Lecture 5

ISOKANN theory

CONTENTS

I. TRANSFER OPERATORS

A. Infinitesimal generator and Koopman operator

Given an observable function $f_t(x) \in L^\infty = \{f : \|f\|_\infty < \infty\}$ the infinitesimal generator $\mathcal{Q}$ acts on $f_t(x)$ as

$$\frac{\partial f_t(x)}{\partial t} = \mathcal{Q} f_t(x) \,. \tag{1}$$

A formal solution of eq. 1 is written as

$$f_{t+\tau}(x) = \exp\left(\mathcal{Q}\,\tau\right) f_t(x) \tag{2}$$

$$= \mathcal{K}_\tau f_t(x) \,, \tag{3}$$

where $\mathcal{K}_\tau$ is the Koopman operator.

1. *Spectral decomposition*

The operators $\mathcal{Q}$ and K have eigenfunctions and eigenvalues that solve the eigenproblems

$$\mathcal{Q}\psi_i(x) = \kappa_i \psi_i(x)\,, \tag{4}$$

and

$$\mathcal{K}_\tau \psi_i(x) = \lambda_i(\tau)\psi_i(x)\,. \tag{5}$$

Eigenfunctions and eigenvalues satisfy the following properties

- The eigenfunctions form orthonormal basis:

$$\langle \psi_i, \psi_j \rangle_\pi = \delta_{ij}\,, \tag{6}$$

- The first eigenfunction is

$$\psi_0(x) = 1\,, \tag{7}$$

- Eigenvalues are real:

$$\kappa_0 = 0 > \kappa_1 \geq \kappa_2 \geq \cdots > -\infty\,, \tag{8}$$

$$\lambda_0(\tau) = 1 > \lambda_1(\tau) \geq \lambda_2(\tau) \geq \cdots > 0\,. \tag{9}$$

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

$$\lambda_i(\tau) = \exp(\tau\kappa_i)\,. \tag{10}$$

II. MEMBERSHIP FUNCTIONS BY PCCA+

Consider a system with two metastable macro-states as in fig. 1, the membership functions are written as

$$\begin{cases} \chi_0(x) = \dfrac{\max_x \psi_1(x)}{\max_x \psi_1(x) - \min_x \psi_1(x)} - \dfrac{\psi_1(x)}{\max_x \psi_1(x) - \min_x \psi_1(x)}\,, \\ \chi_1(x) = \dfrac{\psi_1(x)}{\max_x \psi_1(x) - \min_x \psi_1(x)} - \dfrac{\min_x \psi_1(x)}{\max_x \psi_1(x) - \min_x \psi_1(x)} = 1 - \chi_0(x)\,. \end{cases} \tag{11}$$

