How to construct stochastic models? Theory and numerics

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Why we need stochastic systems? some examples

I- Construction of stochastic models
The stochastisation problem
Stochastic differential equations
Invariance problems
First integrals
Invariant manifolds

II- Validation of models: numerics
Position of the problem
Ghost equilibrium points
Stability/instability artefacts
Invariance
Position of the problem

Why Stochastic models?

In many cases, we have well established deterministic models which are described by differential or a partial differential equations. For some reasons, one has to take into account stochastic phenomenons or perturbations.

Stochastic: randomness depending on time.
Hodgekin-Huxley model for neuronal dynamics\textsuperscript{1,2}

Biology

- Hodgekin-Huxley model for neuronal dynamics\textsuperscript{1,2}
  - Due to the stochasticity of stochastic behavior of neurons and voltage-dependent ion channel

Virology

- HIV dynamics\(^3\)\(^4\)


HIV dynamics\textsuperscript{3,4}

- **stochastic** effects arise by virtue of nature in the **infection process** when virions bind to receptors and interact with uninfected cells.

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Virology

- HIV dynamics\(^3\)\(^4\)
  - stochastic effects arise by virtue of nature in the *infection process* when virions bind to receptors and interact with uninfected cells
  - randomness is also assumed in the transition of uninfected cells into latently infected or actively infected cells and described by the transition probabilities \(p\) and \(1 - p\), respectively\(^5\).

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Population dynamics

- Population dynamics\textsuperscript{6}


\textsuperscript{7} Lisei, Julitz, A stochastic model for the growth of cancer tumors, Studia Univ. Babes-Bolyai, (2008).
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  - Due to an \textit{environment} that is subject to \textit{random fluctuations}.


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- Tumour growth, chemotherapy and optimal therapy strategy\textsuperscript{7}

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Population dynamics

- Population dynamics
  - Due to an environment that is subject to random fluctuations.
- Tumour growth, chemotherapy and optimal therapy strategy
  - The basic tumor growth kinetics is stochastically perturbed by the cytotoxic drug due to the chemotherapy

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Physics

- Landau-Lipshitz model for ferromagnetism

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  - Due to stochastic behavior of the magnetic field

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- Landau-Lipshitz model for ferromagnetism
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- Stochastic climate and weather modelling\(^8\)

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Physics

- Landau-Lipshitz model for ferromagnetism
  - Due to stochastic behavior of the magnetic field
- Stochastic climate and weather modelling
  - Due to unknown processes and multi scale phenomenon

Astronomy

- Two-body problem\textsuperscript{9,10}

\textsuperscript{9} N. Sharma and H. Parthasarathy, Dynamics of a stochastically perturbed two-body problem, Proc. R. Soc. A 2007 463, 979-1003

Two-body problem\textsuperscript{9,10}

Due to the stochastic fluctuations of the zodiacal dust around the sun

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{dust_sphere.png}
\caption{The dust sphere}
\end{figure}

\textsuperscript{9} N. Sharma and H. Parthasarathy, Dynamics of a stochastically perturbed two-body problem, Proc. R. Soc. A 2007 463, 979-1003

Motion of a satellite around an oblate planet: $J_2$ problem

Motion of a satellite around an oblate planet: $J_2$ problem

Due to the stochastic fluctuations of the shape of the Earth.

Figure: Shape of the Earth

Figure: Earth’s second degree zonal harmonic

The stochastisation problem

Give a sense to
\[
\frac{dx}{dt} = f(x, t) + "\text{noise}" \]

**Problem**: What do we mean by "noise"?

- **Construction of the stochastic model**?

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12. Not all constraints are interesting. We must consider constraints which are present independently of the modelling
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  - Find a suitable **framework** to deal with **stochasticity and dynamics** so to define the "noise".

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- Construction of the stochastic model?
  - Find a suitable framework to deal with stochasticity and dynamics so to define the "noise".
  - In this framework, define the suitable stochastic analogue of classical constraints \(^{12}\).

