# MultilayerNeuralNetworks

January 1, 2025

# 1 Multi-layer Neural Network

# 2 Modeling complex functions with artificial neural networks

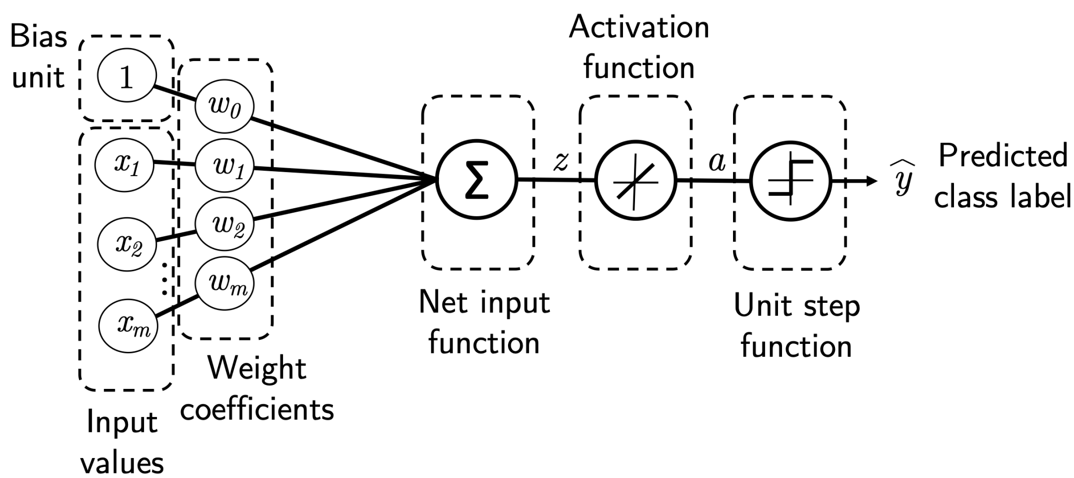
…

## 2.1 Single-layer neural network recap

[3]:

```
Image(filename='images/12_01.png', width=600)
```

[3]:

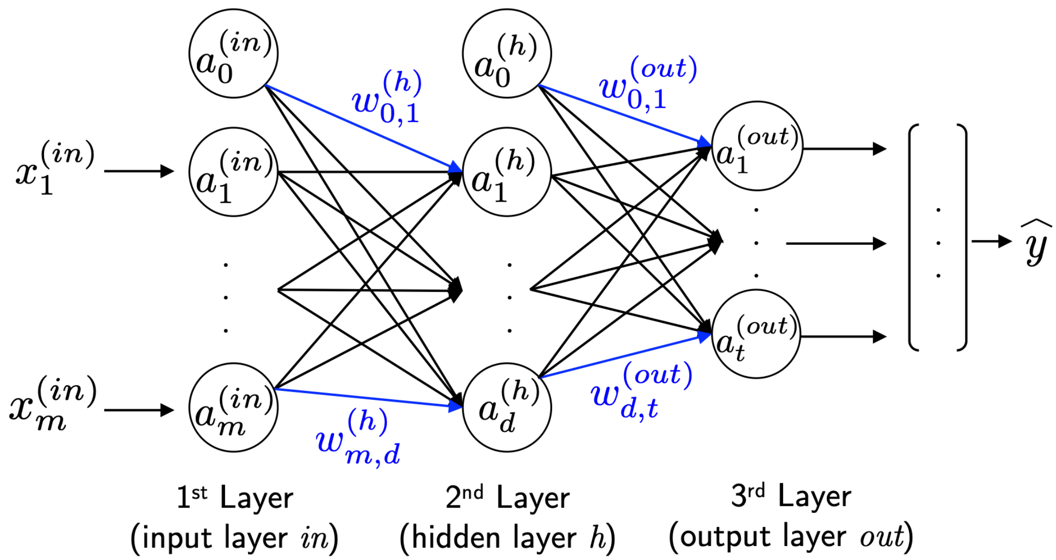



## 2.2 Introducing the multi-layer neural network architecture

[4]:

