



Convex Analysis of Mean Field Langevin Dynamics

^{1,2,3} Atsushi Nitanda, ^{4,5} Denny Wu, and ^{2,6} Taiji Suzuki



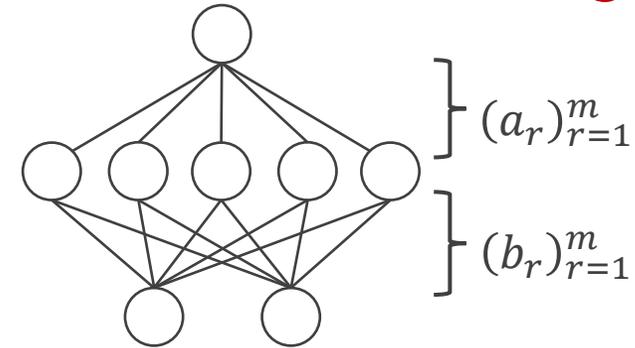
AISTATS2022 (Online)

Outline

Topic: Convergence analysis of **mean-field Langevin dynamics**.

Example: **noisy gradient descent for neural networks in mean-field regime:**

$$h_{\Theta}(x) = \frac{1}{m} \sum_{r=1}^m a_r \sigma(b_r^{\top} x).$$

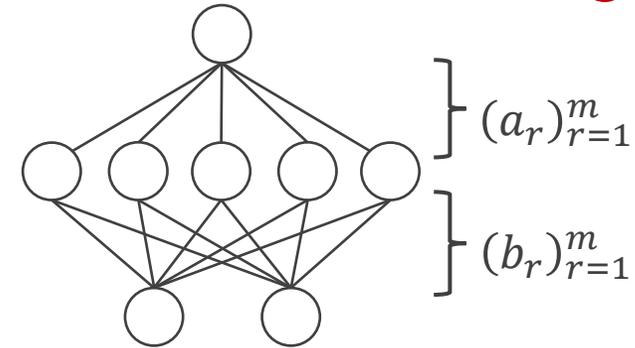


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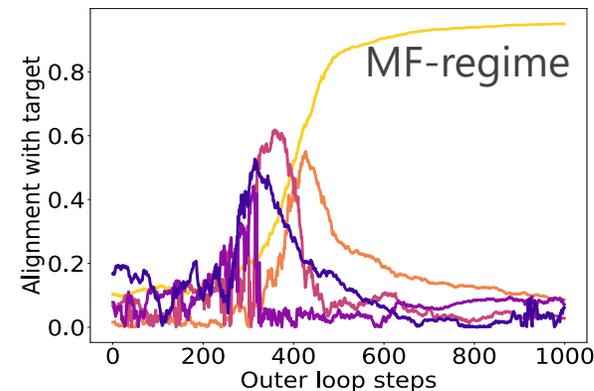
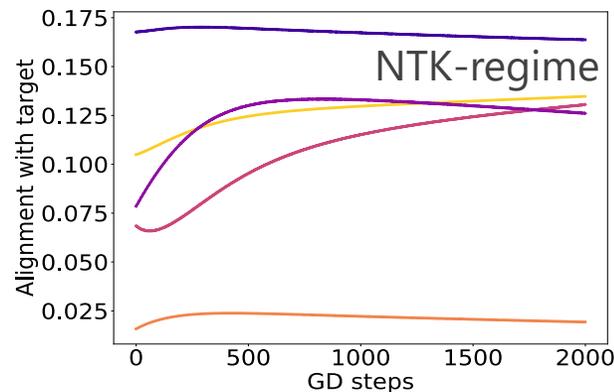
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Mean field neural networks exhibit **global convergence** and **adaptivity**.



