1 Lyapunov Function

Notation 1. *Overall notations in this section are:*

- $\mathcal{M}$ *a manifold, and* μ *its measure, e.g.* $\mu(x) = \sqrt{g(x)}$ *if* $\mathcal{M}$ *is Riemannian with metric* g_{ab}*;*
- *if* $p(x)$ *the distribution of random variable* X*, then*

$$\langle f\rangle_p = \langle f\rangle_X := \int_{\mathcal{M}} \mathrm{d}\mu(x)\, p(x)\, f(x);$$

- *if* D *is a set of samples, then*

$$\langle f\rangle_D := \frac{1}{|D|}\sum_{x\in D} f(x);$$

- *let* $\mathcal{N}(\mu,\sigma)$ *denotes normal distribution with mean* μ *and standard derivative* σ*;*
- *given function* g*, let* $f\{g\}$*, or* $f_{\{g\}}$*, denote a function constructed out of* g*, that is,*

$$f\{\cdot\}\colon (\mathcal{M}\to A)\to(\mathcal{M}\to B).$$

1.1 Relaxation

Next, we illustrate how, during a non-equilibrium process, a distribution p relaxes to its stationary distribution q, and how this process relates to the variational inference. Further, we try to find the most generic dynamics that underlies the non-equilibrium to equilibrium process, on both macroscopic (distribution) and microscopic ("particle") viewpoints.

First, we shall define what relaxation is, via free energy.

Definition 2. [*Free Energy*]

Let $E(x)\colon \mathcal{M}\to\mathbb{R}$*. Define stationary distribution*

$$q_E(x) := \frac{\exp(-E(x)/T)}{Z},$$

where $T>0$ *and* $Z := \int_{\mathcal{M}} \mathrm{d}\mu(x)\exp(-E(x)/T)$*. Given* E*, for any time-dependent distribution* $p(x,t)$*, define free energy as*

$$F_E[p(\cdot,t)] := T D_{\mathrm{KL}}(p\|q_E) - T\ln Z = T\int_{\mathcal{M}} \mathrm{d}\mu(x)\, p(x,t)\ln\frac{p(x,t)}{q_E(x)} - T\ln Z.$$

Or, equivalently,

$$F_E[p(\cdot,t)] := \langle E\rangle_{p(\cdot,t)} - TH[p(\cdot,t)],$$

where entropy functional $H[p(\cdot,t)] := \langle -\ln p(\cdot,t)\rangle_p$*.*

Definition 3. [*Relaxation*]

For a time-dependent distribution $p(x,t)$ *on* $\mathcal{M}$*, we say* p *relaxes to* q_E *if and only if the free energy* $F_E[p(\cdot,t)]$ *monotonically decreases to its minimum, where* $p(\cdot,t) = q_E$*.*

We can visualize this relaxation process by an imaginary ensemble of juggling "particles" (or "bees"). Initially, they are arbitrarily positioned. This forms a distribution of "particles" p. With some underlying dynamics, these "particles" moves and finally the distribution relaxes, if it can, to a stationary distribution q_E. Apparently, the underlying dynamics and the E are correlated. We first provide a way of peeping the underlying dynamics, that is, the "flux".

Theorem 4. [*Conservation of "Mass"*]

For any time-dependent distribution $p(x,t)$*, there exists a "flux"* $f^a\{p\}(x,t)$ *s.t.*

$$\frac{\partial p}{\partial t}(x,t) + \nabla_a(f^a\{p\}(x,t)\, p(x,t)) = 0.$$

What is the dynamics of p by which any initial p will finally relax to q_E? That is, what is the sufficient (and essential) condition of relaxing to q_E for any p? Because of the conservation of "mass", the dynamics of p, i.e. $\partial p/\partial t$, is determined by a "flux", f^a. Thus, this sufficient (and essential) condition must be about the f^a.