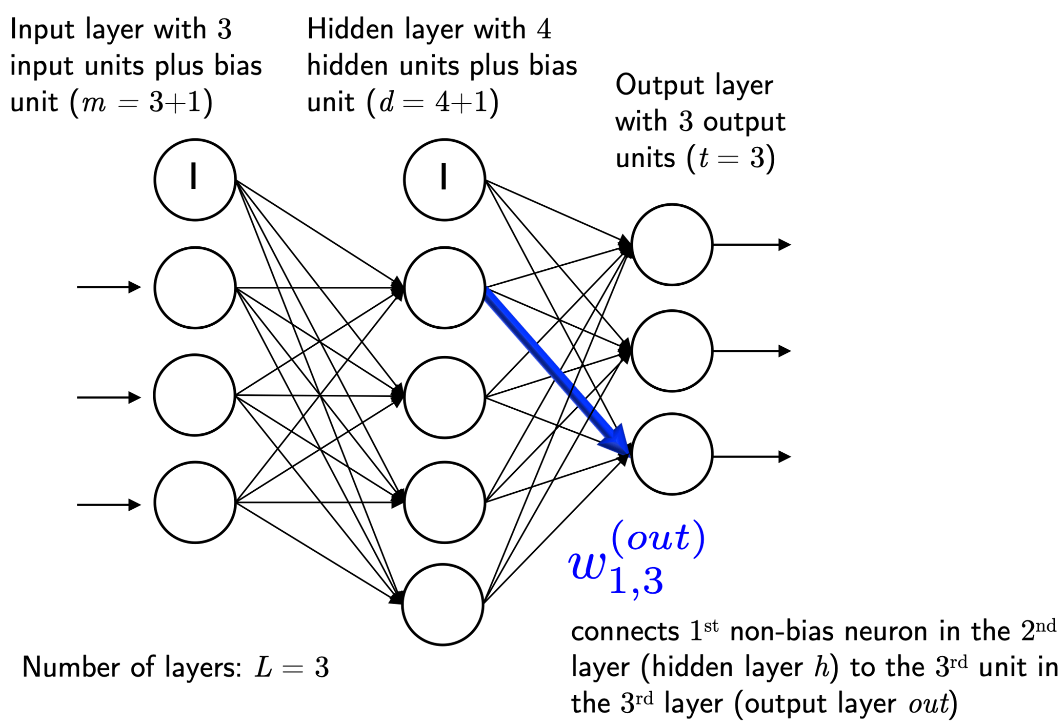
```
Image(filename='images/12_02.png', width=600)
```

[4]:




[5]:
```
Image(filename='images/12_03.png', width=500)
```

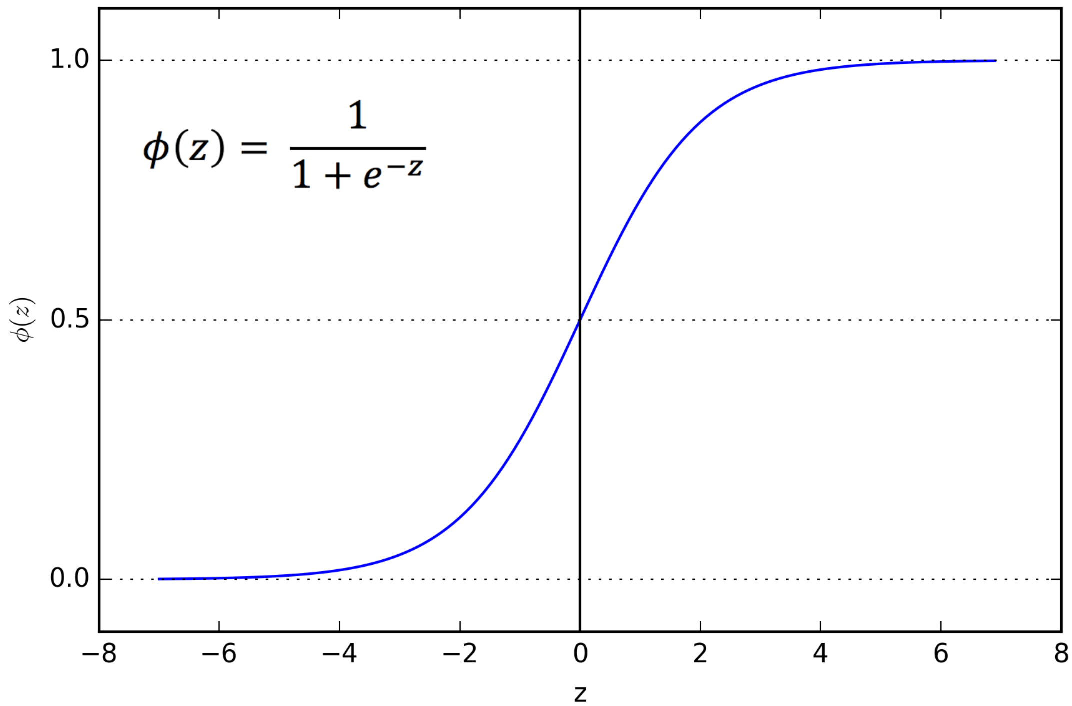
[5]:



## 2.3 Activating a neural network via forward propagation

[6]:
```
Image(filename='images/12_04.png', width=500)
```

[6]:




To use the scikit-learn API for loading MNIST, please uncomment the follwing code below.

