Introduction to stochastic modelling in Mathematical Biology

Tomás Alarcón

Computational & Mathematical Biology Group
Centre de Recerca Matemàtica

Outline

Motivation

Master Equation

Law of mass action

Steady vs absorbing states

Analytical methods: Characteristic function

General bibliography

General references on stochastic processes

1. N. Van Kampen. *Stochastic processes in physics and chemistry*. Elsevier (2007)
2. C.W. Gardiner. *Stochastic methods*. Springer-Verlag (2009)

Specific to mathematical biology

1. L.J.S. Allen. *An introduction to stochastic processes with applications to biology*. CRC Press. (2003)

References to specialised literature relevant to specific issues will be given as we go

Outline

Motivation

Master Equation

Law of mass action

Steady vs absorbing states

Analytical methods: Characteristic function

Motivation

- There exists the general idea that randomness and noise simply add an unsystematic perturbation to a well-defined average behaviour
- I will present several examples of systems in which noise contributes to the behaviour of the system in a non-trivial manner and it is fundamental to understanding the system
- From these examples I will extract rules of thumb for ascertaining when randomness plays a fundamental roles

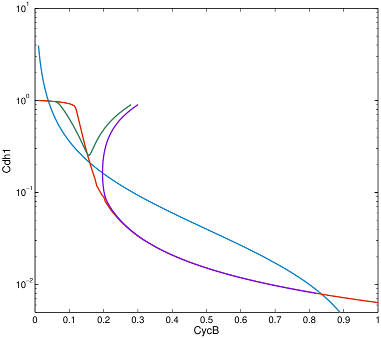
Large fluctuations in bistable systems

Mean-field model of the G_1/S transition model[a]

[a] Tyson & Novak. JTB. **210**, 249-263 (2001)

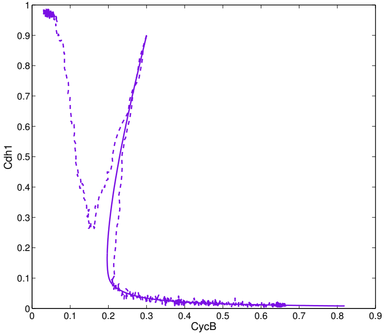
$$\frac{dy}{dt} = k_1 - (k_2' + k_2'' x) y$$

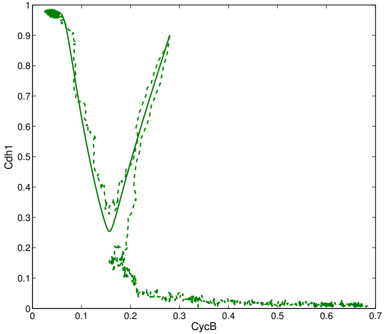
$$\frac{dx}{dt} = \frac{k_3'(1-x)}{J_3 + (1-x)} - \frac{k_4 m y x}{J_4 + x}$$



Finite-size Tyson-Novak system

Separatrix turns into a barrier

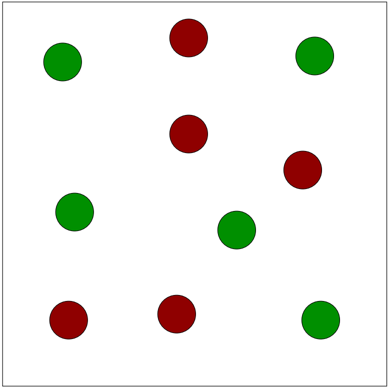




The Moran process

The Moran process, named after the australian statistician Pat Moran, is a widely-used variant of the Wright-Fisher model and is commonly used in population genetics

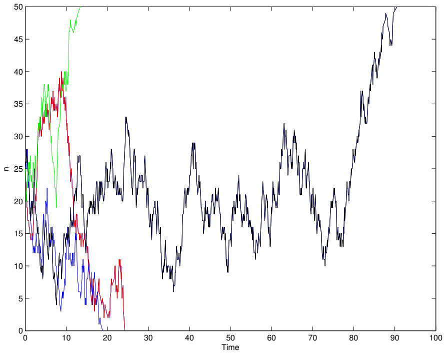
Moran process



- N individuals of two types. N is kept fixed.
- n: number of *normal* individuals. m: number of mutant individuals. $N = n + m$
- At each time step:
  1. $n \to n+1$ and $m \to m-1$ with probability rate $W_+(n) = \frac{n}{N}\left(1 - \frac{n}{N}\right)$
  2. $n \to n-1$ and $m \to m+1$ with probability rate $W_-(n) = \left(1 - \frac{n}{N}\right)\frac{n}{N}$

