

EE3700 Introduction to Machine Learning

Implementing a Multilayer Artificial Neural Network from Scratch

Hsi-Pin Ma 馬席彬

http://lms.nthu.edu.tw/course/40724 Department of Electrical Engineering National Tsing Hua University



Outline

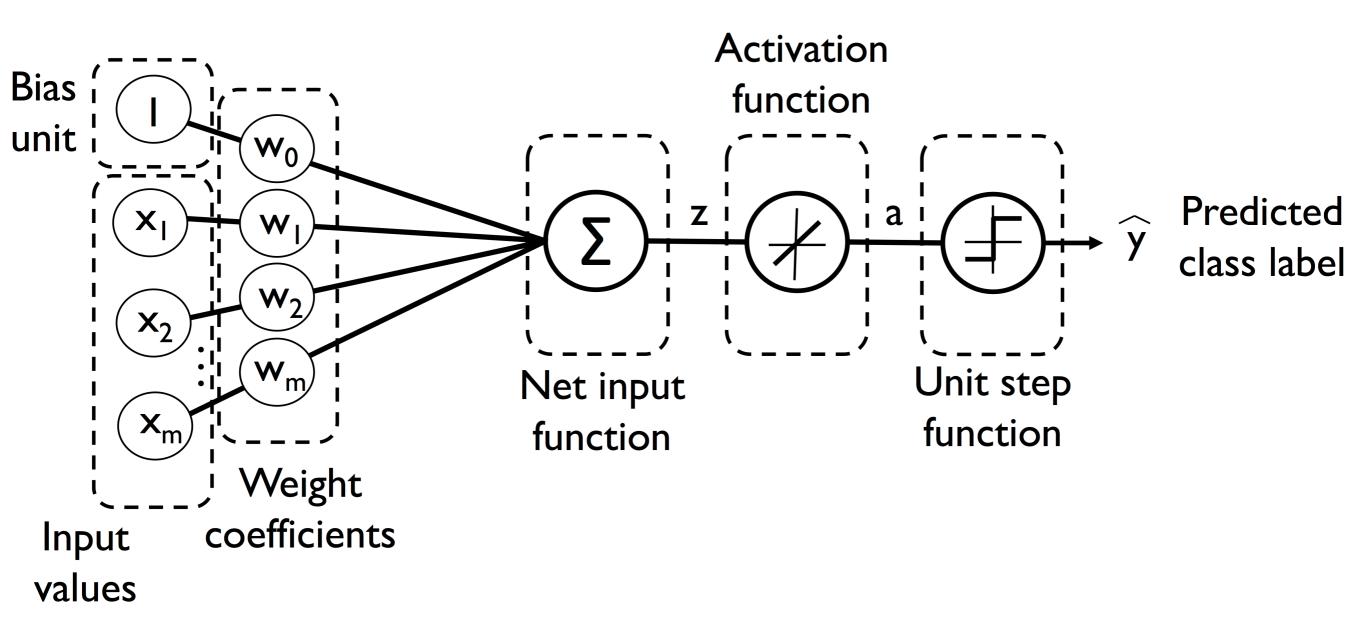
- Modeling complex functions with artificial neural networks
- Classifying handwritten digits
- Training an artificial neural network
- Convergence in neural networks



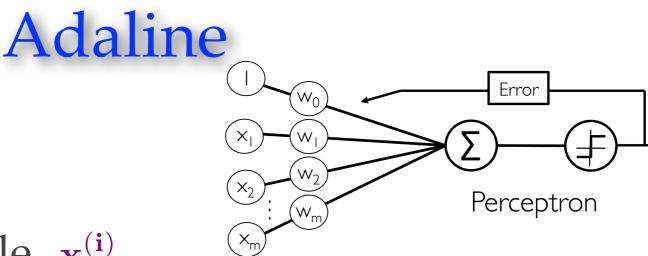
Modeling Complex Functions with Artificial Neural Networks



Single Layer Neural Network Recap







Output

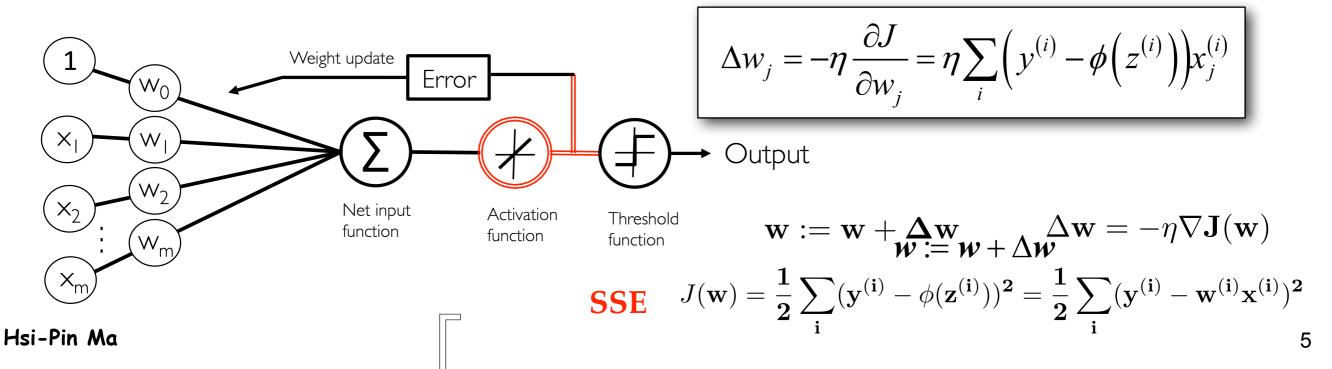
Perceptron

- For each training sample $\mathbf{x}^{(i)}$
 - compute the prediction value $\hat{y}^{(i)}$ with current vector $\mathbf{w}^{(i)}$
 - Update the weights

$$\Delta \mathbf{w}^{(\mathbf{i})} = \eta (\mathbf{y}^{(\mathbf{i})} - \hat{\mathbf{y}}^{(\mathbf{i})}) \mathbf{x}^{(\mathbf{i})}$$

Adaline

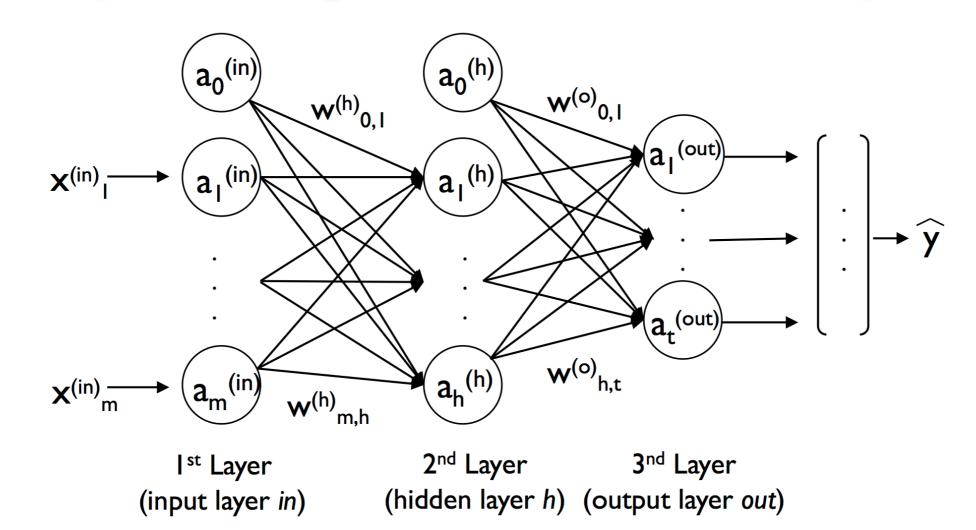
-Weight update done after entire training set has been seen