[7]:
```
"""
from sklearn.datasets import fetch_openml
from sklearn.model_selection import train_test_split


X, y = fetch_openml('mnist_784', version=1, return_X_y=True)
y = y.astype(int)
X = ((X / 255.) - .5) * 2
X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=10000, random_state=123, stratify=y)
"""
```

[7]:
```
"\nfrom sklearn.datasets import fetch_openml\nfrom sklearn.model_selection
import train_test_split\n\n\nX, y = fetch_openml('mnist_784', version=1,
return_X_y=True)\ny = y.astype(int)\nX = ((X / 255.) - .5) * 2\nX_train, X_test,
y_train, y_test = train_test_split(\n    X, y, test_size=10000,
random_state=123, stratify=y)\n"
```

# 3 Classifying handwritten digits

...

## 3.1 Obtaining and preparing the MNIST dataset

The MNIST dataset is publicly available at http://yann.lecun.com/exdb/mnist/ and consists of the following four parts:

- Training set images: train-images-idx3-ubyte.gz (9.9 MB, 47 MB unzipped, 60,000 examples)
- Training set labels: train-labels-idx1-ubyte.gz (29 KB, 60 KB unzipped, 60,000 labels)
- Test set images: t10k-images-idx3-ubyte.gz (1.6 MB, 7.8 MB, 10,000 examples)
- Test set labels: t10k-labels-idx1-ubyte.gz (5 KB, 10 KB unzipped, 10,000 labels)

In this section, we will only be working with a subset of MNIST, thus, we only need to download the training set images and training set labels.

After downloading the files, simply run the next code cell to unzip the files.

[8]:
```
# this code cell unzips mnist

import sys
import gzip
import shutil
import os

if (sys.version_info > (3, 0)):
    writemode = 'wb'
else:
    writemode = 'w'

zipped_mnist = [f for f in os.listdir() if f.endswith('ubyte.gz')]
for z in zipped_mnist:
    with gzip.GzipFile(z, mode='rb') as decompressed, open(z[:-3], writemode)␣
 ↪as outfile:
        outfile.write(decompressed.read())
```

---

IGNORE IF THE CODE CELL ABOVE EXECUTED WITHOUT PROBLEMS:

If you have issues with the code cell above, I recommend unzipping the files using the Unix/Linux gzip tool from the terminal for efficiency, e.g., using the command

`gzip *ubyte.gz -d`

in your local MNIST download directory, or, using your favorite unzipping tool if you are working with a machine running on Microsoft Windows. The images are stored in byte form, and using the following function, we will read them into NumPy arrays that we will use to train our MLP.

Please note that if you are **not** using gzip, please make sure tha the files are named

- train-images-idx3-ubyte

- train-labels-idx1-ubyte
- t10k-images-idx3-ubyte
- t10k-labels-idx1-ubyte

If a file is e.g., named `train-images.idx3-ubyte` after unzipping (this is due to the fact that certain tools try to guess a file suffix), please rename it to `train-images-idx3-ubyte` before proceeding.

---

[9]:

```
import os
import struct
import numpy as np

def load_mnist(path, kind='train'):
    """Load MNIST data from `path`"""
    labels_path = os.path.join(path,
                               '%s-labels-idx1-ubyte' % kind)
    images_path = os.path.join(path,
                               '%s-images-idx3-ubyte' % kind)

    with open(labels_path, 'rb') as lbpath:
        magic, n = struct.unpack('>II',
                                 lbpath.read(8))
        labels = np.fromfile(lbpath,
                             dtype=np.uint8)

    with open(images_path, 'rb') as imgpath:
        magic, num, rows, cols = struct.unpack(">IIII",
                                               imgpath.read(16))
        images = np.fromfile(imgpath,
                             dtype=np.uint8).reshape(len(labels), 784)
        images = ((images / 255.) - .5) * 2

    return images, labels
```

[10]:

```
!ls
```

```
README.md                   t10k-images-idx3-ubyte.gz
ch12.ipynb                  t10k-labels-idx1-ubyte
ch12.py                     t10k-labels-idx1-ubyte.gz
images                      train-images-idx3-ubyte
mnist_scaled.npz            train-images-idx3-ubyte.gz
neuralnet.py                train-labels-idx1-ubyte
t10k-images-idx3-ubyte      train-labels-idx1-ubyte.gz
```