The Moran process

Simulation results



- Note that $W_+(n) = W_-(n)$, i.e. $\langle \Delta n \rangle = \langle (n(t+\Delta t) - n(t)) \rangle = 0$
- This implies that:

$$\frac{d\langle n \rangle}{dt} = 0 \qquad (1)$$

- The system has two absorbing states: $W_+(n=0) = W_-(n=0) = 0$ and $W_+(n=N) = W_-(n=N) = 0$
- This means that

$$\lim_{t\to\infty} P(n(t) = 0 \cup n(t) = N) = 1 \qquad (2)$$

- This behaviour is not at all captured by the deterministic equation (1) which predicts that the population will stay constant

Stochastic logistic growth

- The logistic equation,

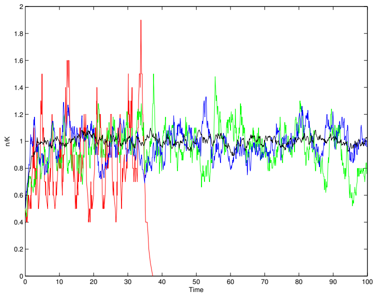
$$\frac{dm}{dt} = m\left(1 - \frac{m}{K}\right), \tag{3}$$

has two steady states: $m = 0$ unstable and $m = K$ stable, i.e. regardless of the value of K and for any initial condition such that $m(t = 0) > 0$, $m(t)$ will asymptotically approach K.

- Consider now a continuous-time Markov process n_t whose dynamics are given by the following transition rate:
  1. $n \to n + 1$ with probability rate $W_+(n) = n$
  2. $n \to n - 1$ with probability rate $W_-(n) = \frac{n(n-1)}{K}$
- This stochastic process has a unique absorbing state: $n = 0$, and therefore we expect the stochastic dynamics to show strong discrepancies with Eq. (8) when randomness is dominant

Stochastic logistic growth

Simulation results



- Red line $K = 10$, green $K = 50$, blue $K = 100$, black $K = 1000$
- For small K fluctuations dominate the behaviour of the system. Extinctions are common for small K, in contradiction to the behaviour predicted by the logistic equation Eq. (8), and become rarer as K is allowed to increase.

Summary

- We have seen two examples in which two different mathematical descriptions of the same physical/biological process give different answers as to what is their behaviour

Summary

- We have seen two examples in which two different mathematical descriptions of the same physical/biological process give different answers as to what is their behaviour
- We have seen a model (the Moran model) where the deterministic description predicts the population to stay constant. To the contrary, the stochastic description predicts that the population never stays constant: Eventually, the system evolves to $n = 0$ or $n = N$

Summary

- We have seen two examples in which two different mathematical descriptions of the same physical/biological process give different answers as to what is their behaviour
- We have seen a model (the Moran model) where the deterministic description predicts the population to stay constant. To the contrary, the stochastic description predicts that the population never stays constant: Eventually, the system evolves to $n = 0$ or $n = N$
- Another model (logistic growth) presents the same dilemma: Its deterministic description preditcs that $n = 0$ is always unstable, whereas the stochastic formulation shows that very often the system evolves to $n = 0$

Summary

- We have seen two examples in which two different mathematical descriptions of the same physical/biological process give different answers as to what is their behaviour
- We have seen a model (the Moran model) where the deterministic description predicts the population to stay constant. To the contrary, the stochastic description predicts that the population never stays constant: Eventually, the system evolves to $n = 0$ or $n = N$
- Another model (logistic growth) presents the same dilemma: Its deterministic description preditcs that $n = 0$ is always unstable, whereas the stochastic formulation shows that very often the system evolves to $n = 0$
- The question naturally arises: How is this possible? How come two mathematical descriptions of the same phenomenon offers so different answers?

