the evolution of the species. In particular, the above mentioned entropy production, that is strictly correlated with the irreversibility of the system's temporal evolution, will be the entropy production of the environment.

Chapter 5: In the last chapter we summarize the main results obtained and we provide some future possibilities of study for systems like the one explored here.

Chapter 1

Ecological models and stability

Here we present the Lotka-Volterra model, which will emerge in the following chapters of this thesis and we show the main properties that belong to these systems' framework.

1.1 Stability of ecological systems

As starting point, in order to introduce concepts useful for this thesis, we give a definition of the term *stability*. Following the distinctions made by J. Hofbauer [15], while a physicist intends the stable equilibrium of a population as a steady state that is constantly re-assumed after a small perturbation, a biologist will certainly identify as equilibrium a random process evolving with time, i.e. stochastic, that never becomes extinct over time, where the populations fluctuate around average values with defined variances. We also distinguish between *inner stability*, that regards the stability of a system under little fluctuations. Thanks to self-regulation, and the *outer stability*, which deals with the introduction (like migration from the surrounding environment) of a new species in the considered system. A quantity that usually is relevant in ecology is the *Time to extinction* parameter T_e and its related index of stability $\xi = \ln(T_e)$. Sometimes it is a relevant number to quantify the stability of a system.

We start with the main definitions and concepts about stability in dynamical systems.

Definition 1.1 (Ordinary Differential Equations ODE)**.** Given a vector field $\mathbf{f} : \mathbb{R}^n \to \mathbb{R}^n$ we define a system of ODE as

$$\dot{\mathbf{x}}(t) = \mathbf{f}(t, \mathbf{x}) \tag{1.1}$$

A *solution* of a ODE is a map

$$t \to \mathbf{x}(t) = (x_1(t), \ldots, x_n(t))$$

where $t \in I$ some interval in $\mathbb{R}$ to $\mathbb{R}^n$, that satisfies the former equation.

An *initial condition* is a particular value of the solution at a given time, and the theorem of uniqueness of solution tells us that there can be only one solution for each initial condition. A particular case (that we will consider most) of ODE is the *time-independent*: $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$. The solutions of the form $\mathbf{x}(t) = \mathbf{c}$; $\mathbf{c} \in \mathbb{R}^n$ are known as *equilibrium points*. Recalling the concept (in Lyapunov sense) of stable equilibrium point we define:

Definition 1.2 (Stable equilibrium point)**.** An equilibrium point $\mathbf{c} \in \mathbb{R}^n$ is defined to be *stable* if for every neighborhood U of $\mathbf{c}$, $\exists$ a neighbourhood V of $\mathbf{c}$, such that the solution $\mathbf{x}(\mathbf{x_0}, t)$ with $\mathbf{x_0} = \mathbf{x}(t_0)$ will stay in U for every time.

Definition 1.3 (Asymptotically stable equilibrium point)**.** If the orbits of the latter definition converge to $\mathbf{c}$ (i.e. $\mathbf{x}(t)$ converge to $\mathbf{c}$) then the stable point is *asymptotically stable*. The set of points $\mathbf{x}$ whose orbits converge to $\mathbf{c}$ is called *basin of attraction* of $\mathbf{c}$ (and it is an open invariant set).

If we act on the system by producing a perturbation, it can be that the solution will stay stationary in the perturbed condition or that it will oscillate with fixed amplitude. In these cases we refer to a *neutral stability point*.
Let us introduce the object that defines the asymptotic properties of a solution $\mathbf{x}(t)$: The *ω-limit* of a solution $\mathbf{x}$ for a time-independent ODE, is the set of all accumulation points of $\mathbf{x}(t)$ for $t \to +\infty$:

$$\omega(\mathbf{x}) = \{\mathbf{y} \in \mathbb{R}^n : \mathbf{x}(t_k) \to \mathbf{y} \text{ for some sequence } \mathrm{t_k} \to +\infty\}$$

The converse limit for $t_k \to -\infty$ is called *α-limit*. Of course this set can be empty, and all the points in the *ω-limit* have their neighbourhood visited constantly by $\mathbf{x}(t)$ for $t > 0$. This set has the property of being *closed*, since it is a set of accumulation points. It is also *invariant* and also it can be write the *ω-limit* as an intersection of closed sets:

$$\omega(\mathbf{x}) = \bigcap_{t \geq 0} \overline{\{\mathbf{x}(s) : s \geq t\}}$$

Other features are that rest points and periodic orbits constitute their own ω-limits and if $\omega(\mathbf{x})$ is compact, it is also connected, that is any two points that belong to $\omega(\mathbf{x})$ can be joined by a continuous path in $\omega(\mathbf{x})$ itself. Thank to the *Lyapunov Theorem* we can deal with ω-limit also lacking of the explicit solution (but it does not tell us how to find a proper V):

Theorem 1.1.1 (Lyapunov theorem)**.**
Let $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$ a time- independent ODE defined on some subset G of $\mathbb{R}^n$. Let $V : G \to \mathbb{R}$ be continuously differentiable. If for some solution $\mathbf{x}(t)$ the derivative of $\dot{V}$ of the map $t \to V(\mathbf{x}(t))$ satisfies the inequality $\dot{V} \geq 0$ (or $\dot{V}(\mathbf{x}) \leq 0$), then $\omega(\mathbf{x}) \bigcap G$ is contained in the set $\{\mathbf{x} \in G : \dot{V} = 0\}$ (and so is $\alpha(\mathbf{x}) \bigcap G$).

Proof. If $\mathbf{y} \in \omega(\mathbf{x}) \bigcap G$, there is a sequence $t_k \to +\infty$ with $\mathbf{x}(t_k) \to \mathbf{y}$. Since $\dot{V} \geq 0$ along the orbit of $\mathbf{x}$, one has $\dot{V}(\mathbf{y}) \geq 0$ by continuity. Suppose that $\dot{V}(\mathbf{y}) = 0$ does

not hold. Then $\dot{V}(\mathbf{y}) > 0$. Since the value of V can never decrease along an orbit, this implies

$$V(\mathbf{y}(t)) > V(\mathbf{y})$$

for $t > 0$. The function $V(\mathbf{x}(t))$ is monotonically increasing. Since V is continuous, $V(\mathbf{x}(t))$ converges to $V(\mathbf{y})$, and hence

$$V(\mathbf{x}(t)) \leq V(\mathbf{y})$$

for very $t \in \mathbb{R}$. From $\mathbf{t}_k \to \mathbf{y}$ it follows that $\mathbf{x}(t_k + t) \to \mathbf{y}(t)$ and hence

$$V(\mathbf{x}(t)_k + t) \to V(\mathbf{y}(t))$$

and thanks to the first relation $V(\mathbf{y}(t)) > V(\mathbf{y})$ we get

$$V(\mathbf{x}(t_k + t)) > V(\mathbf{y})$$

for k sufficiently large. This contradicts the fact that $V(\mathbf{x}(t)) \leq V(\mathbf{y})$. □

Note that this theorem does not tell us how to find a *Laypunov function* V, and in general this is a tough task.

If we consider a two dimensional differential Lotka-Volterra equation, then any solution is a curve γ that divides the plain in an exterior and interior. Thanks to this property we can show the

Theorem 1.1.2 (Poincarè-Brendixon theorem)**.**
Let $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$ be an ODE defined on an open set $G \subseteq \mathbb{R}^2$. Let $\omega(\mathbf{x})$ be a nonempty compact ω-limit set. Then if $\omega(\mathbf{x})$ contains no equilibrium point, it must be a periodic orbit.

This means that if $K \subseteq G$ is nonempty, compact and forward invariant, then K must contain a rest point or a periodic orbit. If γ is a periodic orbit which, together with its interior Γ, is contained in G, then Γ contains a rest point.

1.1.1 Linearisation

One of the most used techniques in the study of differential equations is the process of linearisation. In fact locally, thanks to the Grobman-Hartman theorem [11, 12, 13], the orbits near the fixed point of the non-linear equation look like those of the linear ones in the origin of the transformed coordinates. Considering the equation 1.1, that have an equilibrium in $\mathbf{x}^*$, and then expanding it with Taylor around the fix point $\mathbf{x}^*$, brings the linear equation

$$\dot{\mathbf{y}} = A\mathbf{y}$$

where $\mathbf{y} = \mathbf{x} - \mathbf{x}^*$, and A is the Jacobian matrix with entries $A_{ij} = \frac{\partial f_i}{\partial x_j}$. The study of this matrix gives the local behavior of 1.1.
If A is a real real matrix and has complex eigenvalues, they occur in conjugated pairs. Indeed the solution of the linear equation is a combination of the following objects:

1. $e^{\lambda t}$, if λ is a real eigenvalue of A;
2. $e^{at}\cos bt$ and $e^{at}\sin bt$, where $\mu = a + ib$ is a complex eigenvalue of A;
3. $t^j e^{\lambda t}$, or $t^j e^{at}\cos bt$ and $t^j e^{at}\sin bt$, with $0 \leq j < m$,if the eigenvalue λ or μ occurs with multiplicity m.

With complex eigenvalues, the term introduces an oscillatory component, that will be damped only if $a < 0$. The origin $\mathbf{0}$ is a fixed point of the differential equation. The complex eigenvalues μ introduce an oscillatory component to the solutions, that are damped only if $a < 0$.
The origin $\mathbf{0}$ is a fix point and is called:

- a *sink*, if the real parts of all the eigenvalues are all negative. Then $\mathbf{0}$ is the ω-limit of every orbits.
- a *source*, if the real parts of all the eigenvalues are all positive. Then $\mathbf{0}$ is the α-limit of every orbits.
- a *saddle*, if some eigenvalues are in the right half of the complex plane and some are in the left half of it, but non stands on the imaginary axis. The orbits whose ω-limit (α-limit) is $\mathbf{0}$ form a linear submanifold in $\mathbb{R}^n$ called "stable (unstable) manifold"
- *hyperbolic*, if no eigenvalue has null real part (it is a source, a saddle or a sink).
- a *center*, if alla eigenvalues are on the imaginary axes.

We presented this topic in the most brief way possible and as we see in Chapter 4, these results sketched here will be useful.

1.1.2 The community matrix

We now show that the matrix A that follows from linearisation is a useful object that describes the biological features of the specific system and contains the mathematical features that describe its stability.
If we consider a set of n equations for the relative $N_i(t)$ species of the ecological system [19] that we are taking in account

$$\frac{dN_i(t)}{dt} = f_i(N_1(t), \ldots, N_n(t)) \tag{1.2}$$

where the growth rate is given by the f_i functions, that also gives us the equilibrium points of the system

$$f_i(N_1^*, \ldots, N_n^*) = 0$$

To get a local information of the stability of these points we perform a linear expansion near the equilibrium

$$N_i(t) = N_i^* + x_i(t)$$

where x_i is a small perturbation of the i-th species. Substituting the latter equation in 1.2 and ignoring the terms of second (or higher) order gives

$$\frac{dx_i(t)}{dt} = \sum_{j=1}^{n} a_{ij} x_j(t) \tag{1.3}$$

and the set of n equations describes the dynamics close to $\vec{N}^*$

$$\frac{d\vec{x}(t)}{dt} = A\,\vec{x}(t) \tag{1.4}$$

Here the $n \times n$ matrix A is called "community matrix" (CM) (Levins 1968a) whose elements $(A)_{ij} = a_{ij}$, describe the effect of species j on the i near equilibrium and that has a prominent role on the system's stability

$$a_{ij} = \left(\frac{\partial f_i}{\partial N_j} \right) \Bigg|_{\vec{N}^*} \tag{1.5}$$

The solutions of equation 1.3 can be written as

$$x_i(t) = \sum_{j=1}^{n} C_{ij} \exp(\lambda_j t)$$

where the coefficients C_{ij} are given by the initial conditions and λ_i are the relative eigenvalues of A with $i = 1, \ldots, n$ that in general takes the form $\lambda = \zeta + i\xi$. Depending of the sign of ζ we will have an oscillatory exponential oscillation that will depend on the imaginary part ξ. This means that a little perturbation from the equilibrium point will be dumped only if all the eigenvalues have negative real parts, so that we can claim that an equilibrium point will be locally stable if the eingenvalues of the system lie on the negative demiplane of the complex numbers. If only one λ has positive real part, then the equilibrium is unstable. In the latter case, at first perturbations will grow, but we cannot say much more because we must consider the terms of second (or higher) order and nonlinearities will have the last word on the dynamics of the system.
We stress the fact that in the linear case, the elements of the CM describe the real interactions between species, but in the nonlinear case, it describes the behavior of the system only near the equilibrium points.

Qualitative study of CM

As first described by Odum [16], the signs of the elements of the CM are related to the interactions between the species of the system. If the effect of the j-th species is to favor contrast or ignore the i-th species, then the relative signs of the Odum's scheme will be respectively positive, negative or zero. Below we present the table of all possible interaction types:

We can distinguish between five categories of interaction between species (where the symbols $+, -, 0$ are relative to the signs of the elements a_{ij}) and they are: commensalism $(+0)$, amensalism (-0), mutualism or symbiosis $(++)$, competition $(--)$

i to j/ j to i	+	0	-
+	++	+0	+-
0	0+	00	0-
-	-+	-0	–

Table 1.1: Odum's scheme for interacting species.

and general predator-prey interaction $(+-)$. Even a qualitative study of the community matrix gives important information about the stability of the system that we are considering. The *qualitative stability* is defined as the stability that is determined without considering the intensities of the elements of the matrix itself. Sometimes it can be that one, looking at the food web diagram of a particular biological system, may determine the sign of the community matrix elements. This means that it can be given a sketch of how the system will evolve without sophisticated techniques. In 1965, it was proposed [17] that there exists a set of necessary and sufficient conditions for a matrix A of $n \times n$ elements a_{ij} to be qualitative stable:

1. $a_{ii} \leq 0$, for all i.
   This first criterion requires the fact that the interactions inside the same species did not produce positive destabilizing feedback effect.

2. $a_{ii} \neq 0$, at least for one i.
   This means that inside the whole system, one of the species presents an autostabilizing effect.

3. $a_{ij}a_{ji} \leq 0$ for all $i \neq j$.
   That is the mutualistic $(++)$ and competitive $(--)$ interactions does not contribute to the stability of the system.

4. For each sequence of three or more indices $i, j, k, \ldots, p, q$ (with $i \neq j \neq k \neq \cdots \neq p \neq q$), the product $a_{ij}a_{jk}, \ldots, a_{pq}a_{qi} = 0$. This means that the closed circle contributes negatively to the stability of the system.

5. $\det(A) \neq 0$.
   It is required that the matrix A must be non-singular otherwise there would be more species than equations, and the system would be indetermined.

1.2 The Lotka-Volterra model

As we said this was the first model proposed about the evolutionary dynamics of population numbers that compete with each other in their relative niche, in particular it describes asymmetrical interactions between predator-prey or resource-consumers systems.

Of course, the stochastic form of L-V will certainly drive one of the species to extinction[1], meanwhile oscillations in the populations can be induced by imposing a limit to the preys population (Volterra model). Thus the deterministic L-V model and the stochastic Volterra model have similar features. In the deterministic L-V model, the evolution of the species involved is characterized by a positive growth rate of the preys (H) in absence of predators, and by a negative rate depending of the predator population. Instead for the predator (P), we have a negative rate in absence of preys and a positive rate that multiplies the preys population[2] [19],

$$\begin{cases} \frac{dH(t))}{dt} & = [a - \alpha P(t)]\, H(t) \\ \\ \frac{dP(t))}{dt} & = [-b + \beta H(t)]\, P(t) \end{cases} \tag{1.6}$$

The stable point of 1.6 is easy to find by imposing null derivatives (the trivial solution $P^* = 0$ and $H^* = 0$ will not be considered)

$$\begin{cases} [a - \alpha P(t)]\, H(t) = 0 & \Rightarrow P^* = a/\alpha \\ [-b + \beta H(t)]\, P(t) = 0 & \Rightarrow H^* = b/\beta \end{cases} \tag{1.7}$$

so that the CM has the form $A = \begin{pmatrix} 0 & -\alpha b/\beta \\ \beta a/\alpha & 0 \end{pmatrix}$. The eigenvalues of A are $\lambda = \pm i\sqrt{ab}$ that indicate neutral stability, and a local study of the dynamics around (H^*, P^*) gives us the period of the oscillations around the equilibrium point with $T = 2\pi/\sqrt{ab}$. Now we show some examples of the closed curves and two different examples of the time-dependent solutions of this system.

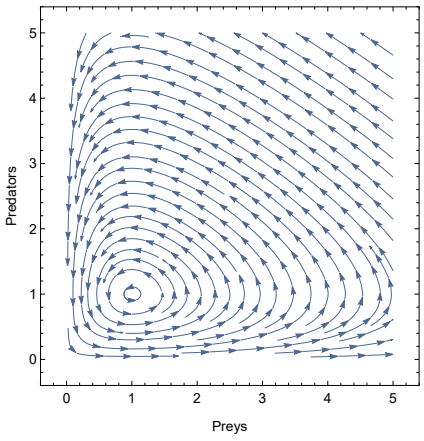


Figure 1.1: Representation of the closed curves of the coupled equations.

[1] Since the model does not contain a spatial component.

[2] The classical deterministic L-V model has been criticized by many for its non-realistic feature of the oscillations, since they are completely determined by the system's initial conditions. Another weak point is the lack of robustness of the marginally stable neutral cycle against perturbations [18].

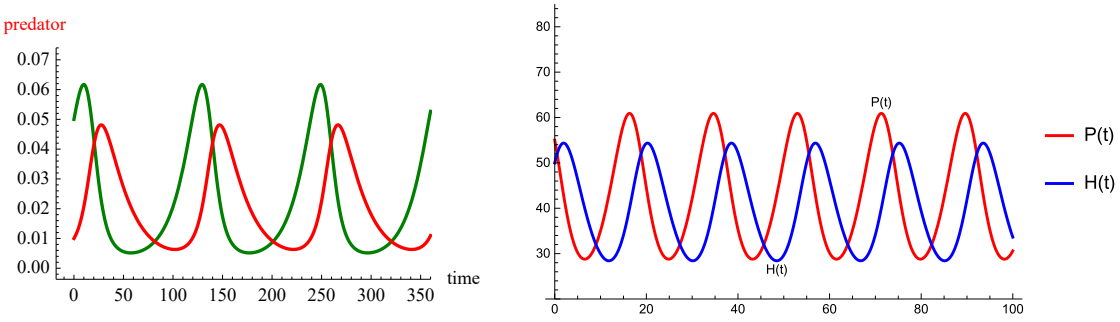


Figure 1.2: Some examples of Lotka-Volterra realisation with different initial conditions and parameters.

As we anticipated above, these quantities will oscillate with a relative frequencies[3] around (P^*, H^*). Denoting T the period of the solution we have

$$\frac{1}{T}\int_0^T H(t)dt = H^*\,, \qquad \frac{1}{T}\int_0^T P(t)dt = P^*$$

thus by rearranging and integrating 1.6 we get

$$\frac{d}{dt}\ln\, H(t)dt = \frac{\dot{H}}{H} = a - \alpha P(t) \;\Rightarrow\; \int_0^T \frac{d}{dt} log\, H(t)dt = \int_0^T (a - \alpha P(t))dt$$

and using the fact that $H(T) = H(0)$ we have $\ln H(T) = \ln H(0)$ and then

$$\frac{1}{T}\int_0^T P(t)\,dt = \frac{a}{\alpha} = P^*$$

As anticipated before, by a simple manipulation of the equations 1.6 it is possible to show that the dynamic is given by periodic close curves. In fact, integrating with the separation of the variables we get

$$\frac{dH}{dP} = \frac{[a - \alpha P]\,H}{[-b + \beta H]\,P} \quad \Rightarrow \quad b\ln H - \beta H + a\ln P - \alpha P = cost.$$

These equations are closed curves that are determined by the initial condition $(H(0), P(0))$. Following Hofbauer, another common way to represent a Lotka-Volterra system is

$$\dot{x}_i = x_i\left(r_i + \sum_{j=1}^{n} a_{ij}x_j\right)$$

where $i = 1, \ldots, n$. Where the matrix $\tilde{A} = (a_{ij})$ is called *interaction matrix*[4]. The topic relative to these equations is very vast, so there are plenty of results that have relevance. In this framework, it is important to show a theorem that will be verified

[3] Depending on the initial conditions.

[4] Do not make mistake by confusing these coefficient with those of the community matrix. From now on is used only the interaction matrix with the above defined entries.

immediately by our simulation in chapter 4, which implies that if there exists a rest point $\mathbf{p}$, and if the solution $\mathbf{x}(t)$ converges neither to the boundary nor to infinity, then its time average converges to $\mathbf{p}$:

Theorem 1.2.1.
If there exist positive constant a and A such that $a < x_i(t) < A$ for all $i = 1, \ldots, n$ and all $t > 0$, and $\mathbf{p}$ is the only fixed point in the positive real demiplan, then $\lim_{T\to\infty} \frac{1}{T} \int_0^T x_i(t)dt = p_i$.

Proof. Let us write the differential equation

$$(\log x_i)' = r_i + \sum_i a_{ij} x_j$$

and integrate it from 0 to T. After dividing by T, we obtain

$$\frac{\log x_i(T) - \log x_i(0)}{T} = r_i + \sum a_{ij} z_j(T) \tag{1.8}$$

where

$$z_j(T) = \frac{1}{T} \int_0^T x_j(t)dt.$$

Obviously $a < z_j(T) < A$ for all j and all $T > 0$. Now consider any sequence T_k converging to $+\infty$. The bounded sequence $z_j(T_k)$ admits a convergent subsequence. By diagonalisation we obtain a sequence (which we are calling T_k again) such that $z_j(T_k)$ converges for every j towards some limit which we shall denote by $\overline{z}_j$. The subsequence $\log x_i(T_k) - \log x_i(0)$ are also bounded. Passage to the limit in eq. 1.8 thus leads to

$$0 = r_i + \sum a_{ij} \bar{z}_j$$

The point $\bar{z} = (\bar{z}_1, \ldots, \bar{z}_n)$ is therefore a rest point. Since $\overline{z}_j \geq a > 0$, belongs to $int\ \mathbb{R}^n$, hence it coincides with $\mathbf{p}$. □

1.2.1 Lotka-Volterra model for $2n$ species

It is now easy to extend the model to the case of $2n$ species, where now there are n predators $P_(i)$, $[i = 1, 2, \ldots, n]$ and n preys $H_i(t)$, $[i = 1, \ldots, n]$. The extended model now takes the form of equation 1.9.

$$\begin{cases} \frac{dH_i(t))}{dt} & = H_i(t) \left[a_i - \sum_{j=1}^n \alpha_{ij} P_j(t) \right] \\ \\ \frac{dP_i(t))}{dt} & = P_i(t) \left[-b_i + \sum_{j=1}^n \beta_{ij} H_j(t) \right] \end{cases} \tag{1.9}$$

Where $i = 1, \ldots, n$ and all the parameters are positive. In order to find the equilibrium points for both predators and preys populations, the square brackets in equation 1.9 must be set to zero. Then we get to deal with a set of n linear equations that can be expressed in the compact form

$$\alpha \mathbf{P}^* = \mathbf{a} \tag{1.10}$$

Where α is a $n \times n$ matrix and $\mathbf{P}^*$ is the vector with n components P_i^* and $\mathbf{a}$ the vector with a_i. In the same way we have the equilibrium point for H_i we have

$$\beta \mathbf{H}^* = \mathbf{b} \tag{1.11}$$

Where the only bound for the parameters must be such that the equilibrium points must be positive for every populations.
The community matrix (CM) is then a $2n \times 2n$ matrix of this form [19],

$$A = \begin{pmatrix} \mathbf{0} & -\alpha^* \\ \beta & \mathbf{0} \end{pmatrix} \tag{1.12}$$

Where α^* and β^* are $n \times n$ matrices with these elements

$$\alpha_{ij}^* = H_i^* \alpha_{ij}, \quad \beta_{ij}^* = P_i^* \beta_{ij}$$

The $2n$ eigenvalues of this matrix are found to be in n pairs

$$\lambda = \zeta + i\xi \qquad \lambda = -\zeta - i\xi$$

This means that all the eigenvalues have real parts equal to zero, which indicates a neutrally stable behaviour, or at least one eigenvalue has positive real parts and then we are in the unstable system. In Fig.1.3 we show a particular realisation for this latter case in which one of the two prey species goes extinct. This observation tells us that systems with more than 2 populations are in general equal or less stable.

This model can be generalised taking in account of a more general type of (diagonal[5]) interaction between the species involved. In fact considering the rate factors members as a generic function of the popilation N_i, where $i = 1, \ldots, n$:

$$\frac{dN_i}{dt} = f_i(N_i) g_i(N_1, \ldots, N_j, \ldots, N_n) \; ; \; j \neq i$$

This means that the dependence of the species itself (F_i) can be put as a multiplying factor. As before, to get the equilibrium points we impose $g_i = 0$ for each i. Setting $f_i(N_i) = N_i$ and a simple linear G, we recover equation 1.9. As shown in [20] such systems will drive the some populations to extinction in order to get the stability.

Lotka-Volterra equations with antisymmetric matrix

The Lotka-Volterra equations can be studied more easily if the matrix elements undergo some symmetries. A particular case can be an *antysimmetric* matrix. In this case we deal with an equation like

[5] The diagonal elements of the community matrix will be $a_{ii} = 0$.

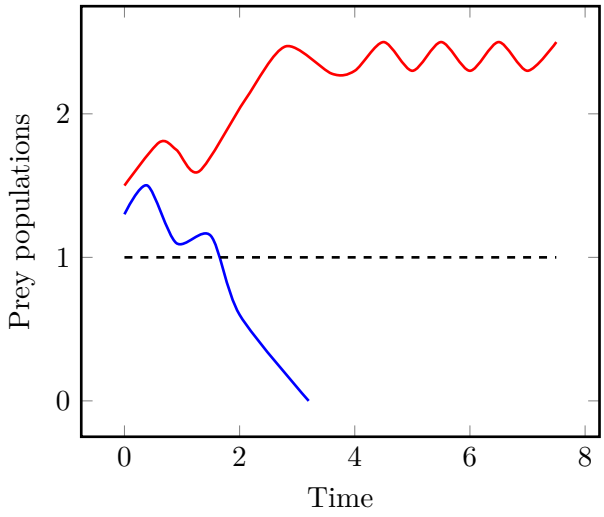


Figure 1.3: Simulation with 2 prey populations. Red (blue) lines are respectively H_1, (H_2). The initial conditions of this system are $H_1(0) = 1.5$(red) and $H_2(0) = 1.3$(blue), where the dashed lines represent the normalised equilibrium populations H_1^*, H_2^*.

$$\frac{dN_i(t)}{dt} = N_i(t)\left[a_i - \sum_{j=1}^{n} \alpha_{ij} N_j(t)\right] \tag{1.13}$$

where of course the non-diagonal coefficients are antisymmetric and the diagonal are zero

$$\alpha_{ij} = -\alpha_{ji} \quad \text{and} \quad \alpha_{ii} = 0.$$

In this case, the relative biological modeling depends on the sign of α_{ij}: if $\alpha > 0$, then the jth species is the prey of the ith one, while if $\alpha < 0$ then the ith species is the prey of the jth one. Thus a certain species can be both a predator and a prey in its interactions inside the system. We see also that setting in equation 1.9 the parameters $\alpha_{ji} = \beta_{ij}$ we recover equation 1.13, and we get the the equilibrium point in the usual way

$$a_i = \sum_{j=1}^{n} a_{ij} N_j^*.$$

Due to the properties of the antisymmetric matrices, its eigenvalues are forced to be imaginary[6], so that the systems have purely oscillatory behavior when displaced from equilibrium i.e. neutral stability.

[6]Since the eigenvalues occur as conjugated purely imaginary numbers $\pm i\omega$, it follows that with a odd number of species, the relative eigenvalue must be zero.

