A general framework for the mean field limit of multilayer neural networks

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(Joint with Phan-Minh Nguyen)

One World Seminar on the Mathematics of Machine Learning July 25, 2020

The setting

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Data distribution:

$$(y,x) \sim \mathbb{P}$$
.

Model:

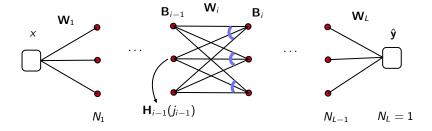
$$\hat{y} = f(x; \theta).$$

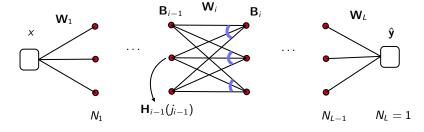
We are interested in the class of models given by deep neural networks.

Optimization problem:

$$\min_{\theta \in \Theta} \mathbb{E}[\ell(\hat{y}, y)].$$

We are interested in solving the optimization problem using stochastic gradient descent.





The model:

$$\begin{aligned} \mathbf{H}_{1}(x,j_{1}) &= \phi_{1}(\mathbf{w}_{1}(j_{1}),x), \qquad \forall j_{1} \in [N_{1}], \\ \mathbf{H}_{i}(x,j_{i}) &= \frac{1}{N_{i-1}} \sum_{j_{i-1}=1}^{N_{i-1}} \phi_{i}(\mathbf{w}_{i}(j_{i-1},j_{i}),\mathbf{b}_{i}(j_{i}),\mathbf{H}_{i-1}(x,j_{i-1})), \\ \forall j_{i} \in [N_{i}], i \in [2,L], \\ \mathbf{\hat{y}}(x) &= \phi_{L+1}(\mathbf{H}_{L}(x,1)). \end{aligned}$$

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•
$$\mathbf{H}_{1}(x) = \mathbf{W}_{1}x \quad \forall j_{1} \in [N_{1}],$$
 $\mathbf{H}_{1}(x, j_{1}) = \mathbf{w}_{1}(j_{1}) \cdot x,$
• $\mathbf{H}_{i}(x) = \mathbf{B}_{i} + \frac{1}{N_{i-1}} \mathbf{W}_{i} \sigma_{i-1}(\mathbf{H}_{i-1}(x)) \quad \forall j_{i} \in [N_{i}], i \in [2, L],$
 $\mathbf{H}_{i}(x, j_{i}) = \frac{1}{N_{i-1}} \sum_{j_{i-1}=1}^{N_{i-1}} \mathbf{b}_{i}(j_{i}) + \mathbf{w}_{i}(j_{i-1}, j_{i}) \sigma_{i-1}(\mathbf{H}_{i-1}(x, j_{i-1})),$
• $\hat{\mathbf{y}}(x) = \sigma_{L}(\mathbf{H}_{L}(x, 1)),$

where

$$\mathbf{W}_1 \in \mathbb{R}^{N_1 \times d}, \qquad \mathbf{W}_i \in \mathbb{R}^{N_{i-1} \times N_i}, \ \mathbf{B}_i \in \mathbb{R}^{N_i} \qquad \forall i \in [2, L].$$

$$\begin{split} \mathbf{w}_1(t+1,j_1) &= \mathbf{w}_1(t,j_1) - \varepsilon \textcolor{red}{N_1} \nabla_{\mathbf{w}_1(j_1)} \ell(\hat{\mathbf{y}}(t,x(t)),y(t)), \\ \mathbf{w}_i(t+1,j_{i-1},j_i) &= \mathbf{w}_i(t,j_{i-1},j_i) - \varepsilon \textcolor{red}{N_{i-1}} \textcolor{red}{N_i} \nabla_{\mathbf{w}_i(j_{i-1},j_i)} \ell(\hat{\mathbf{y}}(t,x(t)),y(t)), \\ \mathbf{b}_i(t+1,j_i) &= \mathbf{b}_i(t,j_i) - \varepsilon \textcolor{red}{N_i} \nabla_{\mathbf{b}_i(j_i)} \ell(\hat{\mathbf{y}}(t,x(t)),y(t)). \end{split}$$

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Remarks.

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• The gradients are scaled so that weight movement is of order 1.

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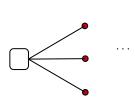
- The gradients are scaled so that weight movement is of order 1.
- The derivation of the mean field limit applies to more general dynamics.

