Evaluation of Sustained Stochastic Oscillations
by Means of a System of Differential Equations

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Abstract

Several approaches exist to model the evolution of dynamical systems with large populations. These approaches can be roughly divided into microscopic ones, which are usually stochastic and discrete, and macroscopic ones, which are obtained as the limit behavior when the populations tend to infinity and are usually deterministic and continuous. We study the dynamics obtained by both approaches in systems with one deterministic equilibrium. We show that such dynamics can exhibit rather different behavior around the deterministic equilibrium, in particular, the limit behavior can tend to an equilibrium while the stochastic discrete dynamics oscillates indefinitely. To evaluate such stochastic oscillations quantitatively, we propose a system of differential equations on polar coordinates. The solution of this system provides several measures of interest related to the stochastic oscillations, such as average amplitude and frequency.

Key Words: Population dynamics, stochastic oscillations, limiting behavior, steady state, polar coordinates

1 Introduction

The population dynamics of many biochemical systems can be naturally modelled by continuous-time Markov chains (CTMCs). In these processes, the population of each species is given by an integer number and the occurrence of a reaction is represented by an event (or jump). The time to the next event follows an exponential distribution whose mean depends on the rate associated to the reaction and the population of each species that takes part in the reaction. The resulting dynamics are therefore stochastic.

Alternatively, the dynamics of such systems can be described by considering population densities instead of absolute populations. When the size (or volume) of the system is significantly large, limit theorems [15, 9, 12] offer an appealing mathematical tool to compute the average behavior of the system densities. In particular, limit theorems provide a system of ordinary differential equations (ODEs) whose solution is the limiting behavior of the densities when the system size tends to infinity. In contrast to the CTMC dynamics, the trajectory described by an ODE is continuous and deterministic.

Although the use of ODEs is straightforward and they represent a mathematically proven average behavior (continuous and deterministic), they might also provide a somewhat myopic view of the original discrete and stochastic system since only the average behavior is being considered. This can lead to conclusions about the dynamics in which important properties such as oscillations, commutations, stochastic resonance, etc. are passed over [10, 2, 7, 1, 5].

This paper is an extension of previous work [13] and focuses on evaluating stochastic oscillations that are frequently seen as equilibrium points in the limiting ODE. Identifying oscillatory behavior and estimating quantitative properties like amplitude and frequency is crucial to correctly analyze real biological systems where such behavior is essential [8, 11], e.g., reactions associated to circadian rhythm.

The method proposed here to evaluate stochastic oscillations is based on the design of an ODE that expresses the system behavior in polar coordinates. The method is also applicable to

other application domains in which similar stochastic models are considered, e.g., population dynamics, chemical reactions, ecological models, etc.

The main feature of the proposed ODE is its ability to correctly average quantitative values of the stochastic oscillations such as amplitude and frequency. In contrast to approaches that make use of probabilistic model checking [4, 3] that can suffer from the state explosion problem and has had limited success in both analyzing and identifying oscillating behavior, and approaches that require ad hoc Lyapunov functions to check stability [2], the approach proposed here does not suffer from the state explosion problem and can be systematically applied to processes modelled as continuous-time Markov chains. The overall approach to design the mentioned ODE on polar coordinates can be summarized in three steps:

(1) Definition of the ODE for the limiting behavior: The ODE for the limiting behavior, as the size of the system tends to infinity, can be straightforwardly obtained from the definition of the considered continuous-time Markov chain by applying well known results related to limit theorems [15, 12].

(2) Computation of the deterministic equilibrium point: A state is said to be a deterministic equilibrium point if at that state all populations remain constant indefinitely. More formally, the derivatives of the ODE representing the limiting behavior of the system are null at deterministic equilibrium points. Thus, equilibrium points can be obtained by computing the points that make the derivatives equal to zero. In the remainder of the paper we will assume that the system under study has a unique deterministic equilibrium point.

(3) Definition of the ODE on polar coordinates and evaluation of oscillations: In order to describe the average behavior of a system around a given point we will use polar coordinates instead of cartesian ones. More precisely, the (unique) deterministic equilibrium point will be taken as the origin for the polar coordinates. For each event of the system, the increments produced by the occurrence of such an event on each polar coordinate will be computed. This allows us to compute the expected increment of each variable and in turn to define the average dynamic behavior of those variables over time. This results in an ODE for the polar coordinates. Such an ODE can be used to compute the amplitude and frequency of the system around the considered equilibrium point in the steady state.

Running example. As a running example a simple population dynamics system described in [2, 17] is considered. The system is similar to those arising when modelling biochemical reactions [16] and predator-prey systems [19]. The state of the system is given by two populations (integer variables) S and I representing the number of susceptible and infected individuals. There are three events, *Birth*, *Contagion*, *Death*, that modify the state of the system. Table 1 shows the effect and rates of each event, e.g., event *Contagion* decreases the number of susceptible individuals by one, increases the number of infected individuals by one and has rate $w_c = (\beta \cdot S \cdot I)/V$. Parameters a, b and β are related to the rates of *Birth*, *Death* and *Contagion* respectively, and V represents the size (or volume) of the system.

Table 1: Events and rates of the running example

Event	Effect	Transition rate
Birth	$\{S, I\} \rightarrow \{S+1, I\}$	$w_b = a \cdot V$
Contagion	$\{S, I\} \rightarrow \{S-1, I+1\}$	$w_c = (\beta \cdot S \cdot I)/V$
Death	$\{S, I\} \rightarrow \{S, I-1\}$	$w_d = b \cdot I$

The described system dynamics can be expressed by means of the following chemical reactions:

$$\emptyset \xrightarrow{w_b} S \qquad S + I \xrightarrow{w_c} 2I \quad I \xrightarrow{w_d} \emptyset$$
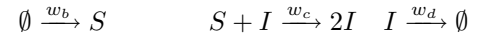
Let us focus on the concentrations $x_1 = \frac{S}{V}$ and $x_2 = \frac{I}{V}$ of the populations of susceptible and infected individuals. When the parameters of the CTMC satisfy some convergence conditions, its limiting behavior as V tends to infinity can be expressed as an ODE [15, 6]. In the Appendix it is shown that these conditions are satisfied by the CTMC under consideration. The limiting behavior of the CTMC can be expressed by the following ODE:

$$\begin{aligned} \frac{dx_1}{dt} &= -\beta \cdot x_1 \cdot x_2 \\ \frac{dx_2}{dt} &= \beta \cdot x_1 \cdot x_2 - b \cdot x_2 \end{aligned} \tag{1}$$

Figure 1 shows the time evolution of $S = V \cdot x_1$ given by both the solution of ODE (1) and just one stochastic simulation run of the CTMC. The parameters used in Figure 1 are $a=1$, $b=10$, $\beta=10$ and $V=10^4$. For these parameters the ODE dynamics has a unique equilibrium point $(x_1^{eq}, x_2^{eq})=(1, 0.1)$, thus in terms of populations the equilibrium point is $(S^{eq}, I^{eq})=(10^4, 10^3)$.