Given the equilibrium point N_i^*, it has been shown (Kerner, 1957) that the quantity

$$\Phi \equiv \sum_{i=1}^{m} \{N_i(t) - N_i^* \ln N_i(t)\} \tag{1.14}$$

and if we derive it in time we obtain

$$\frac{d\Phi}{dt} = - \sum_{i,j=1}^{m} (N_i(t) - N_i^*)\, \alpha_{ij} \left(N_j(t) - N_j^*\right) \tag{1.15}$$

the summation all over the indicies implies that the equation 1.15 is equal to zero if $\alpha_{ij} = -\alpha_{ji}$. This conservation law is associated with the oscillatory behavior of the system.

Chapter 2

Non-equilibrium and Markov processes

2.1 Presenting the non-equilibrium

As we know, at first the aim of statistical mechanics was that of creating a bridge between the microscopical description of a system and thermodynamics. Indeed it considers only the macroscopical properties and features of the specific system in which the fluctuations (typically Gaussian) could be neglected for big enough systems since they are $\sim 1/\sqrt{N}$, with N the number of particles. By taking into account fluctuations, statistical mechanics gives us mathematical relations that are not reachable with standard thermodynamic. The corner stone of this framework was that all the considerations and results achieved along the years were obtained at *equilibrium*, i.e. for system state in which all observable quantities do not depend on time and where there are no currents. Time, as is pointed out later, plays a central role for non-equilibrium thermodynamic.
In this chapter we will show that the thermodynamic equilibrium is linked with the time-reversal invariance. A macroscopic system is said to reach thermodynamic equilibrium if it reaches thermal, mechanical and chemical equilibrium, i.e. temperature, pressure and chemical potential of different parts are the same [21]. In conclusion, the thermodynamic equilibrium is characterized by the fact that the average values of all the fluxes exchanged between the different components of the system and its environment identically vanish.
The non-equilibrium concept subverts the last statement and can be applied in a broad cases of systems, such as: chemical reactions, electrical circuits, systems in contact with many reservoirs with different temperatures, biological systems that have internal fluxes or with fluxes exchanged with the environment like probabilistic cellular automata [22, 23, 24]. Citing Gallavotti [25], the essential difference between equilibrium and non-equilibrium is that in the first case, time evolution is conservative and Hamiltonian while in the second case time evolution takes place under the action of external agents which could be, for instance, external non-conservative

forces. This means that in non-equilibrium processes a privileged direction of time emerges, and time-reversibility is prohibited. A non-equilibrium state can be reached because of a change of the environment state or because of time (in)dependent forces. In the latter case the system (does) does not reach a non-equilibrium stationary state (NESS), and the system performs like a biased random walk in its own configuration space, leading to non-vanishing probability currents, and this is exactly what our model concerns about [42].
Thus by definition, a NESS is a stationary state of the system in which the mean values of its observables are constant and there are non-zero currents in it. Here in this thesis, we are interested in systems with "driving forces". Furthermore, we are mainly interested in the time-invariant stationary behavior of such systems. To sum up, the non-equilibrium steady state[1] is characterized in terms of several key notions: time irreversibility, breakdown of detailed balance, free energy dissipation, and positive entropy production rate [21].

2.2 Stochastic and Markov Processes

The processes that usually happen in nature are not at equilibrium, and in general they cannot be well described by deterministic equations (this comes evident just thinking about quantum mechanics and the theory of chaos arised in the last century). The fundamental tool for studying these processes require the introduction of a definition of an aleatory variable, i.e. whose values occurs with a certain probability along its observation. This means that forward we do not consider anymore the ensamble theory for a certain state, but we focus on the probabilistic trajectory done by our system in its phase-space volume.
Since we assume that the model that describes our system follows a microscopic stochastic dynamics, we can say that the system is described by a continuous-time Markovian stochastic process. Considering for example a discrete space of states, this assumption means that the time evolution equation is set up once transition rates are given. Thus transition rates play a central role in the present approach and we can certainly say that a system is considered to be theoretically defined once this quantities are given a priori (and this is exactly what we are going to do in Chapter 4). Given the transition rates, the probability $P(x;t)$ of state being in x at time t is obtained by solving its evolution equations. In this chapter is presented the concept of stochastic process, of Markovian dynamics and will be derived the master equation[27]. Then is discussed the Van Kampen's systems size expansion that allow us in Chapter 4 to derive the deterministic equations for the model itself. At the end we treat the Fokker-Planck equations and its main features.

A *random variable* X is defined by a set Ω of possible values (that can be either

[1] An interesting point is what I. Prigogine [26] said in his books, claiming that non-equilibrium systems can generate self-organized order even without introducing external mechanical forces.

discrete or continuous) and a probability distribution $P_X(x)$ over this set[2]. We note that $P_X(x)\,dx$ is the probability of variable X to have a value between x and $x+dx$. In case of continuous variable we have that $P_X(x) \geq 0$ and that $\int P_X(x)dx = 1$. If we consider a stochastic variable X, is possible to define a transformation of variable X using a function $Y = f(X)$ so that

$$P_Y(y) = \int P_X(x)\delta(f(x) - y)dx.$$

If now we consider a transformation of the stochastic variable X that have a dependence in time t we get

$$Y_X(t) = f(X, t)$$

and if we consider a particular value $x = X$ for the function f the evolution of this process along time is called a *realization of a stochastic process*

$$Y_x(t) = f(x, t).$$

In order not to be much dispersive, we do not report the definitions of n-th moments, the autocorrelation function or of the generating function.
The probability density for $Y_X(t)$ to take the value y at time t is

$$P_1(y, t) = \int \delta(y - Y_x(t))P_X(x)\,dx$$

and the joint probability density that the variable Y has the value y_1 at t_1, the value y_2 at t_2 and o on is

$$P_n(y_1, t_1; y_2, t_2; \ldots; y_n, t_n) = \int dx P_X(x)\delta(y_1 - Y_x(t_1))\delta(y_2 - Y_x(t_2)) \cdots \delta(y_n - Y_x(t_n)) \tag{2.1}$$

In this way have defined an infinite hierarchy of probabilities densities P_n and with that we can have the averages mentioned before

$$\langle Y(t_1)Y(t_2) \cdots Y(t_n)\rangle = \int y_1 y_2 \cdots y_n P_n(y_1, t_1; y_2, t_2; \ldots; y_n, t_n)dy_1 dy_2 \ldots dy_n$$

If we consider P_n where all the times are different (and ordinated by $t_1 \leq t_2 \leq \ldots \leq t_n$), then the hierarchy of function P_n

$$P_1(y_1, t_1)\,, \quad P_2(y_1, t_1; y_2, t_2)\ \ldots\ P_n(y_1, t_1; y_2, t_2; \ldots; y_n, t_n)$$

defined follows this conditions:

- $P_n \geq 0$;
- P_n does not change by swapping two pairs: $(y_k, t_k) \rightleftarrows (y_m, t_m)$;
- $\int P_n(y_1, t_1; y_2, t_2; \ldots; y_{n-1}, t_{n-1}; y_n, t_n)dy_n = P_{n-1}(y_1, t_1; y_2, t_2; \ldots; y_{n-1}, t_{n-1})$;

[2]Sometimes $P_X(x)$ will be called $P(x)$, omitting the X variable.

- $\int P_1(y_1, t_1)dy_1 = 1$;

Kolmogorov proved that since P_n allows to calculate averages, then the constitute completely a stochastic process $Y(t)$. The *conditional probability* for the probability density function Y to take the values y_2 at t_2, given the fact that it was in y_1 at t_1 is

$$\int P_{1|1}(y-2, t_2|y_1, t_1)dy_2 = 1 \tag{2.2}$$

and in a general way we can define the conditional probability with many different times:

$$P_{l|k}(y_{k+1}, t_{k+1}; \ldots; y_{k+l}, t_{k+l}|y_1, t_1; \ldots; y_k, t_k) = \\ = \frac{P_{k+l}(y_1, t_1; \ldots; y_k, t_k; y_{k+1}, t_{k+1}; \ldots; y_{k+l}, t_{k+l})}{P_k(y_1, t_1; \ldots; y_k, t_k)} \tag{2.3}$$

where by definition $P_{l|k}$ is both symmetric in the set of k and l variables.
A stochastic process is called *stationary* when all the P_n depend only on the differences on time

$$P_n(y_1, t_1 + \tau; y_2, t_2 + \tau; \ldots; y_n, t_n + \tau) = P_n(y_1, t_1; y_2, t_2; \ldots; y_n, t_n)$$

thus the moments will not be affected by a shift in time $\langle Y(t_1 + \tau)Y(t_2 + \tau) \cdots Y(t_n + \tau)\rangle = \langle Y(t_1)Y(t_2) \cdots Y(t_n)\rangle, \quad \forall \tau, t_i, n$. Now we are ready to define a Markov process.

2.3 Markov processes

In literature exist plenty of way to introduce and define a Markov chain or process, but here we follow Van Kampen's book [27] since it is one of the most concise and less technical from the mathematical point of view.
A *Markov process* is defined as a stochastic process with n successive time $t_1 < t_2 < \ldots < t_n$ and with the fundamental property

$$P_{1|n-1}(y_n, t_n|y_1, t_1; y_2, t_2; \ldots; y_{n-1}, t_{n-1}) = P_{1|1}(y_n, t_n|y_{n-1}, t_{n-1}) \tag{2.4}$$

or equivalently

$$P_{l|k}(y_{k+1}, t_{k+1}; \ldots; y_{k+l}, t_{k+l}|y_1, t_1; \ldots; y_k, t_k) = P_{l|1}(y_{k+1}, t_{k+1}; \ldots; y_{k+l}, t_{k+l}|y_k, t_k) \tag{2.5}$$

which means that a process like this has "no memory"[3]. To be more precise, the memory history of the process has a role in the evolution of itself but what we are stating here is that the probability of going in the next configuration (continuous or discrete that it is) depends only on the last configuration assumed by it.
Here we present a simple classification of different Markov processes based on the kind of its states and indices:

[3]The oldest Markov process identified in nature is the Brownian motion, in which a heavy particle immersed in a fluid randomly collides with the molecules of the medium. The markovianity of this process is due to the fact that the particle's velocity at each collision depends only on its velocity before being totally changed with another collision.

states/indicies	continuous	discrete
continuous	Markov processes at continuous time	Markov processes at discrete time
discrete	Markov chains at continuous time	Markov chains at discrete time

The definition just presented is very powerful, since it allows to describe the entire Markov process knowing only the probability $P_1(y_1, t_1)$ and $P_{1|1}(y_2, t_2|y_1, t_1)$ i.e. we can reconstruct the entire hierarchy from those. As useful example, we "decompose" a three step process P_3 with $t_1 < t_2 < t_3$ by using the Markov property:

$$\begin{aligned} P_3(y_1, t_1; y_2, t_2; y_3, t_3) &= P_2(y_1, t_1; y_2, t_2) P_{1|1}(y_3, t_3|y_2, t_2) \\ &= P_1(y_1, t_1) P_{1|1}(y_2, t_2|y_1, t_1) P_{1|1}(y_3, t_3|y_2, t_2) \end{aligned} \tag{2.6}$$

where we have used equation 2.3 and 2.4. If one iterates this procedure can obtains all P_n.

Chapman-Kolmogorov equation

Now that we have defined the basic notions of our framework, it is possible to derive a fundamental equation for a Markov process, named the *Chapman-Kolmogorov equation*. Again we consider a three step process with temporal ordering $t_1 < t_2 < t_3$. As seen above we have

$$P_3(y_1, t_1; y_2, t_2; y_3, t_3) = P_1(y_1, t_1) P_{1|1}(y_2, t_2|y_1, t_1) P_{1|1}(y_3, t_3|y_2, t_2).$$

Integrating this equation for dy_2 we get

$$\begin{aligned} \int dy_2 P_3(y_1, t_1; y_2, t_2; y_3, t_3) = P_2(y_1, t_1; y_3, t_3) &= \cancel{P_1(y_1, t_1)} P_{1|1}(y_3, t_3|y_1, t_1) \\ &= \cancel{P_1(y_1, t_1)} \int dy_2 P_{1|1}(y_2, t_2|y_1, t_1) P_{1|1}(y_3, t_3|y_2, t_2) \end{aligned} \tag{2.7}$$

so that

$$P_{1|1}(y_3, t_3|y_1, t_1) = \int P_{1|1}(y_3, t_3|y_2, t_2) P_{1|1}(y_2, t_2|y_1, t_1) dy_2. \tag{2.8}$$

This is the Chapman-Kolmogorov equation. It says that a process starting at t_1 in y_1, reaches y_1 at t_1 via all the possible space-time configuration between the first and the final point. Of course the functions P_1 and $P_{1|1}$ must not only obey the Chapman-Kolmogorov equation, but also the consistency relation

$$P_1(y_2, t_2) = \int dy_1 P_{1|1}(y_2, t_2|y_1, t_1) P_1(y_1, t_1). \tag{2.9}$$

Note that 2.9 actually contains the profound claim that for the step from 2 to 3 its previous position at 1 has no relevance.
From the Chapman-Kolmogorov equation is possible to verify that it is satisfied by the Weiner process, a fundamental process in this field.

2.3.1 Stationary Markov process

Furthermore, if a Markov process is stationary, it becomes a useful tool for describing fluctuations at equilibrium. A Markov process is called *stationary* if the transition probability $P_{1|1}$ depends only on time interval:

$$P_{1|1}(y_2, t_2|y_1, t_1) \equiv T_\tau(y_2|y_1) \; ; \quad \tau = t_2 - t_1$$

so that the Chapman-Kolmogorov equation has the form

$$T_{\tau+\tau'}(y_3|y_2) \int T_{\tau'}(y_3|y_2) T_\tau(y_2|y_1) dy_2$$

and if we read the integral as a production of two matrices we have

$$T_{\tau+\tau'} = T_\tau \cdot T_{\tau'} \quad (\tau, \tau' \geq 0).$$

Homogeneous process

If we consider a stationary Markov process given by the probabilities $P_1(y_1)$ and $T_\tau(y_2|y_1)$, a non-stationary Markov process can be defined by taking a fixed time t_0 and fixed variable y_0 writing

$$P_1^*(y_1, t_1) = T_{t_1 - t_0}(y_1|y_0)\,,$$

$$P_{1|1}(y_2, t_2|y_1, t_1) = T_{t_2 - t_1}(y_2|y_1)\,.$$

This procedure is nothing than extracting a "sub-ensamble" from the initial process considered. Of course, these processes cannot be stationary since it has been selected a particular time t_0. Anyway its transition probability depends only on time interval just like the transition probability of the starting stationary process. These non-stationary Markov processes are called *homogeneous*. From the physical point of view the extraction of a sub-ensamble means three things:

1. The system derived from the extraction of a sub-ensamble implies that it is set in a non-equilibrium condition.

2. After long time enough, the system returns to equilibrium:

$$P_1^*(y_1, t_1) \to P_1(y_1) \quad \text{for } t \to \infty$$

3. From the above equation this means also that

$$T_{t_1 - t_0}(y_1|y_0) \to P_1(y_1)$$

In practice, we have a stochastic variable that at time t_0 is fixed on having value y_0 and, with the passing of time it evolves to the stationary configuration. This is a usual method of creating in practice stationary systems.

2.3.2 Master Equation

Now we want to derive an equation for Markov processes that is equivalent to the Chapman-Kolmogorov ones, with the advantages of being more easy to use, and which describe the temporal evolution of the probability of the system to be in a certain state. That should concern a differential equation obtained by a taking the limit of the time difference $\tau \to 0$. This means that a master equation is nothing that a continuous-time version of a Markov chain. For convenience we take an homogeneous Markov process with continuous time [29]. We recover the Chapman-Kolmogorov equation derived above for a homogeneous process

$$T_{\tau+\tau'}(y_3|y_1) = \int dy_2 T_{\tau'}(y_3|y_2) T_\tau(y_2|y_1) \tag{2.10}$$

where $\tau = t_2 - t_1$ and $\tau' = t_3 - t_2$. Then we differentiate respect to τ' and take the limit $\tau' \to 0$.
As τ' tends to zero, the transition rate $T'_\tau(y_3|y_2)$ at first order in τ' is $T_{\tau'}(y_3|y_2)$ con:

$$T_{\tau'}(y_3|y_2) = (1 - \tau' a_0(y_2))\delta(y_3 - y_2) + \tau' W(y_3|y_2) + \cdots \tag{2.11}$$

Note that the δ-function is here in order to take account of the possibility of the state to stay in its starting state during τ' and $W(y_3|y_2) \geq 0$ is the transition probability *per unit time* $W(y_3|y_2) = \lim_{\tau' \to 0} \frac{T_{\tau'}(y_3|y_2)}{\tau'}$.
Using the normalisation condition

$$\int T_\tau(y_2|y_1) dy_2 = 1 \tag{2.12}$$

we integrate by dy_3 so that

$$\begin{aligned} \cancel{1} = \int dy_3 T_{\tau'}(y_3|y_2) = \\ = \int dy_3 \left[(1 - \tau' a_0(y_2))\delta(y_3 - y_2) + \tau' W(y_3|y_2)\right] = \\ = \cancel{1} - \tau' a_0(y_2) + \tau' \int dy_3 W(y_3|y_2) \end{aligned} \tag{2.13}$$

$$\cancel{\tau'} a_0(y_2) = \cancel{\tau'} \int dy_3 W(y_3|y_2) \quad \Rightarrow \quad a_0(y_2) = \int dy_3 W(y_3|y_2)$$

Renaming the variable $y_2 \to y_3$ and vice-versa, we get

$$a_0(y_3) = \int dy_2 W(y_2|y_3).$$

Then if we replace equation 2.11 in 2.10 and integrate in dy_2, we obtain

$$\begin{aligned} T_{\tau+\tau'}(y_3|y_1) = \int \left\{[1 - \tau' a_0(y_2)]\delta(y_3 - y_2) T_\tau(y_2|y_1) + \tau' W(y_3|y_2) T_\tau(y_2|y_1)\right\} dy_2 = \\ = T_\tau(y_3|y_1) - \tau' a_0(y_3) T_\tau(y_3|y_1) + \tau' \int W(y_3|y_2) T_\tau(y_2|y_1) dy_2 \end{aligned}$$

Rearranging the last equation and dividing by τ' and finally taking the limit $\tau' \to 0$ comes the definition of partial derivative $\partial/\partial\tau$ one obtains

$$\lim_{\tau'\to 0} \frac{T_{\tau+\tau'}(y_3|y_1) - T_\tau(y_3|y_1)}{\tau'} = \int dy_2 \left[W(y_3|y_2)T_\tau(y_2|y_1) - W(y_2|y_3)T_\tau(y_3|y_1)\right]$$

thus we have derived the so-called *Master Equation*:

$$\frac{\partial}{\partial\tau}T_\tau(y_3|y_1) = \int dy_2 \left[W(y_3|y_2)T_\tau(y_2|y_1) - W(y_2|y_3)T_\tau(y_3|y_1)\right] \tag{2.14}$$

This equation is usually written in this fashion:

$$\frac{\partial P(y,t)}{\partial t} = \int \left\{W(y|y')P(y',t) - W(y'|y)P(y,t)\right\} dy' \tag{2.15}$$

But it must be stressed the fact that 2.15 is not meant as an equation for the single-time distribution $P_1(y,t)$. In fact, if we take a time t_1 and an y_1, and consider the solution of 2.23 (that is determined for $t \geq t_1$ by the initial condition $P(y,t_1) = \delta(t-t_1)$, then we have the solution $T_{t-t_1}(y|y_1)$. This equation is the starting point in our model, since it gives a chance to study the dynamics of a Markov process directly from its microscopic interactions. Concluding, if the probability density function $T(y_3|y_1;\tau)$ is known, one can multiply by $P_1(y_1,t_1)$ and integrate over y_1

$$P_1(y_3,t_1+\tau) = \int dy_1 T_\tau(y_3|y_1)P_1(y_1,t_1)$$

so that

$$\partial_\tau P_1(y_3,t_1+\tau) = \int dy_2 \left\{W(y_3|y_2)P_1(y_2,t_1+\tau) - W(y_2|y_3)P_1(y_3,t_1+\tau)\right\}.$$

2.3.3 Definition of a continuous Markov process

From a theoretical point of view, we need to have a strong definition of whether and how a Markov process can be defined *continuous*. As shown in literature [30], the sample path of a Markov process are *continuous* functions of it with probability one if (uniformly in $\vec{z}$, t and Δt) for any $\varepsilon > 0$ is valid the so-called Lindeberg condition:

$$\lim_{\Delta t\to 0} \frac{1}{\Delta t} \int_{|\vec{x}-\vec{z}|>\varepsilon} d\vec{x}\; p(\vec{x},t+\Delta t|\vec{z},t) = 0$$

which means that the probability for the ending position $\vec{x}$ to be finitely different from $\vec{z}$ goes to zero faster than Δt as Δt goes to zero.

2.3.4 The Fokker-Planck equation

From the master equation can be derived an important relation, that gives the deterministic evolution of the considered system's probability $P_t(C)$. In particular it is used as an approximation of a "real" process or as a general description model for the Markov processes, in which the individual jumps are very small. Using the

notation that will be used in 2.26, the Fokker-Planck equation is a master equation in which the Markov operator is a second order differential operator which brings to:

$$\frac{\partial P(y,t)}{\partial t} = -\frac{\partial}{\partial y}A(y)P(y,t) + \frac{1}{2}\frac{\partial^2}{\partial y^2}B(y)P(y,t) \tag{2.16}$$

where the range of y is continuous and the coefficients $A(y)$ and $B(y)$ are called respectively *drift term* and *diffusion term*[4]. Indeed, consistently with what said in the last paragraph, the solution of equation 2.16 for $t \geq t_1$ is $P(y,t|y_1,t_1)$ which assumes the form of a $\delta(y-y_1)$ when $t = t_1$. The Fokker-Planck equation can be written in terms of a diffusion equation by choosing

$$J(y,t) = A(y)P - \frac{1}{2}\frac{\partial}{\partial y}B(y)P$$

so that

$$\frac{\partial P(y,t)}{\partial t} = -\frac{\partial J(y,t)}{\partial y}$$

and it can be shown that the solution of a Markov process that is described by a linear[5] Fokker-Planck equation (with $A_1 < 0$) is the Ornstein-Uhlenbeck process (a Gaussian) [27]. Let's now derivate the expression of the Fokker-Planck: First we write transition rate as function of the starting point and of the jump

$$W(y|y') = W(y';r), \quad r = y - y'.$$

Thus the master equation now has the following form

$$\frac{\partial P(y,t)}{\partial t} = \int W(y-r;r)P(y-r,t)dr - P(y,t)\int dr\, W(y;-r) \tag{2.17}$$

we now make two fundamental assumptions:

1. Only *small* jumps occur i.e. $W(y';r)$ is a sharply peaked function of r that varies slowly with y'.

2. Also the solution $P(y,t)$ varies slowly with y, so that is possible to use $y-r$ instead of y in the first piece of 2.17 by expanding with Taylor until second order as follow:

$$\begin{aligned}\frac{\partial P(y,t)}{\partial t} = \int W(y;r)P(y,t)dy - \int r\,\frac{\partial}{\partial y}\left\{W(y;-r)P(y,t)\right\} + \\ + \frac{1}{2}\int r^2\frac{\partial^2}{\partial y^2}\left\{W(y;r)P(y,t)\right\}dr - P(y,t)\int W(y;-r)\,dr\end{aligned} \tag{2.18}$$

[4]It is interesting to note that tis equation does not require a complete knowledge of the rate $W(y|y')$ but only the functions $A(y)$ and $B(y)$.

[5]We shall call the Fokker-Planck equation *linear* if A is a linear function of y: $A(y) = A_0 + A_1 y$ and B is a constant.

Note that an expansion with respect to the r-argument is not allowed as W varies rapidly with r. Indeed the first and last term in the right member cancel out each others[6]:

$$\frac{\partial P(y,t)}{\partial t} = \cancel{\int W(y;r)P(y,t)dy} - \int r\,\frac{\partial}{\partial y}\left\{W(y;-r)P(y,t)\right\} + \\ + \frac{1}{2}\int r^2\frac{\partial^2}{\partial y^2}\left\{W(y;r)P(y,t)\right\}dr - \cancel{P(y,t)\int W(y;-r)\,dr}.$$

Finally, using the definition of the n-th jump moment:

$$a_\nu(y) = \int_{-\infty}^{+\infty} r^\nu W(y;r)dr \tag{2.19}$$

We get the *Fokker-Planck equation*:

$$\frac{\partial P(y,t)}{\partial t} = -\frac{\partial}{\partial y}\left\{a_1(y)P(y,t)\right\} + \frac{1}{2}\frac{\partial^2}{\partial y^2}\left\{a_2(y)P(y,t)\right\} \tag{2.20}$$

This equation regulates the mean's broadening position as time increase, or equivalently it describes the dynamics of the Gaussian fluctuations around the deterministic solution. The generalisation of the Fokker-Planck equation in case of multiple (m) variable gives the following expression:

$$\frac{\partial P(y,t)}{\partial t} = -\sum_{i=1}^{m}\frac{\partial}{\partial y_i}A_i(y)P(y,t) + \frac{1}{2}\sum_{i,j=1}^{m}\frac{\partial^2}{\partial y_i\partial y_j}B_{ij}(y)P(y,t)$$

where the coefficients A_i and B_{ij} are real differentiable functions and B_{ij} is taken symmetric and positive definite, or more precisely, $\sum_{i,j=1}^{m} B_{ij}x_ix_j \geq 0$ for each vector $\{x_i\}$.

Kramers-Moyal expansion

It is not difficult to insert all the orders of the Taylor expansion in equation 2.20. This leads us to the so-called *Kramers-Moyal expansion* [28]:

$$\frac{\partial P(y,t)}{\partial t} = \sum_{\nu=1}\frac{(-1)^\nu}{\nu!}\left(\frac{\partial}{\partial y}\right)^\nu\left\{a_\nu(y)P\right\} \tag{2.21}$$

This equation is nothing else than an alternative expression of the master equation and it is often used in literature since if we stop at the second order, we obtain the F-K equation. At last, we specify that in order to make the Fokker-Planck equation exact instead of an approximation, one must make the rate W to depend on a parameter ε in such a way the two assumption made above are exact when $\lim_{\varepsilon\to 0}$.

[6] We rename the variable of integration and we know that $P \sim const.$ in r.

2.3.5 Differential Chapman-Kolmogorov equation

In order to get a separation of the differentiability condition into a part concerning the continuous motion and another one considering the discontinuous one, we make the following requirements for all $\varepsilon > 0$:

i) $\lim_{\Delta t\to 0} p(\vec{x}, t+\Delta t|\vec{z}, t)/\Delta t = W(\vec{x}|\vec{z}, t)$; uniformly in $\vec{x}, \vec{z}$ and t for $|\vec{x}-\vec{z}| \geq \varepsilon$

ii) $\lim_{\Delta t\to 0} \frac{1}{\Delta t} \int_{|\vec{x}-\vec{z}|>\varepsilon} d\vec{x}(x_i - z_i)p(\vec{x}, t + \Delta t|\vec{z}, t) = A_i(\vec{z}, t) + O(\varepsilon)$

iii) $\lim_{\Delta t\to 0} \frac{1}{\Delta t} \int_{|\vec{x}-\vec{z}|>\varepsilon} d\vec{x}(x_i - z_i)(x_j - z_j)p(\vec{x}, t + \Delta t|\vec{z}, t) = B_{ij}(\vec{z}, t) + O(\varepsilon)$

Where ii) and iii) must be uniform in $\vec{z}$,ε ant t.

It is possible to show that the higher order of ii) and iii) must vanish.

We are not interested in the proof of this result (which uses Lindeberg condition enounced before), and that can be entirely found in [28]. At the end we can say that for all $\vec{z}$ in the *interior* of R (a region in which the whole process is confined) we have:

$$\begin{aligned}\partial_t p(\vec{z}, t|\vec{y}, t') = &-\sum_i \frac{\partial}{\partial z_i} \left[A_i(\vec{z}, t)p(\vec{z}, t|\vec{y}, t'))\right] \\ &+ \sum_{i,j} \frac{1}{2} \frac{\partial^2}{\partial z_i \partial z_j} \left[B_{ij}(\vec{z}, t)p(\vec{z}, t|\vec{y}, t'))\right] \\ &+ \int d\vec{x} \left[W(\vec{z}|\vec{x}, t)p(\vec{x}, t|\vec{y}, t\,') - W(\vec{x}|\vec{z}, t)p(\vec{z}, t|\vec{y}, t\,')\right]\end{aligned} \tag{2.22}$$

Furthermore, it was shown that if we have $A(\vec{x}, t)$ and $B(\vec{x}, t)$ semi-definite positive, and $W(\vec{x}|\vec{y}, t)$ non-negative, that exists a non-negative solution of the Chapman-Kolmogorov equation and the differential's one. Clearly the requirements that need to be satisfied are the initial conditions: $p(\vec{z}, t|\vec{y}, t) = \delta(\vec{y} - \vec{z})$.