\(^{12}\) Not all constraints are interesting. We must consider constraints which are present independently of the modelling.
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  - Explain how to preserve the constraints.

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  - Explain how to **preserve** the **constraints**.

- **Validation of the stochastic model?**

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  - In this framework, define the suitable stochastic analogue of classical constraints.\(^\text{12}\).
  - Explain how to preserve the constraints.

- Validation of the stochastic model?
  - Find a numerical methods adapted to stochastic systems and preserving the specific constraints of the model.

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Stochastic framework

As we are dealing initially with differential or partial differential equations, we want to consider a stochastic framework including these objects. A common framework is given by

**Stochastic differential or partial differential equations**¹³

(SDEs or SPDEs)

Itô and Stratonovich formalisms

We consider systems of Itô’s equations

\[ dX_t = f(t, X_t)dt + \sigma(t, X_t)dW_t, \]
\[ X|_{t=0} = X_0, \]

where \( X = (X_1, \ldots, X_d) \), \( f = (f_1, \ldots, f_d) \) and \( \sigma = (\sigma_1, \ldots, \sigma_d) \) and \( dW_t \) are "Brownian" increments.

This notation is formally defined by the integral relation

\[ X_t = X_0 + \int_0^t f(s, X_s) \, ds + \int_0^t \sigma(s, X_s) \, dW_s, \]

where the second integral is an Itô integral.
Chain rule in Itô stochastic calculus: Itô formula

\[
 df(t, X_t) = \frac{\partial f}{\partial t} \, dt + (\nabla_X^T f) \, dX_t + \frac{1}{2} (dX_t^T)(\nabla_X^2 f) \, dX_t, 
\]

where \( \nabla_X f = \frac{\partial f}{\partial X} \) is the gradient of \( f \) w.r.t. \( X \), \( \nabla_X^2 f = \nabla_X \nabla_X^T f \) is the Hessian matrix of \( f \) w.r.t. \( X \), \( \delta \) is the Kronecker symbol and the following rules of computation are used: \( dt \, dt = 0 \), \( dt \, dW_{t,i} = 0 \), \( dW_{t,i} \, dB_{t,j} = \delta_{ij} \, dt \).
Stratonovich stochastic differential equations

\[ dX_t = \mu(t, X_t)\, dt + \sigma(t, X_t) \circ dW_t, \]  

\[ X_t = x + \int_0^t \mu(s, X_s)\, ds + \int_0^t \sigma(s, X_s) \circ dW_t, \]

where the second integral is a Stratonovich integral.
Transformation formula

Solutions of the Stratonovich differential equation (3) corresponds to solutions of a modified \( \text{d}\dot{X} \) equation:

\[
dX_t = \mu_{\text{cor}}(t, X_t)dt + \sigma(t, X_t)dW_t,
\]

where

\[
\mu_{\text{cor}}(t, x) = \left[ \mu(t, x) + \frac{1}{2} \sigma'(t, x)\sigma(t, x) \right].
\]

The correction term is also called the Wong-Zakai correction term.

\[
\mu_{\text{cor},i}(t, x) = \mu_i(t, x) + \frac{1}{2} \sum_{j=1}^{p} \sum_{k=1}^{n} \frac{\partial \sigma_{i,j}}{\partial x_k} \sigma_{k,j}, \quad 1 \leq i \leq n.
\]

Advantage of the Stratonovich integral: the chain rule formulas is the classical one!
Invariance

This is an ubiquitous property of many deterministic models: a set of variables remain in a fixed set under the dynamical evolution of the system.