Lemma 5. *Given p and (x,t), for any $f^a\{p\}(x,t)$, we can always construct a $K^{ab}\{p\}(x,t)$ s.t.*

$$f^a\{p\}(x,t) = -K^{ab}\{p\}(x,t)\,\nabla_b\{T\ln p(x,t) + E(x)\}.$$

Proof. For any vector f^a and v_a, we can always construct a tensor K^{ab} s.t. $f^a = K^{ab}v_b$. Indeed, we can rotate v_a to the direction of f^a and then dimension-wise recale to f^a. This rotation and dimension-wise rescaling compose the linear transform K^{ab}. Now, letting

$$v_a = -\nabla_a\{T\ln p(x,t) + E(x)\},$$

we arrive at the conclusion. □

Now, we claim a sufficient condition of relaxing to q_E for any p.

Theorem 6. [*Fokker-Planck Equation*]

If the symmetric part of $K^{ab}\{p\}(x,t)$ is positive definite for any p and (x,t), then any p evolves by this "flux" will relax to q_E.

Proof. Directly

$$\begin{aligned}\frac{\mathrm{d}F_E}{\mathrm{d}t}[p(\cdot,t)] &= T\int_{\mathcal{M}}\mathrm{d}\mu(x)\,\frac{\partial p}{\partial t}(x,t)\left[\ln\frac{p(x,t)}{q(x)}+1\right]\\ \{\text{Conservation of mass}\} &= -T\int_{\mathcal{M}}\mathrm{d}\mu(x)\,\nabla_a[f^a\{p\}(x,t)\,p(x,t)]\left[\ln\frac{p(x,t)}{q(x)}+1\right].\end{aligned}$$

Since

$$\nabla_a[f^a\{p\}(x,t)\,p(x,t)]\left[\ln\frac{p(x,t)}{q(x)}+1\right] = \nabla_a\left\{[f^a\{p\}(x,t)\,p(x,t)]\left[\ln\frac{p(x,t)}{q(x)}+1\right]\right\} - [f^a\{p\}(x,t)\,p(x,t)]\nabla_a\left[\ln\frac{p(x,t)}{q(x)}+1\right],$$

we have

$$\begin{aligned}\frac{\mathrm{d}F_E}{\mathrm{d}t}[p(\cdot,t)] &= -T\int_{\mathcal{M}}\mathrm{d}\mu(x)\,\nabla_a[f^a\{p\}(x,t)\,p(x,t)]\left[\ln\frac{p(x,t)}{q(x)}+1\right]\\ &= -T\int_{\mathcal{M}}\mathrm{d}\mu(x)\,\nabla_a\left\{[f^a\{p\}(x,t)\,p(x,t)]\left[\ln\frac{p(x,t)}{q(x)}+1\right]\right\} + T\int_{\mathcal{M}}\mathrm{d}\mu(x)\,[f^a\{p\}(x,t)\,p(x,t)]\nabla_a\left[\ln\frac{p(x,t)}{q(x)}+1\right]\\ \{\text{Divergence theorem}\} &= -T\int_{\partial\mathcal{M}}\mathrm{d}S_a\,p(x,t)\,f^a\{p\}(x,t)\left[\ln\frac{p(x,t)}{q(x)}+1\right] + T\int_{\mathcal{M}}\mathrm{d}\mu(x)\,p(x,t)\,f^a\{p\}(x,t)\nabla_a\left[\ln\frac{p(x,t)}{q(x)}+1\right]\end{aligned}$$

The first term vanishes.[1] Then, direct calculus shows

$$\begin{aligned}\frac{\mathrm{d}F_E}{\mathrm{d}t}[p(\cdot,t)] &= T\int_{\mathcal{M}}\mathrm{d}\mu(x)\,p(x,t)\,f^a\{p\}(x,t)\nabla_a\left[\ln\frac{p(x,t)}{q(x)}+1\right]\\ &= T\int_{\mathcal{M}}\mathrm{d}\mu(x)\,p(x,t)\,f^a\{p\}(x,t)[\nabla_a\ln p(x,t) - \nabla_a\ln q(x)]\\ \{q(x) := \cdots\} &= \int_{\mathcal{M}}\mathrm{d}\mu(x)\,p(x,t)\,f^a\{p\}(x,t)[T\nabla_a\ln p(x,t) + \nabla_a E(x)]\\ &= \int_{\mathcal{M}}\mathrm{d}\mu(x)p(x,t)\,f^a\{p\}(x,t)\,\nabla_a\{T\ln p(x,t) + E(x)\}.\end{aligned}$$