Outline

Motivation

Master Equation

Law of mass action

Steady vs absorbing states

Analytical methods: Characteristic function

The Master Equation

- The Master Equation is our fundamental mathematical description of an stochastic process and the starting point for any attempt to analyse a particular model

The Master Equation

- The Master Equation is our fundamental mathematical description of an stochastic process and the starting point for any attempt to analyse a particular model
- It is obtained as a probability balance for all the events that can occur during the time interval $(t, t + \Delta t)$

The Master Equation

- The Master Equation is our fundamental mathematical description of an stochastic process and the starting point for any attempt to analyse a particular model
- It is obtained as a probability balance for all the events that can occur during the time interval $(t, t + \Delta t)$
- Mathematically, it is a set of ordinary differential equations for the probability distribution $P(X, t)$ i.e. the probability that the number of individuals in the population at time t to be X

The Master Equation

$$\frac{dP(X,t)}{dt} = \sum_{i=1}^{R} \left(W_i(X - r_i, t) P(X - r_i, t) - W_i(x, t) P(X, t) \right) \quad (4)$$

where:

- X is a (vector-valued) Markov process

The Master Equation can be interpreted as a balance equation where the first term corresponds to positive flux into state X from every allowed state and the second term as negative flux from state X into every possible state

The Master Equation

$$\frac{dP(X,t)}{dt} = \sum_{i=1}^{R} \left(W_i(X - r_i, t)P(X - r_i, t) - W_i(x, t)P(X, t) \right) \tag{4}$$

where:

- X is a (vector-valued) Markov process
- R is the number of possible processes (e.g. birth, death, mutation)

The Master Equation can be interpreted as a balance equation where the first term corresponds to positive flux into state X from every allowed state and the second term as negative flux from state X into every possible state

The Master Equation

$$\frac{dP(X,t)}{dt} = \sum_{i=1}^{R} \left(W_i(X - r_i, t) P(X - r_i, t) - W_i(x,t) P(X,t) \right) \tag{4}$$

where:

- X is a (vector-valued) Markov process
- R is the number of possible processes (e.g. birth, death, mutation)
- $W_i(X, t)$ is the probability rate of event i to occur

The Master Equation can be interpreted as a balance equation where the first term corresponds to positive flux into state X from every allowed state and the second term as negative flux from state X into every possible state

The Master Equation

$$\frac{dP(X,t)}{dt} = \sum_{i=1}^{R} \left(W_i(X - r_i, t)P(X - r_i, t) - W_i(x, t)P(X, t) \right) \tag{4}$$

where:

- X is a (vector-valued) Markov process
- R is the number of possible processes (e.g. birth, death, mutation)
- $W_i(X, t)$ is the probability rate of event i to occur
- r_i is the change in the value of X when event i occurs, i.e.

The Master Equation can be interpreted as a balance equation where the first term corresponds to positive flux into state X from every allowed state and the second term as negative flux from state X into every possible state

The Master Equation

$$\frac{dP(X,t)}{dt} = \sum_{i=1}^{R} \left(W_i(X - r_i, t) P(X - r_i, t) - W_i(x,t) P(X,t) \right) \quad (4)$$

where:

- X is a (vector-valued) Markov process
- R is the number of possible processes (e.g. birth, death, mutation)
- $W_i(X,t)$ is the probability rate of event i to occur
- r_i is the change in the value of X when event i occurs, i.e.
    - $P(X(t+dt) = X(t) + r_i | X(t)) = W_i(X,t)dt$

The Master Equation can be interpreted as a balance equation where the first term corresponds to positive flux into state X from every allowed state and the second term as negative flux from state X into every possible state

Outline

Motivation

Master Equation

Law of mass action

Steady vs absorbing states

Analytical methods: Characteristic function

Modelling the transition rates: The law of mass action

- To specify an stochastic model we need to give an expression for the probability rate for each of the events involved in the dynamics of the system (for example, birth and death)

