Introduction to stochastic modelling in Mathematical Biology

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Outline

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Markov property & the Chapman-Kolmogorov equation

The Master Equation

Asymptotic methods and rare events

Some basic definitions

Conditional probability and Bayes Theorem

$$P(A|B) = \frac{P(A \cap B)}{P(B)} = \frac{P(B|A)P(A)}{P(B)}$$

Probability density function (PDF)

Let X be a random variable taking values in $\mathbb{R}$. The probability that $X \in (x, x + dx)$ is given by $p(x)dx$ where $p(x)$ is the PDF of X. Some properties of the PDF are:

1. $$\int_{-\infty}^{\infty} p(x)dx = 1$$
2. $$P(x_1 \leq X \leq x_2) = \int_{x_1}^{x_2} p(x)dx = 1$$

Markov processes[1]

- In an informal sense, we can define a stochastic process as a system whose time evolution proceeds in a probabilistic manner and for which a random variable $X(t)$ exists which determines the state of the system at time t

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- Such systems are described in terms of an infinite set of joint probability densities:

$$P(x_n t_n, x_{n-1} t_{n-1}, \ldots, x_1, t_1)$$

or, equivalently, by a set of joint conditional probability densities:

$$P(x_n t_n, x_{n-1} t_{n-1}, \ldots, x_{k+1} t_{k+1} | t_k t_k, \ldots, x_1, t_1)$$

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- Obviously such a system is not possible to deal with in practice and, therefore, additional conditions must be imposed in order to make the system tractable

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Markov processes: The Markov property[2]

The Markov Property: Lack of long-term memory

- The Markov Property is an additional condition whereby we assume that the system looses memory of all its past history except for the most recent event

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- This property allows us to write any joint PDF in the infinite hierarchy in terms of just one: the one-step PDF $P(x_n t_n | x_{n-1} t_{n-1})$:

$$P(x_n t_n, x_{n-1} t_{n-1}, \ldots, x_2 t_2 | x_1, t_1) = \Pi_{i=2}^{n} P(x_i t_i | x_{i-1} t_{i-1})$$

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The Chapman-Kolmogorov Equation

The Chapman-Kolmogorov equation (CKE) is a direct consequence of the Markov property and provides a first step towards writing an equation for the time evolution of the probability density

The Chapman-Kolmogorov Equation

- Consider the identity

$$P(x_3 t_3 | x_1 t_1) = \int P(x_3 t_3, x_2 t_2 | x_1, t_1) dx_2$$

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- By the Markov property:

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Markov property & the Chapman-Kolmogorov equation

The Master Equation

Asymptotic methods and rare events

The Master Equation

The Master Equation is a reformulation of the CKE that is easier to handle and more directly related to physical models.

- Consider $P(x_3 t_3 | x_2 t_2)$ and let $dt \equiv t_3 - t_2$

$$P(x_3 t_3 | x_2 t_2) = (1 - a_0(x_2) dt)\delta(x_3 - x_2) + W(x_3 | x_2) dt$$

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- $W(x_3|x_2)$ is the transition rate (probability per unit time) of the transition $x_2 \to x_3$ and $1 - a_0 dt$ is the probability of no transition occurring. Therefore

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- According to the CKE

$$\frac{P(x_3 t_2 + dt|x_1 t_1) - P(x_2 t_2|x_1 t_1)}{dt} = \int W(x_3|x_2)P(x_2 t_2|x_1, t_1)dx_2 - a_0(x_3)P(x_3 t_2|x_1 t_1)$$

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- Using the definition of $a_0(x_3)$ and taking $dt \rightarrow 0$, we obtain:

$$\frac{dP(x_3 t|x_1 t_1)}{dt} = \int \left(W(x_3|x_2)P(x_2 t|x_1, t_1) - W(x_2|x_3)P(x_3 t|x_1 t_1)\right) dx_2$$

The Master Equation

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- Which can be re-written in the following form:

$$\frac{dP(X,t)}{dt} = \sum_i \left(e^{-r_i \partial_X} - 1 \right) W_i(X)P(X,t)$$

Outline

Rare events in stochastic dynamics[3]

- Rare events are noise-induced transitions between different attractors (equilibrium points) in multi-stable systems or between an attractor and an absorbing state (e.g. extinctions) in systems far away from a phase transition

[3] Hong Qian. Nonlinearity. **24**, R19 (2011). V. Elgart & A. Kamenev. Phys. Rev. E. **70**, 041106 (2004)

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- Therefore, these events are intrinsically non-Gaussian and we need to resort to methods other than diffusive limits of the Master Equation (see Van Kampen (2007) and Gardiner (2009))

