Machine Learning 2016

HW-3：Neural Network

Deadlines: **2016.05.10**-23:59:59

In this homework, you are asked to build **neural network** models for the classification problem of the **hand-written numbers** $\boldsymbol{x}$. Before doing so, the following layers need to be implemented as a Matlab function respectively:

- **Inner-product layer**
- **Activation layer**
- **Softmax layer**

Besides, it is required to use different types of the **activation function** for the tasks:

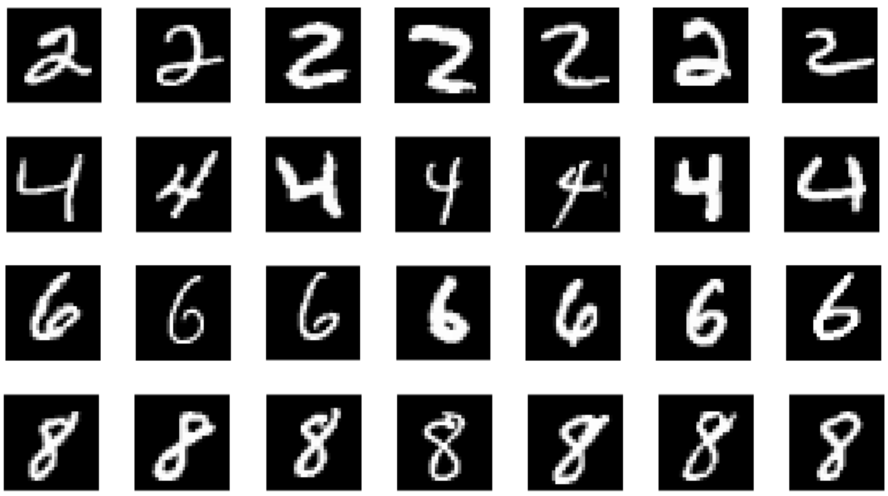
- **Sigmoid function**
- **Rectified function**

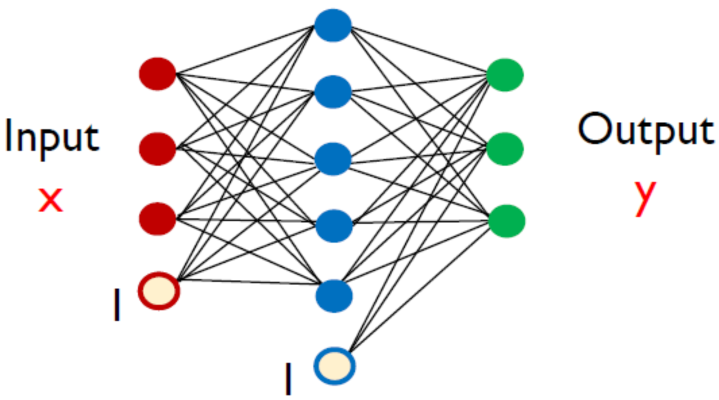
C_1 = **Handwritten 2**

C_2 = **Handwritten 4**

C_3 = **Handwritten 6**

C_4 = **Handwritten 8**





◆ Data

Input data are the extracted information from the picture of the hand-written numbers (**MNIST** Database). There are two data files offered: **Training _data_hw3.mat** file and one **Test_data1_hw3.mat** file.

Training _data_hw3.mat:

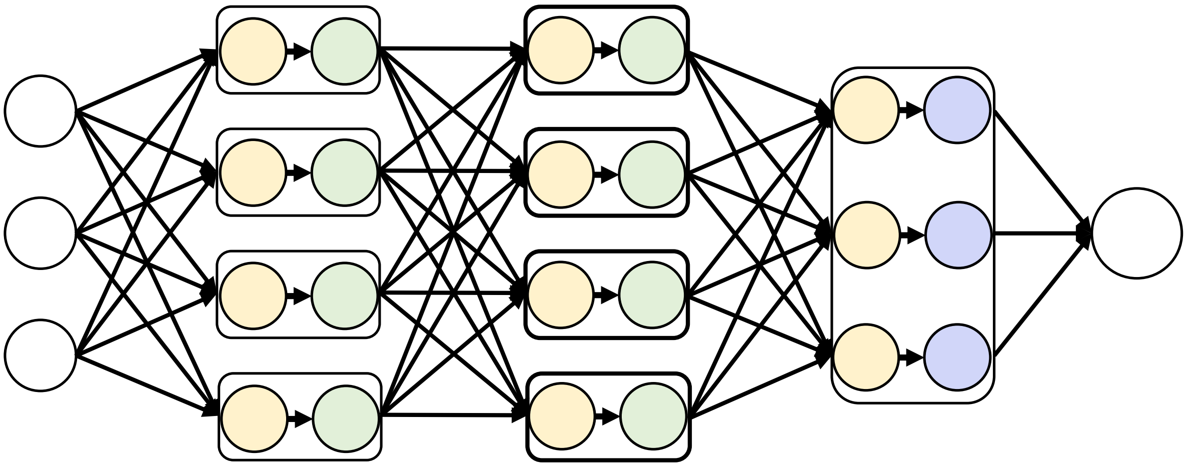
- ➢ **X_train** is a 4000x784 matrix. Every row corresponds to a 28x28 gray-scale image.
- ➢ **T_train** is a 4000x4 matrix, which records the target values of the training samples.

