C++ Assn3 Neural Network for MNIST

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1 Introduction

In this assignment, you will implement basic neural network consists of 3 layers which classifies handwritten digits provided by MNIST dataset. By the assignment, you will understand following concepts:

- Class and inheritance in cpp
- How neural network & backpropagation works

2 Background

2.1 MNIST dataset

MNIST(Modified National Institute of Standards and Technology database) dataset is a large database of handwritten digits, which is widely used for training and testing image processing systems based on deep learning / machine learning model. Since 1998, lots of computer scientists tried to implement AI which can classify the images, and recently the researchers from University of Virginia announced the model which achieved 99.82% accuracy.



MNIST dataset

MNIST contains 60,000 training images and 10,000 test images, and they're provided in mnist directory. Also, accessing and reading files is already implemented, hence you only need to focus on implementing neural network which receives the data from MNIST as input.

2.2 Brief History

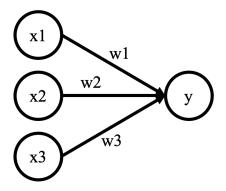
In the early stage of AI(Artificial Intelligence), it was mostly rule-based. Researchers extracted the patterns from data and tried to heuristically encode them as rules. However, the strategy was quite not successful, as it was hard to extract every underlying pattern from data.

On the other hand, in 1970-80s, several researchers including Geoffrey Hinton, David Rumelhart, Yoshua Bengio tried other approach: Artificial neural network. Their approach mainly aimed to mimic the neuron & synapse structure of human brain. However, due to it's high computation requirement, the approach was extremely inefficient and was discarded for decades; we now call this era as AI winter.

However, as the computation power had come a long way, the time and resource usage for Artificial Neural Network decreased significantly, and it showed overwhelming performance. Moreover, as now researchers can collect unlimited data from internet, it got the opportunity to be adopted in various domains. Therefore, in nowadays, AI became one of the most important modern technologies, and learning AI & neural network is now an essential course for the researchers in engineering or science field.

2.3 Perceptron

Perceptron is an algorithm offered by Frank Rosenblatt in 1957, and now used as a fundamental element in many complex nerual networks. The structure is quite simple: it combines several input, and generates single output.



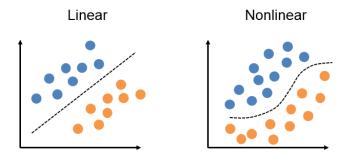
Single perceptron

The y value is determined like this:

$$y = 1$$
 if $x_1w_1 + x_2y_2 + x_3y_3 > \theta$
 $y = 0$ if $x_1w_1 + x_2y_2 + x_3y_3 < \theta$

where θ is a threshold. However, a single-layer perceptron can only classify the space linearly, it cannot be applied to complex non-linear situation. To solve the problem, researchers constructed neural network as sophisticated multi-layer perceptron.

In this assignment, you'll implement multi-layer perceptron. For the detailed explanation for our neural network, refer next section.

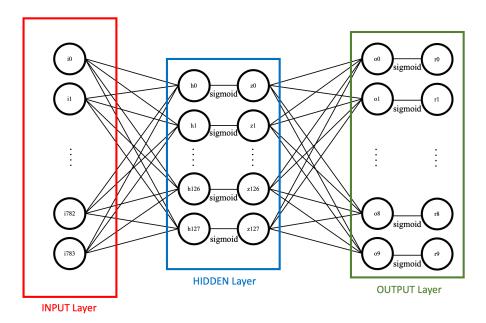


 $\begin{array}{c} Linear\ vs.\ Nonlinear\ perceptron \\ (Reference:\ https://jtsulliv.github.io/perceptron/) \end{array}$

3 Explanation

3.1 Neural network

As I mentioned above, our neural network will consists of 3 layers: input, hidden, and output, which are *fully connected* each other. The structure overview and specification for each part is as follows.



Neural network structure overview

As the MNIST image size is $28 \times 28 = 784$, There are total 784 nodes in input layer. Hidden layer initially has 128 nodes, but you can modify it freely. At last, output layer has 10 nodes, where each represents corresponding digit (0-9).