Notice that whereas the ODE shows damped oscillations tending toward its equilibrium point $(S^{eq}=10^4, I^{eq}=10^3)$, the CTMC dynamics exhibits sustained oscillations [2, 18]. Thus, for this example, the ODE representing the limiting behavior does not capture the sustained oscillations of the CTMC.

Figure 2 shows the frequency spectrum of the stochastic trajectory of Figure 1, i.e., it represents the signal in the frequency domain. A clear peak appears around the frequency 0.5. This phenomenon cannot be observed if the results of several runs of the CTMC are then averaged. In other words, the averaged populations converge to the solution of the ODE, but the ODE does not imitate the oscillations present in the CTMC dynamics around the equilibrium. Further explanations on this phenomenon are provided in the next section.

The goal of the paper is to develop an ODE that provides a complementary view of the dynamics of the CTMC that correctly averages sustained oscillations. The paper is organized as follows: Section 2.1 describes the stochastic and
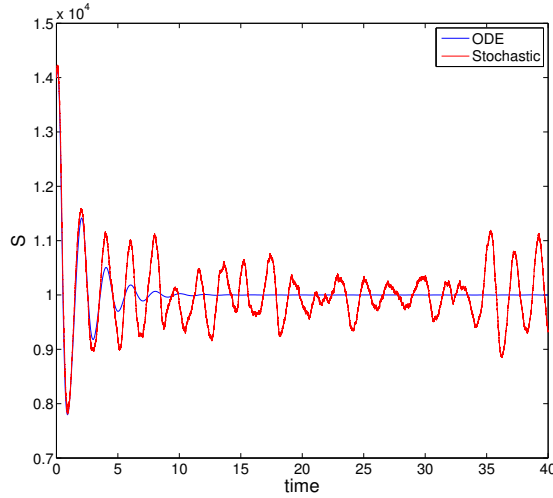
Figure 1: Trajectory S according to the ODE (1) and the CTMC
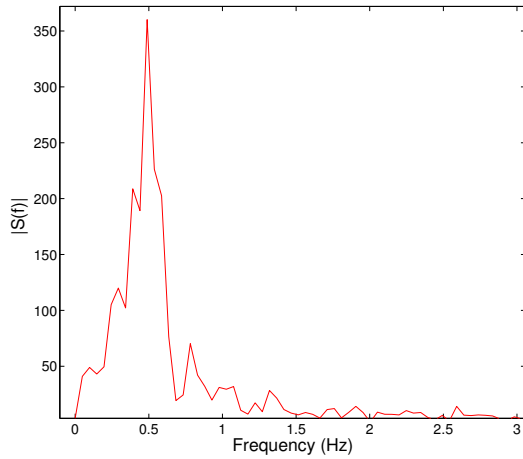
Figure 2: Frequency spectrum of the trajectory of S

deterministic models for the systems under consideration. The behavior of both models around the deterministic equilibrium point is analyzed in Section 3. Section 4 proposes an ODE based on polar coordinates to average stochastic oscillations. An epidemic system is described and analyzed in Section 5. Section 6 concludes the paper.

2 Stochastic and Deterministic Models

2.1 Stochastic Models

The dynamics of many biological systems with discrete populations can be naturally expressed in terms of CTMCs. The following parameters allow us to describe the dynamics of the concentrations of the populations over time. In the following, $\mathbb{N}$ denotes the set of natural numbers, $\mathbb{R}$ the set of real numbers and $\mathbb{Z}$ the set of integers.

Definition 1 (System parameters).

- $V \in \mathbb{R}_{>0}$ is the size (or volume);
- $q \in \mathbb{N}$ is the number of species;

- $n_0 \in \mathbb{Z}_{\geq 0}^q$ is the initial population of the q species;
- $\boldsymbol{\alpha} = \{\alpha_1, \ldots, \alpha_E\}$ is a set of $E \in \mathbb{N}$ events;
- $\boldsymbol{\delta} = \{\delta_1, \ldots, \delta_E\}$ defines the system change after the occurrence of events, i.e., $\delta_j \in \mathbb{R}^q$ determines the population density change produced by α_j;
- $\mathbf{w} = \{w_1, \ldots, w_E\}$ is a set of functions such that $w_j : \mathbb{R}_{\geq 0}^q \to \mathbb{R}_{\geq 0}$ defines the transition rate of event α_j, i.e., $w_j(x)$ is the transition rate of α_j when the population density is x.

For a population $n \in \mathbb{Z}_{\geq 0}^q$, its density (or concentration) is $x=n/V$. The exact meaning of V can depend on the application domain: in physics and chemistry it usually represents volume; in epidemiological models it often means the overall population or the size of the environment being considered. Although some variables, such as x, depend on time, for readability we will use x rather than $x(t)$.

For the running example, the system parameters, where numerical subindices are substituted by letters for clarity, are:

- $V=10^4$ and $q=2$;

- $n_0=(S_0, I_0)$, where $S_0=14000$ and $I_0=500$ are the initial numbers of susceptible and infected individuals respectively,;

- $\boldsymbol{\alpha} = \{\alpha_b, \alpha_c, \alpha_d\} = \{Birth, Contagion, Death\}$;

- $\boldsymbol{\delta} = \{\delta_b, \delta_c, \delta_d\} = \left\{ \left(\frac{1}{V}, 0\right), \left(-\frac{1}{V}, \frac{1}{V}\right), \left(0, -\frac{1}{V}\right) \right\}$;

- $\mathbf{w} = \{w_b, w_c, w_d\} = \{a \cdot V, \beta \cdot x_1 \cdot x_2 \cdot V, b \cdot x_2\}$ where $a=1$, $b=10$ and $\beta=10$.

The system evolution follows the usual dynamics of a CTMC: when an event α_j takes place, the population density is updated from x to $x+\delta_j$. The time to the next event is exponentially distributed. For a given density x, the mean of the exponential distribution associated to event α_j is $1/w_j(x)$. We will restrict our attention to CTMCs that satisfy the mass-action law, i.e., those processes whose reaction rates are proportional to the product of the concentrations of the participating species.

