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Stocasthic Modeling and Simulation

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Abstract

As a student of Scientific and Data Intensive Computing, I've created these notes while attending the **Stochastic Modeling and Simulation** course.
The course covers a wide range of topics, including Stochastic Nonlinear Models in different application fields (as physics, biomedicine, mathematics, ...), Stochastic Differential Equations, and Stochastic Simulation.

The topics covered in these notes include:
- Recap of Deterministic Models
- Stochastic Differential Equations and White Noise
- Fokker Planck Equation
- Noise-induced Transitions
- Colored noises
- Bounded Stochastic Processes
- Spatio-temporal Stochastic Processes
- Parameter Estimation form Data
- Stochasticity …
- …
- Continuous state space-discrete time Stochastic Processes
- Discrete Time Markov Chains
- Continuous Time Markov Chains
- Mean Field Approximation

While these notes were primarily created for my personal study, they may serve as a valuable resource for fellow students and professionals interested in Stochastic Modeling and Simulation.

Contents

1 Introduction

Different fields as Epidemics spreading, Cancer growth, and many others, can be modeled using Stochastic Differential Equations (SDEs).
An example is SIR model for epidemics spreading, formulized during a huge cholera infection in early 19th century. The model is based on three compartments: Susceptible, Infected, and Recovered individuals. This is modeled using a system of SDEs.
Often stochastic models represents well the problem, but real data are noisy and chaotic. For instance often we have to deal with data varying spatially and temporally, and we have to deal with the problem of parameter estimation.
Example: Oscillating chemical system

$$A+Y \xrightarrow{k_1} X+P, \quad X \xrightarrow{k_2} 2P$$
$$A+X \xrightarrow{k_3} 2Z, \quad X+Z \xrightarrow{k_4} 2A$$

Other examples are preys and predators models,
…
Renewable energies introduces a high volatility and unpredictability in energy production
If the demand of energy exceedes the production, we need to activate standard plans, to reduce consumption by switching off devices (e.g. water boilers remotely controlled), or to activate additional production plants. All these scenarios are complex systems.

Definition: ***Complex System***

A **complex system** is a system composed of interconnected parts that as a whole exhibit one or more properties (behavior among the possible properties) not obvious from the properties of the individual parts.

Emergent behavior is a property of complex systems, and it is not predictable from the behavior of the individual parts.

Definition: ***Adaptivity and self-organization***

- **Adaption** meand achieving a fit between the system and its environment.
- **Self-organization** is the process where a system changes its structure spontaneously, in order to adapt to the environment.

An instance of self-organization is the formation of a flock of birds, where each bird follows simple rules, but the flock as a whole exhibits a complex behavior.

Observation: ***Noise and Nonlinearities***

Noise and nonlinearities can (sometimes) favor the emergence of ”order”.

1.1 Modelling complex systems

Math for quantitatve models

We will be interersted in the temporal behavior of the system, and we will use some key ingredients for the maths:

- **Entities** can be modelled as *discrete* objects or *continuous* quantities.
- **...** ...
- **Time** can be *discrete* or *continuous*.

...

Data-Based vs Model-Based Approaches

Will data approaches make the kind of modelling obsolete?
Hybrid approacehs are possible:

1. Math models can be joined/hcybrized with machine learning models.
2. Deep Network to learn modules aor whole math models
   An exampleis *Physics-informed neural networks*: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations
3. ...

Definition: ***Dynamical System***

A **dynamical system** is a system whose state evolves over time according to a rule that depends on the current state.

[definition of differential equations]

Definition: ***Differential Equation***

A **differential equation** is an equation that relates one or more unknown functions and their derivatives.

In practice, differential equations are mathemathical instruments that describves the world around us. A note differential equation (maybe the first ever invented) is the Newton law:

$$F = ma \quad \Rightarrow \quad m\frac{d^2x}{dt^2} = F(x(t))$$

1.2 Tumor Size over Time

Let's consider an example case of a tumor growth. Let's assume that $X(t)$ is the size of a tumor at time t.
The differential equation that describes the growth of the tumor is:

$$X(t+dt) = X(t) + \Phi X(t) - MX(t)$$

where Φ is the growth rate and M is the decay rate.
We can rewrite the equation as:

$$\frac{X(t+dt)-X(t)}{dt} = X(t)\frac{(\Phi - M)}{dt}$$

Let's rewrite Φ and M as:

$$\begin{aligned} \Phi &= bdt + \cancel{O(dt^2)} \\ M &= mdt + \cancel{O(dt^2)} \end{aligned} \qquad \text{(We neglect the higher order terms)}$$

