Mean-Field Theory of Two-Layers Neural Networks: dimension free bounds and examples

Theodor Misiakiewicz

Stanford University

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Dynamics and Discretization: PDEs, Sampling, and Optimization workshop

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Joint work with Song Mei (UC Berkeley) and Andrea Montanari (Stanford)

A. *Approximation theory for two-layers NNs.*

B. *Mean-Field description of SGD on two-layers NNs.*

C. *Example: classifying centered anisotropic Gaussians.*

D. *Dimension-free bounds between SGD dynamics and mean-field PDE.*

E. *Outline of the proof of the dimension-free bounds.*

Setting

Classical supervised learning setting:

- Given n i.i.d. samples $\{(y_i, x_i)\}_{i \in [n]}$:
  - $x_i \in \mathbb{R}^d$ vector of covariates.
  - $y_i \in \mathbb{R}$ response variable.
  - Common probability distribution $(y_i, x_i) \sim_{i.i.d.} \mathbb{P} \in \mathcal{P}(\mathbb{R} \times \mathbb{R}^d)$.

- Learn model $\hat{f} : \mathbb{R}^d \to \mathbb{R}$ s.t. given a new data point $x_{\mathbf{new}}$ predicts $y_{\mathbf{new}}$ via $\hat{f}(x_{\mathbf{new}})$. Measure the quality of the prediction via the squared error loss:

$$R(\mathbb{P}, \hat{f}) := \mathbb{E}_{(y,x)\sim\mathbb{P}}\left\{ \left(y - \hat{f}(x)\right)^2 \right\}.$$

- Take $\hat{f}$ parametrized by a vector of parameters $\theta \in \mathbb{R}^p$, i.e., $\hat{f} : (x, \theta) \to \hat{f}(x; \theta)$.

- E.g., fit $\hat{\theta}$ by minimizing the empirical risk

$$\hat{R}^{(n)}(\theta) := \frac{1}{n} \sum_{i=1}^{n} \left[y_i - \hat{f}(x_i; \theta) \right]^2.$$

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Two-layers neural networks

- Need a rich enough class of functions to fit complex data.

- Consider two-layers neural networks:

$$\hat{f}_N(x;\boldsymbol{\theta}) := \frac{1}{N}\sum_{i=1}^{N}\sigma_*(x;\boldsymbol{\theta}_i)\,.$$

  - N: number of hidden units (neurons).
  - $\sigma_* : \mathbb{R}^d \times \mathbb{R}^D$ is an activation function.
  - $\boldsymbol{\theta}_i \in \mathbb{R}^D$ parameters which we denote collectively $\boldsymbol{\theta} = (\boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_N) \in \mathbb{R}^{ND}$.

- Standard choice: $\boldsymbol{\theta}_i = (a_i, b_i, \boldsymbol{w}_i)$ with $a_i \in \mathbb{R}, b_i \in \mathbb{R}, \boldsymbol{w}_i \in \mathbb{R}^d$, $D = d + 2$,

$$\sigma_*(x;\boldsymbol{\theta}_i) = a_i\sigma(\langle \boldsymbol{w}_i, x\rangle + b_i)\,,$$

where $\sigma : \mathbb{R} \to \mathbb{R}$, e.g.: $\sigma(x) = \max(x, 0)$ (ReLU) or $\sigma(x) = \frac{1}{1+e^{-2x}}$ (sigmoid).

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Approximation properties

- *Is the function class of two-layers NNs rich enough?*

- Universal Approximation [Cybenko, 1989]: Take $\sigma : \mathbb{R} \to \mathbb{R}$ continuous with $\lim_{x\to\infty} \sigma(x) = 1$ and $\lim_{x\to-\infty} \sigma(x) = 0$. For any $\mathbb{E}\{f(x)^2\} < \infty$ and $\varepsilon > 0$, there exists $N = N(\varepsilon, f)$ such that

$$R_{\text{approx}}(f; N) := \inf_{\{(a_i, b_i, w_i)\}} \mathbb{E}\Big\{\Big[f(x) - \frac{1}{N}\sum_{i=1}^{N} a_i \sigma(\langle w_i, x\rangle + b_i)\Big]^2\Big\} \le \varepsilon .$$