3.2 Activation function

You might noticed that both Hidden layer and Output layer have single edge named Sigmoid. It is an Activation function for our neural network. So what is activation function? To understand activation function, you must recall that the single-layer perceptron generates linear classification, and multi-layer approach had arrived to solve the problem. However, if we overlap multiple linear perceptrons successively, it still produces linear classification. Simple example might help you: overlapping y = ax and z = by just generates $z = b \cdot ax$, which is still linear.

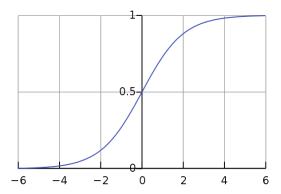
Therefore, a non-linear function should be located between linear perceptrons, and activation function serves the role. There exists various modern non-linear activation functions: ReLU, Leaky ReLU, tanh, Softmax, Swish....

Activation function has one more important property: it controls the power of signal. Let's remind that basic perceptron generates only two kinds of signal: 0 to 1 (transfer or not). However, researchers found that transferring the signal value is more effective to solve complex problems. But to transfer continuous value, output of the perceptron should be post-processed to maintain consistency. Activation function helps neural network to achieve the goal. For instance, Sigmoid normalizes the input value to a value between 0 and 1.

Sigmoid

Sigmoid, or logistic regression, which you'll implement, is a quite old strategy. The function and its graph are like this:

$$Sigmoid(x) = \frac{e^x}{1 + e^x}$$



As represented in the graph, Sigmoid sends large positive number to 1 and the opposite to -1. Sigmoid has some critical problems: exponential function inside it requires high computation, and sometimes extremely slows down the training. Nevertheless, it is easy to implement and also fits to our problem. You'll notice the benefit of Sigmoid in **backpropagation section**.

3.3 Training

The training step of typical neural networks, including our network, follows the process:

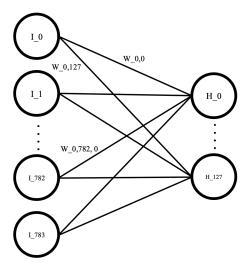
1. Get current input

- 2. Perform feed-forward computation through the network
- 3. Calculate Loss
- 4. Backpropagate the loss and update weights
- 5. Go back to step 1 with next input

Let's see the detail with our neural network.

Feed-Forward

Our network starts with the connection between Input layer and Hidden layer.



Let's denote each input value(node) as I_i and hidden layer input value as H_i . Then the overall computation across Input and Hidden layer is as follows:

$$H_i = W_{0,i}I_0 + W_{1,i}I_1 + \dots + W_{782,i}I_{782} + W_{783,i}I_{783} + b_i$$

where i: 0 to 127 (128 hidden nodes), $W_{a,b}$ corresponds to the edge connecting I_a and H_b , and b_i denotes the bias.

Hidden layer also contains Sigmoid. Let's denote Sigmoid as ϕ and it's result as Z_i . Then we can just say $\phi(H_i) = Z_i$ where i: 0 to 127.

Now only the connection between Hidden / Output layer and the final Sigmoid are left. These computations are like this:

$$O_i = W_{0,i}' Z_0 + W_{1,i}' Z_1 + \dots + W_{126,i}' Z_{126} + W_{127,i}' Z_{127} + b_i'$$

$$R_i = \phi(O_i)$$
 $i:0$ to 9

where O_i : Output layer input value, and R_i : Final result value.

Loss function

As final result R_i s are the output of Sigmoid, their value is in between zero and one. Next step is to calculate loss. In this assignment, you'll implement $MSE(Mean\ Squared\ Error)$:

$$MSE = \frac{1}{2} \sum_{i=0}^{9} (\hat{R}_i - R_i)^2$$

$$\hat{R}_i = 0 \text{ if } label == i \text{ else } 0$$

as loss function, where \hat{R}_i denotes the real result. The value of real result vector \hat{R} is defined as above. For example, if the input image represents digit 7, \hat{R} will be (0,0,0,0,0,0,0,1,0,0).