[11]:

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

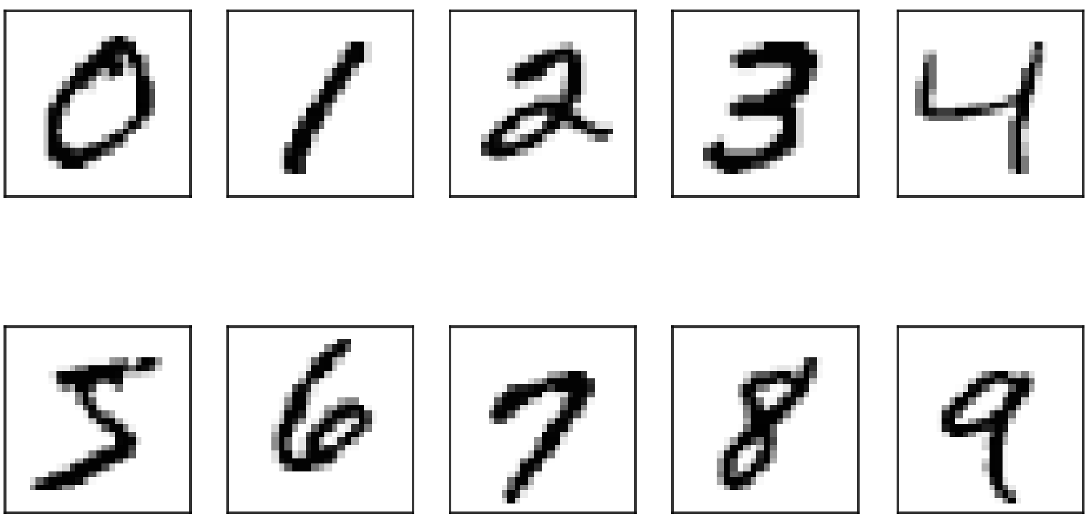
```
Rows: 60000, columns: 784
```

[12]:
```python
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:

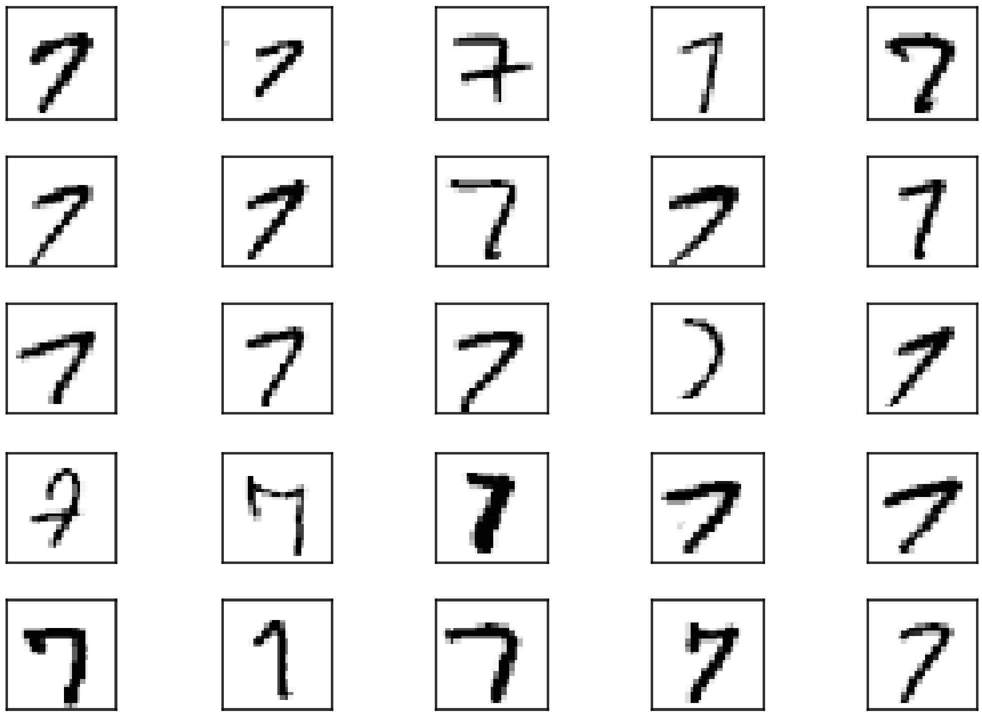
[13]:
```python
import matplotlib.pyplot as plt

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”:

[14]:
```python
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()
```



[15]:
```
import numpy as np

np.savez_compressed('mnist_scaled.npz',
                    X_train=X_train,
                    y_train=y_train,
                    X_test=X_test,
                    y_test=y_test)
```

[16]:
```
mnist = np.load('mnist_scaled.npz')
mnist.files
```

[16]: ['X_train', 'y_train', 'X_test', 'y_test']

[17]:
```
X_train, y_train, X_test, y_test = [mnist[f] for f in ['X_train', 'y_train',
                                    'X_test', 'y_test']]


del mnist
```

```
X_train.shape
```

[17]: (60000, 784)

### 3.2 Implementing a multi-layer perceptron

[18]:
```
import numpy as np
import sys


class NeuralNetMLP(object):
    """ Feedforward neural network / Multi-layer perceptron classifier.

    Parameters
    ------------
    n_hidden : int (default: 30)
        Number of hidden units.
    l2 : float (default: 0.)
        Lambda value for L2-regularization.
        No regularization if l2=0. (default)
    epochs : int (default: 100)
        Number of passes over the training set.
    eta : float (default: 0.001)
        Learning rate.
    shuffle : bool (default: True)
        Shuffles training data every epoch if True to prevent circles.
    minibatch_size : int (default: 1)
        Number of training examples per minibatch.
    seed : int (default: None)
        Random seed for initializing weights and shuffling.

    Attributes
    -----------
    eval_ : dict
      Dictionary collecting the cost, training accuracy,
      and validation accuracy for each epoch during training.

    """
    def __init__(self, n_hidden=30,
                 l2=0., epochs=100, eta=0.001,
                 shuffle=True, minibatch_size=1, seed=None):

        self.random = np.random.RandomState(seed)
        self.n_hidden = n_hidden
        self.l2 = l2
        self.epochs = epochs
        self.eta = eta
```

```python
        self.shuffle = shuffle
        self.minibatch_size = minibatch_size

    def _onehot(self, y, n_classes):
        """Encode labels into one-hot representation

        Parameters
        ------------
        y : array, shape = [n_examples]
            Target values.
        n_classes : int
            Number of classes

        Returns
        -----------
        onehot : array, shape = (n_examples, n_labels)

        """
        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)))

    def _forward(self, X):
        """Compute forward propagation step"""

        # step 1: net input of hidden layer
        # [n_examples, n_features] dot [n_features, n_hidden]
        # -> [n_examples, 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_examples, n_hidden] dot [n_hidden, n_classlabels]
        # -> [n_examples, 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

    def _compute_cost(self, y_enc, output):
        """Compute cost function.

        Parameters
        ----------
        y_enc : array, shape = (n_examples, n_labels)
            one-hot encoded class labels.
        output : array, shape = [n_examples, n_output_units]
            Activation of the output layer (forward propagation)

        Returns
        ---------
        cost : float
            Regularized cost

        """
        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

        # If you are applying this cost function to other
        # datasets where activation
        # values maybe become more extreme (closer to zero or 1)
        # you may encounter "ZeroDivisionError"s due to numerical
        # instabilities in Python & NumPy for the current implementation.
        # I.e., the code tries to evaluate log(0), which is undefined.
        # To address this issue, you could add a small constant to the
        # activation values that are passed to the log function.
        #
        # For example:
        #
        # term1 = -y_enc * (np.log(output + 1e-5))
        # term2 = (1. - y_enc) * np.log(1. - output + 1e-5)

        return cost

    def predict(self, X):
        """Predict class labels

        Parameters
        -----------
```

```
        X : array, shape = [n_examples, n_features]
            Input layer with original features.

        Returns:
        ----------
        y_pred : array, shape = [n_examples]
            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

    def fit(self, X_train, y_train, X_valid, y_valid):
        """ Learn weights from training data.

        Parameters
        -----------
        X_train : array, shape = [n_examples, n_features]
            Input layer with original features.
        y_train : array, shape = [n_examples]
            Target class labels.
        X_valid : array, shape = [n_examples, n_features]
            Sample features for validation during training
        y_valid : array, shape = [n_examples]
            Sample labels for validation during training

        Returns:
        ----------
        self

        """
        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)

        # 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])

                ##################
                # Backpropagation
                ##################

                # [n_examples, n_classlabels]
                delta_out = a_out - y_train_enc[batch_idx]

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

                # [n_examples, n_classlabels] dot [n_classlabels, n_hidden]
                # -> [n_examples, n_hidden]
                delta_h = (np.dot(delta_out, self.w_out.T) *
                           sigmoid_derivative_h)

                # [n_features, n_examples] dot [n_examples, n_hidden]
                # -> [n_features, n_hidden]
                grad_w_h = np.dot(X_train[batch_idx].T, delta_h)
                grad_b_h = np.sum(delta_h, axis=0)

                # [n_hidden, n_examples] dot [n_examples, n_classlabels]
                # -> [n_hidden, n_classlabels]
                grad_w_out = np.dot(a_h.T, delta_out)
                grad_b_out = np.sum(delta_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)

            cost = self._compute_cost(y_enc=y_train_enc,
                                      output=a_out)

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

            train_acc = ((np.sum(y_train == y_train_pred)).astype(np.float) /
                         X_train.shape[0])
            valid_acc = ((np.sum(y_valid == y_valid_pred)).astype(np.float) /
                         X_valid.shape[0])

            sys.stderr.write('\r%0*d/%d | Cost: %.2f '
                             '| Train/Valid Acc.: %.2f%%/%.2f%% ' %
                             (epoch_strlen, i+1, self.epochs, cost,
                              train_acc*100, valid_acc*100))
            sys.stderr.flush()

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

        return self
```

