Provable convergence of NN training in the overparametrized setting

Banach Center – Oberwolfach Graduate Seminar: Mathematics of Deep Learning

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November 21, 2019

University of Vienna

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Introduction and Overview

Introduction

- overparametrized setting: #neurons >> #samples
- convergence of SGD with high probability (over the initialization)
- zero training loss: globally optimal solution
- related literature: [1, 2, 4, 5, 6, 8]

Overview

- training data $((x_i, y_i))_{i=1}^m \subseteq (\mathbb{R}^d \times \mathbb{R})^m$ and label vector $y := (y_i)_{i=1}^m$.
- prediction map $\mathcal{R}\colon \mathbb{R}^P \mapsto \mathbb{R}^m$ of, e.g. a neural network, mapping parameters $\Phi \in \mathbb{R}^P$ to the corresponding prediction, e.g.

$$\mathcal{R}\Phi = \big((W_L \circ \varrho \dots \varrho \circ W_1)(x_i)\big)_{i=1}^m \in \mathbb{R}^m.$$

- consider optimization via gradient flow using squared loss $\mathcal{L}(\hat{y}) := \frac{1}{2}\|\hat{y} - y\|^2$ (for simplicity)

gradient flow

$$\Phi'(t) := -\nabla_\Phi\big[\mathcal{L}(\mathcal{R}\Phi(t))\big] = -\nabla\mathcal{R}\Phi(t)^T(\mathcal{R}\Phi(t) - y)$$

with $\Phi(0) = \Phi_0$ initialized (randomly).

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Dynamics

- linearized prediction model $\bar{\mathcal{R}}\colon \mathbb{R}^P \to \mathbb{R}^m$ at initialization

$$\bar{\mathcal{R}}\Phi := \mathcal{R}(\Phi_0) + \nabla\mathcal{R}(\Phi_0)(\Phi - \Phi_0)$$

- evolve parameter $\bar{\Phi}(t)$ via gradient flow using the same initialization $\bar{\Phi}(0) = \Phi_0$

dynamics of the predictions

1. exact model : $\frac{d\mathcal{R}\Phi(t)}{dt} := -H(t)(\mathcal{R}\Phi(t) - y)$
2. linearized model : $\frac{d\bar{\mathcal{R}}\bar{\Phi}(t)}{dt} := -H(0)(\bar{\mathcal{R}}\bar{\Phi}(t) - y)$

where $H(t) := \nabla\mathcal{R}\Phi(t)\nabla\mathcal{R}\Phi(t)^T \in \mathbb{R}^{m\times m}$

- Proof:

1. $\frac{d\mathcal{R}\Phi(t)}{dt} = \nabla\mathcal{R}\Phi(t)\Phi'(t) = -\underbrace{\nabla\mathcal{R}\Phi(t)\nabla\mathcal{R}\Phi(t)^T}_{:=H(t)}(\mathcal{R}\Phi(t) - y)$

2. $\nabla\bar{\mathcal{R}}\bar{\Phi}(t) = \nabla\mathcal{R}(\Phi_0)$

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Lazy Training

- $\mathcal{L}(\bar{\mathcal{R}}\bar{\Phi}(t)) \approx \mathcal{L}(\mathcal{R}\Phi(t))$ for sufficiently small t
- "lazy training regime": this holds until algorithm stops
- linear model well understood: linear convergence to global minimizer with speed depending on smallest EV $\lambda = \lambda_{min}(H(0))$
- Proof idea:

$$\frac{d\|\bar{\mathcal{R}}\bar{\Phi}(t)-y\|^2}{dt} = -2(\bar{\mathcal{R}}\bar{\Phi}(t) - y)^T H(0)(\bar{\mathcal{R}}\bar{\Phi}(t) - y) \leq -2\lambda\|\bar{\mathcal{R}}\bar{\Phi}(t) - y\|^2$$

$\rightarrow$ Grönwall: $\|\bar{\mathcal{R}}\bar{\Phi}(t) - y\|^2 \leq e^{-2\lambda t}\|\bar{\mathcal{R}}\Phi_0 - y\|^2$

- under suitable conditions this regime can be achieved by scaling the prediction function [2]

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Example

Definitions

- for illustration: Du et al. - Gradient Descent Provably Optimizes Over-parameterized Neural Networks (ICLR '19) [5]