Examples:

▸ densities must belong to the interval $[0, 1]$
▸ the oblateness of a planet must remain in a given admissible interval
▸ a population remains positive

These invariance constraints are independent of the underlying nature of the dynamics: deterministic or stochastic.
Invariance for deterministic systems
Stochastic invariance: a definition

Definition
We call the subset $K \subset \mathbb{R}^m$ invariant for the stochastic system $(f, g)$ if for every initial data $X_0 \in K$ and initial time $t_0 \geq 0$ the corresponding solution $X(t), t \geq t_0$, satisfies

$$P(\{X(t) \in K, \ t \in [t_0, \infty[\}) = 1,$$

i.e., the solution almost surely attains values within the set $K$. 
Additive noise

\[
\begin{aligned}
\begin{cases}
du &= 0 \, dt + dW_t \\
u(0) &= u_0,
\end{cases}
\end{aligned}
\]  \hspace{1cm} (8)

- The positivity is not preserved by the solutions of the perturbed stochastic system (8).
Additive noise

\[
\begin{cases}
    du = 0 \, dt + dW_t \\
    u(0) = u_0,
\end{cases}
\]

(8)

- The positivity is not preserved by the solutions of the perturbed stochastic system (8).
- \( u(t) = u(0) + W_t \).
Multiplicative noise

We consider a **linear, multiplicative noise** of the form

\[
\begin{cases}
    du = 0 \, dt + \alpha u \circ dW_t \\
    u(0) = u_0,
\end{cases}
\]  

(9)

where the constant \( \alpha \in \mathbb{R} \).

- The stochastic problem (9) preserves positivity.
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- The stochastic problem (9) preserves positivity.

\[
u(\omega, t) = u_0 e^{-\left(\frac{\alpha^2}{2} t - \alpha W_t(\omega)\right)}
\]
Invariance for stochastic systems\textsuperscript{14}

**Theorem**

Let $I \subset \{1, \ldots, m\}$ be a non-empty subset. Then, the set

$$K^+ := \{ x \in \mathbb{R}^m : x_i \geq 0, \ i \in I \}$$

is invariant for the stochastic system $(f, \sigma)$ if and only if

$$f_i(t, x) \geq 0 \quad \text{for } x \in K^+ \text{ such that } x_i = 0,$$

$$\sigma_{i,j}(t, x) = 0 \quad \text{for } x \in K^+ \text{ such that } x_i = 0, \ j = 1, \ldots, r,$$

for all $t \geq 0$ and $i \in I$.

*This result is valid independently of Itô’s or Stratonovich’s interpretations.*

The model studied by H.C. Tuckwell and E. Le Corfec is the following system of SDEs

\begin{align}
    dT &= (\lambda - \mu T - k_1 TV)dt - \sqrt{k_1 TV}dW_1, \\
    dL &= (k_1 p TV - \mu L - \alpha L)dt + \sqrt{k_1 p TV}dW_2, \\
    dI &= (k_1 (1 - p) TV + \alpha L - aI)dt + \sqrt{k_1 (1 - p) TV}dW_3, \\
    dV &= (cI - \gamma V - k_2 TV)dt - \sqrt{k_2 TV}dW_4. 
\end{align}

(10)

The constants \(a, c, k_1, k_2, \alpha, \gamma, \lambda\) and \(\mu\) are positive and \(p \in (0, 1)\). The model variables \(T, L, I\) and \(V\) represent cell densities, which are necessarily non-negative.

The positivity of solutions is preserved by the deterministic model. What about the stochastic version?
Proposition

The stochastic model for HIV-1 population dynamics (10) has the following properties:

(i) The solutions of the underlying deterministic system remain non-negative.

(ii) For any constant \( k_1 \neq 0 \) the stochastic model does not preserve the positivity of solutions, independent of Itô’s or Stratonovich’s interpretation of SDEs.

As a consequence, this model is not viable!

Simulations

**Figure:** Variable $T$ and $I$
Figure: Variable $L$ and $V$
The authors of this model was aware that it does not work! In (\cite{16} p.454, Section 3):
"In the simulations we found it expeditious to insert reflecting barriers at very small uninfected cells and virions numbers [...]. This prevented the random fluctuation terms from taking these variables to unphysical negative values [...]."