Modelling the transition rates: The law of mass action

- To specify an stochastic model we need to give an expression for the probability rate for each of the events involved in the dynamics of the system (for example, birth and death)
- The standard modelling assumption used to write down expressions for these rates is the so called Law of Mass Action

Modelling the transition rates: The law of mass action

- To specify an stochastic model we need to give an expression for the probability rate for each of the events involved in the dynamics of the system (for example, birth and death)
- The standard modelling assumption used to write down expressions for these rates is the so called Law of Mass Action
- This assumption, which originates in chamical kinetics, consists of assuming that the probability rate of a particular event involving j molecular species, of the same type or of different types, is proportional to (i) the number of ways in which the corresponding molecular species can combine and (ii) a rate constant which accounts for the probability that an encounter of the elements participating in the reaction actually produces the corresponding product

Examples

- $X \rightarrow$ Product: $W(x) = k_1 X$

Examples

- $X \to$ Product: $W(x) = k_1 X$
- $X + Y \to$ Product: $W(x) = k_2 \frac{XY}{2}$

Examples

- $X \to$ Product: $W(x) = k_1 X$
- $X + Y \to$ Product: $W(x) = k_2 \frac{XY}{2}$
- $X + X \to$ Product: $W(x) = k_2 \frac{X(X-1)}{2}$

Examples

- $X \to$ Product: $W(x) = k_1 X$
- $X + Y \to$ Product: $W(x) = k_2 \frac{XY}{2}$
- $X + X \to$ Product: $W(x) = k_2 \frac{X(X-1)}{2}$
- $X + Y + Z \to$ Product: $W(x) = k_3 \frac{XYZ}{3!}$

Examples

- $X \to$ Product: $W(x) = k_1 X$
- $X + Y \to$ Product: $W(x) = k_2 \frac{XY}{2}$
- $X + X \to$ Product: $W(x) = k_2 \frac{X(X-1)}{2}$
- $X + Y + Z \to$ Product: $W(x) = k_3 \frac{XYZ}{3!}$
- $X + X + X \to$ Product: $W(x) = k_3 \frac{X(X-2)(X-3)}{3!}$

Example: Birth-and-death process

1. Birth: $n \to n+1$ with probability rate $W_+(n) = \lambda n$. Death: $n \to n-1$ with probability rate $W_-(n) = \sigma n$
2. Probability balance:

$$P(n, t+\Delta t) = \lambda(n-1)\Delta t P(n-1, t) + \sigma(n+1)\Delta t P(n+1, t) + (1-(\lambda n \Delta t + \sigma n \Delta t))P(n, t) \tag{5}$$

3. When $\Delta t \to 0$:

$$\frac{dP(n,t)}{dt} = \lambda(n-1)P(n-1,t) + \sigma(n+1)P(n+1,t) - (\lambda n + \sigma n)P(n,t) \tag{6}$$

Outline

Motivation

Master Equation

Law of mass action

Steady vs absorbing states

Analytical methods: Characteristic function

Steady states in stochastic systems

- The definition of equilibrium states in stochastic systems is a bit technical and there are several definitions of equilibrium (with or without detailed balance, equilibrium or non-equilibrium, etc.)

Steady states in stochastic systems

- The definition of equilibrium states in stochastic systems is a bit technical and there are several definitions of equilibrium (with or without detailed balance, equilibrium or non-equilibrium, etc.)
- We will avoid these technicalities, at least for the moment, and adopt a more intuitive and practical approach (although not terribly rigorous)

Steady states in stochastic systems

- The definition of equilibrium states in stochastic systems is a bit technical and there are several definitions of equilibrium (with or without detailed balance, equilibrium or non-equilibrium, etc.)
- We will avoid these technicalities, at least for the moment, and adopt a more intuitive and practical approach (although not terribly rigorous)
- For concreteness, consider (again) the stochastic logistic growth, i.e. a process n_t such that:
  1. $n \rightarrow n+1$ with probability rate $W_+(n) = n$
  2. $n \rightarrow n-1$ with probability rate $W_-(n) = \frac{n(n-1)}{K}$

Steady states in stochastic systems

- The definition of equilibrium states in stochastic systems is a bit technical and there are several definitions of equilibrium (with or without detailed balance, equilibrium or non-equilibrium, etc.)
- We will avoid these technicalities, at least for the moment, and adopt a more intuitive and practical approach (although not terribly rigorous)
- For concreteness, consider (again) the stochastic logistic growth, i.e. a process n_t such that:
    1. $n \to n+1$ with probability rate $W_+(n) = n$
    2. $n \to n-1$ with probability rate $W_-(n) = \frac{n(n-1)}{K}$
- Consider a state of the system, n_s, is, roughly speaking, a state of the process such that $W_+(n_s) = W_-(n_s)$.

