# Section 16 Neural Network (and Deep Learning)

### **Basic Structures of Neural Network (NN)**

Intuitively, Neural Network is nothing but the construction of one nonlinear (vector-valued) function  $\mathbf{h}(\mathbf{x}; W, b) \in \mathbb{R}^p \to \mathbb{R}^k$  with a series of composite functions (layers). For the interactive visualization and exploration of NN, you can refer here.

The layers can be further classified into three categories:

- Input layer: p nodes representing the input sample  $x \in \mathbb{R}^p$
- **Hidden layers**: Calculate the values on the nodes of (l+1)-th layers based on those on the l-th layer as

$$egin{aligned} \mathbf{z}^{(l+1)} &= W^{(l)} \mathbf{a}^{(l)} + \mathbf{b}^{(l)} \ \mathbf{a}^{(l+1)} &= \sigma(\mathbf{z}^{(l+1)}) \end{aligned}$$

where  $\sigma$  is the nonlinear activation function (common choices include sigmoid, tanh or ReLU), and the second equation is element-wize.

*Note*: Suppose there are m nodes in layer l and n nodes in layer (l+1). Then there are  $(m+1)\times n$  trainable parameters between the two layers, or sometimes by convention, we just say they are the parameters are on the (l+1)-th layer.

- Output layer: k nodes representing the output, and dependent on the problem can be
  - 1) For regression problem, just as another regular hidden layer of k nodes
  - 2) For classification problem, apply the softmax function on the vector  $\mathbf{z}$  to ensure that the output is the probability vector for k classes.

After constructing the mapping, in supervised problem, the loss function  $J(W,b;\mathbf{x},y)$  can be choosed the same as other machine learning models.

- For regression: MSE (mean squared error)
- For classification: Cross Entropy

#### **Interesting Facts** (not required in exam):

- Logistic regression can be viewed as "the simplest" NN with only the input layer (p nodes) and output layer (softmax output). Because it only has "one layer of parameters", sometimes it is also called single-layer NN.
- NN can also be used in unsupervised tasks, such as Autoencoder for dimension reduction.

## Training Algorithms: BP (Back Propagation) and SGD (or other optimization method)

As we've known well, training the machine learning model is largely dependent on minimizing the loss function, where its gradient provides the important information.

Intuitively speaking, **back propagation** is just the right algorithm to find such gradient for the training of NN, which is based on the **chain-rule** of derivatives in hierarchical network-structured composite function.

In detail, the backpropagation algorithm for NN training can be described as (not required):

Step 1: Perform a **forward pass**, computing the values for layers  $L_2$ ,  $L_3$ , and so on up to the output layer  $L_{n_l}$ . We take the loss of MSE in regression as example.

Step 2: For each output unit i in layer  $n_l$  (the output layer), set

$$\delta_i^{(n_l)} := rac{\partial}{\partial z_i^{(n_l)}} \left. J(W,b;\mathbf{x},y) = rac{\partial}{\partial z_i^{(n_l)}} rac{1}{2} \left\| y - h(\mathbf{x};W,b) 
ight\|^2 = -(y-a_i^{(n_l)}) \cdot \sigma'(z_i^{(n_l)})$$

Step 3: For  $l=n_l-1, n_l-2, n_l-3, \ldots, 2$  For each node i in layer l, set

$$\delta_i^{(l)} := rac{\partial}{\partial z_i^{(l)}} \ J(W,b;\mathbf{x},y) = rac{\partial}{\partial a_i^{(l)}} \ J(W,b;\mathbf{x},y) rac{\partial a_i^{(l)}}{\partial z_i^{(l)}} = \left(\sum_{j=1}^{s_{l+1}} w_{ji}^{(l)} \delta_j^{(l+1)}
ight) \sigma'(z_i^{(l)})$$

Step 4: the desired partial derivatives are computed as:

$$egin{align} rac{\partial}{\partial w_{ij}^{(l)}} J(W,b;\mathbf{x},y) &= a_j^{(l)} \delta_i^{(l+1)} \ rac{\partial}{\partial b_i^{(l)}} J(W,b;\mathbf{x},y) &= \delta_i^{(l+1)}. \end{align}$$

After obtaining the gradient with BP, we can then use stochastic gradient descent (SGD, or other methods) to minimize the loss function.