Fokker-Planck and deterministic equation

If we set $W(\vec{z}|\vec{x}, t) = 0$, then equation 2.22 reduces to the *Fokker-Planck* equation, that corresponds to a diffusion process equation. This equation describes a process in which are involved continuous paths. It can also be shown that if the W and the matrix elements are both set to zero, then 2.22 describe a deterministic process, i.e. an ordinary differential equation. Thus its solution is a particular elementary form of Markov Process.

Furthermore, it can be show [28] that if $B = 0$, then we handle a deterministic equation

$$\frac{dx_i(\vec{x}, t)}{dt} = A_i\left[\vec{x}(t), t\right]$$

Again on master equation

In equation 2.22 we can obtain the m.e. by setting $A_i(\vec{z}, t) = B_{ij}(\vec{z}, t) = 0$ we have recovered the Master Equation

$$\partial_t p(\vec{z},t\,|\vec{y},t') = \int d\vec{x}\,[W(\vec{z}\,|\,\vec{x},t)p(\vec{x},t\,|\,\vec{y},t\,') - W(\vec{x}\,|\,\vec{z},t)p(\vec{z},t\,|\,\vec{y},t\,')] \tag{2.23}$$

Since this integro-differential equation has only the contributes of the discontinuous jumps, a sample of a process ruled by this equation will be made-up by straight lines over time with jumps that denote that our system has gone from a state to another one. If we handle with discrete states then our equation gets the form

$$\partial_t P(\vec{n},t|\vec{n}',t') = \sum_m [W(\vec{n}\,|\,\vec{m},t)P(\vec{m},t\,|\,\vec{n}',t\,') - W(\vec{m}\,|\,\vec{n},t)P(\vec{n},t\,|\,\vec{n}',t\,')] \tag{2.24}$$

Here W can be seen as the rates at a given time to go from one state to another. The use of these probabilistic tools are very useful for describing systems out of equilibrium.
There are more compact ways [31] to express 2.24, enumerating the microstates of the system $\{C_1, C_2, \ldots\}$ and calling $P_t(C)$ the probability of the system of being in the state C at time t, and $W(C',C)dt$ the probability of a transition $C \to C'$ between time t and $t+dt$ we get

$$\frac{d}{dt}P_t(C) = \sum_{C'\neq C} W(C,C')P_t(C') - \left\{\sum_{C'\neq C} W(C',C)\right\} P_t(C) \tag{2.25}$$

This is a linear equation in the probability vector P_t whose components are given by $\{P_t(C)\}$. Thus, a possible evolution of a system that start at time t_0 in a configuration C_0 and that evolve until a time T is $C_0 \xrightarrow{t_1} C_1 \xrightarrow{t_2} \cdots \xrightarrow{t_i} C_i \xrightarrow{t_{i+1}} \cdots \xrightarrow{t_T} C_T$ (Note that we can define a function $C(t)$.

Connection to thermodynamics and Detailed balance

If we define the *Markov operator* $\mathbb{W}$, the master equation can be recasted as

$$\frac{d}{dt}P_t(C) = \mathbb{W}\cdot P_t(C) \tag{2.26}$$

where the Markov operator $\mathbb{W}$ has the following structure:

- For elements $C \neq C'$ the entries are the usual $W(C,C')$.
- For diagonal elements are defined by $W(C,C) = -\sum_{C'\neq C} W(C',C)$.
- A stationary vector P_∞ in kernel of $\mathbb{W}$ is a stationary state. This means $\dfrac{dP_\infty}{dt} = 0$. And thanks to Perron-Frobenius theorem it can be shown that this state is unique [27] *and* that all other eigenvalues of $\mathbb{W}$ have strictly negative real parts; the inverse of these real parts correspond to the intrinsic system's relaxation times towards its stationary state and the imaginary parts (if existing) characterize the oscillations during relaxation. This behavior will be tested in our numerical simulations in Chapter 4.

Then the stationary state is obtained through $\frac{d}{dt}P_t(C) = 0$ and the connection with thermodynamics is obtained by the condition that the stationary state of Markovian dynamics P_∞ is given by the Boltzmann-Gibbs canonical formula which describes a system in thermal equilibrium: the requirement for having thermal equilibrium is verified to be [31]:

$$\sum_{C' \neq C} W(C, C') e^{-\frac{E(C')}{k_B T}} = e^{-\frac{E(C)}{k_B T}} \left\{ \sum_{C' \neq C} W(C', C) \right\}$$

where[7] $P_\infty(C) = P_{\text{eq}}(C) \equiv e^{-\beta E(C)}/Z$. This condition means that a system described by the stochastic dynamics reaches ultimately a state of thermodynamic equilibrium. Note that for systems far from equilibrium with a non-thermodynamic stationary state, this relation does not hold anymore. Using the fact that the system's microscopic dynamics (which is represented by an effective Markovian model) is Hamiltonian and that Hamiltonian dynamics is in general time-reversible, Onsager derived the following, much stronger, constraint:

$$W(C, C') P_{\text{eq}}(C') = W(C', C) P_{\text{eq}}(C) \tag{2.27}$$

This important relation, known as *detailed balance*, is a consequence of time-reversal symmetry of the system's microscopic dynamics and it holds for systems at thermodynamic equilibrium and implies also annihilation of the currents inside the system itself. We stress that if we only ask for the Gibbs-Boltzmann distribution to be stationary, we need only that 2.27 holds added over configurations as seen above, and not term by term (from here comes the term 'detailed') [38]. The detailed balance[8] condition is a fundamental dynamic property of equilibrium systems that holds also for laws that do not concern classical thermodynamics.
If a system has an invariant probability distribution $P_*(C)$, such that $\dot{P}_*(C) = 0$, but the equality is not satisfied for each term:

$$W(C, C') P_*(C') \neq W(C', C) P_*(C) \tag{2.28}$$

i.e. detailed balance is broken, then the system is said to be in a NESS. Usually in this case P_* is not a Boltzmann-Gibbs distribution but exists examples that lack of detailed balance but still have a B-G distribution [40].
There is an interesting way to write the detail balance as the hermiticity of the Markov operator $\mathbb{W}$ by dividing equation 2.27 at both members for $P_{\text{eq}}(C)^{1/2} P_{\text{eq}}(C')^{1/2}$ we get

$$P_{\text{eq}}(C)^{-1/2} W(C, C') P_{\text{eq}}(C')^{1/2} = P_{\text{eq}}(C')^{-1/2} W(C', C) P_{\text{eq}}(C)^{1/2} \tag{2.29}$$

[7] Z is the usual partition function of canonical ensemble and $E(C)$ is the energy given by Boltzmann-Gibbs canonical law.

[8] Sometimes a systems that reaches this condition is said to *thermalise*.

By defining the diagonal matrix Q as follows

$$Q = \begin{pmatrix} \ddots & & \\ & P_{\text{eq}}(C_2)^{1/2} & \\ & & \ddots \end{pmatrix} = \begin{pmatrix} P_{\text{eq}}(C_1)^{1/2} & 0 & \cdots & 0 \\ 0 & P_{\text{eq}}(C_2)^{1/2} & \cdots & \vdots \\ \vdots & 0 & \ddots & 0 \\ 0 & \cdots & 0 & P_{\text{eq}}(C_T)^{1/2} \end{pmatrix}$$

and

$$\mathcal{W} = Q^{-1}\mathbb{W}Q$$

then the detailed balance implies the hermiticity of the matrix $\mathcal{W}$:

$$\mathcal{W} = \mathcal{W}^{\dagger}. \tag{2.30}$$

Before continuing, we want to stress the fact that a system at thermodynamic equilibrium fulfill the detailed balance as a consequence of time-reversal symmetry of the system's microscopic dynamics, but if the system's steady state is not in equilibrium i.e. is in a non-equilibrium steady state, then detailed balance is broken and the state is necessary out of equilibrium.
Now, the master equation can be rewritten in the following way:

$$\frac{d}{dt}P_t(C) = \sum_{C'} \{W(C, C')P_t(C') - W(C', C)P_t(C)\} := \sum_{C'} J_t(C, C') \tag{2.31}$$

where J is defined as the probability flux from C' to C.From this definition we can lists some main properties:

- The cumulative probability is conserved then

$$\sum_{C'} J_t(C, C') = 0 \tag{2.32}$$

- The probability flux is symmetric

$$J_t(C, C') = -J_t(C', C) \tag{2.33}$$

- For a stationary state must hold the following

$$\sum_{C'} J_{\infty}(C, C') = 0 \tag{2.34}$$

Let's see a picture that better gives an idea of the trajectory $P(C; t)$ that evolve until a time T:

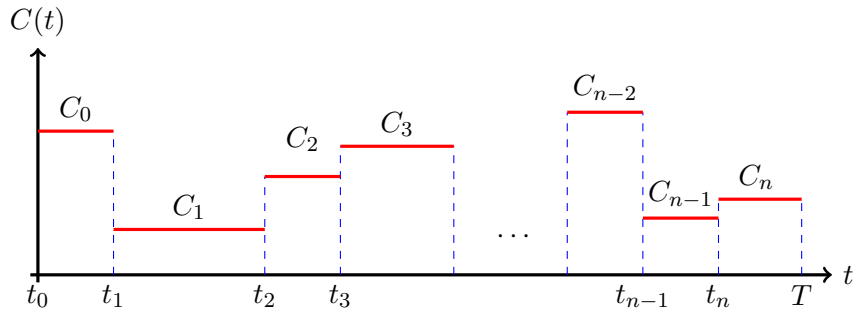


Figure 2.1: The red lines represent the jumps occurred along the stochastic system's trajectory for a continuous time Markov process (chain) with discrete state.

Let's show here that the equilibrium state of a system which satisfies the detailed balance, is necessarily invariant by time reversal.
In order to determine the probability of the trajectory, it must be determined the state's probability to remain in C for a time τ; in general, since $W(C,C) < 0$, the probability that a trajectory would not change in a time dt is $1 + W(C,C)dt$. Using then the markovian property of the system, we can calculate the probability for state C to remain in it for a time τ by multiplying the same term and taking the limit $dt \to 0$:

$$\lim_{dt\to 0} [1 + W(C,C)dt]^{\frac{\tau}{dt}} = e^{W(C,C)\tau} \tag{2.35}$$

At time τ, the system goes in C', bringing a probability $W(C',C)d\tau$. In general, the probability of going from C to C' during an interval dt is: $W(C';C)dt$. Then, going along the whole trajectory (see Fig. 2.1), we have the probability

$$\begin{aligned}\Pr\{C(t)\} = e^{W(C_n,C_n)(T-t_n)}W(C_n,C_{n-1})dt_n\, e^{W(C_1,C_1)(t_2-t_1)}W(C_2,C_1)dt_2\ldots \\ \ldots e^{W(C_0,C_0)t_1}W(C_1,C_0)dt_1 P_{\text{eq}}(C_0)\end{aligned}$$

The inverse trajectory is called $\widehat{C}(t) \equiv C(T-t)$ and its probability is

$$\begin{aligned}\Pr\{\widehat{C}(t)\} = e^{W(C_0,C_0)(t_1-t_0)}W(C_0,C_1)dt_1\ldots \\ \ldots e^{W(C_{n-1},C_{n-1})(t_n-t_{n-1})}W(C_{n-1},C_n)dt_n e^{W(C_n,C_n)(T-t_n)}P_{\text{eq}}(C_n)\end{aligned}$$

If we consider the division of the members

$$\frac{\Pr\{C(t)\}}{\Pr\{\widehat{C}(t)\}} = \frac{W(C_n,C_{n-1})W(C_{n-1},C_{n-2})\ldots W(C_2,C_1)W(C_1,C_0)P_{\text{eq}}(C_0)}{W(C_0,C_1)W(C_1,C_2)\ldots W(C_{n-2},C_{n-1})W(C_{n-1},C_n)P_{\text{eq}}(C_n)}$$

Now we assume the equilibrium and the related detailed balance, which brings a great semplification

$$\frac{\Pr\{C(t)\}}{\Pr\{\widehat{C}(t)\}} = \frac{P_{\text{eq}}(C_0)}{P_{\text{eq}}(C_n)}\cdot\frac{P_{\text{eq}}(C_1)}{P_{\text{eq}}(C_0)}\cdot\frac{P_{\text{eq}}(C_2)}{P_{\text{eq}}(C_1)}\cdots\frac{P_{\text{eq}}(C_n)}{P_{\text{eq}}(C_{n-1})} = 1 \tag{2.36}$$

As we wanted to show, at equilibrium, the probability of a certain trajectory is the same of its time reversed one

$$\Pr\{C(t)\} = \Pr\{\widehat{C}(t)\}$$

We know that the predictive power of equilibrium statistical mechanics relies on the fact that the stationary probability distribution of a thermalized system is universal and can be classified into a small number of thermodynamic ensembles [33]. In particular, an isolated system will thermalize in such a way that each available configuration is visited with the same probability. This fundamental equal *a priori probability* postulate is the core of equilibrium statistical mechanics, from which all other thermodynamic ensembles can be derived. Recalling what we have said about the non-equilibrium condition, we see then that if the detailed balance law is broken, then the probability currents do not vanish at the stationary state.
In a NESS [34], the probability distribution of the microscopic trajectories inside the system differs from the probability distribution of the time-reversed trajectories so that the system is in an (stochastic) irreversible state (and this is directley connected with entropy production). The irreversibility of a NESS thus finds its origin in a selection of the initial conditions for the trajectories incoming the open system. In fact, most trajectories have an initial condition which is different from the initial condition of the timereversed trajectory and, moreover, the stationary probability distribution of a NESS gives a different weight to the forward and backward trajectories. Therefore, the selection of initial conditions by the flux boundary conditions explicitly breaks the time-reversal symmetry of the model considered. In this context, the irreversibility of a NESS is commonly characterized by the production of entropy inside the system and we will give a formula for its measure in Chapter 3.

2.4 Van Kampen's system size expansion

As we have said before, the master equation describe the system completely, taking into account its intrinsic stochastic nature. This induces a lot of complexities in the description of its evolution, given a specific initial condition. This means that solving exactly the master equation can be done only in very few cases. Thus is required a general method for expanding the equation, and this should give (with the correct assumptions) the results given by the Fokker-Planck equation or the Langevin's description (which we not develop here) [27]. Here we want to introduce the theoretical approach to this procedure that will be used in Chapter 4 to obtain the deterministic equations. The Van Kampen's system size expansion is, as suggested by the name, a perturbative expansion of the master equation, by considering that the fluctuations around the macroscopic value that describe the system, are small. Even if the nature has a stochastic behavior, it is also true that a great ensamble of particles often follow a deterministic description. In fact, has been well shown that a system of N particles usually present fluctuations of order $\sim N^{1/2}$, this means

that the macroscopic properties are $\sim N^{-1/2}$.
Thus, we now define a parameter Ω that must:

1. Be present inside the master equation in the formulation of the problem.
2. Govern the size of fluctuations around the peak of the system variable.
3. Determine the size of the relative jumps at each instant in which the system evolves. For high Ω we require that the respective jump size will be small, and usually Ω is the size of the system itself.

It is now necessary to make the assumption for the proper expansion of Ω. For example, following what we said before, defining P_n the solution of the master equation involved to have a certain variable n at time t with a certain probability, one expects that P_n would be peaked around its macroscopic value $\phi(t)$ with a width that is

$$n \sim \Omega\, \phi(t) + \Omega^{1/2}\xi$$

where ξ is the new variable replacing n.
Being more general, we see that the parameter Ω creates on one side a point of view in which the size of jumps, that will be denoted by the extensive variable X, that remains the same even if Ω changes. On the other side, it creates a point of view in which the macroscopic properties can be studied by a parameter $x = X/\Omega$, that is an intensive variable. Of course the limit of interest is at large Ω and fixed x.
The starting point of our derivation is to write the transition rates as functions of the starting point and jump length, so that the master equation (in which we will specify the parameter dependence in the rates) is

$$\dot{P}(X,t) = \int \left\{ W_\Omega(X|X')P(X',t) - W_\Omega(X'|X)P(X,t) \right\} dX' \tag{2.37}$$

and the rate can be expressed as function of the starting point and of the jump length $r \equiv \Delta X = X - X'$:

$$W_\Omega(X|X') = W_\Omega(X'; X - X') = W_\Omega(X'; r). \tag{2.38}$$

Here the dependence on r give the probability measure of the possible jumps length inside the system, while the dependence on X' gives the general probability. Some author like Gardiner then immediately make the following assumption

$$W(X'; r) = \Omega\psi\left(x' \equiv \frac{X'}{\Omega}; r\right)$$

and starts with the procedure of expansion. We follow the Van-Kampen's way, which in general affirms that there is a function of two variables r and x':

$$W_\Omega(X'; X - X') = \Phi\left(\frac{X'}{\Omega}; X - X'\right) \equiv \Phi\left(x'; r\right) \text{ and } W_\Omega(X'|X) = \Phi(x; -r) \tag{2.39}$$

We note that there can be present a positive factor $f(\Omega)$ which can be deleted by a simple redefinition of the time coordinate (the system will evolve faster or slowly). The expansion then reads

$$W_\Omega(X|X') = f(\Omega)\left\{\Phi_0\left(\frac{X'}{\Omega};r\right) + \Omega^{-1}\Phi_1\left(\frac{X'}{\Omega};r\right) + \Omega^{-2}\Phi_2\left(\frac{X'}{\Omega};r\right) + \cdots\right\} \tag{2.40}$$

This expression takes the name of *canonical form* and occur in most of the natural cases. We then substitute 2.40 inside 2.37 so that

$$\begin{aligned}\dot{P}(X,t) = f(\Omega)\int\left\{\Phi_0\left(\frac{X-r}{\Omega};r\right) + \Omega^{-1}\Phi_1\left(\frac{X-r}{\Omega};r\right) + \cdots\right\}P(X-r,t)\,dr \\ - f(\Omega)\int\left\{\Phi_0\left(\frac{X}{\Omega};-r\right) + \Omega^{-1}\Phi_1\left(\frac{X}{\Omega};-r\right) + \cdots\right\}P(X,t)\,dr\end{aligned} \tag{2.41}$$

As we anticipated at the beginning of the paragraph, we now need to anticipate how the solution will depend on Ω. At time 0, one expects that the solution of the master equation $P(X,0) = \delta(X - X_0)$. As time passes, P will be sharply peaked on a position of order Ω, but it will still have a width of order $\Omega^{1/2}$. Explicitly this means that X have a first macroscopic term plus a noise:

$$X = \Omega\phi(t) + \Omega^{1/2}\xi \tag{2.42}$$

where the function $\phi(t)$ evolves as the peak does. Note that 2.42 is the only expansion that justifies a deterministic description that have a natural stochasticity. Thus we have the following expansion:

$$P(X,t) = P(\Omega\phi(t) + \Omega^{1/2}\xi, t) = \Pi(\xi,t) \tag{2.43}$$

The respective transformations of the derivatives are:

$$\frac{\partial^\nu \Pi}{\partial \xi^\nu} = \Omega^{\frac{\nu}{2}}\frac{\partial^\nu P}{\partial X^\nu} \tag{2.44}$$

$$\frac{\partial \Pi}{\partial t} = \frac{\partial P}{\partial t} + \Omega\frac{d\phi}{dt}\frac{\partial P}{\partial X} = \frac{\partial P}{\partial t} + \Omega^{1/2}\frac{d\phi}{dt}\frac{\partial \Pi}{\partial \xi} \tag{2.45}$$

Thus, the master equation 2.41 is

$$\begin{aligned}\frac{\partial \Pi(\xi,t)}{\partial t} - \Omega^{1/2}\frac{d\phi}{dt}\frac{\partial \Pi}{\partial \xi} = \\ = f(\Omega)\int \Phi_0(\phi(t) + \Omega^{-1/2}(\xi - \Omega^{-1/2}r;r))\Pi(\xi - \Omega^{-1/2}r,t)dr + \\ + \Omega^{-1}f(\Omega)\int \Phi_1(\phi(t) + \Omega^{-1/2}(\xi - \Omega^{-1/2}r;r))\Pi(\xi - \Omega^{-1/2}r,t)dr + \cdots \\ - f(\Omega)\int \Phi_0(\phi(t) + \Omega^{-1/2}\xi;-r)\Pi(\xi,t) \\ - \Omega^{-1}f(\Omega)\int \Phi_1(\phi(t) + \Omega^{-1/2}\xi;-r)\Pi(\xi,t) - \cdots .\end{aligned} \tag{2.46}$$

we can now follow the steps of the expansion done during the derivation of the Fokker-Planck equation, but now are visible the order terms in $\Omega^{-1/2}$. Expanding with Taylor the first two terms of the second member (note that ξ is shifted by -$\Omega^{-1/2}$) we get a semplification of the first two terms with the last two of the member.

$$\begin{aligned}\frac{\partial\Pi(\xi,t)}{\partial t} - \Omega^{1/2}\frac{d\phi}{dt}\frac{\partial\Pi}{\partial\xi} = \\ = -\Omega^{-1/2}f(\Omega)\frac{\partial}{\partial\xi}\int r\Phi_0(\phi(t)+\Omega^{-1/2}\xi;r)\Pi(\xi,t)dr + \\ + \frac{1}{2}\Omega^{-1}f(\Omega)\frac{\partial^2}{\partial\xi^2}\int r^2\Phi_0(\phi(t)+\Omega^{-1/2}\xi;r)\Pi(\xi,t)dr \\ - \frac{1}{3!}\Omega^{-3/2}f(\Omega)\frac{\partial^3}{\partial\xi^3}\int r^3\Phi_0(\phi(t)+\Omega^{-1/2}\xi;r)\Pi(\xi,t)dr + \\ - \Omega^{-3/2}f(\Omega)\frac{\partial}{\partial\xi}\int r\Phi_1(\phi(t)+\Omega^{-1/2}\xi;r)\Pi(\xi,t)dr + \mathcal{O}(\Omega^{-2}). \quad (2.47)\end{aligned}$$

To simplify this expression we can define the jump moments

$$\alpha_{\nu,\lambda}(x) = \int r^\nu\Phi_\lambda(x;r)dr \quad (2.48)$$

and rescaling the time as follow

$$\Omega^{-1}f(\Omega)t = \tau$$

by doing that we get

$$\begin{aligned}\frac{\partial\Pi(\xi,t)}{\partial t} - \Omega^{1/2}\frac{d\phi}{dt}\frac{\partial\Pi}{\partial\xi} = &- \Omega^{1/2}\frac{\partial}{\partial\xi}\alpha_{1,0}(\phi(\tau)+\Omega^{-1/2}\xi)\Pi \\ &+ \frac{1}{2}\frac{\partial^2}{\partial\xi^2}\alpha_{2,0}(\phi(\tau)+\Omega^{-1/2}\xi)\Pi \\ &- \frac{1}{3!}\Omega^{-1/2}\frac{\partial^3}{\partial\xi^3}\alpha_{3,0}(\phi(\tau)+\Omega^{-1/2}\xi)\Pi \\ &- \Omega^{-1/2}\frac{\partial}{\partial\xi}\alpha_{1,1}(\phi(\tau)+\Omega^{-1/2}\xi)\Pi + \mathcal{O}(\Omega^{-1})\end{aligned} \quad (2.49)$$

we now expand the jump moments and we get (note that the primes indicates the

derivatives)[9]:

$$\begin{aligned}\frac{\partial\Pi(\xi,t)}{\partial t}-\Omega^{1/2}\frac{d\phi(\tau)}{dt}\frac{\partial\Pi}{\partial\xi} =& -\Omega^{1/2}\alpha_{1,0}(\phi(\tau))\frac{\partial\Pi}{\partial\xi}-\alpha'_{1,0}\frac{\partial}{\partial\xi}\xi\Pi-\frac{1}{2}\Omega^{-1/2}\alpha''_{1,0}(\phi(\tau))\frac{\partial}{\partial\xi}\xi^2\Pi\\ &+\frac{1}{2}\alpha_{2,0}(\phi(\tau))\frac{\partial^2\Pi}{\partial\xi^2}+\frac{1}{2}\Omega^{-1/2}\alpha'_{2,0}(\phi(\tau))\frac{\partial^2}{\partial\xi^2}\xi\Pi\\ &-\frac{1}{3!}\Omega^{-1/2}\alpha_{3,0}(\phi(\tau))\frac{\partial^3\Pi}{\partial\xi^3}\\ &-\Omega^{-1/2}\alpha_{1,1}(\phi(\tau))\frac{\partial\Pi}{\partial\xi}+\mathcal{O}(\Omega^{-1})\end{aligned} \tag{2.50}$$

The same result could be obtained via Kramers-Moyal expansion.
At first one could rebut that the expansion performed is incorrect, since it presents terms of order $\Omega^{1/2}$. We can make them cancel out if we impose that the system fulfill the equation

$$\frac{d\phi}{d\tau}=\alpha_{1,0}(\phi(\tau)) \tag{2.51}$$

The solution of 2.51 is given by the initial condition: $P(X,0)=\delta(X-X_0)$; and the initial value X_0 which is given by $\phi(0)=X_0/\Omega=x_0$. This equation is nothing that the *deterministic equations*.
After we have considered the terms of order $\Omega^{1/2}$, we now can consider the terms of order Ω^0. This brings to

$$\frac{\partial\Pi(\xi,t)}{\partial t}=-\alpha'_{1,0}(\phi(\tau))\frac{\partial}{\partial\xi}\xi\Pi+\frac{1}{2}\alpha_{2,0}(\phi(\tau))\frac{\partial^2\Pi}{\partial\xi^2}. \tag{2.52}$$

that's a *linear Fokker-Planck equation* whose coefficients depends on time, since ϕ depends on it. All this procedure has given the so-called *linear noise approximation* that is obtained thanks to a systematic expansion in Ω^{-1}, and it is also called *the Gaussian approximation* because if the Fokker-Planck equation describes a linear process, its solution is a Gaussian. This fact implies that the distribution $\Pi(\xi,t)$ is completely specified by the first two moments $\langle\xi\rangle_t$ and $\langle\xi^2\rangle_t$. To obtain that, one must multiply equation 2.52 by ξ and ξ^2 and integrate over ξ:

$$\partial_\tau\langle\xi\rangle=\alpha'_{1,0}(\phi)\langle\xi\rangle$$

$$\partial_\tau\left\langle\xi^2\right\rangle=2\alpha'_{1,0}(\phi)\left\langle\xi^2\right\rangle+\alpha_{2,0}(\phi)$$

and the variance obeys the following

$$\partial_\tau\left\langle\left\langle\xi^2\right\rangle\right\rangle=2\alpha'_{1,0}(\phi)\left\langle\left\langle\xi^2\right\rangle\right\rangle+\alpha_{2,0}(\phi)$$

[9]The relation between the old jump moments a_ν and the new $\alpha_{\nu,\lambda}$:

$$a_\nu(X)=f(\Omega)\left[\alpha_{\nu,0}(\frac{X}{\Omega})+\frac{1}{\Omega}\alpha_{\nu,1}\left(\frac{X}{\Omega}\right)+\cdots\right]$$

Of course, since we want to start with a solution that is a delta-function and we want x_0 to be the starting value of the macroscopic quantity, then the initial fluctuation will be zero: $\langle\xi\rangle_0 = \langle\xi^2\rangle_0 = \langle\langle\xi^2\rangle\rangle = 0$. Integrating the first equation brings to

$$\langle\xi\rangle_\tau = \underbrace{\langle\xi\rangle_0}_{0} \exp \int_0^t d\tau\, \alpha'_{1,0}(\phi(\tau))$$

This implies that $\langle\xi\rangle_\tau = 0$ and then

$$\langle X\rangle_\tau = \Omega\phi(\tau|x_0) + \Omega^{1/2}\underbrace{\langle\xi\rangle_\tau}_{0}$$

so that in the linear noise approximation the average $\langle x\rangle = \langle X\rangle_\tau / \Omega$ follows the deterministic equations

$$\partial_\tau \langle x\rangle = \alpha_{1,0}(\langle x\rangle) + \mathcal{O}(\Omega^{-1})$$

It is important to stress the fact that the expansion proposed in 2.42 is not one of the possible approximations, but it will match with the common postulate of using a Gaussian noise as first approximation going beyond the mean-field description. Finally, we want to give an *a posteriori* reason from the Ansatz 2.42. The equation 2.52 does not contain Ω, this implies the fairness of 2.42 since the fluctuation emerges in the right order.

