Lecture-12: Stein's method

1 Stein's method for rate of convergence

Definition 1.1. We define the inner product of $x, y \in \mathbb{R}^d$ as $\langle x, y\rangle \triangleq \sum_{i=1}^d x_i y_i$, and the 2-norm for any $x \in \mathbb{R}^d$ as $\|x\| \triangleq \sqrt{\langle x, x\rangle} = \sqrt{\sum_{i=1}^d x_i^2}$.

Definition 1.2. Any vector in $\mathbb{R}^d$ will be denoted by its row vector, and hence the inner product for any two vectors $x, y \in \mathbb{R}^d$ can be written as $\langle x, y\rangle = xy^T = yx^T$.

Definition 1.3. For any differentiable function $g : \mathbb{R}^d \to \mathbb{R}$, we denote its gradient by $\nabla g : \mathbb{R}^d \to \mathbb{R}^d$ and define it in terms of unit row vectors $(e_i : i \in [d])$, as $\nabla g(x) \triangleq \sum_{i=1}^d e_i \frac{\partial g(x)}{\partial x_i}$. The inner product of $\nabla g : \mathbb{R}^d \to \mathbb{R}^d$ and $y \in \mathbb{R}^d$ is given by

$$\langle \nabla g(x), y\rangle = \sum_{i=1}^d \frac{\partial g(x)}{\partial x_i} y_i = \nabla g(x) y^T = y(\nabla g(x))^T.$$

For any function $f : \mathbb{R}^d \to \mathbb{R}^d$, we denote its gradient in terms of unit row vectors $(e_i : i \in [d])$, by matrix

$$\nabla f(x) \triangleq \sum_{i,j=1}^d e_j^T \frac{\partial f_i(x)}{\partial x_j} e_i = \sum_{i=1}^d (\nabla f_i(x))^T e_i.$$

For a vector $y \in \mathbb{R}^d$ and function $f : \mathbb{R}^d \to \mathbb{R}^d$, we can write the row vector

$$\sum_{i=1}^d (\sum_{j=1}^d \frac{\partial f_i(x)}{\partial x_j} y_j) e_i = \sum_{i=1}^d \langle \nabla f_i(x), y\rangle e_i = y \sum_{i=1}^d (\nabla f_i(x))^T e_i = y \nabla f(x).$$

For a function $f : \mathbb{R}^d \to \mathbb{R}^d$ and $x : \mathbb{R}_+ \to \mathbb{R}^d$, we can derivative of the norm

$$\frac{d}{dt} \|f(x(t))\|^2 = 2 \sum_{i,j=1}^d f_i(x) \frac{\partial f_i(x)}{\partial x_j} \dot{x}_j(t) = \left\langle f(x), \sum_{i=1}^d e_i \langle \nabla f_i(x), \dot{x}\rangle \right\rangle = \langle f(x), \dot{x}\nabla f(x)\rangle = f(x)(\dot{x}\nabla f(x))^T.$$

Definition 1.4 (Locally exponentially stable). A mean-field model $\dot{a} = f(a)$ is said to be **locally exponentially stable** if there exist positive constants $\epsilon, \alpha, \kappa > 0$, such that if initial condition $\|a(0)\| \leqslant \epsilon$, then

$$\|a(t) - a^*\| \leqslant \kappa \|a(0)\| e^{-\alpha t}.$$

Definition 1.5 (Poisson). For a mean field model $\dot{a} = f(a)$ where $a \in \mathcal{M}(\mathcal{Z})$ and a^* is a rest point and $d \triangleq |\mathcal{Z}|$, we define $g : \mathcal{M}(\mathcal{Z}) \to \mathbb{R}$ be the solution to the Poisson equation

$$\langle \nabla g(a), \dot{a}\rangle = \langle \nabla g(a), f(a)\rangle = \|\Phi_t(a) - a^*\|^2. \tag{1}$$

Remark 1. We note that $\frac{\partial g(a)}{\partial t} = 0$, and hence the total derivative of g with respect to t is given by

$$\frac{dg(a)}{dt} = \langle \nabla g(a), \dot{a}\rangle + \frac{\partial g(a)}{\partial t} = \|\Phi_t(a) - a^*\|^2.$$

Since $a(\infty) = a^*$, it follows that the solution to the Poisson equation is given by $g(a) \triangleq -\int_{t \in \mathbb{R}_+} \|\Phi_t(a) - a^*\|^2 dt$, when the integral exists and is finite. The integral is finite when the mean-field model is asymptotically stable and locally exponentially stable. Note that $-g(a)$ can be viewed as the cumulative square deviation of the system state from the equilibrium point when the initial condition is a.