#### Deep Learning: What packages/platforms to choose?

By making the NN "deeper" (increase the hidden layers and add other complex structures), we have the deep learning models. Of course, deep NN will face the serious problem of overfitting (can be alleviated by regularization or dropout) and huge computation cost (can be solved by using GPU instead of CPU).

The neural network models in scikit-learn does not provide the flexible support for large-scale deep learning applications.

For beginners, Keras (high-level API that supports tensorflow, which developed by Google) and Pytorch (developed by Facebook) are the most accessible and popular deep learning packages in Python.

To get acess to free GPU resources for training deep learning models (see here for why GPU is widely applied in deep learning), you can use the online notebook provided by Kaggle or google colab. If you are using very basic Keras or Pytorch, there's no need to change the code much to adopt to GPU computation. With GPU, you can even give up sklearn and replace much of your codes using the GPU-version machine learning algorithms with the package cuml.

### **Exploring Deep Learning with Keras**

Let's build our first "deep learning" model (indeed a simple Neural Network model trained with deep learning package)

```
In [ ]:
         pip install tensorflow # you can also setup the apu if it is supported in your local co
In [1]:
         import numpy as np
         import tensorflow as tf
         from tensorflow import keras
         from tensorflow.keras import layers
         mnist = tf.keras.datasets.mnist
         (x_train, y_train),(x_test, y_test) = mnist.load_data()
         x_train, x_test = x_train / 255.0, x_test / 255.0
In [ ]:
         # sequential model to define a graph of neural network
         model = tf.keras.models.Sequential([
           tf.keras.layers.Flatten(input shape=(28, 28)),# input layer
           tf.keras.layers.Dense(128, activation='relu'), # hidden Layer
           tf.keras.layers.Dense(64, activation='relu'), # hidden Layer
           tf.keras.layers.Dense(10, activation='softmax') # output layer for classification
         1)
In [ ]:
         model.summary()
In [ ]:
         model.compile(optimizer='adam',
                       loss='sparse categorical crossentropy',
                       metrics=['accuracy'])
In [ ]:
         model.fit(x_train, y_train, epochs=100, batch_size = 2048)
         model.evaluate(x_test, y_test)
       We can also try autoencoder for the dimension reduction
In [2]:
         from keras import layers
         # functional API to define a graph of neural network -- more flexible than sequential
         input img = keras.Input(shape=(784,)) # input layer
         encoded = layers.Dense(128, activation='relu')(input_img)
         encoded = layers.Dense(32, activation='relu')(encoded)
```

```
encoded = layers.Dense(8, activation='relu')(encoded)
encoded = layers.Dense(2, activation='relu')(encoded)

decoded = layers.Dense(8, activation='relu')(encoded)
decoded = layers.Dense(32, activation='relu')(decoded)
decoded = layers.Dense(128, activation='relu')(decoded)
decoded = layers.Dense(784, activation='sigmoid')(decoded)
```

In [3]:

autoencoder = keras.Model(input\_img, decoded) # builds up the model
autoencoder.summary()

Model: "functional\_1"

Layer (type)	Output Shape	Param #
input_1 (InputLayer)	[(None, 784)]	0
dense (Dense)	(None, 128)	100480
dense_1 (Dense)	(None, 32)	4128
dense_2 (Dense)	(None, 8)	264
dense_3 (Dense)	(None, 2)	18
dense_4 (Dense)	(None, 8)	24
dense_5 (Dense)	(None, 32)	288
dense_6 (Dense)	(None, 128)	4224
dense_7 (Dense)	(None, 784)	101136

