FU course: Mathematical Strategies for Complex Stochastic Dynamics

April-July 2025

Lecturer: Wei Zhang (ZIB)

Course Information

Schedule

Lectures:

- T9/053 Seminarraum (Takustr. 9)
- Wed. from 14:00-16:00
- Last lecture: July 16, 2025

Practice:

- T9/046 Seminarraum (Takustr. 9)
- Fri. from 10:00-12:00
- Last course: July 18, 2025

Note: no meetings on June 4 and 6 due to conference.

Course Information

1. lecture notes:

   https://weizhang.userpage.fu-berlin.de/teach.html
2. jupyter notebooks

   https://github.com/zwpku/course-FUB-summer2025

Course Information

Format:

- Lectures: slides + black board
- Practice:
  - analytical examples: slides + black board
  - numerical examples: Python, Jupyter, Pytorch

Course Information

Tentative plan for grading:

1. **Solve problems**: Each week, I will provide questions/problems. You choose one of them to solve. In total, 10 questions shall be solved.
2. **a short report**: I provide several topics for numerical experiment. Select 1 topics to conduct numerical experiement and write a short report:
   - length: 4-6 pages recommended
   - problem description and goal
   - method and algorithm
   - details about numerical experiment
3. optional: 5-10 min presentation of your numerical experiment

Introduction

ODEs

ODE in $\mathbb{R}^d$

$$\frac{dx(t)}{dt} = f(x(t)) \quad s \in [0, T] , \quad x(0) = x , \tag{1}$$

where $f : \mathbb{R}^d \to \mathbb{R}^d$.

ODEs

ODE in $\mathbb{R}^d$

$$\frac{dx(t)}{dt} = f(x(t)) \quad s \in [0, T]\,, \quad x(0) = x\,, \tag{1}$$

where $f : \mathbb{R}^d \to \mathbb{R}^d$.

Known facts:

- trajectory $x(t)$ is C^1-differentiable.
- given $x(0)$, $x(t)$ is determinstic.
- explicit Euler scheme: $\Delta t = \frac{T}{N}$,

$$x_{n+1} = x_n + f(x_n)\Delta t\,, \quad n = 0, 1, 2, \ldots\,.$$

- Runge-Kutta scheme

Stochastic processes

Markovian processes:

1. Markov chain
2. Markov jump process
3. Diffusion process: continous time and space

SDEs

Stochastic differential equations in $\mathbb{R}^d$

$$dx(t) = f(x(t))\,dt + \Sigma dw(t)\,, \quad t \in [0, T]\,. \tag{2}$$

where $f : \mathbb{R}^d \to \mathbb{R}^d$, Σ is a constant matrix, $w(t)$ is a d-dimensional Browian motion.

SDEs

Stochastic differential equations in $\mathbb{R}^d$

$$dx(t) = f(x(t))\,dt + \Sigma dw(t)\,, \quad t \in [0, T]\,. \tag{2}$$

where $f : \mathbb{R}^d \to \mathbb{R}^d$, Σ is a constant matrix, $w(t)$ is a d-dimensional Browian motion.

The meaning of (2):

- SDE = ODE + noise
- (continuous-time) limit of the scheme:

$$x_{n+1} = x_n + f(x_n)\Delta t + \sqrt{\Delta t}\Sigma\eta_n, \tag{3}$$

  where η_n are i.i.d. standard Gaussian random variables in $\mathbb{R}^d$.

Complex stochastic dynamics

Main application areas:

- molecular dynamics
- material sciences
- climate

Main study approaches:

- theoretical analysis
- numerical computing

Complex stochastic dynamics: Multiple time-scales

- molecular dynamics:
  atom vibration v.s. conformational changes
- climate:
  weather forcast from next hours to next days, climate changes in the coming years
- finance: stock prices
- ...

Complex stochastic dynamics: Multiple time-scales

Consider SDE

$$\begin{aligned} dx(t) =& f(x(t), y(t))\, dt + dw_1(t) \\ dy(t) =& \frac{1}{\epsilon} g(x(t), y(t))\, dt + \frac{1}{\sqrt{\epsilon}} dw_2(t)\,, \end{aligned} \tag{4}$$

where $\epsilon > 0$ is a small parameter.

In this case, $x(t)$ is a slow variable, $y(t)$ is a fast variable.

Complex stochastic dynamics: Multiple time-scales

Consider SDE

$$\begin{aligned} dx(t) =& f(x(t), y(t))\,dt + dw_1(t) \\ dy(t) =& \frac{1}{\epsilon} g(x(t), y(t))\,dt + \frac{1}{\sqrt{\epsilon}} dw_2(t)\,, \end{aligned} \tag{4}$$

where $\epsilon > 0$ is a small parameter.

In this case, $x(t)$ is a slow variable, $y(t)$ is a fast variable.

Difficulty:

In numerical simulations, step-size Δt has to be very small, e.g. $O(\epsilon)$.

$\Longrightarrow$ large computational cost, e.g. $\mathcal{O}(\frac{T}{\epsilon})$.

Complex stochastic dynamics: Metastability

Consider the SDE

$$dx(t) = -\nabla V(x(t))\, ds + \sqrt{2\epsilon} dw(t)\,, \tag{5}$$

where V is a potential function with **multiple** local minima.

Complex stochastic dynamics: Metastability

Consider the SDE

$$dx(t) = -\nabla V(x(t))\, ds + \sqrt{2\epsilon} dw(t)\,, \tag{5}$$

where V is a potential function with **multiple** local minima.