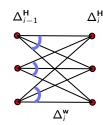
In the standard model:

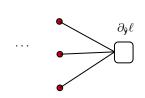
$$\begin{split} & \textcolor{red}{\mathsf{N}_1 \nabla_{\mathbf{w}_1(j_1)} \ell(\hat{\mathbf{y}}(t,x(t)),y(t))} = \Delta_1^\mathsf{H}(y,x,j_1)x, \\ & \textcolor{red}{\mathsf{N}_{i-1} \mathsf{N}_i \nabla_{\mathbf{w}_i(j_{i-1},j_i)} \ell(\hat{\mathbf{y}}(t,x(t)),y(t))} = \Delta_i^\mathsf{H}(y,x,j_i)\sigma_{i-1}(\mathsf{H}_{i-1}(x,j_{i-1})), \\ & \textcolor{red}{\mathsf{N}_i \nabla_{\mathbf{b}_i(j_i)} \ell(\hat{\mathbf{y}}(t,x(t)),y(t))} = \Delta_i^\mathsf{H}(y,x,j_i), \end{split}$$

where

$$\begin{split} & \Delta_L^{\mathsf{H}}(y,x,j_L) = \partial_{\hat{\mathbf{y}}}\ell(y,\hat{\mathbf{y}}(x))\sigma_L'(\mathsf{H}_L(x,j_L)), \\ & \Delta_{i-1}^{\mathsf{H}}(y,x,j_{i-1}) = \frac{1}{N_i}\sum_{j_i=1}^{N_i}\Delta_i^{\mathsf{H}}(y,x,j_i)\mathsf{w}_i(t,j_{i-1},j_i)\sigma_{i-1}'(\mathsf{H}_{i-1}(x,j_{i-1})). \end{split}$$







In the general model:

$$N_{1}\nabla_{\mathbf{w}_{1}(j_{1})}\ell(\hat{\mathbf{y}}(t,x(t)),y(t)) = \Delta_{1}^{\mathsf{H}}(y,x,j_{1})x,$$

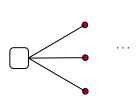
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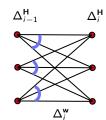
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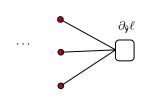
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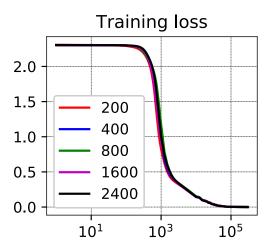
$$\Delta_{i-1}^{\mathsf{H}}(y,x,j_{i-1}) = \frac{1}{N_i} \sum_{i-1}^{N_i} \psi(\Delta_i^{\mathsf{H}}(y,x,j_i), \mathbf{w}_i(t,j_{i-1},j_i), \mathbf{H}_{i-1}(x,j_{i-1})).$$







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MNIST, 3-layer nets, $N_1 = N_2 = 200, 400, ...$

In the large width limit, the mean field limit is obtained in the setting of i.i.d. initialization by Araújo-Oliveira-Yukimura and Sirignano-Spiliopoulos. The i.i.d. initialization plays an important role, and the limit formulation hinges on certain degeneracy in the dynamics.

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- Our formulation of the mean field limit applies to general initialization distributions where there is no degeneracy in the dynamics.
- The limit formulation is based on an infinite width representation that factors out the symmetries of the neurons in the hidden layer, and applies to general dynamics on systems with mean-field interactions.

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- Our formulation of the mean field limit applies to general initialization distributions where there is no degeneracy in the dynamics.
- The limit formulation is based on an infinite width representation that
 factors out the symmetries of the neurons in the hidden layer, and applies
 to general dynamics on systems with mean-field interactions.
- Specializing to i.i.d. initializations, the degeneracy properties of the dynamics can be readily recovered from the framework.

D. Araújo, R. Oliveira, D. Yukimura, arXiv:1906.00193 (2019).

J. Sirignano, K. Spiliopoulos, arXiv:1903.04440 (2019).

P.-M. Nguyen, arXiv:1902.02880 (2019).

'Neuronal embedding'

Plan of the talk Description of the infinite width limit

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Equivalent description:

$$\hat{\mathbf{y}}(x) = \mathbf{E}_{w \sim \rho_N} [\sigma(w, x)],$$

where $\rho_N = \frac{1}{N} \sum_{i=1}^N \delta_{\mathbf{w}_i}$ is the empirical measure of the neurons.