[Nitanda, Denny, & Suzuki (NeurIPS2021)]

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We consider **noisy gradient descent** for mean-field neural networks:

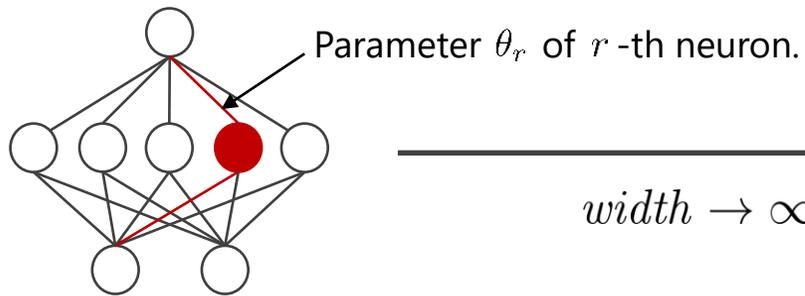
$$\theta_r^{(k+1)} \leftarrow \underbrace{(1 - 2\eta\lambda')\theta_r^{(k)}}_{L_2\text{-regularization}} - \underbrace{\eta\mathbb{E}[\partial_z \ell(h_{\Theta^{(k)}}(X), Y) \partial_{\theta_r} h(\theta_r^{(k)}, X)]}_{\text{Gradient of loss}} + \underbrace{\sqrt{2\eta\lambda}\zeta_r^{(k)}}_{\text{Gauss noise}}.$$

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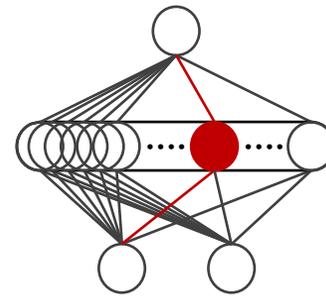
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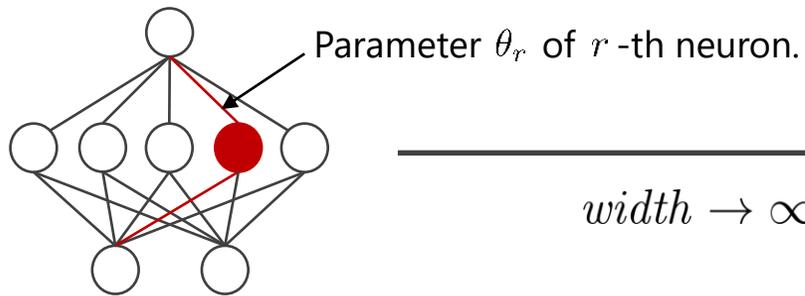
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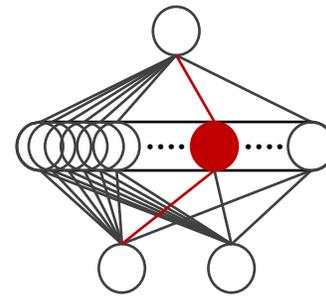
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Mean-field Langevin dynamics:

$$d\theta_t = -\nabla_{\theta} g_{q_t}(\theta_t)dt + \sqrt{2\lambda}dW_t. \quad q_t(\theta_t)dt \text{ is a probability distribution of } \theta_t.$$

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We analyze the noisy gradient descent via mean-field Langevin dynamics:

$$d\theta_t = -\underbrace{\nabla_{\theta} g_{q_t}(\theta_t)}_{\text{Drift term}} dt + \sqrt{2\lambda} dW_t$$

Drift term

The drift term involves the distribution unlike normal Langevin dynamics. This difference makes the convergence analysis difficult.

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- We show the *global convergence with the rate* for KL-regularized problems.
- *Prima-dual viewpoint* of proximal Gibbs distribution.

Regularized Risk Minimization

KL-regularized empirical risk minimization over the probability space:

$$\min_{q \in \mathcal{P}} \left\{ \mathcal{L}(q) = \frac{1}{n} \sum_{i=1}^n \ell(h_q(x_i), y_i) + \underbrace{\lambda' \mathbb{E}_q[\|\theta\|_2^2] + \lambda \mathbb{E}_q[\log(q(\theta))]}_{\propto \lambda \text{KL} \left(q \parallel \mathcal{N} \left(0, \frac{\lambda}{2\lambda'} I \right) \right)} \right\}.$$

Kullback-Leibler divergence to zero-mean Gaussian.