Steady states in stochastic systems

- The definition of equilibrium states in stochastic systems is a bit technical and there are several definitions of equilibrium (with or without detailed balance, equilibrium or non-equilibrium, etc.)
- We will avoid these technicalities, at least for the moment, and adopt a more intuitive and practical approach (although not terribly rigorous)
- For concreteness, consider (again) the stochastic logistic growth, i.e. a process n_t such that:
  1. $n \rightarrow n+1$ with probability rate $W_+(n) = n$
  2. $n \rightarrow n-1$ with probability rate $W_-(n) = \frac{n(n-1)}{K}$
- Consider a state of the system, n_s, is, roughly speaking, a state of the process such that $W_+(n_s) = W_-(n_s)$.
  1. $W_+(n_s)$ is the number of births within a population of n_s individuals
  2. Likewise, $W_-(n_s) =$ the number of deaths within a population of n_s individuals
  3. So an steady state of our population dynamics is reached when $n_t = n_s$, since death rate is balanced by birth rates and therefore the population stays roughly constant

Steady states in stochastic systems

- The definition of equilibrium states in stochastic systems is a bit technical and there are several definitions of equilibrium (with or without detailed balance, equilibrium or non-equilibrium, etc.)
- We will avoid these technicalities, at least for the moment, and adopt a more intuitive and practical approach (although not terribly rigorous)
- For concreteness, consider (again) the stochastic logistic growth, i.e. a process n_t such that:
  1. $n \to n+1$ with probability rate $W_+(n) = n$
  2. $n \to n-1$ with probability rate $W_-(n) = \frac{n(n-1)}{K}$
- Consider a state of the system, n_s, is, roughly speaking, a state of the process such that $W_+(n_s) = W_-(n_s)$.
  1. $W_+(n_s)$ is the number of births within a population of n_s individuals
  2. Likewise, $W_-(n_s)$ = the number of deaths within a population of n_s individuals
  3. So an steady state of our population dynamics is reached when $n_t = n_s$, since death rate is balanced by birth rates and therefore the population stays roughly constant
- $n_s = K + 1$ which coincides with the deterministic stable fixed point (if $K \gg 1$)

Steady states in stochastic systems

- The definition of equilibrium states in stochastic systems is a bit technical and there are several definitions of equilibrium (with or without detailed balance, equilibrium or non-equilibrium, etc.)
- We will avoid these technicalities, at least for the moment, and adopt a more intuitive and practical approach (although not terribly rigorous)
- For concreteness, consider (again) the stochastic logistic growth, i.e. a process n_t such that:
  1. $n \to n+1$ with probability rate $W_+(n) = n$
  2. $n \to n-1$ with probability rate $W_-(n) = \frac{n(n-1)}{K}$
- Consider a state of the system, n_s, is, roughly speaking, a state of the process such that $W_+(n_s) = W_-(n_s)$.
  1. $W_+(n_s)$ is the number of births within a population of n_s individuals
  2. Likewise, $W_-(n_s)$ = the number of deaths within a population of n_s individuals
  3. So an steady state of our population dynamics is reached when $n_t = n_s$, since death rate is balanced by birth rates and therefore the population stays roughly constant
- $n_s = K + 1$ which coincides with the deterministic stable fixed point (if $K \gg 1$)
- Note that $W_+(n) - W_-(n) > 0$ if $n < n_s$ and $W_+(n) - W_-(n) < 0$ if $n > n_s$

Absorbing states in stochastic systems

- The concept of absorbing state is the stochastic equivalent of the concept of attractor in deterministic systems

