Mean-Field Langevin Dynamics and Neural Networks

Zhenjie Ren

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joint works with Giovanni Conforti, Kaitong Hu, Anna Kazeykina, David Siska, Lukasz Szpruch, Xiaolu Tan, Junjian Yang

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MF Langevin

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The Langevin dynamics was first introduced in statistical physics to describe the motion of a particle with position X and velocity V in a potential field $\nabla_x f$ subject to damping and random collision.

Overdamped Langevin dynamics

 $dX_t = -\nabla_x f(X_t) dt + \sigma dW_t$

Underdamped Langevin dynamics

$$dX_t = V_t dt dV_t = (-\nabla_x f(X_t) - \gamma V_t) dt + \sigma dW_t$$

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Under mild conditions, the two Markov diffusions admits unique invariant measures whose densities read:

Overdamped Langevin dynamics $m^*(x) = Ce^{-\frac{2}{\sigma^2}f(x)}$

Underdamped Langevin dynamics

$$\int f(x) = \frac{2}{2} \left(f(x) + \frac{1}{2} |y|^2 \right)$$

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$$m^*(x,v) = Ce^{-\frac{2}{\sigma^2}(f(x)+\frac{1}{2}|v|^2)}$$

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In particular, f does NOT need to be convex.

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One may diminish $\sigma \downarrow 0$ along the simulation \Rightarrow Simulation annealing.

The deep neural networks have won and continue gaining impressive success in various applications. Mathematically speaking, we may approximate a given function f with the parametrized function:

$$f(z) pprox arphi_n \circ \cdots \circ arphi_1(z), \quad ext{where} \quad arphi_i(z) := \sum_{k=1}^{n_i} c_k^i arphi(A_k^i z + b_k^i)$$

and φ is a given non-constant, bounded, continuous activation function. The expressiveness of the neural network is ensured by the universal representation theorem. However, the efficiency of such over-parametrized, non-convex optimization is still a mystery for mathematical analysis.

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It is natural to study this problem using Mean-field Langevin equations.

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In the work with *K. Hu, D. Siska, L. Szpruch* '19, we focused on the two-layer network, and aimed at minimizing

$$\inf_{n,(c_k,A_k,b_k)} \mathbf{E}\Big[\big|f(Z) - \sum_{k=1}^n c_k \varphi(A_k Z + b_k)\big|^2\Big],$$

where Z represents the data and **E** is the expectation under the law of the data.

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How to characterize the minimizer of a function of probabilities ?

Let $F : \mathcal{P}(\mathbb{R}^d) \to \mathbb{R}$. Denote its derivative by $\frac{\delta F}{\delta m} : \mathcal{P}(\mathbb{R}^d) \times \mathbb{R}^d \to \mathbb{R}$.

• given m, m', denote $m^{\lambda} := (1 - \lambda)m + \lambda m'$ we have $F(m^{\varepsilon}) - F(m) = \int_0^{\varepsilon} \int_{\mathbb{R}^d} \frac{\delta F}{\delta m}(m^{\lambda}, x)(m' - m)(dx)d\lambda$

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- e.g. (a) $F(m) := \mathbb{E}^{m}[\varphi(X)]$, then $\frac{\delta F}{\delta m}(m, x) = \varphi(x)$ (b) $F(m) := g(\mathbb{E}^{m}[\varphi(X)])$, then $\frac{\delta F}{\delta m}(m, x) = \dot{g}(\mathbb{E}^{m}[\varphi(X)])\varphi(x)$

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$$\varepsilon \Big(F(m') - F(m) \Big) \geq F(m^{\varepsilon}) - F(m)$$

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$$F(m') - F(m) \geq \int_{\mathbb{R}^d} \frac{\delta F}{\delta m}(m, x)(m' - m)(dx)$$

Therefore, a sufficient condition for m being a minimizer would be

$$\frac{\delta F}{\delta m}(m,x) = C \quad \text{for all } x$$

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Intrinsic derivative
$$D_m F(m, x) = \nabla \frac{\delta F}{\delta m}(m, x) = 0$$
 for all x

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First order condition of minimizers

Under the presence of the entropy regularizer, we can also prove the first order equation is a necessary condition for being minimizer.