Chapter 3

Entropy and entropy production

As in thermal equilibrium there are no flows of free energy, which mean no expendable work for the system, life relies on non-equilibrium thermodynamics. Biological systems are usually open systems[1], i.e. a system where its constituents are in contact with an environment, and energy flows inside and outside them. However, in ecology sometimes the systems are treated as approximately closed, and they can approach to equilibrium before being disrupted in one way or another. This can happen in a multitude of cases such as an evolutionary population (or a chemical reaction) that reaches its stable state. All these events have in common the fact that all constantly tend to increase their entropy [39, 21]. The breaking of time-reversal symmetry is certainly an important feature of non-equilibrium systems. While the underlying microscopic dynamics is (under usual circumstances) time-reversal symmetric, the plausibility of the time-reversed history of mesoscopic or even more macroscopic conditions can greatly differ from that of the original history. This means that out of equilibrium a particular sequence of macrostates and its time-reversal can have a very different plausibility and these considerations are very much linked with the concept of entropy and its production. As written by Max Planck in 1926 [20]: "...there is no other general measure for the irreversibility of a process than the amount of increase of entropy". In Chapter 2, we dealt with stochastic systems in non-equilibrium conditions. Here we want to introduce the idea of entropy and its main features, since it is the fundamental quantity of study in this work of thesis. Specifically we are interested in the entropy production in a framework of Markovian processes. Historically, the notion of entropy emerged in conceptually distinct contexts, we will present entropy by its three main different perspective and conceptions, that are:

- Entropy seen as irreversibility of a certain transformation that occurs inside a system.

[1] Note that in open systems the increment of entropy may be negative (and free energy increment may be positive), this because the system is driven by the environment: energy is pumped into the system. In the steady state of an open system, it is now the entropy production rate that must be nonnegative [21].

- Entropy seen as a measure of disorder of a system.
- Entropy seen as a measure of the lack of information about a system.

3.1 Entropy and non-equilibrium entropy

Let's start discussing the first time in which the concept of entropy emerged in literature [32].

Entropy as irreversibility

During the experiments on the steam engines in the early '800, scientists started realising that some of the heat energy involved in the transformations was lost into a cold reservoir due to vibration, friction etc. This fact showed that energy conservation (that is expressed thermodynamically by the first law $dU = \delta Q - \delta W$) cannot be the only principle that must be valid for heat engines. In 1824 Carnot published a treatise in which was stated that the efficiency of n engine could not never reach 100% efficiency i.e. it is not possible to convert all the usable heat of a reservoir in work and found that the most efficient engines are the *reversible* one's, named Carnot's engine. In a Carnot's cycle he found that, named Q_1, Q_2 the heat flux inside/outside the piston and T_1, T_2 its relative temperature, the following law holds

$$\frac{Q_1}{T_1} = \frac{Q_2}{T_2}$$

and ater scientists decided to call this ratio the "entropy change"[2]

$$\Delta S_{therm} = \frac{Q}{T} \tag{3.1}$$

The notion of entropy was defined by Clausius in 1850–1865 as an extensive quantity that links temperature with heat

$$dS = \frac{\delta Q}{T} \quad \Rightarrow \quad \Delta S = \int \frac{\delta Q}{T} \tag{3.2}$$

where T is the temperature and Q is the heat flowed into the system. Of course if the process is irreversible, then we have the second law of thermodynamics: $\Delta S \geq \int \frac{\delta Q}{T}$ where the total entropy of an isolated system always increase until a maximum is reached. For more general time-dependent processes from an equilibrium state A to another equilibrium state B, holds the inequality

$$S(B) - S(A) = \int_{t_A}^{t_B} \frac{Q(t)}{T(t)} dt \tag{3.3}$$

where $T(t)$ is the temperature of a single heat bath in contact with a system, and $Q(t)$ is a heat flux i.e. the energy transfer from the heat bath at time t.

[2] This means that in a Carnot's engine cycle no entropy is produced.

Entropy as disorder

Another interpretation of entropy is as a measure of the disorder in a system. Following the usual procedure describing the microcanocical ensemble, remembering the fundamental claim that all points in phase space (with a given energy) are a priori equally likely, we arrive at the probability of a system having a certain phase-space volume $\Omega(E)$ in a shell of energy E

$$\Omega(E) = \int dE_1 \Omega_1(E_1)\Omega_2(E - E_1) \tag{3.4}$$

where the subscripts 1 and 2 indicate the respective two subsystems. Thus by normalisation we can obtain the probability density of the subsystem with E_1 of being in any of the compatible state with that energy that is

$$\rho(E_1) = \frac{\Omega_1(E_1)\Omega_2(E - E_1)}{\Omega(E)}$$

taking the maximum of the derivative in the integrand above gives the energy of the first subsystem. Then we can define the *equilibrium entropy* as done at first in 1887 by Boltzmann, that creates a bridge between the statistical mechanics and thermodynamics:

$$S_{eq}(E) = k_B \log(\Omega(E)) \tag{3.5}$$

The condition of thermal equilibrium is then reached by an extremum of entropy, and it can be seen by taking its derivative d/dE_1 for both subsystems. Now, if we consider a system with N particles of two types, and we mix them, the entropy will be given, by following equation

$$S = k_B \log(W)$$

where W is the discrete number of possible configurations. A much disordered system has obviously a greater number of possible configurations W which implies a greater values of S.

Entropy as lack of information

Another interpretation of entropy is as a measure of our ignorance about a system. If we consider an equilibrium state following this interpretation, then we see that it reaches the maximum of entropy because we have lost all the information about the initial condition of the state except for the conserved quantities. The entropy of a certain mixture of atoms in a box is nothing but a measure of the possible states in which these atoms could be arranged inside the box, given our ignorance about the real arrangement[3]. So, in information theory, the entropy of a system is defined as the amount of information which is necessary to describe the configuration of the system. Since an ordered system requires less information to be described than a

[3]We note that the many possible arrangement of these particles are defined by statistical mechanics by the ensamble theory.

disordered one, the entroy can be seen as a measure of disorder.
This definition of entropy was given by Shannon [47] in the context of information theory and, since in this particular case we are not interested in the connection with temperature, instead of using the Boltzmann's constant it uses the constant $k_S = 1/\log(2)$

$$S_S = -k_S \sum_i^{\Upsilon} p_i \log p_i \,.$$

We note that the definition of k_S is necessary if we want to measure the entropy in bits, as was done by Shannon. In this framework, in a low-entropy set of data it is easy to predict, so that in information theory it is necessary only to transmit those data that violates our predictions.

Non-Equilibrium entropy

An extension of entropy outside of equilibrium has been done, and in literature this definition is named in several ways. We start from a discrete probability distribution $\{P_t(C)\}$, and we define the entropy as a functional of the set of probabilities just introduced for finding a given system in a state C (where $C = C_1, C_2, \ldots, \Upsilon$) at time t:

$$S\,[P] = -k_B \left\langle \log(P_t(C)) \right\rangle = -k_B \sum_C P_t(C) \log(P_t(C)) \tag{3.6}$$

In this definition the stochasticity properties of a system emerge naturally and it is easy to see that, if we consider all the possible state Ω as equally probable so that $P = 1/\Omega$, then we recover equation 3.5. We can then extend this definition in the continuous case considered as a quantity derived by many ensamble of the system's constituents, that often is called *Boltzmann-Gibbs entropy*:

$$\begin{aligned} S_{neq} &= -k_B \left\langle \log(\rho) \right\rangle = \\ &= -k_B \int \rho \log \rho = -k_B \int_{E<H(p,q<E+\delta E)} \frac{dp\,dq}{h^{3N}} \rho(p,q) \log \rho(p,q) \end{aligned} \tag{3.7}$$

where $\rho(p,q)$ is the probability density in the continuous phase space Υ with $(p,q) \in \Upsilon$. It is interesting to note that, even if all the notions presented are conceptually different, the functional form behind these definitions is the same.

3.2 Entropy production on Markov processes

Entropy is probably the most fundamental concept of statistical physics. From the information/theoretic point of view, as we have seen, the entropy of a system can be defined as the amount of information which is necessary to describe the configuration of the system. Since the description of a highly ordered configuration requires less information than a disordered one, entropy can be viewed as a measure of disorder. The amount of information which is necessary to describe a configuration depends on

the already existing partial knowledge of the observer at a given time. For example, deterministic systems with a given initial configuration have no entropy because the observer can compute the entire trajectory in advance, having complete knowledge of the configuration as a function of time even without measuring it. Contrarily, in stochastic systems the observer has only a partial knowledge about the system expressed in terms of the probability distribution $P_t(C)$.[33].
In order to give the right framework in which we operate, it is fundamental presenting the main concepts of Stochastic Thermodynamics (ST) of single trajectories . In the last decades this field has been introduced by the works of Crooks, Sekimoto, Seifert and Schnakenberg [41]-[43]. We summarize here ST and the most important results for our purposes of work, taking into account that we are interested mainly on the applications of these concept in the master equation formalism. Because of that many results that do not pertain to our goals will not be presented below.

3.2.1 Stochastic Thermodynamics

Stochastic Thermodynamics, is usually introduced as the combination of stochastic energetics [41] with the possibility of assigning in a consistent way an entropy to a single fluctuating trajectory. Instead, stochastic energetics can be seen as the link between the usual thermodynamics and the stochastic dynamics, that concerns the so-called Brownian motion and thermal fluctuations. We know that one of the first systems of the non-equilibrium statistical mechanics is based on a colloidal particle which is well described by the Langevin equation. For this reason we will follow some detail of this equation in [42].
If we imagine a particle immersed in a heat bath, it is clear how to assign an entropy change, it is less obvious to do that for the particle itself. Starting from a overdamped motion $x(\tau)$ of a particle with mobility μ along a one-dimensional coordinate in the time-interval $0 \leq \tau \leq t$ subject to a force

$$F(x,l) = -\frac{\partial}{\partial x}V(x,l) + f(x,l)$$

where the force can come from a conservative potential $V(x,l)$ or from the particle itatvself $f(x,l)$. For these sources of the force can be defined a control-parameter $\lambda(t)$ that varies coherently with the experimental prescriptions. Thus the motion is controlled by the Langevin equation

$$\dot{x} = \mu F(x,l) + \zeta$$

The stochastic term is given by a Gaussian white noise[4] with
$\langle \zeta(\tau)\zeta(\tau')\rangle = 2D\delta(\tau - \tau')$ where D is the diffusion constant.At the equilibrium, D and μ are related by the Einstein relation $D = T\mu$ where T is the temperature of the medium in which the particle is immersed[5]. In order to get a good definition

[4]The term *white* means that the respective Fourier transformation of ζ has a flat spectrum.
[5]Up to now we will se the Boltzmann constant $k_B = 1$ so that the entropy results dimensionless.

of the entropy along a single trajectory, we use the Fokker-Planck equation for the probability $p(x,\tau)$ to find the particle at a specific point in time and space

$$\partial_\tau p(x,\tau) = -\partial_x j(x,\tau) = -\partial_x(\mu F(x,l) - D\partial_x p(x,\tau) \tag{3.8}$$

where the initial condition is set as $p(x,0) \equiv p_0(x)$.

As specified in the previous paragraph, the non-equiibrium Gibbs entropy can be stated as

$$S(\tau) \equiv -\int dx\, p(x,\tau) \ln p(x,\tau) \equiv \langle s(\tau) \rangle$$

and suggested that a possible definition of the entropy of a single-trajectory is

$$s(\tau) = -\ln p(x(\tau),\tau) \tag{3.9}$$

where the probability $p(x,\tau)$ is obtained by the solutions of the Fokker-Planck equation evaluated along the trajectory $x(\tau)$. From what said, the entropy $s(\tau)$ depends on the initial condition $p_0(x)$, which means that it contains informations of the whole ensamble and for an equilibrium Boltzmann distribution at fixed l, this definition gives the following

$$s(x) = (V(x,l) - \mathcal{F}(l))/T$$

with the free energy $\mathcal{F}(l) \equiv -T \int dx\, e^{-V(x,l)/T}$.
Following this framework it is possible to show the entropy production $\dot{s}(\tau)$ of the particle, the $\dot{s}_m(\tau)$ of the medium and the Fluctuation Theorem for the total change of entropy. In our model we are interested in a generalisation of these concepts for more than one degree of freedom, in which enter the master equation.

3.2.2 Entropy production and master equation

In this framework, we want to present a well defined entropy production rate for a single trajectory taking into account that there is not (conversley to a colloidal particle) the concept of heat that makes easily to define entropy production in the medium. Firstly, we want to sketch the way in which Schnakenberg defined the entropy production rate. The concept of time reversal as previously seen, is central in this framework since it ditinguishes the flow of a particular event in a sense or in the other and we will use it to get a good definition of entropy production.
Considering equation 2.25, it can be rewritten in the following fashion[6]

$$\frac{d}{dt}P_t(C) = \sum_{C' \neq C} \left[W_{C,C'}P_t(C') - W_{C',C}P_t(C)\right] \tag{3.10}$$

where the quantities $W_{C',C}$ are the usual transition rates defined in the past chapter. By taking the bilinear expression

$$\dot{S} = \frac{1}{2}\sum_{C,C'} J_{C',C}A_{C',C}$$

[6]In the next pages the rates $W_{C',C}$ will also benne expressed by the notation: $\Gamma(C \to C') \equiv \Gamma_t(C \to C') \equiv \Gamma_{C',C}(t)$.

with $A_{C',C}$ being the generalise thermodynamic force of the processes involved and $J_{C',C}$ the fluxes of the system itself [7] gives

$$\dot{S} = \frac{1}{2}\sum_{C,C'}\left[W_{C',C}P_t(C) - W_{C,C'}P_t(C')\right]\ln\frac{W_{C',C}P_t(C)}{W_{C,C'}P_t(C')} \tag{3.11}$$

We note that in this case the transition rates were indipendent of time t and that $J_t(C,C') = W_{C',C}P_t(C) - W_{C,C'}P_t(C')$. Following [44], we introduce the time-reversed trajectory defined by

$$C_{rev} \equiv \widehat{C} = \{C(t-\tau), 0 \leq \tau \leq t\}$$

Again, the non-equilibrium ensamble entropy of a stochastic system is the Gibbs' one [47, 33], noting that below the average is taken since an observer lacks of information about the probability function (that would be known only by solving the F-P equation 3.8):

$$\langle S(t)\rangle = -\sum_{C} P(C;t)\ln P(C;t) = -\langle \ln P(C;t)\rangle \tag{3.12}$$

and we see that is the average of the entropy associated to the system in 3.9 Indeed, we take the definition 3.12, and we operate to it in order to obtain two component of the entropy: one dealing with the internal entropy production and the other with the exchange (flow) of entropy per unit time in the environment. We will see that for the ensemble-averaged rate of total entropy production in a non-equilibrium process that assures the important condition $\langle S_{tot} \geq 0\rangle$.
Let us start taking the time-derivative of equation 3.12 and using the master equation and defining $\tilde{J}_{C',C} := W(C,C')P_{C'}(t)$ so that the master equation can be written as $\dot{P}_C = \sum_{C'}\left[\tilde{J}_{C',C} - \tilde{J}_{C,C'}\right]$:

$$\begin{aligned}
\left\langle \dot{S}(t)\right\rangle &= -\sum_{C}\dot{P}_C(t)\log P_C(t) + \sum_{C}\dot{P}_C(t) \\
&= -\sum_{C}\dot{P}_C(t)\log P_C(t) + \frac{d}{dt}\{\underbrace{\sum_{C}P_C(t)}_{1}\} \\
&= -\sum_{C,C'}\left[\tilde{J}_{C',C} - \tilde{J}_{C,C'}\right]\log P_C(t) = \sum_{C,C'}\left[\tilde{J}_{C,C'} - \tilde{J}_{C',C}\right]\log P_C(t)
\end{aligned} \tag{3.13}$$

$$\begin{aligned}
&= \frac{1}{2}\sum_{C,C'}\left[\tilde{J}_{C,C'} - \tilde{J}_{C',C}\right]\log P_C(t) + \frac{1}{2}\sum_{C,C'}\left[\tilde{J}_{C',C} - \tilde{J}_{C,C'}\right]\log P_{C'}(t) \\
&= \frac{1}{2}\sum_{C,C'}\tilde{J}_{C,C'}\log\frac{P_C(t)}{P_{C'}(t)} + \left\{\frac{1}{2}\sum_{C,C'}\tilde{J}_{C,C'}\log P_C(t) - \frac{1}{2}\sum_{C,C'}\tilde{J}_{C,C'}\log P_{C'}(t)\right\} \\
&= \sum_{C,C'}\tilde{J}_{C,C'}\log\frac{P_C(t)}{P_{C'}(t)} = \sum_{C,C'}P_C(t)W(C',C)\log\frac{P_C(t)}{P_{C'}(t)}.
\end{aligned} \tag{3.14}$$

[7] In the following we will consider $\{C\}$ as the trajectory of the particle, meanwhile the bare symbol C will indicates the particular states in which the particle lies at that time.

where in certain passages we changed $C \leftrightarrows C'$.
In accordance to what will be derived in 3.20, this entropy production (generated by the interaction of the system with particle/heat reservoirs which leads to the stochastic jumps) can be divided into terms representing the total entropy production of the stochastic system itself and an entropy flow that leads to a change of the entropy of the environment (the reservoirs). In fact, multiplying and dividing $\log \frac{P_C(t)}{P_{C'}(t)}$ in 3.13 for $\frac{W_{C',C}}{W_{C,C'}}$ we obtain the internal entropy production

$$\left\langle \dot{S}_{tot}(t) \right\rangle \equiv \sum_{C',C} W_{C',C}(t) P_C(t) \ln \frac{W_{C',C}(t) P_C(t)}{W_{C,C'}(t) P_{C'}(t)} \tag{3.15}$$

note that this quantity is zero if the detailed balance holds. Indeed the flow of entropy in the environment i.e. the variation of entropy due to the interaction with the environment or equivalently the heat exchange with the surroundings of the system:

$$\left\langle \dot{S}_{env}(t) \right\rangle \equiv \sum_{C',C} W_{C',C}(t) P_C(t) \log \frac{W_{C,C'}(t)}{W_{C',C}(t)} \tag{3.16}$$

note that is exactly this term that prevents the system to reach an equilibrium state. And of course holds $\langle \dot{S}_{tot} \rangle + \langle \dot{S}_{env} \rangle = \langle \dot{S} \rangle$. These ensemble averages can be given in a microscopic meaning in terms of the entropy change along a single stochastic trajectory. Thus, we can go back from the ensemble-averaged Gibbs entropy to microscopic configurations and assigns an 'entropy' in the following way[8]

$$\mathcal{S} = -\ln P(C_k; t) \qquad \text{for} \quad t_k \leq t \leq t_{k+1}$$

$$\mathcal{S} = -\log P(C; t) \qquad \text{for} \quad 0 \leq t \leq T$$

for the configurations of the trajectory $\{C\}$. Therefore, $\mathcal{S}(t)$ is time-dependent due to two contributions:

- There can be a time-dependence in $P(C_k; t)$ even if the system doen't effectuate jumps because there can be a possible relaxation from a non-stationary initial state.
- There can be time-dependent rates that imply a direct dependence in time for $P(C_k; t)$.

Including th jumps, the rate of change of entropy is

$$\dot{\mathcal{S}}(t) = -\frac{\partial_t P(C(t); t)}{P(C(t); t)} - \sum_{k=1}^{n} \delta(t - t_k) \ln \left[\frac{P(C_k; t_k)}{P(C_{k-1}; t_k)} \right] \tag{3.17}$$

and that can be split in two parts:

[8] From the notational point of view, now $\mathcal{S}$ represents the same of the $s(t)$ that was used in the previous paragraph.

$$\dot{\mathcal{S}}_{tot} \equiv -\frac{\partial_t P(C(t);t)}{P(C(t);t)} - \sum_{k=1}^{n} \delta(t-t_k) \ln \left[\frac{W_{C_{k-1},C_k}(t_k) P(C_k;t_k)}{W_{C_k,C_{k-1}(t_k)} P(C_{k-1};t_k)} \right] \tag{3.18}$$

$$\dot{\mathcal{S}}_{env} \equiv \sum_{k=1}^{n} \delta(t-t_k) \ln \left[\frac{W_{C_k,C_{k-1}(t_k)}}{W_{C_{k-1},C_k(t_k)}} \right] \tag{3.19}$$

with $\dot{\mathcal{S}} = \dot{\mathcal{S}}_{tot} - \dot{\mathcal{S}}_{env}$, where by taking the ensamble averages bring back the equation presented before. In order to take the average, it is needed the probability for a jump that occurs at $t = t_k$ from C_{k-1} to C_k that is $P(C_{k-1};t_k)W_{C_k,C_{k-1}}(t_k)$, thus we have

$$\left\langle \dot{S}_{env}(t) \right\rangle = \sum_{C',C} P(C;t) W_{C',C}(t) \ln \frac{W_{C',C}(t)}{W_{C,C'}(t)} \tag{3.20}$$

and same for the other relation. Of course adding these quantities we have $\langle \dot{S}_{tot}(t) \rangle = \langle \dot{S}_{env}(t) \rangle + \langle \dot{S}(t) \rangle$ with $\langle \dot{S}_{tot}(t) \rangle \geq 0$.
Therefore we have shown that dS/dt can be written by the sum of two term: the first correspond to dS, and the second to dS_{env}, that can be interpreted also as the *heat dissipation rate* (h.d.r.) called $-h_d$.
The first term is indeed $dS \geq 0$, unless it holds the law of detail balance, where in that case $dS = 0$. We regard that if the system is in a NESS, then we have

$$dS_{tot} \stackrel{!}{=} 0 = dS + dS_{env} \equiv dS - h_d$$

so that the heat dissipation rate equals the entropy production of the system[9]. We note that since

$$dS + dS_{env} \equiv dS + dS_{env} = dS + \frac{\delta Q}{T} \geq \frac{\delta Q}{T}$$

if the system is adiabatically isolated, then $\delta Q = 0$ (there's no exchange of heat with the environment of the system, preventing a contribution for the entropy). This means that

$$dS_{tot} = dS \geq 0\,.$$

It is interesting to show [46] that if we integrate for a time interval the follow equation we get

$$\frac{dS_{tot}}{dt} = \frac{dS}{dt} + \frac{dS_{env}}{dt} \tag{3.21}$$

thus we recover the Clausius relation, by simply interpreting (as we suggested before) $\frac{dS_{env}}{dt}$ as the ratio between the heat flux $\frac{dQ}{dt}$ and the temperature T of the environment so that

$$\Delta S_{tot} = \int dS\, dt + \int dS_{env}\, dt$$

[9] Usually the scientific papers define the entropy production like $dS/dt = \Pi - \Phi$, where Π stands for the entropy production rate and Φ stands for the flux of entropy from inside the system to the environment.

then since $\frac{dS}{dt} \geq 0$ we get

$$\int dS_{env}\, dt = -\int \frac{dQ}{T} \quad \Rightarrow \quad \Delta S_{tot} \geq \int \frac{dQ}{T}$$

and this is exactly the Clausius relation briefly discussed before. The difference between ΔS_{tot} and $\int \frac{dQ}{T}$ is the production of entropy.
Thus, the results presented above tell us a concrete (and computational) way to calculate the entropy production of a certain system. This is done by performing the logarithm of the ratio between the rates of the forward jump and its reversed one. Of course this is also strictly related to the concept of irreversibility since if the two rates were equal at each step, then the entropy production would be zero and there would not be a privileged choice for the system to realize a particular path induced by non-symmetric probabilities. As in Fig. 3.1, in nature isolated systems are expected to thermalize, we can conclude that conversely a non-thermalizing system must always interact with the environment [33].

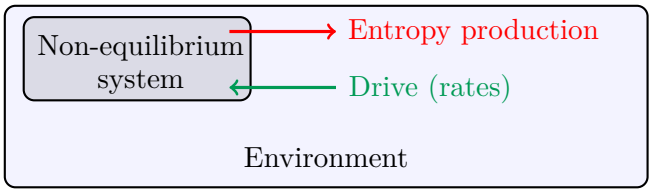


Figure 3.1: Scheme of the relations between the Non-equilibrium system and the Environment.

This means that an external drive is needed to prevent the system from thermalizing by driving it from the outside, maintaining its non-vanishing probability currents which can be seen as the forces that (coupling with the system) allow its rates to be maintained in the defined analytical form through time. The external drive, that keeps the system away from thermal equilibrium, inevitably increases the entropy in the environment. We point out that thermalizing systems (i.e. systems with balanced rates relaxing into thermal equilibrium) can contain subsystems which are out of thermal equilibrium in the sense that the transition rates do not obey detailed balance i.e. they are antisymmetric. This apparent contradiction is resolved by observing that the rates in the subsystem are generally time-dependent and will eventually be adjusted in such a way that the subsystem thermalizes as well with the rest of the environment, but later in time. However, for a limited time interval (that can also be long) it is possible to keep them constant in order to make them violating the detailed balance. This is exactly what happens in experiments and simulations far from equilibrium – typically they depend on external power and will quickly thermalize just it is turned off.
To conclude, there is another interesting way to derive the entropy production of a system [35, 36, 37], by assuming the so-called *local detailed balance* condition. Starting from a condition of equilibrium which holds the detailed balance condition, the

equilibrium probability

$$P_{\text{eq}}(C) = \frac{e^{-U(C)/(k_B\,T)}}{Z}$$

which means that the ratio

$$\frac{W(C',C)}{W(C,C')} = e^{-\beta(U(C')-U(C))} = e^{-\beta\Delta U} = e^{\Delta S/k_B}$$

where as usual S is the entropy change of the environment in the transition $C \to C'$. Upon now the system was considered at equilibrium, and out of equilibrium this relation cannot still hold. Here comes the local detailed balance condition: if it is assumed that for a sufficiently short time and space, the system equilibrates locally with the reservoirs interacting singularly with one of them at a time (but the reservoirs does not interact each other), then we can use the relation above.

Then, without making any assumptions on the time-dependent transition rates, we can decompose them in two parts, one (time) symmetric and the other one (time) antisymmetric:

$$W(C',C) \equiv W(C \to C') = a(C',C)\; e^{\dfrac{F(C',C)}{2}} \tag{3.22}$$

and the reverse rate that is

$$W(C,C') \equiv W(C' \to C) = a(C,C')\; e^{-\dfrac{F(C',C)}{2}} \tag{3.23}$$

where $a(C',C) = \sqrt{W(C',C)W(C,C')} = a(C,C')$ are called *activity parameters* and reflects the accessibility to the respective channel: they are frequencies and can depend both on intensive parameters of the environment or on external forces. Since a is symmetric in time, implies that it is a non-dissipative element in the decomposition of W. The term $F(C',C)$, due to its asymmetry, can be seen as the driving force of the system (we omitted the k_B factor). Indeed, taking the ratio between 3.22 and 3.22 we get

$$F(C',C) = \log\frac{W(C',C)}{W(C,C')} = -F(C,C'). \tag{3.24}$$

Thus we can interpret F as the entropy production on the environment due to its coupling to the system.

