RELAXATION

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,

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

- for conditional maps f, let f(x|y) denotes the map of x with y given and fixed, and f(x;y) denotes the map of x with y given but mutable;
- r.v. is short for random variable, i.i.d. for independent identically distributed, s.t. for such that, and a.e. for almost every.

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

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

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.

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

2 Section 1

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, for any p and t, the symmetric part of $K^{ab}\{p\}(x,t)$ is a.e. positive definite on \mathcal{M} , 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

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

The first term vanishes. 1 Then, direct calculus shows

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

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,

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

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

Relaxation 3

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 $(dF_E/dt)[p(\cdot,t)]$ 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"², is as follow.

Theorem 8. [Stochastic Dynamics]

If K^{ab} is symmetric, independent of p and almost everywhere smooth on \mathcal{M}^3 , then Fokker-Planck equation is equivalent to the stochastic dynamics

$$dx^a = [T \nabla_b K^{ab}(x,t) - K^{ab}(x,t) \nabla_b E(x)] dt + \sqrt{2T} dW^a(x,t),$$

where

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

Proof. By the lemma 22, we find

$$\mu^{a}(x,t) = T \nabla_{b} K^{ab}(x,t) - K^{ab}(x,t) \nabla_{b} E(x)$$

and

$$\Sigma^{ab}(x,t) = 2TK^{ab}(x,t).$$

Then, directly,

$$\begin{split} \frac{\partial p}{\partial t}(x,t) &= -\nabla_a \{p(x,t) \ \mu^a(x,t)\} + \frac{1}{2} \nabla_a \nabla_b (p(x,t) \Sigma^{ab}(x,t)) \\ &= \nabla_a \{p(x,t) \left[K^{ab}(x,t) \ \nabla_b E(x) - T \nabla_b K^{ab}(x,t)\right]\} + \nabla_a \nabla_b \{T p(x,t) K^{ab}(x,t)\} \\ \{\text{Expand}\} &= \nabla_a \{K^{ab}(x,t) \ \nabla_b E(x) \ p(x,t)\} - \nabla_a \{T \nabla_b K^{ab}(x,t) \ p(x,t)\} \\ &+ \nabla_a \{T K^{ab}(x,t) \nabla_b p(x,t)\} + \nabla_a \{T \nabla_b K^{ab}(x,t) p(x,t)\} \\ &= \nabla_a \{K^{ab}(x,t) \ \nabla_b E(x) \ p(x,t)\} + \nabla_a \{T K^{ab}(x,t) \nabla_b p(x,t)\}, \end{split}$$

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

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

exactly the same. Thus proof ends.

Question 1. Given a stochastic dynamics, 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 $(dx^a/dt) = h^a(x,t)$, how can we reconstruct the E and find a positive definite K^{ab} , s.t. $h^a(x) = K^{ab}(x,t)\nabla_b E(x)$?

The scalar function E is called Lyapunov function. Given an autonomous dynamical system⁴, along the phase trajectory, Lyapunov function will monomotically decrease. So, it reflects the stability of the dynamical system. Next, we investigate, for any autonomous dynamical system, if there's a Lyapunov function, s.t.

$$\frac{\mathrm{d}x^a}{\mathrm{d}t} = f^a(x) = K^{ab}(x) \, \nabla_b E(x),$$

Notice that, this is an autonomous stocastical dynamics with $T \rightarrow 0$.

^{2.} For the conception of stochastic dynamics, c.f. B.2.

^{3.} TODO: Check this.

^{4.} That is, ordinary differential equations that do not explicitly depend on time. The word autonomous means independent of time.

4 Section 3

Definition 9. [Phase Tape]

Given an autonomous dynamical system $dx^a/dt = f^a(x)$ on \mathcal{M} and a hypersurface \mathcal{S} with $\dim(\mathcal{S}) < \dim(\mathcal{M})$. A phase tape $\operatorname{PT}(\mathcal{S},t) := \{x^a(s): s \in [0,t], x^a(0) \in \mathcal{S}\}$.

Theorem 10. [Existance of Lyapunov Function]

If there's no limit cycle, then there exists a Lyapunov function, constructed as follow. First

2 Ambient & Latent Variables

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 extend the free energy to

Definition 11. [Conditional Free Energy]

Given v, if define

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

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

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

Directly, we have

Lemma 12.

$$q_E(h|v) = \frac{\exp(-E(v,h)/T)}{\int_{\mathcal{H}} \mathrm{d}\mu(h) \exp(-E(v,h)/T)},$$

which is simply the q_E with the v in the E(v,h) fixed.