Infinite width limit

The infinite width limit of a two-layer network can be captured by a general distribution over \mathbb{R}^d .

$$\hat{y}(x) = \mathbf{E}_{w \sim \rho_N}[\sigma(w, x)] \longrightarrow \hat{y} = \mathbf{E}_{w \sim \rho}[\sigma(w, x)].$$

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This does not generalize to networks with more than two layers:

• For *L*-layer networks, the symmetry group acts as follows: For permutation matrices Π_1, \ldots, Π_{L-1} ,

$$\hat{\mathbf{y}}(x; \mathbf{W}_1, \dots, \mathbf{W}_L) = \hat{\mathbf{y}}(x; \Pi_1 \mathbf{W}_1, \Pi_2 \mathbf{W}_2 \Pi_1^T, \dots, \mathbf{W}_L \Pi_{L-1}^T).$$

• Difficult to factor out symmetry to a distributional representation due to complex interaction with $\mathbf{W}_2, \dots, \mathbf{W}_{L-1}$.

Constructing the infinite width network - Two-layer case

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Claim

There exists a probability space (Ω, P) such that any two-layer network can be written as

$$\hat{\mathbf{y}}(x) = \mathbf{E}_{C \sim P}[\sigma(w(C), x)],$$

for a measurable function w on (Ω, P) .

Finite width:

$$\mathbf{H}_{i}(x,j_{i}) = \frac{1}{N_{i-1}} \sum_{j_{i-1}=1}^{N_{i-1}} \phi_{i}(\mathbf{b}_{i}(j_{i}), \mathbf{w}_{i}(j_{i-1},j_{i}), \mathbf{H}_{i-1}(x,j_{i-1})),$$

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Infinite width:

For (c_1, \ldots, c_L) in some probability space $(\Omega_1 \times \cdots \times \Omega_L, P_1 \times \cdots \times P_L)$ with $\Omega_L = \{1\}$, and functions $w_i : \Omega_{i-1} \times \Omega_i \to \mathbb{W}_i$, $b_i : \Omega_i \to \mathbb{B}_i$, let

$$H_i(x,c_i) = \mathbb{E}_{C_{i-1} \sim P_{i-1}} [\phi_i(b_i(c_i), w_i(C_{i-1}, c_i), H_{i-1}(x, C_{i-1}))],$$

$$\hat{y}(x; w, b) = \phi_{L+1}(H_L(x, c_L)).$$

Claim

There exists a probability space $(\Omega_1 \times \cdots \times \Omega_L, P_1 \times \cdots \times P_L)$ and measurable functions $w_i : \Omega_{i-1} \times \Omega_i \to \mathbb{W}_i$, $b_i : \Omega_i \to \mathbb{B}_i$, such that any depth L network can be written as

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This talk: focus on optimization aspect (would be interesting to study generalization, approximation, etc.).

Dynamics of the infinite width network

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$$\begin{split} \partial_t w_i(t,c_{i-1},c_i) &= -\mathbb{E}_{(y,x)}[\nabla_{w_i(c_{i-1},c_i)}\ell(\hat{y},y)] \\ &= -\mathbb{E}_{(y,x)}[\mathbb{E}_{C_{i+1}\sim P_{i+1}}[\psi_i^w(w_i(t,c_{i-1},c_i),w_{i+1}(t,c_i,C_{i+1}),\\ &\qquad \qquad H_{i+1}(x,C_{i+1}),H_{i-1}(x,c_{i-1}))]].\\ \partial_t b_i(t,c_i) &= -\mathbb{E}_{(y,x)}[\nabla_{b_i(c_i)}\ell(\hat{y},y)] \\ &= -\mathbb{E}_{(y,x)}[\mathbb{E}_{C_{i+1}\sim P_{i+1}}[\psi_i^b(b_i(t,c_i),w_{i+1}(t,c_i,C_{i+1}),H_{i+1}(x,C_{i+1}))]]. \end{split}$$

In the standard model:

$$\begin{split} \partial_t w_i(t,c_{i-1},c_i) &= -\mathbb{E}_{(y,x)}[\Delta_i^w(y,x,c_{i-1},c_i)], \\ \partial_t b_i(t,c_i) &= -\mathbb{E}_{(y,x)}[\Delta_i^b(y,x,c_i)], \end{split}$$