However, the use of reflecting barriers lead to difficulties. In particular:

- Can we rely on the numerical simulations to validate the model behaviour and deduce biological interpretations?

\par

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However, the use of reflecting barriers lead to difficulties. In particular:

- Can we rely on the numerical simulations to validate the model behaviour and deduce biological interpretations?
- What is the relation between the simulations and the original model? Could we formulate a modified stochastic model that reflects the absorbing barriers used in the simulations?

A viable model

Using our result, we can describe a class of viable models:

\[
\begin{align*}
    dT &= (\lambda - \mu T - k_1 TV)dt - \sqrt{k_1 TV}dW_1, \\
    dL &= (k_1 p TV - \mu L - \alpha L)dt + h_1(L)\sqrt{k_1 p TV}dW_2, \\
    dI &= (k_1 (1-p) TV + \alpha L - aI)dt + h_2(I)\sqrt{k_1 (1-p) TV}dW_3, \\
    dV &= (cI - \gamma V - k_2 TV)dt - \sqrt{k_2 TV}dW_4,
\end{align*}
\]

(11)

where \(h_1\) and \(h_2\) are two functions satisfying \(h_1(0) = h_2(0) = 0\). The conditions on \(h_1\) and \(h_2\) imply that the solutions of our modified model (11) remain non-negative for both, Itô’s and Stratonovich’s interpretation of SDEs. One simple choice are the functions

\[
    h_1(L) = \sqrt{aL}, \quad h_2(I) = \sqrt{bI}
\]

where \(a\) and \(b\) are two positive constants. The intensities of the stochastic perturbations in the equations for \(L\) and \(I\) then depend on these variables and not only on the cell densities \(T\) and \(V\).
simulations

Figure: Variable $T$ and $I$
Figure: Variable $L$ and $V$
Invariance: make your own stochastic perturbation

Classical theory for precession and nutation: movement of the geographic pole

due to the non-spherical form of the Earth but...he real movement of the pole is:
Stochastic $J_2$ problem: produce a stochastic deformation of a planet
Easy with the invariance characterisation! We define a "tyo-model" with an ad-hoc stochastic viable perturbation...

Strange coincidence with the real behaviour!
Conservation laws for stochastic systems

The classical definition:

Definition
A function $I : \mathbb{R}^n \mapsto \mathbb{R}$ is called a \textit{first integral} if for all solutions $x_t$ of the equation we have $I(x_t) = I(x_0)$ for all $t$. If $I$ is sufficiently smooth we deduce $\frac{dI(x_t)}{dt} = 0$.

What is the stochastic analogue of a first integral?
Two possibilities$^{17}$

Definition (Strong first integral)
A function $I : \mathbb{R}^n \rightarrow \mathbb{R}$ is a \textit{strong first integral} of (1) if for all solutions $X_t$ of (1), the stochastic process $I(X_t)$ is a constant process, i.e. $I(X_t) = I(X_0)$ a.s. (almost surely) or $d(I(X_t)) = 0$.

Very strong property! Most of the time not satisfied!

---

A weaker property is:

**Definition (Weak stochastic first integral)**

A function $I : \mathbb{R}^n \rightarrow \mathbb{R}$ is a weak stochastic first integral of (1) if for all solutions $X_t$ of (1), the stochastic process $I(X_t)$ satisfies $E(I(X_t)) = E(I(X_0))$ where $E$ denotes the expectation.

Many deterministic systems are preserving first integrals in the weak sense under stochastisation!
Example: the stochastic two-body problem

Classical conserved quantities: angular momentum and energy defined by

\[ M = mr^2w, \quad H = \frac{1}{2}m(v^2 + r^2w^2) - \frac{k}{r}. \]

\[ dM(X_t) = m\sigma_\phi dB^\phi_t, \quad dH(X_t) = mr\sigma_r dB^r_t + mrw\sigma_\phi dB^\phi_t + \frac{m}{2} \left[ \sigma_r^2 r^2 + \sigma_\phi^2 \right] dt. \]

Lemma

The angular momentum is a weak first integral of the stochastic two-body problem.

