# ML HW3

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### **Problem 1: Explanation to The Lemma**

1. Reading and Explaining Lemmas:

Your task is to read Ryck et al., On the approximation of function by tanh neural networks[1]. Focus on Lemma 3.1 and Lemma 3.2.

**Setup:** Before stating the explanation, we define the following terms:

#### Definition 1: $L^p$ Space

The **Lebesgue space** is defined as:

$$\mathrm{L}^p(\Omega) = \left\{ f : \Omega \to \overline{\mathbb{R}} : \int_{\Omega} |f|^p \, \mathrm{d}\mu < +\infty \right\},$$

where  $\Omega \subseteq \mathbb{R}^d$ ,  $p, d \in \mathbb{Z}^+$ ,  $\mu(\cdot)$  be the **Lebesgue measure**.

$$L^{\infty}(\Omega) = \left\{ f : \Omega \to \overline{\mathbb{R}} : \ \mu\{x \in \Omega : \ |f(x)| = \infty\} = 0 \right\},\,$$

where  $\Omega \subseteq \mathbb{R}^d$ ,  $d \in \mathbb{Z}^+$ ,  $\mu(\cdot)$  be the **Lebesgue measure**.

### **Definition 2: L**<sup>p</sup> Norm

Given  $d \in \mathbb{Z}^+$ , function  $f : \Omega \subseteq \mathbb{R}^d \to \overline{\mathbb{R}}$ . For  $p \in \mathbb{Z}^+$ , the norm is defined as:

$$||f||_{\mathrm{L}^p} = \left(\int_{\Omega} |f|^p \,\mathrm{d}\mu\right)^{\frac{1}{p}},$$

for  $p = +\infty$ , the norm is defined as:

$$||f||_{\mathcal{L}^{\infty}} = \sup_{x \in \Omega} |f(x)|$$

#### **Definition 3: Sobolev Space**

Let  $d \in \mathbb{Z}^+$ ,  $p \in \mathbb{Z}^+ \cup \{+\infty\}$  and let  $\Omega \subseteq \mathbb{R}^d$  be open,  $L^p(\Omega)$  be the Lebesgue space. For  $k \in \mathbb{N}$ , we define **Sobolev space** as:

$$W^{k,p}(\Omega) = \left\{ f \in \mathcal{L}^p(\Omega) : D^{\alpha} f \in \mathcal{L}^p(\Omega), \ \forall \alpha \in \mathbb{N}^d, \ |\alpha| \le k \right\},$$

where  $\alpha = (\alpha_1, \dots, \alpha_d), \ D^{\alpha} = \partial_1^{\alpha_1} \cdots \partial_d^{\alpha_d}$ .

### **Definition 4: Seminorm on Sobolev Space**

For  $p \in \mathbb{Z}^+$ , the seminorm of f on  $W^{k,p}(\Omega)$  is

$$|f|_{W^{m,p}(\Omega)} = \left(\sum_{|\alpha|=m} \left\| D^{\alpha} f \right\|_{\mathrm{L}^p(\Omega)}^p \right)^{1/p}, \text{ for } m = 0, \dots, k.$$

For  $p = +\infty$ , we define the seminorm:

$$|f|_{W^{k,\infty}(\Omega)} = \max_{|\alpha|=m} \left\| D^{\alpha} f \right\|_{L^{\infty}(\Omega)}, \text{ for } m = 0, \dots, k.$$

### **Definition 5: Norm on Sobolev Space**

Based on **definition 3**, we define norm of f for  $p \in \mathbb{Z}^+$ :

$$||f||_{W^{k,p}(\Omega)} = \left(\sum_{m=0}^{k} |f|_{W^{m,p}(\Omega)}^{p}\right)^{1/p},$$

for  $p = +\infty$ , we define as

$$||f||_{W^{k,\infty}(\Omega)} = \max_{0 \le m \le k} |f|_{W^{m,\infty}(\Omega)}$$

In **Section 2.3. Neural network**, it is mentioned in this paper that:  $\Psi_{\Theta}$  is a neural network for which activation function is  $\tanh x$ , where  $\Theta$  is the set of parameters (weight matrices  $W_k$ , biases  $b_k$ ).

Neural networks  $\Psi_{\Theta}$ , in this paper, can be categorised into 2 classes:

- Shallow neural network: For neural networks who have only 1 hidden layer.
- Deep neural network: For neural networks who have more than 1 hidden layers.

In this paper, for  $p \in \mathbb{Z}^+$ ,  $M \in \mathbb{R}^+$ , the monomials  $f_p : [-M, M] \to \mathbb{R}$  is defined as

$$f_p(y) := y^p$$
; for instance,  $f_3(y) = y^3$ ,  $f_3(2) = 2^3 = 8$ .