Theorem (Hu, R., Siska, Szpruch, '19)

Under mild conditions, if $m^* = \arg \min_m \{F(m) + \frac{\sigma^2}{2} \operatorname{Ent}(m)\}$, then

$$D_m F(m^*, x) + \frac{\sigma^2}{2} \nabla \ln m^*(x) = 0, \quad \text{for all } x.$$
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Conversely, if F to be convex, (1) implies m^* is the minimizer.

Note that the density of m^* satisfies:

$$m^*(x) = Ce^{-\frac{2}{\sigma^2}\frac{\delta F}{\delta m}(m^*,x)}$$

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$$D_m F(m^*, x) + \frac{\sigma^2}{2} \frac{\nabla m^*(x)}{m^*(x)} = 0$$

Image: A math a math

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$$D_m F(m^*, x) m^*(x) + \frac{\sigma^2}{2} \nabla m^*(x) = 0$$

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$$\partial_t m = \nabla \cdot \left(D_m F(m, \cdot) m + \frac{\sigma^2}{2} \nabla m \right)$$
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It is well-known that the equation (2) characterizes the marginal law of the mean-field Langevin (MFL) dynamics:

$$dX_t = -D_m F(m_t, X_t) dt + \sigma dW_t, \quad m_t = \text{Law}(X_t)$$

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Link to Underdamped Mean-field Langevin equation

Different from above, introduce the velocity variable V and consider the minimization:

$$\inf_{m=\text{Law}(X,V)} F(m^X) + \frac{1}{2} \mathbb{E}^m \left[|V|^2 \right] + \frac{\sigma^2}{2\gamma} \text{Ent}(m)$$

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One can again directly verify that the minimizer is an invariant measure of the underdamped MFL equation:

$$\begin{cases} dX_t = V_t, \\ dV_t = (-D_m F(m_t^X, X_t) - \gamma V_t) dt + \sigma dW_t \end{cases}$$

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For the mean-field diffusion, the existence and uniqueness of the invariant measures is non-trivial, and the convergence of the marginal laws towards the invariant measure, if exists, is one of the long-standing problems in probability.

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A simple example: mean-field Ornstein-Uhlenbeck process $dX_t = (\alpha \mathbb{E}[X_t] - X_t)dt + dW_t$

- $\alpha < 1 \Longrightarrow \exists$ unique invariant measure
- $\alpha > 1 \Longrightarrow$ no invariant measure
- $\alpha = 1 \Longrightarrow \exists$ multiple invariant measures

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Given a convex F, the existence and uniqueness of the invariant measure of MFL is due to that of the minimizer m^* , thanks to the first order condition.

It remains to study the convergence of the marginal laws to the invariant measure.

Gradient flow and its analog

Define the energy functions for both overdamped and underdamped cases

$$U(m) = F(m) + \frac{\sigma^2}{2} \operatorname{Ent}(m), \quad \widehat{U}(m) = F(m^X) + \frac{1}{2} \mathbb{E}^m[|V|^2] + \frac{\sigma^2}{2\gamma} \operatorname{Ent}(m)$$

For the convergence towards the invariant measure, it is crucial to observe

Theorem (*Overdamped MFL*, Hu, R., Siska, Szpruch, '19) $dU(m_t) = -\mathbb{E}\Big[\left| D_m F(m_t, X_t) + \frac{\sigma^2}{2} \nabla_x \ln m_t(X_t) \right|^2 \Big] dt \quad \text{for all } t > 0$

Theorem (Underdamped MFL, Kazeykina, R., Tan, Yang, '20) $d\widehat{U}(m_t) = -\gamma \mathbb{E}\Big[|V_t + \frac{\sigma^2}{2\gamma} \nabla_v \ln m_t(X_t, V_t)|^2 \Big] dt \quad \text{for all } t > 0$

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Gradient flow and its analog

Define the energy functions for both overdamped and underdamped cases

$$U(m) = F(m) + \frac{\sigma^2}{2} \operatorname{Ent}(m), \quad \widehat{U}(m) = F(m^X) + \frac{1}{2} \mathbb{E}^m[|V|^2] + \frac{\sigma^2}{2\gamma} \operatorname{Ent}(m)$$

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Due to the generalized Itô calculus and time-reversal of diffusions.