By the previous lemma, we have

$$\begin{aligned}\frac{\mathrm{d}F_E}{\mathrm{d}t}[p(\cdot,t)] &= \int_{\mathcal{M}}\mathrm{d}\mu(x)p(x,t)\,f^a\{p\}(x,t)\,\nabla_a\{T\ln p(x,t) + E(x)\}\\ \{f^a = \cdots\} &= -\int_{\mathcal{M}}\mathrm{d}\mu(x)p(x,t)K^{ab}\{p\}(x,t)\,\nabla_a\{T\ln p(x,t) + E(x)\}\,\nabla_b\{T\ln p(x,t) + E(x)\}.\end{aligned}$$

Letting $S^{ab} := (K^{ab} + K^{ba})/2$ and $A^{ab} := (K^{ab} - K^{ba})/2$, we have $K^{ab} = S^{ab} + A^{ab}$, where S^{ab} is symmetric and A^{ab} anti-symmetric. Then,

$$\begin{aligned}\frac{\mathrm{d}F_E}{\mathrm{d}t}[p(\cdot,t)] &= -\int_{\mathcal{M}}\mathrm{d}\mu(x)p(x,t)[S^{ab}\{p\}(x,t) + A^{ab}\{p\}(x,t)]\,\nabla_a\{T\ln p(x,t) + E(x)\}\,\nabla_b\{T\ln p(x,t) + E(x)\}\\ \{A^{ab} = A^{ba}\} &= -\int_{\mathcal{M}}\mathrm{d}\mu(x)p(x,t)S^{ab}\{p\}(x,t)\,\nabla_a\{T\ln p(x,t) + E(x)\}\,\nabla_b\{T\ln p(x,t) + E(x)\}.\end{aligned}$$

The condition claims that $S^{ab}\{p\}(x,t)$ is positive definite for any p and (x,t). Then, the integrad is a positive definite quadratic form, being positive if and only if $\nabla_a\{T\ln p(x,t) + E(x)\} \neq 0$. Then, we find $(\mathrm{d}F_E/\mathrm{d}t)[p(\cdot,t)] < 0$ as long as $\nabla_a\{T\ln p(x,t) + E(x)\} \neq 0$ at some x, i.e. $p \neq q$, and $(\mathrm{d}F_E/\mathrm{d}t)[p(\cdot,t)] = 0$ if and only if $\nabla_a\{T\ln p(x,t) + E(x)\} = 0$ for $\forall x$, i.e. $p = q$. Thus proof ends. □

Remark 7. [Sufficent but Not Essential]

However, this is not an essntial condition of relaxing to q_E for any p. Indeed, we proved the integrand of $(\mathrm{d}F_E/\mathrm{d}t)[p(\cdot,t)]$ is negative everywhere, which implies the integral, i.e. $(\mathrm{d}F_E/\mathrm{d}t)[p(\cdot,t)]$, is negative. But, we cannot exclude the case where the integrand is not negative everywhere, whereas the integral is still negative. During the proof, this is the only place that leads to the non-essential-ness, which is hard to overcome.

1. To-do: Explain the reason explicitly.

As the dynamics of distribution is a macroscopic viewpoint, the microscopic viewpoint, i.e. the stochastic dynamics of single "particle", is as follow.