Multilayer Feedforward Neural Network

• Multilayer Perceptron (MLP) with 3 layers



• Deep artificial neural network

– A network has more than one hidden layer



Notation

()

• *i*th activation unit in the *l*th layer as $a_i^{(l)}$

(1)

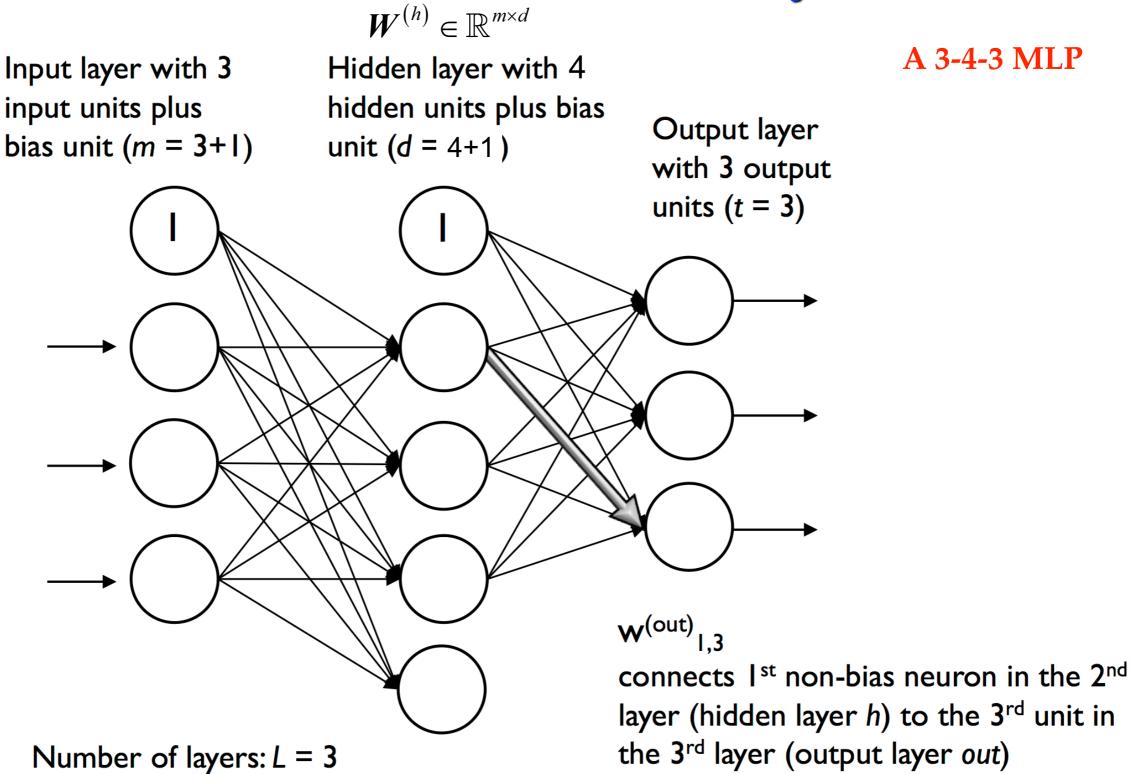
- The activation units $a_0^{(in)}$ and $b_0^{(in)}$ are the *bias units*, respectively, which we set equal to 1
- The activation of the units in the input layer

$$a^{(in)} = \begin{bmatrix} a_0^{(in)} \\ a_1^{(in)} \\ \vdots \\ a_m^{(in)} \end{bmatrix} = \begin{bmatrix} 1 \\ x_1^{(in)} \\ \vdots \\ x_m^{(in)} \end{bmatrix}$$

• The connection between *k*th unit in layer *l* to the *j*th unit in layer *l*+1 written as $w_{\kappa,j}^{(l)}$



Notation Summary



A 3-4-3 MLP



MLP Learning Procedure

Three steps

- Starting at the input layer, forward propagate the training data $x^{(i)}$ to generate an output
- -Calculate the error we want to minimize with a cost function
- -Backpropagate the error, find its derivative with respective to each weight, and update the model
- After repeating the steps, use *forward propagation* to calculate the network output and apply a threshold function to obtain the predict the class label in 1-hot representation



Forward Propagation

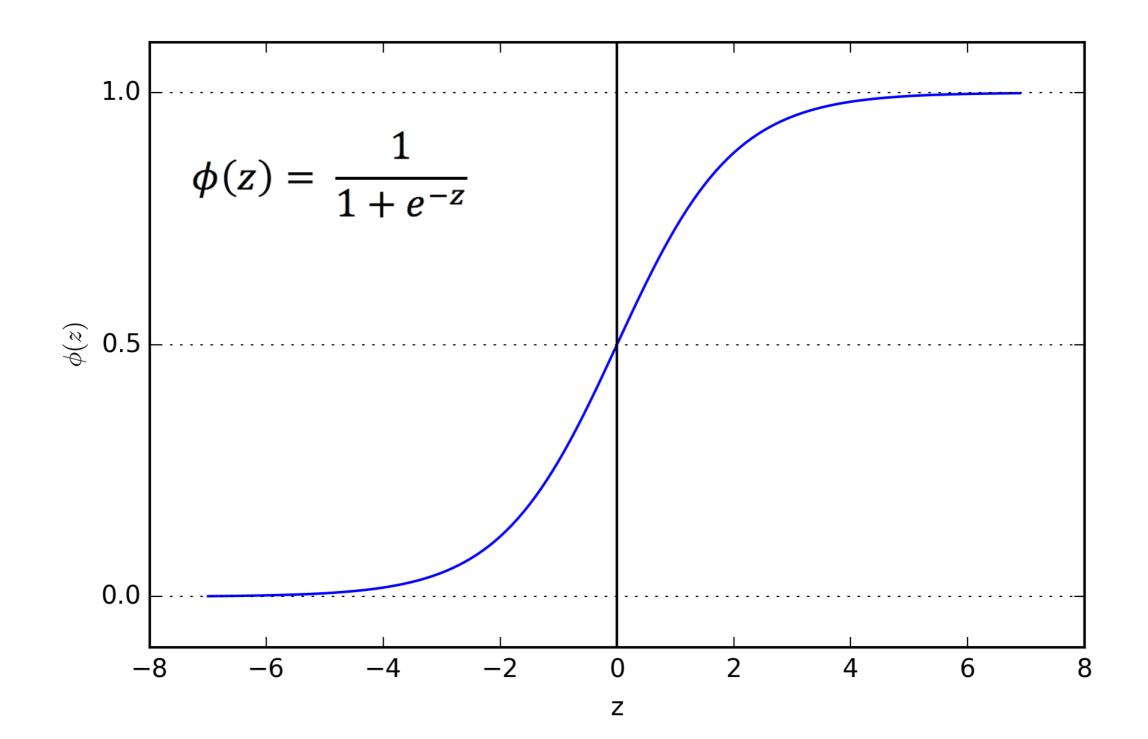
 Calculate the net input for unit 1 in the hidden layer (in) (h) (in) (h)(h)(in)(h) $z_1^{(h)} = a_0^{(in)} w_{0,1}^{(h)} + a_1^{(in)} w_{1,1}^{(h)} + \dots + a_m^{(in)} w_{m,1}^{(h)}$ • Calculate he(i) activation for $y(\cdot)$ in the hidden layer $\begin{array}{c} q_{\mathbf{h}}^{(h)} = \phi \left(z_{1}^{(h)} \right) \\ \phi^{(h)} = \phi \left(z_{1}^{(h)} \right) \end{array}$ () $f_{1}^{()}$ – To be able to solve complex problems such as image classification, we need non-linear activation functions