#### Lemma 3.1

Let  $k \in \mathbb{N}$  and  $s \in 2\mathbb{Z}^+ - 1$ . Then it holds that for all  $\varepsilon \in \mathbb{R}^+$ , there exists a shallow tanh neural network  $\Psi_{s,\varepsilon} : [-M, M] \to \mathbb{R}^{\frac{s+1}{2}}$  of width  $\frac{s+1}{2}$  such that

$$\max_{\substack{p \le s, \\ p \text{ odd}}} \left\| f_p - (\Psi_{s,\varepsilon})_{\frac{p+1}{2}} \right\|_{W^{k,\infty}} \le \varepsilon.$$

Moreover, the weights of  $\Psi_{s,\varepsilon}$  scale as  $\mathcal{O}\left(\varepsilon^{-\frac{s}{2}}(2(s+2)\sqrt{2M})^{s(s+3)}\right)$  for small  $\varepsilon$  and large s.

## What to notice?

- $\Psi_{s,\varepsilon}$  is a **single-hidden-layer** neural network with  $\frac{s+1}{2}$  neurons.
- The lemma only holds for closed interval [-M, M], instead of  $\mathbb{R}$ .
- The norm used is **Sobolev space norm**, which is stronger than  $L^{\infty}$  norm.
- Taking **max** ensures for all odd  $p \leq s$  the inequality holds.

#### What does the lemma tell us?

The lemma tells us that under a compact interval [-M, M],  $s \in 2\mathbb{Z}^+ - 1$ , error  $\varepsilon \in \mathbb{R}^+$ , we can always find a **one-layer**- $\frac{s+1}{2}$ -**neuron neural network**  $\Psi_{s,\varepsilon}$  to approximate all the **odd** term monomial up to order s within the error  $\varepsilon$  in the sense of **Sobolev norm**, which also ensures the **derivative**  $D_y^n \Psi_{s,\varepsilon}$  is close to the **derivative of the object function**  $D_y^n y^p$  for  $0 \le n \le k$ .

Moreover, we can also predict the **growth speed of weights**, they grow as fast as  $\varepsilon^{-\frac{s}{2}}(2(s+2)\sqrt{2M})^{s(s+3)}$  for large number of neurons s and small enough error  $\varepsilon$ .

Excellent, let's move on to the lemma 3.2, which is very similar to lemma 3.1.

#### Lemma 3.2

Let  $k \in \mathbb{N}$  and  $s \in 2\mathbb{Z}^+ - 1$ . Then it holds that for all  $\varepsilon \in \mathbb{R}^+$ , there exists a shallow tanh neural network  $\psi_{s,\varepsilon} : [-M, M] \to \mathbb{R}^s$  of width  $\frac{3(s+1)}{2}$  such that

$$\max_{p < s} \left\| f_p - (\psi_{s,\varepsilon})_p \right\|_{W^{k,\infty}} \le \varepsilon.$$

Moreover, the weights of  $\psi_{s,\varepsilon}$  scale as  $\mathcal{O}\left(\varepsilon^{-\frac{s}{2}}((s+2)\sqrt{M})^{\frac{3s(s+3)}{2}}\right)$  for small  $\varepsilon$  and large s.

## What does the lemma tell us?

Similar to lemma 3.1, under a compact interval [-M, M],  $s \in 2\mathbb{Z}^+ - 1$ , error  $\varepsilon \in \mathbb{R}^+$ , we can always find a **one-layer**- $\frac{3(s+1)}{2}$  **neuron-neural network**  $\psi_{s,\varepsilon}$  to approximate all the monomial up to order s within the error  $\varepsilon$  in the sense of **Sobolev norm**, which also ensures the **derivative**  $D_y^n \psi_{s,\varepsilon}$  is close to the **derivative of the object function**  $D_y^n y^p$  for  $0 \le n \le k$ .

Moreover, we can also predict the **growth speed of weights**, they grow as fast as  $\varepsilon^{-\frac{s}{2}}((s+2)\sqrt{M})^{\frac{3s(s+3)}{2}}$  for large number of neurons s and small enough error  $\varepsilon$ .

#### What is it different from lemma 3.1?

**Lemma 3.2** is an enhanced version of **lemma 3.1**, it shows that using s + 1 more neurons can let us approximate the even monomials. Overall, to approximate an order n polynomial, we need  $\frac{3(n+1)}{2}$  neurons.

## How does it work in practice?

We then look at an example of how it work theoretically.