Total params: 210,562 Trainable params: 210,562 Non-trainable params: 0

In [10]:

```
Epoch 1/100
Epoch 2/100
10/10 [============== ] - 0s 8ms/step - loss: 0.0431
Epoch 3/100
10/10 [==========] - 0s 8ms/step - loss: 0.0429
Epoch 4/100
10/10 [============== ] - 0s 9ms/step - loss: 0.0428
Epoch 5/100
10/10 [============ ] - 0s 9ms/step - loss: 0.0428
Epoch 6/100
10/10 [============== ] - 0s 8ms/step - loss: 0.0427
Epoch 7/100
Epoch 8/100
10/10 [============== ] - 0s 8ms/step - loss: 0.0427
Epoch 9/100
```

```
Epoch 10/100
10/10 [============] - 0s 7ms/step - loss: 0.0427
Epoch 11/100
Epoch 12/100
Epoch 13/100
Epoch 14/100
Epoch 15/100
Epoch 16/100
10/10 [============== ] - 0s 9ms/step - loss: 0.0426
Epoch 17/100
10/10 [============== ] - 0s 10ms/step - loss: 0.0425
Epoch 18/100
10/10 [============== ] - 0s 8ms/step - loss: 0.0425
Epoch 19/100
Epoch 20/100
10/10 [============= ] - 0s 9ms/step - loss: 0.0425
Epoch 21/100
Epoch 22/100
10/10 [============= ] - 0s 9ms/step - loss: 0.0425
Epoch 23/100
Epoch 24/100
Epoch 25/100
Epoch 26/100
Epoch 27/100
Epoch 28/100
Epoch 29/100
10/10 [============== ] - 0s 9ms/step - loss: 0.0423
Epoch 30/100
Epoch 31/100
10/10 [============= ] - 0s 9ms/step - loss: 0.0423
Epoch 32/100
Epoch 33/100
10/10 [============== ] - 0s 9ms/step - loss: 0.0423
Epoch 34/100
Epoch 35/100
Epoch 36/100
Epoch 37/100
Epoch 38/100
10/10 [============ - - 0s 10ms/step - loss: 0.0422
Epoch 39/100
10/10 [============== ] - 0s 9ms/step - loss: 0.0422
Epoch 40/100
10/10 [============== ] - 0s 8ms/step - loss: 0.0421
Epoch 41/100
10/10 [============== ] - 0s 9ms/step - loss: 0.0421
```