- *How big should $N(\varepsilon, f)$ be for reasonable functions?*

- Barron's Theorem [Barron, 1993]: $\|x\|_2 \le r$ on the support of $\mathbb{P}$ and $f : \mathbb{R}^d \to \mathbb{R}$ has Fourier transform F such that $f(x) = \int e^{i\langle x, w\rangle} F(w) \mathrm{d}w$. Then

$$R_{\text{approx}}(f; N) \le \frac{\Delta(f)^2}{N}, \qquad \Delta(f) := 2r \int \|w\|_2 |F(w)| \mathrm{d}w .$$

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Insights from approximation theory

- Suggest that we should *represent two-layers NN with distribution* $\rho \in \mathcal{P}(\mathbb{R}^D)$:

$$\hat{f}(x;\rho) = \int \sigma_*(x;\boldsymbol{\theta})\rho(\mathrm{d}\boldsymbol{\theta}) .$$

E.g., take $\hat{\rho}^{(N)} = N^{-1}\sum_{i\le N}\delta_{\boldsymbol{\theta}_i}$ for finite networks: $\hat{f}_N(x;\boldsymbol{\theta}) = \hat{f}(x;\hat{\rho}^{(N)})$.

- *Small population risk achieved by many NNs*: what matters is ρ, not $\boldsymbol{\theta}_1,\ldots,\boldsymbol{\theta}_N$. Behavior is insensitive to the number of neurons N, as long as it is large enough for $\hat{\rho}^{(N)}$ to approximate ρ.

- Minimum number of neurons to achieve certain accuracy depends on the *intrinsic regularity* of f (e.g., $\Delta(f)$) and not on the dimension d.

These insights concern *ideal representations*.

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Training with SGD

- In practice, the parameters of NNs are learned by SGD or its variants.

- SGD: initialize weights $\boldsymbol{\theta}_i \sim_{iid} \rho_0$. At each step k, sample (x_k, y_k) and update

$$\boldsymbol{\theta}_i^{k+1} = \boldsymbol{\theta}_i^k + \varepsilon\big(y_k - \hat{f}_N(x_k; \boldsymbol{\theta}^k)\big)\nabla_{\boldsymbol{\theta}_i}\sigma_*(x_k; \boldsymbol{\theta}_i^k)\,.$$

ε: step size; $\boldsymbol{\theta}^k = (\boldsymbol{\theta}_i^k)_{i\le N}$: parameters after k iterations.

What are the properties of NNs reached by SGD?

- Do they have small test error? Are they fairly insensitive to the number N of neurons (as long as N is large enough) and the dimension d, as in approximation theory?

- Recent analysis connects naturally SGD dynamics and approximation theory.
  [Mei,Montanari,Nguyen,'18], [Chizat,Bach,'18], [Sirignano,Spiliopoulos,'18], [Rotskoff,Vanden-Eijnden,'18]

  Mean-field theory: SGD dynamics admits an asymptotic description as $N \to \infty, \varepsilon \to 0$ in terms of a PDE in the space of probability distributions on $\mathbb{R}^D$.

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Mean-field limit

- One-pass SGD: training examples are never revisited, i.e., $\{(x_k, y_k)\}_{k\geq 1}$ are iid.
- Denote $\hat{\rho}_k^{(N)} = N^{-1}\sum_{i\leq N}\delta_{\theta_i^k}$ after k SGD steps with step size ε and $\theta_i^0 \sim_{iid} \rho_0$:

$$\hat{\rho}_{t/\varepsilon}^{(N)} \Rightarrow \rho_t, \qquad \text{as } N\to\infty,\ \varepsilon\to 0\,.$$

- Evolution of ρ_t given by the following PDE (of *McKean-Vlasov* type):

$$\partial_t\rho_t = \nabla_{\theta}\cdot\Big(\rho_t\nabla_{\theta}\Psi(\theta;\rho_t)\Big)\,,$$
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This is referred to as the *mean-field* description, or *distributional dynamics* (DD).

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- Evolution of ρ_t given by the following PDE (of *McKean-Vlasov* type):

$$\partial_t\rho_t = \nabla_{\boldsymbol{\theta}}\cdot\Big(\rho_t\nabla_{\boldsymbol{\theta}}\Psi(\boldsymbol{\theta};\rho_t)\Big)\,,$$

$$\Psi(\boldsymbol{\theta};\rho_t) \equiv V(\boldsymbol{\theta}) + \int U(\boldsymbol{\theta},\boldsymbol{\theta}')\rho(\mathrm{d}\boldsymbol{\theta}')\,,$$

where $V(\boldsymbol{\theta}) := -\mathbb{E}\{y\sigma_*(x;\boldsymbol{\theta})\}$ and $U(\boldsymbol{\theta}_1,\boldsymbol{\theta}_2) := \mathbb{E}_x\{\sigma_*(x;\boldsymbol{\theta}_1)\sigma_*(x;\boldsymbol{\theta}_2.)\}$.