-sigmoid (logistic) activation function $\phi(z) = \frac{1}{1 + e^{-z}}$

Ф



Sigmoid Function





Forward Propagation

• MLP is a typical feedforward ANN

- Feedforward: each layer serves as the input to the next layer without loops, in contrast to recurrent neural networks
- Neurons are typically sigmoid units, not perceptrons
 - Intuitively consider neurons in MLP as logistic regression units



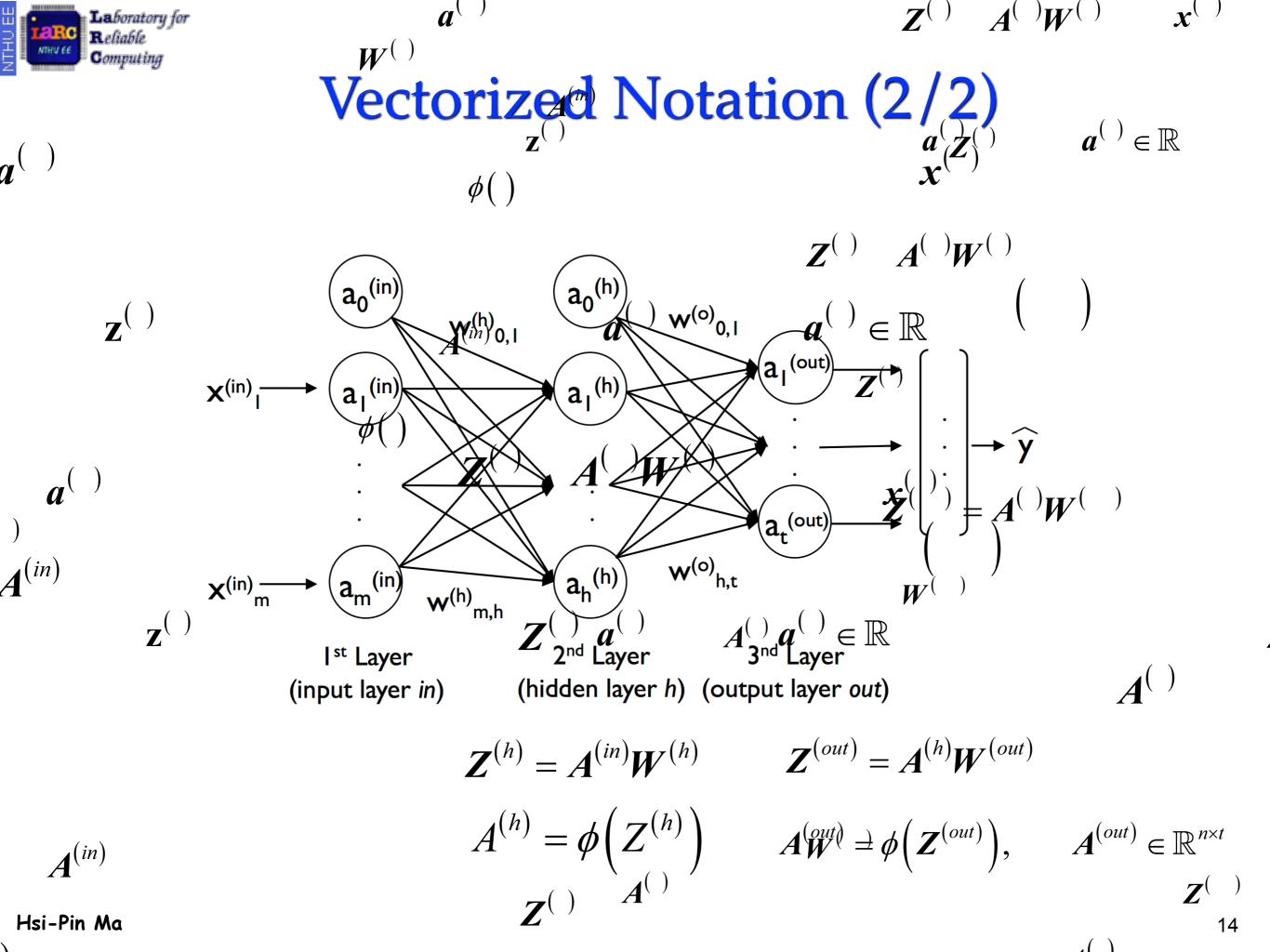
Vectorized Notation (1/2)

- Write activation in a matrix form
- Readability + more efficient code
- Net inputs for the hidden layer

 $\boldsymbol{z}^{(h)} = \boldsymbol{a}^{(in)} \boldsymbol{W}^{(h)}$

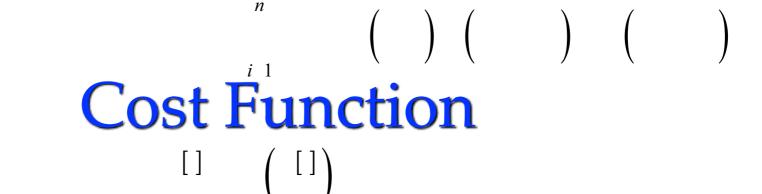
- Dimensions (ignøre) bias unit for simplicity) -[h x 1] = [h x m] [m x 1]
- Activations for the hidden layer

$$\boldsymbol{a}^{(h)} = \boldsymbol{\phi}\left(\boldsymbol{z}^{(h)}\right)$$





Training an Artificial Neural Network



• The logistic cost function is the same we used for logistic regression

$$J(w) = -\sum_{i=1}^{n} y^{[i]} log(a^{[i]}) + (1-y^{[i]}) log(1-a^{[i]})$$

- $a^{[i]}$ is the sigmoid activation of the *i*th sample in the dataset $a^{[i]} = \phi(z^{[i]})$
- **Regularization: use** $\mathbf{L}^{[1]} \left\{ \mathcal{L}^{[1]} \right\} \| \mathbf{w} \|_{2}^{2} = \lambda \sum_{j=1}^{m} w_{j}^{2}$
- Final cost function