where

$$\begin{split} & \Delta_{L}^{H}(y,x,c_{L}) = \partial_{\hat{y}}\ell(\hat{y},y)\phi_{L}'(H_{L}(x,c_{L})), \\ & \Delta_{i-1}^{H}(y,x,c_{i-1}) = \mathbb{E}_{c_{i}}[\Delta_{i}^{H}(y,x,C_{i})w_{i}(t,c_{i-1},C_{i})\phi_{i-1}'(H_{i-1}(x,c_{i-1}))], \\ & \Delta_{i}^{w}(y,x,c_{i-1},c_{i}) = \Delta_{i}^{H}(y,x,c_{i})\phi_{i-1}(H_{i-1}(x,c_{i-1})), \\ & \Delta_{i}^{b}(y,x,c_{i}) = \Delta_{i}^{H}(y,x,c_{i}), \\ & \Delta_{1}^{w}(y,x,c_{1}) = \Delta_{1}^{H}(y,x,c_{1})x. \end{split}$$

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Sampling procedure

• Consider a neuronal ensemble $(\Omega_1 \times \cdots \times \Omega_L, P_1 \times \cdots \times P_L)$ and measurable functions

$$w_i^0: \Omega_{i-1} \times \Omega_i \to \mathbb{W}_i, \qquad b_i^0: \Omega_i \to \mathbb{B}_i.$$

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• For $i \in [L]$ and $j_i = 1, 2, ..., N_i$, sample $C_i(j_i)$ independently at random from (Ω_i, P_i) .

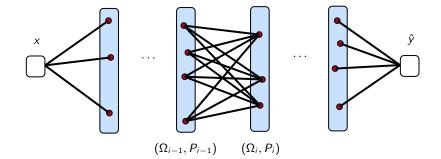
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- For $i \in [L]$ and $j_i = 1, 2, ..., N_i$, sample $C_i(j_i)$ independently at random from (Ω_i, P_i) .
- Construct the neural network of widths (N_1, \ldots, N_L) with weights initialized at

$$\mathbf{w}_i(0,j_{i-1},j_i) = w_i^0(C_{i-1}(j_{i-1}),C_i(j_i)), \qquad \mathbf{b}_i(0,j_i) = b_i^0(C_i(j_i)).$$



Neuronal embedding

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Definition (Neuronal embedding)

Consider an L-layer neural network with initialization distribution ρ . A neuronal embedding is a tuple

$$((\Omega_1 \times \cdots \times \Omega_L, P_1 \times \cdots \times P_L), (w_i^0, b_i^0)_{i=1}^L)$$

such that following the sampling procedure for this tuple, the constructed finite width network has the same initialization distribution as ρ .

• The neuronal embedding allows to embed all finite size networks into an infinite width limit.

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- Consider a neuronal embedding

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- The neuronal embedding allows to embed all finite size networks into an infinite width limit.
- Consider a neuronal embedding

$$(\Omega_1 \times \cdots \times \Omega_L, P_1 \times \cdots \times P_L, (w_i^0, b_i^0)_{i=1}^L).$$

• Run the infinite width network dynamics initialized at $(w_i^0, b_i^0)_{i=1}^L$. We refer to $(w_i(t, c_{i-1}, c_i), b_i(t, c_i))_{i=1}^L$ as the mean field limit.

• Consider the sampled neural network with hidden widths N_i :

$$\mathbf{w}_i(0,j_{i-1},j_i) = w_i^0(C_{i-1}(j_{i-1}),C_i(j_i)), \qquad \mathbf{b}_i(0,j_i) = b_i^0(C_i(j_i)).$$

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• Run stochastic gradient descent on the network with step-size ε in time T/ε .

• Consider the sampled neural network with hidden widths N_i :

$$\mathbf{w}_i(0,j_{i-1},j_i) = w_i^0(C_{i-1}(j_{i-1}),C_i(j_i)), \qquad \mathbf{b}_i(0,j_i) = b_i^0(C_i(j_i)).$$

- Run stochastic gradient descent on the network with step-size ε in time T/ε .
- Let

$$\begin{aligned} &\|\mathbf{w} - w\|_{t,\infty} \\ &= \max_{i \in [L], j_{i-1} \in [N_{i-1}], j_i \in [N_i]} \|\mathbf{w}_i(t, j_{i-1}, j_i) - w_i(\varepsilon t, C_{i-1}(j_{i-1}), C_i(j_i))\|, \\ &\|\mathbf{b} - b\|_{t,\infty} \\ &= \max_{i \in [L], j_i \in [N_i]} \|\mathbf{b}_i(t, j_i) - b_i(\varepsilon t, C_i(j_i))\|. \end{aligned}$$

Theorem (Nguyen-P. 2020)

Under some regularity properties of the activations, then with probability at least $1-\delta$, we have

$$\sup_{t \leq T/\varepsilon} \|\mathbf{w} - w\|_{t,\infty} = O_T \left(\sqrt{\log(\max N_i/\delta)} \left(\frac{1}{\sqrt{\min N_i}} + \sqrt{\varepsilon} \right) \right).$$

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- Description of the infinite width limit
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- **5** Global convergence: General *L*-layer network

Theorem (Nguyen-P. 2020)

There exists a neuronal embedding of the neural network whose weights are i.i.d. with law $\mathbf{w}_i \sim \rho_i^w$, $\mathbf{b}_i \sim \rho_i^b$.