2.2 Deterministic Models

The vector field for species $i \in \{1, \ldots, q\}$ is given by [18]:

$$F_i(x^c) = \sum_{j=1}^{E} \delta_j \cdot w_j(x^c) \qquad (2)$$

where $x^c \in \mathbb{R}_{\geq 0}^q$ denotes the state of the process. In the deterministic model the state x^c represents the average behavior of the stochastic model, that is the reason why the different notations x and x^c are used for the Markovian and the deterministic models respectively.

When the parameters of the CTMC satisfy certain conditions [15, 6], its limiting behavior is given by the following set of differential equations:

$$\frac{dx^c}{dt} = \sum_{j=1}^{E} \delta_j \cdot w_j(x^c) \qquad (3)$$
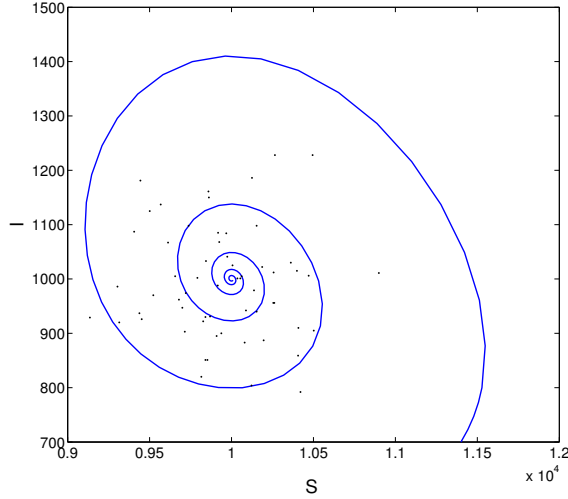
Figure 3: ODE (1) trajectory and final states of simulations

A state x^{eq} is said to be a deterministic equilibrium point if it holds that $\sum_{j=1}^{E} \delta_j \cdot w_j(x^{eq}) = 0$. As already mentioned, this paper focuses on systems having a unique deterministic equilibrium. The ODE given in (3) is a deterministic approximation for the densities of the species in the system. For the particular system parameters of the running example ODE (3) corresponds to ODE (1).

Figure 3 shows the evolution of the ODE (1) in the phase space over 20 time units. Each dot in the figure corresponds to the state of a simulation run of the CTMC after 20 time units. Conversely, as Figure 1 demonstrates, at time 20 the deterministic trajectory has already reached its equilibrium point. It can be observed that the *center of mass* of the black dots lies on the equilibrium point towards which the ODE converges. This is an expected result since the system satisfies the conditions of the limit theorems [15].
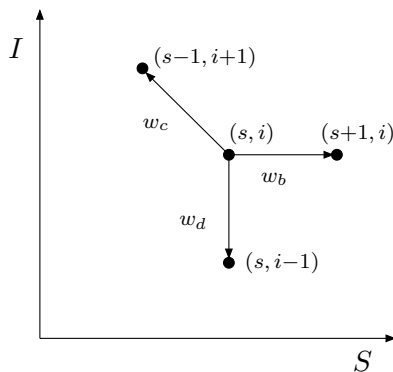

Figure 4: Phase space evolution of the CTMC

The static picture of Figure 3 does not show that each particular run is not tending to the deterministic equilibrium point. This at first glance surprising phenomenon can be intuitively explained. Figure 4 shows the potential evolutions, i.e., changes produced by the events, of the state of the CTMC together with the rates associated to them. If (s^{eq}, i^{eq}) is

a deterministic equilibrium point, all the components of the vector field cancel out, i.e., (2) becomes null, and therefore the solution ODE remains at (s^{eq}, i^{eq}). However, the CTMC does not remain at the deterministic equilibrium indefinitely since the rates of the events at this point are positive. Moreover, at the deterministic equilibrium all three rates are equal, hence the CTMC will evolve similarly to a random walk in a neighborhood close to the equilibrium. In fact, as pointed out in [18], non-extinction deterministic equilibria have associated a region of stochastic instability. This intuitive explanation is developed mathematically in the next section.

3　System Behavior around the Equilibrium Point

This section compares the evolution, with respect to a deterministic equilibrium point, of ODE (3) and the CTMC. In particular, we focus on the evolution of the euclidian distance squared from the system state to the equilibrium point.

Let $x^{eq} \in \mathbb{R}^q$ be a deterministic equilibrium point, i.e., $\sum_{j=1}^{E} \delta_j \cdot w_j(x^{eq}) = 0$. Let us define the distance of a point $x \in \mathbb{R}^q$ to x^{eq} as:

$$D(x, x^{eq}) = \sum_{i=1}^{q} (x_i - x_i^{eq})^2 \qquad (4)$$

The variation of $D(x^c, x^{eq})$ per time unit, where x^c is the continuous trajectory provided by (3), is given by:

$$\frac{dD(x^c, x^{eq})}{dt} = \sum_{i=1}^{q} \frac{d(x_i^c - x_i^{eq})^2}{dt} \qquad (5a)$$

$$= \sum_{i=1}^{q} 2 \cdot (x_i^c - x_i^{eq}) \cdot \frac{dx_i^c}{dt} \qquad (5b)$$

$$= \sum_{i=1}^{q} \left(2 \cdot (x_i^c - x_i^{eq}) \cdot \sum_{i=1}^{E} \delta_{ji} \cdot w_j(x^c) \right) \qquad (5c)$$

where δ_{ji} is the density change of the ith species due to the occurrence of event α_j. The expression in (5b) is obtained by applying the chain rule, and (5c) is obtained by using Equation (3).

In order to compute the time evolution of (4) on the CTMC, we will first obtain an expression for the expected change of $D(x, x^{eq})$ after the occurrence of an event. To obtain such an expression, the embedded Markov chain is used. In the following, all the expressions related to expected values depend on the current state x, i.e., they are conditional expectations. For brevity, the current state will be omitted in the expressions, e.g., $\mathbb{E}[\Delta D(x, x^{eq}) \,|\, x]$ will be shortened to $\mathbb{E}[\Delta D(x, x^{eq})]$. Let us define $R(x)$ as the average number of events per time unit:

$$R(x) = \sum_{j=1}^{E} w_j(x)$$

By the product rule of the difference operator we have:

$$\Delta(x_i - x_i^{eq})^2 = 2 \cdot (x_i - x_i^{eq}) \cdot \Delta x_i + (\Delta x_i)^2$$

and hence the expected increment of $D(x, x^{eq})$ after an event is:

$$\mathbb{E}[\Delta D(x, x^{eq})] = \mathbb{E}\left[\sum_{i=1}^{q} \Delta(x_i - x_i^{eq})^2\right] \qquad (6a)$$

$$= \mathbb{E}\left[\sum_{i=1}^{q}\left(2\cdot(x_i - x_i^{eq})\cdot\Delta x_i + (\Delta x_i)^2\right)\right] \qquad (6b)$$

$$= \sum_{i=1}^{q}\mathbb{E}[(\Delta x_i)^2] + \sum_{i=1}^{q} 2\cdot(x_i - x_i^{eq})\cdot\mathbb{E}[\Delta x_i] \qquad (6c)$$

$$= \sum_{i=1}^{q}\mathbb{E}[(\Delta x_i)^2] + \sum_{i=1}^{q}\left(2\cdot(x_i - x_i^{eq})\cdot\frac{\sum_{j=1}^{E}\delta_{ji}\cdot w_j(x)}{R(x)}\right) \qquad (6d)$$