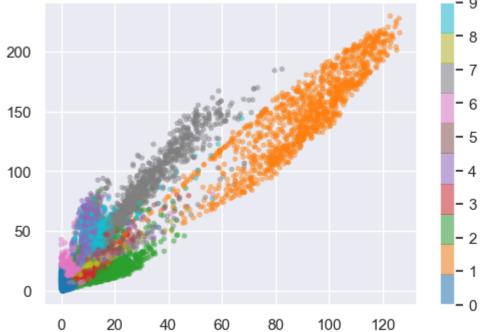
```
Epoch 42/100
10/10 [============== ] - 0s 9ms/step - loss: 0.0421
Epoch 43/100
Epoch 44/100
Epoch 45/100
Epoch 46/100
Epoch 47/100
Epoch 48/100
Epoch 49/100
Epoch 50/100
Epoch 51/100
Epoch 52/100
Epoch 53/100
Epoch 54/100
10/10 [============== ] - 0s 9ms/step - loss: 0.0419
Epoch 55/100
Epoch 56/100
10/10 [============== ] - 0s 9ms/step - loss: 0.0419
Epoch 57/100
Epoch 58/100
Epoch 59/100
10/10 [============ ] - 0s 9ms/step - loss: 0.0418
Epoch 60/100
Epoch 61/100
Epoch 62/100
10/10 [============== ] - 0s 9ms/step - loss: 0.0418
Epoch 63/100
Epoch 64/100
10/10 [============= ] - 0s 9ms/step - loss: 0.0417
Epoch 65/100
10/10 [=============== ] - 0s 9ms/step - loss: 0.0417
Epoch 66/100
10/10 [============== ] - 0s 8ms/step - loss: 0.0417
Epoch 67/100
Epoch 68/100
10/10 [=============== ] - 0s 9ms/step - loss: 0.0417
Epoch 69/100
Epoch 70/100
Epoch 71/100
Epoch 72/100
Epoch 73/100
10/10 [============== ] - 0s 9ms/step - loss: 0.0416
Epoch 74/100
```

```
Epoch 75/100
     10/10 [============== ] - 0s 9ms/step - loss: 0.0415
     Epoch 76/100
     Epoch 77/100
     10/10 [============== ] - 0s 9ms/step - loss: 0.0415
     Epoch 78/100
     10/10 [============== ] - 0s 9ms/step - loss: 0.0415
     Epoch 79/100
     Epoch 80/100
     Epoch 81/100
     10/10 [============== ] - 0s 9ms/step - loss: 0.0414
     Epoch 82/100
     10/10 [============== ] - 0s 10ms/step - loss: 0.0414
     Epoch 83/100
     10/10 [============== ] - 0s 10ms/step - loss: 0.0414
     Epoch 84/100
     10/10 [============ - - 0s 10ms/step - loss: 0.0414
     Epoch 85/100
     Epoch 86/100
     10/10 [============== ] - 0s 11ms/step - loss: 0.0414
     Epoch 87/100
     Epoch 88/100
     10/10 [============= - - os 10ms/step - loss: 0.0414
     Epoch 89/100
     Epoch 90/100
     10/10 [============= ] - 0s 10ms/step - loss: 0.0413
     Epoch 91/100
     10/10 [============= ] - 0s 10ms/step - loss: 0.0413
     Epoch 92/100
     Epoch 93/100
     10/10 [============= ] - 0s 10ms/step - loss: 0.0413
     Epoch 94/100
     Epoch 95/100
     Epoch 96/100
     Epoch 97/100
     Epoch 98/100
     Epoch 99/100
     Epoch 100/100
     Out[10]: <tensorflow.python.keras.callbacks.History at 0x7ffb282a3390>
In [11]:
     encoder = keras.Model(input_img, encoded) # also define the encoder part
     encoder.get weights()
Out[11]: [array([[-0.05947556, 0.02999774, 0.03496894, ..., 0.06997635,
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         [-0.00772542, 0.01606809, 0.00638994, ..., -0.0793802,
```

```
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        2.66798466e-01, 5.87142520e-02, -1.74439456e-02, -1.40925134e-02,
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       -2.07967479e-02, 6.67532953e-03, -1.54011518e-01, 3.65302563e-01,
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        8.29982042e-01, 2.00706646e-01, -1.60036981e-02, -1.79883260e-02,
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       [ 0.09728131, 0.1213326 , 0.1580048 , ..., -0.09850125,
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        0.6506759 \;\; , \quad 0.13108687, \quad 0.4883804 \;\; , \quad 0.15848926, \quad 0.00482019, \\
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       -0.00471628, 0.11195443, 0.1449951, 0.26420838, 0.0942094,
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```

```
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        0.14867495, -0.20313665, -0.14027984],
       [-0.14774525, -0.00727039, 0.31838563, -0.01514569, -0.6983138,
        -0.31751183, -0.1617338 , -0.09526449],
       [-0.5374191 , -0.10106187, -0.10516742, -0.49867204, 0.31834292,
        -0.3419259 , -0.30635524, 0.02560506],
       [-0.7228207 , -0.2751459 , -0.24725819, -0.7852104 , 0.78232145,
        -0.33753145, -0.19054532, -0.12788124]], dtype=float32),
array([ 9.0897024e-02, -3.0559542e-02, -8.3352752e-05, 8.8079989e-02,
       5.4166859e-01, -8.6392006e-03, -1.1247671e-02, 8.6889137e-03],
     dtype=float32),
array([[-0.2846781 , 0.53235614],
       [ 0.5957006 , -0.37706986],
```

```
0.34214923, -0.22898577],
                  [-0.2685487 , 0.6061868 ],
                  0.83776647, 0.4639623 ],
                  [ 0.42550644, -0.7541872 ],
                  [ 0.45924413, -0.05488669],
                  [ 0.5632348 , 0.23399091]], dtype=float32),
          array([0.30013943, 0.01383021], dtype=float32)]
In [12]:
          encoded_coord = encoder.predict(x_test.reshape((len(x_test), np.prod(x_test.shape[1:]))
In [13]:
          import matplotlib.pyplot as plt
          import seaborn as sns; sns.set()
          fig = plt.figure(dpi=100)
          plt.scatter(encoded_coord[:, 0], encoded_coord[:, 1],c=y_test, s=15, edgecolor='none',
          plt.colorbar()
Out[13]: <matplotlib.colorbar.Colorbar at 0x7ffb2d469610>
                                                                           . 9
```

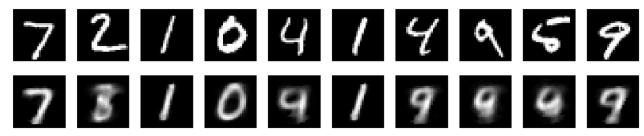