[19]:

```
n_epochs = 200

## @Readers: PLEASE IGNORE IF-STATEMENT BELOW
##
## This cell is meant to run fewer epochs when
```

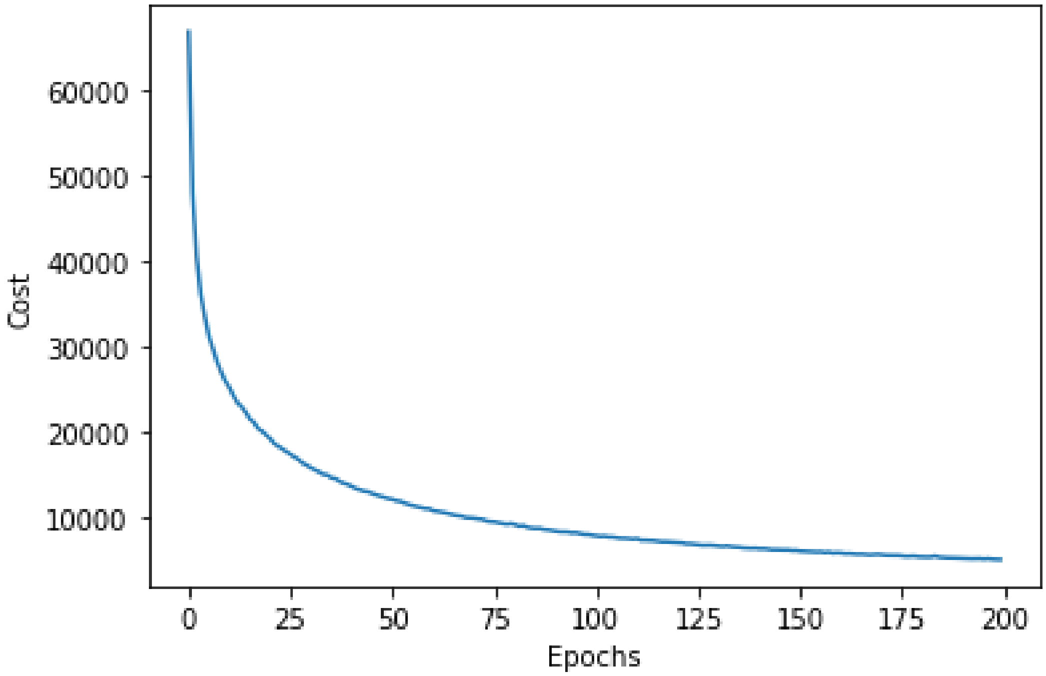
```
## the notebook is run on the Travis Continuous Integration
## platform to test the code on a smaller dataset
## to prevent timeout errors; it just serves a debugging tool

if 'TRAVIS' in os.environ:
    n_epochs = 20
```

[20]:
```
nn = NeuralNetMLP(n_hidden=100,
                  l2=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:])
```