Since at state x, the average number of events per time unit is $R(x)$, the average change of the distance squared per time unit is given by:

$$\frac{d\mathbb{E}[\Delta D(x, x^{eq})]}{dt} = R(x)\cdot\mathbb{E}[\Delta D(x, x^{eq})] \qquad (7a)$$

$$= R(x)\cdot\sum_{i=1}^{n}\mathbb{E}[(\Delta x_i)^2] + \sum_{i=1}^{q}\left(2\cdot(x_i - x_i^{eq})\cdot\sum_{j=1}^{E}\delta_{ji}\cdot w_j(x)\right) \qquad (7b)$$

By making use of Equations (5c) and (7b), the following equality for the same concentrations of the continuous and discrete trajectories, $x^c = x$, is obtained:

$$\frac{d\mathbb{E}[\Delta D(x, x^{eq})]}{dt} = R(x)\cdot\sum_{i=1}^{n}\mathbb{E}[(\Delta x_i)^2] + \frac{dD(x^c, x^{eq})}{dt}$$

More precisely, if x is not a deadlock point, i.e., there is at least one event α_j with strictly positive $w_j(x)$, then $R(x)\cdot\sum_{i=1}^{n}\mathbb{E}[(\Delta x_i)^2] > 0$ and it holds that:

$$\frac{d\mathbb{E}[\Delta D(x, x^{eq})]}{dt} > \frac{dD(x^c, x^{eq})}{dt} \qquad (8)$$

Equation (8) implies that ODE (3) is not averaging correctly the distance to the equilibrium point of the CTMC dynamics.

Due to the mass-action law, $R(x)$ is proportional to V for a given concentration x, i.e., $R(x) = \mathcal{O}(V)$ where $\mathcal{O}(V)$ is the Landau notation to describe limiting behaviors. On the other hand, the changes in the concentration x produced by events are $\mathcal{O}(1/V)$, hence $\sum_{i=1}^{q}\mathbb{E}[(\Delta x_i)^2] = \mathcal{O}(1/V^2)$ implying that:

$$R(x)\cdot\left(\sum_{i=1}^{q}\mathbb{E}[(\Delta x_i)^2]\right) = \mathcal{O}\left(\frac{1}{V}\right)$$

Therefore as V tends to infinity, $R(x)\cdot\sum_{i=1}^{q}\mathbb{E}[(\Delta x_i)^2]$ vanishes and the ODE (3) improves its quality with respect to the average distance to equilibrium. Nevertheless, in many practical cases V is finite, and the term $R(x)\cdot\sum_{i=1}^{q}\mathbb{E}[(\Delta x_i)^2]$ cannot be ignored, since it can cause interesting oscillatory behaviors.
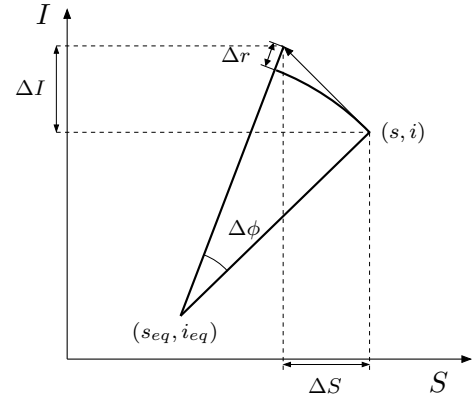

Figure 5: System evolution from event *Contagion*

4 Stochastic Oscillations

4.1 Polar ODE

The previous section showed that, while stable behavior can occur in the solution of the ODE (3), the Markov process can exhibit sustained stochastic oscillations around the deterministic equilibrium. In order to study the behavior of the CTMC around the deterministic equilibrium, we propose to average the distance to the deterministic equilibrium for the different potential evolutions, i.e., events, of the CTMC. To achieve this goal, an ODE based on polar coordinates is designed. The origin of such coordinates is the deterministic equilibrium x^{eq} around which the system dynamics is to be studied. Recall that deterministic equilibrium points can be easily computed by solving the system of equations $\sum_{j=1}^{E}\delta_j\cdot w_j(x^{eq}) = 0$ (see Equation (3)). In contrast to the classical approach that focuses on the cartesian coordinates, polar coordinates explicitly refer to the distance to an equilibrium state. After some mathematical considerations, an ODE that averages the distance and angle to the deterministic equilibrium is obtained. We will constrain our attention to systems with two species, i.e., $q=2$.

Figure 5 shows the system evolution after the event *Contagion* for the cartesian (S, I) and polar (r, ϕ) coordinates. For the polar coordinates the deterministic equilibrium (s^{eq}, i^{eq}) is taken as the origin. The choice of (s^{eq}, i^{eq}) as origin is quite natural since we desire to study the system dynamics around this point.

In order to define the state of the process in polar coordinates, radial and angular coordinates are required. The distance, or radial coordinate, of a point x to the equilibrium point x^{eq} is given by the function $rad(x)$:

$$r = rad(x) = \sqrt{(x_1 - x_1^{eq})^2 + (x_2 - x_2^{eq})^2} \qquad (9)$$

For a given x, the angular coordinate of ϕ is given by:

$$\phi = \text{atan}(x_2 - x_2^{eq}, x_1 - x_1^{eq}) \qquad (10)$$

where $\text{atan}(y, x) : \mathbb{R}\times\mathbb{R} \to \mathbb{R}$ is the arctangent of a point with cartesian coordinates (x, y). The range of $\text{atan}(y, x)$ is

$(-\pi, \pi]$.

For the running example, the expected increment at state x of the radial coordinate is given by:

$$\mathbb{E}[\Delta r] = \frac{\sum_{j=1}^{E} w_j(x) \cdot rad(x + \delta_j)}{R(x)} - rad(x) \qquad (11)$$

and the expected increment of the angle ϕ is:

$$\mathbb{E}[\Delta \phi] = \frac{\sum_{j=1}^{E} w_j(x) \cdot \mathrm{atan}(x + \delta_j)}{R(x)} - \mathrm{atan}(x) \qquad (12)$$

where $\mathtt{atan}$ is as in (10) but now has one bidimensional argument instead of two unidimensional ones.