Test_data2_hw3.mat:

- ➢ **X_test** is a 2000x784 matrix. Every row corresponds to a 28x28 gray-scale image.

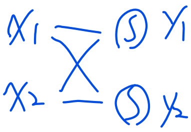
◆ Models

A simple neural network can be decomposed into the input layer, hidden layer(s) and output layer. A hidden layer is usually composed of an **inner-product layer** and an **activation layer**. Likewise, an output layer normally contains an **inner-product layer** and a **softmax layer**.



Let the m-by-1 vector $\boldsymbol{x}$ and n-by-1 vector $\boldsymbol{y}(\boldsymbol{x})$ be the input and output of a layer respectively, the forward-propagation and back-propagation can be inferred as bellow:

● Inner-product layer



$y_1 = x_1 w_a + x_2 w_b + b$

$y_2 = x_1 w_c + x_2 w_d + b$

✧ Forward-propagation

$W^T = \begin{bmatrix} w_1^T \\ w_2^T \end{bmatrix}$, $b = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$

$$\boldsymbol{y}(\boldsymbol{x}) = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} \boldsymbol{w}_1^T\boldsymbol{x} + b_1 \\ \vdots \\ \boldsymbol{w}_n^T\boldsymbol{x} + b_n \end{bmatrix} = [\boldsymbol{w}_1 \dots \boldsymbol{w}_n] \cdot \boldsymbol{x} + \begin{bmatrix} b_1 \\ \vdots \\ b_n \end{bmatrix} = \boldsymbol{W}^T\boldsymbol{x} + \boldsymbol{b}$$

$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$, $w_1 = \begin{bmatrix} w_a \\ w_b \end{bmatrix}$, $w_2 = \begin{bmatrix} w_c \\ w_d \end{bmatrix}$ $\Rightarrow$ $\underbrace{\begin{bmatrix} w_a & w_b \\ w_c & w_d \end{bmatrix}}_{W^T} \cdot \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \underbrace{\begin{bmatrix} b_1 \\ b_2 \end{bmatrix}}_{b}$

$x_1, x_2 \to y_1, y_2$

對 Loss來說, y_1, y_2 都有影響 → 要 sum 起來

if x有2個
y有2個

$y_1 = w_a x_1 + w_b x_2$

$y_2 = w_c x_1 + w_d x_2$

$$A = \begin{bmatrix} w_a & w_b \\ w_c & w_d \end{bmatrix} = W^T$$

✧ **Back-propagation**

這邊的 y 是經過 w, b 的 z

$$\nabla_x E = \begin{bmatrix} \frac{\partial E}{\partial x_1} \\ \vdots \\ \frac{\partial E}{\partial x_m} \end{bmatrix} = \begin{bmatrix} \frac{\partial E}{\partial y_1}\frac{\partial y_1}{\partial x_1} + \cdots + \frac{\partial E}{\partial y_n}\frac{\partial y_n}{\partial x_1} \\ \vdots \\ \frac{\partial E}{\partial y_1}\frac{\partial y_1}{\partial x_m} + \cdots + \frac{\partial E}{\partial y_n}\frac{\partial y_n}{\partial x_m} \end{bmatrix} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \cdots & \frac{\partial y_n}{\partial x_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_1}{\partial x_m} & \cdots & \frac{\partial y_n}{\partial x_m} \end{bmatrix} \begin{bmatrix} \frac{\partial E}{\partial y_1} \\ \vdots \\ \frac{\partial E}{\partial y_n} \end{bmatrix} = \boldsymbol{A} \begin{bmatrix} \frac{\partial E}{\partial y_1} \\ \vdots \\ \frac{\partial E}{\partial y_n} \end{bmatrix}$$