Convergence for convex F

• Overdamped: $dU(m_t) = -\mathbb{E}\left[\left|D_m F(m_t, X_t) + \frac{\sigma^2}{2} \nabla_x \ln m_t(X_t)\right|^2\right] dt$. Heuristically, $U(m_t)$ decreases till m_t hits m^* s.t.

$$D_m F(m^*, x) + \frac{\sigma^2}{2} \nabla_x \ln m^*(x) = 0$$

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$$m^* = rg \min_m U(m)$$

and $m_t \equiv m^*$ afterwards.

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$$m^* = rg\min_m U(m)$$

and $m_t \equiv m^*$ afterwards.

• Underdamped: $d\widehat{U}(m_t) = -\gamma \mathbb{E}\left[\left|V_t + \frac{\sigma^2}{2\gamma} \nabla_v \ln m_t(X_t, V_t)\right|^2\right] dt$ Similarly, $\widehat{U}(m_t)$ shall decrease till m_t hits m^* s.t.

$$v + rac{\sigma^2}{2\gamma}
abla_v \ln m^*(x, v) = 0$$

The intuition above can be materialized by the LaSalle's invariance principle and the functional inequalities. Define the set of cluster points

$$w(m_0) := \{m: \exists (m_{t_n})_{n \in \mathbb{N}} \text{ s.t. } \lim_{n \to \infty} \mathcal{W}_1(m_{t_n}, m) = 0\}$$

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Invariance Principle says:

$$\operatorname{Law}(X_0) \in w(m_0) \Longrightarrow \operatorname{Law}(X_t) \in w(m_0) \text{ for all } t > 0$$

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• Overdamped: $m^* \in w(m_0) \Longrightarrow m_t \to \arg\min_m U(m)$ in \mathcal{W}_1

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Recall that

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Consider any smooth function h with compact support. Let $Law(X_0) \in w(m_0)$.

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$$dV_t h(X_t) = \left(\left(\dot{h}(X_t) \cdot V_t \right) V_t + h(X_t) (-D_m F(m_t^X, X_t) - \gamma V_t) \right) dt + dM_t$$

Recall that

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$$\Rightarrow \frac{\sigma^2}{2\gamma}\nabla_x \ln m_t(X_t, V_t) + D_mF(m_t^X, X_t) = 0$$

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$$\Rightarrow \frac{\sigma^2}{2\gamma}\nabla_x \ln m_t(X_t, V_t) + D_mF(m_t^X, X_t) = 0$$

$$\Rightarrow m_t \equiv \arg\min_m \widehat{U}(m)$$

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$$\Rightarrow \frac{\sigma^2}{2\gamma}\nabla_x \ln m_t(X_t, V_t) + D_mF(m_t^X, X_t) = 0$$

$$\Rightarrow w(m_0) = \{\arg\min_m \widehat{U}(m)\}$$

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Convergence rate for special case

For possibly non-convex F such that $D_m F(m, x)$ bearing small mean-field dependence, we can prove the contraction results using synchronous-reflection couplings.

Theorem (Overdamped MFL, Hu, R., Siska, Szpruch, '19)

 $\mathcal{W}_1(m_t, m_t') \leq C e^{-\lambda t} \mathcal{W}_1(m_0, m_0').$

Theorem (Underdamped MFL, Kazeykina, R., Tan, Yang, '20)

$$\begin{split} \mathcal{W}_{\psi}(m_t, m'_t) &\leq C e^{-\lambda t} \mathcal{W}_{\psi}(m_0, m'_0), \text{ with the semi-metric} \\ \mathcal{W}_{\psi}(m, m') &= \inf \{ \int \psi((x, v), (x', v')) \pi(dx, dy) : \pi \text{ is a coupling of } m, m' \} \end{split}$$

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Regretfully, the small mean-field dependence assumption is corresponding to the over-regularized problem in the context of neural networks.