There are two problems associated with equation (12). First, when the state is close to angle $\phi = \pi$, the function $\mathtt{atan}$ might yield values close to π for the angle after a given event, and close to $-\pi$ for the angle after another event if the abscissa is crossed. The average of those angles will be close to 0, which is not meaningful. Second, the angular coordinate ϕ might be used not only to localize the state of the system but also to evaluate the overall number of degrees traveled by the system around the equilibrium. To cope with these two issues $\mathbb{E}[\Delta \phi]$ is redefined as follows:

$$\mathbb{E}[\Delta \phi] = \frac{\sum_{j=1}^{E} w_j(x) \cdot \big(\mathrm{atan}(x + \delta_j) + g(x, \delta_j)\big)}{R(x)} - \mathrm{atan}(x) \qquad (13)$$

where $g(x, \delta_j)$ equals:

$$\begin{cases} -2 \cdot \pi & \text{if } \mathrm{atan}(x) < -\frac{\pi}{2} \text{ and } \mathrm{atan}(x + \delta_j) > \frac{\pi}{2} \\ +2 \cdot \pi & \text{if } \mathrm{atan}(x) > \frac{\pi}{2} \text{ and } \mathrm{atan}(x + \delta_j) < -\frac{\pi}{2} \\ 0 & \text{otherwise} \end{cases} \qquad (14)$$

The term $g(x, \delta_j)$ is used to check whether ϕ has crossed the value π. If the crossing is clockwise, then $g(x, x + \delta_j) = -2 \cdot \pi$, while if it is counterclockwise, then $g(x, x + \delta_j) = 2 \cdot \pi$. Thus, $g(x, x + \delta_j)$ allows the increments of $\mathbb{E}[\Delta \phi]$ to be smooth.

More precisely, the inclusion of $g(x, x + \delta_j)$ in the computation of $\mathbb{E}[\Delta \phi]$ solves the two mentioned problems: a) the average of angles close to π is now ensured to be close to π; b) if ϕ is updated according to its increments computed with $g(x, x + \delta_j)$ it will record the number of degrees traveled by the system around the equilibrum.

At a given state x, the average number of events per time unit is $R(x)$. Hence, the term $R(x) \cdot \mathbb{E}[\Delta r]$ is the average speed of change of r. Given that the same reasoning applies to ϕ, the following ODE can be used to describe the behavior over time of r and ϕ:

$$\begin{aligned} \frac{dr}{dt} &= R(x) \cdot \mathbb{E}[\Delta r] \\ \frac{d\phi}{dt} &= R(x) \cdot \mathbb{E}[\Delta \phi] \end{aligned} \qquad (15)$$

where $\mathbb{E}[\Delta r]$ and $\mathbb{E}[\Delta \phi]$ are given by Equations (11) and (13) respectively. Given that x is just the cartesian coordinate of (r, ϕ), ODE (15) is composed of 2 equations and 2 variables.
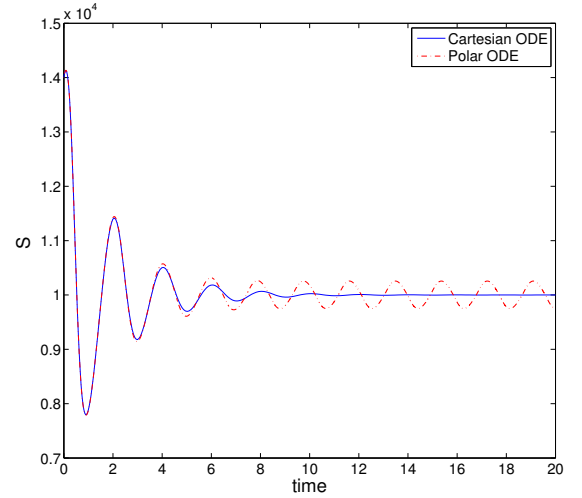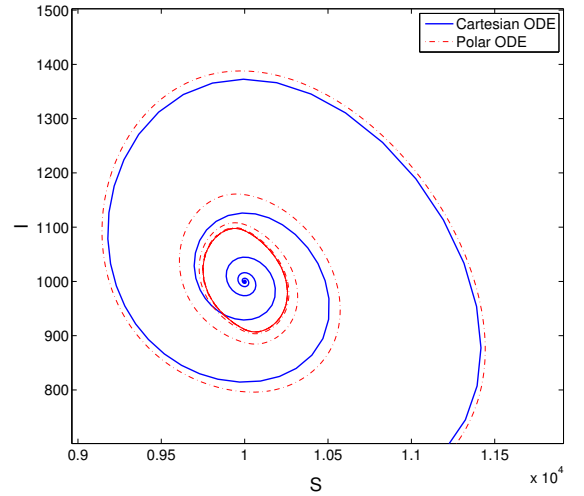

Figure 6: Time evolution of ODEs (3) and (15)

Figure 7: Phase space evolution of ODEs (3) and (15)

4.2 Averaging Stochastic Oscillations

Consider again the running example. Figures 6 and 7 show the evolution of both ODEs, (3) (labelled cartesian ODE) and (15) (labelled polar ODE), over time and in the phase space. It can be observed that, while (3) exhibits damped oscillations, (15) tends to a limit cycle with clear sustained oscillations.

The ODEs present complementary views both useful for analyzing the CTMC dynamics. While (3) focuses on the limiting behavior of the concentrations as V goes to infinity, (15) describes the dynamics in terms of polar coordinates for a given V which uncovers the oscillating behavior around the equilibrium.

The ODE (15) can be used to evaluate the average oscillations of the CTMC. To compute the average distance to the equilibrium, $\bar{r}$, of the oscillation in the steady state, the

following formula can be used:

$$\bar{r} = \lim_{\tau \to \infty} \frac{1}{\tau} \cdot \int_0^\tau r \, dt \qquad (16)$$

For the running example $\bar{r} = 1.801 \cdot 10^{-2}$, thus the average distance in terms of populations (not densities) to the deterministic equilibrium is $\bar{r} \cdot V = 180.1$. This value is in good agreement with the average distance to the equilibrium of the dots shown in Figure 3.