 $a^{[]}$

$$J(\mathbf{w}) = -\left[\sum_{i=1}^{n} y^{[i]} log(a^{[i]}) + (1 - y^{[i]}) log(1 - a^{[i]})\right] + \frac{\lambda}{2} \|\mathbf{w}\|_{2}^{2}$$



Cost Function for All Units in Output Layer

• The activation of the 3rd layer and the target class (class 2) for a particular sample may look like $a^{(out)} = \begin{bmatrix} 0.1\\0.9\\\vdots\\0.3 \end{bmatrix}, y = \begin{bmatrix} 0\\1\\\vdots\\0 \end{bmatrix}$

• Need to generalize the logistic cost function to all *t* activation units (without regularization)

$$J(W) = -\sum_{i=1}^{n} \sum_{j=1}^{t} y_{j}^{[i]} log(a_{j}^{[i]}) + (1 - y_{j}^{[i]}) log(1 - a_{j}^{[i]})$$



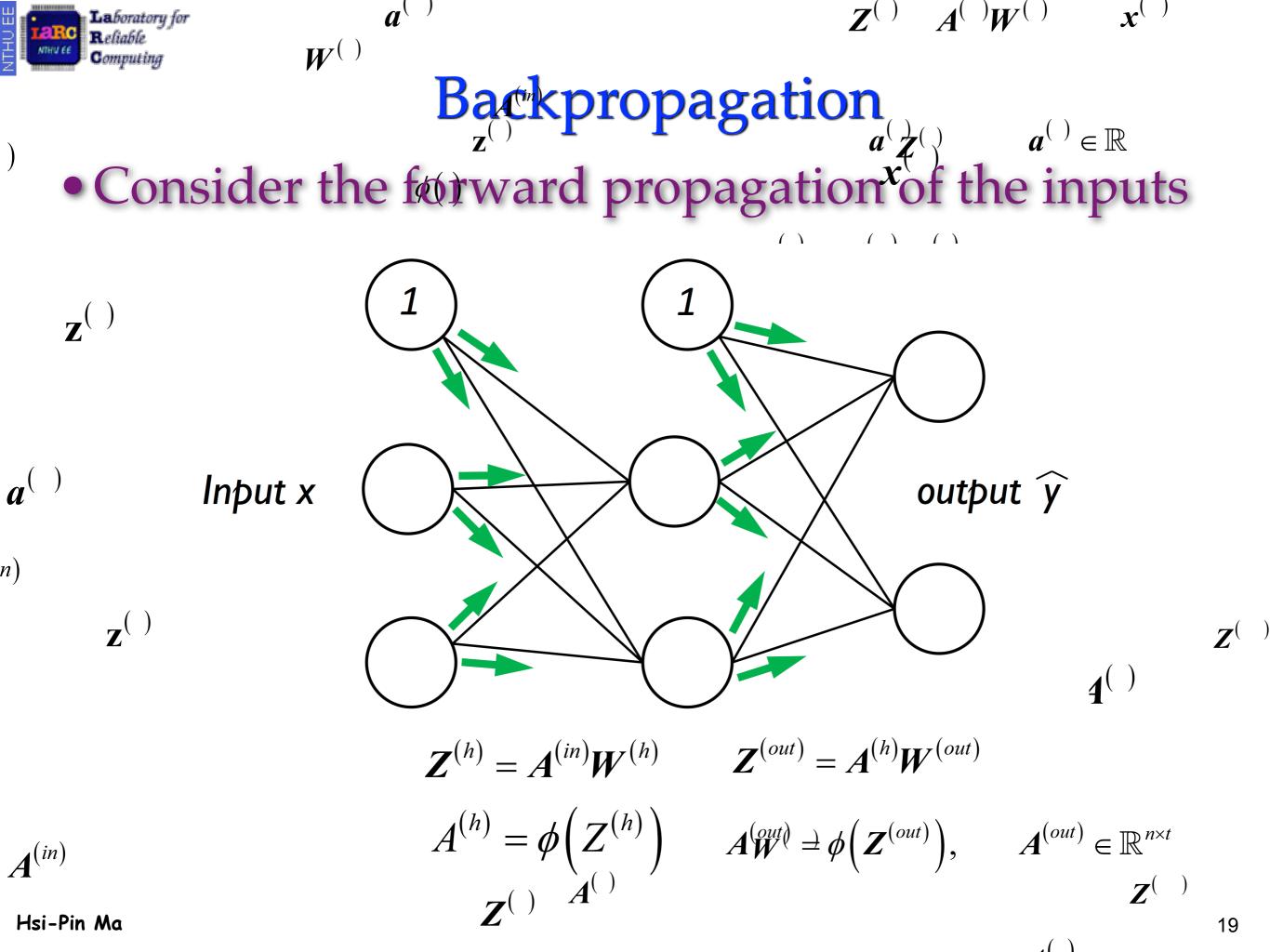
Cost Function for the Entire Network

• Sum all the weights in the entire network in the regularization term L2 penalty term

$$J(\boldsymbol{W}) = -\left[\sum_{i=1}^{n} \sum_{j=1}^{t} y_{j}^{[i]} log(a_{j}^{[i]}) + (1 - y_{j}^{[i]}) log(1 - a_{j}^{[i]})\right] + \frac{\lambda}{2} \sum_{l=1}^{L-1} \sum_{i=1}^{u_{l}} \sum_{j=1}^{u_{l+1}} (w_{j,i}^{(l)})^{2}$$
()

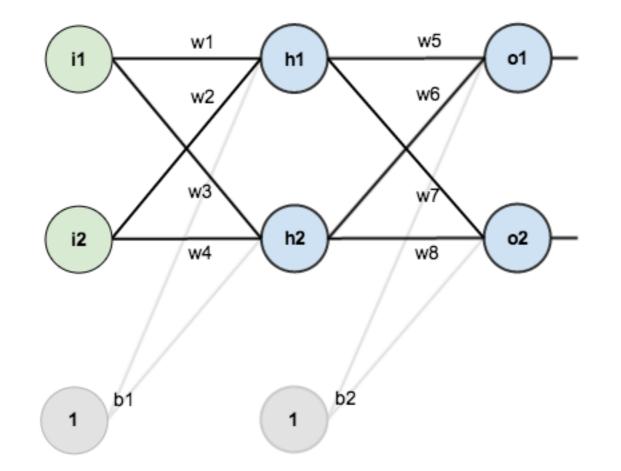
- u₁ refers to the number of units in a given layer 1
- To minimize the cost function – Use back propagation algorithm