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1

The Generative Adversary Network aims at sampling a target a probability measure $\hat{\mu} \in \mathcal{P}(\mathbb{R}^{n^1})$ only empirically known.

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$$\begin{split} \min_{\mu} \mathcal{W}_{1}(\mu, \hat{\mu}) \\ &= \min_{\mu} \sup_{f \in \operatorname{Lip}_{1}} \int f(x)(\mu - \hat{\mu})(dx) \\ &\approx \min_{\mu} \sup_{f \in \mathcal{E}} \int f(x)(\mu - \hat{\mu})(dx) \\ \end{split}$$
where $\mathcal{E} = \left\{ z \mapsto \mathbb{E}^{m} \big[\varphi(X, z) \big] : \ X \sim m \in \mathcal{P}(\mathbb{R}^{n^{2}}) \right\}$

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GAN and zero-sum game

The Generative Adversary Network aims at sampling a target a probability measure $\hat{\mu} \in \mathcal{P}(\mathbb{R}^{n^1})$ only empirically known. Taking Wasserstein distance as example, we aim at sampling $\hat{\mu}$ by

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where $\mathcal{E} = \left\{ z \mapsto \mathbb{E}^m [\varphi(X, z)] : X \sim m \in \mathcal{P}(\mathbb{R}^{n^2}) \right\}$ GAN can be viewed as a zero-sum game between the generator and the discriminator:

$$\begin{cases} \text{Gen.}: & \inf_{\mu \in \mathcal{P}(\mathbb{R}^{n^1})} \int \mathbb{E}^m [\varphi(X, z)](\mu - \hat{\mu})(dz) + \frac{\sigma^2}{2} (\text{Ent}(\mu) - \text{Ent}(m)) \\ \text{Discr.}: & \inf_{m \in \mathcal{P}(\mathbb{R}^{n^2})} - \int \mathbb{E}^m [\varphi(X, z)](\mu - \hat{\mu})(dz) + \frac{\sigma^2}{2} (\text{Ent}(m) - \text{Ent}(\mu)) \end{cases}$$

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In particular, $\mu, m \mapsto F(\mu, m) := \int \mathbb{E}^m [\varphi(X, z)](\mu - \hat{\mu})(dz)$ are linear.

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The feedback of the generator

Due to the linearity, the solution to the generator given m (choice of discriminator) is explicit:

$$\mu^*[m](z) = C(m)^{-1} e^{-\frac{2}{\sigma^2} \left(\mathbb{E}^m[\varphi(X,z)] \right)},$$

where C(m) is the normalization constant.

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where C(m) is the normalization constant. Therefore the value of the game can be rewritten as

$$\min_{m} \max_{\mu} -F(\mu, m) + \frac{\sigma^2}{2} (\operatorname{Ent}(m) - \operatorname{Ent}(\mu)) = \min_{m} G(m) + \frac{\sigma^2}{2} \operatorname{Ent}(m)$$
where $G(m) := -F(\mu^*[m], m) - \frac{\sigma^2}{2} \operatorname{Ent}(\mu^*[m])$ is convex

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Therefore the choice of the discriminator at the equilibrium is the invariant measure of the MFL dynamics:

$$dX_t = -D_m G(m_t, X_t) dt + \sigma dW_t$$

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Therefore the choice of the discriminator at the equilibrium is the invariant measure of the MFL dynamics:

$$dX_t = -D_m G(m_t, X_t) dt + \sigma dW_t$$

and the intrinsic derivative can be computed explicitly:

$$G(m) = -\int \mathbb{E}^{m}[\varphi(X,z)](\mu^{*}-\hat{\mu})(dz) - \frac{\sigma^{2}}{2}\mathsf{Ent}(\mu^{*}[m])$$