In (15) the term $d\phi/dt$ is the angular speed ω of the system for angle ϕ. Thus the average angular speed of the system in steady state is given by:

$$\bar{\omega} = \lim_{\tau \to \infty} \frac{1}{\tau} \cdot \int_0^\tau \omega \, dt = \lim_{\tau \to \infty} \frac{\phi}{\tau} \qquad (17)$$

For the running example $f = \omega/(2 \cdot \pi) = 0.535$ which matches the peak exhibited in Figure 2. This can be interpreted as if the dots in Figure 3 were orbiting around the equilibrium point at an average frequency of 0.535. The next section shows that other values of interest can also be obtained from the ODE on polar coordinates.

5 Case Study

This section applies the ideas developed in the previous sections to an epidemic system [18] that is a more realistic version of the running example. First, the system parameters are defined, then the suggested approach to evaluate stochastic oscillations is applied.

5.1 Description of the System

With respect to the running example, two new events are included: an event *Death S* associated to the death of susceptible individuals, and an event *Recovery*, meaning that an infected individual is restored to health. Moreover, a more realistic rate for event *Birth* is considered. Table 2 summarizes the existing events, their effect and their rate.

Table 2: Events of the epidemic system

Event	Effect	Transition rate
Birth	$\{S,I\} \to \{S+1,I\}$	$w_b = \frac{S+I}{1+(b \cdot (S+I))/V}$
Death S	$\{S,I\} \to \{S-1,I\}$	$w_{dS} = m_S \cdot S$
Contagion	$\{S,I\} \to \{S-1,I+1\}$	$w_c = \beta \cdot S \cdot \frac{I}{V}$
Recovery	$\{S,I\} \to \{S+1,I-1\}$	$w_r = r \cdot I$
Death I	$\{S,I\} \to \{S,I-1\}$	$w_{dI} = m_I \cdot I$

Let the size of the system be $V = 5 \cdot 10^3$ and the initial populations be $n_0 = (7000, 250)$, i.e., the initial concentrations are $x_0 = (1.4, 0.05)$. We will consider the following values for the constants: $b=0.4$, $\beta=10$, $m_S=0.2$, $m_I=5$ and $r=3$. This way the stochastic system is fully defined: the number of species is $q=2$ (susceptible and infected), $\boldsymbol{\alpha}$ is a set of 5 events, $\boldsymbol{\delta}$ and $\mathbf{w}$ are determined by the values in Table 2.
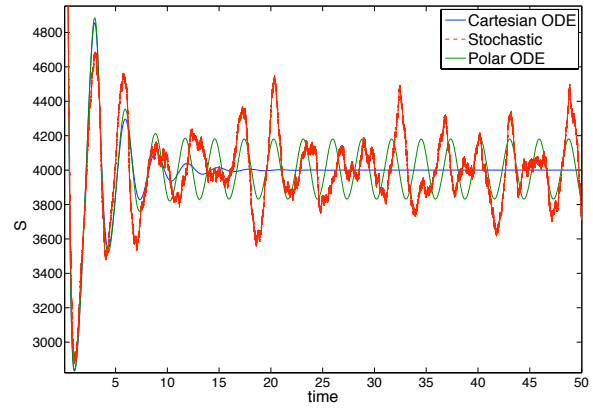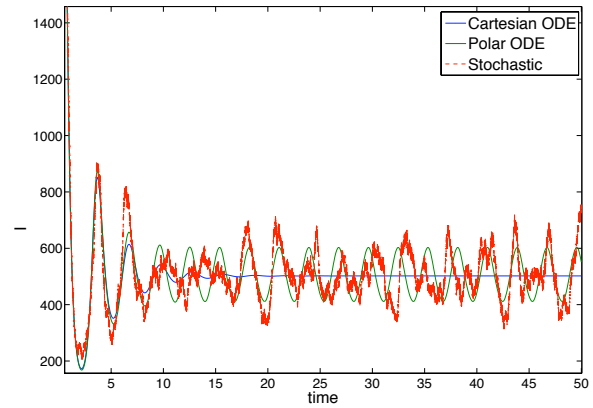

Figure 8: Time evolution of variable S

Figure 9: Time evolution of variable I

The time trajectory of variables S and I of the stochastic system are shown by the skewed lines in Figure 8 and Figure 9 respectively. Figure 10 shows the frequency spectrum of S. The highest peaks appear for values of the frequency in the interval $(0.2, 0.5)$.

In order to evaluate the oscillations, the following three steps will be followed: 1. Definition of ODE (3) for the limiting behavior of the system; 2. Computation of the deterministic equilibrium point for such ODE; 3. Evaluation of oscillations by using ODE (15) describing the evolution of polar coordinates and Equations (16) and (17).

5.2 ODE for the Limiting Behavior

As for the running example, it is quite straightforward to write down an ODE that defines the limiting behavior of the extended system as V tends to infinity. The proof for the obtained ODE is very similar to the one presented in the Appendix for the running example. For the concentrations $x_1 = S/V$ and $x_2 = I/V$, the equations of the ODE are given
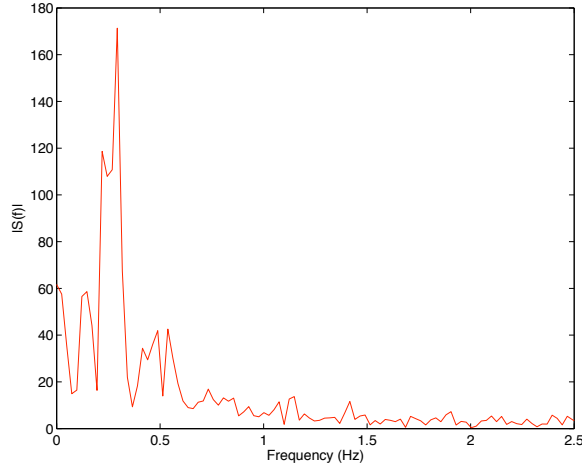
Figure 10: Frequency spectrum of S of the epidemic example

by:

$$\frac{dx_1}{dt} = \frac{x_1+x_2}{1+b\cdot(x_1+x_2)} - m_S \cdot x_1 - \beta\cdot x_1\cdot x_2 + r\cdot x_2$$

$$\frac{dx_2}{dt} = \beta\cdot x_1\cdot x_2 - m_I\cdot x_2 - r\cdot x_2 \qquad (18)$$

The trajectories of S and I given by ODE (18) are shown as the plots labelled "Cartesian ODE" in Figures 8 and 9. Notice that these eventually reach a constant value, the so called deterministic equilibrium point. This can be better appreciated in the phase space plot of Figure 11.