**Example:** Approximate  $g(x) = 5x^5 - 3x^3 + x^2 - x$  on [-2, 2] within error  $= 10^{-4}$ .

**Step 1:** Notice that g is a degree 5 polynomial, we choose s = 5, also k = 1.

**Step 2:** Our neural network will have  $\frac{3(5+1)}{2} = 9$  neurons in the hidden layer.

**Step 3:** Since for all  $p \leq 5$ , we have

$$||f_p - (\psi_{s,\varepsilon})_p||_{W^{k,\infty}} \le \varepsilon;$$

by the triangular inequality,

$$||g - \psi_{s,\varepsilon}||_{L^{\infty}} \le ||g - \psi_{s,\varepsilon}||_{W^{k,\infty}} \le 5||f_5 - (\psi_{s,\epsilon})_5||_{W^{k,\infty}} + 3||f_3 - (\psi_{s,\epsilon})_3||_{W^{k,\infty}} + ||f_2 - (\psi_{s,\epsilon})_2||_{W^{k,\infty}} + ||f_1 - (\psi_{s,\epsilon})_1||_{W^{k,\infty}}$$

$$\le (5 + 3 + 1 + 1)\varepsilon$$

$$= 10\varepsilon$$

$$< 10^{-4}$$

we choose  $\varepsilon = 10^{-5}$ .

Step 4: By setting  $k=1,\ s=5,\ \varepsilon=10^{-5},$  lemma 3.2 renders the theoretical existence of neural network  $\psi_{5,10^{-5}}$  that approximate g(x) on  $[-2,\ 2]$  with error no more than  $10^{-4}$ .

Moreover, since we set k = 1, the error between their derivatives will be less than  $10^{-4}$ .

$$\|g' - (\psi_{s,\varepsilon})'\|_{L^{\infty}} \le \|g - (\psi_{s,\varepsilon})\|_{W^{k,\infty}} \le 10^{-4}$$

This is the reason why we say **Sobolev norm** is stronger than  $L^{\infty}$  **norm** and use **Sobolev norm** instead of  $L^{\infty}$  **norm**.

## **Proof Insights:**

**Taylor Theorem** states for any given **smooth** function at x = a, we have:

$$f(x) = \sum_{k=0}^{n} \frac{f^{(k)}(a)}{k!} (x-a)^k + \frac{f^{(n+1)}(\xi(x,a))}{(n+1)!} (x-a)^{n+1},$$

where  $n \in \mathbb{Z}^+$ ,  $\xi(x, a)$  lies between x and a.

We can apply this to the finite difference method, we get Stirling formula:

$$P_{n}(x) = P_{2m+1}(x) = f[x_{0}] + \frac{sh}{2}(f[x_{-1}, x_{0}] + f[x_{0}, x_{1}]) + s^{2}h^{2}f[x_{-1}, x_{0}, x_{1}]$$

$$+ \frac{s(s^{2} - 1)h^{3}}{2}(f[x_{-2}, x_{-1}, x_{0}, x_{1}] + f[x_{-1}, x_{0}, x_{1}, x_{2}]) + \cdots$$

$$+ s^{2}(s^{2} - 1)(s^{2} - 4)(s^{2} - (m - 1)^{2})h^{2m}f[x_{-m}, \dots, x_{m}]$$

$$+ \frac{s(s^{2} - 1)\cdots(s^{2} - m^{2})h^{2m+1}}{2}(f[x_{-m-1}, \dots, x_{m}] + f[x_{-m}, \dots, x_{m+1}]),$$

for s=1, h the step size, for  $P_{2m}$ , we wipe out the last term.

For the term  $f[x_l, \ldots, x_k]$ , we have the recurrence formula [2]:

$$f[x_l, \dots, x_k] = \frac{f[x_{l+1}, \dots, x_k] - f[x_l, \dots, x_{k-1}]}{x_k - x_l}; \quad f[x_k] = f(x_k)$$

This is my brief explanation of lemma 3.1 and lemma 3.2, hope you find it easy to read.

## **Problem 2: Runge Function Derivatives**

- 1. Use the same code from Assignment 2 programming assignment 1 to calculate the error in approximating the derivative of the given function.
- 2. In this assignment, you will use a neural network to approximate both the Runge function and its derivative. Your task is to train a neural network that approximates:
  - a. The function f(x) itself.
  - b. The derivative f'(x).

You should define a loss function consisting of two components:

- 1) Function loss: the error between the predicted f(x) and the true f(x).
- 2) **Derivative loss**: the error between the predicted f'(x) and the true f'(x).