\mathcal{P} : the set of probability densities.

\mathbb{E}_q : expectation w.r.t $\theta \sim q(\theta)d\theta$.

$h_q(x) = \mathbb{E}_q[h(\theta, x)]$: mean-field neural network.

$(h(\theta, x) = a\sigma(b^\top x), \theta = (a, b))$

Proximal Gibbs Distribution

Definition (Proximal Gibbs distribution):

For a distribution q , we define p_q as

$$p_q(\theta) \propto \exp\left(-\frac{1}{\lambda}g_q(\theta)\right).$$

$$\begin{aligned}g_q(\theta) &= \frac{1}{n} \sum_{i=1}^n \partial_z \ell(h_q(X), Y) h(\theta, X) + \lambda' \|\theta\|_2^2 \\ &= \frac{\delta}{\delta q} \left\{ \frac{1}{n} \sum_{i=1}^n \ell(h_q(X), Y) + \lambda' \mathbb{E}_q[\|\theta\|_2^2] \right\}.\end{aligned}$$

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Entropy sandwich: $\lambda \text{KL}(q \| p_q) \geq \mathcal{L}(q) - \mathcal{L}(q_*) \geq \lambda \text{KL}(q \| q_*).$

- This formula is derived by the convex argument on the space of probability distributions.
- p_q plays as a cushion to absorb difference from the analysis of normal Langevin dynamics.
- As a result, we can develop convergence analysis in the mean-field regime, which mirrors the classical convex optimization analysis.

Assumption

Assumption (modified log Sobolev inequality (LSI)): Let $\alpha > 0$ be a constant.

For any q , the distribution p_q satisfies the following with

$$\text{KL}(q||p_q) \leq \frac{1}{2\alpha} \mathbb{E}_q \left[\left\| \nabla \log \frac{q}{p_q} \right\|_2^2 \right].$$

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Holley and Stroock (1987) argument guarantees the LSI of

$$p_q(\theta) \propto \exp \left(-\frac{1}{\lambda} g_q(\theta) \right)$$

when the potential g_q is the sum of strongly convex and bounded functions.

Example (mean-field neural networks):

For uniformly bounded $h(\theta, x)$, the modified LSI is satisfied with the constant $\frac{2\lambda'}{\lambda \exp(C\lambda^{-1})}$.

Convergence Analysis

Theorem: Let $\{q_t\}_{t \geq 0}$ be the evolution of mean-field Langevin dynamics. Under LSI assumption with $\alpha > 0$ and smoothness assumptions,

$$\mathcal{L}(q_t) - \mathcal{L}(q_*) \leq \exp(-2\alpha\lambda t)(\mathcal{L}(q_0) - \mathcal{L}(q_*)).$$

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Proof.
$$\begin{aligned} \frac{d}{dt}(\mathcal{L}(q_t) - \mathcal{L}(q_*)) &= \int \frac{\delta \mathcal{L}}{\delta q}(q_t)(\theta) \frac{\partial q_t}{\partial t}(\theta) d\theta \\ &= \lambda \int \frac{\delta \mathcal{L}}{\delta q}(q_t)(\theta) \nabla \cdot \left(q_t(\theta) \nabla \log \frac{q_t}{p_{q_t}}(\theta) \right) d\theta \\ &= -\lambda \int q_t(\theta) \nabla \frac{\delta \mathcal{L}}{\delta q}(q_t)(\theta)^\top \nabla \log \frac{q_t}{p_{q_t}}(\theta) d\theta \\ &= -\lambda^2 \int q_t(\theta) \|\nabla \log \frac{q_t}{p_{q_t}}(\theta)\|_2^2 d\theta \\ &\leq -2\alpha\lambda^2 \text{KL}(q_t \| p_{q_t}) \\ &\leq -2\alpha\lambda(\mathcal{L}(q_t) - \mathcal{L}(q_*)). \end{aligned}$$

The Grönwall's inequality finishes the proof.