This is referred to as the *mean-field* description, or *distributional dynamics* (DD).

- Wasserstein gradient flow on risk $R(\rho) := \mathbb{E}\{(y-\hat{f}(x;\rho))^2\}$, with $\rho\in\mathcal{P}(\mathbb{R}^D)$

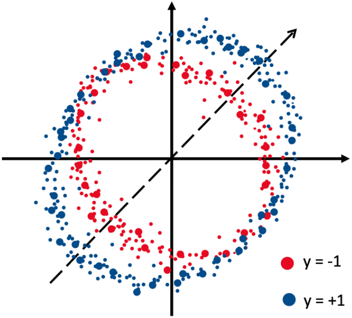
Example: classifying centered anisotropic Gaussians (I)

Data distribution (y, x):

With proba $1/2$: $y = +1$, $x \sim N(0, \Sigma_+)$,

With proba $1/2$: $y = -1$, $x \sim N(0, \Sigma_-)$,

- $\Sigma_\pm = U \mathrm{diag}((1 \pm \Delta)^2 \cdot \mathrm{Id}_{s_0}, \mathrm{Id}_{d-s_0}) U^\mathsf{T}$.
- $U \in \mathbb{R}^{d \times d}$ orthogonal matrix.
- $P_\mathcal{V}$: projection on the subspace $\mathcal{V} = \mathrm{span}(U_{1:s_0})$.



Consider activation function $\sigma_*(x; \theta) = \sigma(\langle x, w \rangle)$ (i.e., $\theta = w \in \mathbb{R}^d$).

Goal: study SGD on

$$R_N(\theta) = \mathbb{E}\left\{ \left(y - \frac{1}{N} \sum_{i=1}^{N} \sigma(\langle x, w_i \rangle) \right)^2 \right\}.$$

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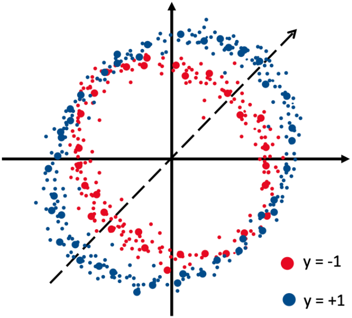

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Mean-field description of SGD in this problem:

- $(x, y) \sim \mathbb{P}$ is invariant under $\mathcal{O}(\mathcal{V}) \times \mathcal{O}(\mathcal{V}^\perp)$.
- Denote $r_1 := \|P_\mathcal{V} w\|_2$ and $r_2 := \|(\mathrm{Id} - P_\mathcal{V})w\|_2$. If ρ_0 is spherically symmetric, solution ρ_t of DD remains uniform conditional on r_1, r_2:

$$\rho_t(w) = \bar{\rho}_t(r_1, r_2) \times \mu_{s_0}(P_\mathcal{V} w / r_1) \times \mu_{d-s_0}((\mathrm{Id} - P_\mathcal{V})w / r_2), \qquad \mu_p \equiv \mathrm{Unif}(\mathbb{S}^{p-1}).$$

  (global optimum must be of this form by Jensen's inequality).
- PDE on $\rho_t \in \mathcal{P}(\mathbb{R}^d)$ simplifies to PDE on $\bar{\rho}_t \in \mathcal{P}([0, \infty)^2)$:

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- PDE in 2 dimensions: efficient to solve numerically, can classify stationary points...

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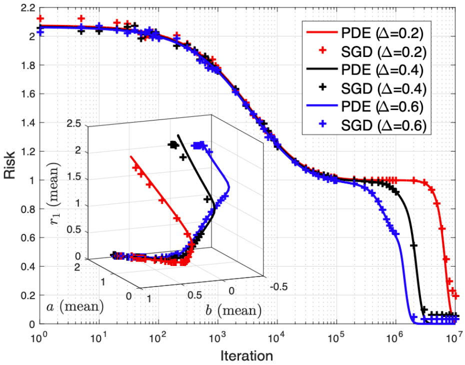
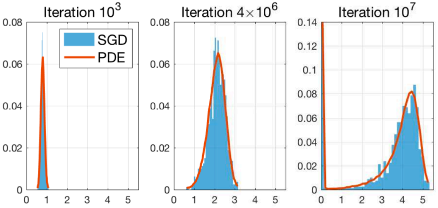
Example: classifying centered anisotropic Gaussians (III)





