1. Introduction

In this paper, we are interested in understanding certain models of deep network architectures. We consider a regression task where $(X,Y) \in \mathbb{R}^{d_X} \times \mathbb{R}^{d_Y}$ is a random pair. As is standard, we consider a network with L hidden layers. The parameters of the network are defined via a choice of dimensions

$$d_0 := d_X, D_0, d_1, D_1, d_2, D_2, \dots, d_L, D_L, d_{L+1} = d_Y,$$

of numbers of units for layers $1, \ldots, L$

$$\vec{N} := (N_1, \dots, N_L) \in \mathbb{N}^L \setminus \{0\}.$$

We set $N_0 = N_{L+1} = 1$ as the number of units in the input and output. We also select functions:

$$\eta^{(\ell)} : \mathbb{R}^{d_{\ell}} \times \mathbb{R}^{D_{\ell}} \to \mathbb{R}^{d_{\ell+1}}, \sigma^{(\ell+1)} : \mathbb{R}^{d_{\ell+1}} \to \mathbb{R}^{d_{\ell+1}} \ (\ell = 0, \dots, L).$$

We consider networks with L internal layers and full connections between layers.

This gives us a model with parameters:

$$\theta_{i_{\ell},i_{\ell+1}}^{(\ell)}: \ell=0,\ldots,L, (i_{\ell},i_{\ell+1}) \in [N_{\ell}] \times [N_{\ell+1}]$$

each representing a connection between unit i_{ℓ} in layer ℓ and unit $i_{\ell+1}$ in layer $\ell+1$. Our total vector of parameters $\vec{\theta}_{\vec{N}}$ lives in dimension

$$p_{\vec{N}} := \sum_{\ell=0}^{L} N_{\ell} N_{\ell+1} D_{\ell}.$$

The function computed by our network is given by:

$$\widehat{y}_N = \widehat{y}_N : \mathbb{R}^{d_X} \times \mathbb{R}^{p_{\vec{N}}} \to \mathbb{R}^{d_Y}$$

that takes as input an element $x \in \mathbb{R}^{d_X}$ and a setting or parameters $\vec{\theta}_{\vec{N}}$ and produces a sequence of values as follows. For $1 \le i_1 \le N$,

(1)
$$a_{i_1}^{(1)}(x,\vec{\theta}_N) := \eta^{(0)}(x,\theta_{1,i_1}^{(0)}).$$

For $\ell = 1, ..., L$, $1 \le i_{\ell+1} \le N_{\ell+1}$:

(2)
$$z_{i_{\ell+1}}^{(\ell+1)}(x,\vec{\theta}_{\vec{N}}) := \frac{1}{N_{\ell}} \sum_{i_{\ell}=1}^{N_{\ell}} \eta^{(\ell)}(a_{i_{\ell}}^{\ell}(x,\vec{\theta}_{\vec{N}}), \theta_{i_{\ell},i_{\ell+1}}^{(\ell)});$$

(3)
$$a_{i_{\ell+1}}^{(\ell+1)}(x,\vec{\theta}_{\vec{N}}) := \sigma^{(\ell+1)}(z_{i_{\ell+1}}^{(\ell+1)}(x,\vec{\theta}_{\vec{N}})).$$

The output is $\widehat{y}(x, \vec{\theta}_{\vec{N}}) = a_1^{(L+1)}$.

Our model defines a very general version of a neural network with fully connected layers, where the internal units (with activations $a_{i_\ell}^{(\ell)}$) may have dimension greater than 1. This is convenient because it allows us to carry bias terms and consider more general versions of these units.

The derivatives of \widehat{y} with respect to the $\theta_{i_\ell,i_{\ell+1}}^{(\ell)}$ can be computed via standard backpropagation. In what follows, we assume that all functions σ and \underline{eta} are C^1 -Fréchet differentiable. We let $D\sigma^{(\ell)}(z)$ denote the derivative of $\sigma^{(\ell)}$ and $D_a\eta^{(\ell)}(a,\theta)$, $D_\theta\eta^{(\ell)}(a,\theta)$ denote the partial derivatives of η with respect to the variables a and θ (respectively).

The derivative with respect to the weights $\theta_{i_L,1}^{(L)}$ is most easily computed. Omitting the $(x, \vec{\theta}_{\vec{N}})$ for simplicity,

(4)
$$\partial_{\underline{\theta}_{i_L,1}^{(L)}} \widehat{y} = \frac{1}{N_{\ell}} D\sigma^{(L+1)}(z_1^{(L+1)}).$$

For other weights, we define:

$$M_{i_L}(x, \vec{\theta}_N) := D\sigma^{(L+1)}(z_1^{(L+1)}) D_a \eta^{(L)}(a_{i_L}^{(L)}, \theta_{i_L, 1}^{(L)}) D\sigma^{(L)}(z_{i_L}^{(L)})$$

and for $1 \le \ell \le L - 1$, $1 \le i_{\ell} \le N$:

$$M_{i_{\ell},i_{\ell+1},\dots,i_L}(x,\vec{\theta}_N) := M_{i_{\ell+1},\dots,i_L}(x,\vec{\theta}_N) D_a \eta^{(\ell)}(a_{i_{\ell}}^{(\ell)},\theta_{i_{\ell},i_{\ell+1}}^{(\ell)}) D\sigma^{(\ell)}(z_{i_{\ell}}^{(\ell)}).$$