Chapter 4

Our model of interactive species

4.1 The stochastic model and master equation

In the introduction, we enounced that our goal in this thesis is to study a particular model of interaction between species. There exist various examples of systems which consist of elements that influence each other through competition or cooperation. Some important cases are: populations of various biological species, political parties, businesses, countries, coupled reacting chemical components in bodies of water, and in organisms, components of the nervous system and so on [48]. Specifically, we want to use the theoretical tools introduced in the previous Chapters (2-3) to give information about the evolution of the system. Furthermore, we are interested in performing a study of its entropy production in different conditions that will be expressed by various values of the parameter on which the system depends. These values must be interpreted as the intrinsic definition of the biological relationships between the species of the relative ecosystem and they may depend on external or internal factors. The procedure that will be followed here consists first by a description of the model that has been chosen for this thesis and then of the method used to simulate the processes involved, then a mathematical analysis is presented in which the deterministic equations (when $N \gg 1$) are derived via Van Kampen's system size expansion and the Fokker-Planck equation (linear noise approximation). The populations evolutions is modelled in a stochastic way by an instantaneous random births-deaths process (Moran Process). Finally, we perform the numerical simulations, plus a comparison between the deterministic and the high population model and we study for which cases (values of the rates entries) the entropy production of the system is higher.

As we said, it is a consolidated procedure to describe these ecological process as stochastic Markov processes (regulated by a master equation) of discrete variables (that represent the single individuals). These kind of formulations are called "Individual-Based-Model" (IBM) where the noise/stochasticity stems from the discreteness of the system itself and not from an external noise. The IBM strength lives in the possibility of a numerical and analytical study, instead of the so called

"Agent-Based-Models" (ABM), that use algorithms, preventing further studies in depth [49].
The model from which we start is that of an ecological system composed of a defined number of species that mutually interact and compete between each other with birth-death processes [14]. Specifically, we handle with a system of m different states E_i, $i = 1, \dots, m$, each of them occupied by $N_i \geq 0$ individuals of that particular state. Of course each state represents its respective species in our model. The configuration of the system, that is nothing that the vector whose entries are the occupation number of all the m species, is

$$C = \begin{bmatrix} N_1 \\ N_2 \\ N_3 \\ \vdots \\ N_{m-1} \\ N_m \end{bmatrix} \tag{4.1}$$

This configuration, as time passes, changes its entries due to the competition process that happens.
Furthermore, the system will have the total number N of individuals *constant*, that is

$$N = \sum_{i=1}^{m} N_i(t), \quad \forall\, t \geq 0. \tag{4.2}$$

Note that this is a strict condition *imposed a priori.* In fact, there are plenty of models that violate equation 4.2; for example, removing the conservation law gives rise to spiral conformation of members of the same species that does not occur if the total density is conserved [50]. Thus one could ask if this bound is legitimate or not. In our case we are interested only in the competitive mechanisms between the species, but we are not interested in the spatial variant of this model where the total number of species cannot be conserved through time, so it is reasonable to make a request like 4.2.
The microscopic interactions between the members of the system are described in time by the following master equation[1], which describe the time evolution of the probability distribution $P(C, t)$

$$\partial_t P(\vec{N}, t) = \sum_{\substack{i,j=1 \\ i \neq j}}^{m} \left[\Gamma_{i \leftarrow j}(N_i - 1, N_j + 1) P(\vec{N} - e_i + e_j, t) - \Gamma_{i \leftarrow j}(N_i, N_j) P(\vec{N}, t) \right] \tag{4.3}$$

where $e_i \in \mathbb{Z}^m$ denotes the unit vector in direction i: $e_i = (0, \dots, \underbrace{1}_{\text{position } i}, \dots, 0)$ and the rate $\Gamma_{i \leftarrow j}$ pertains the specific "jump" of a unit from the j-th species to the i-th one. Thus a jump implies that the new state of the system will be a C'

[1] This kind of model are very popular in literature and have been studied in depth during the last decades.

vector where the state E_j lose a particle that goes to E_i. These jumps are given by a predation or mutation process of the relative species considered. Indeed, the other fundamental definition that is set *a priori* concerns the transition rate per unit time $\Gamma_{i\leftarrow j}$: we make them depend linearly on the number of individual in the departure and in the arrival state:

$$\Gamma_{i\leftarrow j} = r_{ij} N_j (N_i + \sigma_{ij}) \,; \quad r_{ij} \geq 0, \quad \sigma_{ij} \geq 0. \tag{4.4}$$

There are two possible events for the competition process that are defined by the predation rates r_{ij} and the mutation rates σ_{ij} and their dimension is

$$[r_{ij}] = \left[\frac{1}{T}\right], \quad [\sigma_{ij}] = \left[\frac{1}{T}\right] \quad \forall\, i,j = 1,\dots,m. \tag{4.5}$$

These are two $m \times m$ matrices which describe the respective probability contribution to the jump of a certain member on a specific time when the predation|mutation happens:

$$r = \begin{pmatrix} 0 & r_{1,2} & \cdots & r_{1,m} \\ \vdots & 0 & \cdots & \vdots \\ r_{m-1,1} & r_{m-1,2} & \ddots & r_{m-1,m} \\ r_{m,1} & r_{m,2} & \cdots & 0 \end{pmatrix} \quad \sigma = \begin{pmatrix} 0 & \sigma_{1,2} & \cdots & \sigma_{1,m} \\ \vdots & 0 & \cdots & \vdots \\ \sigma_{m-1,1} & \sigma_{m-1,2} & \ddots & \sigma_{m-1,m} \\ \sigma_{m,1} & \sigma_{m,2} & \cdots & 0 \end{pmatrix} \tag{4.6}$$

The diagonal terms ($\Gamma_{i\leftarrow i}$) are set to 0 because we do not consider any auto-interaction.
Solving a master equation is usually very difficult, this is the reason why one adopts two general methods that complement each other:

1. Starting from the master equation it is performed a Kramers-Moyal or a Van Kampen's expansion in order to recover the deterministic equations (taking $N \to \infty$) and the Fokker-Planck ones that include the deterministic part plus a correction term for the demographic stochasticity.

2. Through the so-called *Stochastic Simulation Algorithm* (SSA) also called *Gillespie algorithm* [51], it is a Monte Carlo method, which provides a computational method to simulate a single-realisation of a master equation regulated process. We stress that our system is, in few words, a master equation on a network of accessible states.

We now describe in detail how the Gillespie algorithm works and next we will show the particular model that we have chosen for this master thesis. For completeness, in [52] is shown the equivalence between the continuous master equation and the discrete simulation of the process.

4.2 The Gillespie algorithm for our model

Based on the assumption of a homogeneous and well-mixed system, Gillespie in the 70-ies [51] proposed an exact stochastic simulation algorithm to simulate directly the time evolution of a master equation. At each time, the system is precisely situated in a state C and the possible states reachable by the system are determined by the number m of the ecological species. A particular way to represent the process we want to simulate, is to consider the above cited network of states. The system will start at a given initial condition, at a state C and it will jump from one state to another at a time that will be calculated in a probabilistic way depending on different rates as in Figure 4.1:

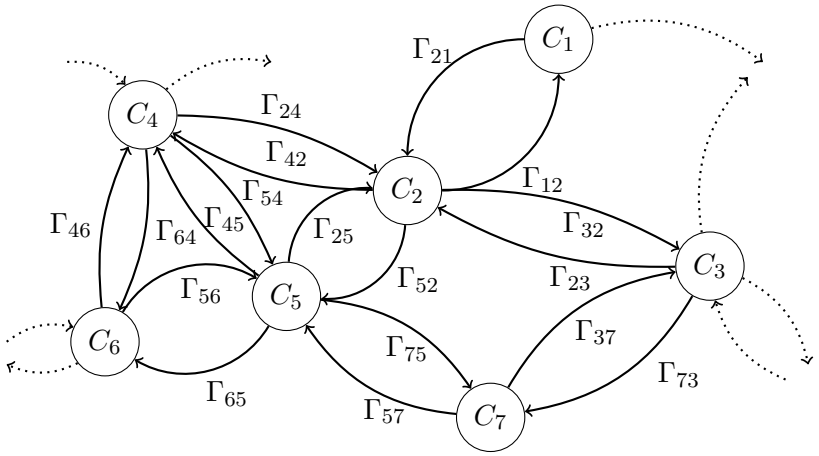


Figure 4.1: Graphical representation of the system's network of states $\{C_1, C_2, C_3, \ldots\}$ that are connected to each other with the appropriate rate constants that bring the stochasticity of the evolution of the path, where for more clarity $\Gamma_{21} \equiv \Gamma(C_1 \to C_2)$.

Specifically, the algorithm determines the new state C' in which the system will jump and also the time interval Δt at which this happens, given that at time t it was in C. These two occurrences are determined in a stochastic way [53] i.e. the algorithm determines which reaction occurs and at what time. We stress the fact that these two steps do not depend on one another so they can be presented in an arbitrary way and from a notational point of view we will represent the rates with $\Gamma_t(C \to C')$.

Choice of the time interval

In order to choose the time interval of the system at each step, we define the sum of all the transition rate from a state C to all the possible communicating states C':

$$\lambda(C) = \sum_{C' \neq C} \Gamma(C \to C') \tag{4.7}$$

this is the *Total Escape Rate* from the state C.
Considering the dimensions of the rates involved in 4.5, we see immediately that all together, they can bring a *Time-scale* χ that will be the inverse of $\lambda(C)$. In fact, the dimension of $\lambda(C)$ is the same of the rate Γ, this means that by inversion one can easily obtain the time scale

$$\chi(C) = \frac{1}{\lambda(C)}\,, \tag{4.8}$$

Considering the state being at C at time t, the probability $P(\tau, \psi)d\tau$ that the next reaction[2] ψ will occur in the time interval $[t+\tau, t+\tau+d\tau]$ and that there will be a reaction ψ. This means that

- no reaction occurs during $[t, t+\tau]$
- the reaction ψ occurs in the interval $[t+\tau, t+\tau+d\tau]$.

The probability that the reaction ψ will occur in the interval $[t+\tau, t+\tau+d\tau]$ is

$$P(\psi, [t+\tau, t+\tau+d\tau]) = \Gamma_\psi d\tau \tag{4.9}$$

If we denote with

$$P_0(\tau' + d\tau') = P_0(\tau')(1 - \lambda(C)) \tag{4.10}$$

indeed the probability that no reaction occurs during $[t, t+\tau'+d\tau']$ is equal to the probability to have no reaction in $[t, t+\tau']\,(= P(\tau'))$ multiplied by the probability to have no reaction in $[t+\tau', t+\tau'+d\tau']$, $(1-\lambda(C)d\tau')$ where $\lambda(C)d\tau'$ is the probability to have one reaction in the time interval $[t, t+\tau'+d\tau']$. Dividing by $d\tau'$ we get

$$\frac{P_0(\tau'+d\tau') - P_0(\tau')}{d\tau'} = -\lambda(C)P_0(\tau'),$$

so that when we take the limit $d\tau' \to 0$, $P_0(\tau')$ is

$$P_0(\tau') = \exp(-\lambda(C) \cdot P_0(\tau'))$$

From this we obtain $P(\psi, \tau)$

$$P(\psi, \tau)d\tau = P_0(\tau') \cdot P(\psi, [t+\tau, t+\tau+d\tau])d\tau \tag{4.11}$$

At the end we have

$$P_C(\psi, \tau) = \Gamma_\psi \exp(-\lambda(C)\tau). \tag{4.12}$$

Summing all over the possible reactions we have that the next reaction takes place with the following distribution:

$$P_C(\tau) = \lambda(C) \exp(-\lambda(C)\tau). \tag{4.13}$$

[2]For example ψ can be a jump of the system in which an individual goes from N_3 to N_1. Thus it will be regulated by the rate $\Gamma_{1\leftarrow 3} \equiv \Gamma_\psi$.

Our goal now is to obtain for each step the value τ. This can be done using a Monte Carlo method. In fact, since $P_C(\tau)$ is a probability, it has a value between 0 and 1. Thus we generate a random number $r_1 \in [0;1]$ and thanks to the *inversion method* we can extract the associated random number τ from its probability distribution function (see Fig.4.2):

$$P_C(\tau) \mapsto r_1 \quad \Rightarrow \quad \tau = -\chi \ln(r_1). \tag{4.14}$$

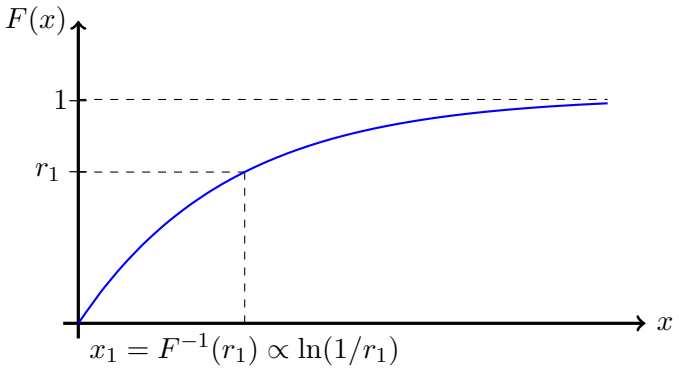


Figure 4.2: In this figure is sketched the inversion method that allows to obtain the time τ at each step, where $F(x) = 1 - \exp(-Ax)$ is $F(x) = \int_{-\infty}^{x} P(s)\, ds$, with A= const.

Thus at each iteration we have to compute τ, that is a different random number. This means that each temporal jump, is usually not equal to the previous one and it depends on the state C.

Choice of the new state

Now that we know for how long the system stays in a particular state, it is necessary to know what its further step is. To do this, a *cumulative probability function* is often used. In detail, starting from the transition rates $\Gamma(C \to C')$ we derive a probability

$$P(C \to C') = \frac{\Gamma(C \to C')}{\lambda(C)} \tag{4.15}$$

and obviously this quantity has the right properties of a probability, since:

(i) It has both a value between 0 and 1, plus it has
(ii) The summation all over the probabilities gives $1 = \sum_{C' \neq C} P(C \to C')$. A strategy that is similar to the one just used, is to consider a random number $r_2 \in [0;1]$ and see if, defining the partial cumulative function[3] as

$$\Lambda_\Theta = \sum_{C'_i}^{\Theta} P(C \to C'_i)$$

[3]Where Θ is the considered (not all) number of reachable state from C.

hold the relation

$$\Lambda_{\Theta-1} < r_2 < \Lambda_{\Theta}.$$

When that happens, it means that the state has privileged that particular jump and this procedure can be now iterated.

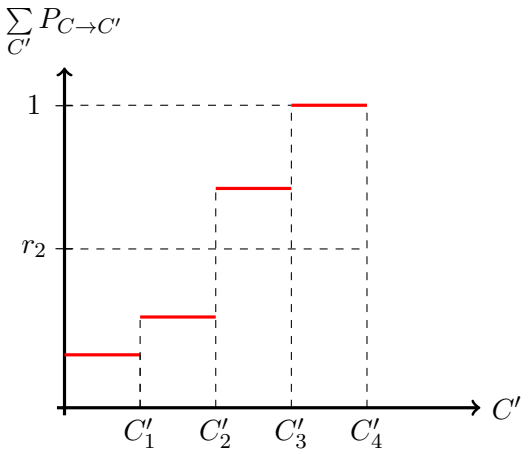


Figure 4.3: The cumulative function method for determining the next system's state. In this example we see that the state has fallen in C'_3. In this figure $\Theta = 4$.

4.3 The cyclic three species model.

The model that we have introduced in the previous section is very general since we have not specified how many species we are interested in and we did not point out some very of its significant properties.

As we said before, the microscopic birth-death interactions between the species imply that at each jump a global state C evolves in a C' state like in this example:

$$C = \begin{bmatrix} N_1 \\ N_2 \\ N_3 \\ \vdots \\ N_{m-1} \\ N_m \end{bmatrix} \quad \Rightarrow \quad C' = \begin{bmatrix} N_1 \\ N_2 + 1 \\ N_3 \\ \vdots \\ N_{m-1} - 1 \\ N_m \end{bmatrix} \tag{4.16}$$

This kind of models are called *Moran processes* [54, 55] (that are known since the end of '50) and they are the most simple in order to study reproduction/selection in a finite population [56]. Since the gain of a species in compensated by the loss of another, these systems are named also *zero-sum games*. In particular we are considering the frequency-dependent Moran process, that follows these steps:

1. In each time step, following their respective fitness (that depends on the actual global state C of the system), two different members are chosen.

2. One member will die and it will be replaced by the off-spring of the one that has been chosen for the reproduction.

This model does not take in account the spatiality of the system, but considers it as a *well-mixed* homogeneous system in which all the particles can interact with each other without spatial limitations. In Fig.4.4 there's a graphical representation of what we said.

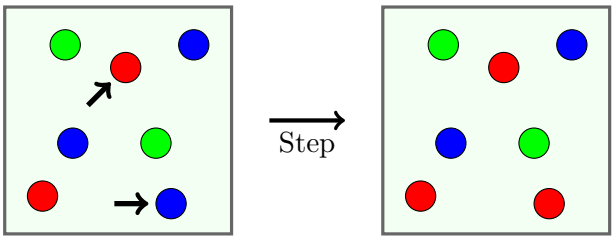


Figure 4.4: Graphical description of the Moran process.

It must be clarified that this mechanism of competition between the species from the biological point of view can be questioned by many sides [57, 58], here are some of them:

- There is no account of the finiteness of food or resources for the species.
- Predator reproduction is immediately coupled to predation. It is not ecologically reasonable to assume a direct conversion of prey to predator, it is too simple.
- The individuals of the population do not react instantaneously between themselves and to any change in the environment, a time-lag should be taken in account.
- The mortality of single predators is uniform and does not depend on the abundance of prey.

Since in the next section from this system, taking the limit of $N \to \infty$, we will recover the deterministic equations that will be Antisymmetric Lotka-Volterra ones, it follows that these criticisms lead to a limited applicability of these equations to a real ecological predator-prey system. Some experiments have shown that the sustenance of biodiversity can often be achieved introducing a spatial structure: In vitro experiments with Escherichia Coli, for example, have shown that the spatial arrangement of the bacteria is crucial for keeping all three competing strands alive [59] and in vivo experiments with bacterial colonies in the intestines of mice can be considered as locally well-mixed populations, and showed that the mobility is

sufficient to maintain coexistence of the species and give rise to traveling waves (Igoshin et al., 2004), and can bring to the self-organization of individuals into spirals in bacteria aggregation. The high mobility imply then a well-mixed system with a spatially uniform configuration. Conversely to a well-mixed population, a spatial system allows us to introduce an additional microscopic process that has no effect if everybody interacts with everybody else: that is site exchange between an individual and an empty site[4]. This gives rise to mobility, which arguably has a profound impact on the outcome of the system's evolution as it can both promote and impede biodiversity [60, 50].
In this thesis we will concentrate on a model of only $\mathbf{m = 3}$ species.The number of the possible interactions between the species can be easily calculated and corresponds to $\Xi(m) = m(m-1)$, thus for $m = 3 \Rightarrow \Xi = 6$. Following the fact that $\Xi = 6$, this means that each state C is surrounded by six states C' (or C_i) and then the abstract figure 4.1 for $m = 3$ is shown in Fig.4.6. The set of death-birth processes contains six elements, described by the rate equations 4.18:

$$\begin{array}{ll} 3+1 \to 1\ ,\ 1; & 2+1 \to 1\ ,\ 1; \\ 1+2 \to 2\ ,\ 2; & 3+2 \to 2\ ,\ 2; \\ 1+3 \to 3\ ,\ 3; & 2+3 \to 3\ ,\ 3; \end{array} \tag{4.17}$$

note that the numbers indicates the interacting species. This interaction leads to a decrease of the first species by one unit which increase the second one. Since r embodies multiplicative factors in the rates, it is the "driving force" of the cyclic mechanism:

$$\begin{array}{ll} \Gamma_{1\leftarrow 2} = r_{12}N_2(N_1+\sigma_{12}); & \Gamma_{1\leftarrow 3} = r_{13}N_3(N_1+\sigma_{13}) \\ \Gamma_{2\leftarrow 1} = r_{21}N_1(N_2+\sigma_{21}); & \Gamma_{2\leftarrow 3} = r_{23}N_3(N_2+\sigma_{23}) \\ \Gamma_{3\leftarrow 1} = r_{31}N_1(N_3+\sigma_{31}); & \Gamma_{3\leftarrow 2} = r_{32}N_2(N_3+\sigma_{32}) \end{array} \tag{4.18}$$

The possible interactions between the species are represented as in Fig.4.5 below:

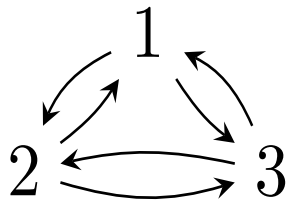


Figure 4.5: Diagram of the possible interactions between the species.

The choice of m has been done for the reason that the increase of the species involved in a system, leads to a significant increment of the computational time at each simulation, and since all of them have been performed on our computer, the computational capacity was not extremely high. From literature [61, 62], we

[4]There exist models that does not permit to have empty sites.

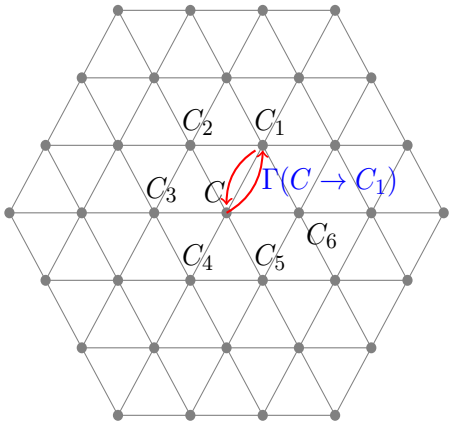


Figure 4.6: Time continuous Markov chain with $m = 3$. It is represented a single jump of the system from the starting state to the next one.

know that cases in which $m = 4, 5, \ldots$ are interesting and give rise to unexpected phenomenologies like the formation of spatial cluster, complicated extinction probabilities, the birth of alliance pairs between the two non directly interacting species or the existence of $2(N+1)$ fixed point where N is the total number of the individuals.

Even if we have well defined the mathematical structure of our model, we do not indicate the specific competitive mechanism between the species 1,2,3. Of course **all** this information is encoded in the entries of the matrices r_{ij} and σ_{ij}.
Our purpose is to study a non-equilibrium ecological system, and one of the most common phenomena in nature and in particular in biological systems is characterized by **cyclic competition**, where different species compete with each other with a cyclic dominance relation in which each species has an advantage over *one* of its opponents but *not* the other. This cyclic dynamics embody the non-equilibrium property of the species interactions. In nature, systems are frequently out of equilibrium and relax to a NESS through time. In the numerical simulations we will try to see if this is our case or not. In nature, exist plenty examples with this cyclicity. For example, dominance of three male strategies has been reported in side-blotched lizards in the inner Coast Range of California [63, 64]: Orange-throated males establish large territories holding several females. These populations are invaded by males with yellow-striped throats, which do not contribute to the defense of the territory but sneak on the females. Such a population of yellow-striped males can be invaded by blue-throated males, which defend territories large enough to hold one female which they defend against sneakers. Once yellow-striped sneakers are rare, it is advantageous to defend a large territory with several females and the cycle starts with orange-throated males again. Other interesting examples can be found in the coral reef invertebrates (Jackson and Buss, 1975) and rodents in the high-Arctic tundra in Greenland (Gilg et al., 2001) or in evolutionary public-good game [65, 66]. Cyclic competition is a very common phenomenon in nature and society and usually

it takes the name of Rock-Scissors-Paper (RSP) game[5].
Therefore the prescription that we need to get accomplished a cyclical behavior of our system is to set the entries of the 3×3 matrices r and s:

$$r = \begin{pmatrix} 0 & r_{1,2} & R_{1,3} \\ R_{2,1} & 0 & r_{2,3} \\ r_{3,1} & R_{3,2} & 0 \end{pmatrix} \quad s = \begin{pmatrix} 0 & \sigma_{1,2} & \sigma_{1,3} \\ \sigma_{2,1} & 0 & \sigma_{2,3} \\ \sigma_{3,1} & \sigma_{3,2} & 0 \end{pmatrix} \tag{4.19}$$

where the factors $R_{ij} > r_{ij} \forall\ i, j = 1, 2, 3$. In many of the following analysis and in the computational simulation we will set $r_{ij} = 1$ and $R_{ij} = R$.
Could we set the factors $r_{ij} = 0$ (leaving $R_{ij} \neq 0$)? That choice would not harm the cyclical property of the system, but it would break its microscopic reversibility and, considering that we are interested in the study of entropy production of the system, the stochastic possibility *must* be included in the next step of the system to return back to the previous state. Furthermore this should happen with a different (lower) rate in order to preserve the cyclicity, otherwise the entropy production per time would be equally zero at each time. Regarding the entries of the matrix σ, they are usually expressed as a set of all equal values, this means: $\sigma_{ij} = \sigma_{ji} \equiv \sigma$ in eq. 4.19.

4.4 Analytical results

Recalling what we said before, solving a master equation cannot be done very easily. The main approach used then is try to obtain the ODE deterministic equation in terms of the fraction populations of the stochastic system considered when $N \to \infty$. This means that all the stochasticity of the system is neglected and we are only considering the collective behaviors of the species i.e. the driving force of the system. We now proceed doing the Van-Kampen system size expansion in order to get those equations. At first we write the extended form of the master equation we are handling with as

$$\begin{aligned} \partial_t P(\vec{N}, t) = &\Big[\Gamma_{1\leftarrow 2}(N_1 - 1, N_2 + 1)P(\vec{N} - e_1 + e_2, t) - \Gamma_{1\leftarrow 2}(N_1, N_2)P(\vec{N}, t)\Big] \\ &+ \Big[\Gamma_{1\leftarrow 3}(N_1 - 1, N_3 + 1)P(\vec{N} - e_1 + e_3, t) - \Gamma_{1\leftarrow 3}(N_1, N_3)P(\vec{N}, t)\Big] \\ &+ \Big[\Gamma_{2\leftarrow 3}(N_2 - 1, N_3 + 1)P(\vec{N} - e_2 + e_3, t) - \Gamma_{2\leftarrow 3}(N_2, N_3)P(\vec{N}, t)\Big] \\ &+ \Big[\Gamma_{2\leftarrow 1}(N_2 - 1, N_1 + 1)P(\vec{N} - e_2 + e_1, t) - \Gamma_{2\leftarrow 1}(N_2, N_1)P(\vec{N}, t)\Big] \\ &+ \Big[\Gamma_{3\leftarrow 1}(N_3 - 1, N_1 + 1)P(\vec{N} - e_3 + e_1, t) - \Gamma_{3\leftarrow 1}(N_3, N_1)P(\vec{N}, t)\Big] \\ &+ \Big[\Gamma_{3\leftarrow 2}(N_3 - 1, N_2 + 1)P(\vec{N} - e_3 + e_2, t) - \Gamma_{3\leftarrow 2}(N_3, N_2)P(\vec{N}, t)\Big]. \end{aligned} \tag{4.20}$$

[5] A vast field of research is the so called Evolutionary Games Theory (EGT). It study the relationships between a group of players, that play some strategies and that evolves usually with time. We are not interested here in this arguments, but let us say that exists a conceptual (and operative) mapping between the evolution of the strategies implemented by the players and the evolution of the species of an ecological system.