We obtain the following differential equation:

$$\frac{X(t+dt)-X(t)}{dt} = X(t)(b-m) \quad \Rightarrow \quad \frac{dX}{dt} = X(b-m)$$

Often we have a starting condition $X(0) = X_0$. Defining $a = b - m$, the sistem becomes:

$$\begin{cases} \frac{dX}{dt} = aX \\ X(0) = X_0 \end{cases}$$

Since makes no sense to have a negative time or tumor size, we have the constraints:

$$\begin{cases} t \in \mathbb{R}^+ \cup \{0\} \\ X \in \mathbb{R}^+ \cup \{0\} \end{cases}$$

The solution is given by:

$$X(t) = X_0 e^{at}$$

$$X(t+dt) = X(t) + bdtX - mdtX - \theta dtX$$

$$\left\{ \dot{X} = (a-\theta)XX(0) = X_0 \right.$$

dunque la soluzione è:

$$X(t) = X_0 e^{(a-\theta)t}$$

In questo caso, per $a > \theta$, il tumore cresce esponenzialmente, mentre per $a < \theta$, il tumore decresce esponenzialmente.
Nella realtà però il valore θ non è costante nel tempo, ma varia nel tempo. In tal caso il sistema diventa:

$$\begin{cases} \dot{X} = (a - \theta(t))X \\ X(0) = X_0 \end{cases}$$

e la soluzione è:

$$X(t) = X_0 e^{\int_0^t (a-\theta(s))ds}$$

Più in generale, un sistema del tipo:

$$z(y) = e^{G(y)} b$$

si ha

$$\frac{dz}{dy} = \frac{d}{dy} e^{G(y)} b = e^{G(y)} b \frac{dG}{dy} = G'(y) z(y)$$

Esempio:

$$\begin{cases} Z'(t) = \sin(t) Z(t) \\ Z(0) = Z_0 \end{cases}$$

Si ha:

$$\begin{cases} Z(t) = e^{-\cos(t)} B \\ Z_0 = e^{-1} B \end{cases} \qquad \Rightarrow \qquad Z(t) = e^{1-\cos(t)} z_0$$

1.3 Stabily and Eq. Points

1.3.1 Equilibrium Points

Given the system:

$$\begin{cases} \dot{x} = f(x) \\ x \in \mathbb{R}^n \end{cases}$$

An equilibrium point is a point x^* such that $f(x^*) = 0$.

Tip: *Eq. points*

A system can have multiple equilibrium points.

We have three kinds of equilibrium:

- **Stable equilibrium**: if the system is in the neighborhood of the equilibrium point, it will remain there.
- **Neutral equilibrium**: if the system is in the neighborhood of the equilibrium point, it will remain there, but it will not return to it.
- **Unstable equilibrium**: if the system is in the neighborhood of the equilibrium point, it will move away from it.

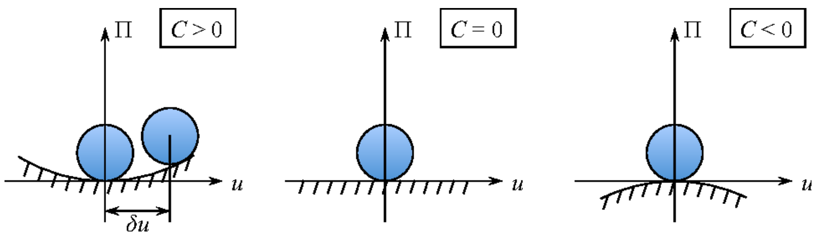

Figure 1.1: Stable, Natural and Unstable Equilibrium Points [1]

1.3.2 Stability

We say that a system is ***Globally Asymptotically Stable*** (or *Globally Attractive*) if it is stable and if it converges to the equilibrium point from any initial condition.

1.4 Local Analysis Near the Equilibrium Point

In this section, we study the system in the neighborhood of the equilibrium point. Let the initial condition be a small perturbation around the equilibrium:

$$X(0) = X_e + \varepsilon.$$

We introduce a deviation function $U(t)$ defined by

$$X(t) = X_e + U(t),$$

with the initial condition

$$U(0) = \varepsilon.$$

Thus, the evolution of the perturbation is governed by

$$\begin{cases} \dot{U} = f(X_e + U), \\ U(0) = \varepsilon. \end{cases}$$

Assume that the dynamics of the system are given by

$$\dot{X} = X(b(X) - m(X)).$$

Then the perturbed system becomes

$$\dot{U} = (b(X_e + U) - m(X_e + U))(X_e + U).$$

Expanding $b(X_e + U)$ and $m(X_e + U)$ in a Taylor series around X_e, we have:

$$b(X_e + U) \approx b(X_e) + b'(X_e)U,$$
$$m(X_e + U) \approx m(X_e) + m'(X_e)U.$$