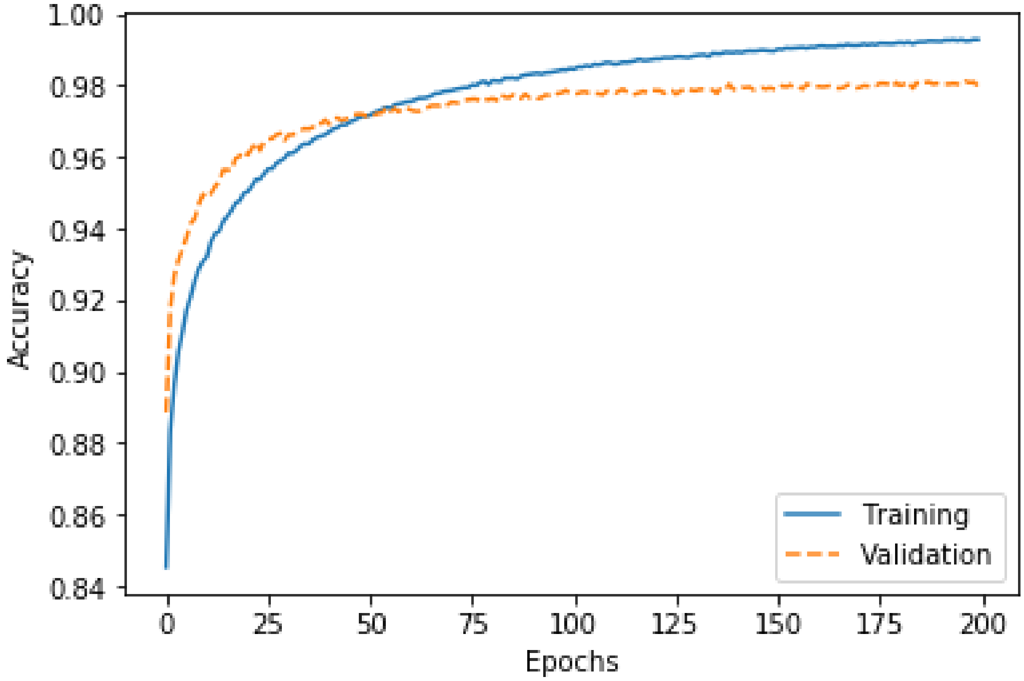
```
200/200 | Cost: 5065.78 | Train/Valid Acc.: 99.28%/97.98%
```

[20]:
```
<__main__.NeuralNetMLP at 0x7fdfc8463518>
```

[21]:
```
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()
```



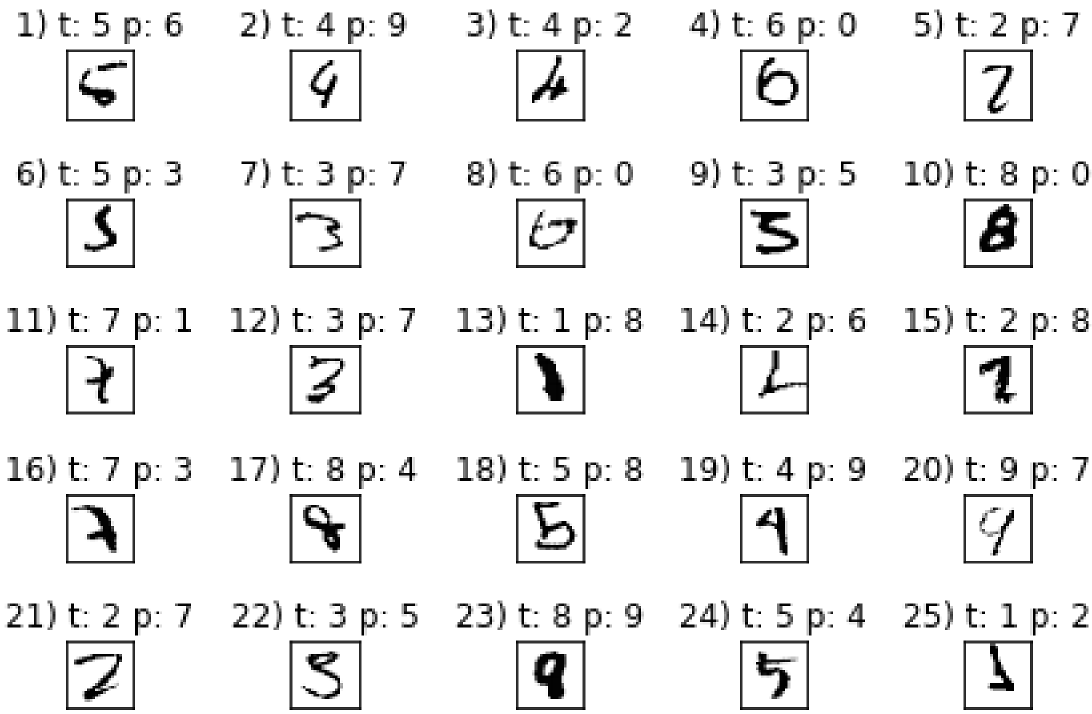

[22]:
```
plt.plot(range(nn.epochs), nn.eval_['train_acc'],
         label='Training')
plt.plot(range(nn.epochs), nn.eval_['valid_acc'],
         label='Validation', linestyle='--')
plt.ylabel('Accuracy')
plt.xlabel('Epochs')
plt.legend(loc='lower right')
plt.savefig('images/12_08.png', dpi=300)
plt.show()
```