Can be used to test a numerical simulation!
stochastic two-body problem

Using a stochastic Runge-Kutta method developed by Kasdin and al\textsuperscript{18}.

Rapid divergence between the perturbed and unperturbed case!

**Is the simulation accurate?**

Simulations two-body problem

Good preservation of the weak first integral!

Figure: Left: $E(M(X_t))$. Right: $E(H(X_t))$. 
Invariant manifolds and conservation laws

Definition
A deterministic system leaves a given manifold of $\mathbb{R}^d$, denoted by $M$, invariant if for all initial condition $x_0 \in M$, the maximal solution $x_t(x_0)$ starting in $x_0$ when $t = 0$ remains in $M$, i.e. satisfied $x_t(x_0) \in M$ for all $t \in \mathbb{R}^+$. Let $M$ be defined by

$$M = \{x \in \mathbb{R}^n, F(x) = 0\},$$

where $F : \mathbb{R}^d \to \mathbb{R}$ is $C^1$.

If $F$ is a first integral then for all $x_0 \in M$, $F(x_t) = F(x_0) = 0$ and the manifold $M$ is invariant.

What about the stochastic case?
Invariant manifolds: the Itô case

The multidimensional Itô formula gives

\[
d[F(x_t)] = \nabla F(x_t)f(t, x_t) dt + \nabla F(x_t)\sigma(t, x_t) dW_t \\
+ \sum_{i,j} \frac{\partial^2 F}{\partial x_i \partial x_j}(x_t) \sum_{l=1}^{k} \sigma_{i,l}(t, x_t)\sigma_{l,j}(t, x_t) dt.
\]

The gradient of \(F\) always being normal to the manifold

\[
\nabla F(x_t) \cdot f(t, x_t) = 0
\]
Two kinds of notions can be developed in the stochastic case:

- **strong persistence** of the invariant manifold: \( dF = 0 \).
- **weak persistence**: persistence in expectation.
We always have:

$$E \left[ \int_{0}^{t} \nabla F(x_{s}) \cdot \sigma(s, x_{s})dW_{s} \right] = 0.$$  

The stochastic term has no influences!

but

$$E \left[ \int_{0}^{t} \sum_{i,j} \frac{\partial^{2}F}{\partial x_{i} \partial x_{j}}(x_{t}) \sum_{l=1}^{k} \sigma_{i,l}(t, x_{t})\sigma_{l,j}(t, x_{t})dt \right] \neq 0$$

in general!

We have generically no weak-persistence!

What about strong persistence?
Strong invariance: Itô case

We must have:
\[ \nabla F(x_t) \sigma(t, x_t) = 0. \]

Which is the **deterministic invariance** condition.

We obtain
\[
d[F(x_t)] = \sum_{i,j} \frac{\partial^2 F}{\partial x_i \partial x_j} (x_t) \sum_{l=1}^k \sigma_{i,l}(t, x_t) \sigma_{l,j}(t, x_t) dt.
\]

Simplest case: \( \sigma_{i,j} = \delta_{i}^{j}. \)

\[
d[F(x_t)] = \sum_{i=1}^n \frac{\partial^2 F}{\partial^2 x_i} [\sigma_{i,i}(t, x_t)]^2 dt.
\]

**Theorem (Invariance-Itô case)**

The manifold \( M \) is invariant by the flow of the stochastic system (1) in the Itô sense if and only if

\[
\sum_{i=1}^n \frac{\partial^2 F}{\partial x_i^2} [\sigma_{i,i}(t, x_t)]^2 dt = 0, \forall (t, x) \in \mathbb{R}^+ \times M.
\]
We can specialize this result in the case of the sphere.