Then the Fréchet derivatives of \widehat{y} with respect to $\theta_{i_\ell,i_{\ell+1}}^{(\ell)}$ for $0\leq \ell \leq L-1$ is

$$\partial_{\theta_{i_L,i_{L+1}}^{(L-1)}} \widehat{y}_N(x,\vec{\theta}_N) = \frac{1}{N_L N_{L-1}} M_{i_L}(x,\vec{\theta}_N) D_{\theta} \eta^{(L-1)}(a_{i_{L-1}}^{(L-1)}, \theta_{i_{L-1},i_L}^{(L-1)})$$

and

$$\partial_{\theta_{i_{\ell},i_{\ell+1}}^{(\ell)}} \widehat{y}_{N}(x,\vec{\theta}_{N}) = \frac{1}{\prod_{j=\ell}^{L} N_{j}} \sum_{i_{\ell+2},\dots,i_{L}=1}^{N} M_{i_{\ell+2},\dots,i_{L}}(x,\vec{\theta}_{N}) D_{\theta} \eta^{(\ell)}(a_{i_{\ell}}^{(\ell)}(x,\vec{\theta}_{N}), \theta_{i_{\ell},i_{\ell+1}}^{(\ell)}).$$

If we define our population loss function $L_{\vec{N}}: \mathbb{R}^{p_{\vec{N}}} \to \mathbb{R}$ as:

$$L_{\vec{N}}(\vec{\theta}_{\vec{N}}) := \frac{1}{2} \mathbb{E}_{(X,Y) \sim P} \left[||Y - \widehat{y}_{\vec{N}}(X, \vec{\theta}_{\vec{N}})||^2 \right],$$

then one can study an evolution

$$\frac{d\vec{\theta}_{\vec{N}}}{dt}(t) = -\alpha_{\vec{N}}(t)\nabla L_{\vec{N}}(\vec{\theta}_{\vec{N}}(t))$$

via the partial derivatives of \hat{y} .

A few preliminary comments on these derivatives are in order. One of them is on differing time scales across layers at least when $N_1 = \cdots = N_L = N$. In this case formula (4) suggests the weights between layers L and L-1 and the weights between layers 0 and 1 move at rate N^{-1} , whereas other weights move at speed N^{-2} .

2. GOAL AND ASSUMPTIONS

Our goal is to analyse the evolution of the weight vector $\vec{\theta}_N(t)$ for $t \geq 0$ under a special setting of parameters $\vec{N} = (N, \dots, N)$ with

$$\frac{d\vec{\theta}_N(t)}{dt} = -N^2 \alpha(t) \, \nabla L_N(\vec{\theta}_N(t)).$$

This implies in particular that

We will study this evolution under the following assumptions.

Assumption 1. At time 0, the weights $\theta_{i_{\ell},i_{\ell+1}}^{(\ell)}(0) \in \mathbb{R}^{D_{\ell}}$ ($10 \leq \ell \leq L$, $(i_{\ell},i_{\ell+1}) \in [N_{\ell}] \times [N_{\ell+1}]$) are all independent. Moreover, there are probability laws $\mu_0^{(\ell)}$ over $\mathbb{R}^{D_{\ell}}$ (for $0 \leq \ell \leq L$) such that $\theta_{i_{\ell},i_{\ell+1}}^{(\ell)}(0) \sim \mu_0^{(\ell)}$ for each $0 \leq \ell \leq L$, $(i_{\ell},i_{\ell+1}) \in [N_{\ell}] \times [N_{\ell+1}]$. The distributions $\mu_0^{(\ell)}$ defined above all have bounded support contained in balls of radius R around the origins of their respective domains.

Assumption 2. There exists a C>0 such that the Fréchet derivatives of the $\sigma^{(\ell+1)}$ and $\eta^{(\ell)}$ satisfy:

$$\forall z \in \mathbb{R}^{d_{\ell+1}} \|D\sigma^{(\ell)}(z)\| \leq C$$

$$\forall (a,\theta) \in \mathbb{R}^{d_{\ell}} \times \mathbb{R}^{D_{\ell}} : \|D_a\eta^{(\ell)}(a,\theta)\| \leq C(1+\|\theta\|) \text{ and } \|D_{\theta}\eta^{(\ell)}(a,\theta)\| \leq C(1+\|a\|).$$
Moreover, $D\sigma^{(\ell)}(z)$

3. THE MEAN FIELD APPROXIMATION DISTRIBUTION

We now construct a mean-field approximating distribution for our problem. By this we mean that we will construct random continuous functions