Absorbing states in stochastic systems

- The concept of absorbing state is the stochastic equivalent of the concept of attractor in deterministic systems
- An absorbing state, n_0, is characterised by $W_i(n_0) = 0$, i.e. once the system has reached the absorbing state, it cannot leave anymore

Absorbing states in stochastic systems

- The concept of absorbing state is the stochastic equivalent of the concept of attractor in deterministic systems
- An absorbing state, n_0, is characterised by $W_i(n_0) = 0$, i.e. once the system has reached the absorbing state, it cannot leave anymore
- The set of accessible states of the abosrbing state is the equivalent of the basin of attraction of an attractor in deterministic systems: If n_a is an accessible state of n_0 the stochastic dynamics will take the system from n_a to n_0 with probability one

Absorbing states in stochastic systems

- The concept of absorbing state is the stochastic equivalent of the concept of attractor in deterministic systems
- An absorbing state, n_0, is characterised by $W_i(n_0) = 0$, i.e. once the system has reached the absorbing state, it cannot leave anymore
- The set of accessible states of the abosrbing state is the equivalent of the basin of attraction of an attractor in deterministic systems: If n_a is an accessible state of n_0 the stochastic dynamics will take the system from n_a to n_0 with probability one
- Consider again, the stochastic logistic growth:

Absorbing states in stochastic systems

- The concept of absorbing state is the stochastic equivalent of the concept of attractor in deterministic systems
- An absorbing state, n_0, is characterised by $W_i(n_0) = 0$, i.e. once the system has reached the absorbing state, it cannot leave anymore
- The set of accessible states of the abosrbing state is the equivalent of the basin of attraction of an attractor in deterministic systems: If n_a is an accessible state of n_0 the stochastic dynamics will take the system from n_a to n_0 with probability one
- Consider again, the stochastic logistic growth:
    1. Steady states are in general not absorbing states

Absorbing states in stochastic systems

- The concept of absorbing state is the stochastic equivalent of the concept of attractor in deterministic systems
- An absorbing state, n_0, is characterised by $W_i(n_0) = 0$, i.e. once the system has reached the absorbing state, it cannot leave anymore
- The set of accessible states of the abosrbing state is the equivalent of the basin of attraction of an attractor in deterministic systems: If n_a is an accessible state of n_0 the stochastic dynamics will take the system from n_a to n_0 with probability one
- Consider again, the stochastic logistic growth:
  1. Steady states are in general not absorbing states
  2. $W_+(n_s) \neq 0$ and $W_+(n_s) \neq 0$

Absorbing states in stochastic systems

- The concept of absorbing state is the stochastic equivalent of the concept of attractor in deterministic systems
- An absorbing state, n_0, is characterised by $W_i(n_0) = 0$, i.e. once the system has reached the absorbing state, it cannot leave anymore
- The set of accessible states of the abosrbing state is the equivalent of the basin of attraction of an attractor in deterministic systems: If n_a is an accessible state of n_0 the stochastic dynamics will take the system from n_a to n_0 with probability one
- Consider again, the stochastic logistic growth:
  1. Steady states are in general not absorbing states
  2. $W_+(n_s) \neq 0$ and $W_+(n_s) \neq 0$
  3. If $n = 0$ then $W_+(0) = W_-(0) = 0$ therefore $n = 0$ is an abosrbing state

Absorbing states in stochastic systems

- The concept of absorbing state is the stochastic equivalent of the concept of attractor in deterministic systems
- An absorbing state, n_0, is characterised by $W_i(n_0) = 0$, i.e. once the system has reached the absorbing state, it cannot leave anymore
- The set of accessible states of the abosrbing state is the equivalent of the basin of attraction of an attractor in deterministic systems: If n_a is an accessible state of n_0 the stochastic dynamics will take the system from n_a to n_0 with probability one
- Consider again, the stochastic logistic growth:
  1. Steady states are in general not absorbing states
  2. $W_+(n_s) \neq 0$ and $W_+(n_s) \neq 0$
  3. If $n = 0$ then $W_+(0) = W_-(0) = 0$ therefore $n = 0$ is an abosrbing state
  4. Also, n_s belongs to the set of accessible states of $n = 0$