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- Therefore, these events are intrinsically non-Gaussian and we need to resort to methods other than diffusive limits of the Master Equation (see Van Kampen (2007) and Gardiner (2009))
- Statistics of rare events: Typically their frequency $\sim e^{-\phi/\epsilon}$ where $\epsilon \ll 1$ is a measure of noise intensity

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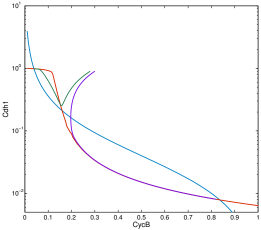
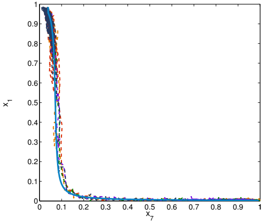
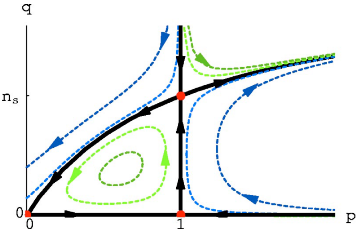
Rare events in stochastic dynamics

Two examples







WKB/Large deviations approximation

In this context, we introduce a set of asymptotic methods which are particularly well-suited for the study of rare events: WKB/Large deviations approximation

- We have seen that Markov stochastic processes can be described in terms of either a Master Equation for P(x,t):

$$\frac{\partial P(x,t)}{\partial t} = \Omega H_P(x, \partial_x) P(x,t)$$

where $x = X/\Omega$, $H_P(p,x) = \sum_i \left(e^{-r_i p} - 1\right) w_i(x)$, and $W_i(X) = \Omega w_i(x)$

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- or in terms of the corresponding characteristic function $G(p,t) = \sum_X P(X,t)p^X$ whose equation is derived from the Master Equation:

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- The operators $H_P(p,x)$ and $H_G(p,q)$ are both Shrödinger-like operators since the pairs (p,x) and (p,q), respectively, satisfy the following the canonical communtation relations for the position-momentum operators:
  - For H_P: $[x,p] = 1$ since $p = \partial_x$
  - For H_G: $[q,p] = 1$ since $q = -\partial_p$

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This asymptotic methods exploit the analogy to the Schrödinger equation to provide a low-noise asymptotic approximation that allows to study the statistics of rare events

The Path Integral Approach

The solution of this Schrödinger-like equations can be given in terms of path integrals[4]

- The solution for the characteristic function equation is given by:

$$G(p,t) = \int_0^t e^{-\mathcal{S}(p,q)} \mathcal{D}q(s)\mathcal{D}p(s)$$

where

$$\mathcal{S}(p,q) = \int_0^t \left(-H_G(p,q) + p(s)\dot{q}(s)\right) ds + S(p, t=0)$$

[4] R.P. Feynman & A.R. Hibbs. *Quantum mechanics & path integrals*. Emended ed. (2005)

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- By using the Laplace method, we can approximate the above path integral by:

$$G(p,t) = e^{-S(p,t)}$$

where $S(p,t)$ is the action integral calculated on the path that minimises the action functional $\mathcal{S}$, which corresponds to the solution of the Hamilton equations:

$$\frac{dp}{dt} = -\frac{\partial H}{\partial q}, \quad \frac{dq}{dt} = \frac{\partial H}{\partial p}$$

[4] R.P. Feynman & A.R. Hibbs. *Quantum mechanics & path integrals*. Emended ed. (2005)

The Path Integral Approach

This approach has been rediscovered several times in Human history:

1. Martin, Siggia, Rose Phys Rev A (1973) (field theory)
2. Kubo, Matsuo, Kitahara J. Stat. Phys. (1973) (WKB singular perturbation analysis)
3. Doi. J Phys. A (1976) (second quantisation)
4. Peliti J. Phys (1984) (second quantisation)
5. Freidlin & Wentzell. *Random perturbations of dynamical systems.* (1984). (Large deviation theory)

Analytical mechanics in stochastic dynamics[5]

- Hamilton equations:

$$\frac{dp}{dt} = -\frac{\partial H}{\partial q}, \ \frac{dq}{dt} = \frac{\partial H}{\partial p}$$

The solution to these equations provide a great amount of information about rare event statistics

[5] H. Ge & H. Qian. Int. J. Mod. Phys. B. **26**, 1230012 (2012). H. Qian. Nonlinearity. **24**, R19 (2011).

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- These trajectories live on a surface constant energy. Rare events are characterised by the trajectory on the corresponding phase space which connect the two states

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- These trajectories live on a surface constant energy. Rare events are characterised by the trajectory on the corresponding phase space which connect the two states
- Finally, the rate of the rare event is proportional to e^{-S}, where S is the classical action on the unique trajectory that fulfils the boundary conditions, thus reducing the problem of rare events to solving the evolution of a classical Hamiltonian system, a task much simpler than tackling the full Master Equation

[5] H. Ge & H. Qian. Int. J. Mod. Phys. B. **26**, 1230012 (2012). H. Qian. Nonlinearity. **24**, R19 (2011).