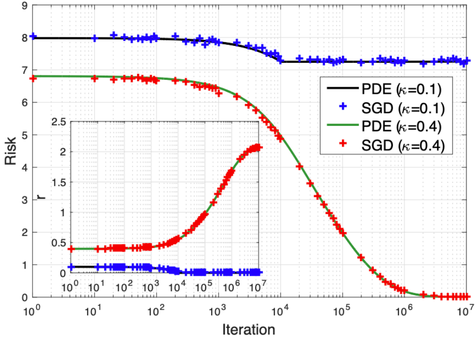
ReLu activation:
$\sigma_*(x;\boldsymbol{\theta}_i) = a_i(\langle x, w_i\rangle + b_i)_+$.

Evolution of some statistics:
$d = 320$, $s_0 = 60$, $N = 800$,
$\varepsilon = 2\times 10^{-4}$.

Evolution of $\bar{\rho}(r_1)$ for $d = s_0 = 40$,
$N = 800$, $\Delta = 0.8$, $\varepsilon = 10^{-6}$,
$\rho_0 = N(0, 0.8^2 \mathrm{Id}_d/d)$.

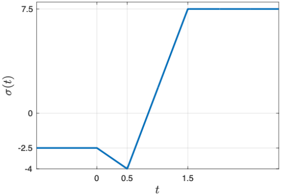
[Mei, Montanari, Nguyen, 2018]

Example: classifying centered anisotropic Gaussians (IV)



Evolution of the risk for $d = s_0 = 320$, $\Delta = 0.5$, $N = 800$.

Starting at two initializations: $N(0, \kappa^2 \mathrm{Id}_d/d)$ with $\kappa \in \{0.1, 0.4\}$.



Non-monotonic activation function.

[Mei, Montanari, Nguyen, 2018]

Mean-field: good theory for SGD?

Mean-field description:

- Independent of N (as long as N is large enough).

Simplify the analysis of SGD:

- Factors-out some landscape complexities of NNs (e.g., permutation invariance).
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Concentration of SGD process on PDE

More precisely:

- $\boldsymbol{\theta}^k = (\boldsymbol{\theta}_i^k)_{i \le N}$: weights after k steps of one-pass SGD with step-size ε and $(\boldsymbol{\theta}_i^0)_{i \le N} \sim_{iid} \rho_0$.
- $(\rho_t)_{t \ge 0}$: solution of the *distribution dynamics* with initialization ρ_0.

Goal: compare population risks $R_N(\boldsymbol{\theta}^k)$ and $R(\rho_t)$.

Show that for $T \ge 0$ and with probability at least $1 - \delta$,

$$\sup_{k \in [0, T/\varepsilon] \cup \mathbb{N}} \left| R_N(\boldsymbol{\theta}^k) - R(\rho_{k\varepsilon}) \right| \le \mathrm{Error}(T, \varepsilon, N, \delta, \ldots) .$$

Assumptions

Take $\boldsymbol{\theta} = (a, w)$ with $a \in \mathbb{R}$ and $w \in \mathbb{R}^{D-1}$ and activation $\sigma_*(x; \boldsymbol{\theta}) = a\sigma(x; w)$.

Denote $V(\boldsymbol{\theta}) = av(w)$ and $U(\boldsymbol{\theta}_1, \boldsymbol{\theta}_2) = a_1 a_2 u(w_1, w_2)$ where

$$v(w) = -\mathbb{E}\{y\sigma(x; w)\}, \qquad u(w_1, w_2) = \mathbb{E}_x\{\sigma(x; w_1)\sigma(x; w_2)\}.$$

Assumptions:

A1. $\sigma : \mathbb{R}^d \times \mathbb{R}^{D-1}$ and y are bounded, i.e., $\|\sigma\|_\infty, |y| \leq K_1$.
For any w, $\nabla_w \sigma(x; w)$ is K_1-sub-Gaussian with respect to $x \sim \mathbb{P}$.