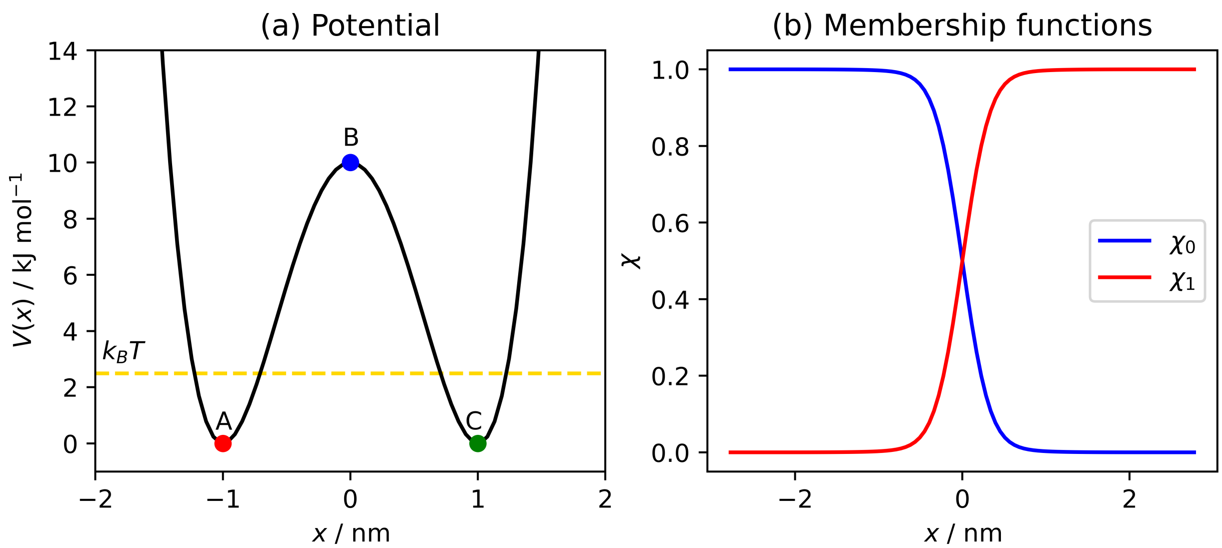

FIG. 1. System with two metastable macro-states.

III. ISOKANN THEORY

In this section, we derive the main equations described in Ref. [1].

A. ISOKANN equation

From now on, we consider just one membership function, and will use the notation

$$\chi := \chi_0(x) = c_0 + c_1\psi_1\,, \tag{12}$$

with

$$\begin{cases} c_0 = \dfrac{\max_x \psi_1(x)}{\max_x \psi_1(x) - \min_x \psi_1(x)} \\ c_1 = -\dfrac{1}{\max_x \psi_1(x) - \min_x \psi_1(x)}\,. \end{cases} \tag{13}$$

Note that $c_0 > 0$ and $c_1 < 0$. Additionally, we rewrite ψ_1 as function of χ:

$$\psi_1 = \frac{\chi}{c_1} - \frac{c_0}{c_1}\,. \tag{14}$$

Applying the operator $\mathcal{Q}$ to the membership function yields

$$\mathcal{Q}\chi = \mathcal{Q}\left(c_0\psi_0 + c_1\psi_1\right) \tag{15}$$

$$= c_0\kappa_0\psi_0 + c_1\kappa_1\psi_1 \tag{16}$$

$$= c_1\kappa_1\psi_1\,. \tag{17}$$

We insert eq. 14 into eq. 17 and we obtain

$$\begin{aligned}
\mathcal{Q}\chi &= \kappa_1\chi - c_0\kappa_1 && (18)\\
&= \kappa_1\chi - c_0\kappa_1 + c_0\kappa_1\chi - c_0\kappa_1\chi && (19)\\
&= \kappa_1\chi(1-c_0) - c_0\kappa_1(1-\chi)\,. && (20)
\end{aligned}$$

or

$$\mathcal{Q}\chi = -\epsilon_1\chi + \epsilon_2(1-\chi)\,, \tag{21}$$

with

$$\begin{cases}\epsilon_1 = -\kappa_1(1-c_0) > 0\\ \epsilon_2 = -c_0\kappa_1 > 0\end{cases}, \tag{22}$$

where the signs are chosen such that ϵ_1 and ϵ_2 are positive. Note that ϵ_1 and ϵ_2 have units $[\text{time}]^{-1}$.

Using the definition of infinitesimal generator in eq. 1, eq. 21 is rewritten as

$$\boxed{\dot{\chi} = -\epsilon_1\chi + \epsilon_2(1-\chi)\,,} \tag{23}$$

with $\dot{\chi} = {}^{d\chi}/_{dt}$. Eq. 23 is known as ISOKANN equation, it is a rate equation, and describes the time evolution of χ. It depends on the parameters ϵ_1 and ϵ_2 which describe the reaction rates between the two metastable macro-states.

