Lecture 10

Transfer operator formalism

CONTENTS

I. Transfer operators 1
A. Langevin equation 1
B. Fokker-Planck operator and propagator 2
C. Infinitesimal generator and Koopman operator 3
D. Adjointness relationships 3

II. Dynamics properties 4
A. Equilibrium distribution 4
The overdamped Langevin equation 6
B. Reversibility 6
1. Self-adjointness relationships 7
2. Spectral decomposition 7
C. Ergodicity 9
D. Example 9

I. TRANSFER OPERATORS

A. Langevin equation

Consider a one-dimensional system represented by the variable $x_t \in \Gamma \subset \mathbb{R}$, whose dynamics evolves according to the stochastic differential equation

$$dx_t = -D_1(x_t)dt + \sqrt{2D_2(x_t)}\,\eta_t \tag{1}$$

where

- Γ is the state-space;
- $D_1(x)$ is a position-dependent drift;

- $D_2(x)$ is a position-dependent diffusion function;
- η_t is a Gaussian white noise that satisfies

$$\begin{cases} \langle \eta_t \rangle = 0 \,, \\ \langle \eta_t,\, \eta_{t'} \rangle = \delta(t - t') \,, \end{cases} \tag{2}$$

As $D_1(x)$ and $D_2(x)$ do not explicitly depend on the time variable t, the process x_t is time-homogeneous. Furthermore, the process x_t is Markovian, as we do not consider memory terms (as for example in the generalised Langevin equation).

B. Fokker-Planck operator and propagator

The dynamics defined by eq. 1 is equivalently described by the Fokker-Planck equation, or forward Kolmogorov equation:

$$\frac{\partial \rho_t(x)}{\partial t} = -\frac{\partial}{\partial x}\left[D_1(x)\,\rho_t(x)\right] + \frac{\partial^2}{\partial x^2}\left[D_2(x)\,\rho_t(x)\right] \,, \tag{3}$$

where $\rho_t(x)$ is a time-dependent probability density that describes the probability to find the system in the state x at time t. Eq. 3 can be rewritten in terms of the Fokker-Planck operator $\mathcal{Q}^*$ as

$$\frac{\partial \rho_t(x)}{\partial t} = \mathcal{Q}^* \rho_t(x) \,, \tag{4}$$

where $\mathcal{Q}^*$ acts on probability densities defined on the Lebesgue space $L^1 = \{f : \int_\Gamma |f(x)|dx < \infty\}$. Solutions of eq. 4 are formally written as

$$\rho_{t+\tau}(x) = \exp\left(\mathcal{Q}^* \,\tau\right) \rho_t(x) \tag{5}$$

$$= \mathcal{P}_\tau \rho_t(x) \,, \tag{6}$$

where we introduced the propagator, or Perron-Frobenius operator, $\mathcal{P}_\tau$. Applying the Chapman-Kolmogorov equation, one finds that $\mathcal{P}_\tau$ acts on probability densities as

$$\rho_{t+\tau}(x) = \int_\Gamma p_\tau(y, x) \rho_t(y)\, dy \tag{7}$$

where $p_\tau(y, x) := p(x, t + \tau | y, t)$ is the conditional probability of finding the system in state x at time $t + \tau$, given it was in state y at time t. Note that in eq. 7 the integral is over the variable y, representing the starting state in the conditional probability.

C. Infinitesimal generator and Koopman operator

We now introduce the backward Kolmogorov equation

$$\frac{\partial f_t(x)}{\partial t} = D_1(x)\,\frac{\partial f_t(x)}{\partial x} + D_2(x)\,\frac{\partial^2 f_t(x)}{\partial x^2}\,, \tag{8}$$

where $f_t(x) \in L^\infty = \{f : \|f\|_\infty < \infty\}$ is an observable function, i.e. a function that represents a physical property or physical quantity that can be measured. Eq. 8 is written equivalently as

$$\frac{\partial f_t(x)}{\partial t} = \mathcal{Q} f_t(x)\,. \tag{9}$$

where the operator $\mathcal{Q}$ is called infinitesimal generator.