Theorem 8. [*Langevin Equation*]

If K^{ab} is symmetric, then TODO

$$\mathrm{d}x^a = K^{ab}(x,t)\,\nabla_b E(x)\,\mathrm{d}t + \sqrt{2T}\,\mathrm{d}W^a(x,t),$$

where

$$\langle \mathrm{d}W^a(x,t)\,\mathrm{d}W^b(x,t)\rangle_{\mathrm{d}W} = K^{ab}(x,t).$$

Question 1. Given a Langevin-like equaiton, how can we determine if there exists the E, or the stationary distribution q_E?

Question 2. Further, if it exists, then how can we reveal it? Precisely, in the case $T \to 0$, given $(\mathrm{d}x^a/\mathrm{d}t) = h^a(x,t)$, how can we reconstruct the E and find a positive definite K^{ab}, s.t. $h^a(x) = K^{ab}(x,t)\nabla_b E(x)$?

1.2 Minimize Free Energy Principle

In the real world, there can be two types of variables: ambient and latent. The ambient variables are those observed directly, like sensory inputs or experimental observations. While the latent are usually more simple and basic aspects, like wave-function in QM.

We formulate the E as a funciton of $(v,h) \in \mathcal{V}\times\mathcal{H}$, where v, for visible, represents the ambient and h, for hidden, represents the latent. Then we have

Lemma 9. [*Conditional Free Energy*]

Given v, if define

$$Z(v) := \int_{\mathcal{H}} \mathrm{d}h \exp(-E(v,h)/T),$$

then we have a (conditional) free energy of distribution $p(h)$

$$\begin{aligned} F_E[p|v] &:= TD_{\mathrm{KL}}(p\|q_E(\cdot|v)) - T\ln Z(v) \\ &= \langle E(v,\cdot)\rangle_p - TH[p]. \end{aligned}$$

Ansatz 10. [*Minimize Free Energy Principle*]

Let $p(h)$ the latent distribution. On one hand, we want to locate it to the minimum of E. That is, given the ambient v, we want to minimize $\langle E(v,\cdot)\rangle_p$, where we have marginalized the latent. On the other hand, we shall keep the minimal prior knowledge on the latent, that is, maximize $H[p]$. So, we minimize $\langle E(v,\cdot)\rangle_p - TH[p]$, where the positive constant T balances the two aspects. This happens to be the (conditional) free energy.

Lemma 11. *If E is in a function family parameterized by $\theta \in \mathbb{R}^N$, then we have*

$$\frac{\partial}{\partial\theta^\alpha}\{-T\ln Z(v)\} = \left\langle \frac{\partial E}{\partial\theta^\alpha}(v,\cdot)\right\rangle_{q_E(\cdot|v)}.$$

Thus, we propose an EM-like algorithm that minimizes the free energy, as

Theorem 12. [*Recall-and-Learn*]

To minimize free energy $F_E[p|v]$, we have two steps:

1. *minimize $\langle E(v,\cdot)\rangle_p - TH[p]$ by Langevin dynamics until relaxation, where $p = q_E(\cdot|v)$; then*
2. *minimize $-T\ln Z(v)$ by gradient descent and replacing $\langle(\partial E/\partial\theta^\alpha)(v,\cdot)\rangle_{q_E(\cdot|v)} \to \langle(\partial E/\partial\theta^\alpha)(v,\cdot)\rangle_p$.*

By repeating these two steps, we get smaller and smaller free energy.

For instance, in a brain, the first step can be illustrated as recalling, and the second as learning (searching for a more proper memory).