Remark 2. We define $h : \mathbb{R}_+ \times \mathcal{M}(\mathcal{Z}) \times \mathcal{M}(\mathcal{Z}) \to \mathbb{R}^d$ as $h(t,a,b) \triangleq (b-a)\nabla\Phi_t(a)$. Since $\Phi_t(a), a^* \in \mathcal{M}(\mathcal{Z})$, we have $\|\Phi_t(a) - a^*\|_\infty \leqslant 1$. From Hölder's inequality for inner product $|\langle a, b\rangle| \leqslant \|a\|_\infty \|b\|_1$, we obtain

$$\int_{t\in\mathbb{R}_+} 2\left\langle(\Phi_t(a)-a^*), (b-a)\nabla\Phi_t(a)\right\rangle dt \leqslant 2\int_{t\in\mathbb{R}_+} \|h(t,a,b)\|_1\, dt \leqslant 2\sqrt{d}\int_{t\in\mathbb{R}_+} \|h(t,a,b)\|_2\, dt \leqslant \frac{2c\sqrt{d}}{\sigma}.$$

We will show the last inequality later. Recall that $\nabla\Phi_t(a) = \sum_{i=1}^d e_i(\nabla\Phi_t(a)_i)^T$, and hence $\left\langle b, (\nabla\Phi_t(a))^T\right\rangle = \sum_{i=1}^d b_i \nabla\Phi_t(a)_i$. Since the integral is bounded, we can exchange differentiation and integration to write

$$\nabla g(a) = -\int_{t\in\mathbb{R}_+} 2\sum_{i=1}^d (\Phi_t(a)_i - a_i^*)\nabla\Phi_t(a)_i dt = -\int_{t\in\mathbb{R}_+} 2(\Phi_t(a)-a^*)(\nabla\Phi_t(a))^T dt.$$

Remark 3. Recall that Q^{A^N} is the generator matrix for the empirical distribution of interacting-particle CTMC with N particles. If A^N is irreducible, then it is positive recurrent with equilibrium distribution $\pi^{A^N(\infty)}$ such that $\pi^{A^N(\infty)}Q^{A^N} = 0$. If the initial distribution $\pi^{A^N(0)} = \pi^{A^N(\infty)}$, then $\pi^{A^N(t)} = \pi^{A^N(\infty)}$ for all $t \in \mathbb{R}_+$. In particular, we have

$$\mathbb{E}_{\pi^{A^N(\infty)}} \sum_{b:b\neq a} Q^{A^N}_{A^N(\infty),b}(g(b) - g(A^N(\infty))) = \sum_{a,b\in\mathcal{M}_N(\mathcal{Z})} \pi_a^{A^N(\infty)} Q^{A^N}_{a,b}(g(b)-g(a)) = 0. \tag{2}$$

Substituting random variable $A^N(\infty)$ into the Poisson equation, taking expectation with respect to stationary distribution $\pi^{A^N(\infty)}$, and recalling that $\pi^{A^N(\infty)}$ remains invariant under map Φ_t for all $t \in \mathbb{R}_+$, we obtain

$$\mathbb{E}_{\pi^{A^N(\infty)}} \left\langle \nabla g(A^N(\infty)), f(A^N(\infty))\right\rangle = \mathbb{E}_{\pi^{A^N(\infty)}} \left\|\Phi_t(A^N(\infty)) - a^*\right\|^2 = \mathbb{E}_{\pi^{A^N(\infty)}} \left\|A^N(\infty) - a^*\right\|^2. \tag{3}$$

Subtracting (2) to the left hand side, adding and subtracting $f(A^N(\infty)) = \sum_{b:b\neq A^N(\infty)} Q^{A^N}_{A^N(\infty),b}(b - A^N(\infty))$ inside the inner product in the left hand side term of (3), and using the fact that $\dot{a} = f(a)$, we obtain

$$\begin{aligned}\mathbb{E}_{\pi^{A^N(\infty)}} \left\|A^N(\infty) - a^*\right\|^2 = \mathbb{E}_{\pi^{A^N(\infty)}} \Bigg[\Bigg\langle \nabla g(A^N(\infty)), \Big(f(A^N(\infty)) - \sum_{b:b\neq A^N(\infty)} Q^{A^N}_{A^N(\infty),b}(b - A^N(\infty))\Big)\Bigg\rangle \\ - \sum_{b:b\neq A^N(\infty)} Q^{A^N}_{A^N(\infty),b}\Big(g(b) - g(A^N(\infty)) - \left\langle\nabla g(A^N(\infty)), (b - A^N(\infty))\right\rangle\Big)\Bigg].\end{aligned} \tag{4}$$

From the equality above, it appears that $\lim_{N\to\infty} \mathbb{E}\left\|A^N(\infty) - a^*\right\|^2 = 0$, if the following are true.

