Lyapunov Function

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 covariance Σ ;
- given function g, let $f\{g\}$, or $f_{\{g\}}$, denote a function constructed out of g, that is,

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

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

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

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

$$F_{E}[p(\cdot,t)] := TD_{KL}(p||q_{E}) - T \ln Z = T \int_{\mathcal{M}} d\mu(x) \ p(x,t) \ln \frac{p(x,t)}{q_{E}(x)} - T \ln Z.$$

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".

Lemma 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 .

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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

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

Since

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

we have

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

The first term vanishes. 1 Then, direct calculus shows

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

By the previous lemma, we have

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

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} antisymmetric. Then,

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

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.

^{1.} To-do: Explain the reason explicitly.

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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 $(dF_E/dt)[p(\cdot,t)]$ is negative everywhere, which implies the integral, i.e. $(dF_E/dt)[p(\cdot,t)]$, 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.

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. [Stochastic Dynamics]

If K^{ab} is symmetric and independent of p, then Fokker-Planck equation is equivalent to the stochastic dynamics

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

where

$$dW \sim \mathcal{N}(0, K(x, t) dt).$$

Proof. From the difference of the stochastic dynamics,

$$\Delta x^a = \left[T \nabla_b K^{ab}(x,t) - K^{ab}(x,t) \nabla_b E(x)\right] \Delta t + \sqrt{2T} \Delta W^a(x,t),$$

by Kramers-Moyal expansion 16, we have

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

For n=1, since $\langle \mathrm{d} W^a(x,t) \rangle_{\mathrm{d} W} = 0$, the term is $-\nabla_a[p(x,t)\langle \Delta x^a \rangle_{\Delta x}] = \nabla_a\{p(x,t)[K^{ab}(x,t)\,\nabla_b E(x) - T\nabla_b K^{ab}(x,t)]\}\Delta t$. And for n=2, up to $o(\Delta t)$, only $T\nabla_a\nabla_b[p(x,t)K^{ab}(x,t)]\,\Delta t$ left. For $n\geqslant 3$, all are $o(\Delta t)$. So, we have

$$\frac{p(x,t+\Delta t)-p(x,t)}{\Delta t} = \nabla_a \left\{ p(x,t) \left[K^{ab}(x,t) \; \nabla_b E(x) - T \, \nabla_b K^{ab}(x,t) \right] \right\} + T \, \nabla_a \nabla_b \left\{ p(x,t) K^{ab}(x,t) \right\} + o(\Delta t).$$

Letting $\Delta t \rightarrow 0$, we find

$$\begin{split} \frac{\partial p}{\partial t}(x,t) &= \nabla_a \{p(x,t) \left[K^{ab}(x,t) \, \nabla_b E(x) - T \nabla_b K^{ab}(x,t)\right]\} + T \nabla_a \nabla_b (p(x,t) K^{ab}(x,t)) \\ \{\text{Expand}\} &= \nabla_a \{K^{ab}(x,t) \, \nabla_b E(x) \, p(x,t)\} - \nabla_a \{T \nabla_b K^{ab}(x,t) \, p(x,t)\} \\ &+ \nabla_a \{T K^{ab}(x,t) \nabla_b p(x,t)\} + \nabla_a \{T \nabla_b K^{ab}(x,t) p(x,t)\} \\ &= \nabla_a \{K^{ab}(x,t) \, \nabla_b E(x) \, p(x,t)\} + \nabla_a \{T K^{ab}(x,t) \nabla_b p(x,t)\}, \end{split}$$

which is just the Fokker-Planck equation. Indeed, the Fokker-Planck equation 6 is

$$\begin{split} \frac{\partial p}{\partial t}(x,t) &= -\nabla_a (f^a \{p\}(x,t) \, p(x,t)) \\ \{f^a &= \cdots\} &= \nabla_a (K^{ab} \{p\}(x,t) \, \nabla_b \{T \ln p(x,t) + E(x)\} \, p(x,t)) \\ \{K^{ab} \, \text{independent of} \, p\} &= \nabla_a (K^{ab}(x,t) \, \nabla_b \{T \ln p(x,t) + E(x)\} \, p(x,t)) \\ \{\text{Expand}\} &= \nabla_a \{K^{ab}(x,t) \, \nabla_b E(x) \, p(x,t)\} + \nabla_a (TK^{ab}(x,t) \, \nabla_b p(x,t)). \end{split}$$

Thus proof ends.

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

Question 2. Further, if it exists, then how can we reveal it? Precisely, in the case $T \to 0$, given $(dx^a/dt) = h^a(x,t)$, 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 function 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

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

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

$$F_E[p|v] := TD_{\mathrm{KL}}(p||q_E(\cdot|v)) - T \ln Z(v)$$

= $\langle E(v, \cdot) \rangle_p - TH[p].$

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

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

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

Algorithm 12. [Recall and Learn (RL)]

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 $\langle (\partial E/\partial \theta^{\alpha})(v,\cdot) \rangle_{\mathbf{gr}(\cdot|v)} \rightarrow \langle (\partial E/\partial \theta^{\alpha})(v,\cdot) \rangle_{\mathbf{gr}}$.

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

Here, we provide a biological inspired example, for illustrating both the stochastic dynamics 8 and the RL algorithm 12.