**Corollary**

The sphere $S^{d-1}$ is invariant under the flow of the stochastic system (1) if and only if the stochastic perturbation is null on the sphere i.e.

$$
\sum_{i=1}^{d} [\sigma_{i,i}(t, x_t)]^2 = 0.
$$

The perturbation is identically null on the sphere!
Example of a stochastic Landau-Lifshitz model

We use the model defined by P. Etoré, S. Labbé and J. Lelong:\footnote{P. Etoré, S. Labbé and J. Lelong. Long time behaviour of a stochastic nano particle, Journal of Differential Equations, 257(6), 2014.}

\[
d\mu_t = [-\mu_t \wedge b - \alpha \mu_t \wedge (\mu_t \wedge b)] dt - \varepsilon [-\mu_t \wedge dW_t - \alpha \mu_t \wedge \mu_t \wedge dW_t],
\]

The vector \( b \) is the magnetic field and \( \alpha > 0 \) is the magnitude of damping term.

Is this model viable?
No! By symmetries arguments and physical arguments, the magnetic field must remains of norm one, i.e. belongs to the sphere independently of the nature of the modelling.

**Figure:** Behaviour of the magnetic field-Itô case

This stochastic model is not viable!
The Stratonovich case

Computations with the Stratonovich integral behave as the usual differential calculus.

\[ d[F(x_t)] = \nabla F(x_t) \cdot f(t, x_t) dt + \nabla F(x_t) \cdot \sigma(t, x_t) dW_t. \]

**Theorem (Stochastic invariance for manifolds)**

The manifold \( M \) is invariant under the flow of the stochastic system in the Stratonovich sense if and only if

\[ f(t, x) \in T_x M \text{ and } \sigma(t, x) \in T_x M, \text{ for all } (t, x) \in \mathbb{R}^+ \times M. \]
Invariant sphere - the Stratonovich case

**Theorem**

The sphere $S$ is invariant under the flow of the stochastic system (3) if and only if

$$x \cdot f(t, x) = x \cdot \sigma(t, x) = 0, \forall (t, x) \in \mathbb{R}^+ \times M.$$ 

The Stratonovich version of the stochastic Landau-Lifshitz example is viable!
Behaviour of the magnetic field - Stratonovich case
Stochastic Hamiltonian systems

Introduced by J-M. Bismut in his book *Mécanique aléatoire*,
Stochastic Hamiltonian systems are formally defined as:

**Definition**

A stochastic differential equation is called stochastic Hamiltonian
system if we can find a finite family of smooth functions
\( H = \{ H_r \}_{r=0,...,m}, \ H_r : \mathbb{R}^{2n} \rightarrow \mathbb{R}, \ r = 0, \ldots, m \) such that

\[
\begin{align*}
    dP^i &= -\frac{\partial H}{\partial q_i} \ dt - \sum_{r=1}^{m} \frac{\partial H_r}{\partial q_i} (t, P, Q) \circ dB^r_t, \\
    dQ^i &= \frac{\partial H}{\partial p_i} \ dt + \sum_{r=1}^{m} \frac{\partial H_r}{\partial p_i} (t, P, Q) \circ dB^r_t. 
\end{align*}
\]

(12)

We recover the classical **algebraic structure** of Hamiltonian
systems. What more?
**Liouville's property**: Let \((P, Q) \in \mathbb{R}^{2n}\), we consider the stochastic differential equation

\[
\begin{align*}
    dP &= f(t, P, Q)dt + \sum_{r=1}^{m} \sigma_r(t, P, Q) \circ dB_t^r, \\
    dQ &= g(t, P, Q)dt + \sum_{r=1}^{m} \gamma_r(t, P, Q) \circ dB_t^r.
\end{align*}
\] (13)

The phase flow of (13) preserves the symplectic structure if and only if it is a stochastic Hamiltonian system.