$$\frac{\partial}{\partial w_{j,i}^{(l)}}J(\boldsymbol{W})$$





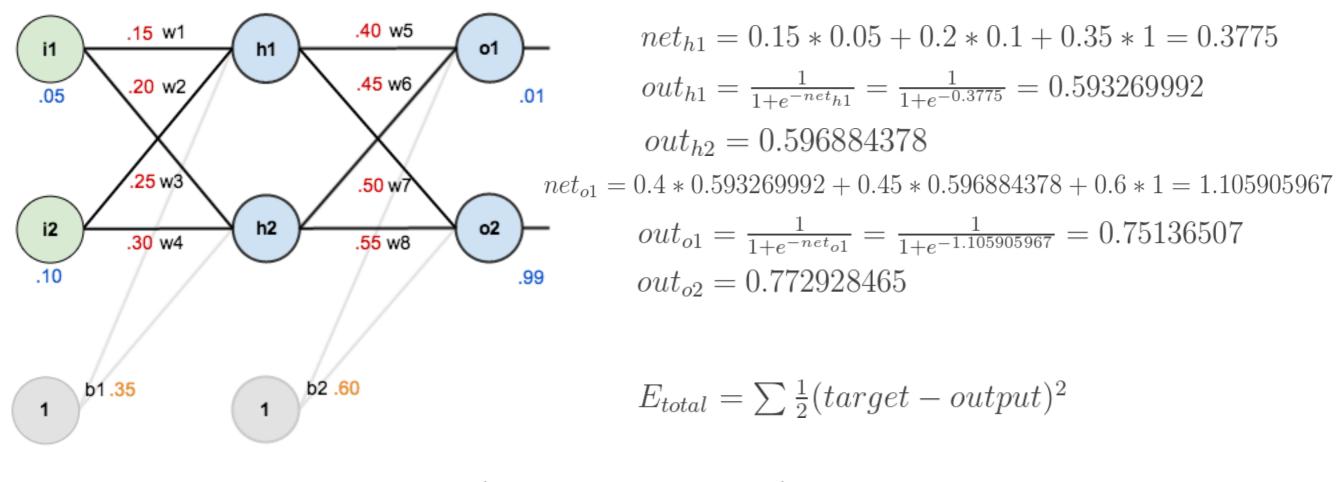
Example



[https://mattmazur.com/2015/03/17/a-step-by-step-backpropagation-example/]



Feedforward

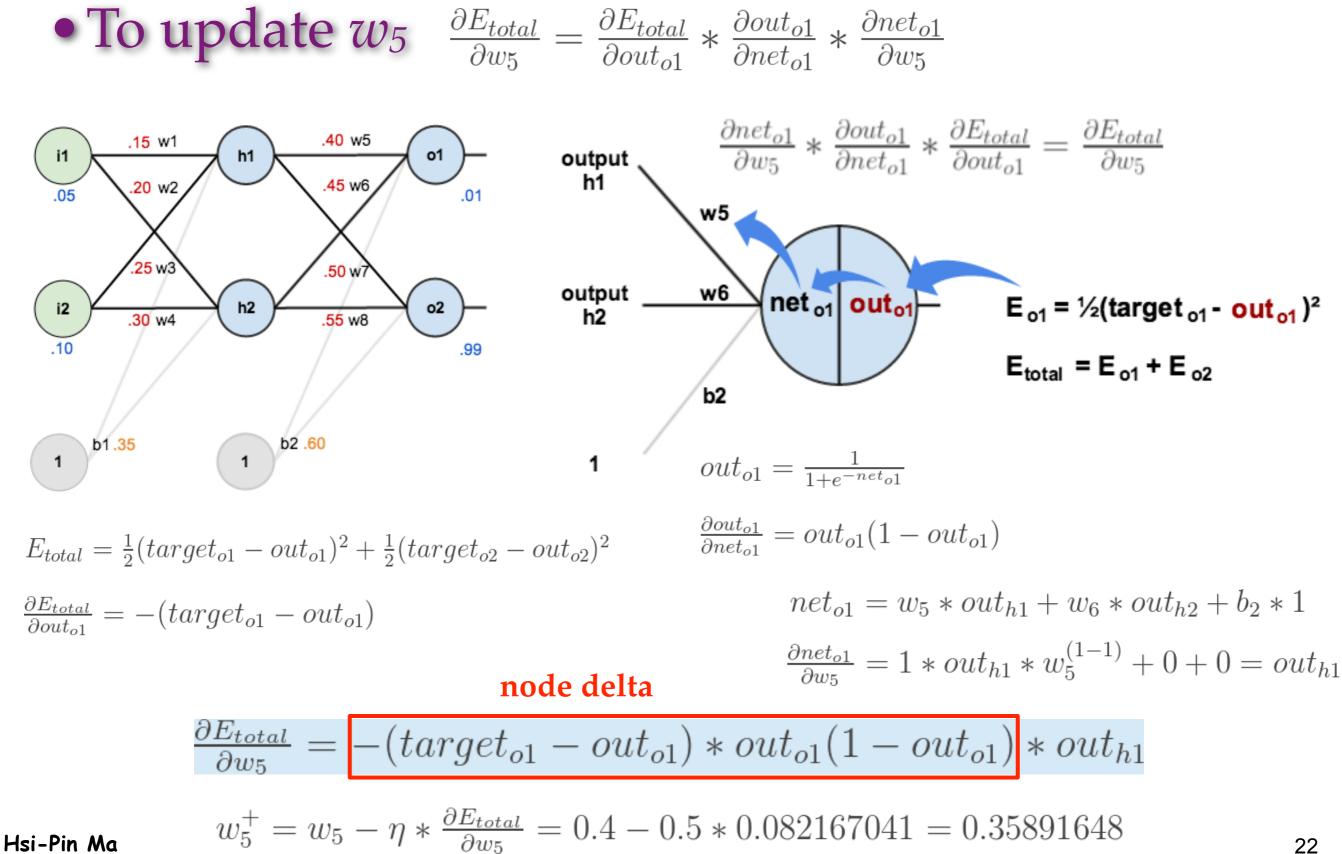


$$E_{o1} = \frac{1}{2} (target_{o1} - out_{o1})^2 = \frac{1}{2} (0.01 - 0.75136507)^2 = 0.274811083$$
$$E_{o2} = 0.023560026$$
$$E_{total} = E_{o1} + E_{o2} = 0.274811083 + 0.023560026 = 0.298371109$$