For the given parameters of the epidemic system, the point $(x_1^{eq}, x_2^{eq}) = (4000/V, 502/V)$ is the unique equilibrium point in which both populations are positive. We will study the oscillating behavior of the system around this point.
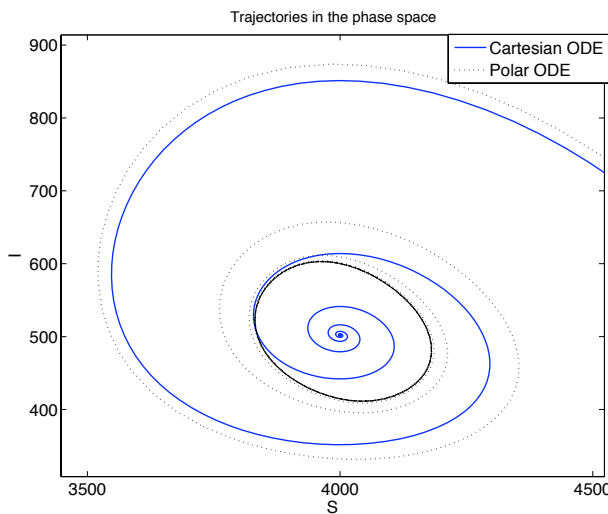

Figure 11: Trajectories in phase space of ODEs (18) and (15)

5.3 Evaluation of Oscillations

According to Section 4, ODE (15) describes the average time evolution of the distance and angle with respect to the equilibrium point (x_1^{eq}, x_2^{eq}). The time trajectories of S and I given by (15) are shown by the plots labelled "Polar ODE" in Figure 8 and Figure 9 respectively. We see that, using this approach, the sustained oscillations of the system are clearly visible. The trajectory in the phase space is the line representing a limit cycle in Figure 11. The limit cycle towards which the trajectory tends can be examined to obtain the amplitude of the oscillations. Variables S and I oscillate in the interval $[3831, 4186]$ and $[411, 603]$ respectively, thus, the amplitudes of both variables are 177.5 and 96 respectively.
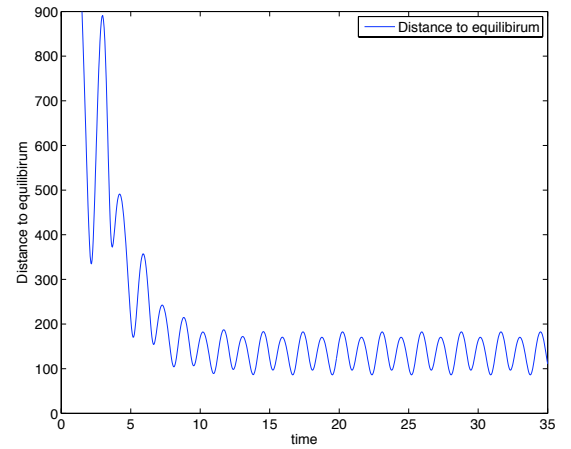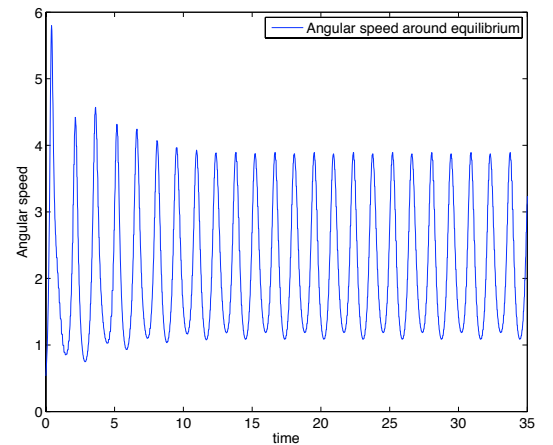

Figure 12: Time trajectory of $r \cdot V$ to the equilibrium

Figure 13: Average angular speed $\left(\frac{d\phi}{dt}\right)$ according to ODE (15)

Figure 12 and Figure 13 show the time evolution of the average distance, $r\cdot V$, to the deterministic equilibrium and the average angular speed $\left(\frac{d\phi}{dt}\right)$ around this point respectively. From these plots, it can be determined that, once the system is oscillating, the maximum (minimum) distance to the deter-

ministic equilibrium is 86.1 (182.5), and that the maximum (minimum) angular speed is 3.875 (1.087).

By means of (16) and (17), the average distance to the equilibrium and frequency of the oscillations can be obtained. For the epidemic system the average distance is $\bar{r}\cdot V = 136$ and the average frequency is $f = \bar{\omega}/(2\cdot\pi) = 0.352$.

6 Conclusions

Macroscopic models have been widely used in different application areas as biology, chemistry and ecology. Such models enjoy a solid mathematical grounding in the theory of limit theorems which provide the conditions required to approximate a large stochastic discrete system by a system of ordinary differential equations (ODE). Although important conclusions can be obtained from the solution of such a system of equations, it must be taken into account that it might also mask interesting features of the system dynamics as oscillations.

The paper focuses on systems with a unique deterministic equilibrium point, and the dynamics of the original stochastic discrete model and its limiting behavior around that equilibrium have been studied. It has been shown that the ODE associated to the limiting behavior does not average correctly the variations of the distance to a deterministic equilibrium point. More precisely, while the solution of the ODE is stable at such a point, the original continuous-time Markov chain is unstable in a neighborhood of this point.

In order to average correctly the evolution of the distance to the equilibrium and the angular speed, an ODE based on polar coordinates has been developed. This ODE can be used to compute several measures of interest related to the oscillations, such as time evolution of the average distance to the equilibrium, time evolution of the angular speed, average amplitude and frequency of each variable, etc. The developed ODE must be understood as a complementary tool to understand the behavior of the stochastic discrete model: while the initial ODE describes the overall *cartesian* tendency of populations, the proposed ODE describes the oscillating behavior of the populations. This way, the proposed ODE represents a systematic way of evaluating quantitatively the behavior of the system around an equilibrium point.

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Appendix

This appendix first reports the main Theorem in [6], and then applies it to the Markov process of the running example presented in Section 1.

A.1 Fluid Limit of a Pure Jump Markov Process

Assume that for each $N>1$ we have a Markov chain $\langle X_n^N \rangle_{n\geq 0}$, on a state space $I_N \subseteq E$ (where E is an euclidian space), whose increments have mean $\mu_N[x] = \mathbb{E}[X_{n+1}-X_n \mid X_n=x]$ and covariance $\Sigma_N[x] = \text{Var}[X_{n+1}-X_n \mid X_n=x]$ respectively.