Difficulty: transition events are rare.

$\Longrightarrow$ Long-time simulation

$\Longrightarrow$ large computational cost.

Example: potential $V(x) = \frac{1}{4}(x^2 - 1)^2$.

$$dx(t) = -\nabla V(x(t))\, ds + \sqrt{2\epsilon} dw(t)\,, \tag{6}$$

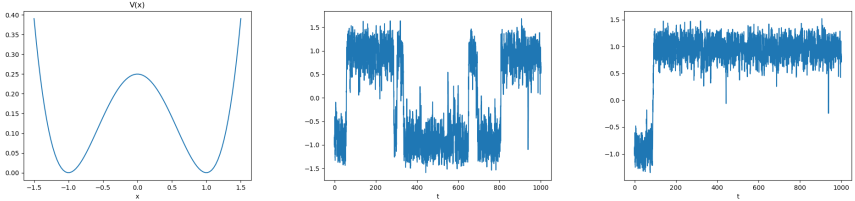


Figure: left: potential. middle: $\epsilon = 0.1$, right: $\epsilon = 0.05$.

Complex stochastic dynamics: High-dimensionality

$$dx(t) = f(x(t))\,ds + \Sigma dw(t)\,, \quad t \in [0, T]\,. \tag{7}$$

Common features:

- large number of particles in systems: m
- high dimension: $d = 3m$
- complicated interaction forces f.

Complex stochastic dynamics: High-dimensionality

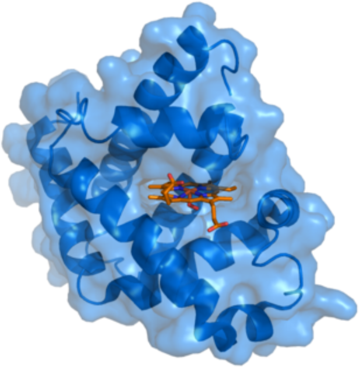
$$dx(t) = f(x(t))\, ds + \Sigma dw(t)\,, \quad t \in [0, T]\,. \tag{7}$$

Common features:

- large number of particles in systems: m
- high dimension: $d = 3m$
- complicated interaction forces f.

As a result, (7) is in a high-dimensional space and f is highly complicate.

Examples: molecular dynamics in biophysics



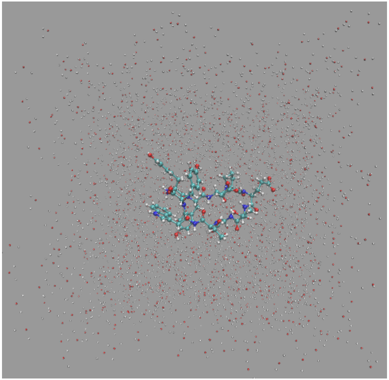


Figure: left: protein (myoglobine). right: MD simulation

Common goal

Common research goal is to better understand these complex dynamics (e.g. protein dynamics, climate, materials) by

- analyzing the dynamics
- building simplified surrogate model
- developing efficient numerical simulation method

Research questions

- averaging system:

$$
\begin{aligned}
dx(t) =& f(x(t), y(t))\, dt + dw_1(t) \\
dy(t) =& \frac{1}{\epsilon} g(x(t), y(t))\, dt + \frac{1}{\sqrt{\epsilon}} dw_2(t)\,,
\end{aligned}
\tag{8}
$$

  Questions:

  1. What is the limiting behavior when $\epsilon \to 0$?
  2. Can we elimenate the fast variable $y(s)$, and obtain an effective dynamics for the slow variable $x(t)$?

- metastable system:

$$
dx(t) = -\nabla V(x(t))\, ds + \sqrt{2\epsilon} dw(t)\,, \tag{9}
$$

  Questions:

  1. How to characterize the transition events (jumps from one well to another)?
  2. How to reduce the dimensionality and obtain equation of some observables?

Goal of this course

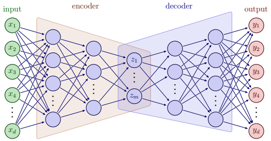
Provide both **theoretical** and **numerical** tools to study SDEs with multiple time scales or metastabilty.

Related topics in machine learning

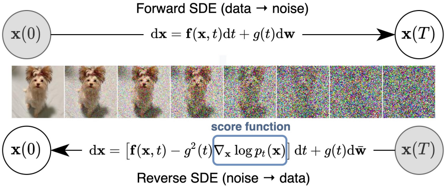
- stochastic gradient descent

$$\mathrm{Loss}(\theta_n) = \frac{1}{B}\sum_{l=1}^{B} \ell(x_{i_l}, \theta_n), \quad \theta_{n+1} = \theta_n - r\nabla_\theta \mathrm{Loss}(\theta_n) \tag{10}$$

- Autoencoder for dimensionality reduction



- Diffusion models for generative modeling



Contents

To summarize, we will discuss the following topics in this course.

1. Basic of stochastic processes (4 weeks)

   Langevin dynamics, Markov chains, generators, Fokker-Planck equation, convergence to equilibrium, Ito's formula

2. Model reduction for stochastic dynamics (4 weeks)

   averaging, collective variables, effective dynamics, Markov state modeling

3. Machine learning techniques (4 weeks)

   stochastic gradient descent, autoencoders, PDE eigenvalue problems by deep learning, diffusion models, continuous normalizing flow, flow-matching

Questions?