Substituting these into the equation for $\dot{U}$, we get:

$$\begin{aligned} \dot{U} &= \big[b(X_e) + b'(X_e)U\big] - \big[m(X_e) + m'(X_e)U\big](X_e + U) \\ &= \big[b(X_e) + b'(X_e)U\big] - \big[m(X_e)X_e + m(X_e)U + m'(X_e)X_eU + m'(X_e)U^2\big]. \end{aligned}$$

Since the equilibrium condition implies that

$$(b(X_e) - m(X_e))X_e = 0,$$

the above expression simplifies (neglecting the higher-order term $m'(X_e)U^2$) to:

$$\dot{U} \approx [b'(X_e) - m(X_e) - m'(X_e)X_e]\,U.$$

Under the assumption that $b'(X_e)$ is negative, we can express this as

$$\dot{U} \approx -X_e\Big(|b'(X_e)| + m'(X_e)\Big)U.$$

The solution of this linearized differential equation is given by:

$$U(t) = U(0)\,e^{-X_e(|b'(X_e)| + m'(X_e))t}.$$

Hence, we identify the decay rate (or the inverse of the characteristic time constant) as

$$X_e\Big(|b'(X_e)|+m'(X_e)\Big),$$

and the characteristic time τ is:

$$\tau=\frac{1}{X_e\left(|b'(X_e)|+m'(X_e)\right)}.$$

This time constant represents the rate at which perturbations decay in the vicinity of the equilibrium point.

$$X(t) = X_e + U(t) \Rightarrow \dot{U} = f(X_e + U) = \underbrace{f(X_e)}_{=0} + f'(X_e)U + O(U^2)$$

$$\dot{U} = f'(X_e)U \Rightarrow U(t) = U(0)e^{f'(X_e)t}$$

So we have:

$$\begin{cases} f'(X_e) < 0 & \Rightarrow & X_e \text{ is Locally Asintotically stable} \\ f'(X_e) > 0 & \Rightarrow & X_e \text{ is Unstable} \end{cases}$$

1.5 Non-scalar Systems

Consider the system:

$$\begin{cases} \dot{x} = f(x) \\ x \in \{ \subseteq \mathbb{R}^n \end{cases}$$

As in the scalar case, we can linearize the system around the equilibrium point x_e:

$$f(X_e) = 0$$

$$X = X_e + U, \qquad |U| \ll 1$$

We have to consider the Jacobian matrix of f:

...

1.6 Exponential of a Matrix

Let's consider a linear system of the form:

$$\dot{x} = Ax$$

where $A \in \mathbb{R}^{n \times n}$ is a matrix. The solution of this system is given by:

$$x(t) = e^{At} x(0)$$

where e^{At} is the exponential of the matrix A.

Definition: ***Exponential of a Matrix***

Given a matrix $A \in \mathbb{R}^{n \times n}$, the exponential of A is defined as:

$$e^A = I + A + \frac{A^2}{2!} + \frac{A^3}{3!} + \cdots = \sum_{k=0}^{\infty} \frac{A^k}{k!}$$

This comes from the Taylor series expansion of the exponential function.

$$\frac{d}{dt} e^{At} = \sum_{m=1}^{\infty} A^m m \frac{t^{m-1}}{m(m-1)!} = \sum_{k=0}^{\infty} A A^k \frac{t^k}{k!} = A e^{At}$$

$$\begin{array}{lcl} A & = & H \cdot \text{Diag}(\lambda_1, \lambda_2, \ldots, \lambda_n) \cdot H^{-1} \\ A^2 & = & H \cdot \text{Diag}(\lambda_1^2, \lambda_2^2, \ldots, \lambda_n^2) \cdot H^{-1} \\ A^m & = & H \cdot \text{Diag}(\lambda_1^m, \lambda_2^m, \ldots, \lambda_n^m) \cdot H^{-1} \end{array}$$

So we have:

$$e^{At} = \sum_{m=0}^{\infty} \frac{A^m t^m}{m!} =$$

An example of a matrix exponential is given by the Newton's law:

$$m\ddot{x} = F$$

Let's consider a more complex case with air resistance γ:

$$m\ddot{x} = -\gamma\dot{x} - F(x)$$

We can rewrite this system as:

2 Lecture 10/03/2024

Last lecture we saw that we can approximate a non-linear system with a linear one, locally in an equilibrium point.
Let's consider an electric circuit, if the elecrical field is not static, it generates a variable magnetic field and viceversa.