Analytical mechanics in stochastic dynamics[6]

Some properties

- The Hamiltonian dynamics generated by $H_G(p, q)$ is conservative. In fact, we will see that $H_G(p(t), q(t)) = 0$.
- $S(p = 1, t) = 0$. Normalisation $G(p = 1, t) = 1 \Rightarrow S(p = 1, t) = 0$
- $S(p, t) > 0$ for all $p \neq 1$
- $$\frac{dq}{dt} = \left.\frac{\partial H_G}{\partial p}\right|_{p(t)=1} \tag{1}$$

  corresponds to the mean-field, deterministic dynamics

[6] V. Elgart & A. Kamenev. Phys. Rev. E. **70**,041106 (2004). H. Qian. Nonlinearity. **24**, R19 (2011).

Example: Branching and binary annihilation[7]

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

$$\begin{aligned} P(n, t+\Delta t) = \quad & \Delta t\,(\sigma(n-1)P(n-1,t) + (\lambda(n+2)(n+1)/2)P(n+2,t)) \\ & +(1-\Delta t(\sigma n + (\lambda n(n-1)/2)))P(n,t) \end{aligned}$$

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

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

4. Which leads to the Hamiltonian $H_G(p,q) = \sigma(p-1)pq - \frac{\lambda}{2}(p^2-1)q^2$

[7] V. Elgart & A. Kamenev. Phys. Rev. E. **70**, 041106 (2004)

Hamilton equations and phase portrait[8]

- Hamilton equations:

$$\frac{dq}{dt} = -\lambda p q^2 + \sigma(2p-1)q$$

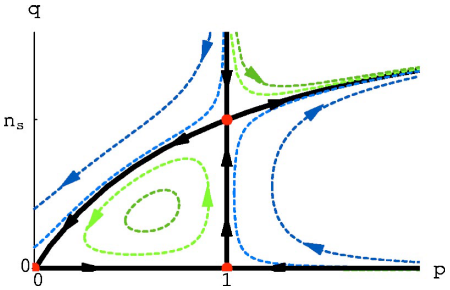
$$\frac{dp}{dt} = \lambda(p^2-1)q - \sigma(p-1)p$$

- Mean-field equation, i.e. $p(t) = 1$:

$$\frac{dq_{mf}}{dt} = \sigma q_{mf}\left(1 - \frac{\lambda}{\sigma} q_{mf}\right),$$

  i.e. a logistic growth model with carrying capacity $n_s = \sigma/\lambda$

- Conservative system: Thick lines show the lines of $H_G(p,q) = 0$ which implies $q(p) = 2n_s p/(p+1)$



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Extinction probability[9]

- From the analysis of the phase protrait we conclude that the optimal fluctuation path to extinction from the mean-field stable steady-state, $(p = 1, q = n_s)$, is

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which connects the mean-field stable steady-state with the absorbing state $(p = 0, q = 0)$

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- The action calculated along this trajectory is given by (recall that, on this trajectory, $H_G = 0$):

$$S_0 = \int_0^1 q(p)dp = n_s 2(1 - \log 2) \qquad (2)$$

[9] V. Elgart & A. Kamenev. Phys. Rev. E. **70**, 041106 (2004)

Extinction probability[9]

- From the analysis of the phase protrait we conclude that the optimal fluctuation path to extinction from the mean-field stable steady-state, $(p = 1, q = n_s)$, is

$$q(p) = 2n_s p/(p+1),$$

which connects the mean-field stable steady-state with the absorbing state $(p = 0, q = 0)$

- The action calculated along this trajectory is given by (recall that, on this trajectory, $H_G = 0$):

$$S_0 = \int_0^1 q(p)dp = n_s 2(1 - \log 2) \quad (2)$$

- The extinction rate, τ_E^{-1} is thus given by

$$\tau_E^{-1} = e^{-S_0} = e^{-n_s 2(1-\log 2)}$$

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Summary

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- We have seen that the study of the solutions of corresponding Hamilton equations and its phase portrait yields a wealth of useful information regarding rare event statistics
- Sometimes, however, the information provided by the classical Hamiltonian is not enough to predict rare events statistics to the accuracy demanded by certain applications, and one needs to resort to the statistical analysis of the ensemble of transition paths. Such analisys is beyond the scope of these lectures. If interested, consult the reviews C.P. Dellago & P.G. Bolhuis. Adv. Polymer Sci. (2008) or W. E and E. Vanden-Eijnden. Ann Rev. Phys. Chem. (2012).

Outline of next lecture

1. Numerical methods I: Gillespie stochastic simulation algrithm
2. Numerical methods II: The τ-leap method