ML HW2

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Problem 1: Algorithm Construction

1. Read Deep Learning: An Introduction for Applied Mathematicians. Consider a network as defined in (3.1) and (3.2).

$$a^{[1]} = x \in \mathbb{R}^{n_1}$$

(3.2)
$$a^{[l]} = \sigma\left(W^{[l]}a^{[l-1]} + b^{[l]}\right) \in \mathbb{R}^{n_l}, \quad \text{for } l = 2, 3, \dots, L.$$

Assume that $n_L = 1$, find an algorithm to calculate $\nabla a^{[L]}(x)$.

Sol: Recall that we have a powerful tool —Chain Rule.

Theorem 1: Recurrence Formula on δ Function

$$\delta^{[k]} = \frac{\partial C}{\partial z^{[k]}} = \frac{\partial C}{\partial z^{[k+1]}} \frac{\partial z^{[k+1]}}{\partial z^{[k]}} = \delta^{[k+1]} \frac{\partial z^{[k+1]}}{\partial z^{[k]}} = \delta^{[l]} \frac{\partial z^{[l]}}{\partial z^{[l-1]}} \cdots \frac{\partial z^{[k+1]}}{\partial z^{[k]}}$$

where $2 \le k < l \le L$.

Since $n_L = 1$, $a^{[L]} \in \mathbb{R}$. Hence we can replace the role of C by $a^{[L]}$. We get:

$$\xi^{[k]} := \frac{\partial a^{[L]}}{\partial z^{[k]}} = \frac{\partial a^{[L]}}{\partial z^{[k+1]}} \frac{\partial z^{[k+1]}}{\partial z^{k}} = \xi^{[k+1]} \frac{\partial z^{[k+1]}}{\partial z^{[k]}}, \quad 2 \le k < L; \qquad \xi^{[L]} := \sigma'(z^{[L]}),$$

where $2 \le k < L$. Note that

$$\frac{\partial z^{[k+1]}}{\partial z^{[k]}} = \frac{\partial z^{[k+1]}}{\partial a^{[k]}} \frac{\partial a^{[k]}}{\partial z^{[k]}} = W^{[k+1]} \sigma'(z^{[k]}), \quad 2 \le k < L;$$

therefore

$$\xi^{[k]} = \sigma'(z^{[k]}) \circ \left[(W^{[k+1]})^\top \xi^{[k+1]} \right], \quad 2 \leq k < L.$$

Lastly, $\frac{\partial z^{[2]}}{\partial x} = W^{[2]}$, the last puzzle of the algorithm is finally done.

The algorithm is as follow:

Step 1: Calculate $\xi^{[L]} = \sigma'(z^{[L]})$

Step 2: Use recurrence formula:

$$\xi^{[k]} = \sigma'(z^{[k]}) \circ \left[(W^{[k+1]})^\top \xi^{[k+1]} \right], \quad 2 \leq k < L,$$

to compute $\xi^{[2]}$.

Step 3:
$$\nabla a^{[L]} = \xi^{[2]} \frac{\partial z^{[2]}}{\partial x} = (W^{[2]})^{\top} \xi^{[2]}.$$

Problem 3: Runge Phenomena

1. Use a neural network to approximate the Runge function

$$f(x) = \frac{1}{1 + 25x^2}, \quad x \in [-1, 1].$$

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: The full Jupyter file is here.

- Basic Setup
 - 1. The training set and validation/training set are sampled 100 and 20 uniformly in the interval [-1, 1] respectively.
 - 2. The neural network has 2 layers and each has 50 neurons.
 - 3. Activation function is chosen as $\tanh x$.
 - 4. Two optimisers are tested for the comparison:
 - Regular MSE
 - Sup-norm (also p-norm for p = 20)
 - 5. Epoch is set 5000.
- Result Presentation
 - 1. Loss of MSE.