A2. Functions $w \mapsto v(w)$ and $(w_1, w_2) \mapsto u(w_1, w_2)$ are differentiable with bounded and Lipschitz gradients: $\|\nabla v(w)\|_2 \leq K_2$, $\|\nabla u(w_1, w_2)\|_2 \leq K_2$,

$$\|\nabla v(w) - \nabla v(w')\|_2 \leq K_2 \|w - w'\|_2,$$
$$\|\nabla u(w_1, w_2) - \nabla u(w_1', w_2')\|_2 \leq K_2 \|(w_1, w_2) - (w_1', w_2')\|_2.$$

A3. Initialization $\rho_0 \in \mathcal{P}(\mathbb{R}^D)$ is supported on $|a_i| \leq K_3$.

Dimension-free bound (I)

Consider two cases:

- General coe□cients: initialize parameters $\boldsymbol{\theta}_i^0 = (a_i^0, w_i^0)$ as $(\boldsymbol{\theta}_i^0)_{i \le N} \sim_{iid} \rho_0$. Update both a_i and w_i during the dynamics.

- Fixed coe□cients: same initialization but only update w_i during the dynamics.

Theorem (Mei, Misiakiewicz, Montanari, 2019)

Let σ_* verifies assumptions A1-A3. Take $T \ge 1$.

Fixed coe□cients: $\exists K$ depending only on K_1-K_3 such that with proba at least $1 - e^{-z^2}$,

$$\sup_{k \in [0, T/\varepsilon] \cup \mathbb{N}} \left| R_N(\boldsymbol{\theta}^k) - R(\rho_{k\varepsilon}) \right| \le K e^{KT} \frac{1}{\sqrt{N}} [\sqrt{\log N} + z] + K e^{KT} [\sqrt{D + \log(N)} + z] \sqrt{\varepsilon}\,.$$

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Dimension-free bound (II)

With probability at least $1 - 1/N$:

$$\sup_{k \in [0, T/\varepsilon] \cup \mathbb{N}} \left| R_N(\boldsymbol{\theta}^k) - R(\rho_{k\varepsilon}) \right| \leq \underbrace{Ke^{KT} \sqrt{\frac{\log N}{N}}}_{\text{error due to finite } N} + \underbrace{Ke^{KT} \sqrt{D + \log(N)} \sqrt{\varepsilon}}_{\text{error due to discretization } \varepsilon > 0} .$$

Provided $T, K = O(1)$, the mean-field approximation is accurate for

- *Number of neurons:* $N \gg 1$ independent of D, and only depends on intrinsic properties of the activation and data distribution.
- *Step-size:* $\varepsilon \ll 1/D$.

'Dimension-free bound': N does not depend directly on D.
The K_i's in the assumption can potentially depend on D. However in a number of setting of interests, the K_i's are independent of D.

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Application: classifying centered anisotropic Gaussians (V)

- $\Sigma_{\pm} = U\mathrm{diag}((1 \pm \Delta)^2 \cdot \mathrm{Id}_{s_0}, \mathrm{Id}_{d-s_0})U^{\mathsf{T}}$ with $s_0 = \gamma d$ and $\gamma \in (0, 1)$.
- $\sigma(t) = 0$ for $t \leq 0$, $\sigma(t) = 1$ for $t \geq 1$, and $\sigma(t) = t$ for $0 \leq t \leq 1$ (truncated ReLu).
- $(w_i^0)_{i \leq N} \sim_{iid} \bar{\rho}_0 \times \mathrm{Unif}(\mathbb{S}^{d-1})$ with $\bar{\rho}_0$ with bounded density and $R_{d=\infty}(\bar{\rho}_0) < 1$.

Theorem (Mei, Misiakiewicz, Montanari, 2019)

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such that for $d \geq d_0$, $N \geq C_0$ and $\varepsilon \leq 1/(C_0 d)$, we have at $k = T/\varepsilon$ with probability at least $1 - \delta$,

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Theorem (Mei, Misiakiewicz, Montanari, 2019)

For any $\eta, \Delta, \delta > 0$, there exists

$$d_0 \equiv d_0(\eta, \bar{\rho}_0, \Delta, \gamma), \qquad C_0 \equiv C_0(\eta, \bar{\rho}_0, \Delta, \gamma), \qquad T \equiv T(\eta, \bar{\rho}_0, \Delta, \gamma)\,,$$

such that for $d \geq d_0$, $N \geq C_0$ and $\varepsilon \leq 1/(C_0 d)$, we have at $k = T/\varepsilon$ with probability at least $1 - \delta$,

$$R_N(\boldsymbol{\theta}^k) \leq \inf_{\rho} R(\rho) + \eta/2 \leq \inf_{\boldsymbol{\theta} \in \mathbb{R}^{N \times d}} R_N(\boldsymbol{\theta}) + \eta\,.$$

For $N = O(1)$ and $n = O(d)$, one-pass SGD finds a near global minimizer of the population risk (near global minimizer over all two-layers neural networks).