2-layer biasless ReLU predictions

Let ϱ be the ReLU activation function and fix weights $a \in \mathbb{R}^{1\times N}$ (specified later). For weights $W = \begin{bmatrix} w_1 \\ \vdots \\ w_N \end{bmatrix} \in \mathbb{R}^{N\times d}$ we identify $W \in \mathbb{R}^{N\times d} \sim \mathbb{R}^P$ and define the predictions of the corresponding ReLU network

$$\mathcal{R}W := (a\varrho(Wx_i))_{i=1}^m \in \mathbb{R}^m.$$

- for the ease of presentation we do not train $a \in \mathbb{R}^{1\times N}$ (convex optimization problem w.r.t. the weights in the last layer)

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Omitting Bias

- omission of bias weights is standard in NN optimization literature [3, 4, 7, 8]
- severely limits the functions that can be realized with a given architecture
- BUT: augmenting the input data $x_i := (\tilde{x}_i, 1)$ and defining

$$W^{biasless} := \begin{bmatrix} W & b \\ 0 & 1 \end{bmatrix}$$

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Gram/Kernel Matrix H and its Expectation

- $\nabla_{w_n} \mathcal{R}W(t)_i = a_n \varrho'(w_n x_i) x_i^T$

$$\to H_{ij}(t) = \nabla \mathcal{R}W(t)_i \nabla \mathcal{R}W(t)_j^T = x_i^T x_j \sum_{n=1}^{N} a_n^2 \varrho'(w_n(t)x_i)\varrho'(w_n(t)x_j)$$

$$= \sum_{n=1}^{N} a_n^2 g_i^T(w_n(t)) g_j(w_n(t))$$

where $g_i(w) := x_i \varrho'(w x_i)$

Assumptions

(1) assume $\|x_i\| = 1$ (normalized input data)
(2) independent $w_n(0) = w_0 \sim \mathcal{N}(0, I)$, $n = 1, \dots, N$
(3) assume $a \sim \mathcal{U}\left(\{-\frac{1}{\sqrt{N}}, \frac{1}{\sqrt{N}}\}^N\right)$ independent of W_0

$\to$ $H_{ij}(0)$ is Monte-Carlo approximation of

$$H_{ij}^{\infty} := \mathbb{E}[H_{ij}(0)] = \mathbb{E}_{w \sim \mathcal{N}(0,I)}\left[g_i^T(w) g_j(w)\right]$$

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High-Level Overview

Assumptions

(4) assume $x_i \not\parallel x_j$ for $i \neq j$

Steps: | **Proof Idea:**

(A) $\lambda = \lambda_{min}(H^\infty) > 0$ (smallest EV) — $(g_i)_i$ lin. indep.

(B) $\|H^\infty - H(0)\|_2 \leq \frac{\lambda}{4}$ — Concentration ineq.

(C) W close to $W(0) \implies \|H^W - H(0)\|_2 \leq \frac{\lambda}{4}$ — scaled ridge func.

(D) $\lambda_{min}(H(t)) \geq \frac{1}{2}\lambda \quad (0 \leq s \leq t)$ — Grönwall's ineq.

$$\implies \begin{cases} W(t) \text{ close to } W(0) \\ \|\mathcal{R}W(t) - y\|^2 \leq e^{-\lambda t}\|\mathcal{R}W_0 - y\|^2 \end{cases}$$

....for suff. large N w.h.p., where $H^W := \frac{1}{N}\sum_{n=1}^{N} g_i^T(w_n)g_j(w_n)$.

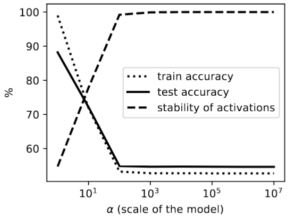
Result

Theorem: Zero NN Training Loss with Linear Convergence Rate

For every $\delta \in (0,1)$ and $N \gtrsim \frac{m^6}{\lambda^4 \delta^3}$ it holds that

$$\mathbb{P}\Big[\forall t \geq 0 : \|\mathcal{R}W(t) - y\|^2 \leq e^{-\lambda t}\|\mathcal{R}W_0 - y\|^2\Big] \geq 1 - \delta.$$

Performance in the Lazy Regime [2]



(a)

Model	Train acc.	Test acc.
ResNet wide, linearized	55.0	56.7
VGG-11 wide, linearized	61.0	61.7
Prior features [31]	-	82.3
Random features [36]	-	84.2
VGG-11 wide, standard	99.9	89.7
ResNet wide, standard	99.4	91.0

(b)

Figure 3: (a) Accuracies on CIFAR10 as a function of the scaling α. The stability of activations suggest a linearized regime when high. (b) Accuracies on CIFAR10 obtained for $\alpha = 1$ (standard, non-linear) and $\alpha = 10^7$ (linearized) compared to those reported for some linear methods without data augmentation: random features and prior features based on the scattering transform.

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