CMPUT 654 Fa 23: Theoretical Foundations of Machine Learning Fall 2023

Lecture 22: November 28

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## 22.1 Outline

- Introduction to neural networks.
- Function approximation.
- Depth vs width in neural networks.

## 22.2 Neural Networks

A two-layered (one hidden and one output layer) fully connected neural network with *m* units in the hidden layer is a map  $f : \mathbb{R}^d \to \mathbb{R}$  given by

$$
f_w(x) = \sum_{i=1}^m u_i h(\theta_i^\top x + b_i),
$$

where  $h : \mathbb{R} \to \mathbb{R}$  is the activation function,  $x \in \mathbb{R}^d$  is the input vector,  $\theta_i \in \mathbb{R}^d$  is the weight vector,  $b_i \in \mathbb{R}$  is the bias/threshold,  $u_i \in \mathbb{R}$  is the weight to the output, and  $w = (\theta, u, b) \in \mathbb{R}^{m(d+2)}$  are the parameters.

## 22.2.1 Function Approximation with Neural Networks

Let  $\mathcal{F}_m^{(h)} = \{f_w : w \in \mathcal{W}_m\}$ , where  $\mathcal{W}_m = \mathbb{R}^{m(d+2)}$ , be the two-layered neural network function class with  $m$ hidden units and activation function *h*. The next theorem shows that  $f \in \mathcal{F}_m$  is a universal approximator.

In this section, we will see how well we can approximate functions of different kinds with neural networks.

**Theorem 22.1** (Leshno, 1993). Let  $h : \mathbb{R} \to \mathbb{R}$  be such that  $h \notin \mathbb{R}[x]$  (not a polynomial). Let  $K \subset \mathbb{R}^d$  be compact. *Then*  $\mathcal{F}_m^{(h)}|_K = \left\{ f|_K : f \in \mathcal{F}_m^{(h)} \right\}$  is dense in  $C(K)$ .

To state the next result, let us introduce a set of functions

$$
\Gamma_r = \left\{ f : \mathbb{R}^d \to R : \exists \tilde{f} : \mathbb{R}^d \to C \text{ s.t. } f(x) = \int e^{i\omega^\top x} \tilde{f}(\omega) d\omega, \forall x \in B_r \right\},\
$$

where  $B_r = \{x^d : ||x||_2 \le r\}$  is a ball of radius *r*. The function  $\tilde{f}$  is the Fourier transform of  $f$  up to constant factors. We have a complexity/smoothness measure/coefficient for  $f \in \Gamma_r$  (assuming there exists a unique  $\tilde{f}$  for  $f$ ):

$$
C(f) = \int \|\omega\|_2 |\tilde{f}(\omega)| d\omega.
$$

<span id="page-0-0"></span>The quantity  $C(f)$  roughly measures the "energy" of f at high frequency. Thus, f is smooth if  $C(f)$  is small. With  $C(f)$  in hand, we state our next result:



<span id="page-1-0"></span>Figure 22.1: Barron's theorem (Theorem [22.2\)](#page-0-0) does not hold for all smooth functions but only a "slice".

**Theorem 22.2** (Barron, 1993). Let  $h : \mathbb{R} \to \mathbb{R}$  be a measurable bounded function such that  $\lim_{z\to -\infty} h(z) = 0$ *and*  $\lim_{z\to\infty}$   $h(z) = 1$ *. Let*  $f \in \Gamma_r$  *such that*  $C(f) < \infty$  *and*  $\mu \in M_1(B_r)$ *. Then for all*  $m \ge 1$ 

$$
\inf_{w \in \mathcal{W}_m} \|f - f(0) - f_w\|_{L_2(\mu)} \le \frac{(2rC(f))^2}{m}.
$$

Remark 22.3. Note that the above result is independent of *d*. When we approximate a smooth function with polynomial, we get a rate of roughly (1*/m*) *s/d*, where *s* is the number of continuous derivative of the target function *f*. So the above result does not tell us that for any smooth function, the approximation error goes down with 1*/m* rate. But functions with finite *C*(*f*) creates a subset of smooth functions for which we get the 1*/m* rate (see Fig. [22.1\)](#page-1-0).

**Remark 22.4.** Some of the common choices of the activation function are sigmoid  $(h(z) = 1/(1+e^{-z}))$  and ReLU  $(h(z) = \max(0, z))$ . Note that while sigmoid satisfies the condition of Theorem [22.2,](#page-0-0) ReLU does not. However, for ReLU, we can write  $s(z) = h(z) - h(z - 1)$  such that *s* satisfies the condition.

**Does depth in neurals networks give some advantage?** For the next result, let  $d = 1$  and the activation function is ReLU. We also index the neural network class with number of layers:

 $\mathcal{F}_{k,m} = \{f : [0,1] \to \mathbb{R} : f$  can be implemented by a NN with  $\leq k$  layers and  $\leq m$  hidden units}.

**Theorem 22.5** (Telgarsky, 2016). Let  $k \geq 3$ . Then

$$
\sup_{f \in \mathcal{F}_{2k^2,2}} \inf_{g \in \mathcal{F}_{k,2^{k-2}}} \|f - g\|_{\infty} \ge \frac{1}{16} \, .
$$

*Proof intuition.* The proof is done by constructing a function  $f_k$  which is difficult to approximate using shallow networks. Let  $f_0(x) = \max(0, \min(2x, 2(1-x)))$  on [0,1]. Note that  $f_0(x)$  can be implemented by a 2 layer neural network with  $m = 2$ ,  $\theta_1 = 2$ ,  $\theta_2 = -4$ ,  $b_1 = 0$ , and  $b_2 = -0.5$  so that

$$
f_0(x) = 2\max(0, x) - 4\max(0, x - 0.5) = w_1h(x) + w_2h(x - 0.5).
$$

Let  $f_k(x) = f_0(f_{k-1}(x))$  with  $k \ge 1$ . Then  $f_k(x)$  can be represented by a 2*k* layer neural network with 2 units in each hidden layer. Fig. [22.2](#page-2-0) shows  $f_k$  for  $k = 0, 1, 2$ .

**Definition 22.6** (Crossing Number). The crossing number of a function  $f : [0, 1] \rightarrow [0, 1]$  is the number of segments in the graph on which *f* is above the line  $y = \frac{1}{2}$ .

Combining the below two claims gives us the result.

**Claim 22.7.** For every measurable  $g : [0,1] \to [0,1]$  such that  $C(g) < 2^{k-1}$ ,  $||f_k - g||_{L_1} \ge \frac{1}{16}$ .

Claim 22.8. *We have that*

$$
\max \left\{C(g) : g \in \mathcal{F}_{l,m}\right\} \leq 2(2m)^l.
$$

<span id="page-2-0"></span>

**Figure 22.2:**  $f_k(x)$  for  $k = 0, 1, 2$ .