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$$G(m) = -\int \mathbb{E}^{m}[\varphi(X,z)](\mu^{*}-\hat{\mu})(dz) + \frac{\sigma^{2}}{2}\int \big(\ln C(m) + \frac{2}{\sigma^{2}}\mathbb{E}^{m}[\varphi(X,z)]\big)\mu^{*}(dz)$$

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Recall $C(m) = \int e^{-\frac{2}{\sigma^2}\mathbb{E}^m[\varphi(X,z)]} dz$, and thus

Therefore the choice of the discriminator at the equilibrium is the invariant measure of the MFL dynamics:

$$dX_t = -D_m G(m_t, X_t) dt + \sigma dW_t$$

and the intrinsic derivative can be computed explicitly:

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$$\frac{\delta G}{\delta m} = \int \varphi(x,z)\hat{\mu}(dz) - \frac{\sigma^2}{2C(m)} \int e^{-\frac{2}{\sigma^2}\mathbb{E}^m[\varphi(X,z)]} \frac{2}{\sigma^2}\varphi(x,z)dz$$

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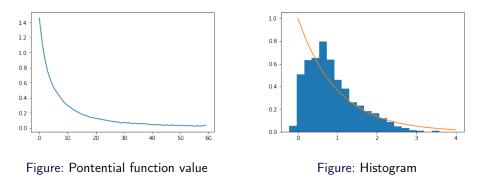
$$D_m G(m,x) = \int \nabla_x \varphi(x,z) (\hat{\mu} - \mu^*[m])(dz)$$

Finally note that $\mu^*[m]$ can be sampled by MCMC.

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A toy example

Here we sample the law $\hat{\mu} = \exp(1)$ with $\mu_0 = \mathcal{N}(0, 1)$.



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Toy example with underdamped MFL

Similarly, we can train the discriminator by the underdamped MFL dynamics.

$$\begin{cases} dX_t = V_t \\ dV_t = \left(-D_m G(m_t^X, X_t) - \gamma V_t\right) dt + \sigma dW_t \end{cases}$$

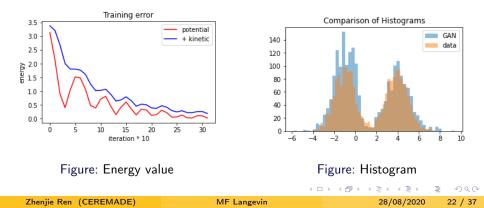


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Optimization on random environment/with marginal constraint

More recently, with *G. Conforti* and *A. Kazeykina*, we discover that the previous analysis can be generalized to the optimization on random environment.

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Optimization on random environment/with marginal constraint

More recently, with *G. Conforti* and *A. Kazeykina*, we discover that the previous analysis can be generalized to the optimization on random environment. Consider the optimization over $\pi \in \mathcal{P}(\mathbb{R}^d \times \mathbb{Y})$:

$$\min_{\pi: \pi_{Y}=\mathsf{m}} F(\pi) + \frac{\sigma^{2}}{2} \mathsf{Ent}(\pi | \mathrm{Leb} \times \mathsf{m})$$

where m is a fixed law on the environment \mathbb{Y} (Polish).

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It is crucial to observe : for F convex we have

$$F(\pi') - F(\pi) \geq \int_{\mathbb{R}^d} \frac{\delta F}{\delta m}(\pi, x, y)(\pi' - \pi)(dx, dy) d\lambda$$

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Since $\pi_Y = \pi'_Y = m$, a sufficient condition for *m* to be a minimizer is: $\frac{\delta F}{\delta m}(\pi, x, y) \text{ does NOT depend on } x$

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Theorem (Conforti, Kazeykina, R., '20)

Under mild conditions, if $\pi^* \in \arg \min_{\pi_Y=m} \left\{ F(\pi) + \frac{\sigma^2}{2} \operatorname{Ent}(\pi | \operatorname{Leb} \times m) \right\}$ and let $\pi^*(dx, dy) = \pi^*(x|y) dxm(dy)$, then

$$\nabla_x \frac{\delta F}{\delta m}(\pi^*, x, y) + \frac{\sigma^2}{2} \nabla_x \ln \pi^*(x|y) = 0, \quad \text{for all } x, \text{ m-a.s. y.}$$
(3)

Conversely, if F to be convex, (3) implies m^* is the minimizer.