$$\begin{cases} \Phi = Li \\ Ri = -\dfrac{d\Phi(\vec{B})}{dt} = -\dfrac{d(Li)}{dt} \end{cases}$$

We can write this system in the cauchy form:

$$\begin{cases} \dfrac{di}{dt} = -\dfrac{R}{L}i \\ i(0) = i_0 \end{cases}$$

The solution is:

$$i(t) = i_0 e^{-\frac{R}{t}}$$

$$L\frac{di}{dt} + Ri + V_c = 0$$

$$VC = Q$$

$$y = \begin{bmatrix} i \\ q \end{bmatrix}, \quad A = \begin{bmatrix} -\dfrac{R}{L} & -\dfrac{1}{LC} \\ 1 & 0 \end{bmatrix}$$

$$m\ddot{x} = \gamma\dot{x} + kx$$

2.1 Dirak Delta

If ypu consider a foorball player that kicks a ball, the force is not constant, and it is not possible to model it with a constant force. We can model it with a Dirak Delta function.

$$\begin{cases} m\ddot{x} = m\dot{v} = F(t) \\ v(0) = 0 \end{cases} \quad \Rightarrow \quad mv_{after} = \int_0^a F(t)dt \quad \Rightarrow \quad \boxed{v_{after} = \frac{1}{m}\int_0^a F(t)dt}$$

So the Dirak Delta function is a function that is zero everywhere except in zero, where it is infinite. It is used to model impulses.

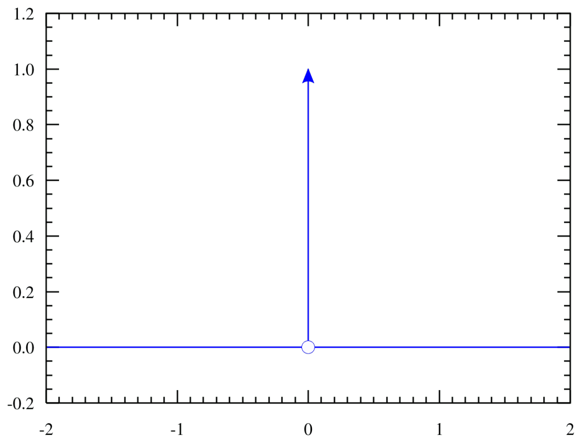

Figure 2.1: Dirak Delta Function

…

Let's consider a function $f(t)$ such that $f(0) < \infty$ and $f'(0) < \infty$. We can calculate:

$$\int_{\mathbb{R}} \delta(t)f(t)dt = \int_{\mathbb{R}} \delta(t)[f(0) + f'(0)t]dt = \int_{\mathbb{R}} \delta(t)f(0)dt + \int_{\mathbb{R}} \delta(t)f'(0)tdt$$

Now, we use two key properties of the Dirac delta function:

1. **Sifting Property:**
$$\int_{\mathbb{R}} \delta(t)\,dt = 1.$$
2. **First Moment:**
$$\int_{\mathbb{R}} \delta(t)t\,dt = 0,$$
which follows because $t\delta(t)$ is an odd function.

Substituting these results, we obtain:

$$\int_{\mathbb{R}} \delta(t)f(t)\,dt = f(0)\cdot 1 + f'(0)\cdot 0 = f(0).$$

…

2.2 Random Processes

$$< x(t) >= \frac{1}{N}\sum_{i=1}^{N} x_{Ri}(t)$$

$$m_i\ddot{x}_i = -\gamma\dot{x}_i \quad \Rightarrow \quad m_i\dot{v}_i = -\gamma v_i \quad \Rightarrow \quad \dot{v}_i = -\frac{\gamma}{m_i}v_i \quad \Rightarrow \quad \boxed{v_i(t) = v_i(0)e^{-(\gamma/m_i)t}}$$

$$\boxed{m\dot{v} = -\gamma v + \hat{F}_s(t)}$$

$$\begin{gathered}
m\ddot{x} = -k\dot{x} + \hat{F}_p(x) + \hat{F}_s(t) \\
m\ddot{x} = -k\dot{x} + kf(x) + kf_s(t) \\
\frac{m}{k}\ddot{x} = -\dot{x} + f(x) + f_s(t) \\
\frac{m}{k}\ddot{x} \ll 1 \quad \Rightarrow \quad \frac{m}{k}\ddot{x} \approx 0 \\
\dot{x} \simeq f(x) + f_s(t) = f(x) + \omega\xi(t)
\end{gathered}$$

Bibliography

[1] "2.080 Structural Mechanics Stability of Elastic Structures". In: 2014. URL: https://api.semanticscholar.org/CorpusID:30595920.