1.3 Example: Continuous Hopfield Network

Let $U^{\alpha\beta}$ and I^α constants, and L_v and L_h scalar functions. Define $f_\alpha(h) := \partial L_h/\partial h^\alpha$, $g_\alpha(v) := \partial L_v/\partial v^\alpha$. Then the deterministic version of continuous Hopfield network is

$$\frac{\mathrm{d}v^\alpha}{\mathrm{d}t} = U^{\alpha\beta} f_\beta(h) - v^\alpha + I^\alpha;$$
$$\frac{\mathrm{d}h^\alpha}{\mathrm{d}t} = (U^T)^{\alpha\beta} g_\beta(v) - h^\alpha,$$

where U describes the strength of connection between neurons, and f, g the activation functions of latent and ambient, respectively. Further, we have the E constructed as

$$E(v,h) = [(v^\alpha - I^\alpha)\, g_\alpha(v) - L_v(v)] + [h^\alpha f_\alpha(h) - L_h(h)] - U_{\alpha\beta}\, g^\alpha(v)\, f^\beta(h),$$

which implies

$$K = \begin{pmatrix} K_v & 0 \\ 0 & K_h \end{pmatrix},$$

where $K_v(v) = \partial^2 L_v(v)^{-1}$, $K_h(h) = \partial^2 L_h(h)^{-1}$. Then we find the stochastic version, as

$$\frac{\mathrm{d}v^\alpha}{\mathrm{d}t} = U^{\alpha\beta} f_\beta(h) - v^\alpha + I^\alpha + \sqrt{2T}\, \mathrm{d}W_v^\alpha(v);$$
$$\frac{\mathrm{d}h^\alpha}{\mathrm{d}t} = (U^T)^{\alpha\beta} g_\beta(v) - h^\alpha + \sqrt{2T}\, \mathrm{d}W_h^\alpha(h),$$

where

$$\langle \mathrm{d}W_v^\alpha(v)\, \mathrm{d}W_v^\alpha(v)\rangle = [\partial^2 L_v(v)^{-1}]^{\alpha\beta};$$
$$\left\langle \mathrm{d}W_h^\alpha(h)\, \mathrm{d}W_h^\beta(h)\right\rangle = [\partial^2 L_h(h)^{-1}]^{\alpha\beta}.$$

In addition, we find, along the gradient descent trajectory of U, the difference is

$$\Delta U^{\alpha\beta} \propto \left\langle -\frac{\partial E}{\partial U_{\alpha\beta}}(v,h)\right\rangle_{q_E(\cdot|v)} = \langle g^\alpha(v)\, f^\alpha(h)\rangle_{q_E(\cdot|v)}.$$

Since f and g are activation functions, we recover the Hebbian rule, that is, neurons that fire together wire together.

Appendix A Useful Lemmas

Lemma 13. [*Kramers–Moyal Expansion*]

Given random variable X and time parameter t, consider random variable ϵ whose distribution is (x,t)-dependent. After Δt, particles in position x jump to $x+\epsilon$. Then, we have

$$p(x,t+\Delta t) - p(x,t) = \sum_{n=1}^{+\infty} \frac{(-1)^n}{n!} \nabla_{a_1}\cdots\nabla_{a_n}[p(x,t) M^{a_1\cdots a_n}(x,t)]\,,$$

where $M^{a_1\cdots a_n}(x,t)$ represents the n-order moments of ϵ

$$M^{a_1\cdots a_n}(x,t) := \langle \epsilon^{a_1}\cdots\epsilon^{a_n}\rangle_\epsilon.$$

Proof. The trick is introducing a smooth test function, $h(x)$. Denote

$$I_{\Delta t}[h] := \int \mathrm{d}\mu(x)\, p(x,t+\Delta t) h(x). \qquad \square$$

The transition probability from x at t to y at $t+\Delta t$ is $\int \mathrm{d}\mu(\epsilon)\, p_\epsilon(\epsilon;x,t)\, \delta(x+\epsilon-y)$. This implies

$$p(y,t+\Delta t) = \int \mathrm{d}\mu(x)\, p(x,t) \left[\int \mathrm{d}\mu(\epsilon)\, p_\epsilon(\epsilon;x,t)\, \delta(x+\epsilon-y)\right].$$