Due to the first order condition, the minimizer of V^{σ} is closely related to the invariant measure of the overdamped MFL system:

$$dX_t = -
abla_x rac{\delta F}{\delta m}(\pi_t, X_t, Y) + \sigma dW_t, \quad \pi_t = \operatorname{Law}(X_t, Y)$$

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In particular, we know

- if F is convex, $\pi^* = \arg \min_{\pi_Y=m} V^{\sigma}(\pi)$ iff π^* is the invariant measure
- for general *F*, if MFL system has unique invariant measure π^* , then $\pi^* = \arg \min_{\pi_Y=m} V^{\sigma}(\pi)$

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Theorem (Conforti, Kazeykina, R., '20)

Under mild conditions, the MFL system admits unique strong solution and

$$dV^{\sigma}(\pi_t) = -\mathbb{E}\Big[\big| \nabla_x \frac{\delta F}{\delta m}(\pi_t, X_t, Y) + \nabla_x \ln \pi_t(X_t|Y) \big|^2 \Big] dt, \quad \text{for } t > 0$$

Convergence towards the invariant measure

• In case F convex, the V^{σ} again serves as Lyapunov function for the dynamic system (m_t) . Provided that \mathbb{Y} is countable or \mathbb{R}^n , we can show π_t converges to π^* in \mathcal{W}_2 based on Lasalle's invariant principle.

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- For possibly non-convex but with small MF-dependence *F*, we can prove the contraction result:

Theorem (Conforti, Kazeykina, R., '20)

Under particular conditions, we have

$$\begin{split} \overline{\mathcal{W}}_{1}(\pi_{t},\pi_{t}') &\leq C e^{-\gamma t} \overline{\mathcal{W}}_{1}(\pi_{0},\pi_{0}'), \\ \textit{where} \quad \overline{\mathcal{W}}_{1}(\pi,\pi') &= \int \mathcal{W}_{1}\big(\pi(\cdot|\mathsf{y}),\pi'(\cdot|\mathsf{y})\big)\mathsf{m}(d\mathsf{y}) \end{split}$$

The constant γ can be computed, and once $\gamma > 0$ the MFL has a unique invariant measure, equal to the minimizer of V^{σ} , towards which the marginal laws converge.

Let $\mathbb{Y} = [0, T]$ and $m = \operatorname{Leb}[0, T].$ Consider the relaxed optimal control

$$\inf_{\pi_{Y}=m} \int_{0}^{T} \int L(\mathbf{y}, S_{\mathbf{y}}, \mathbf{x}) \pi(\mathbf{x}|\mathbf{y}) d\mathbf{y} + g(S_{T}) + \frac{\sigma^{2}}{2} \mathsf{Ent}(\pi|\mathrm{Leb}),$$
where $S_{\mathbf{y}} = S_{0} + \int_{0}^{\mathbf{y}} \int \varphi(u, S_{u}, \mathbf{x}) \pi(\mathbf{x}|u) du$

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Define the Hamiltonian function $H(y, s, x, p) = L(y, s, x) + p \cdot \varphi(y, s, x)$. We may compute $\frac{\delta F}{\delta m}(\pi, x, y) = H(y, S_y, x, P_y)$, where

$$P_{y} = \nabla_{s}g(S_{T}) + \int_{y}^{T} \int \nabla_{s}H(u, S_{u}, x, P_{u})\pi(x|u)du$$

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The paper with *K*. *Hu and A*. *Kazeykina*, '19 was devoted to this example and connect it to the deep neural network.

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Deep neural network associated to relaxed controlled process

The Euler scheme introduces a forward propagation of a neural network: $S_{t_{i+1}} \approx S_{t_i} + \frac{\delta t}{n_{t_{i+1}}} \sum_{j=1}^{n_{t_{i+1}}} \varphi(t_i, S_{t_i}, X_{t_{i+1}}^j, Z)$, where Z is the data.

