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*

$$\langle f \rangle_p = \langle f \rangle_X = \mathbb{E}_{x \sim p}[f(x)] := \int_{\mathcal{M}} \mathrm{d}\mu(x)\, p(x)\, f(x);$$

- *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 Lyapunov Function

Definition 2. *[Lyapunov Function]*

Given an autonomous dynamics[1]*,*

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

a Lyapunov function of this dynamics, $V(x)$*, is a scalar function s.t.* $\nabla_a V(x)\, f^a(x) \leqslant 0$ *and the equality holds if and only if* $f^a(x) = 0$*.*

Along the phase trajectory, a Lyapunov function will monomotically decrease. So, it reflects the stability of the dynamics.

The problem is how to find a Lyapunov function for a given autonomous dynamics, if there is any. Here we propose a simulation based method that furnishes a criterion on whether a Lyapunov function for this autonomous dynamics exists or not, and then to reveal an analytic approximation to the true Lyapunov function if it exists.

We first extend the autonomous (determinate) dynamics to a stochastical dynamics[2], as

$$\mathrm{d}X^a = f^a(X)\, \mathrm{d}t + \mathrm{d}W^a,$$

where $\mathrm{d}W^a \sim \mathcal{N}(0, 2T\delta^{ab}\mathrm{d}t)$ and parameter $T > 0$. Then, we sample an essemble of particles independently evolving along this stochastic dynamics. As a set of Markov chains, this simulation will reach a stationary distribution. This is true if the Markov chain is irreducible and recurrent. These condition is hard to check. But, in practice, there is criterion that if the chains have converged at a finite time.[3] If it has converged, we get an empirical distribution, denoted as p_D, that approximates to the true stationary distribution.

Now, we to find an analytic approximation to the empirical distribution p_D. This can be done by any universal approximator, such as neural network. Say, an universal approximator $E(\cdot; \theta)$ parameterized by θ, and define q_E as

$$q_E(x; \theta) := \frac{\exp(-E(x; \theta)/T)}{Z_{E(\cdot; \theta)}},$$

where $Z_{E(\cdot;\theta)} := \int_{\mathcal{M}} \mathrm{d}\mu(x) \exp(-E(x; \theta)/T)$.

1. That is, ordinary differential equations that do not explicitly depend on time. The word autonomous means independent of time.
2. Stochastic dynamics is defined in 6.
3. E.g., Gelman-Rubin-Brooks plot.

Then, we construct the loss as

$$L(\theta) := T D_{\mathrm{KL}}(p_D \| q_E(\cdot;\theta)) = T\int_{\mathcal{M}} \mathrm{d}\mu(x)\, p_D(x) \ln p_D(x) - T\int_{\mathcal{M}} \mathrm{d}\mu(x)\, p_D(x) \ln q_E(x;\theta).$$

The first term is independent of θ, thus omitable. Thus, the loss becomes

$$\begin{aligned} L(\theta) &= -T\int_{\mathcal{M}} \mathrm{d}\mu(x)\, p_D(x) \ln q_E(x;\theta) \\ &= \int_{\mathcal{M}} \mathrm{d}\mu(x)\, p_D(x)\, E(x;\theta) + T\int_{\mathcal{M}} \mathrm{d}\mu(x)\, p_D(x) \ln Z_{E(\cdot;\theta)} \\ [p_D \text{ is empirical}] &= \mathbb{E}_{x\sim p_D}[E(x;\theta)] \\ \left[\int_{\mathcal{M}} \mathrm{d}\mu(x)\, p_D(x) = 1\right] &+ \ln Z_{E(\cdot;\theta)}. \end{aligned}$$

Lemma 3.

$$T\frac{\partial}{\partial\theta^\alpha} \ln Z_{E(\cdot;\theta)} = -\mathbb{E}_{x\sim q_E(\cdot;\theta)}\left[\frac{\partial E}{\partial\theta^\alpha}(\cdot;\theta)\right].$$