B. Holding probability

We now multiply by $e^{-\epsilon_1 t}$ eq. 21 and we obtain

$$\begin{aligned}
\mathcal{Q}\chi e^{-\epsilon_1 t} &= -\epsilon_1\chi e^{-\epsilon_1 t} + \epsilon_2(1-\chi)e^{-\epsilon_1 t} && (24)\\
&= -\epsilon_1\chi e^{-\epsilon_1 t} + \epsilon_2\frac{1-\chi}{\chi}\chi e^{-\epsilon_1 t}\,. && (25)
\end{aligned}$$

Introducing the quantity

$$p_\chi := p_\chi(x,t) = \chi(x)e^{-\epsilon_1 t}\,, \tag{26}$$

we obtain

$$\mathcal{Q}p_\chi = -\epsilon_1 p_\chi + \epsilon_2\frac{1-\chi}{\chi}p_\chi\,, \tag{27}$$

or

$$-\epsilon_1 p_\chi = \mathcal{Q} p_\chi - \epsilon_2 \frac{1-\chi}{\chi} p_\chi \,, \tag{28}$$

The quantity p_χ introduced in eq. 26 is solution of the ordinary equation

$$\frac{\partial p_\chi}{\partial t} = -\epsilon_1 p_\chi \,, \tag{29}$$

with initial condition

$$p_\chi(x, 0) = \chi(x) \,. \tag{30}$$

Then, comparing eq. 29 with eq. 28, we obtain

$$\frac{\partial p_\chi}{\partial t} = \mathcal{Q} p_\chi - \epsilon_2 \frac{1-\chi}{\chi} p_\chi \tag{31}$$

Applying the Feynman-Kac formula (see Appendix 1), we obtain a solution for eq. 31

$$p_\chi(x,t) = \mathbb{E}\left[\chi(X_t) \exp\left(-\epsilon_2 \int_0^t \frac{1-\chi(X_s)}{\chi(X_s)}\, ds\right)\right]_{x_0=x} \,. \tag{32}$$

Eq. 32 is analogous to

$$p_{\mathbb{1}_S}(x,t) = \mathbb{E}\left[\mathbb{1}_S(X_t) \delta_0 \left(\int_0^t \left(1 - \mathbb{1}_S(x_s)\right)\, ds\right)\right]_{x_0=x} \,, \tag{33}$$

with

$$\mathbb{1}_S(x) = \begin{cases} 1 & \text{if } \; x \in S \;, \\ 0 & \text{if } \; x \notin S \;, \end{cases} \tag{34}$$

and

$$\delta_0(x) = \begin{cases} 1 & \text{if } \; x = 0, \\ 0 & \text{if } \; x \neq 0 \,. \end{cases} \tag{35}$$

Eq. 33 describes the holding probability of the subset $S \subset \Gamma$, i.e. the percentage of solutions of the Langevin equation starting in $x_0 = x$ which have never left the subset S until time t.

From this analogy, we conclude that the quantity $p_\chi(x,t)$ describes the χ-holding probability of the fuzzy set identified by the membership function χ.