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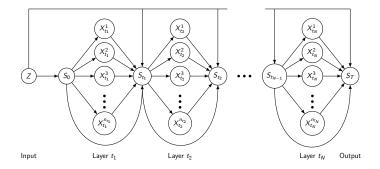


Figure: Neural network corresponding to the relaxed controlled process

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Mean-field Langevin system \approx Backward propagation

The architecture of the network is characterized by the average pooling after each layer!

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Mean-field Langevin system \approx Backward propagation

The architecture of the network is characterized by the average pooling after each layer!

The gradients of the parameters are easy to compute, due to the chain rule (or backward propagation):

$$\begin{aligned} X_{s_{j+1}}^{y} &= X_{s_{j}}^{y} - \delta s \mathsf{E} \big[\nabla_{a} H(\mathsf{y}, S_{s_{j}}^{y}, X_{s_{j}}^{y}, P_{s_{j}}^{y}, Z) \big] + \sigma \delta W_{s_{j}}, \text{ with } \delta s &= s_{j+1} - s_{j}, \\ \text{where } P_{s}^{\mathsf{y}_{i-1}} &= P_{s}^{\mathsf{y}_{i}} - \delta \mathsf{y} \sum_{j=1}^{n_{\mathsf{y}_{i+1}}} \nabla_{s} H\big(\mathsf{y}_{i}, S_{s}^{\mathsf{y}_{i}}, X_{s}^{\mathsf{y}_{i}, j}, P_{s}^{\mathsf{y}_{i}}, Z\big), \ P_{s}^{\mathsf{T}} &= \nabla_{s} g(S_{s}^{\mathsf{T}}, Z), \end{aligned}$$

 (δW_{s_i}) are independent copies of $\mathcal{N}(0, \delta s)$.

Mean-field Langevin system \approx Backward propagation

The architecture of the network is characterized by the average pooling after each layer!

The gradients of the parameters are easy to compute, due to the chain rule (or backward propagation):

$$dX_{s}^{y} = -\mathbb{E}\left[\nabla_{a}H(y, S_{s}^{y}, X_{s}^{y}, P_{s}^{y}, Z)\right]ds + \sigma dW_{s},$$

where $dP_{s}^{y} = -\mathbb{E}\left[\nabla_{s}H(y, S_{s}^{y}, X_{s}^{y}, P_{s}^{y}, Z)\right]dy, P_{s}^{T} = \nabla_{s}g(S_{s}^{T}, Z),$

 (δW_{s_j}) are independent copies of $\mathcal{N}(0, \delta s)$. Clearly, it is a discretization of the MF Langevin system.

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Nash equilibirum

Consider the game in which the *i*-th player chooses the probability measure π^i on $\mathbb{R}^{n^i} \times \mathbb{Y}$ as strategy to minimize his objective function $F^i(\pi^i, \pi^{-i})$, where π^{-i} is the joint strategy of other players on $\prod_{j \neq i} \mathbb{R}^{n^j} \times \mathbb{Y}$. We urge that the marginal law of π^i on \mathbb{Y} is equal to the fixed law $m \in \mathcal{P}(\mathbb{Y})$.

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$$\pi^* \text{ is Nash eq:} \quad \pi^{*,i} \in \arg\min_{\pi^i: \ \pi^i_y = \mathsf{m}} \mathsf{F}^i(\pi^i,\pi^{*,-i}) + \frac{\sigma^2}{2}\mathsf{Ent}(\pi^i | \mathrm{Leb} \times \mathsf{m}), \ \forall i$$

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Due to the previous first order condition we have

Theorem (Conforti, Kazeykina, R., '20)

If π is a Nash equilibrium, we have for $i = 1, \cdots, n$,

$$\nabla_{x^{i}} \frac{\delta F^{i}}{\delta \nu} (\pi^{i}, \pi^{-i}, x^{i}, \mathsf{y}) + \frac{\sigma^{2}}{2} \nabla_{x^{i}} \ln \left(\pi^{i} (x^{i} | \mathsf{y}) \right) = 0 \quad \forall x^{i} \in \mathbb{R}^{n^{i}}, \text{ m-a.s. } \mathsf{y} \in \mathbb{Y}.$$