Proof. Directly,

$$\begin{aligned} T\frac{\partial}{\partial\theta^\alpha} \ln Z_{E(\cdot;\theta)} &= T\frac{1}{Z_{E(\cdot;\theta)}} \frac{\partial}{\partial\theta^\alpha} Z_{E(\cdot;\theta)} \\ \{Z_E := \cdots\} &= T\frac{1}{Z_{E(\cdot;\theta)}} \frac{\partial}{\partial\theta^\alpha} \int_{\mathcal{M}} \mathrm{d}\mu(x)\, \mathrm{e}^{-E(x;\theta)/T} \\ &= -\int_{\mathcal{M}} \mathrm{d}\mu(x)\, \frac{\mathrm{e}^{-E(x;\theta)/T}}{Z_{E(\cdot;\theta)}} \frac{\partial E}{\partial\theta^\alpha}(x;\theta) \\ \{q_E := \cdots\} &= -\int_{\mathcal{M}} \mathrm{d}\mu(x)\, q_E(x;\theta) \frac{\partial E}{\partial\theta^\alpha}(x;\theta). \\ &= -\mathbb{E}_{x\sim q_E(\cdot;\theta)}\left[\frac{\partial E}{\partial\theta^\alpha}(\cdot;\theta)\right]. \end{aligned}$$

Thus, proof ends. □

This implies

$$\frac{\partial L}{\partial\theta^\alpha}(\theta) = \mathbb{E}_{x\sim p_D}\left[\frac{\partial E}{\partial\theta^\alpha}(\cdot;\theta)\right] - \mathbb{E}_{x\sim q_E(\cdot;\theta)}\left[\frac{\partial E}{\partial\theta^\alpha}(\cdot;\theta)\right],$$

where the second term can be computed via persistent MCMC. So, during this computation, we employ two different sets of Markov chains that are consistently evolving. The first is constructed by the stochastic dynamics, and the second by the persistent MCMC of q_E. Along the gradient descent steps of θ, on the chains of p_D E is sunk, while on the chains of q_E E is elevated. Gradient descent stops when the two parts balance, where q_E fits p_D best.

Finally, we claim that the E we find at the best fit θ is a Lyapunov of the original autonomous (determinate) dynamics. We first claim that the evolution of the distribution of the stochastic dynamics, $p(x,t)$, by lemma 7, is

$$\frac{\partial p}{\partial t}(x,t) = -\nabla_a[p(x,t)\, f^a(x)] + T\,\Delta p(x,t),$$

where Laplacian $\Delta := \delta^{ab}\nabla_a\nabla_b$. In the end, $p \to q_E$ where $\partial p/\partial t \to 0$. Here, it becomes

$$0 = -\nabla_a E(x)\, f^a(x) - \delta^{ab}\, \nabla_a E\,(x) \nabla_b E(x) + T\,[\nabla_a f^a(x) + \Delta E(x)].$$

As $T \to 0$, the stochastic dynamics reduces to the original, and we arrive at

$$\nabla_a E(x)\, f^a(x) = -\delta^{ab}\, \nabla_a E\,(x) \nabla_b E(x) \leqslant 0,$$

where equality holds if and only if $\nabla_a E(x) = 0$. Thus, $E(x)$ is a Lyapunov function.

Appendix A Useful Lemmas

A.1 Kramers–Moyal Expansion

Kramers–Moyal Expansion relates the microscopic landscape, i.e. the dynamics of Brownian particles, and the macroscopic landscape, i.e. the evolution of distribution.

Lemma 4. *[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 $\int \mathrm{d}\mu(\epsilon)\;p_\epsilon(\epsilon;x,t)\;\delta(x+\epsilon-y)$. This implies

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

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

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

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

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

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

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

$$\{\varepsilon_i^a\colon i=1\ldots n(t)\},$$

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

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

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

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

Then, we have

Theorem 5. *[Brownian Motion]*
As $\mathrm{d}n/\mathrm{d}t \to +\infty$*,*

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

where

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

Proof. 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 $\mathrm{d}n/\mathrm{d}t \to +\infty$, 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

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

In reality, the space cannot be infinite, we live in a box, no matter how large it is.

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 6. *[Stochastic Dynamics]*
Given $\mu^a(x,t)$ *and* $\Sigma^{ab}(x,t)$ *on* $\mathcal{M} \times \mathbb{R}$*,*

$$\mathrm{d}x^a = \mu^a(x,t)\, \mathrm{d}t + \mathrm{d}W^a(x,t),$$

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

Lemma 7. *[Macroscopic Landscape]*
Consider an ensemble of particles, randomly sampled at an initial time, evolving along a stochastic dynamics 6. By saying "ensemble", we mean that the number of particles has the order of Avogadro's constant, s.t. the distribution of the particles can be viewed as smooth. Let $p(x,t)$ *denotes the distribution. Then we have*

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

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 4, 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

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

Letting $\Delta t \to 0$, 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. □