Thus,

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

3 Minimize Free Energy Principle

If E is in a function family parameterized by $\theta \in \mathbb{R}^N$, denoted as $E(x;\theta)$, then we want to find the most generic distribution q_E in the function family of E s.t. the expection $\langle E(\cdot;\theta)\rangle_{q_{E(\cdot;\theta)}}$ is minimized. For instance, given ambient v, we want to locates v on the minimum of E, that is $\langle E(v,\cdot;\theta)\rangle_{q_E(\cdot|v;\theta)}$ (c.f. lemma 12).

On one hand, we want to minimize $\langle E(\cdot;\theta)\rangle_{q_{E(\cdot;\theta)}}$; on the other hand, we shall keep the minimal prior knowledge on $q_{E(\cdot;\theta)}$, that is, maximize $H[q_{E(\cdot;\theta)}]$. So, we find the θ that minimizes $\langle E(\cdot;\theta)\rangle_{q_{E(\cdot;\theta)}} - TH[q_{E(\cdot;\theta)}]$, where the positive constant T balances the two aspects. This happens to be the free energy.

Next, we propose an algorithm that establishes the free energy minimization. First, notice the relation

Lemma 14.
$$\frac{\partial}{\partial \theta^{\alpha}} \{ -T \ln Z_{E(\cdot;\theta)} \} = \left\langle \frac{\partial E}{\partial \theta^{\alpha}} (\cdot;\theta) \right\rangle_{q_{E(\cdot;\theta)}}.$$

So, we have an EM-like algorithm, as

Algorithm 15. [Recall and Learn (RL)]

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

1. minimize $\langle E(\cdot;\theta)\rangle_p - TH[p]$ by the stochastic dynamics until relaxation, where $p = q_{E(\cdot;\theta)}$; then

2. minimize $-T \ln Z_{E(\cdot;\theta)}$ by gradient descent and replacing $\left\langle \frac{\partial E}{\partial \theta^{\alpha}}(\cdot;\theta) \right\rangle_{q_{E(\cdot,\theta)}} \rightarrow \left\langle \frac{\partial E}{\partial \theta^{\alpha}}(\cdot;\theta) \right\rangle_{p}$.

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, or code of information). So we call this algorithm *recall and learn*.

During the optimization, the first term minimizes the expectation of $E(\cdot;\theta)$, while the second term smoothes $E(\cdot;\theta)$. Since the $q_E(\cdot;\theta)$ is invariant for $E(x;\theta) \to E(x;\theta) + \text{Const}$, we shall eliminate this symmetry by re-defining

$$E(x;\theta) \rightarrow E(x;\theta) - E(x_{\star};\theta),$$

for any $x_{\star} \in \mathcal{M}$ given.

4 Example: Continuous Hopfield Network

Here, we provide a biological inspired example, for illustrating both the stochastic dynamics 8 and the RL algorithm 15.

Definition 16. [Continuous Hopfield Network]

Let $U^{\alpha\beta}$ and I^{α} constants, and $L_v(v)$ and $L_h(h)$ scalar functions. Define $f_{\alpha} := \partial_{\alpha} L_h$, $g_{\alpha} := \partial_{\alpha} L_v$. Then the dynamics of continuous Hopfield network is defined as⁵

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

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

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

Next, we convert this deterministic dynamics to its stochastic version.

Theorem 17. If $f = \partial L_h$ and $g = \partial L_v$ are linear functions, and the Hessian matrix of L_v and L_h are positive definite, then the stochastic dynamics of the continuous Hopfield network is

$$\begin{split} \frac{\mathrm{d}v^{\alpha}}{\mathrm{d}t} &= K_{v}^{\alpha\beta} \left[U_{\beta\gamma} f^{\gamma}(h) - v_{\beta} + I_{\beta} \right] + \sqrt{2T} \, \mathrm{d}W_{v}^{\alpha}; \\ \frac{\mathrm{d}h^{\alpha}}{\mathrm{d}t} &= K_{h}^{\alpha\beta} \left[U_{\gamma\beta} g^{\gamma}(v) - h^{\beta} \right] + \sqrt{2T} \, \mathrm{d}W_{h}^{\alpha}, \end{split}$$

where $K_v := [\partial^2 L_v(v)]^{-1}$ and $K_h := [\partial^2 L_h(h)]^{-1}$ are constant matrices.