Uniqueness: Monotonicity condition

Theorem (Conforti, Kazeykina, R., '20)

Denote $\bar{x} = (x, y)$. The functions $(F^i)_{i=1,\dots,n}$ satisfy the monotonicity condition, if for π, π' we have

$$\sum_{i=1}^n \int \left(rac{\delta {\sf F}^i}{\delta
u}(\pi^i,\pi^{-i},ar x^i)-rac{\delta {\sf F}^i}{\delta
u}(\pi'^i,\pi'^{-i},ar x^i)
ight)(\pi-\pi')(dar x)\geq 0.$$

We have the following results:

- (i) if n = 1, a function F satisfies the monotonicity condition iff it is convex.
- (ii) in general $(n \ge 1)$, if $(F^i)_{i=1,\dots,n}$ satisfy the monotonicity condition, then for any two Nash equilibria $\pi^*, \pi'^* \in \Pi$ we have $(\pi^*)^i = (\pi'^*)^i$ for all $i = 1, \dots, n$.

3

Proof of uniqueness

Sketch of proof: Since (F^i) is monotone,

$$\sum_{i=1}^n \int \left(\frac{\delta F^i}{\delta \nu} (\pi^i, \pi^{-i}, \bar{x}^i) - \frac{\delta F^i}{\delta \nu} (\pi'^i, \pi'^{-i}, \bar{x}^i) \right) (\pi - \pi') (d\bar{x}) \geq 0.$$

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Together with the first order condition of equilibrium, we obtain

$$\sum_{i=1}^n \int ig(-\lnig(\pi^i(x^i|\mathsf{y})ig)+\lnig(\pi'^i(x^i|\mathsf{y})ig)ig)(\pi-\pi')(dar{x})\geq 0.$$

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Together with the first order condition of equilibrium, we obtain

$$-\sum_{i=1}^{n} \left(\mathsf{Ent}\big(\pi^{i}|\pi^{\prime i}\big) + \mathsf{Ent}\big(\pi^{\prime i}|\pi^{i}\big) \right) \geq 0.$$

Therefore $\pi^i = \pi'^i$ for all *i*.

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Again the FOC inspires the form of MFL dynamics:

$$dX_t^{i,y} = \nabla_{x^i} \frac{\delta F^i}{\delta \nu} (\pi_t^i, \pi_t^{-i}, X_t^{i,y}, y) dt + \sigma dW_t^i$$

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In particular, if the game admits at least one Nash equilibrium and the MFL system has a unique invariant measure, then the invariant measure is an equilibrium.

- In the context of game, in general it is hard to find Lyapunov function.
- If the coefficient $\nabla_{x^i} \frac{\delta F^i}{\delta \nu}(\pi^i, \pi^{-i}, x^i, y)$ bears small mean-field dependence, we still can prove the contraction result, namely,

$$\overline{\mathcal{W}}_1(\pi_t, \pi_t') \leq C e^{-\gamma t} \overline{\mathcal{W}}_1(\pi_0, \pi_0')$$

References: One layer: Mei, Montanari, Nguyen '18, Hu, R., Siska, Szpruch '19; Deep/Neuron ODE: Hu, R., Kazeykina, '19, Jabir, Siska, Szpruch '19; Game on random environment: Conforti, R., Kazeykina, '20; Stochastic control: Siska, Szpruch, '20; Underdamped MFL: Kazeykina, R., Tan, Yang, '20 ...

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• Mean-field Langevin dynamics is a natural model to analyze the (Hamiltonian) gradient descent for the overparametrized nonconvex optimization

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- The calculus involving the measure derivatives characterizes the first order conditions, as well as allows the Itô-type calculus
- The relaxed control (continuous time or discrete time) can be viewed as an optimization with marginal constraint.

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Thank you for your attention!

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