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By specializing the general framework to initialization distributions with certain symmetries, we can also characterize the symmetries in the mean field limit.

Theorem - simplified (Nguyen-P. 2020)

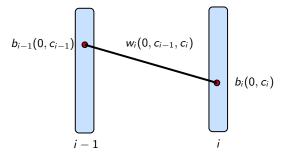
Consider the neural network whose weights are i.i.d. with law $\mathbf{w}_i \sim \rho_i^w$, $\mathbf{b}_i \sim \rho_i^b$. Then for $3 \le i \le L - 2$:

- The middle layer weight $w_i(t, c_{i-1}, c_i)$ is a Borel function of its initial value $w_i(0, c_{i-1}, c_i)$ and the initial biases $b_{i-1}(0, c_{i-1}), b_i(0, c_i)$.
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Theorem (Nguyen-P. 2020)

• For $3 \le i \le L - 2$,

$$w_i(t, c_{i-1}, c_i) = w_i^*(t, w_i(0, c_{i-1}, c_i), b_{i-1}^0(c_{i-1}), b_i^0(c_i)),$$

$$b_i(t, c_i) = b_i^*(t, b_i(0, c_i)).$$

• For i = 1, L,

$$\begin{split} w_1(t,c_1) &= w_1^*(t,w_1(0,c_1),b_1(0,c_1)), \\ b_1(t,c_1) &= b_1^*(t,b_1(0,c_1)), \\ w_L(t,c_{L-1},c_L) &= w_L^*(t,w_L(0,c_{L-1},c_L),b_{L-1}(0,c_{L-1}),b_L(0,c_L)), \\ b_L(t,c_L) &= b_L^*(t,b_L(0,c_L)). \end{split}$$

• For i = 2, L - 1,

$$\begin{split} w_2(t,c_1,c_2) &= w_2^*(t,w_2(0,c_1,c_2),b_2(0,c_2),w_1(0,c_1),b_1(0,c_1)),\\ b_2(t,c_2) &= b_2^*(t,b_2(0,c_2)),\\ w_{L-1}(t,c_{L-2},c_{L-1}) &= w_{L-1}^*(t,w_{L-1}(0,c_{L-2},c_{L-1}),b_{L-1}(0,c_{L-1}),\\ &\qquad \qquad w_L(0,c_{L-1},c_L),b_{L-2}(0,c_{L-2})),\\ b_{L-1}(t,c_{L-1}) &= b_{L-1}^*(t,b_{L-1}(0,c_{L-1}),w_L(0,c_{L-1},c_L)). \end{split}$$

Remark. The Borel functions w^* , b^* can be obtained by solving a self-contained system of ODEs.

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Corollary (Nguyen-P. 2020)

If the biases are initialized to be constants, then the weight w_i at time t only depends on its value at initialization for $3 \le i \le L-2$. Thus, for any positive time t, the middle layer weights $w_i(t,c_{i-1},c_i)$ for $3 \le i \le L-2$ remain i.i.d. random variables.

Furthermore, the pre-activations $H_i(t, c_i)$ are equal for all $2 \le i \le L - 2$.

Corollary (Nguyen-P. 2020)

If we assume the standard model of the neural network with the biases initialized to be constants, then there exists functions $\Delta_i^*:[0,\infty)\to\mathbb{R}$ such that for $3\leq i\leq L-2$,

$$w_i(t, c_{i-1}, c_i) = w_i(0, c_{i-1}, c_i) + \Delta_i^*(t).$$

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Thus, in the standard architecture with no bias, each of the middle layers of the network degenerates to a single translation parameter.

