CMPUT 654 Fa 23: Theoretical Foundations of Machine Learning

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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):

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

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:

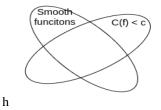


Figure 22.1: Barron's theorem (Theorem 22.2) does not hold for all smooth functions but only a "slice".

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 $\mu \in \mathcal{M}_1(B_r)$. 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).

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, 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:

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

Theorem 22.5 (Telgarsky, 2016). Let $k \ge 3$. 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 2k layer neural network with 2 units in each hidden layer. Fig. 22.2 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

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

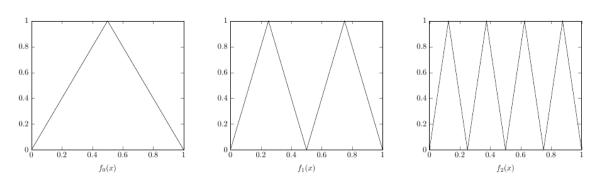


Figure 22.2: $f_k(x)$ for k = 0, 1, 2.