Let $\langle \nu^N[t] \rangle_{t\geq 0}$ be a Poisson process, with event times $\tau_1 < \tau_2 < \cdots$, which is dependent on $\langle X_n^N \rangle_{n\geq 0}$ in the following sense: there is some bounded rate function $c_N : I_N \to \mathbb{R}_{>0}$, such that each inter-event time $\tau_{n+1}-\tau_n$ is exponential with mean $\frac{1}{c_N[x]}$ on the event $X_n^N=x$. As in [14], the formula $\Upsilon_t^N \equiv X_{\nu[t]}^N$ defines a pure jump Markov process $\langle \Upsilon_t^N \rangle_{t\geq 0}$. In other words $\Upsilon_{\tau_n}^N=X_n^N$, so $\langle \Upsilon_t^N \rangle_{t\geq 0}$ has the same increments as does $\langle X_n^N \rangle_{n\geq 0}$, and these occur at the random times $\tau_1 < \tau_2 < \cdots$.

Let us define $b_N[x]$ as $b_N[x] = c_N[x]\cdot\mu_N[x]$, and let $D \subseteq E$ be any closed set such that $D \supseteq \cup_{N>2}I_N$. We fix a relatively open set $S \subseteq D$ and define $S_N \equiv S \cap_{N>2} I_N$. In addition, let us assume that the parameters of these processes satisfy the following convergence criteria (in the below $\kappa_1[\delta]$, κ_2, κ_3 denote positive constants, and the inequalities hold uniformly in N).

- *Initial conditions convergence:* assume that there is some $a \in \overline{S}$, the relative closure of S in D, such that for each $\delta>0$:

$$\mathbb{P}[\|\Upsilon_0^N - a\| > \delta] \leq \frac{\kappa_1[\delta]}{N} \qquad (19)$$

- *Mean dynamics convergence:* assume that there is a Lipschitz vector field $b : D \to E$ such that:

$$\sup_{x\in S_N}\|b_N[x] - b[x]\| \to 0 \qquad (20)$$

- *Noise convergence to zero:*

$$\sup_{x\in S_N} c_N[x] \leq \kappa_2\cdot N \qquad (21)$$

$$\sup_{x\in S_N} \left(Trace[\Sigma_N[x]]+\|\mu_N[x]\|^2\right) \leq \frac{\kappa_3}{N^2} \qquad (22)$$

Since b is Lipschitz on $\overline{S} \subseteq D$, there is a unique solution $\langle y[t] \rangle_{0\leq t\leq \zeta[a]}$ in $\overline{S}$, where $\zeta[a] \equiv \inf\{t\leq 0 \mid y[t] \notin S\} \leq \infty$, to the ordinary differential equation:

$$\dot{y}[t] = b[y[t]] \text{ and } y[0] = a. \qquad (23)$$

Theorem 1. Assume the convergence criteria (19), (20), (21) and (22) hold, let $a \in S$ and fix $\delta>0$. For any finite $z<\zeta[a]$ we have:

$$\mathbb{P}\left[\sup_{0\leq t\leq z}\|\Upsilon_t^N-y[t]\| > \delta\right] = \mathcal{O}\left(\frac{1}{N}\right) \qquad (24)$$

A.2 ODE for the Running Example

Recall, for the cartesian description of the running example we have:

- $x_0=(S_0/N, I_0/N)$;
- $A=\{Birth, Death, Contagion\}$;
- $D=\{(1/N,0),(-1/N,1/N),(0,1/N)\}$;
- $W = \{a\cdot N, \beta\cdot x_1\cdot x_2\cdot N, b\cdot x_2\cdot N)$.

The initial condition $\Upsilon_0^N=x_0$ trivially satisfies (19) by choosing $a=x_0$. The expression associated to $\mu_N[x_1,x_2]$ is:

$$\mu_N[x_1,x_2] = \left(\frac{\frac{1}{N}\cdot w_b - \frac{1}{N}\cdot w_c}{w_b+w_c+w_d}, \frac{\frac{1}{N}\cdot w_c - \frac{1}{N}\cdot w_d}{w_b+w_c+w_d}\right)$$
$$= \left(\frac{1}{N}\cdot\frac{w_b - w_c}{w_b+w_c+w_d}, \frac{1}{N}\cdot\frac{w_c - w_d}{w_b+w_c+w_d}\right)$$

The expression for $Trace[\Sigma_N[x_1,x_2]]$ is:

$$Trace[\Sigma_N[x_1,x_2]] = \mathbb{E}[x_1^2] - \mathbb{E}[x_1]^2 + \mathbb{E}[x_2^2] - \mathbb{E}[x_2]^2$$
$$= \frac{\frac{1}{N^2}\cdot w_b + \frac{1}{N^2}\cdot w_c}{w_b+w_c+w_d} - \frac{1}{N^2}\cdot\left(\frac{w_b - w_c}{w_b+w_c+w_d}\right)^2$$
$$+ \frac{\frac{1}{N^2}\cdot w_c + \frac{1}{N^2}\cdot w_d}{w_b+w_c+w_d} - \frac{1}{N^2}\cdot\left(\frac{w_c - w_d}{w_b+w_c+w_d}\right)^2$$
$$= \frac{1}{N^2}\cdot\left(\frac{w_b+w_c}{w_b+w_c+w_d} - \left(\frac{w_b - w_c}{w_b+w_c+w_d}\right)^2\right.$$
$$\left. + \frac{w_c+w_d}{w_b+w_c+w_d} - \left(\frac{w_c - w_d}{w_b+w_c+w_d}\right)^2\right)$$

Finally the expression for $c_N[x_1,x_2]$ is:

$$c_N[x_1,x_2] = w_b+w_c+w_d = a\cdot N + \beta\cdot x_1\cdot x_2\cdot N + b\cdot x_2\cdot N$$

Thus, there exists a set S_N in which (21) and (22) are satisfied. The product $c_N[x_1,x_2]\cdot\mu_N[x_1,x_2]$ is $b_N[x_1,x_2] = (a - \beta\cdot x_1\cdot x_2, \beta\cdot x_1\cdot x_2 - b\cdot x_2)$. Hence, the limiting vector field is $b[x_1,x_2] = (a - \beta\cdot x_1\cdot x_2, \beta\cdot x_1\cdot x_2 - b\cdot x_2)$. Given that $\|b_N[x] - b[x]\| = 0$, (20) is satisfied. Furthermore, b is Lipschitz on D. Thus, all the assumptions of Theorem 1 are verified and the limiting behavior of the Markov process is given by ODE (1).
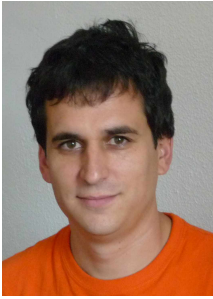
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