With this,

$$\begin{aligned} I_{\Delta t}[h] &:= \int \mathrm{d}\mu(x)\, p(x,t+\Delta t) h(x) \\ \{x\to y\} &= \int \mathrm{d}\mu(y)\, p(y,t+\Delta t) h(y) \\ [p(y,t+\Delta t) = \cdots] &= \int \mathrm{d}\mu(x)\, p(x,t) \int \mathrm{d}\mu(y) \int \mathrm{d}\mu(\epsilon)\, p_\epsilon(\epsilon;x,t)\, \delta(x+\epsilon-y)\, h(y) \\ \{\text{Integrate over } y\} &= \int \mathrm{d}\mu(x)\, p(x,t) \int \mathrm{d}\mu(\epsilon)\, p_\epsilon(\epsilon;x,t)\, h(x+\epsilon). \end{aligned}$$

Taylor expansion $h(x+\epsilon)$ on ϵ gives

$$I_{\Delta t}[h] = \int \mathrm{d}\mu(x)\, p(x,t) h(x) + \sum_{n=1}^{+\infty} \frac{1}{n!} \int \mathrm{d}\mu(x)\, p(x,t)\, [\nabla_{a_1} \cdots \nabla_{a_n} h(x)] \int \mathrm{d}\mu(\epsilon)\, p_\epsilon(\epsilon; x, t)\, \epsilon^{a_1} \cdots \epsilon^{a_n}.$$

Integrating by part on x for the second term, we find

$$I_{\Delta t}[h] = \int \mathrm{d}\mu(x)\, p(x,t) h(x) + \sum_{n=1}^{+\infty} \frac{(-1)^n}{n!} \int \mathrm{d}\mu(x)\, h(x)\, \nabla_{a_1} \cdots \nabla_{a_n} \Big[p(x,t) \int \mathrm{d}\mu(\epsilon)\, p_\epsilon(\epsilon; x, t)\, \epsilon^{a_1} \cdots \epsilon^{a_n} \Big].$$

Denote n-order moments of ϵ as $M^{a_1 \cdots a_n}(x,t) \coloneqq \langle \epsilon^{a_1} \cdots \epsilon^{a_n} \rangle_\epsilon$ and recall the definition of $I_{\Delta t}[h]$, then we arrive at

$$\int \mathrm{d}\mu(x)\, [p(x, t+\Delta t) - p(x,t)]\, h(x) = \sum_{n=1}^{+\infty} \frac{(-1)^n}{n!} \int \mathrm{d}\mu(x)\, h(x)\, \nabla_{a_1} \cdots \nabla_{a_n} [p(x,t) M^{a_1 \cdots a_n}(x,t)].$$

Since $h(x)$ is arbitrary, we conclude that

$$p(x, t+\Delta t) - p(x,t) = \sum_{n=1}^{+\infty} \frac{(-1)^n}{n!} \nabla_{a_1} \cdots \nabla_{a_n} [p(x,t) M^{a_1 \cdots a_n}(x,t)].$$

Appendix B Stochastic Dynamics

B.1 Random Walk

The first step is omitting the deterministic part, considering the stochastic only. Given $\forall x \in \mathcal{M}$ and any time t, during a tiny time interval Δt, consider a list of i.i.d. random variables,

$$\{\varepsilon_i : i = 1 \ldots n\},$$

where, for $\forall i$, $\varepsilon_i \sim P$ for some distribution P, with the mean 0 and standard derivative $\sigma(x,t)$. This series of random walks leads to a difference $\Delta x \coloneqq \sum_{i=1}^{n} \varepsilon_i$. Notice that $\Delta t \propto n$, that is, longer time interval implies longer chain of random walk. With this, we can define

$$\sqrt{\Delta t}\, g(x,t) \coloneqq \lim_{n \to +\infty} \sqrt{n}\, \sigma(x,t).$$

If g exists, then by central limit theorem $\Delta x \sim \mathcal{N}(0, \sqrt{\Delta t}\, g(x,t))$. If define $\Delta W \sim \mathcal{N}(0, \sqrt{\Delta t})$, then $\Delta x = g(x,t)\, \Delta W$.

TODO