Definition 13. [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 dynamics of continuous Hopfield network is defined as

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

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

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

Theorem 14. If $f = \partial L_h$ and $g = \partial L_v$ are piecewise linear functions², then the stochastic dynamics of the continuous Hopfield network is

$$\begin{split} \frac{\mathrm{d}v^{\alpha}}{\mathrm{d}t} &= U^{\alpha\beta}\,f_{\beta}(h) - v^{\alpha} + I^{\alpha} + \sqrt{2T}\;\mathrm{d}W^{\alpha}_{v};\\ \frac{\mathrm{d}h^{\alpha}}{\mathrm{d}t} &= U^{\beta\alpha}\,g_{\beta}(v) - h^{\alpha} + \sqrt{2T}\;\mathrm{d}W^{\alpha}_{h}, \end{split}$$

where

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

^{2.} E.g. ReLU or LeakyReLu.

Useful Lemmas 5

Proof. Directly, we have

$$\begin{split} \frac{\partial E}{\partial v^{\alpha}}(v,h) &= g_{\alpha}(v) + (v^{\beta} - I^{\beta}) \, \frac{\partial g_{\beta}}{\partial v^{\alpha}}(v) - \frac{\partial L_{v}}{\partial v^{\alpha}}(v) - U^{\beta\gamma} \, f_{\gamma}(h) \, \frac{\partial g_{\beta}}{\partial v^{\alpha}}(v) \\ \left\{ g_{\alpha} &= \frac{\partial L_{v}}{\partial v^{\alpha}} \right\} &= -[U^{\beta\gamma} \, f_{\gamma}(h) + v^{\beta} - I^{\beta}] \, \frac{\partial g_{\beta}}{\partial v^{\alpha}}(v); \end{split}$$

and

$$\begin{split} \frac{\partial E}{\partial h^{\alpha}}(v,h) &= f_{\alpha}(h) + h^{\beta}\,\frac{\partial f_{\beta}}{\partial h^{\alpha}}(h) - \frac{\partial L_{h}}{\partial h^{\alpha}}(h) - U^{\gamma\beta}\,g_{\gamma}(v)\,\frac{\partial f_{\beta}}{\partial h^{\alpha}}(h) \\ \left\{ f_{\alpha} &= \frac{\partial L_{h}}{\partial h^{\alpha}} \right\} &= -[U^{\gamma\beta}\,g_{\gamma}(v) + h^{\beta}]\,\frac{\partial f_{\beta}}{\partial h^{\alpha}}(h). \end{split}$$

If f and g are piecewise linear functions, then $\partial^2 f$ and $\partial^2 g$ vanish. Thus, comparing with 8, we find $K_v = \partial^2 L_v(v)^{-1}$, $K_h = \partial^2 L_h(h)^{-1}$, and $\nabla K = 0$. Thus, we get the stochastic version by directly adding a random walk term $\mathrm{d}W$, as

$$\begin{split} \frac{\mathrm{d}v^{\alpha}}{\mathrm{d}t} &= U^{\alpha\beta}\,f_{\beta}(h) - v^{\alpha} + I^{\alpha} + \sqrt{2T}\,\mathrm{d}W_{v}^{\alpha}\,; \\ \frac{\mathrm{d}h^{\alpha}}{\mathrm{d}t} &= U^{\beta\alpha}\,g_{\beta}(v) - h^{\alpha} + \sqrt{2T}\,\mathrm{d}W_{h}^{\alpha}, \end{split}$$

where

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

Thus proof ends.

Remark 15. [Hebbian Rule]

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 16. [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

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

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

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

With this,

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

6 Appendix B

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

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

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

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

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

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

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

Given $\forall x \in \mathcal{M}$ and any time t, consider a series of i.i.d. random variables (random walks),

$$\{\varepsilon_i^a: i=1...n(t)\},\$$

where, for $\forall i, \, \varepsilon_i^a \sim P$ for some distribution P, with the mean 0 and covariance $\Sigma(x,t)$, and the walk steps

$$n(t) = \int_0^t d\tau \, \frac{dn}{dt}(x(\tau), \tau).$$

For any time interval Δt , his series of random walks leads to a difference

$$\Delta x^a := \sum_{i=n(t)}^{n(t+\Delta t)} \varepsilon_i^a.$$

Let

$$\tilde{W}^a(x,t) := \frac{1}{\sqrt{n(t+\Delta t)-n(t)}} \sum_{i=n(t)}^{n(t+\Delta t)} \varepsilon_i^a,$$

we have $\Delta x^a = \sqrt{n(t+\Delta t)-n(t)} \ \tilde{W}^a(x,t)$. Since $n(t+\Delta t)-n(t) = \frac{\mathrm{d}n}{\mathrm{d}t}(x,t) \ \Delta t + o(\Delta t)$, we have

$$\Delta x^a = \sqrt{n(t+\Delta t) - n(t)} \; \tilde{W}^a(x,t) = \sqrt{\frac{\mathrm{d}n}{\mathrm{d}t}(x,t) \; \Delta t} \; \tilde{W}^a(x,t) + o(\Delta t).$$

If

$$\frac{\mathrm{d}n}{\mathrm{d}t}(x,t)\,\Sigma^{ab}(x,t) = \mathcal{O}(1)$$

as $dn/dt \rightarrow +\infty$, that is, more steps per unit time, then, by central limit theorem (for multi-dimension),

$$\Delta x^a = \Delta W^a + o\left(\frac{\mathrm{d}n}{\mathrm{d}t}(x,t)\right),$$

where

$$\Delta W^a \sim \mathcal{N}(0, \Delta t \Sigma^{ab}(x, t)).$$

B.2 Stochastic Dynamics

TODO