$$\nabla_W E = \begin{bmatrix} \frac{\partial E}{\partial w_{11}} & \cdots & \frac{\partial E}{\partial w_{n1}} \\ \vdots & \ddots & \vdots \\ \frac{\partial E}{\partial w_{1m}} & \cdots & \frac{\partial E}{\partial w_{nm}} \end{bmatrix} = \begin{bmatrix} \frac{\partial E}{\partial y_1}\frac{\partial y_1}{\partial w_{11}} & \cdots & \frac{\partial E}{\partial y_n}\frac{\partial y_n}{\partial w_{n1}} \\ \vdots & \ddots & \vdots \\ \frac{\partial E}{\partial y_1}\frac{\partial y_1}{\partial w_{1m}} & \cdots & \frac{\partial E}{\partial y_n}\frac{\partial y_n}{\partial w_{nm}} \end{bmatrix} = \begin{bmatrix} \frac{\partial E}{\partial y_1} \\ \vdots \\ \frac{\partial E}{\partial y_n} \end{bmatrix} \boldsymbol{B}$$

$$\nabla_b E = \begin{bmatrix} \frac{\partial E}{\partial b_1} \\ \vdots \\ \frac{\partial E}{\partial b_n} \end{bmatrix} = \begin{bmatrix} \frac{\partial E}{\partial y_1}\frac{\partial y_1}{\partial b_1} \\ \vdots \\ \frac{\partial E}{\partial y_n}\frac{\partial y_n}{\partial b_n} \end{bmatrix} = \begin{bmatrix} \frac{\partial E}{\partial y_1} \\ \vdots \\ \frac{\partial E}{\partial y_n} \end{bmatrix} \boldsymbol{C}$$

$B = \begin{bmatrix} x_1 & x_2 \end{bmatrix}$

$C = \begin{bmatrix} 1 & 1 \end{bmatrix}$

Please find the matrices **A**, ***B*** and **C** by yourself.

- **Activation layer – Sigmoid function**

✧ **Forward-propagation**

$z_1 \quad \sigma(z_1) = \frac{1}{1+\exp(-z_1)}$

$z_2 \quad \sigma(z_2) = \frac{1}{1+\exp(-z_2)}$

$$\boldsymbol{y}(\boldsymbol{x}) = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1/(1+e^{-x_1}) \\ \vdots \\ 1/(1+e^{-x_n}) \end{bmatrix}$$

$\sigma(z)$

$y_1 = \frac{1}{1+\exp(-x_1)}$

✧ **Back-propagation**

這邊的 y 是經過 sigmoid 的值 a 和 g

$$\nabla_x E = \begin{bmatrix} \frac{\partial E}{\partial x_1} \\ \vdots \\ \frac{\partial E}{\partial x_n} \end{bmatrix} = \begin{bmatrix} \frac{\partial E}{\partial y_1}\frac{\partial y_1}{\partial x_1} \\ \vdots \\ \frac{\partial E}{\partial y_n}\frac{\partial y_n}{\partial x_n} \end{bmatrix} = \cancel{\begin{bmatrix} \frac{\partial E}{\partial y_1} \\ \vdots \\ \frac{\partial E}{\partial y_n} \end{bmatrix} \boldsymbol{D}} = D \begin{bmatrix} \frac{\partial E}{\partial y_1} \\ \frac{\partial E}{\partial y_2} \end{bmatrix}$$

Please find the matrix ***D*** by yourself.

$$D = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & 0 \\ 0 & \frac{\partial y_2}{\partial x_2} \end{bmatrix} = \begin{bmatrix} \sigma(x_1)(1-\sigma(x_1)) & 0 \\ 0 & \sigma(x_2)(1-\sigma(x_2)) \end{bmatrix}$$

- **Activation layer – Rectified function** (optional)

  - **Forward-propagation**

$$\boldsymbol{y}(\boldsymbol{x}) = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} [x_1 > 0] \cdot x_1 \\ \vdots \\ [x_n > 0] \cdot x_n \end{bmatrix}$$

  - **Back-propagation**

$$\nabla_{\boldsymbol{x}} E = \begin{bmatrix} \frac{\partial E}{\partial x_1} \\ \vdots \\ \frac{\partial E}{\partial x_n} \end{bmatrix} = \begin{bmatrix} \frac{\partial E}{\partial y_1} \frac{\partial y_1}{\partial x_1} \\ \vdots \\ \frac{\partial E}{\partial y_n} \frac{\partial y_n}{\partial x_n} \end{bmatrix} = \begin{bmatrix} \frac{\partial E}{\partial y_1} \\ \vdots \\ \frac{\partial E}{\partial y_n} \end{bmatrix} \boldsymbol{E}$$

Please find the matrix $\boldsymbol{E}$ by yourself.