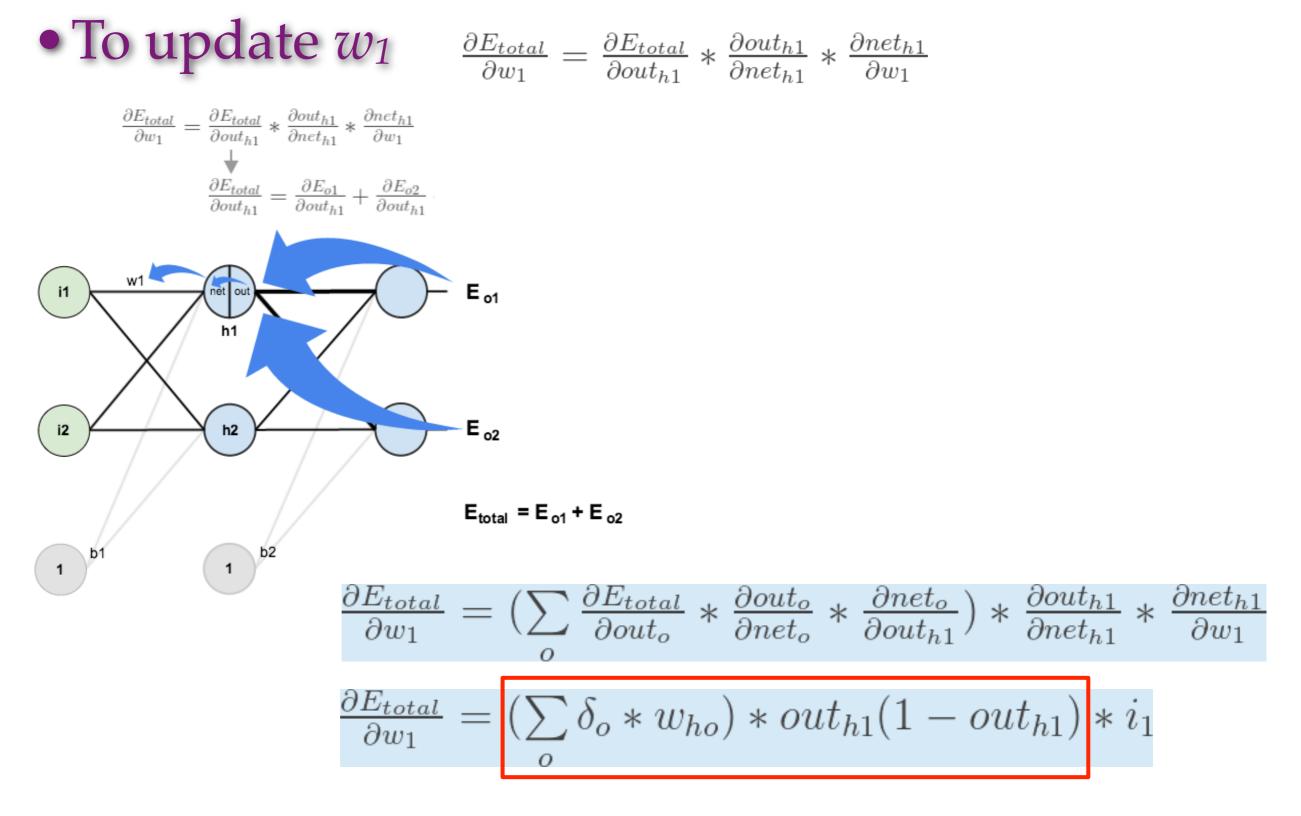
Laboratory for

Computina





Backpropagation (2/2)



$$\mathcal{E} \qquad \mathcal{E} \qquad$$

 δ

• Error vector of the output layer $W^{(out)} = a^{(out)} - y \qquad \partial$ ()

• Error term(of)the hidden & ayer

$$\delta^{(h)} = \delta^{(out)} \left(W^{(out)} \right)^T \odot \frac{\partial \phi(z^{(h)})}{\partial z^{(h)}} \qquad \qquad \delta^{(h)} = \delta^{(out)} \left(W^{(out)} \right)^T \odot \left(a^{(h)} \odot \left(1 - a^{(h)} \right) \right)$$
Derivation of the cost function
$$\delta^{(h)}$$

$$\frac{\partial}{\partial w_{i,j}^{(out)}} J(\boldsymbol{W}) = a_j^{(h)} \delta_i^{(out)}$$

$$\Delta \mathbf{W}^{(h)_{ut}} = \Delta^{(h)} + \left(\mathbf{A}^{(in)}\right)^T \delta^{(h)}$$

$$\frac{\partial \phi \widehat{Q}(z)}{\partial \widehat{W}_{i,j}^{(h)}} J(W) = a_j^{(in)} \delta_i^{(h)}$$

$$\Delta^{(out)} = \Delta^{(out)} + \left(\boldsymbol{A}^{(h)}\right)^T \boldsymbol{\delta}^{(out)}_{\boldsymbol{\delta}^{(-)}}$$



Textbook Version (2/2)

Add the regularization term

 $\Delta^{(l)} \coloneqq \Delta^{(l)} + \lambda^{(l)} (except for the bias term)$

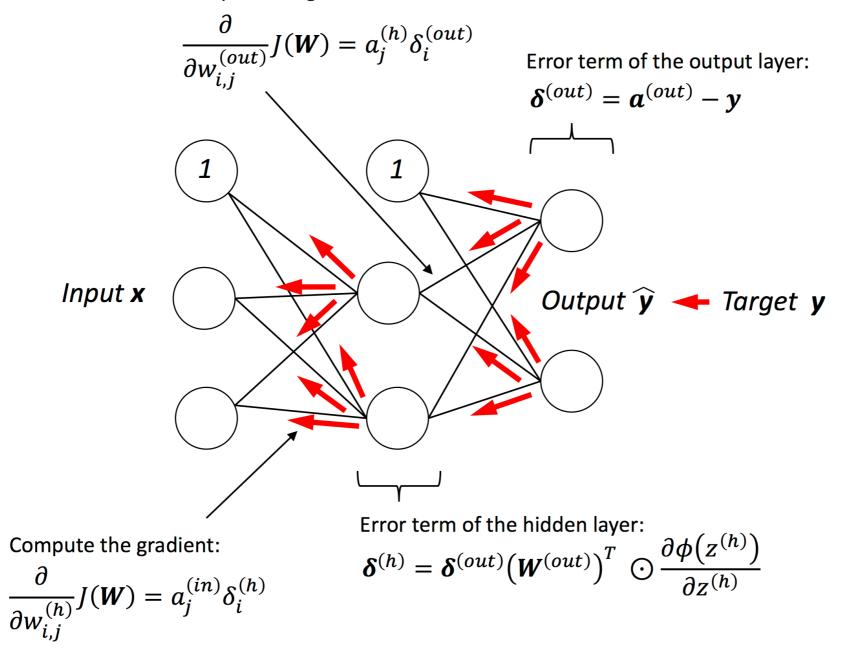
• Final weight update

$$\boldsymbol{W}^{(l)} \coloneqq \boldsymbol{W}^{(l)} - \eta \boldsymbol{\Delta}^{(l)}$$



Summary

Compute the gradient:



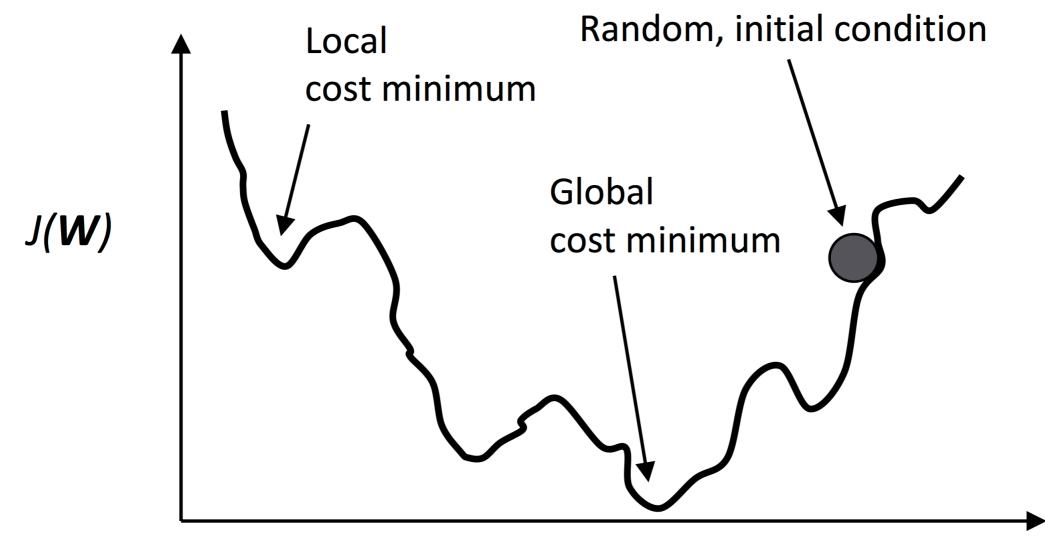


Convergence in Neural Networks



Min-batch Learning

Speed and convergence





Classifying Handwritten Digits



MNIST Dataset

- Mixed National Institute of Standards and Technology (MNIST) dataset
 - Constructed by Yan LeCun and others as a popular benchmark for ML
 - -<u>http://yann.lecun.com/exdb/mnist/</u>
 - Training set images
 - Training set labels
 - Test set images
 - Test set labels
 - was constructed from two datasets of the US NIST
 - handwritten digits from 250 different people, 50% high school students and 50% employees from the Census Bureau



Load Dataset

• load_mnist returns two arrays

- -images: n x m array, n: # of samples, m: # of features(pixels)
 - Each pixel is represented by a grey intensity value (0-255), and is normalized to [-1,1]
- labels: target variable of the class labels (0-9)

```
X_train, y_train = load_mnist('', kind='train')
print('Rows: %d, columns: %d' % (X_train.shape[0], X_train.shape[1]))
```

```
Rows: 60000, columns: 784
```

```
X_test, y_test = load_mnist('', kind='t10k')
print('Rows: %d, columns: %d' % (X_test.shape[0], X_test.shape[1]))
```

```
Rows: 10000, columns: 784
```

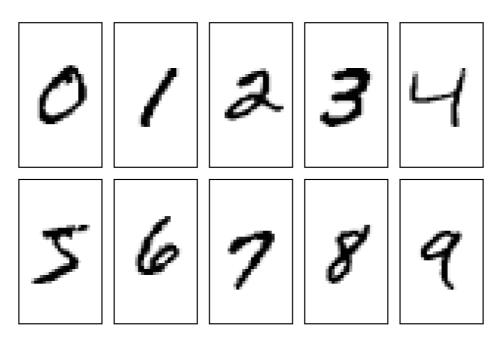


Visualize the First Digit of Each Class

```
import matplotlib.pyplot as plt

fig, ax = plt.subplots(nrows=2, ncols=5, sharex=True, sharey=True,)
ax = ax.flatten()
for i in range(10):
    img = X_train[y_train == i][0].reshape(28, 28)
    ax[i].imshow(img, cmap='Greys')

ax[0].set_xticks([])
ax[0].set_yticks([])
plt.tight_layout()
# plt.savefig('images/12_5.png', dpi=300)
plt.show()
```





Visualize 25 Different Versions of 7

```
fig, ax = plt.subplots(nrows=5, ncols=5, sharex=True, sharey=True,)
ax = ax.flatten()
for i in range(25):
    img = X_train[y_train == 7][i].reshape(28, 28)
    ax[i].imshow(img, cmap='Greys')
ax[0].set_xticks([])
ax[0].set_yticks([])
plt.tight_layout()
# plt.savefig('images/12_6.png', dpi=300)
plt.show()
```



```
mnist = np.load('mnist_scaled.npz')
mnist.files
```

```
['X_train', 'y_train', 'X_test', 'y_test']
```

```
del mnist
```

X_train.shape

(60000, 784)

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```
import numpy as np
import sys
class NeuralNetMLP(object):
    def init (self, n hidden=30,
                 12=0., epochs=100, eta=0.001,
                 shuffle=True, minibatch size=1, seed=None):
        self.random = np.random.RandomState(seed) # Random seed
                                       # number of hidden units
        self.n hidden = n hidden
                                       # Lambda value for L2 regularization
        self.12 = 12
                                       # number of passes over the training set
        self.epochs = epochs
                                       # learning rate
        self.eta = eta
                                       # Shuffles training data every epoch if True to prevent circles
        self.shuffle = shuffle
        self.minibatch size = minibatch size
                                                # number of training samples per mini batch
```



Label Onehot Encoding and Sigmoid

```
def onehot(self, y, n classes):
    """Encode labels into one-hot representation
   Parameters
     -----
   y : array, shape = [n_samples]
       Target values.
   Returns
     _____
   onehot : array, shape = (n samples, n labels)
    0.0.0
   onehot = np.zeros((n_classes, y.shape[0]))
    for idx, val in enumerate(y.astype(int)):
       onehot[val, idx] = 1.
   return onehot.T
def sigmoid(self, z):
    """Compute logistic function (sigmoid)"""
    return 1. / (1. + np.exp(-np.clip(z, -250, 250)))
```



Forward Calculation

```
def _forward(self, X):
    """Compute forward propagation step"""
    # step 1: net input of hidden layer
    # [n_samples, n_features] dot [n_features, n_hidden]
    # -> [n_samples, n_hidden]
    z_h = np.dot(X, self.w_h) + self.b_h

    # step 2: activation of hidden layer
    a_h = self._sigmoid(z_h)
```

```
# step 3: net input of output layer
# [n_samples, n_hidden] dot [n_hidden, n_classlabels]
# -> [n_samples, n_classlabels]
```

z_out = np.dot(a_h, self.w_out) + self.b_out

```
# step 4: activation output layer
a_out = self._sigmoid(z_out)
```

return z_h, a_h, z_out, a_out



Cost Calculation

```
def compute cost(self, y enc, output):
    """Compute cost function.
    Parameters
       _____
   y_enc : array, shape = (n_samples, n_labels)
        one-hot encoded class labels.
    output : array, shape = [n samples, n output units]
        Activation of the output layer (forward propagation)
    Returns
       _____
    cost : float
        Regularized cost
    II II II
   L2 term = (self.l2 *
               (np.sum(self.w h ** 2.) +
                np.sum(self.w out ** 2.)))
   term1 = -y enc * (np.log(output))
   term2 = (1. - y enc) * np.log(1. - output)
    cost = np.sum(term1 - term2) + L2_term
    return cost
```



Prediction