Therefore, if our neural network assigns high value to the index corresponds to the answer and low value to the others, the loss will be small. Therefore, we interpret the final result value vector R as follows: answer = $\arg \max R_i$.

Backpropagation

Now we learned how our neural network generates the answer and the way to calculate the loss. Then, how can we *train* our neural network? Backpropagation, which was first suggested by Rumelhart et al. in their paper published in *Nature*, provides polished way to achieve the goal.

The main concept of backpropagation is to send back the generated loss(or error) toward the input and underlying weights. While sending back the error, the gradient for each weight will be calculated successively and the weights will be updated due to their gradients. So how can we calculate gradient *successively*? The theoretical background for this step is quite simple: *chain rule*.

Maybe you had learned partial derivative and chain rule in the calculus class. For who did not or who forgot the concepts, I'll briefly explain about them. Actually, the former is quite easy concept: a partial derivative of a function of several variables is its derivative with respect to one of those variables, with the others held constant. For example, partial derivative $\partial f/\partial x$ of the function $f(x,y) = ax^2 + bxy + cy^2$ will be:

$$\frac{\partial f}{\partial x} = 2ax + by.$$

This is the only thing you need to know about partial derivative.

Then how about chain rule? Astonishingly, you had noticed the basic concept of the chain rule in high school. Recall the famous derivative rule $(f(g(x))' = f'(g(x)) \cdot g'(x))$, which can be written as

$$\frac{df \circ g}{dx} = \frac{df}{dg} \cdot \frac{dg}{dx}$$

according to the Leibniz's notational system. This directly shows the main idea of the chain rule: the derivative can be calculated through consecutive sequence of inner derivatives. Simple example will help you. Let's think about the composite function f(g(h(i(x)))). The derivative of the

function can be calculated through the sequence:

$$(f(g(h(i(x)))))' = f'(g(h(i(x)))) \cdot (g(h(i(x))))'$$

$$= f'(g(h(i(x)))) \cdot g'(h(i(x))) \cdot (h(i(x)))'$$

$$= f'(g(h(i(x)))) \cdot g'(h(i(x))) \cdot h'(i(x)) \cdot i'(x)$$

which can be expressed as

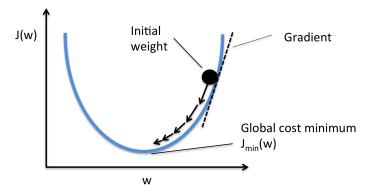
$$\frac{df}{dx} = \frac{df}{dq} \cdot \frac{dg}{dh} \cdot \frac{dh}{di} \cdot \frac{di}{dx},$$

which is the standard form of the chain rule. Of course chain rule can be applied to partial derivative too.

Then how can we apply these concepts to update weights during backpropagation? The main purpose of the backpropagation is to reduce the loss. And our error, MSE, can be expressed as the function of variables W, b, I, where each denotes the set of weight, bias, and input values. Therefore, it is evident that we can calculate the partial derivative of MSE due to each weight and bias, and the value can be evaluated using chain rule. After calculating the gradient, the weight can be updated toward the direction which reduces the loss. The equation below explains the work.

$$w = w - \eta \frac{\partial MSE}{\partial w}$$

In the equation, w denotes the certain weight and η is learning rate. If learning rate is small, the precision of the training will become high but it will take much time to arrive the point. In contrast, big learning rate will ensure both fast training and low precision.



Weight update due to its gradient

Now its time to follow the backpropagation step. Let's first recall the entire feed-forward process.

$$\begin{split} H_i &= W_{0,i}I_0 + W_{1,i}I_1 + \dots + W_{782,i}I_{782} + W_{783,i}I_{783} + b_i \\ Z_i &= \phi(H_i) & i:0 \text{ to } 127 \\ O_j &= W'_{0,j}Z_0 + W'_{1,j}Z_1 + \dots + W'_{126,j}Z_{126} + W'_{127,j}Z_{127} + b'_j \\ R_j &= \phi(O_j) & j:0 \text{ to } 9 \\ MSE &= \frac{1}{2}\Sigma_{k=0}^9 (\hat{R}_k - R_k)^2 & \hat{R}_k = 0 \text{ if } label == k \text{ else } 0 \end{split}$$