- **Softmax layer**

  - **Forward-propagation**

$$x_1 \quad e^{x_1} \quad y_1 = \frac{e^{x_1}}{sum}$$
$$x_2 \Rightarrow e^{x_2} \quad y_2 = \frac{e^{x_2}}{sum}$$
$$x_3 \quad e^{x_3} \quad y_3 = \frac{e^{x_3}}{sum}$$
$$sum = e^{x_1} + e^{x_2} + e^{x_3}$$

$$\boldsymbol{y}(\boldsymbol{x}) = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \frac{1}{\sum_{i=1}^{n} e^{x_i}} \begin{bmatrix} e^{x_1} \\ \vdots \\ e^{x_n} \end{bmatrix}$$

$$loss = (\hat{y}_1 \times \ln y_1) + (\hat{y}_2 \times \ln y_2) + (\hat{y}_3 \times \ln y_3)$$

  - **Back-propagation**

不知道為啥只有一項

大概是[100][010][001]組的關係吧

$$\frac{\partial E}{\partial y_1}\frac{\partial y_1}{\partial x_1} + \frac{\partial E}{\partial y_2}\frac{\partial y_2}{\partial x_1} + \frac{\partial E}{\partial y_3}\frac{\partial y_3}{\partial x_1}$$

$$\begin{bmatrix} (-\hat{y}_1 \times \frac{1}{y_1})(y_1 - e^{2x_1}(sum)^{-2}) \\ (-\hat{y}_2 \times \frac{1}{y_2})(y_2 - e^{2x_2}(sum)^{-2}) \\ (-\hat{y}_3 \times \frac{1}{y_3})(y_3 - e^{2x_3}(sum)^{-2}) \end{bmatrix}$$

$$\nabla_{\boldsymbol{x}} E(\boldsymbol{y}, \boldsymbol{t}) = \begin{bmatrix} \frac{\partial E}{\partial x_1} \\ \vdots \\ \frac{\partial E}{\partial x_n} \end{bmatrix} = \begin{bmatrix} \frac{\partial E}{\partial y_1} \frac{\partial y_1}{\partial x_1} \\ \vdots \\ \frac{\partial E}{\partial y_n} \frac{\partial y_n}{\partial x_n} \end{bmatrix} = \begin{bmatrix} y_1 - t_1 \\ \vdots \\ y_n - t_n \end{bmatrix} = \boldsymbol{y} - \boldsymbol{t}$$

$$\frac{\partial y_1}{\partial x_1} = y_1 - e^{2x_1}(e^{x_1} + e^{x_2} + e^{x_3})^{-2}$$

There is only the inner-product layer containing parameters which need to be optimized. Please follow the **gradient descent** approach to iteratively update the parameters.

$$\boldsymbol{W}^{new} = \boldsymbol{W}^{old} - \eta \nabla_{\boldsymbol{W}} E$$

$$\boldsymbol{b}^{new} = \boldsymbol{b}^{old} - \eta \nabla_{\boldsymbol{b}} E$$

◆ Tasks

1. Layers as Matlab Functions

Implement the forward-propagation and back-propagation of every layer into Matlab functions **(LayerName)_ForProp(.)** and **(LayerName)_BackProp(.)**. You are suggested to modify the templates attached in the HW package to accomplish the task.

2. One-hidden-layer Neural Network

Based on the Matlab functions created in the task 1, you are able to build **one-hidden-layer NNs**. Please use such models to deal with the MNIST classification problem. (Choose the **sigmoid function** as the activation function.) Predict the 2000x4 target matrix **T_test** given the input data **X_test** and save it in the file **OneHidNN_T_test.mat**.

3. Two-hidden-layer Neural Network

One step further, you are asked to build **two-hidden-layer NNs**. Please use such models to deal with the MNIST classification problem. (Choose the **rectified function** as the activation function.) Predict the 2000x4 target matrix **T_test** given the input data **X_test** and save it in the file **TwoHidNN_T_test.mat**.

What should be uploaded?

- ☐ Your Matlab source code with comments.
- ☐ The **OneHidNN_T_test.mat** file which contains **T_test**.
- ☐ The **TwoHidNN_T_test.mat** file which contains **T_test**.
- ☐ The **ReadMe.txt** file which describes how to run your program.
- ☐ Your **report** in the format of .pdf or .doc.

Reminders:

- ☐ There won't be a need for demonstration.
- ☐ Please make sure your source code can be compiled by **Matlab**.
- ☐ **DO NOT COPY!!!（懶人包、考古題亦同）**