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Assume some regularity properties of the activations, and

- $\partial_{\hat{y}}\ell(\hat{y},y)=0 \Rightarrow \ell(\hat{y},y)=0.$
- Diversity: At initialization, w_1 has full support in \mathbb{R}^d .
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- y = y(x).
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$$\mathbb{E}_{(y,x)}[\ell(\hat{y},y)] \to 0 \text{ as } t \to \infty.$$

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- The loss ℓ does not need to be convex.
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• Our first insight is to look at the second layer weights:

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Question

Can we obtain global convergence for deep neural networks without changing the architecture?

Consider the standard model of an L-layer neural network.

Theorem (Global convergence of the mean field dynamics, Nguyen-P. 2020)

Assume some regularity properties of the activations, and

- $\partial_{\hat{y}}\ell(\hat{y},y)=0 \Rightarrow \ell(\hat{y},y)=0$.
- Bidirectional diversity: $(w_1(0, C_1), w_2(0, C_1, c_2))_{C_1 \sim P_1}$ has full support in $\mathbb{R}^d \times L^2(P_2)$ and $(w_i(0, c_{i-1}, C_i), w_{i+1}(0, C_i, c_{i+1}))_{C_i \sim P_i}$ has full support in $L^2(P_{i-1}) \times L^2(P_{i+1})$ for all $2 \leq i \leq L-1$.
- Universal approximation: $\{f_w(x) = \sigma_1(w \cdot x)\}_{w \in \mathbb{R}^d}$ is dense in $L^2(\mathbb{P}_x)$.
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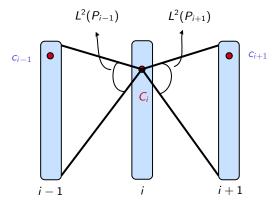
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The bidirectional diversity condition:



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Remarks.

- Global convergence guarantee applies to gradient descent on the fully connected L-layer neural network with no modification to the architecture.
- The bidirectional diversity condition necessitates correlated weight initialization distribution to avoid the degeneracy of the mean field dynamics of i.i.d. initializations.

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• Consider the gradient of the last layer weights:

$$\mathbb{E}_{(y,x)}[\partial_{\hat{y}}\ell(\hat{y},y)\sigma'_L(H_L(t,x,C_L))\sigma_{L-1}(H_{L-1}(t,x,C_{L-1}))] \to 0. \quad \text{(Uniform conv.)}$$

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• Key step. Using a flow argument, we show that at all finite time t: $(w_1(t, \textcolor{red}{C_1}), w_2(t, \textcolor{red}{C_1}, c_2))_{\textcolor{red}{C_1}\sim P_1}$ has full support in $\mathbb{R}^d \times L^2(P_2)$ and $(w_i(t, c_{i-1}, \textcolor{red}{C_i}), w_{i+1}(t, \textcolor{red}{C_i}, c_{i+1}))_{\textcolor{red}{C_i}\sim P_i}$ has full support in $L^2(P_{i-1}) \times L^2(P_{i+1})$ for all $2 \leq i \leq L-1$. (Topological invariance.)

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- The diversity of the weights can be used to show that $H_i(t,x,C_i)$ has full support in $L^2(\mathbb{P}_x)$ for all $i \in [2,L-1]$. Thus, $\sigma_{L-1}(H_{L-1}(t,x,C_{L-1}))$ is dense in $L^2(\mathbb{P}_x)$.

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- The conclusion follows combining the convergence condition with the denseness of $\sigma_{I-1}(H_{I-1}(t,x,C_{I-1}))$.

Our insight on a general scheme for a global convergence mechanism:

 Uniform convergence of the gradient update of an appropriate layer's weights.

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Remarks. The diversity condition is inspired by Chizat-Bach 2018, where global convergence is shown for two-layer networks by a different mechanism.

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- The mean field limit applies to general initialization distributions. When specializing to i.i.d. initializations, it recovers the degeneracy properties of the dynamics.
- The mean field limit can be used to understand global convergence guarantees of stochastic gradient descent.
- For deep fully connected networks, one can obtain global convergence guarantee assuming that the initialization distribution satisfies certain diversity condition that avoids the degeneracy of i.i.d. initializations.

Future directions

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- Quantitative rate of convergence.
- Uniform-in-time coupling with the mean field limit.
- Quantitative effect of depth.

References

A Rigorous Framework for the Mean Field Limit of Multilayer Neural Networks, Phan-Minh Nguyen, Huy Tuan Pham, Jan 2020. arXiv:2001.11443.

A Note on the Global Convergence of Multilayer Neural Networks in the Mean Field Regime, Huy Tuan Pham, Phan-Minh Nguyen, Jun 2020. arXiv:2006.09355.

Thank you!