Global convergence of SGD with mean-field theory

Strategy to prove (quantitative) global convergence of SGD:

- *Global convergence of the PDE* (e.g., [Chizat, Bach, 2018]).
- *Bound the time to convergence* T_c (e.g., [Javanmard, Mondelli, Montanari, 2019]).
- *Bound between SGD and PDE:* unfortunately, current bound is $e^{KT}/\sqrt{N}$, hence it is non-vacuous only if $T_c \ll \log(N)$.

Strategy already applies to some non-trivial examples (e.g., anisotropic Gaussians).

Noisy SGD and entropic regularization

- Noisy SGD:

$$\boldsymbol{\theta}_i^{k+1} = \boldsymbol{\theta}_i^k + \varepsilon(y_k - \hat{f}_N(x_k; \boldsymbol{\theta}^k))\nabla_{\boldsymbol{\theta}_i}\sigma_*(x_k; \boldsymbol{\theta}_i^k) + \sqrt{\varepsilon/\beta} \cdot g_i^k ,$$

where $g_i^k \sim_{iid} N(0, \mathrm{Id}_D)$.

- Mean-field description:

$$\partial_t \rho_t = \nabla_{\boldsymbol{\theta}} \cdot \big(\rho_t \nabla_{\boldsymbol{\theta}} \Psi(\boldsymbol{\theta}; \rho_t)\big) + \frac{1}{\beta}\Delta_{\boldsymbol{\theta}} \rho_t \, .$$

- Wasserstein gradient flow for the free energy: $F_\beta(\rho) = R(\rho) + \frac{1}{\beta}\int \rho(\boldsymbol{\theta}) \log \rho(\boldsymbol{\theta}) \mathrm{d}\boldsymbol{\theta}$.

- [Mei, Montanari, Nguyen, 2018] convergence $\rho_t \Rightarrow \rho_*^\beta$ global minimizer $F_\beta(\rho)$. Under some regularity conditions,

$$R(\rho_*^\beta) \leq \inf_\rho R(\rho) + O\Big(\frac{D}{\beta}\Big) \, .$$

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Bounds with noisy SGD

Theorem (Mei, Misiakiewicz, Montanari, 2019)

Let σ_* verifies assumptions A1-A3, $\tau \leq K_4$ and $T \geq 1$.

Fixed coe□cients: $\exists K$ depending only on K_1-K_4 such that with proba at least $1 - e^{-z^2}$

$$\sup_{k \in [0, T/\varepsilon] \cup \mathbb{N}} \left| R_N(\boldsymbol{\theta}^k) - R(\rho_{k\varepsilon}) \right| \leq K e^{KT} \frac{1}{\sqrt{N}} [\sqrt{\log N} + z] + K e^{KT} [\sqrt{D + \log(N)} + z] \sqrt{\varepsilon} \, .$$

General coe□cients: $\exists K$ depending only on K_1-K_4 such that with proba at least $1 - e^{-z^2}$

$$\sup_{k \in [0, T/\varepsilon] \cup \mathbb{N}} \left| R_N(\boldsymbol{\theta}^k) - R(\rho_{k\varepsilon}) \right| \leq K e^{e^{KT}[\sqrt{\log N} + z^2]} [\sqrt{D \log N} + \log^{3/2}(NT) + z^5] / \sqrt{N}$$

$$+ K e^{e^{KT}[\sqrt{\log N} + z^2]} [\sqrt{D} \log(NT/\varepsilon) + \log^{3/2}(N) + z^6] \sqrt{\varepsilon} \, .$$

General coefficients: harder to control. The bound is not dimension-free and only allows us to control the approximation error up to $T = o(\log \log N)$ instead of $T = o(\log N)$.

Outline of the proof of the non-asymptotic bound (I)

Ingredients: isolating different error terms + coupling + concentration-of-measure.