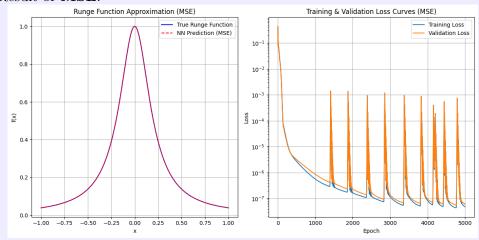
```
--- Training with MSE Loss ---
Epoch [500/5000], Train Loss: 0.000002, Val Loss: 0.000002
Epoch [1000/5000], Train Loss: 0.000000, Val Loss: 0.000001
Epoch [1500/5000], Train Loss: 0.001174, Val Loss: 0.000867
Epoch [2000/5000], Train Loss: 0.000000, Val Loss: 0.000000
Epoch [2500/5000], Train Loss: 0.000000, Val Loss: 0.000000
Epoch [3000/5000], Train Loss: 0.000000, Val Loss: 0.000000
Epoch [3500/5000], Train Loss: 0.000000, Val Loss: 0.000000
Epoch [4000/5000], Train Loss: 0.000000, Val Loss: 0.000000
Epoch [4500/5000], Train Loss: 0.000000, Val Loss: 0.000000
Epoch [5000/5000], Train Loss: 0.000000, Val Loss: 0.000000
```

2. Loss of **sup-norm**.

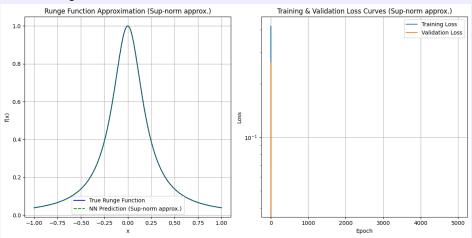
```
--- Training with Sup-norm Approximation Loss (Corrected) ---
Epoch [500/5000], Train Loss: -2.728260, Val Loss: -3.100614
Epoch [1000/5000], Train Loss: -3.279954, Val Loss: -3.616254
Epoch [1500/5000], Train Loss: -3.972852, Val Loss: -4.871111
Epoch [2000/5000], Train Loss: -4.939495, Val Loss: -5.529874
Epoch [2500/5000], Train Loss: -5.252147, Val Loss: -5.487857
Epoch [3000/5000], Train Loss: -5.954085, Val Loss: -6.249280
Epoch [3500/5000], Train Loss: -6.223094, Val Loss: -6.334863
Epoch [4000/5000], Train Loss: -7.161107, Val Loss: -7.228351
Epoch [4500/5000], Train Loss: -7.462693, Val Loss: -7.674273
Epoch [5000/5000], Train Loss: -7.557062, Val Loss: -7.776904
```

• Approximation Result

1. Result of **MSE**:



2. Result of **sup-norm**:



• Conclusion & Comparison

--- Final Results Comparison ---

Metric	 	MSE Method		Sup-Norm Method
Final MSE Final Max Abs Error	 	0.000001 0.002417	 	0.000000 0.000431

Conclusion: The Sup-Norm method achieved a lower maximum absolute error, making it the better method for this specific objective.

• Explanation

Although the loss of the **sup-norm** method may seem high relative to the **MSE** method, the actual loss under the same metric has the opposite result. Not only the runtime but the final loss has shown that **sup-norm** is overall the better option of the two.

My Question 1: Why Is The Approximation Work During The Course?

For the approximation theory mentioned during the class, we know that for continuous function f(x) on a closed interval [a, b], the following must hold:

$$\forall \varepsilon \in \mathbb{R}^+, \ \exists n \in \mathbb{Z}^+, \ p(x) \in \mathbb{P}_n, \ s.t. \ \|f(x) - p(x)\|_{\mathcal{C}^0([a, b])} < \frac{\varepsilon}{2}.$$
 (1)