Absorbing states in stochastic systems

- The concept of absorbing state is the stochastic equivalent of the concept of attractor in deterministic systems
- An absorbing state, n_0, is characterised by $W_i(n_0) = 0$, i.e. once the system has reached the absorbing state, it cannot leave anymore
- The set of accessible states of the abosrbing state is the equivalent of the basin of attraction of an attractor in deterministic systems: If n_a is an accessible state of n_0 the stochastic dynamics will take the system from n_a to n_0 with probability one
- Consider again, the stochastic logistic growth:
  1. Steady states are in general not absorbing states
  2. $W_+(n_s) \neq 0$ and $W_+(n_s) \neq 0$
  3. If $n = 0$ then $W_+(0) = W_-(0) = 0$ therefore $n = 0$ is an abosrbing state
  4. Also, n_s belongs to the set of accessible states of $n = 0$
- n_s belonging to the set of accessible states of $n = 0$ means that there is at least one consecutive set of transitions that connects n_s and n_0. For example: $K \to K-1 \to K-2 \to \cdots 1 \to 0$

Absorbing states in stochastic systems

- The concept of absorbing state is the stochastic equivalent of the concept of attractor in deterministic systems
- An absorbing state, n_0, is characterised by $W_i(n_0) = 0$, i.e. once the system has reached the absorbing state, it cannot leave anymore
- The set of accessible states of the abosrbing state is the equivalent of the basin of attraction of an attractor in deterministic systems: If n_a is an accessible state of n_0 the stochastic dynamics will take the system from n_a to n_0 with probability one
- Consider again, the stochastic logistic growth:
  1. Steady states are in general not absorbing states
  2. $W_+(n_s) \neq 0$ and $W_+(n_s) \neq 0$
  3. If $n = 0$ then $W_+(0) = W_-(0) = 0$ therefore $n = 0$ is an abosrbing state
  4. Also, n_s belongs to the set of accessible states of $n = 0$
- n_s belonging to the set of accessible states of $n = 0$ means that there is at least one consecutive set of transitions that connects n_s and n_0. For example: $K \to K-1 \to K-2 \to \cdots 1 \to 0$
- However, if $K \gg 1$ the probability of such a chain of events is vanishingly small

Summary I

- n_s is an steady state in the sense that births and deaths are balanced. Moreover, $W_+(n) - W_-(n) > 0$ if $n < n_s$ and $W_+(n) - W_-(n) < 0$ if $n > n_s$. This is essentially equivalent to what happens in the deterministic logistic growth model.

Summary I

- n_s is an steady state in the sense that births and deaths are balanced. Moreover, $W_+(n) - W_-(n) > 0$ if $n < n_s$ and $W_+(n) - W_-(n) < 0$ if $n > n_s$. This is essentially equivalent to what happens in the deterministic logistic growth model.
- However, n_s is not an absorbing state of the stochastic dynamics. The only absorbing state is $n = 0$

Summary I

- n_s is an steady state in the sense that births and deaths are balanced. Moreover, $W_+(n) - W_-(n) > 0$ if $n < n_s$ and $W_+(n) - W_-(n) < 0$ if $n > n_s$. This is essentially equivalent to what happens in the deterministic logistic growth model.
- However, n_s is not an absorbing state of the stochastic dynamics. The only absorbing state is $n = 0$
- Stochastic extinctions are relatively rare provided K is big. If this is the case, the deterministic system provides a reasonable approximation to the behaviour of the model.