1. Solution g to the Poisson equation has a bounded gradient, i.e. $\|\nabla g(a)\|$ is bounded by a constant independent of N.
2. Generator f converges, i.e. $\lim_{N\to\infty} \mathbb{E}_{\pi^{A^N(\infty)}} \left\| f(A^N(\infty)) - \sum_{b:b\neq A^N(\infty)} Q^{A^N}_{A^N(\infty),b}(b - A^N(\infty))\right\| = 0$.
3. The CTMC A^N has bounded transition-rates, i.e. $\frac{1}{N}\mathbb{E}_{\pi^{A^N(\infty)}} \sum_{b:b\neq A^N(\infty)} Q^{A^N}_{A^N(\infty),b}$ is bounded.
4. The first-order approximation error for g is diminishing, i.e. $\|g(b) - g(a) - \langle\nabla g(a), (b-a)\rangle\| = O(\frac{1}{N^2})$. Note that $g(a) + \langle\nabla g(a), (b-a)\rangle$ is the first-order Taylor approximation of $g(b)$.

For many CTMCs and the associated mean-field models, the first three conditions mentioned above can be easily verified. In the following theorem, we will prove that the last condition holds when the mean-field model is globally asymptotically stable and locally exponentially stable (see inequality (13)), and then establish the rate of convergence based on that.

Theorem 1.6. *The empirical distribution processes of the density-dependent family of CTMCs* $((X^N : \Omega \to \mathcal{Z}^N) : N \in \mathbb{N})$*, converge to the equilibrium point* a^* *of the mean-field model in the mean-square sense with rate* $\frac{1}{N}$*, i.e.,*

$$\mathbb{E}_{\pi^{A^N(\infty)}} \left\|A^N(\infty) - a^*\right\|^2 = O\Big(\frac{1}{N}\Big),$$

when the following conditions hold.

Condition 1. **Bounded transition-rate.** *There exists a constant $c > 0$ independent of N such that*

$$\mathbb{E}_{\pi^{A^N(\infty)}} \sum_{b:b\neq A^N(\infty)} Q^{A^N}_{A^N(\infty),b} \leqslant Nc.$$

Condition 2. **Bounded state transition.** *There exists a constant $\tilde{c}$ independent of N such that $N\|b-a\| \leqslant \tilde{c}$ for any $a, b \in \mathcal{M}_N(\mathcal{Z})$ such that $Q^{A^N}_{a,b} \neq 0$.*

Condition 3. **Perfect mean-field model.** *The mean-field model is given by $f(a) = \sum_{b:b\neq a} Q^{A^N}_{a,b}(b-a)$ for all $a \in \mathcal{M}(\mathcal{Z})$.*

Condition 4. **Existence of partial derivatives.** *The first order partial derivatives $\frac{\partial f_w}{\partial a_z}$ exist and are Lipschitz for all $w, z \in \mathcal{Z}$.*

Condition 5. **Stability.** *The mean-field model is globally asymptotically stable and is locally exponentially stable.*

Proof. We will first show the theorem assuming that the system is globally exponentially stable, and then extend it to the case of global asymptotically stable and local exponentially stable case. Under perfect mean-field model condition, we can rewrite (4) as

$$\mathbb{E}_{\pi^{A^N(\infty)}} \left\|A^N(\infty) - a^*\right\|^2 = \mathbb{E}_{\pi^{A^N(\infty)}} \left[- \sum_{b:b\neq A^N(\infty)} Q^{A^N}_{A^N(\infty),b} \Big(g(b) - g(A^N(\infty)) - \left\langle \nabla g(A^N(\infty)), (b - A^N(\infty)) \right\rangle \Big) \right].$$

Recall that map $g : \mathcal{M}(\mathcal{Z}) \to \mathbb{R}$ is the solution to Poisson equation (1), and thus we can write

$$-\Big(g(b) - g(a) - \langle \nabla g(a), (b-a)) \rangle \Big) = \int_{t\in\mathbb{R}_+} \Big(\|\Phi_t(b) - a^*\|^2 - \|\Phi_t(a) - a^*\|^2 - 2\left\langle (\Phi_t(a) - a^*)\nabla\Phi_t(a)^T, (b-a) \right\rangle \Big) dt.$$