And the professor said we aim to use machine learning method to use $\tanh x$ to approximate p(x) such that

$$\forall \varepsilon \in \mathbb{R}^+, \exists N \in \mathbb{Z}^+, \ h(x) = \sum_{k=1}^N a_k \sigma(khx) + b, \ s.t. \ \|h(x) - p(x)\|_{\mathcal{C}^0([a, b])} < \frac{\varepsilon}{2}$$
 (2)

Thus combine (1) and (2), we get:

$$\forall \varepsilon \in \mathbb{R}^+, \exists N \in \mathbb{Z}^+, \ h(x) = \sum_{k=1}^N a_k \sigma(khx) + b, \ s.t. \ \|h(x) - f(x)\|_{\mathcal{C}^0([a, b])} < \frac{\varepsilon}{2} + \frac{\varepsilon}{2} = \varepsilon \quad (3)$$

However the process seems legit, I find it a flaw occurs in the equation (2).

The function p(x) in equation (1) is actually $p(x;\varepsilon)$, thus in equation (2), h(x) is $h(x;\varepsilon)$. Meaning that $\forall \varepsilon \in \mathbb{R}^+$, we have a varying, unique objective polynomial $p(x;\varepsilon)$ to approximate, thus the structure of each $h(x;\varepsilon)$ may look very different. It is not just a simple step size h changing process, isn't it?

The Answer Got from AI for Problem 1

You are correct: the polynomial p(x) and the approximating neural network are not fixed. They change depending on the value of ε you choose.

Your observation is exactly right. If you want a more accurate approximation (you choose a smaller ε), the Weierstrass theorem might require a different, possibly higher-degree, polynomial p'(x); then, the equation would require a different, likely larger, neural network to approximate that new polynomial p'(x).

The theorem's power lies in this **guarantee of existence**. It states that for any continuous function f(x) you give me and for any desired level of accuracy ε you specify, I can find a neural network (of sufficient size) that will do the job.

The proof doesn't tell you how to find that specific polynomial or that specific network. That's what the training process in machine learning is for. The theorem simply provides the **theoretical foundation**, assuring us that a sufficiently large neural network has the capacity to represent the function we want to learn.

——— (Answer from Gemini)

My Question 2: Can An Activation Function Be Linear or Identity Function?

Is a non-linear activation function an absolute necessity for a neural network to be a useful model, and what happens if all activation functions are linear? (This question is refined by Gemini.)

The Answer Got from AI for Problem 2

Yes, a non-linear activation function is **absolutely necessary** for a neural network to be a useful and powerful tool for solving complex problems. Without it, the network **cannot learn anything** more complex than a simple **linear** relationship, regardless of how many layers it has.

The Role of Non-Linearity

• The entire purpose of a deep neural network is to learn complex, non-linear patterns in data—the kind of patterns found in images, speech, and text. These patterns cannot be captured by a straight line or a simple plane. Activation functions are the key to introducing this essential non-linearity.

What Happens with Linear Activation Functions?

• If you were to use only linear activation functions (like the identity function) in all hidden layers, the network would **collapse** into a single-layer linear model. The mathematical reason is that the composition of any number of linear functions is always another linear function.

In conclusion, a linear activation function in a hidden layer is a **dead-end**, as it prevents the network from **learning the complex representations** that make it powerful. Non-linear activation functions are the fundamental building blocks that unlock the potential of deep learning.

——— (Answer from Gemini)

What I Want to Propose 1: Importance of One-Hot Encoding

I think the importance of **one-hot encoding** or **dummy variable** can be manifested in the scenario that a variable has 3 or more discrete states. In my current project focusing on the **fraud detection** with machine learning, this occurs quite often; for instance, the transactions can be simply categorized into 5 continents, it is unreasonable to label *Asia* to be 1, *Europe* to be 2, and so on. The solution we come up with is to use dummy variables like **is_asia**, **is_europe**,... functions that give either 0 or 1. This can be seen that a problem under lower-dimensional space cannot find a smooth curve to accommodate, but with higher dimensions, it is feasible. This is my own perspective to the **one-hot encoding** on the implementation.