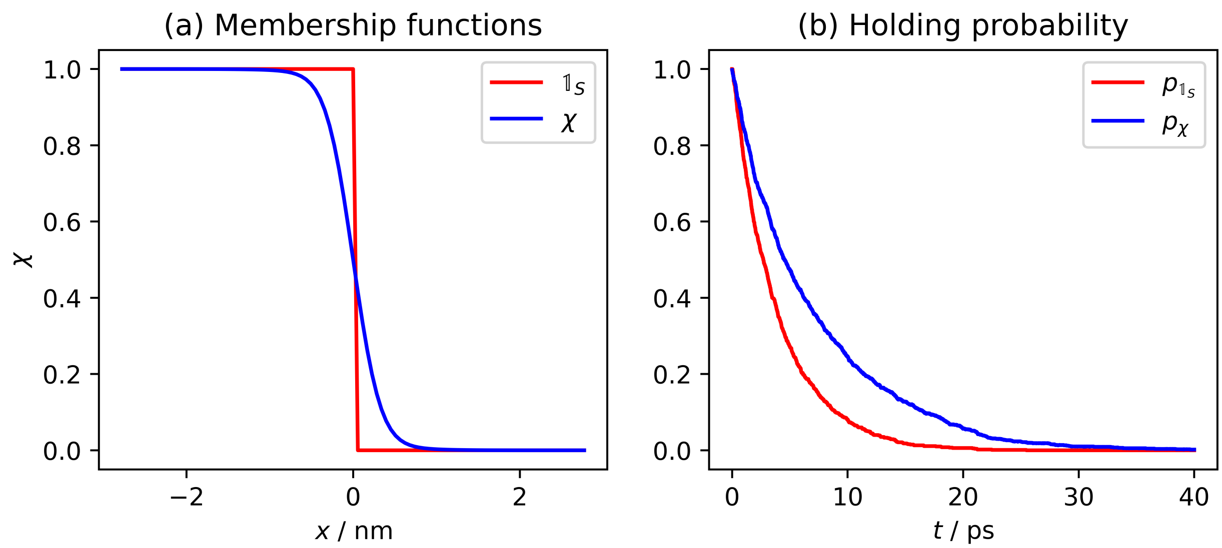

FIG. 2. Holding probabilities.

C. Mean holding time

The mean holding time, or mean first passage time (MFPT), is calculated from the holding probability as

$$\langle \tau_{fp}(x) \rangle \int_0^\infty p_{\mathbb{1}_S}(x, s)\, ds \,, \tag{36}$$

solution of backward Kolmogorov equation

$$\mathcal{Q} \langle \tau_{fp}(x) \rangle = -1 \,. \tag{37}$$

Then, the mean holding time for the membership function is

$$\langle \tau_\chi(x) \rangle = \int_0^\infty p_\chi(x, s)\, ds \,, \tag{38}$$

Solving the integral with p_χ as defined in eq. 26, we obtain

$$\boxed{\langle \tau_\chi(x) \rangle = \frac{\chi(x)}{\epsilon_1} \,,} \tag{39}$$

solution of

$$\boxed{\mathcal{Q} \langle \tau_\chi(x) \rangle = \mathcal{Q} \frac{\chi(x)}{\epsilon_1} = -\chi + \frac{\epsilon_2}{\epsilon_1}(1 - \chi) \,,} \tag{40}$$

where we used the isokann equation defined in eq. 21.

D. Calculation of rates

In order to find an expression to determine the rates ϵ_1 and ϵ_2, we transform the ISOKANN equation, written in terms of the infinitesimal generator, into an equation that depends on the Koopman operator.

First, we rewrite eq. 21 as

$$\mathcal{Q}\chi = -\epsilon_1\chi + \epsilon_2 - \epsilon_2\chi \tag{41}$$

$$= -(\epsilon_1 + \epsilon_2)\chi + \epsilon_2 \tag{42}$$

$$= \alpha\chi + \beta\,, \tag{43}$$

with

$$\begin{cases} \alpha = -(\epsilon_1 + \epsilon_2) \\ \beta = \epsilon_2\,. \end{cases} \tag{44}$$

We multiply eq. 43 by τ:

$$\tau\mathcal{Q}\chi = \tau\alpha\chi + \tau\beta\,, \tag{45}$$

and we apply again $\tau\mathcal{Q}$ to the equation:

$$\tau\mathcal{Q}\left(\tau\mathcal{Q}\chi\right) = \tau\mathcal{Q}\left(\tau\alpha\chi + \tau\beta\right) \tag{46}$$

$$= \tau^2\alpha^2\chi + \tau^2\alpha\beta\,. \tag{47}$$

Applying i times $\tau\mathcal{Q}$, we obtain

$$\left(\tau\mathcal{Q}\right)^i\chi = \left(\tau\alpha\right)^i\chi + \tau^i\alpha^{i-1}\beta\,. \tag{48}$$