```
def predict(self, X):
    """Predict class labels
    Parameters
    _____
    X : array, shape = [n_samples, n_features]
        Input layer with original features.
    Returns:
     _____
    y_pred : array, shape = [n_samples]
       Predicted class labels.
    .....
    z_h, a_h, z_out, a_out = self._forward(X)
    y_pred = np.argmax(z_out, axis=1)
    return y_pred
```



Fit (1/3)

```
def fit(self, X_train, y_train, X_valid, y_valid):
   n output = np.unique(y train).shape[0] # number of class labels
   n features = X train.shape[1]
   # Weight initialization
   # weights for input -> hidden
   self.b_h = np.zeros(self.n_hidden)
   self.w h = self.random.normal(loc=0.0, scale=0.1,
                               size=(n features, self.n hidden))
   # weights for hidden -> output
   self.b out = np.zeros(n output)
   self.w out = self.random.normal(loc=0.0, scale=0.1,
                                 size=(self.n hidden, n output))
   epoch_strlen = len(str(self.epochs)) # for progress formatting
```

```
self.eval_ = {'cost': [], 'train_acc': [], 'valid_acc': []}
```

```
y_train_enc = self._onehot(y_train, n_output)
```



Fit (2/3)

```
# iterate over training epochs
for i in range(self.epochs):
    # iterate over minibatches
    indices = np.arange(X_train.shape[0])
    if self.shuffle:
        self.random.shuffle(indices)
    for start_idx in range(0, indices.shape[0] - self.minibatch_size +
                           1, self.minibatch size):
        batch idx = indices[start idx:start idx + self.minibatch size]
        # forward propagation
        z h, a h, z out, a out = self. forward(X train[batch idx])
```



```
# [n_samples, n_classlabels]
sigma_out = a_out - y_train_enc[batch_idx]
```

```
# [n_samples, n_hidden]
sigmoid_derivative_h = a_h * (1. - a_h)
```

[n_features, n_samples] dot [n_samples, n_hidden]
-> [n_features, n_hidden]
grad_w_h = np.dot(X_train[batch_idx].T, sigma_h)
grad_b_h = np.sum(sigma_h, axis=0)
[n_hidden, n_samples] dot [n_samples, n_classlabels]
-> [n_hidden, n_classlabels]
grad_w_out = np.dot(a_h.T, sigma_out)
grad_b_out = np.sum(sigma_out, axis=0)

Regularization and weight updates delta_w_h = (grad_w_h + self.l2*self.w_h) delta_b_h = grad_b_h # bias is not regularized self.w_h -= self.eta * delta_w_h self.b_h -= self.eta * delta_b_h

delta_w_out = (grad_w_out + self.l2*self.w_out)
delta_b_out = grad_b_out # bias is not regularized
self.w_out -= self.eta * delta_w_out
self.b_out -= self.eta * delta_b_out



Evaluation

```
# Evaluation after each epoch during training
z_h, a_h, z_out, a_out = self._forward(X_train)
```

```
y_train_pred = self.predict(X_train)
y_valid_pred = self.predict(X_valid)
```

```
X_valid.shape[0])
```

```
self.eval_['cost'].append(cost)
self.eval_['train_acc'].append(train_acc)
self.eval_['valid_acc'].append(valid_acc)
return self
```

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Training and Validation

```
n_{epochs} = 200
nn = NeuralNetMLP(n hidden=100,
                  12=0.01,
                  epochs=n_epochs,
                  eta=0.0005,
                  minibatch_size=100,
                  shuffle=True,
                  seed=1)
nn.fit(X_train=X_train[:55000],
       y_train=y_train[:55000],
       X_valid=X_train[55000:],
       y_valid=y_train[55000:])
 200/200 | Cost: 5065.78 | Train/Valid Acc.: 99.28%/97.98%
```

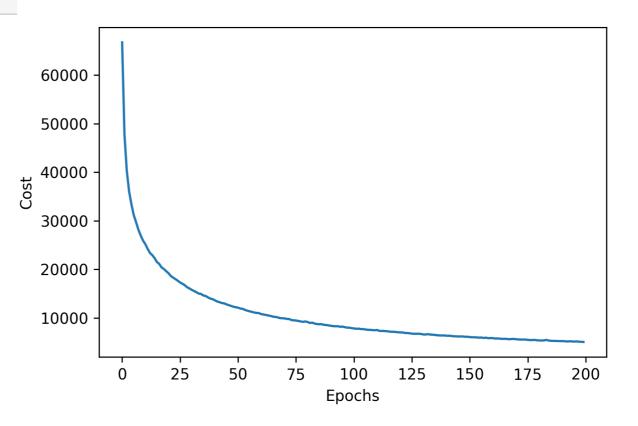


Training Epochs Evaluation

• eval_ attribute

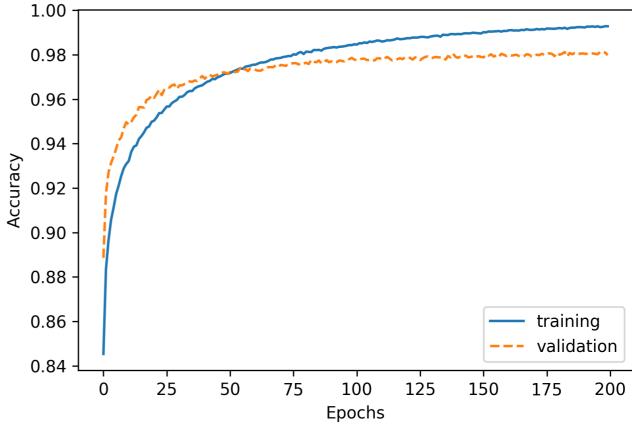
```
import matplotlib.pyplot as plt
```

```
plt.plot(range(nn.epochs), nn.eval_['cost'])
plt.ylabel('Cost')
plt.xlabel('Epochs')
#plt.savefig('images/12_07.png', dpi=300)
plt.show()
```





Model Training





Generalization Performance

```
y_test_pred = nn.predict(X_test)
acc = (np.sum(y_test == y_test_pred)
    .astype(np.float) / X_test.shape[0])
```

print('Test accuracy: %.2f%%' % (acc * 100))

Test accuracy: 97.54%



Check the Misclassified Samples (1/2)

```
miscl img = X test[y test != y test pred][:25]
correct lab = y test[y test != y test pred][:25]
miscl_lab = y_test_pred[y_test != y_test_pred][:25]
fig, ax = plt.subplots(nrows=5, ncols=5, sharex=True, sharey=True,)
ax = ax.flatten()
for i in range(25):
    img = miscl img[i].reshape(28, 28)
    ax[i].imshow(img, cmap='Greys', interpolation='nearest')
    ax[i].set title('%d) t: %d p: %d' % (i+1, correct lab[i], miscl lab[i]))
ax[0].set xticks([])
ax[0].set_yticks([])
plt.tight layout()
#plt.savefig('images/12 09.png', dpi=300)
plt.show()
```



Check the Misclassified Samples (2/2)