Analogously to eq. 6, we write a formal solution of eq. 9 as

$$f_{t+\tau}(x) = \exp\left(\mathcal{Q}\,\tau\right) f_t(x) \tag{10}$$

$$= \mathcal{K}_\tau f_t(x)\,, \tag{11}$$

where $\mathcal{K}_\tau$ is the Koopman operator and acts on functions as

$$f_{t+\tau}(x) = \int_\Gamma p_\tau(x,y) f_t(y)\,dy \tag{12}$$

Note that in eq. 12 the integral is again on the variable y, but here, the variable y represents the target state in the conditional probability function $p_\tau(x,y)$. The integral in eq. 12 is equivalent to the expectation

$$f_{t+\tau}(x) = \mathbb{E}\left[f(x_\tau)|x_0 = x\right]\,. \tag{13}$$

The infinitesimal generator is often written as the time-derivative of the Koopman operator as

$$\mathcal{Q} f(x) = \lim_{\tau\to 0^+} \frac{\mathcal{K}_\tau - \mathcal{I}}{\tau} f(x)\,, \tag{14}$$

where $\mathcal{I}$ is the identity operator.

D. Adjointness relationships

Given two test functions $f, g \in L^\infty$, the four operators $\mathcal{Q}^*$, $\mathcal{Q}$, $\mathcal{P}_\tau$ and $\mathcal{K}_\tau$, satisfy the following adjointness relationships.

$$\langle \mathcal{Q}^* f, g\rangle = \langle f, \mathcal{Q} g\rangle\,, \tag{15}$$

and

$$\langle \mathcal{P}_\tau f, g \rangle = \langle f, \mathcal{K}_\tau g \rangle \,, \tag{16}$$

where we defined the scalar product

$$\langle f, g \rangle = \int_\Gamma f(x) g(x)\, dx \,. \tag{17}$$

II. DYNAMICS PROPERTIES

Studying the dynamics of a system by means of the infinitesimal generator and the Koopman operator makes it possible to transform a non-linear problem, defined in eq. 1, into a linear problem, defined in eq. 9. The drawback is that the problem from being finite-dimensional defined on the space Γ, becomes an infinite-dimensional problem defined in the functional space L^∞. In order to use these operators in applications, we need a finite-dimensional representation. To this end, we require that the dynamic x_t, solution of eq. 1 satisfies certain properties. We already assumed time-homogeneity and Markovianity. Additionally, we require that the system has an equilibrium distribution, is reversible, is ergodic.

A. Equilibrium distribution

In order to find the equilibrium distribution, we rewrite eq. 3 as

$$\frac{\partial \rho_t(x)}{\partial t} = -\frac{\partial J_t(x)}{\partial x} \,, \tag{18}$$

where we introduced the flux, or probability current,

$$J_t(x) = \left[D_1(x)\, \rho_t(x) \right] + \frac{\partial}{\partial x} \left[D_2(x)\, \rho_t(x) \right] \,. \tag{19}$$

The flux is a measure of how the probability density $\rho_t(x)$ passes through the boundaries of a volume in unit time. If we imagine the probability density as a fluid, the flux describes how the fluid flows through a surface, e.g. the cross-section of a pipeline. Eq. 18, also called continuity equation, expresses the fact that the fluid conserves the mass, so the rate at which it enters a volume is balanced by the rate at which it leaves it.

We are interested in solutions of eq. 18 (or eq. 3) such that

$$\frac{\partial \rho_t}{\partial t} = 0\,, \tag{20}$$

then we require that

$$\frac{\partial J_t}{\partial t} = 0\,. \tag{21}$$

We distinguish two cases:

- Steady-state distributions $\rho_{ss}(x)$ such that

$$J(x) = \text{const.}, \tag{22}$$

- Equilibrium distribution $\pi(x)$ such that

$$J_t(x) = 0\,. \tag{23}$$

Steady-state distributions, or stationary distributions, describe distributions that do not change over time, but have a constant flux. Referring again to the example of fluids, a liquid that flows uniformly (e.g. by opening a tap), is a representation of a distribution that is stationary, but whose flux is not zero. To construct stationary distributions, it is necessary to introduce sources and sinks in the system. For example, Kramers, to construct his model, imagines a situation in which particles are created in the left well and removed once they reach the right well. This results in a constant flux $J(x)$ and a steady-state distribution $\rho_{ss}(x)$ that does not change over time.

Instead, equilibrium distributions, represent situations where the distribution does not change over time and there is no mass transport, then the flux is zero. For example, a basin in which the liquid relaxes until it homogeneously occupies all available space and no macroscopic movement takes place.