Next, we divide by $i!$:

$$\frac{\left(\tau\mathcal{Q}\right)^i\chi}{i!} = \frac{\left(\tau\alpha\right)^i}{i!}\chi + \frac{\tau^i\alpha^{i-1}\beta}{i!} \tag{49}$$

$$= \frac{\left(\tau\alpha\right)^i}{i!}\chi + \frac{\tau^i\alpha^i}{i!}\frac{\beta}{\alpha}\,. \tag{50}$$

Summing from 1 to ∞, we obtain the series of the exponential function:

$$\sum_{i=1}^{\infty}\frac{\left(\tau\mathcal{Q}\right)^i\chi}{i!} = \sum_{i=1}^{\infty}\frac{\left(\tau\alpha\right)^i}{i!}\chi + \sum_{i=1}^{\infty}\frac{\tau^i\alpha^i}{i!}\frac{\beta}{\alpha} \tag{51}$$

$$. \tag{52}$$

We add χ on both sides:

$$\sum_{i=1}^{\infty}\frac{(\tau\mathcal{Q})^i\chi}{i!}+\chi=\sum_{i=1}^{\infty}\frac{(\tau\alpha)^i}{i!}\chi+\chi+\sum_{i=1}^{\infty}\frac{\tau^i\alpha^i}{i!}\frac{\beta}{\alpha} \tag{53}$$

$$\sum_{i=0}^{\infty}\frac{(\tau\mathcal{Q})^i\chi}{i!}=\sum_{i=0}^{\infty}\frac{(\tau\alpha)^i}{i!}\chi+\sum_{i=1}^{\infty}\frac{\tau^i\alpha^i}{i!}\frac{\beta}{\alpha} \tag{54}$$

$$. \tag{55}$$

Then we change the index of the last series and we subtract the term β/α:

$$\sum_{i=0}^{\infty}\frac{(\tau\mathcal{Q})^i\chi}{i!}=\sum_{i=0}^{\infty}\frac{(\tau\alpha)^i}{i!}\chi+\sum_{i=0}^{\infty}\frac{\tau^i\alpha^i}{i!}\frac{\beta}{\alpha}-\frac{\beta}{\alpha}\,. \tag{56}$$

Finally we have:

$$\exp(\tau\mathcal{Q})\,\chi=e^{\tau\alpha}\chi+\frac{\beta}{\alpha}(e^{\tau\alpha}-1) \tag{57}$$

$$\mathcal{K}_\tau\chi=e^{\tau\alpha}\chi+\frac{\beta}{\alpha}(e^{\tau\alpha}-1) \tag{58}$$

$$=a_1\chi+a_2\,, \tag{59}$$

with

$$\begin{cases} a_1=e^{\tau\alpha}\\ a_2=\dfrac{\beta}{\alpha}(e^{\tau\alpha}-1)\,, \end{cases} \tag{60}$$

Let's imagine to solve the linear regression problem

$$\min_{a_1,a_2}\|\mathcal{K}_\tau\chi(x)-a_1\chi(x)-a_2\|, \tag{61}$$

then, using eqs. 44 and 60, the rate is calculated as

$$\boxed{\epsilon_1=-\frac{1}{\tau}\log(a_1)\left(1+\frac{a_2}{a_1-1}\right)\,.} \tag{62}$$

Appendix A: Feynman-Kac formula

Consider the parabolic partial differential equation

$$\frac{\partial u}{\partial t}=Gu+Vu\,, \tag{A1}$$

where G and V are two functions, with initial condition

$$u(x,0)=f(x)\,, \tag{A2}$$

then the solution is written as

$$u(x,t) = \mathbb{E}\left[f(X_t) \exp\left(\int_0^t V(X_0)\, ds \right) \right]_{x_s = x} , \tag{A3}$$

where X_t are solutions of the Langevin equations.

See Ref. [2] for more details.

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[1] M. Weber and N. Ernst, A fuzzy-set theoretical framework for computing exit rates of rare events in potential-driven diffusion processes, arXiv preprint arXiv:1708.00679 (2017).

[2] H. Gzyl, The feynman-kac formula and the hamilton-jacobi equation, J. Math. Anal. Appl. **142**, 74 (1989).