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 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 $\nabla K = 0$. That is,

$$\begin{split} \frac{\mathrm{d}v^\alpha}{\mathrm{d}t} &= K_v^{\alpha\beta} \left[U_{\beta\gamma} \, f^\gamma(h) - v_\beta + I_\beta \right] + \sqrt{2T} \, \mathrm{d}W_v^\alpha; \\ \frac{\mathrm{d}h^\alpha}{\mathrm{d}t} &= K_h^{\alpha\beta} \left[U_{\gamma\beta} \, g^\gamma(v) - h^\beta \right] + \sqrt{2T} \, \mathrm{d}W_h^\alpha, \end{split}$$

^{5.} Originally illustrated in Large Associative Memory Problem in Neurobiology and Machine Learning, Dmitry Krotov and John Hopfield, 2020.

^{6.} Here the $\partial^2 L$ is the Hessian matrix, and $[\partial^2 L]^{-1}$ the inverse matrix.

6 Appendix A

Thus proof ends. \Box

Remark 18. [Hebbian Rule]

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

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

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

Remark 19. [Simplified Brain]

This model can be viewed as a simplified model of brain. Indeed, in the equation (1) of Dehaene et al. $(2003)^7$, when the V are limited to a small region, and the τ s are large, then the coefficients, i.e. the ms and hs, can be regarded as constants. The equation (1), thus, reduces to the continuous Hopfield network.

Appendix A Useful Lemmas

Lemma 20. [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

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

With this,

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

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

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

^{7.} A neuronal network model linking subjective reports and objective physiological data during conscious perception, Stanislas Dehaene, Claire Sergent, and Jean-Pierre Changeux, 2003.

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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 , this 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

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

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),

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

where

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

B.2 Stochastic Dynamics

A stochastic dynamics is defined by two parts. The first is deterministic, and the second is a random walk. Precisely,

Definition 21. [Stochastic Dynamics]

Given $\mu^a(x,t)$ and $\Sigma^{ab}(x,t)$ on $\mathcal{M} \times \mathbb{R}$,

$$dx^a = \mu^a(x, t) dt + dW^a(x, t),$$

where $dW^a(x,t)$ is a random walk with covariance $\Sigma^{ab}(x,t)$.

Consider an ensemble of particles, each obeys this stochastic dynamics. This ensemble will form a distribution, evolving with time t, say p(t). The equation of this evolution is

Lemma 22. [Macroscopic Landscape]

$$\frac{\partial p}{\partial t}(t) = -\nabla_a \{p(x,t) \; \mu^a(x,t)\} + \frac{1}{2} \, \nabla_a \nabla_b \{p(x,t) \Sigma^{ab}(x,t)\}.$$

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 ${\bf Proof.}$ From the difference of the stochastic dynamics,

$$\Delta x^a = \mu^a(x, t) \, \Delta t + \Delta W^a(x, t),$$

by Kramers-Moyal expansion 20, 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 $\mathrm{d}W^a(x,t)$ is a random walk, $\langle \Delta W^a(x,t) \rangle_{\Delta W(x,t)} = 0$. Then the term is $-\nabla_a[p(x,t)\langle \Delta x^a \rangle_{\Delta x}] = -\nabla_a\{p(x,t)\mu^a(x,t)\}\Delta t$. And for n=2, by noticing that, as a random walk, $\langle \Delta W^a(x,t)\Delta W^b(x,t)\rangle_{\Delta W(x,t)} = \mathcal{O}(\Delta t)$, we have, up to $o(\Delta t)$, only $(1/2)\nabla_a\nabla_b[p(x,t)\Sigma^{ab}(x,t)]\Delta t$ left. For $n\geqslant 3$, all are $o(\Delta t)$. So, we have

$$\frac{p(x,t+\Delta t) - p(x,t)}{\Delta t} = -\nabla_a \{p(x,t) \ \mu^a(x,t)\} + \frac{1}{2} \nabla_a \nabla_b \{p(x,t) \Sigma^{ab}(x,t)\} + o(1).$$

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

$$\frac{\partial p}{\partial t}(x,t) = -\nabla_a \{p(x,t) \; \mu^a(x,t)\} + \frac{1}{2} \nabla_a \nabla_b \{p(x,t) \Sigma^{ab}(x,t)\}.$$

Thus proof ends. \Box