Then it is useful to define the equivalent of the rising/lowering-operator of Quantum Mechanics for the master equation:

$$\begin{cases} \mathbb{E}_i f(\vec{N}) &= f(\vec{N} + e_i) \\ \mathbb{E}_i^{-1} f(\vec{N}) &= f(\vec{N} - e_i) \end{cases} \tag{4.21}$$

where $f(\vec{N})$ is a generic function and $\vec{N} = (N_1, N_2, N_3)$.
Following the procedure of Chapter 2, we now see that what we called Ω now is the total number of individuals $N = N_1 + N_2 + N_3$, and the van Kampen ansatz results to be (we expand in order of $N^{-1/2}$):

$$\begin{aligned} N_1 &= Nx_1 + \sqrt{N}\xi_1 \\ N_2 &= Nx_2 + \sqrt{N}\xi_2 \\ N_3 &= Nx_3 + \sqrt{N}\xi_3 \end{aligned} \tag{4.22}$$

where ξ_i is the i-th component of the 3-dimensional stochastic variable (fluctuations) $\vec{\xi} = (\xi_1, \xi_2, \xi_3)$, and x_i is the i-th component of the 3-dimensional variable $\vec{x} = (x_1, x_2, x_3)$ that are the concentrations of the various species.
Using the operatorial notation, the master equation can be edited in the form:

$$\partial_t P(\vec{N}, t) = \sum_{\substack{i,j=1 \\ i \neq j}}^{3} \left(\mathbb{E}_j \mathbb{E}_i^{-1} - 1 \right) \left[\Gamma_{i \leftarrow j}(N_i, N_j) P(\vec{N}, t) \right] \tag{4.23}$$

Up to now there is no approximations involved. Since $\mathbb{E}_i$ changes N_i in $N_i + 1$ and then ξ_i in $\xi_i + N^{-1/2}$, it can be expanded in power-series

$$\mathbb{E}_i^{\pm 1} = 1 + \sum_{\ell=1}^{\infty} \frac{(\pm 1)^\ell}{\ell!} \frac{1}{N^{\ell/2}} \frac{\partial^\ell}{\partial \xi_i^\ell} \tag{4.24}$$

Of course, we are interested on the first two orders, this brings

$$\begin{cases} \mathbb{E}_i &= 1 + \dfrac{1}{\sqrt{N}} \dfrac{\partial}{\partial \xi_i} + \dfrac{1}{2N} \dfrac{\partial^2}{\partial \xi_i^2} + \cdots \\ \mathbb{E}_i^{-1} &= 1 - \dfrac{1}{\sqrt{N}} \dfrac{\partial}{\partial \xi_i} + \dfrac{1}{2N} \dfrac{\partial^2}{\partial \xi_i^2} + \cdots \end{cases} \tag{4.25}$$

Now we have to write the probability density function in terms of ξ_i: $P(N_1, N_2, N_3, t) \rightarrow \Pi(\xi_1, \xi_2, \xi_3, t)$ which specifically implythese two conditions:

$$\Pi(\{\xi_i\}, t) = N^{3/2} P(N\{x_i + \sqrt{N}\xi_i\}, t) \tag{4.26}$$

$$\frac{\partial P}{\partial t} = \frac{1}{N^{3/2}} \frac{\partial \Pi}{\partial t} - \frac{1}{N} \sum_i \frac{dx_i}{dt} \frac{\partial \Pi}{\partial x_i} \tag{4.27}$$

We substitute eq. 4.22, 4.25, 4.4, 4.26 and 4.27 in 4.23 and we do the calculations:

$$\frac{1}{N^{3/2}}\frac{\partial\Pi}{\partial t}-\frac{1}{N}\sum_i\frac{dx_i}{dt}\frac{\partial\Pi}{\partial x_i}=\sum_i\sum_j\left(\mathbb{E}_j\mathbb{E}_i^{-1}\right)\left[r_{ij}(Nx_j+\sqrt{N}\xi_j)(Nx_i+\sqrt{N}\xi_i+\sigma_{ij})\frac{\Pi}{N^{3/2}}\right]-$$
$$-r_{ij}(Nx_j+\sqrt{N}\xi_j)(Nx_i+\sqrt{N}\xi_i+\sigma_{ij})\frac{\Pi}{N^{3/2}}=$$
$$=\sum_i\sum_j\left\{(\mathbb{E}_j)\left(1-\frac{1}{\sqrt{N}}\frac{\partial}{\partial\xi_j}+\frac{1}{2N}\frac{\partial^2}{\partial\xi_j^2}\right)\left[r_{ij}(Nx_j+\sqrt{N}\xi_j)(Nx_i+\sqrt{N}\xi_i+\sigma_{ij})\frac{\Pi}{N^{3/2}}\right]-\right.$$
$$\left.-r_{ij}(Nx_j+\sqrt{N}\xi_j)(Nx_i+\sqrt{N}\xi_i+\sigma_{ij})\frac{\Pi}{N^{3/2}}\right\}=$$
$$=\sum_i\sum_j\left\{(\mathbb{E}_j)\left[r_{ij}(\cdots)_j(\cdots)_i\frac{\Pi}{N^{3/2}}-\cancel{\frac{1}{\sqrt{N}}}r_{ij}(\cdots)_j\cancel{\sqrt{N}}\frac{\Pi}{N^{3/2}}-\frac{1}{\sqrt{N}}\frac{r_{ij}}{N^{3/2}}(\cdots)_j(\cdots)_i\frac{\partial\Pi}{\partial\xi_i}+\right.\right.$$
$$+\frac{1}{2\sqrt{N}}\cancel{\frac{1}{\sqrt{N}}}\frac{r_{ij}}{N^{3/2}}(\cdots)_j\cancel{\sqrt{N}}\frac{\partial\Pi}{\partial\xi_i}+\frac{1}{2\sqrt{N}}\cancel{\frac{1}{\sqrt{N}}}\frac{r_{ij}}{N^{3/2}}(\cdots)_j\cancel{\sqrt{N}}\frac{\partial\Pi}{\partial\xi_i}+$$
$$\left.\left.+\frac{1}{2\sqrt{N}}\frac{r_{ij}}{N^{3/2}}(\cdots)_j(\cdots)_i\frac{\partial^2\Pi}{\partial\xi_i^2}\frac{1}{\sqrt{N}}\right]\right\}-r_{ij}(\cdots)_j(\cdots)_i\frac{\Pi}{N^{3/2}}=$$

Before continuing, we define (1) all the terms inside the square brackets of the last expression, then:

$$=\sum_i\sum_j\left\{(1)+\cancel{\frac{1}{\sqrt{N}}}\frac{r_{ij}}{N^{3/2}}\cancel{\sqrt{N}}(\cdots)_i\Pi+\frac{1}{\sqrt{N}}\frac{r_{ij}}{N^{3/2}}(\cdots)_j(\cdots)_i\frac{\partial\Pi}{\partial\xi_j}-\frac{r_{ij}}{N^{3/2}}\cancel{\sqrt{N}}\cancel{\frac{1}{\sqrt{N}}}\Pi-\right.$$
$$-\frac{r_{ij}}{N^{3/2}}(\cdots)_j\frac{1}{\sqrt{N}}\frac{\partial\Pi}{\partial\xi_j}-\cancel{\frac{1}{\sqrt{N}}}\frac{r_{ij}}{N^{3/2}}\cancel{\sqrt{N}}(\cdots)_i\frac{\partial\Pi}{\partial\xi_i}-\frac{1}{\sqrt{N}}\frac{1}{\sqrt{N}}\frac{r_{ij}}{N^{3/2}}(\cdots)_j(\cdots)_i\frac{\partial^2\Pi}{\partial\xi_i\xi_j}+$$
$$\cancel{2}\left[\cancel{\frac{1}{\sqrt{N}}}\frac{1}{\cancel{2}\sqrt{N}}\frac{r_{ij}}{N^{3/2}}\cancel{\sqrt{N}}\frac{\partial\Pi}{\partial\xi_i}+\frac{1}{\sqrt{N}}\frac{1}{\cancel{2}\sqrt{N}}\frac{r_{ij}}{N^{3/2}}(\cdots)_j\frac{\partial^2\Pi}{\partial\xi_i\xi_j}+\right]+$$
$$+\cancel{\frac{1}{\sqrt{N}}}\frac{1}{2\sqrt{N}}\frac{r_{ij}}{N^{3/2}}\cancel{\sqrt{N}}(\cdots)_i\frac{\partial^2\Pi}{\partial\xi_i^2}+\ \text{3-rd order derivative in } \xi...\ +$$
$$+\frac{1}{2\sqrt{N}}\frac{r_{ij}}{N^{3/2}}(\cdots)_i\frac{\partial\Pi}{\partial\xi_j}+\frac{1}{2\sqrt{N}}\cancel{\frac{1}{\sqrt{N}}}\frac{r_{ij}}{N^{3/2}}\cancel{\sqrt{N}}(\cdots)_i\frac{\partial\Pi}{\partial\xi_j}+$$
$$+\frac{1}{2\sqrt{N}}\frac{1}{\sqrt{N}}\frac{r_{ij}}{N^{3/2}}(\cdots)_j(\cdots)_i\frac{\partial^2\Pi}{\partial\xi_j^2}-\frac{1}{2\sqrt{N}}\frac{r_{ij}}{N^{3/2}}\frac{\partial\Pi}{\partial\xi_j}-\frac{1}{2\sqrt{N}}\frac{r_{ij}}{N^{3/2}}\cancel{\frac{1}{\sqrt{N}}}\cancel{\sqrt{N}}-\frac{\partial\Pi}{\partial\xi_j}-$$
$$-\frac{1}{2\sqrt{N}}\frac{1}{\sqrt{N}}\frac{r_{ij}}{N^{3/2}}(\cdots)_j\frac{\partial^2\Pi}{\partial\xi_j^2}-\frac{1}{2\sqrt{N}}\frac{1}{\sqrt{N}}\cancel{\frac{1}{\sqrt{N}}}\frac{r_{ij}}{N^{3/2}}\cancel{\sqrt{N}}(\cdots)_i\frac{\partial^2\Pi}{\partial\xi_i\xi_j}-$$
$$+\ \text{3-rd ord. der. in } \xi...\ +\frac{1}{2\sqrt{N}}\frac{1}{\sqrt{N}}\frac{r_{ij}}{N^{3/2}}\frac{\partial^2\Pi}{\partial\xi_i\xi_j}+\frac{1}{2\sqrt{N}}\frac{1}{\sqrt{N}}\cancel{\frac{1}{\sqrt{N}}}\frac{r_{ij}}{N^{3/2}}\cancel{\sqrt{N}}\frac{\partial^2\Pi}{\partial\xi_i\xi_j}+$$
$$\left.\text{3-rd order derivatives in } \xi...\right\}-r_{ij}(\cdots)_j(\cdots)_i\frac{\Pi}{N^{3/2}}= \tag{4.28}$$

Following the theoretical prescriptions described in Chapter 2, we have to put equal the terms with $\frac{\partial\Pi}{\partial\xi_{i_{or}j}}$. By doing that, we can exchange the indicies $i\leftrightarrows j$ and thus

we obtain

$$\sum_j -\frac{r_{ij}}{N^2}(\cdots)_j(\cdots)_i\cancel{\frac{\partial \Pi}{\partial \xi_i}} + \frac{r_{ji}}{N^2}(\cdots)_j(\cdots)_i\cancel{\frac{\partial \Pi}{\partial \xi_i}} = -\frac{1}{N}\frac{dx_i}{dt}\cancel{\frac{\partial \Pi}{\partial \xi_i}} \quad \forall i = 1,2,3. \quad (4.29)$$

Now, since

$$(\cdots)_j(\cdots)_i \equiv (Nx_j + \sqrt{N}\xi_j + \sigma_{ij})(Nx_i + \sqrt{N}\xi_i + \sigma_{ij}),$$

we must remember that we have taken the limit $N \to \infty$, this means that the leading order of the product is

$$(\cdots)_j(\cdots)_i \cong (Nx_j)(Nx_i)$$

substituting this last relation in 4.29 brings

$$\sum_j \left[\frac{r_{ij}}{N^2}Nx_jNx_i - \frac{r_{ji}}{N^2}Nx_jNx_i\right] = \frac{1}{N}\frac{dx_i}{dt} \quad (4.30)$$

Finally to get rid of the N, we remember that we can always do a resale of the time calling $Nr_{ij} \Rightarrow r_{ij}$ so we get the deterministic equation of our model:

$$\dot{x}_i = x_i \sum_{j=1}^{m} (r_{ij} - r_{ji})\, x_j, \quad m = 3, \;\; i = 1,2,3. \quad (4.31)$$

We see immediately that, calling $\alpha \equiv r_{ij} - r_{ji}$ we get for example $\alpha_{12} = 1 - R \equiv -\alpha\,;\ \alpha > 0$, we can thus define a matrix $A_{ij} = -\alpha_{ij} = \alpha_{ji}$ and equation 4.31 is seen to be an

Antisymmetric Lotka-Volterra equation (ALVE):

$$\dot{\vec{x}}(t) = \vec{x}(t) \cdot [A\vec{x}(t)] \;\; ; \quad A = \begin{pmatrix} 0 & -\alpha & \alpha \\ \alpha & 0 & -\alpha \\ -\alpha & \alpha & 0 \end{pmatrix} \quad (4.32)$$

The (non-linear) equations written in their explicit form give

$$\begin{cases} \dot{x}_1 = & x_1\,(-\alpha x_2 + \alpha x_3) \\ \dot{x}_2 = & x_2\,(+\alpha x_1 - \alpha x_3) \\ \dot{x}_3 = & x_3\,(-\alpha x_1 + \alpha x_2) \end{cases} \quad (4.33)$$

Below in Fig. 4.7 is shown the solution of equation 4.33:

The classical approach to non-linear equations is to see the behavior of the linearised system near the fixed points. We want now to find if other non-banal fixed points that are the vertices of the plain exist. Let us consider a slightly more general matrix:

$$A = \begin{pmatrix} 0 & a & -b \\ -a & 0 & c \\ b & -c & 0 \end{pmatrix} \quad (4.34)$$

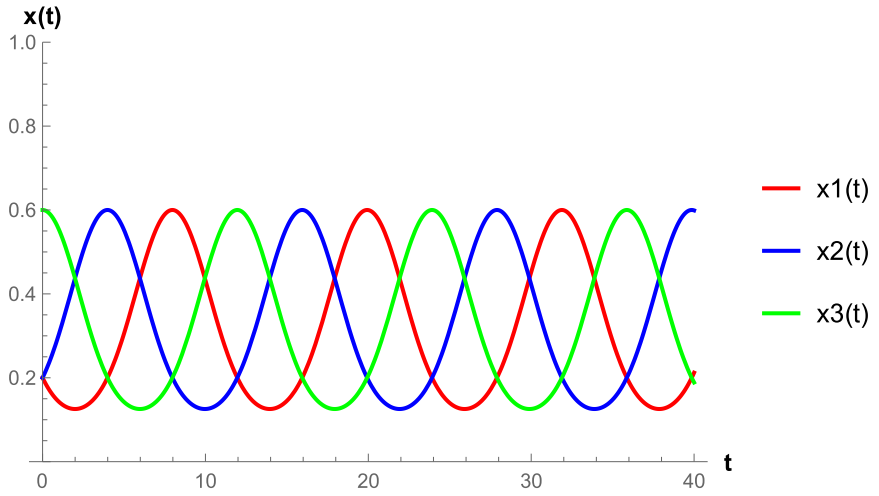


Figure 4.7: Solutions of the 3-species ALVE with initial conditions $(0.2, 0.2, 0.6)$.

Imposing $\dot{\vec{x}} = 0$ of equation 4.32, more that the trivial solution $\vec{x} = 0$ we get the fixed points:

$$\begin{cases} ax_2^* - bx_3^* = 0 \\ -ax_1^* + cx_3^* = 0 \\ ax_1^* - cx_2^* = 0 \end{cases} \Rightarrow \begin{cases} ax_2^* = bx_3^* \\ ax_1^* = cx_3^* \\ ax_1^* = cx_2^* \end{cases} \tag{4.35}$$

then we have

$$x_1^* + x_2^* + x_3^* = 1 = \frac{c}{a}x_3^* + \left(\frac{b+a}{c}x_1^*\right) = \frac{c}{a}x_3^* + \frac{b}{a}x_3^* + x_3^* = \frac{a+b+c}{a}x_3^*$$

and finally we obtain the fixed point

$$\begin{cases} x_3^* = \dfrac{a}{a+b+c} \\ x_2^* = \dfrac{b}{a+b+c} \\ x_1^* = \dfrac{c}{a+b+c} \end{cases} \Rightarrow \quad \text{if } a = b = c = \alpha \quad \Rightarrow \mathbf{p}^* = \begin{pmatrix} 1/3 \\ 1/3 \\ 1/3 \end{pmatrix} \tag{4.36}$$

This result was suggested by the Figures 4.11, in which there are concentric closed curves around $\mathbf{p}^*$. A very interesting representation of the evolution of the system can be performed considering that a mapping between the 3-cartesian-coordinates and the two-coordinates ternary plot in a S_2 simplex[6] exists. Thus, noting Fig. 4.6, the system evolution is represented as a curve on the network inside the simplex S_2 (see Fig.4.8).

In order to do the linearisation we use the constant of motion $N(t) = N$ to symplify the calculations. In fact, once we have determined the motion of two of

[6]It can be shown that for a cartesian point of coordinates (a, b, c) the ternary plot coordiantes are: $\left(\frac{1}{2}\frac{a+2b}{a+b+c}; \frac{\sqrt{3}}{2}\frac{a}{a+b+c}\right)$.

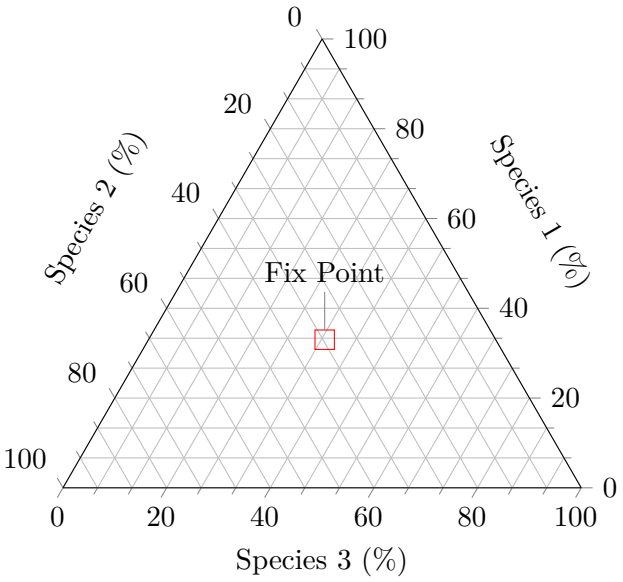


Figure 4.8: Ternary plot in the simplex S_2. Of course in the further simulations the network will be much dense than in this picture.

the variables x_1 and x_2 then the third is determined by $x_3(t) = 1 - x_1(t) - x_2(t)$. Thus defining the new quantities

$$\begin{aligned} \delta x_1 &= x_1 - 1/3 \equiv z \\ \delta x_2 &= x_2 - 1/3 \equiv w \\ \delta x_3 &= x_3 - 1/3 \equiv l \end{aligned} \tag{4.37}$$

we have the linearized system that is

$$\begin{pmatrix} \dot{z} \\ \dot{w} \end{pmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{bmatrix}_{|_{\mathbf{p}^*}} \begin{pmatrix} z \\ w \end{pmatrix} \tag{4.38}$$

so that we have

$$\dot{Z} \equiv \begin{pmatrix} \dot{z} \\ \dot{w} \end{pmatrix} = \begin{bmatrix} 0 & -\frac{\alpha}{3} \\ \frac{\alpha}{3} & 0 \end{bmatrix} \begin{pmatrix} z \\ w \end{pmatrix} \tag{4.39}$$

The eigenvalues of this matrix are $\lambda_{\pm} = \pm i\frac{\alpha}{3}$ and the eigenvectors are $(\pm i, 1)$. Using the matrix $Q = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ we have[7]

$$AQ = Q \begin{pmatrix} 0 & \alpha/3 \\ -\alpha/3 & 0 \end{pmatrix}$$

[7] A is the linearised matrix in $\mathbf{p}^*$. Indeed $Q = Q^{-1}$.

and setting $Y = QZ$ leads to

$$\dot{Y} = Q\dot{Z} \equiv \widetilde{A}Y = Q \begin{pmatrix} 0 & -\frac{\alpha}{3} \\ \frac{\alpha}{3} & 0 \end{pmatrix} \underbrace{Q^{-1}Y}_{Z} \Rightarrow \dot{Y} = \begin{pmatrix} 0 & \frac{\alpha}{3} \\ -\frac{\alpha}{3} & 0 \end{pmatrix} Y$$

Finally, setting $Y_1(t) = r(t)\cos\theta(t)$ and $Y_2(t) = r(t)\sin\theta(t)$ we transform the coupled equations in polar coordinates which gives (multiply by cos and sin respectively second and first line and summing them)

$$\begin{cases} \dot{r}\cos\theta - r\sin\dot{\theta} = & -(\alpha/3)r\sin\theta \\ \dot{r}\sin\theta + r\cos\dot{\theta} = & (\alpha/3)r\cos\theta \end{cases} \Rightarrow \begin{cases} \dot{r} = & 0 \\ \dot{\theta} = & \alpha/3 \end{cases}$$

these are substantially circles around $\mathbf{p}^*$. Now that we know the behavior of the solutions near the fixed point, we show that exist another constant of motion with respect to the total concentration, i.e. $(x(t) = N(t)/N)$

$$N(t) = N_1(t) + N_2(t) + N_3(t) = N \Rightarrow$$

$$\Rightarrow x(t) = x_1(t) + x_2(t) + x_3(t) = 1,$$

so that the solution of our equations will necessarily stay in the plane

$$\Big\{(x_1, x_2, x_3) \in (\mathbb{R}_+)^3 : x_1(t) + x_2(t) + x_3(t) = 1\Big\} \tag{4.40}$$

Note that this is not the only constant of motion that the system has. In effect [67], another one is the following quantity:

$$\Psi(t) \equiv x_1^\alpha(t)x_2^\alpha(t)x_3^\alpha(t) = x_1^\alpha(0)x_2^\alpha(0)x_3^\alpha(0) = const. \tag{4.41}$$

Taking the derivative of Ψ and substituting eq.4.33, we get:

$$\begin{aligned} \dot{\Psi}(t) &= \alpha x_1^{\alpha-1}\dot{x}_1 + \alpha x_2^{\alpha-1}\dot{x}_1 + \alpha x_3^{\alpha-1}\dot{x}_1 \\ &= \alpha\Psi\left[\frac{\dot{x}_1}{x_1} + \frac{\dot{x}_2}{x_2} + \frac{\dot{x}_3}{x_3}\right] \\ &= \alpha\Psi\left[\frac{x_1\left(-\alpha x_2 + \alpha x_3\right)}{x_1} + \frac{x_2\left(\alpha x_1 - \alpha x_3\right)}{x_2} + \frac{x_3\left(-\alpha x_1 + \alpha x_2\right)}{x_2}\right] \\ &= \alpha\Psi\Big[-\alpha x_2 + \alpha x_3 + \alpha x_1 - \alpha x_3 - \alpha x_1 + \alpha x_2\Big] = 0. \end{aligned}$$

This means that the solutions of the ALVE must be the class of curves that emerge from the intersection between the plain 4.40 and different values of the function 4.41 as in Fig. 4.11.

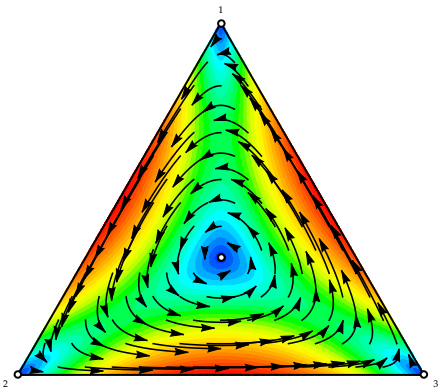


Figure 4.9: Representation of the closed curves of the coupled equations in a ternary plot. This graphics has been obtained using the *Dynamo* package [68].

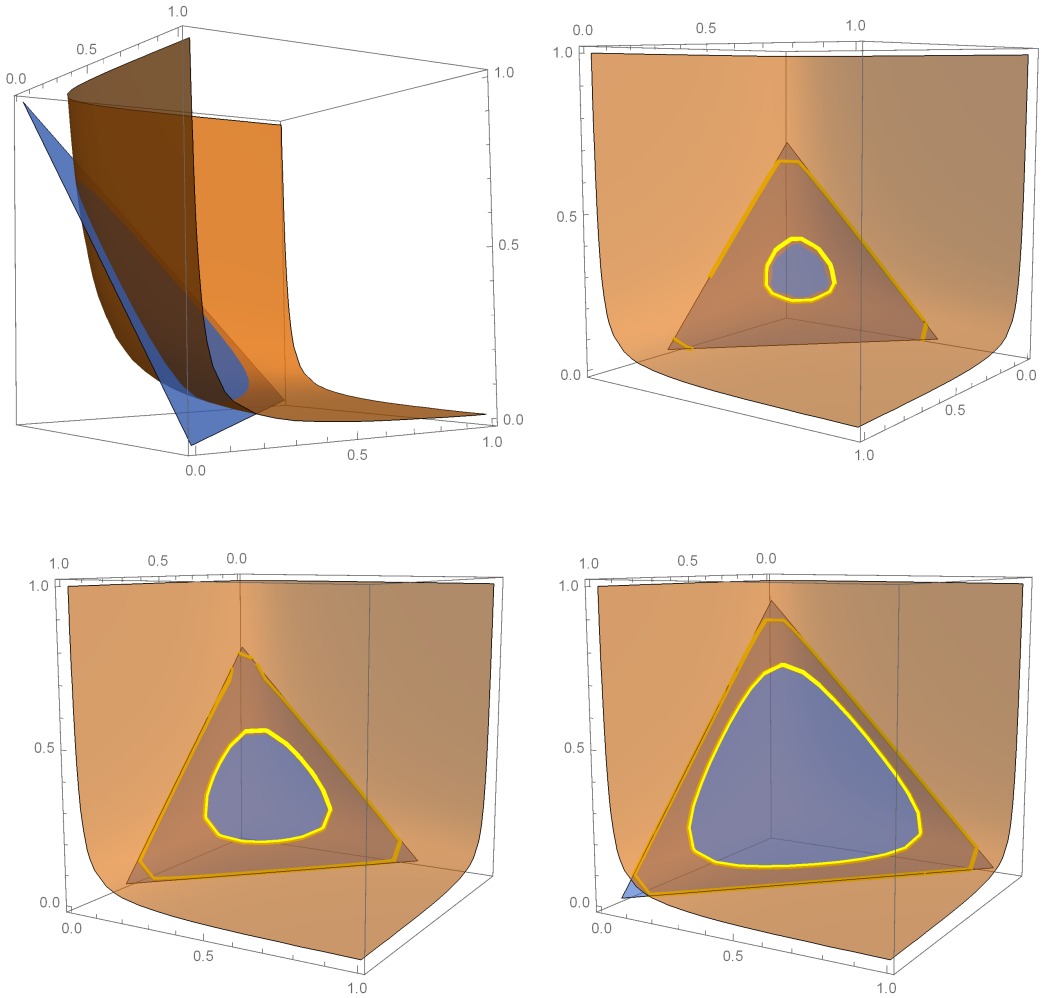


Figure 4.11: Representation of the closed curves of the coupled equations and some examples of solutions of the Antisymmetric Lotka-Volterra equations.