The parameters that should be updated are the weights and bias of the neural network. Let's first investigate $W'_{i,j}$. It is obvious that

$$\frac{\partial MSE}{\partial W_{i,j}'} = \frac{\partial MSE}{\partial R_j} \frac{\partial R_j}{\partial O_j} \frac{\partial O_j}{\partial W_{i,j}'},$$

and each term of the right-hand side is as follows:

$$\begin{split} \frac{\partial MSE}{\partial R_j} &= \frac{1}{2} \frac{\partial}{\partial R_j} (\hat{R}_j - R_j)^2 = (\hat{R}_j - R_j) \\ \frac{\partial R_j}{\partial O_j} &= \frac{\partial \phi(O_j)}{\partial O_j} \\ \frac{\partial O_j}{\partial W_{i,j}^{\prime}} &= Z_i \end{split}$$

Now you might ask; "How can we calculate $\frac{\partial \phi(O_j)}{\partial O_j}$ "? Recall that

$$\phi(x) = \text{Sigmoid}(x) = \frac{e^x}{1 + e^x} = \frac{1}{1 + e^{-x}}.$$

We can easily calculate the derivative using simple derivation rule:

$$\phi'(x) = ((1 + e^{-x})^{-1})'$$

$$= (1 + e^{-x})^{-2} \cdot (1 + e^{-x})'$$

$$= (1 + e^{-x})^{-2} \cdot (-e^{-x})$$

$$= \frac{1}{1 + e^{-x}} \cdot \frac{-e^{-x}}{1 + e^{-x}}$$

$$= (1 - \phi(x))\phi(x)$$

Therefore, we can rewrite the second derivative $\frac{\partial R_j}{\partial O_j}$.

$$\frac{\partial R_j}{\partial O_j} = \frac{\partial \phi(O_j)}{\partial O_j} = (1 - \phi(O_j))\phi(O_j) = (1 - R_j)R_j$$

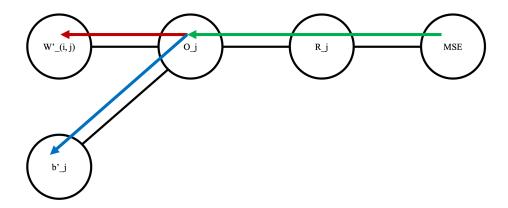
It is easy to notice that $\frac{\partial MSE}{\partial W_{i,j}}$ can be calculated only by using \hat{R}_j, R_j, Z_i , which are the values that can be evaluated during feed-forward step.

Then How about the bias b'_i ? We can simply write the gradient like:

$$\frac{\partial MSE}{\partial b_j'} = \frac{\partial MSE}{\partial R_j} \frac{\partial R_j}{\partial O_j} \frac{\partial O_j}{\partial b_j'},$$

Now you might found the issue; we already calculated $\frac{\partial MSE}{\partial R_j}$ and $\frac{\partial R_j}{\partial O_j}$ while dealing with $W_{i,j}$. Therefore the only thing we need to consider is $\frac{\partial O_j}{\partial b_j^i}$, which is 1.

This fact is one of the most important point during backpropagation. We can reuse the sequence of partial gradients. Above situation can be illustrated like this.



As we already calculated the gradients corresponds to green arrow while going toward red arrow, we don't need to do it again while going toward blue arrow. This technique reduces computation a lot, and therefore accelerates training.

4 Assignments

4.1 Calculation

You may understood how our neural network works. However, I didn't explained everything, so you must first fill up the missing links.

Solve the following problems. It is highly recommended to write the entire process with LATEX.

- 1. In section 3, we only calculated the gradient for the second layer. Calculate the gradients for the first layer.
 - a) Calculate $\frac{\partial MSE}{\partial W_{i,j}}$.
 - b) Calculate $\frac{\partial MSE}{\partial b_j}$.
- 2. Recall that our neural network updates the weight by applying

$$w = w - \eta \frac{\partial MSE}{\partial w}.$$

Prove that this updating strategy ensures the decrease of MSE (hint: focus on ΔMSE).