```
In [8]: decoded_imgs = autoencoder.predict(x_test.reshape((len(x_test), np.prod(x_test.shape[1:
```

```
In [9]:
    n = 10  # How many digits we will display
    plt.figure(figsize=(20, 4))
    for i in range(n):
        # Display original
        ax = plt.subplot(2, n, i + 1)
        plt.imshow(x_test[i])
        plt.gray()
        ax.get_xaxis().set_visible(False)
        ax.get_yaxis().set_visible(False)

# Display reconstruction
        ax = plt.subplot(2, n, i + 1 + n)
        plt.imshow(decoded_imgs[i].reshape(28, 28))
        plt.gray()
```

```
ax.get_xaxis().set_visible(False)
ax.get_yaxis().set_visible(False)
plt.show()
```



Maybe condensing to 2D layer loses too much information. Let's try a more realistic model

```
In [ ]:
         from keras import layers
         input img = keras.Input(shape=(784,))
         encoded = layers.Dense(128, activation='relu')(input img)
         encoded = layers.Dense(64, activation='relu')(encoded)
         encoded = layers.Dense(32, activation='relu')(encoded)
         decoded = layers.Dense(64, activation='relu')(encoded)
         decoded = layers.Dense(128, activation='relu')(decoded)
         decoded = layers.Dense(784, activation='sigmoid')(decoded)
         autoencoder = keras.Model(input img, decoded)
         autoencoder.summary()
In [ ]:
         autoencoder.compile(optimizer='adam', loss= tf.keras.losses.MeanSquaredError())
         autoencoder.fit(x test.reshape((len(x test), np.prod(x test.shape[1:]))), x test.reshape
                         epochs=200,
                         batch size=256)
In [ ]:
         encoder = keras.Model(input_img, encoded)
         encoded coord = encoder.predict(x test.reshape((len(x test), np.prod(x test.shape[1:]))
         encoded coord.shape
In [ ]:
         from sklearn.manifold import TSNE # for GPU acceleration, use the cuml
         tsne = TSNE(n_jobs = -1)
         X tsne = tsne.fit transform(encoded coord)
         import matplotlib.pyplot as plt
         import seaborn as sns; sns.set()
         fig = plt.figure(dpi=100)
         plt.scatter(X_tsne[:, 0], X_tsne[:, 1],c=y_test, s=15, edgecolor='none', alpha=0.5,cmap
         plt.colorbar()
In [ ]:
         decoded imgs = autoencoder.predict(x test.reshape((len(x test), np.prod(x test.shape[1:
         n = 10 # How many digits we will display
         plt.figure(figsize=(20, 4))
         for i in range(n):
```

# Display original

plt.gray()

plt.imshow(x\_test[i])

ax = plt.subplot(2, n, i + 1)

```
ax.get_xaxis().set_visible(False)
ax.get_yaxis().set_visible(False)

# Display reconstruction
ax = plt.subplot(2, n, i + 1 + n)
plt.imshow(decoded_imgs[i].reshape(28, 28))
plt.gray()
ax.get_xaxis().set_visible(False)
ax.get_yaxis().set_visible(False)
plt.show()
```

## Other Useful References and Suggestions for Future Learning in Data Science

#### **Websites for Everyday Practice**

• Python Programming: Leetcode

• Data Science: Kaggle

#### **Courses and Books**

- UCI ICS 31-33 (Python Programming), CS 178 (Machine Learning)
- Berkeley Stat 157
- Stanford CS 231
- The Deep Learning Book

```
In [ ]:
```