With the analysis done until now, it is well clear what the behavior of the drift term is the deterministic behavior of the system. However, it is fundamental having a knowledge of the diffusion term, and this can be obtained only finding the Fokker-Planck equation. This could be obtained following the next order of the van Kampen's expansion. Instead, here we follow the formalism used in [69]. In fact the master equation can be revived in the following form

$$\partial_t P(\vec{x},t) = \sum_{\delta\vec{x}} \{P(\vec{x}+\delta\vec{x},t)\mathcal{W}(\vec{x}+\delta\vec{x}\to\vec{x}) - P(\vec{x},t)\mathcal{W}(\vec{x}\to\vec{x}+\delta\vec{x})\} \tag{4.42}$$

where $\mathcal{W}(\vec{x}\to\vec{x}+\delta\vec{x})$ denotes the transition probability from state $\vec{x}$ to the state $\vec{x}+\delta\vec{x}$ within one time step.
According to Kramers-Moyal expansion to the second order we get the Fokker-Planck equation:

$$\partial_t P(\vec{x},t) = -\partial_i\left[\alpha_i(\vec{x})P(\vec{x},t)\right] + \frac{1}{2N}\partial_i\partial_j\left[\beta_{ij}(\vec{x})P(\vec{x},t)\right] \tag{4.43}$$

where the quantities are the following:

$$\alpha_i(\vec{x}) = \sum_{\delta\vec{x}} \delta x_i \mathcal{W}(\vec{x}\to\vec{x}+\delta\vec{x}) \tag{4.44}$$

$$\beta_{ij}(\vec{x}) = \sum_{\delta\vec{x}} \delta x_i \delta x_j \mathcal{W}(\vec{x}\to\vec{x}+\delta\vec{x}) \tag{4.45}$$

Let us write the explicit form of $\alpha_i(\vec{x})$ and $\beta_{ij}(\vec{x})$ for our system. For example, note that the term $\delta x_i = \pm\frac{1}{N}$ if the rate considered in that term of the summation describes a particle incoming or outgoing from the i-th position. Thus we calculate the drift $\alpha_1(\vec{x})$ term remembering 4.19 and that $N_i = N\,x_i$:

$$\begin{aligned}
\alpha_1(\vec{x}) &= \frac{1}{N}r_{12}N_2(N_1+\sigma_{12}) + \frac{1}{N}r_{13}N_3(N_1+\sigma_{13}) - \frac{1}{N}r_{21}N_1(N_2+\sigma_{21}) - \\
&- \frac{1}{N}r_{31}N_1(N_3+\sigma_{31}) = \\
&= r_{12}Nx_1x_2 + r_{12}x_2\sigma_{12} + r_{13}Nx_3x_1 + r_{13}x_3\sigma_{13} \\
&- r_{21}Nx_1x_2 - r_{21}x_1 + \sigma_{21} - r_{31}Nx_1x_3 - e_{31}\sigma_{31}x_1 = \\
&= (r_{12}-R_{21})Nx_2x_1 + (R_{13}-r_{31})Nx_1x_3 + \\
&+ [r_{12}\sigma_{12}x_2 - R_{21}\sigma_{21}x_1 + R_{13}\sigma_{13}x_3 - r_{31}\sigma_{31}x_1.]
\end{aligned} \tag{4.46}$$

Dividing both members by N, and rescaling the time coordinate $Nt\to t$, we get for a generic indicies:

$$\alpha_i(\vec{x}) = x_i\sum_{j=1}^{m}(r_{ij}-r_{ji})x_j + \frac{1}{N}\sum_{j=1}^{m}(r_{ij}\sigma_{ij}x_j - r_{ji}\sigma_{ji}x_i). \tag{4.47}$$

As we expected, if $N\to\infty$, then we recover the ALVE. The same procedure can be done for the terms $\beta_{ii}(\vec{x})$ and $\beta_{ij}(\vec{x})$ and we obtain the following diffusion expressions

$$\beta_{ii}(\vec{x}) = \sum_{\substack{j=1\\ i\neq j}}^{m}(r_{ij}+r_{ji}) + \frac{1}{N}\sum_{\substack{j=1\\ i\neq j}}^{m}(r_{ij}\sigma_{ij}x_j + r_{ji}\sigma_{ji}x_i) \tag{4.48}$$

$$\beta_{ij}(\vec{x}) = -(r_{ij}+r_{ji})x_ix_j - \frac{1}{N}(r_{ij}\sigma_{ij}x_j + r_{ji}\sigma_{ji}x_i). \tag{4.49}$$

4.5 Numerical simulations and its analysis

As we have just seen, the complexity of the obtained Fokker-Planck equations gives little hope to study analytically the evolution of the system. Therefore in this last section we see some numerical simulations of the SSA of the continuous time Markov process we are dealing with. The SSA was written in C++ programming language. It is our interest to study as the systems behave in different cases of:

1. Total number N, in which we expect an approach to the deterministic behavior as $N \gg 1$.

2. Values of the predation and mutation rates r_{ij} and s_{ij}.

Above all, for these various cases we want to study the entropy production of the system. Indeed individuals of the species produce and exchange entropy in an open stochastic-thermodynamic system. Within the framework of the classical theory of irreversible thermodynamics, and under the condition of constant external constraints, such a system will naturally evolve toward a globally stable thermodynamic stationary state [70].
The entropy production at the i-th step of the system evolution, will be calculated as shown in Chapter 3 by (see also Fig. 4.6):

$$\delta S_i = \log \frac{\Gamma(C \to C')_i}{\Gamma(C' \to C)_i}.$$

It is important to stress that this formula does not require any knowledge about the nature or composition of the environment. It depends exclusively on the stochastic trajectory of the subsystem and the corresponding transition rates that drive it. Indeed the total entropy production will be simply[8]

$$S = \sum_i \delta S_i$$

Furthermore, one of the first things we want to be sure of, is that the systems actually goes to a NESS (from theory one expect this) and how fast it goes to it. We said that this condition should be achieved when the mean of the observables (in this case each of he three species) does not change with time. Since the definition of the mean value of a generic observable O_C (in our case we have $O_C(t) = N_i(t), \quad i = 1, 2, 3.$), function of the states C is by definition

$$\frac{d\langle O \rangle}{dt} := \sum_C O_C \frac{dP_C}{dt}$$

is immediately clear that in a stationary state $\dfrac{d\langle O \rangle}{dt} = 0, \quad \forall\, t$. To be precise, this does not imply that the system effectively reached a NESS, because it could be at equilibrium for example. Anyway, in the model we choose, it is not necessary to prove this since we have by-hand imposed the rates in a way to get the cyclical behavior that surely involves non-zero currents.

[8] Indeed, it is reasonable to expect that, being coupled in an irreversible way to the environment, the system in a NESS continues to 'induce' the entropy of the surrounding medium to increase [71].

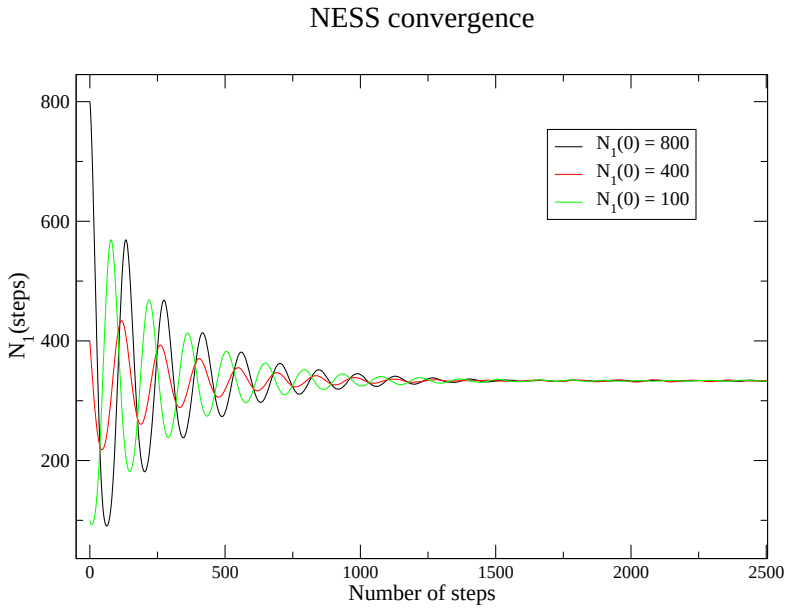


Figure 4.12: Temporal evolution (averaged over 10000 samples) of the system towards a NESS of species 1 with three different initial conditions. Parameters: r=1, R=5, s=S=1.

In order to observe if the system effectively goes towards a NESS, we wrote a program in C++ language which performed thousands of times the simulations of the same process, and took the mean of the values of each species at every x jumps, where usually $x \sim 100$. Of course, we expect a greater reliability of the method if the simulations involved are several thousands. All the simulations effectuated showed that effectively the system goes towards a NESS very fast. Considering that all the simulation performed involves a number of steps that are greater than $\sim 10^6$, it can be assumed that compared to the simulation times, the state goes toward a NESS almost instantly. For example, in Fig.4.12 we show that running the program for 10000 simulations gives a perfect convergence to the NESS, even with different initial conditions of the system. Another interesting result comes from the mathematical structure of the spectrum of the master equation. In fact, if we increase the number of N, then the system itself goes to a NESS in a (slightly) longer time.
In the following sections, different values of N and of parameters will be studied and a study of the irreversibility will be performed (i.e. of the entropy production) for those various conditions.

4.5.1 Case without cyclicity

Before studying the realizations of the SSA in which the cyclicity is present[9], let us see what happens in a case in which the predation rates are all equal $r_{ij} = R_{ji}$. One should expect the evolution to be strongly stochastic. In Fig. 4.13 and 4.14 are

[9]Of course it is imposed by the choice of the constants of the matrices of the rates.

shown different simulations that justify what just stated.

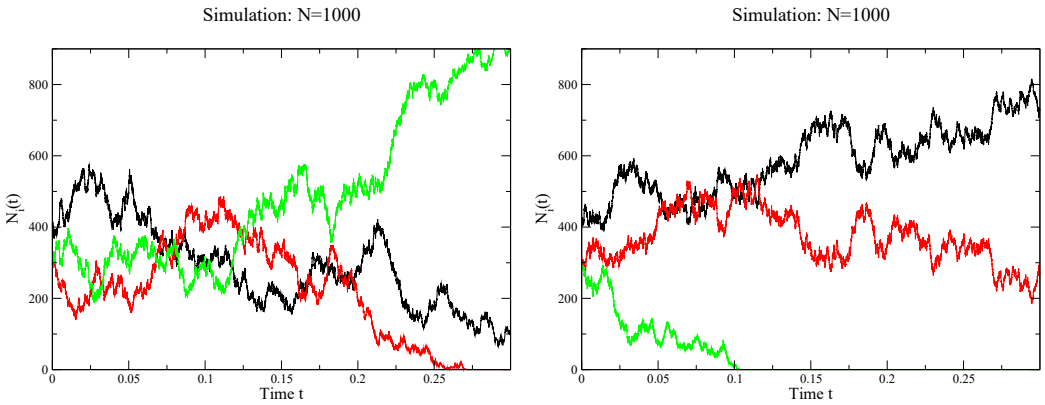


Figure 4.13: Simulations with parameters $r = R = 1$ and $s = S = 0$ with the same initial conditions.

These simulations show that if N increases, the stochasticity of the system's evolution is less prominent.

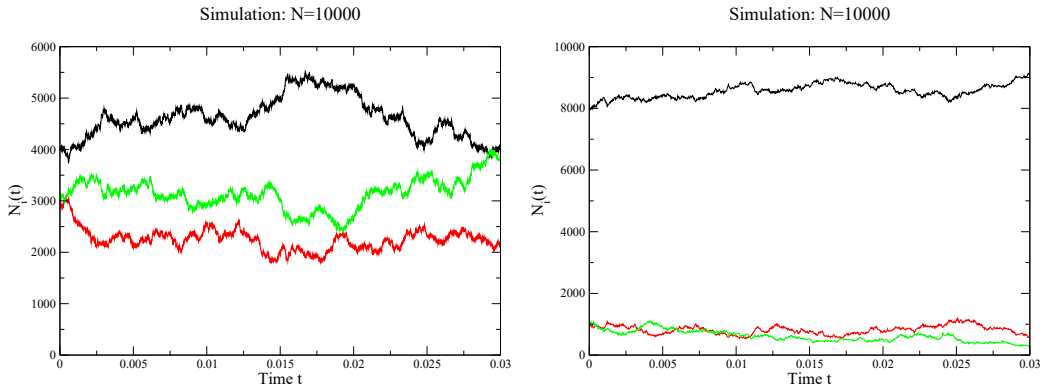


Figure 4.14: Simulations with parameters $r = R = 1$ and $s = S = 0$ with different initial conditions and $N \gg 1$.

4.5.2 Approaching the deterministic model: $N \gg 1$

In this thesis our interest is focused to a system where cyclicity is present, and this implies that the r-matrix must be like in 4.19. In order to retrieve the differential equations described in the analytical calculations, it is necessary to choose a number for the initial condition of the system where N is sufficiently big. So we performed a simulation in which is represented each single variation (step) of the system state for all three species and N was set to 10000. In the following Fig. 4.15 we effectively recover the solution of the ALVE obtained in this chapter (see Fig.4.7). Conversely to what just done, during the run of the SSA we wrote in the data file of the simulations the number N_i, $i = 1, 2, 3$ of the species only at every 500 steps (an

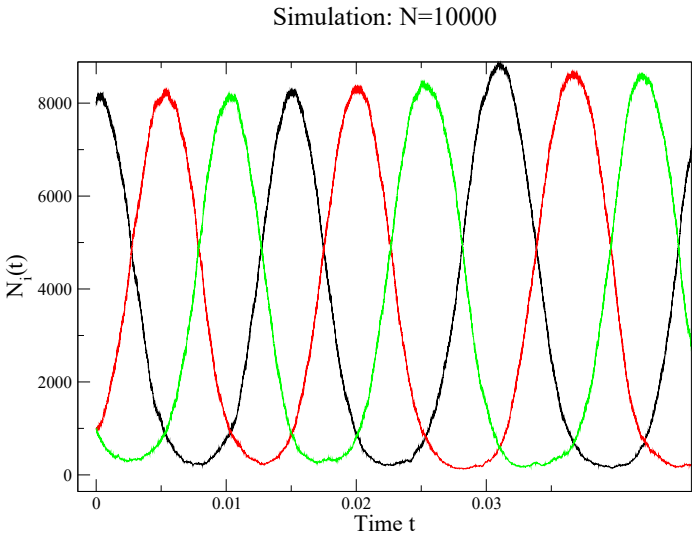


Figure 4.15: Numerical simulation with parameters: $R = 0.5$, $r = 0.4$, $\sigma = 1$.

example of that can be seen in Fig. 4.18). This was done also in further simulations for two central reasons:

1. It could be that we want to focus less on the immanent stochasticity of the system's evolution (except when this is not our specific interest like before) and show its behavior in "coarse grained view", in order to see the main properties of the evolution of the species.

2. By writing the results only at intervals of several hundreds, we overcome the computational problem of getting intractable (too heavy) data-files.

Furthermore, it is interesting to show the ternary plot mapping introduced above for an analogue simulation, which well shows the curves that were discussed previously in the analytical part:

As one would expect, the system's evolution (in part) depends on the initial state condition, and this is more evident when approaching to $N \to \infty$. In Fig.4.17 we show two graphics which start with different initial conditions. In Fig.4.16 it is shown that the paths accomplished by the system approach the condition $N \to \infty$ described in Fig.4.11.

Null mutation: case with $\sigma = 0$

An interesting case is that in which mutation is prevented, and that corresponds to set all the non-diagonal parameters $\sigma_{ij} = 0$. What do we expect by doing this assumption in the simulations? Remembering that the r-matrix has the form of 4.19, we expect that at some time, one of the three species involved will lead the system and this should happen with a probability of $1/3$ for all three species (see Fig. 4.18). Once one of the systems (due to the intrinsic stochasticity of the evolution) takes the total number N of the population, entropy should not be produced anymore since the

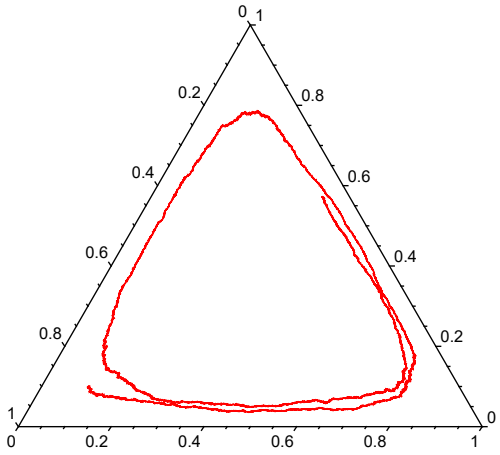
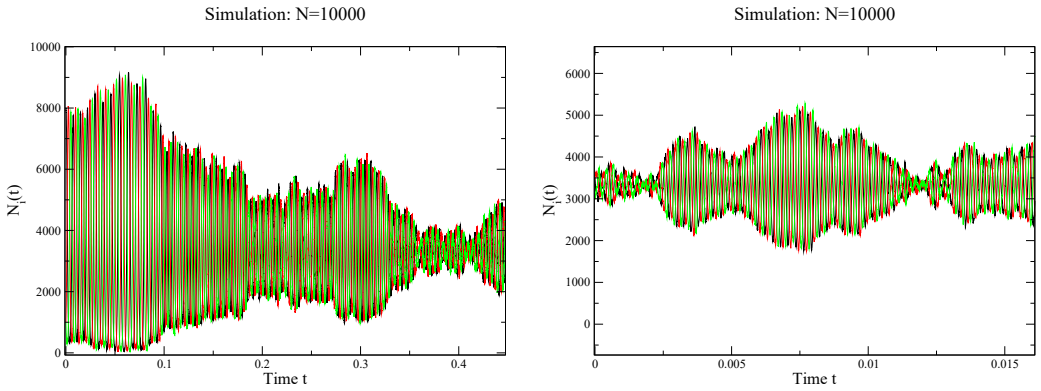


Figure 4.16: Ternary plot for a simulation with N=10000 with initial concentrations $(0.8, 0.1, 0.1)$.



(a) $R = 0.5$, $r = 0.3$, $\sigma = 1$ *(b)* $R = 5$, $r = 1$, $\sigma = 1$

Figure 4.17: Simulations with different initial conditions: a =(8000, 1000, 1000) and b =(3500, 3500, 3500).

system is stuck in a condition with no mutation, where all the other populations are null, which implies null transition rates. In particular doing the simulations we have seen that the system in these conditions tends to reach the bound of the simplex S_2, with a mechanism that seems more influencing than the simple stochasticity. This is well explained in [72], in which it is shown that the constant of motion can be used as a difference from the interior fixed point and its average change is $\langle \Delta\Psi \rangle \propto 1/N^2 \underset{N\gg 1}{\longrightarrow} 0$. Regarding what we said about the entropy production, later we will show that locally in time there can be a negative entropy production, but on average, this quantity must be always positive. A first example is the entropy production in the case of $\sigma = 0$ (see Fig. 4.19).

From this last plot, it is interesting to note that the entropy production rate scales linearly with time, and this will be a general feature of this quantity. More important is that at first sight, near the end of the simulation, where the system

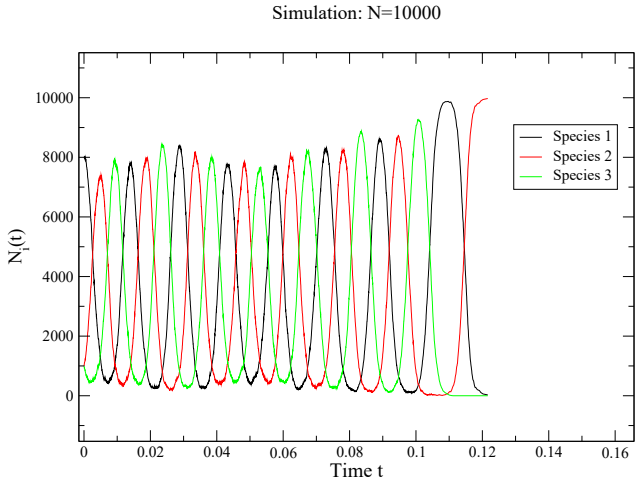


Figure 4.18: Simulation in which $\sigma = 0$, N=10000. The extinction of two species out three and the leading of the left species can happen with a 1/3 probability.

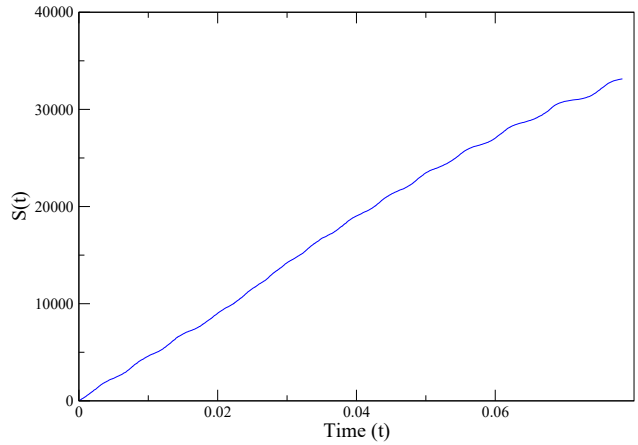


Figure 4.19: Entropy production s=S=0, N=10000.

evolves towards the bound of the simplex S_2, it seems to produce less entropy.This of course means that the system evolves into a state which can be interpreted as "less irreversible".

4.5.3 N= 100

Besides the case for $N \gg 1$, we show also the case in which N is not large ($N \sim 100$), here the effects of the intrinsic stochasticity should be very relevant. An example is shown in Fig. 4.20 where the system's cyclicity is heavily perturbed by the randomness due to the finite size of the three interacting species.

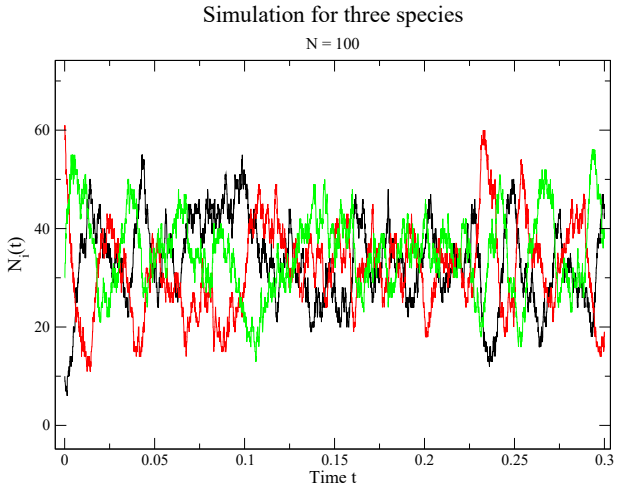


Figure 4.20: Example of the system's evolution for N small. Parameters: $r = 1$, $R = 2$, $\sigma = 5$.

4.5.4 N= 1000

The most interesting condition of analysis for us is when the system's size is neither too much low or high. In fact, in this case the effect of stochasticity is important, but it is not enough effective to overcome the oscillatory mechanism imposed by the transition rates. This can be seen below in Fig.4.21 that an example of evolution of the system for certain parameters. Note that if one zooms in that figure, the cycles appear immediately.

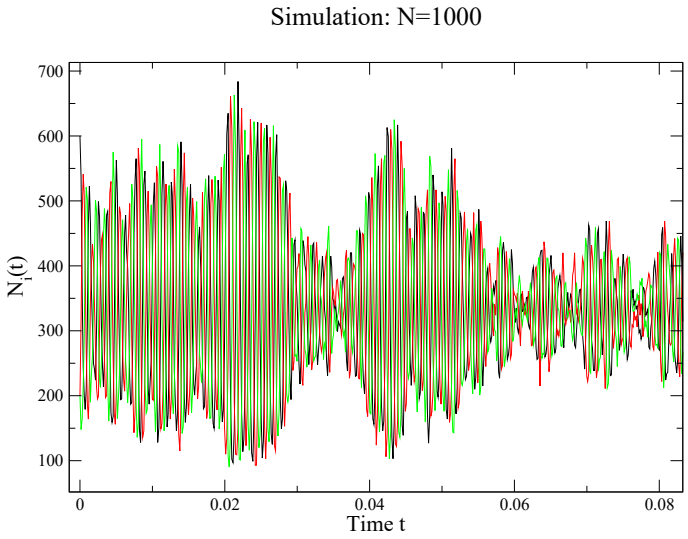


Figure 4.21: Numerical simulation with parameters: $r = 1$, $R = 10$, $\sigma = 5$. Initial condition $(600, 200, 200)$.

Following our study on the entropy production, in Fig.4.22-4.23 is shown the

time-series of the three species in a condition of low mutation rate with a remarkable cyclicity imposed[10].

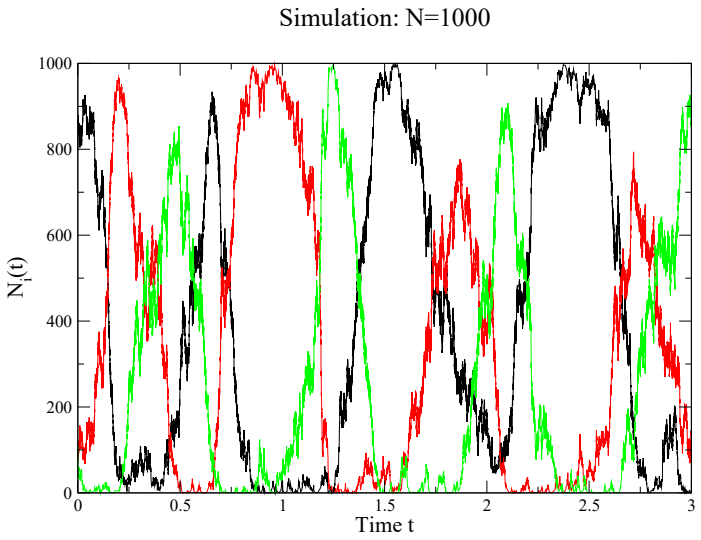


Figure 4.22: Numerical simulation with parameters: $r = 1$, $R = 1.02$, $\sigma = 0.4$.

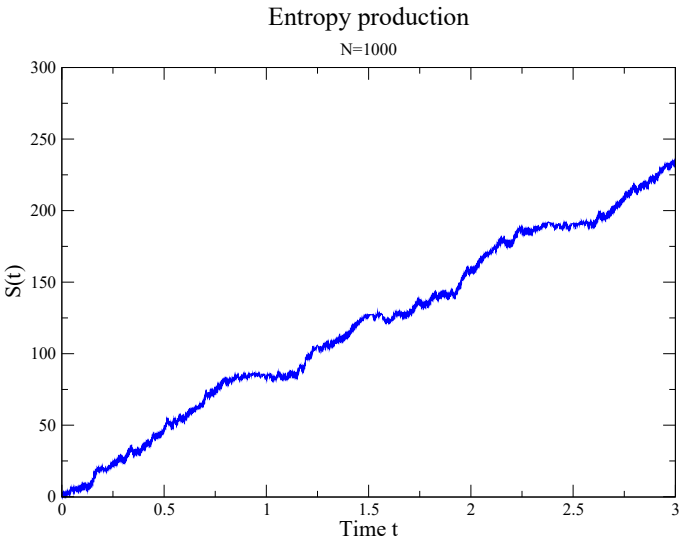


Figure 4.23: Entropy production with parameters: $r = 1$, $R = 1.02$, $\sigma = 0.4$.

In the entropy production figure one immediately sees that there are some regions in which the entropy remains quite constant, i.e. the entropy production is almost null. These regions correspond to a dominance of one species among the others. This behavior goes along with the one of Fig.4.19.
Thus, everything that has been seen until now makes us suppose that the entropy production is lower when the system accomplishes trajectories in which one species

[10] In this simulation every single jump was printed.

is dominant.
To investigate more deeply this fact, it is interesting to evaluate the entropy production for $N \gg 1$. Comparing Fig.4.24 and Fig.4.25, we clearly see that the entropy production decreases more not only when there is a dominance of one species, but when the system itself lives far from the fixed point $N(1/3, 1/3, 1/3)$.

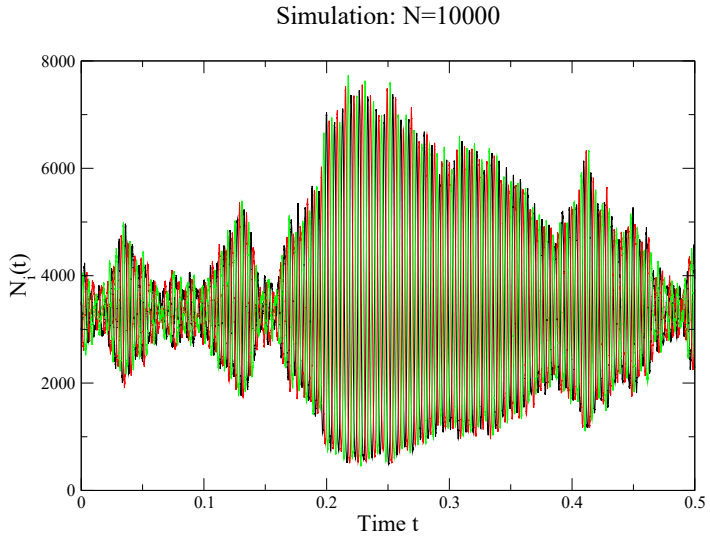


Figure 4.24: Numerical simulation with parameters: $r = 0.3$, $R = 0.5$, $\sigma = 1$.