Consider four coupled dynamics:

- *Nonlinear dynamics (ND):* $\overline{\boldsymbol{\theta}}_i^0 \sim_{iid} \rho_0$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\overline{\boldsymbol{\theta}}_i^t = -\Big[\nabla V(\overline{\boldsymbol{\theta}}_i^t) + \int \nabla_1 U(\overline{\boldsymbol{\theta}}_i^t, \boldsymbol{\theta})\rho_t(\mathrm{d}\boldsymbol{\theta})\Big]\,.$$

- *Particle dynamics (PD):* $\underline{\boldsymbol{\theta}}_i^0 = \overline{\boldsymbol{\theta}}_i^0$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\underline{\boldsymbol{\theta}}_i^t = -\Big[\nabla V(\underline{\boldsymbol{\theta}}_i^t) + \frac{1}{N}\sum_{j=1}^N \nabla_1 U(\underline{\boldsymbol{\theta}}_i^t, \underline{\boldsymbol{\theta}}_j^t)\Big]\,.$$

- *Gradient descent (GD):* $\tilde{\boldsymbol{\theta}}_i^0 = \overline{\boldsymbol{\theta}}_i^0$,

$$\tilde{\boldsymbol{\theta}}_i^{k+1} = \tilde{\boldsymbol{\theta}}_i^k - \varepsilon\Big[\nabla V(\tilde{\boldsymbol{\theta}}_i^k) + \frac{1}{N}\sum_{j=1}^N \nabla_1 U(\tilde{\boldsymbol{\theta}}_i^k, \tilde{\boldsymbol{\theta}}_j^k)\Big]\,.$$

- *Stochastic gradient descent (SGD):* $\boldsymbol{\theta}_i^0 = \overline{\boldsymbol{\theta}}_i^0$,

$$\boldsymbol{\theta}_i^{k+1} = \boldsymbol{\theta}_i^k - \varepsilon\Big[-y_k\nabla_{\boldsymbol{\theta}}\sigma_*(x_k;\boldsymbol{\theta}_i^k) + \frac{1}{N}\sum_{j=1}^N \sigma_*(x_k;\boldsymbol{\theta}_j^k)\nabla_{\boldsymbol{\theta}}\sigma_*(x_k;\boldsymbol{\theta}_i^k)\Big]\,.$$

Outline of the proof of the non-asymptotic bound (II)

$$\left|R(\rho_{k\varepsilon}) - R_N(\boldsymbol{\theta}^k)\right| \le \underbrace{\left|R(\rho_{k\varepsilon}) - R_N(\overline{\boldsymbol{\theta}}^{k\varepsilon})\right|}_{\mathrm{PDE-ND}} + \underbrace{\left|R_N(\overline{\boldsymbol{\theta}}^{k\varepsilon}) - R_N(\underline{\boldsymbol{\theta}}^{k\varepsilon})\right|}_{\mathrm{ND-PD}}$$
$$+ \underbrace{\left|R_N(\underline{\boldsymbol{\theta}}^{k\varepsilon}) - R_N(\tilde{\boldsymbol{\theta}}^k)\right|}_{\mathrm{PD-GD}} + \underbrace{\left|R_N(\tilde{\boldsymbol{\theta}}^k) - R_N(\boldsymbol{\theta}^k)\right|}_{\mathrm{GD-SGD}}.$$

- PDE-ND: $\overline{\boldsymbol{\theta}}^{k\varepsilon} \sim_{iid} \rho_{k\varepsilon}$ + McDiarmid's inequality.
- ND-PD: McDiarmid's inequality + Gronwall's inequality.
- PD-GD: Lipschitzness + Gronwall's lemma.
- GD-SGD: Azuma-Hoeffding inequality + Gronwall's lemma.

Details in:

Mean-field theory of two-layers neural networks: dimension-free bounds and kernel limit.
Mei, Misiakiewicz, Montanari, COLT 2019.

Final remarks

- Mean-field theory: describe SGD for $N \to \infty, \varepsilon \to 0$, in terms of a PDE in the space of probability distributions.
- It allows to focus on key elements of the dynamics (global convergence, stationary points), and in some cases vastly simplifies the analysis of SGD.
- Dimension-free bounds: to approximate the SGD dynamics by the distributional dynamics, we only need $N = O(1)$ that depends on intrinsic properties of the activation and data distribution, and $\varepsilon = O(1/D)$.
- Capturing the correct dimension-dependence is crucial in order to compare neural networks to other learning techniques.
- Lots of open problems: global convergence guarantees, bounding convergence time, improving the exponential dependency in T, multi-layer etc.

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