Summary I

- n_s is an steady state in the sense that births and deaths are balanced. Moreover, $W_+(n) - W_-(n) > 0$ if $n < n_s$ and $W_+(n) - W_-(n) < 0$ if $n > n_s$. This is essentially equivalent to what happens in the deterministic logistic growth model.
- However, n_s is not an absorbing state of the stochastic dynamics. The only absorbing state is $n = 0$
- Stochastic extinctions are relatively rare provided K is big. If this is the case, the deterministic system provides a reasonable approximation to the behaviour of the model.
- If, on the contrary, K is small stochastic extinctions are relatively common and the deterministic description is not an accurate one

Summary II

- We have seen several examples of stochastic systems in which noise and randomness are the dominating factors. Their behaviours are not captured by their deterministic or mean-field conterparts
- In general, we should expect non-trivial random effects for:
  1. Small populations: Large fluctuations/rare events have probability $P \sim e^{-\Omega S}$ for large system size Ω
  2. Dynamics with absorbing states

Outline

Motivation

Master Equation

Law of mass action

Steady vs absorbing states

Analytical methods: Characteristic function

Analytical solutions

- Analytical solutions to the Master Equation are rare. General situations need to be dealt with by means of perturbative methods (Lecture 2) or numerical simulation (Lecture 3)

Analytical solutions

- Analytical solutions to the Master Equation are rare. General situations need to be dealt with by means of perturbative methods (Lecture 2) or numerical simulation (Lecture 3)
- For linear systems, it is possible to write a PDE for the so called probability generating function:

$$G(s,t) = \sum_n P(n,t) s^n \tag{7}$$

Analytical solutions

- Analytical solutions to the Master Equation are rare. General situations need to be dealt with by means of perturbative methods (Lecture 2) or numerical simulation (Lecture 3)
- For linear systems, it is possible to write a PDE for the so called probability generating function:

$$G(s,t) = \sum_n P(n,t) s^n \tag{7}$$

Example: Birth-and-death process

1. Master Equation:

$$\frac{dP(n,t)}{dt} = \lambda(n-1)P(n-1,t) + \sigma(n+1)P(n+1,t) - (\lambda n + \sigma n)P(n,t) \tag{8}$$

2. Multiply by s^n and sum over all n

$$\begin{aligned}\sum_n s^n \frac{dP(n,t)}{dt} = \quad & s^2 \sum_n \lambda(n-1)P(n-1,t)s^{n-2} + \sum_n \sigma(n+1)P(n+1,t)s^n \\ & -s\sum_n (\lambda n + \sigma n)P(n,t)s^{n-1}\end{aligned} \tag{9}$$

Analytical solutions

Example: Birth-and-death process (cont.)

1. PDE for the characteristic function:

$$\frac{\partial G(s,t)}{\partial t} = (\lambda s - \sigma)(s-1)\frac{\partial G(s,t)}{\partial s} \tag{10}$$

2. This PDE can be solved by the method of characteristics. If $G(s, t=0) = s^I$

$$G(s,t) = \left(\frac{\sigma(s-1) - (\sigma - \lambda s)\exp(-t(\lambda-\mu))}{\lambda(s-1) - (\sigma - \lambda s)\exp(-t(\lambda-\mu))} \right)^I \tag{11}$$

3. By Cauchy's formula:

$$P(n,t) = \frac{n!}{2\pi i} \oint \frac{G(z,t)}{z^{n+1}} dz \tag{12}$$

Analytical solutions

Example: Birth-and-death process (cont.)

1. PDE for the characteristic function:

$$\frac{\partial G(s,t)}{\partial t} = (\lambda s - \sigma)(s-1)\frac{\partial G(s,t)}{\partial s} \tag{10}$$

2. This PDE can be solved by the method of characteristics. If $G(s, t=0) = s^I$

$$G(s,t) = \left(\frac{\sigma(s-1) - (\sigma - \lambda s)\exp(-t(\lambda-\mu))}{\lambda(s-1) - (\sigma - \lambda s)\exp(-t(\lambda-\mu))}\right)^I \tag{11}$$

3. By Cauchy's formula:

$$P(n,t) = \frac{n!}{2\pi i}\oint \frac{G(z,t)}{z^{n+1}}dz \tag{12}$$

Note

Even when an analytical, closed solution for the characteristic function is not available, this function and its associated PDE are the corner stone for asymptotic analysis, specially WKB asymptotics

Outline of next lecture

1. Formal definition of a Markov process
   - The Markov property
   - Chapman-Kolmogorov equation
   - Derivation of the Master Equation
2. Asymptotic methods and rare events
   - WKB/large deviations approximation to the solution of the Master Equation
   - Eikonal approximation and analytical mechanics in stochastic processes