We define the error function $e : \mathbb{R}_+ \times \mathcal{M}(\mathcal{Z}) \times \mathcal{M}(\mathcal{Z}) \to \mathbb{R}^d$ for each $t \in \mathbb{R}_+, a, b \in \mathcal{M}(\mathcal{Z})$, as

$$e(t, a, b) \triangleq \Phi_t(b) - \Phi_t(a) - (b-a)\nabla\Phi_t(a).$$

With this definition, we can write

$$\begin{aligned}
&\|\Phi_t(b) - a^*\|^2 - \|\Phi_t(a) - a^*\|^2 - 2\left\langle (\Phi_t(a) - a^*)\nabla\Phi_t(a)^T, (b-a) \right\rangle \\
&= \|e(t,a,b) + \Phi_t(a) - a^* + (b-a)\nabla\Phi_t(a)\|^2 - \|\Phi_t(a) - a^*\|^2 - 2\left\langle (\Phi_t(a) - a^*)\nabla\Phi_t(a)^T, (b-a) \right\rangle \\
&= \|e(t,a,b)\|^2 + \|(b-a)\nabla\Phi_t(a)\|^2 + 2\left\langle e(t,a,b), \Phi_t(a) - a^* + (b-a)\nabla\Phi_t(a) \right\rangle.
\end{aligned}$$

We will show that $\|e(t,a,b)\|_2 = O(\frac{1}{N^2})$, from the bounded state transition condition we have $\|b-a\| \leqslant \frac{\tilde{c}}{N}$, and we will show that $N\|(b-a)\nabla\Phi_t(a)\|_2 \leqslant c$ independent of N and t. Therefore, there exists $\tilde{N} \in \mathbb{N}$ such that for all $N \geqslant \tilde{N}$,

$$\|e(t,a,b) + 2(\Phi_t(a) - a^*) + 2(b-a)\nabla\Phi_t(a)\| \leqslant 3.$$

Substituting this, we can upper bound

$$-(g(b) - g(a) - \langle \nabla g(a), (b-a)) \rangle) \leqslant 3\int_{t\in\mathbb{R}_+} \|e(t,a,b)\|\, dt + \frac{1}{N^2}\int_{t\in\mathbb{R}_+} \|N(b-a)\nabla\Phi_t(a)\|^2\, dt.$$

We will show that $\int_{t\in\mathbb{R}_+} \|e(t,a,b)\|\, dt = O(\frac{1}{N^2})$ and $\int_{t\in\mathbb{R}_+} \|N(b-a)\nabla\Phi_t(a)\|^2\, dt = \Theta(1)$, to obtain that the RHS of the above equation is of order $O(\frac{1}{N^2})$. Together with bounded transition rate condition, we conclude that $\mathbb{E}_{\pi^{A^N(\infty)}} \left\|A^N(\infty) - a^*\right\|^2 = O(\frac{1}{N})$.

Consider the case that the mean-field model is not globally exponentially stable, but is globally asymptotically stable and locally exponentially stable. Recall that $a(t) \in \mathcal{M}(\mathcal{Z}) \subseteq [0,1]^d$ is compact. From the definition of global asymptotic stability, given any $\epsilon > 0$, there exists a finite time t_ϵ such that $\|\Phi_t(a)\| \leqslant \epsilon$ for all $t \geqslant t_\epsilon$. We observe that $\|e(t_\epsilon, a, b)\|_1\, dt = O(\frac{1}{N^2})$ and writing the integration $\int_{t\in\mathbb{R}_+} = \int_{t\leqslant t_\epsilon} + \int_{t>t_\epsilon}$, we get the result. ∎

Proposition 1.7. *A dynamical system has an exponentially stable equilibrium point if and only if the linearized system at the equilibrium is exponentially stable.*

Remark 4. The first four conditions are straightforward to verify, however showing the stability condition requires work. The global asymptotical stability in general is studied using the Lyapunov theorem. The local exponential stability can be verified by computing the eigenvalues of the state matrix of the linearized mean-field model at equilibrium. For given parameters of the mean-field model, one can verify the local exponential stability.

Remark 5. If the mean-field model is unstable but the perfect mean-field model assumption holds, then Kurtz's theorem indicates that the sample paths of the CTMCs converge to the trajectory of the mean-field model for any finite time interval, which implies that the CTMCs are *unstable* as well.

Remark 6. Convergence to the mean-field model in Theorem 1.6 requires a perfect mean-field model and bounded state transitions, both of which can be relaxed.