**Hamilton’s principle**: Solutions of a stochastic Hamiltonian system correspond to critical points of a stochastic functional defined by

\[
\mathcal{L}_H(X) = \int_0^t H_0(s, X_s) + \sum_{r=1}^{m} H_r(s, X_s) \circ dB_t^r.
\] (14)
How to know if a stochastic system is Hamiltonian or not?

Theorem

A $2n$-system of stochastic differential equations of the form

$$
\begin{align*}
    dP &= f(t, P, Q)dt + \sum_{r=1}^{m} \sigma_r(t, P, Q) \circ dB_t^r, \\
    dQ &= g(t, P, Q)dt + \sum_{r=1}^{m} \gamma_r(t, P, Q) \circ dB_t^r,
\end{align*}
$$

(15)

possesses a stochastic Hamiltonian formulation if and only if the coefficients satisfy the following set of conditions

$$
\begin{align*}
    \frac{\partial \sigma_{ir}}{\partial p^\alpha} + \frac{\partial \gamma_{ir}}{\partial q^i} &= 0, \\
    \frac{\partial \sigma_{ir}}{\partial q^\alpha} &= \frac{\partial \sigma_{ir}}{\partial q^i}, \quad \alpha \neq i, \\
    \frac{\partial \gamma_{ir}}{\partial p^\alpha} &= \frac{\partial \gamma_{ir}}{\partial p^i}, \quad \alpha \neq i,
\end{align*}
$$

(16)

for $i, \alpha = 1, \ldots, n$.

The Stratonovich form of the stochastic two-body problem is given by

\[
\begin{align*}
    dr &= \frac{p_r}{mr^2} dt, \\
    d\phi &= \frac{P_\phi}{mr^2} dt, \\
    dp_r &= \left(\frac{P_\phi^2}{mr^3} - \frac{k}{r^2}\right) dt + m\sigma_r r \circ dB_t^r, \\
    dp_\phi &= m\sigma_\phi r \circ dB_t^\phi.
\end{align*}
\]

(17)

We check that the stochastic two-body problem does not possess a stochastic Hamiltonian formulation.

Validation of a stochastic model

How to validate a given stochastic model?
simulations → comparison with the expected behaviour
simulations require an adapted numerical scheme → why?
Numerical problems related to simulations are already present in the deterministic case. For example, use a Runge-Kutta of order 4 method. We have the following well-known problems:

- Creation of ghost equilibrium points
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- Creation of ghost equilibrium points
- Non-preservation of the positivity (more generally invariance)
- Non-preservation of the variational structure
- Non-preservation of conservation laws
We consider the following classical population dynamics model

\[
\frac{dx}{dt} = x \left( b - \left( bx + \frac{ay}{c+x} \right) \right),
\]

\[
\frac{dy}{dt} = y \left( \frac{x}{c+x} - d \right),
\]

where \( a, b, c, d \) are real constants.

For the following simulations, we use \( a = 2, \ b = 1, \ c = 0.5, \ d = 6. \)
Creation of ghost equilibrium points and positivity

Numerical simulations for the initial conditions $x_0 = 15, y_0 = 0.1$.

Figure: $h = 0.2$ and $h = 0.1$
But the correct behaviour is:

Figure: $h = 0.01$
Stability/instability artefacts
Simulations with initial conditions $x_0 = 0.3$, $y_0 = 7.5$.

Figure: $h = 0.01$
Figure: $h = 0.2$

Figure: $h = 0.3$
Consequence:

If you make simulation with an unadapted numerical method, you obtain unphysical results.

No possibilities to test your model!
A possible answer: Construct adapted numerical scheme! Variational integrators for the preservation of variational structures
Mickens non standard methods to preserve invariance and some dynamical properties
More generally topological numerical scheme to preserve specific dynamical properties
Balance between approximation order and dynamical accuracy of the scheme.
In the stochastic case: you need a very high number of simulations to compute expectations: for implementation this is better a low order of approximation but an accurate dynamical scheme.
First step in this direction done by F. Pierret

Thank you for your attention!