Setting $J(x,t) = 0$ in eq. 19 and integrating with natural boundary conditions ($\pi(x) = 0$ at $\pm\infty$), one obtains

$$\pi(x) = \frac{\mathcal{N}}{D_2(x)} \exp\left(\int_{-\infty}^{x} \frac{D_1(x')}{D_2(x')})\, dx'\right)\,, \tag{24}$$

where $\mathcal{N}$ is a normalization constant.

The overdamped Langevin equation

A special case of eq. 1 is the overdamped Langevin equation, where the drift term is written as

$$D_1(x) = -\frac{1}{m\gamma(x)}\frac{dV(x)}{dx}\,, \tag{25}$$

where m is the mass of a particle, $\gamma(x)$ is a position dependent friction coefficient, and $V(x)$ is a smooth potential energy function, and the diffusion term is written as

$$D_2(x) = \frac{k_B T}{m\gamma(x)}\,. \tag{26}$$

Then the equilibrium distribution is written as

$$\pi(x) = \mathcal{N}\gamma(x)\exp\left(-\frac{1}{k_B T}V(x)\right)\,. \tag{27}$$

If the friction coefficient is a constant, then

$$\pi(x) = \mathcal{N}\exp\left(-\frac{1}{k_B T}V(x)\right)\,. \tag{28}$$

B. Reversibility

The zero-flux condition (eq. 23) is equivalent to the detailed balance condition

$$\pi(x)p_\tau(x,y) = \pi(y)p_\tau(y,x)\,, \tag{29}$$

where $\pi(x)$, $\pi(y)$ are equilibrium distributions and $p_\tau(x,y)$, $p_\tau(y,x)$ are conditional probabilities. The detailed balance condition expresses the fact that, at the equilibrium described by the distribution $\pi(x)$, the average number of microscopic transitions (i.e. solution trajectories of eq. 1) from a state x to a state y is equal to the average number of transitions in the opposite direction. If this condition is fulfilled, then we say that the system is reversible. Note, that the reversibility condition is more general than the time-reversibility condition. For example, Hamiltonian dynamics is time-reversible, Langevin dynamics is reversible, but not time-reversible.

Under the reversibility condition, the operators $\mathcal{Q}^*$, $\mathcal{Q}$, $\mathcal{P}_\tau$ and $\mathcal{K}_\tau$ satisfy the following properties:

1. Self-adjointness relationships

$$\langle \mathcal{Q}^* f, g \rangle_{\pi^{-1}} = \langle f, \mathcal{Q}^* g \rangle_{\pi^{-1}} \,, \tag{30}$$

$$\langle \mathcal{Q} f, g \rangle_{\pi} = \langle f, \mathcal{Q} g \rangle_{\pi} \,, \tag{31}$$

$$\langle \mathcal{P}_\tau f, g \rangle_{\pi^{-1}} = \langle f, \mathcal{P}_\tau g \rangle_{\pi^{-1}} \,, \tag{32}$$

and

$$\langle \mathcal{K}_\tau f, g \rangle_{\pi} = \langle f, \mathcal{K}_\tau g \rangle_{\pi} \,, \tag{33}$$

where we defined the weighted scalar products

$$\langle f, g \rangle_{\pi} = \int_\Gamma f(x) g(x)\, \pi(x) dx \,, \tag{34}$$

and

$$\langle f, g \rangle_{\pi^{-1}} = \int_\Gamma f(x) g(x)\, \pi^{-1}(x) dx \,, \tag{35}$$

2. Spectral decomposition

$$\mathcal{Q}^* \varphi_i(x) = \kappa_i \varphi_i(x) \,, \tag{36}$$

$$\mathcal{Q} \psi_i(x) = \kappa_i \psi_i(x) \,, \tag{37}$$

$$\mathcal{P}_\tau \varphi_i(x) = \lambda_i(\tau)_i \varphi_i(x) \,, \tag{38}$$

and

$$\mathcal{K}_\tau \psi_i(x) = \lambda_i(\tau)_i \psi_i(x) \,. \tag{39}$$

- The eigenfunctions form orthonormal basis:

$$\langle \varphi_i, \varphi_j \rangle_{\pi^{-1}} = \delta_{ij} \,, \tag{40}$$

$$\langle \psi_i, \psi_j \rangle_{\pi} = \delta_{ij} \,, \tag{41}$$

- The first eigenfunctions are

$$\varphi_0(x) = \pi(x)\,, \tag{42}$$

$$\psi_0(x) = 1\,, \tag{43}$$

- The eigenfunctions are related by

$$\varphi_i(x) = \psi_i(x)\pi(x)\,. \tag{44}$$

- Eigenvalues are real:

$$\kappa_0 = 0 > \kappa_1 \geq \kappa_2 \geq \cdots > -\infty\,, \tag{45}$$

$$\lambda_0(\tau) = 1 > \lambda_1(\tau) \geq \lambda_2(\tau) \geq \cdots > 0\,. \tag{46}$$

- The eigenvalues $\lambda_i(\tau)$ and κ_i are related by

$$\lambda_i(\tau) = \exp(\tau\kappa_i)\,. \tag{47}$$

We can write solutions of eq. 3 as

$$\rho_{t+\tau}(x) = \sum_{i=0}^{\infty} \lambda_i(\tau)\varphi_i(x) \tag{48}$$

$$= \sum_{i=0}^{\infty} \exp(\tau\kappa_i)\varphi_i(x) \tag{49}$$

$$= \pi(x) + \sum_{i=1}^{\infty} \exp(\tau\kappa_i)\varphi_i(x)\,, \tag{50}$$

and eq. 8 as

$$f_{t+\tau}(x) = \sum_{i=0}^{\infty} \lambda_i(\tau)\psi_i(x) \tag{51}$$

$$= \sum_{i=0}^{\infty} \exp(\tau\kappa_i)\psi_i(x) \tag{52}$$

$$= 1 + \sum_{i=1}^{\infty} \exp(\tau\kappa_i)\psi_i(x)\,. \tag{53}$$

These representations of the solutions of eqs. 3 and 8 express the fact that the dynamics of the system can be decomposed into eigenmodes that at infinite time decay and the solutions converge to the equilibrium distribution. The eigenvalues κ_i have a physical interpretation, they are the rates at which the eigenmodes decay. Equivalently, we can introduce the time scales at which the eigenmodes occur:

$$t_i = -\frac{1}{\kappa_i} = -\frac{\tau}{\log[\lambda_i(\tau)]}\,. \tag{54}$$

C. Ergodicity

If the drift and the diffusion terms $D_1(x)$ and $D_2(x)$ in eq. 1 are smooth functions, then the system is ergodic:

- There are no two subsets of the space Γ dynamically disconnected.
- After an infinite time, each state $x \in \Gamma$ will be visited an infinite number of times proportional to $\pi(x)$.
- The equilibrium distribution $\pi(x)$ is unique.
- Time average are equal to ensemble average:

$$\bar{f}(x) = \mathbb{E}[f(x)] \tag{55}$$

$$\lim_{t\to\infty} \frac{1}{t}\int_0^t f(x_s)\,ds = \int_\Gamma f(x)\,\pi(x)dx\,. \tag{56}$$

D. Example

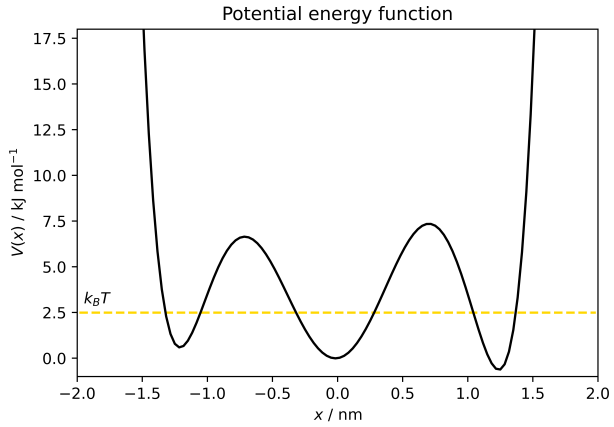

FIG. 1. Triple-well potential energy function.