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We also obtain a **time-discretized version** of this result. See our paper for details.

Primal-Dual Viewpoint

Duality for empirical risk [Oko, Suzuki, Nitanda, and Denny (2022)] :

$$\begin{aligned} & \min_q \left\{ \mathcal{L}(q) = \frac{1}{n} \sum_{i=1}^n \ell(h_q(x_i), y_i) + \lambda' \mathbb{E}_q[\|\theta\|_2^2] + \lambda \mathbb{E}_q[\log(q(\theta))] \right\} \\ & = \max_{g \in \mathbb{R}^n} \left\{ \mathcal{D}(g) = -\frac{1}{n} \sum_{i=1}^n \ell_i^*(g_i) - \lambda \int q_g(\theta) d\theta \right\}. \end{aligned} \quad \begin{aligned} \ell_i(z) &= \ell(z, y_i), \\ q_g(\theta) &= \exp\left(-\frac{1}{n} \left(\frac{1}{n} \sum_{i=1}^n h_\theta(x_i) g_i + \lambda' \|\theta\|_2^2\right)\right). \end{aligned}$$

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Theorem (Duality Theorem): Set $g_q = \{\partial_z \ell(h_q(x_i), y_i)\}_{i=1}^n$.

Suppose $\ell(\cdot, y)$ is convex and differentiable. Then,

$$0 \leq \mathcal{L}(q) - \mathcal{D}(g_q) = \lambda \text{KL}(q \| p_q).$$

Through the round trip: $q \rightarrow g_q \rightarrow q_{g_q} \propto p_q$, $\text{KL}(q \| p_q)$ exactly measures the duality gap.

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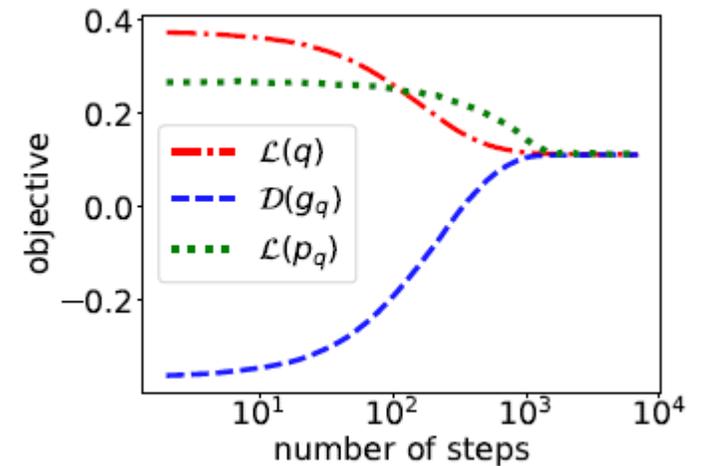
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- **Convergence rate analysis in the continuous-time setting**

[Hu, Ren, Siska, & Szpruch (2019)] shows the linear convergence of mean field Langevin with strong KL-regularization.

- **Quantitative convergence rate analysis under KL-regularization with any strength**

[Nitanda, Denny, & Suzuki (2021)] is the first work that gives the quantitative convergence guarantees by proposing a method which exploits the convexity of the problem.

[Oko, Suzuki, Nitanda, & Denny (2021)] gives an improved guarantee based on the similar idea.

Contribution: global convergence rate analysis for mean field Langevin dynamics with any strength KL-regularization.

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Concurrent work: [Chizat (2022)] also arrived at the same result in continuous time analysis.

Unique contributions in each paper: **time-discretization** and **dual viewpoint** in ours and annealed version in [Chizat (2022)].