4.2 Implementation

The template code is available at the link. The training and testing code are already implemented, so you only need to focus on implementing the feed-forward and backpropagation step.

The functions that you need to implement is like this:

• perceptron.cpp

- Perceptron(int num)

The constructor of a single perceptron, which gets num inputs. Allocate the initial value to the num weights correspond to each input, and a single bias. I recommend to assign random value to weights / bias using rand_Oto1 function in helper.cpp.

- forward(double* input)Feed-forward step for a single perceptron.
- backprop(double delta, double *current_input)
 Backpropagation step for a single perceptron. delta denotes the former gradients which are propagated from the fore, and current_input literally denotes the current input vector for the layer which contains the perceptron.

• sigmoid.cpp

- forward(double input)
- backprop()

• bridge.cpp

This class represents the bridge between a layer to the other layer. It is consists with the set of perceptrons and sigmoids, according to the input / output structure explained in section **3.1**.

- Bridge(int input_num, int output_num)
 Gets input / output number as arguments, and allocates perceptrons and sigmoids due to the values.
- forward(double* input)

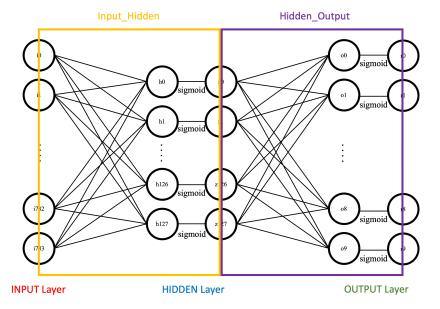
ullet hidden_output.cpp

inherites Bridge class, and represents the bridge from the input layer to the hidden layer.

- backprop(double* delta)
- input_hidden.cpp

inherites Bridge class, and represents the bridge from the input layer to the hidden layer.

- backprop(double* delta)
 Input_Hidden :: backprop() should get the result of Hidden_Output :: backprop()
 as a argument.
- train.cpp
 - loss_function(double* delta) delta denotes the array consists of $\hat{R}_i R_i$, where i = 0 to 9.



The area of Hidden_Output and Input_Hidden are like this.

After implementation, you can generate executable program by make run command. If the program output is like this, it verifies your implementation.

```
Neural Network model for MNIST
   EP0CH: 100
    Learning rate: 0.01
TRAINING START!!
Total dataset size: 60000
Sample ~3000: Average loss is 0.402518
Sample ~6000: Average loss is 0.258591
Sample ~9000: Average loss is 0.217464
Sample ~12000: Average loss is 0.195215
Sample ~15000: Average loss is 0.198591
Sample ~18000: Average loss is 0.178943
Sample ~21000: Average loss is 0.155885
Sample ~24000: Average loss is 0.155108
Sample ~27000: Average loss is 0.15103
Sample ~30000: Average loss is 0.147741
Sample ~30000: Average loss is 0.147741
  Sample ~18000:
Sample ~21000:
Sample ~24000:
Sample ~27000:
Sample ~30000:
Sample ~30000:
Sample ~30000:
                                                                        loss is 0.147/41
loss is 0.154779
loss is 0.12361
loss is 0.128606
loss is 0.131559
loss is 0.126316
loss is 0.127829
                                                Average
                                                Average
   Sample ~39000:
Sample ~42000:
Sample ~45000:
Sample ~48000:
                                                Average
                                                Average
                                                Average
                                                Average
   Sample ~51000:
Sample ~54000:
                                                Average
                                                                        loss is 0.113296
loss is 0.103901
                                                Average
    Sample ~57000:
                                               Average
   Sample ~60000: Average loss is 0.080278
    TESTING...
    Test RESULT
   Test set size: 10000
Correct: 8877
Wrong: 1123
    Accuracy: 0.8877
```

4.3 Tips

- Use the constants in constants.h. For fast test & verification, I recommend you to change the EPOCH
- Remember that you only need to implement about 50 lines.