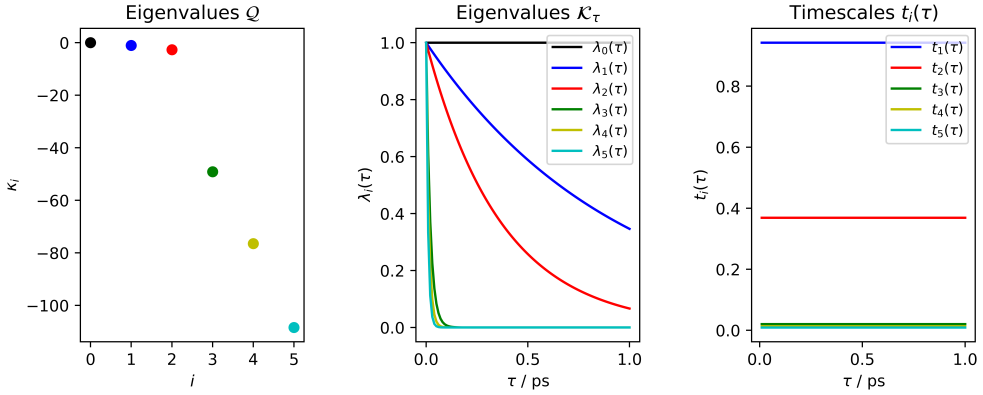

FIG. 2. Eigenvalues and timescales.

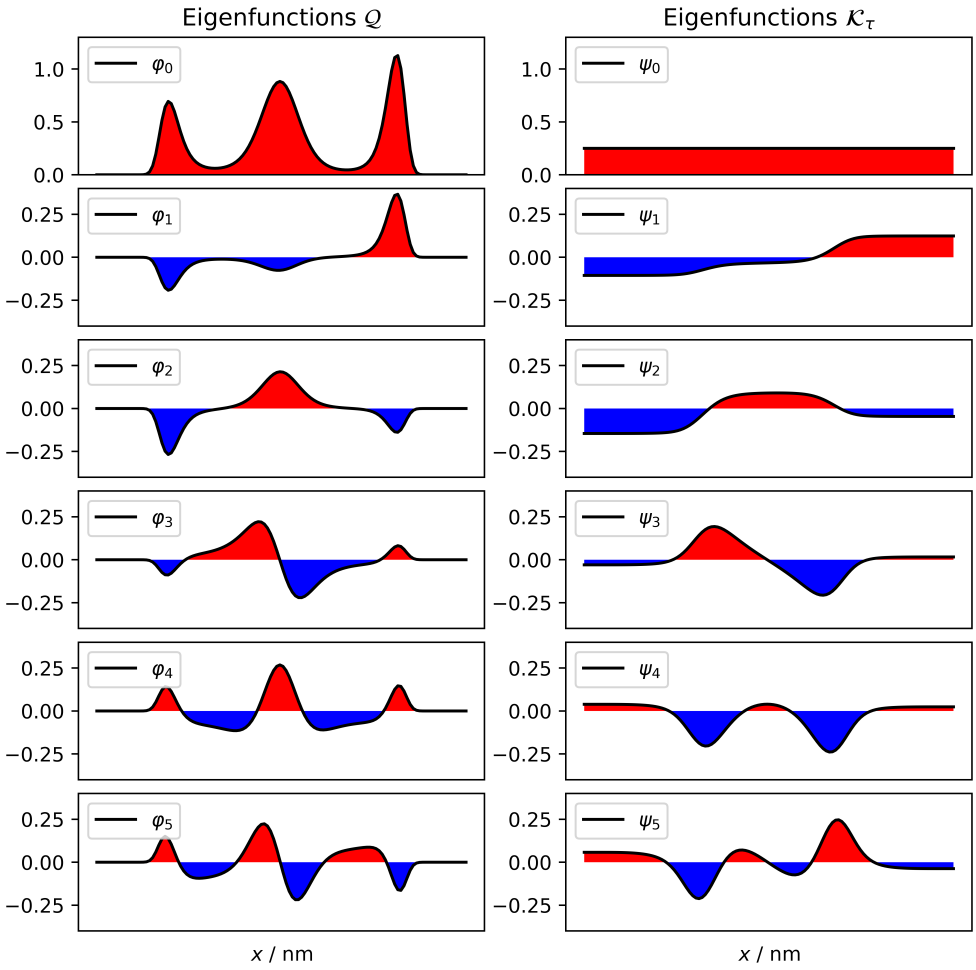

FIG. 3. Eigenfunctions.