Write a short report (1–2 pages) explaining method, results, and discussion including:

- Plot the true function and the neural network prediction together.
- Show the training/validation loss curves.
- Compute and report errors (MSE or max error).

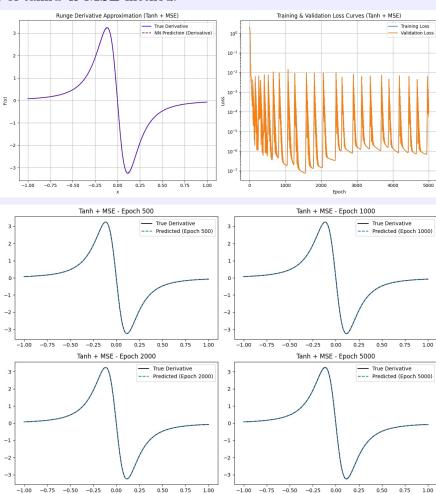
**Sol:** We first setup the neural network as before:

- Training set, validation set and testing set are selected uniformly on [-1, 1] with counts 100, 10 and 40, respectively.
- The neural network has 2 layers and each has 50 neurons.
- We have 3 methods to comparison:
  - $\tanh x$  as activation function & MSE for loss function.
  - $\tanh x$  as activation function & **sup-norm** for loss function.
  - $\cos x$  as activation function & MSE for loss function.
- Optimiser is chosen as **Adam** and the epoch is set 5000.
- Objective function is given  $f(x) = \frac{1}{1 + 25x^2}$ .
- Objective derivative is  $f'(x) = \frac{-50x}{(1+25x^2)^2}$ .

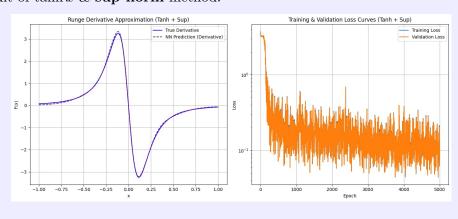
Be clear that we only measure the error between Runge function and the hypothesis function, instead of training the derivatives again with same manner done in assignment 2.

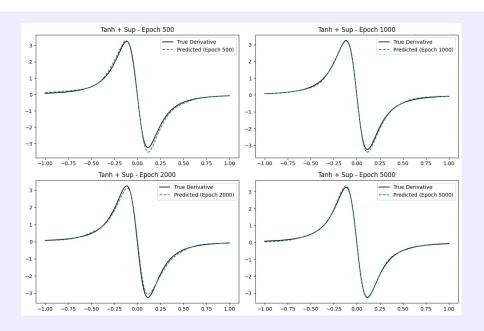
# **Brief results:**

1. Result of  $\tanh x \& \mathbf{MSE}$  method:

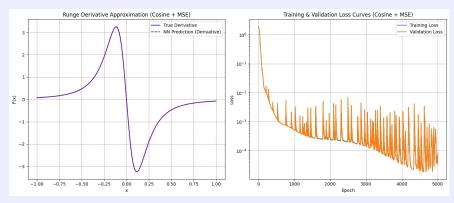


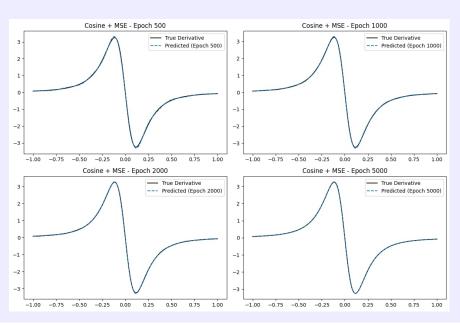
## 2. Result of $\tanh x \& \mathbf{sup\text{-}norm}$ method:





## 3. Result of $\cos x \& \mathbf{MSE}$ method:





## **Result Overview:**

Function	Method	tanh + MSE	tanh + sup	cos + MSE
f(x)	Test MSE	0.000000	0.000000	0.000006
	Test Max Absolute Error	0.000489	0.000564	0.005360
f'(x)	Test MSE	0.000054	0.001418	0.000086
	Test Max Absolute Error	0.019007	0.097872	0.036319

We can see that using  $\tanh x$  as activation function with loss  $\mathbf{MSE}$  is the best option of the three for approximating the Runge function, it performs quite well on both original function and its derivative.

# References

- [1] Tim De Ryck, Samuel Lanthaler, and Siddhartha Mishra. On the approximation of functions by tanh neural networks. *Neural Networks*, 143:732–750, 2021.
- [2] Richard L. Burden, J. Douglas Faires, and Annette M. Burden. *Numerical Analysis*. Cengage Learning, 10 edition, 2015.