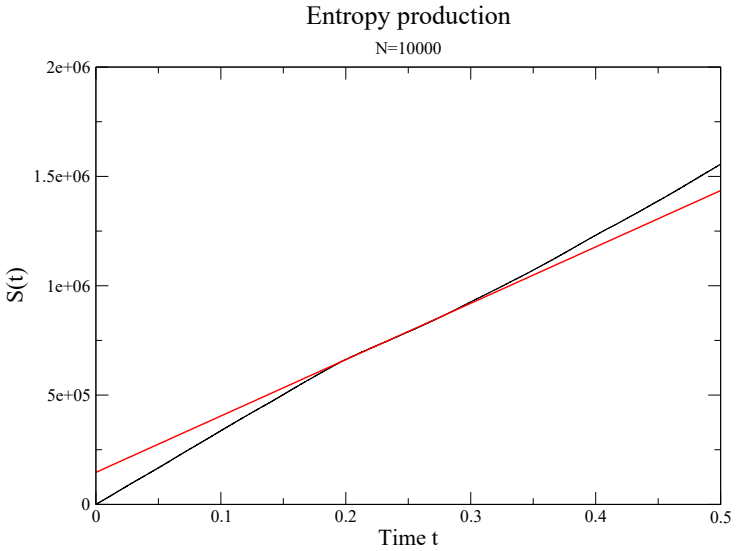


Figure 4.25: Entropy production with parameters: $r = 0.3$, $R = 0.5$, $\sigma = 1$.

In Fig.4.24 a linear fit has been performed in the time range that corresponds to the maximal distance of the vector state from the fix point. Here it is clear what was anticipated before about the different regimes of entropy production associated to different trajectories along through the simplex S_2.

The different entropy production is stressed if we plot the system's entropy production in a condition in which the state evolves far from the fix point and another one that evolves near of it.
First, we have chosen some parameters that allowed the system to be de-localised compared to the fix point, and the relative entropy production.

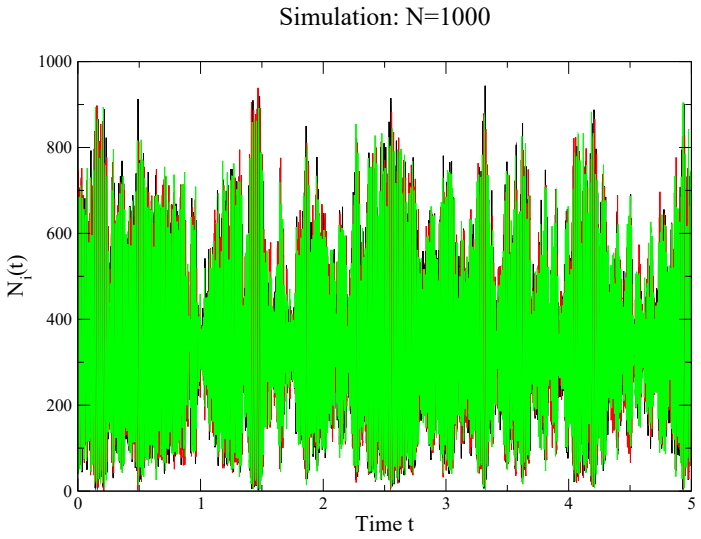


Figure 4.26: Entropy production with parameters: $r = 0.3$, $R = 0.5$, $\sigma = 1$.

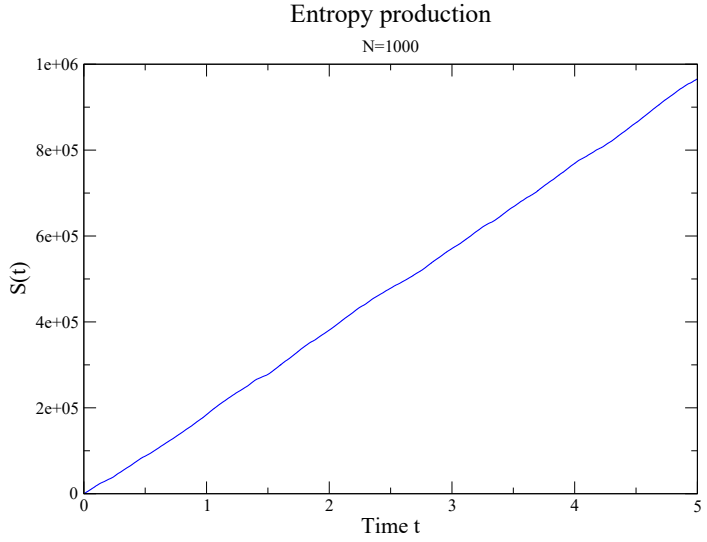


Figure 4.27: Entropy production with parameters: $r = 0.3$, $R = 0.5$, $\sigma = 1$.

Then, a high value of mutation rate is considered (Fig.4.28). Here the action of the mutation forces the system to live near the fix point and this is the reason of the higher entropy produced. The simulation time goes from 0 to 5. In Fig.4.29 it is shown a comparison of the entropy production of the graphics 4.26-4.28 with a high and low value of σ.

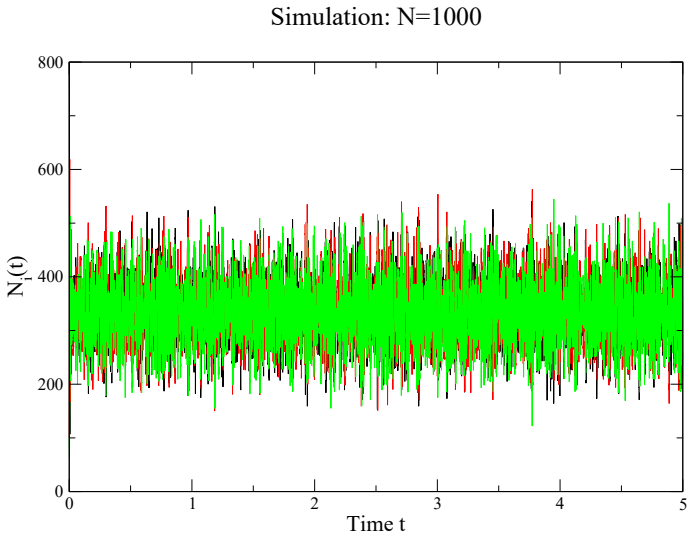


Figure 4.28: Entropy production with parameters: $r = 0.3$, $R = 0.5$, $\sigma = 30$.

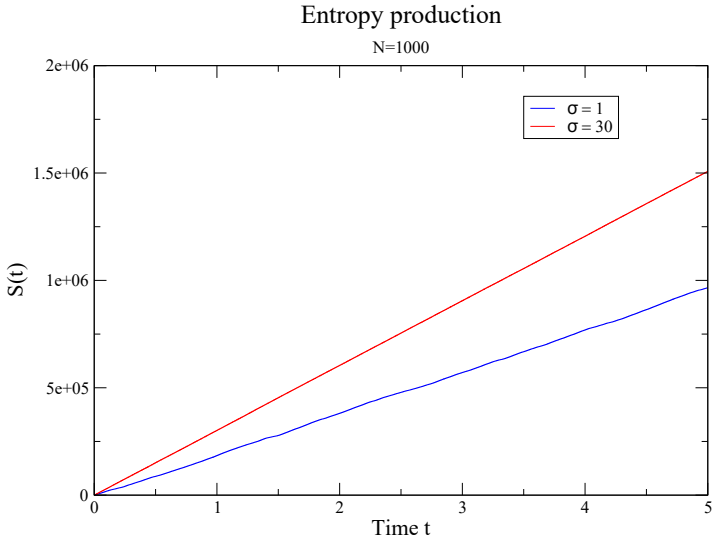
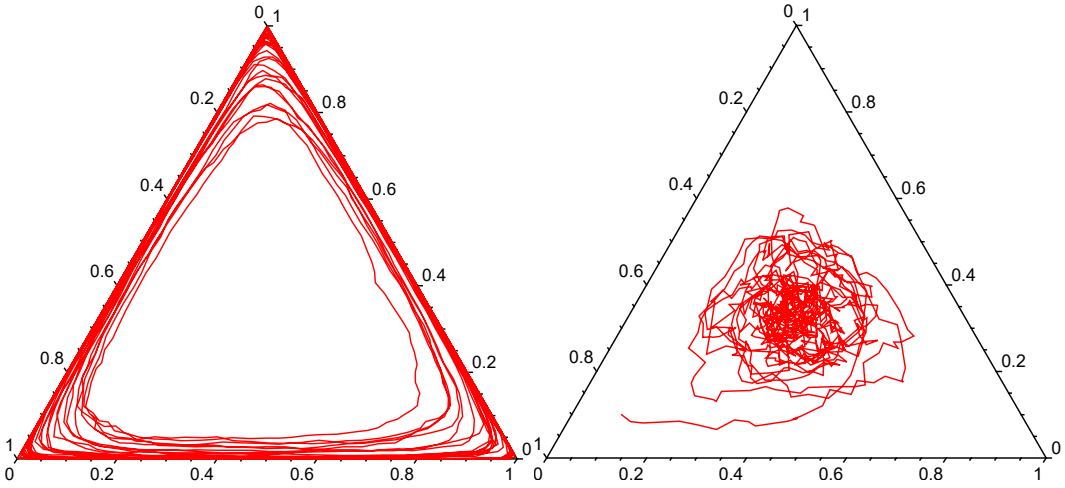


Figure 4.29: Entropy production with different mutational parameters: $r = 0.3$, $R = 0.5$, $\sigma_1 = 1$, $\sigma_2 = 30$, $T = 5$.

The comparison between the entropy produced in both the simulations gives a difference of $S_2(T) - S_1(T) \simeq 5.4 \times 10^5$ which corresponds to the 35% of $S_2(T)$.

An important fact that has not yet been clarified is for what values of the predation/mutation a system behaves in different manners. In particular during the numerical simulations (see Fig.4.30), we saw that for a very small coefficient of mutation σ the system presents large oscillation between the three species and with a great mutation rate σ the system lives near the center of the simplex S_2.



(a) Mutation rate: $\sigma = 0.3$. *(b)* Mutation rate: $\sigma = 5$.

Figure 4.30: Representation of the two different system's behavior depending on the value of the mutation. Where $N = 1000$ with initial condition $(800, 100, 100)$. In these graphics the state was printed every 50 jumps.

Before giving an analytical result that justifies the graphic above, we study the system's mean entropy production at each point in the simplex.

4.5.5 Estimation of the mean entropy production on S_2

Here we want to find an analytical method for determining the average entropy produced at each step by our three species system during its evolution, depending on the state C of the system itself. This means that we have to find an analytical expression that gives us an estimate of the single-step mean entropy production. A good way to do that is writing a weighted average of the usual expression of the logarithm of the jump's rates, where the weight are given by the possible rates surrounding the actual state C. Considering the rates expression $\Gamma_{i \leftarrow j}$ we obtain a function of the three species $\langle S \rangle (N_1, N_2, N_3)$. Expressing this equation through the form of the explicit rates one obtains

$$\langle S \rangle (N_1, N_2, N_3) = \frac{1}{\sum_{\substack{i,j=1 \\ i \neq j}}^{3} r_{ij} N_j (N_j + \sigma_{ij})} \cdot \cdot \sum_{\substack{i,j=1 \\ i \neq j}}^{3} \log \left(\frac{r_{ij} N_j (N_j + \sigma_{ij})}{r_{ji} (N_i + 1)((N_j - 1) + \sigma_{ji})} \right) r_{ij} N_j (N_j + \sigma_{ij}) \quad (4.50)$$

Dividing 4.50 by N^2 both at numerator and denominator, we can write the formula in terms of the concentrations $x_i \in [0,1]$ so that $x_1 + x_2 + x_3 = 1$:

$$\langle S \rangle (x_1, x_2, x_3) = \frac{1}{\sum_{\substack{i,j=1 \\ i \neq j}}^{3} r_{ij} x_j \left(x_j + \frac{\sigma_{ij}}{N} \right)} \cdot \cdot \sum_{\substack{i,j=1 \\ i \neq j}}^{3} \log \left(\frac{r_{ij} x_j \left(x_j + \frac{\sigma_{ij}}{N} \right)}{r_{ji}(x_i + 1/N)((x_j - 1/N) + \frac{\sigma_{ji}}{N})} \right) r_{ij} x_j \left(x_j + \frac{\sigma_{ij}}{N} \right) \quad (4.51)$$

we now evaluate this function along all the possible values of the three coordinates x_i $i = 1, 2, 3$; and with a single mutation rate for all the possible transition $\sigma_{ij} = \sigma$.

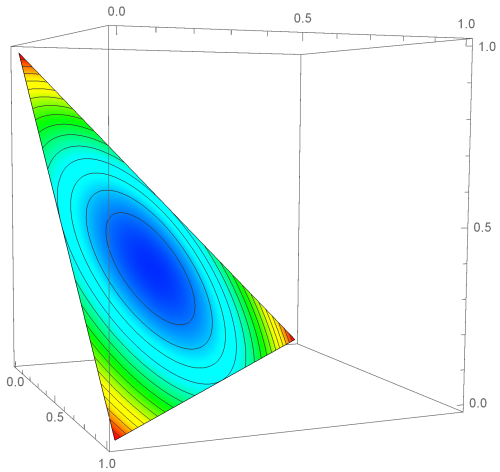


Figure 4.31: A 3 dimensional representation of the function $\langle S \rangle (x_1, x_2, x_3)$ on S_2.

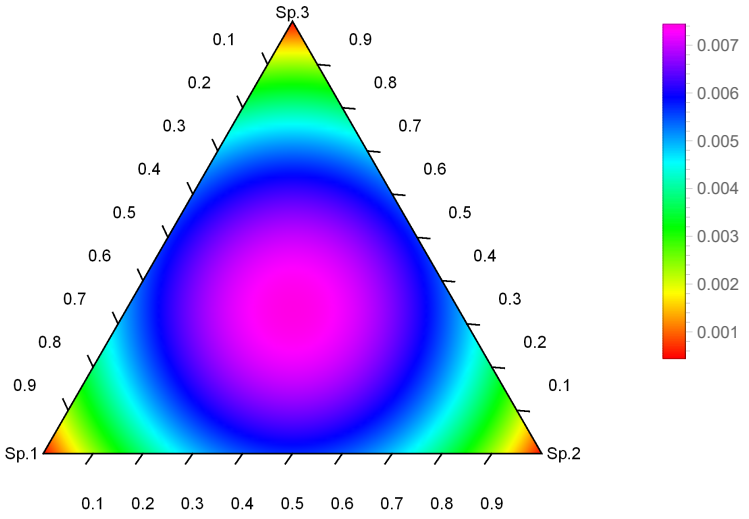


Figure 4.32: A 3 dimensional representation of the function $\langle S \rangle (x_1, x_2, x_3)$ on S_2, after the mapping in Cartesian coordinates.

To show effectively how the entropy production of a system decreases moving off the center of the simplex, the following parametrization of the coordinates of the function $\langle S \rangle$ was used, (see eq.4.51). Using a parameter x we define

$$\begin{cases} x_1(x) = 1/3 + 2x \\ x_2(x) = 1/3 - x \\ x_3(x) = 1/3 - x \end{cases} \tag{4.52}$$

where $x \in [\,0\,;1/3\,]$.
Visually, this means that we calculate the entropy production for that precise jump along the trajectory of figure 4.33

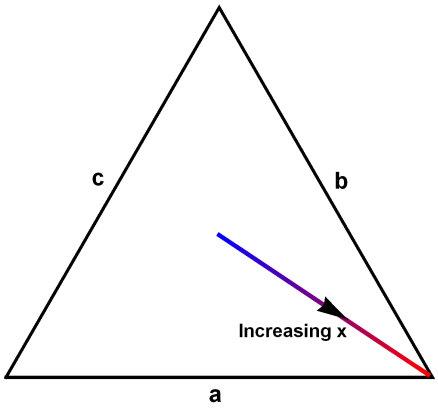


Figure 4.33: Graphical representation of 4.52, i.e. the direction along which the function $\langle S \rangle$ is estimated. Here a, b, and c are the three species concentrations.

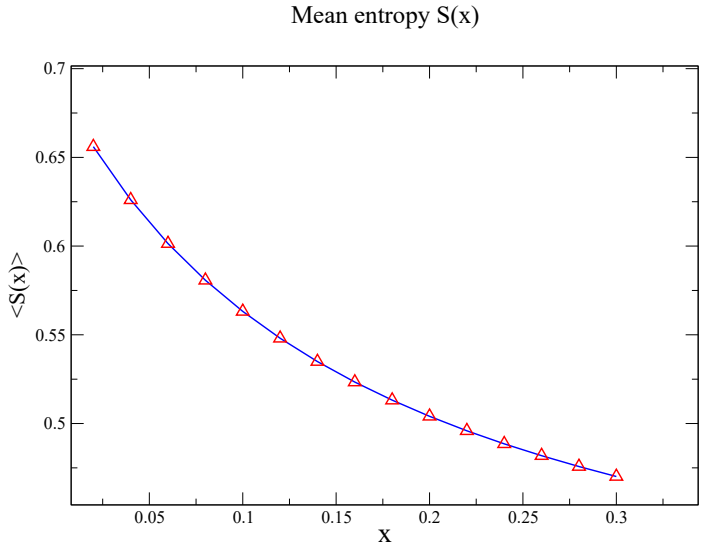


Figure 4.34: Entropy production with parameters: $r = 1$, $R = 2$, $dx = 0.02$ and x starts at 0 and goes up to 0.3.

A program in C++ was written, that for different updated value of x, and the curve obtained has been reported in Fig.4.34.

4.5.6 Calculation of the critical mutation rate

The system's dynamics dependence on the mutation rate σ was shown first in [73], which considered a different model. All the simulations done like the ones in Fig.4.30, suggest that a critical mutation rate σ_c in which the probability of the system is uniform through all the simplex S_2 must exist. Considering that we fall in a NESS practically instantaneously, the temporal derivative of the probability $P(\vec{x},t)$ is zero. Thus we can simplify the probability $P(\vec{x},t)$ and try to find the critical value σ_c such that the following equation holds, i.e. the value in which exist a transition between these two different regimes

$$0 = -\sum_{i=1}^{3}\partial_i\left[\alpha_i(\vec{x})\right] + \frac{1}{2N}\sum_{i=1}^{3}\sum_{j=1}^{3}\partial_i\partial_j\left[\beta_{ij}(\vec{x})\right]\Bigg|_{\sigma=\sigma_c} \tag{4.53}$$

where the coefficients α_i and β_{ij} are those found before in the analytical study. The drift and diffusion terms are the ones found in the analytical calculation paragraph. The first term can be moved to the left which brings the following

$$\sum_{i=1}^{3}\frac{\partial}{\partial x_i}\left[\alpha_i(\vec{x})\right] = \sum_{i=1}^{3}\sum_{m=1}^{3}(r_{im}-r_{mi})x_m - \frac{1}{N}\sum_{i=1}^{3}\sum_{m=1}^{3}r_{mi}\sigma_{mi} \tag{4.54}$$

in the second member we must distinguish for terms with diagonal indices (β_{ii}) and non-diagonal ones (β_{ij}):

$$\begin{aligned}\frac{\partial}{\partial x_i}\frac{\partial}{\partial x_i}\left[\beta_{ii}(\vec{x})\right] = \frac{\partial}{\partial x_i}\Bigg[&\sum_{\substack{m=1\\m\neq i}}^{3}(r_{im}-r_{mi})x_m + \sum_{\substack{m=1\\m\neq i}}^{3}(r_{im}-r_{mi})x_i\delta_{mi} + \\ &+\frac{1}{N}\sum_{\substack{m=1\\m\neq i}}^{3}(r_{mi}\sigma_{mi}\delta_{im}+r_{mi}\sigma_{mi})\Bigg]\end{aligned} \tag{4.55}$$

note that the second and third members are zero due to the presence of the δ symbol and the fact that $m \neq i, \quad \forall i$. We immediately see that acting with the second derivative ∂_i implies that all the terms are zero.
The non-diagonal term (with $i \neq j$) gives

$$\begin{aligned}\frac{\partial}{\partial x_i}\frac{\partial}{\partial x_j}\left[\beta_{ij}(\vec{x})\right] &= \frac{\partial}{\partial x_i}\left[-(r_{ij}+r_{ji})x_i - (r_{ij}+r_{ji})\delta_{ij}x_j - \frac{1}{N}(r_{ij}\sigma_{ij}+r_{ji}\sigma_{ji}\delta_{ij})\right] \\ &= -(r_{ij}+r_{ji}) - (r_{ij}+r_{ji})\delta_{ij}\delta_{ji}\end{aligned}$$

so that

$$\sum_{i=1}^{3}\sum_{m=1}^{3}\partial_i\partial_j\left[\beta_{ij}(\vec{x})\right] = -\sum_{i=1}^{3}\sum_{m=1}^{3}(r_{ij}+r_{ji}). \tag{4.56}$$

Note that the mutation rate has been treated in the most general possible case, but in our case we have $\sigma_{ij} = \sigma \equiv \sigma_c$. Putting all together one obtains

$$\sum_{i=1}^{3}\sum_{m=1}^{3}(r_{im} - r_{mi})x_m - \frac{1}{N}\sigma_c \sum_{i=1}^{3}\sum_{m=1}^{3} r_{mi} = -\frac{1}{2N}\sum_{\substack{i,j=1 \\ i\neq j}}^{3}(r_{ij} + r_{ji}) \tag{4.57}$$

Using the antisymmetric property of the ALVE, we see that the first term is equal to zero. The summing over the indices for the entries of r-matrix gives

$$-\frac{1}{N}\sigma_c 3(r+R) = -\frac{1}{2N}6(r+R) \tag{4.58}$$

$$\Rightarrow \quad \sigma_c = 1\,. \tag{4.59}$$

It is interesting to note that this is a constant value, that does not depend on the parameters r_{ij} or N.
To verify the result just obtained, we performed several sets of simulations for different values of R while the entries r are set to 1 thanks to the property of rescaling time in the master equation. The different values of σ are proposed using the formula $\sigma = 0.1(10^{1/10})^x$ where $x \in \mathbb{N}^+$, which produces values equispaced in log-scale.

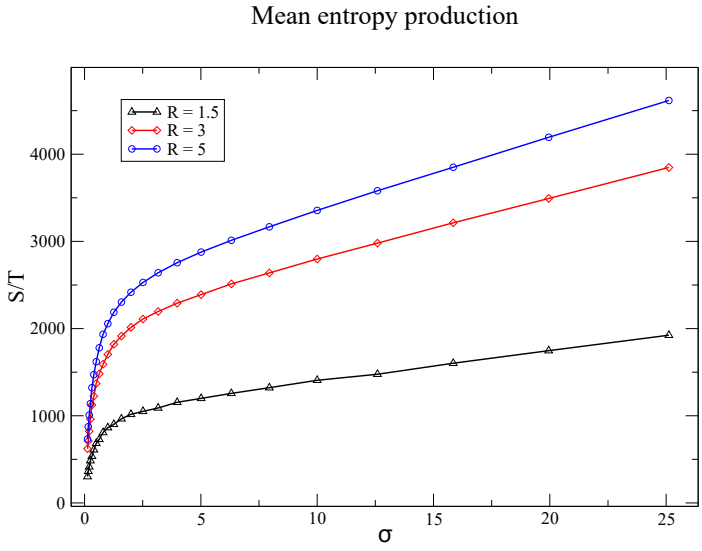


Figure 4.35: Entropy production $\dot{S}$ for different values of R and σ. The time of each simulation is $T = 200$.

In order to have a better visualization in Fig.4.35, the values obtained of $\dot{S}$ are normalized by the factor $R\ln(R)$. Thus at the critical value σ_c there is a *smooth* transition of the entropy produced during the time T. This fact implies that the transition of the system dynamics (varying σ) on S_2 is not discontinuous as we guessed during the analytical simulations.
If we divide each curve for the maximum value of $\dot{S}$, we see that all the different curves in Fig.4.35 appear to have the same structure in Fig.4.36.

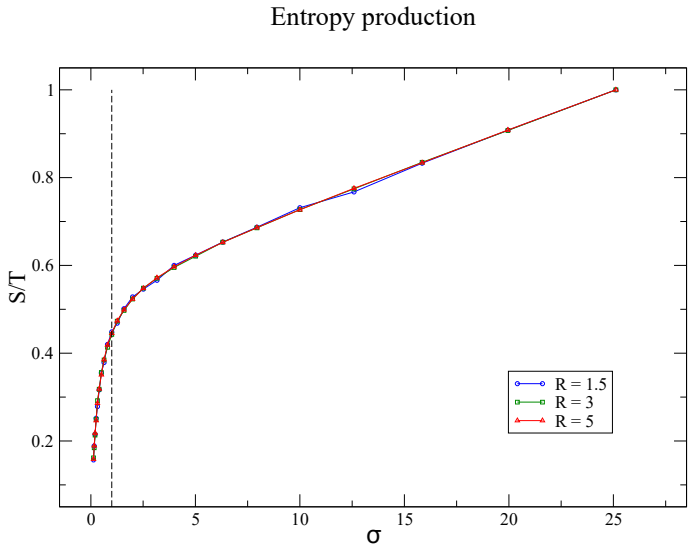


Figure 4.36: Entropy production $\dot{S}$ for different values of R and σ. The time of each simulation is $T = 200$. All the data have been divided by the maximum value of $\dot{S}$.

The dashed line in the plot above represents the point on the abscissa in which $\sigma = \sigma_c = 1$, before and after this point the system shows two different trends, and the entropy production increases linearly with σ for sufficiently high values of the mutation rate.

Chapter 5

Conclusions

In this thesis we have discussed the theoretical framework concerning both the dynamical behavior and the entropy production of an ecological system with three interacting species. In order to perform simulations of the stochastic realizations of the system itself, we have written a program in C++ language, based on the Gillespie algorithm. In Chapter 2 we outlined the procedure of Van Kampen's system's size expansion, which allowed us to get the deterministic equations of the system when its size tends to infinity. In Chapter 3 we retraced the theoretical machinery of Schnakenberg et al. which justifies the formulation of the single-step entropy production in stochastic jumps. Specifically, it was found to be the logarithm of the ratio between the forward and the backward transition rate.

In Chapter 4 we started from the definition of the master equation for our model and it has been recovered that when $N \to \infty$, the evolution is governed by Antisimmetric Lotka-Volterra Equations. We showed how their solutions can be obtained using exclusively its conserved quantities along the solutions of those equations. Using the Kramers-Moyal expansion, we recovered the expression of the Fokker-Planck equations, which embodies a first correction to the deterministic equations in order to take into account the stochasticity. During the simulations we observed that the system's evolution depends on the value of the frequency of random mutations, parametrised by a coefficient σ. For low values of σ the system lives mostly on the boundaries of the simplex S_2, i.e. persist a cyclical domination of one species among the others. For high values of σ the fixed point becomes an asymptotically stable point that is every species has its population near a third of the total considered of the system. Using the Fokker-Planck equation we showed that there exists a critical value of mutation $\sigma_c = 1$ that determines this transition from a cyclical dominance to a mean coexistence condition, and this transition is found to be smooth. Furthermore it was shown that for values of $\sigma > \sigma_c$ we get a higher production of entropy. We also calculated the expected irreversibility (entropy production) of the ecosystem as a function of the partition of its individuals among the various species during each step. In particular it was shown that where one species dominates the others, the mean entropy produced during each step is almost zero, while near the fixed point the system produce respectively more entropy. All this is coherent with the simula-

tions carried out. In the end we showed that σ_c does not depend on the predation coefficient R, since all the different curves converge to the same if we divides all the data for the respective maximum of the entropy produced $\dot{S} = S/T$. To summarize, we performed a study on the irreversibility of the biological system considered, which is strictly linked with the concept of entropy production. It was shown that at coexistence, i.e. close to the fixed point ,where all species have the same success, the system evolve along a more irreversible state contrarily to the case in which one species dominates among the others.

The approach followed in this work is very general and in future investigations it could be applied to more complex systems, which may include a spatial structure (instead of the well mixed ones studied here), environmental stochasticity or more interacting species. It would be interesting to obtain similar results in such more elaborate models, because it would explain the propensity of ecological systems to have a great number of coexisting species that are always subjected to mutational processes.

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