[23]:
```
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%
```

[24]:
```
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()
```




# 4 Training an artificial neural network

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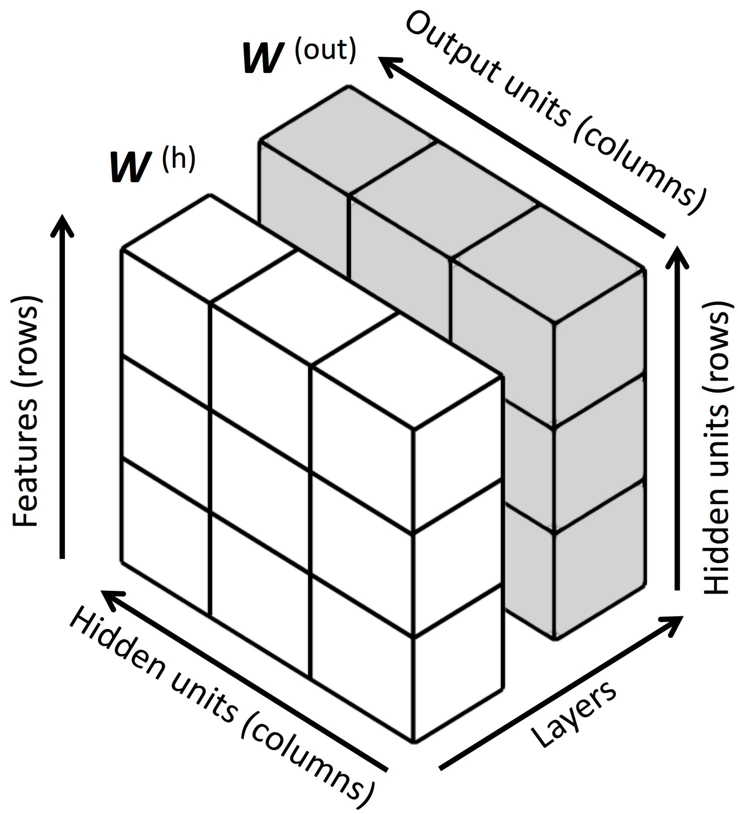
## 4.1 Computing the logistic cost function

[25]:
```
Image(filename='images/12_10.png', width=300)
```

[25]:




### 4.2 Developing your intuition for backpropagation

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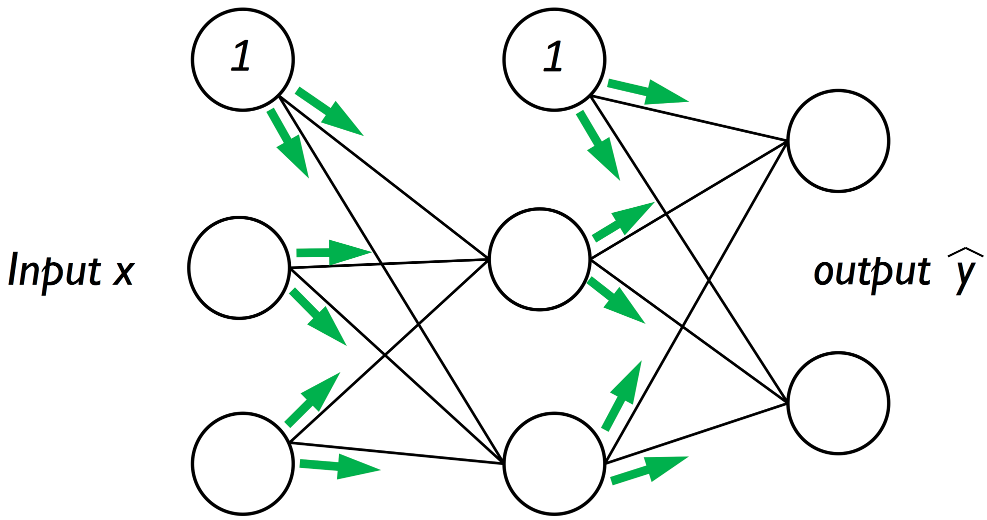
### 4.3 Training neural networks via backpropagation

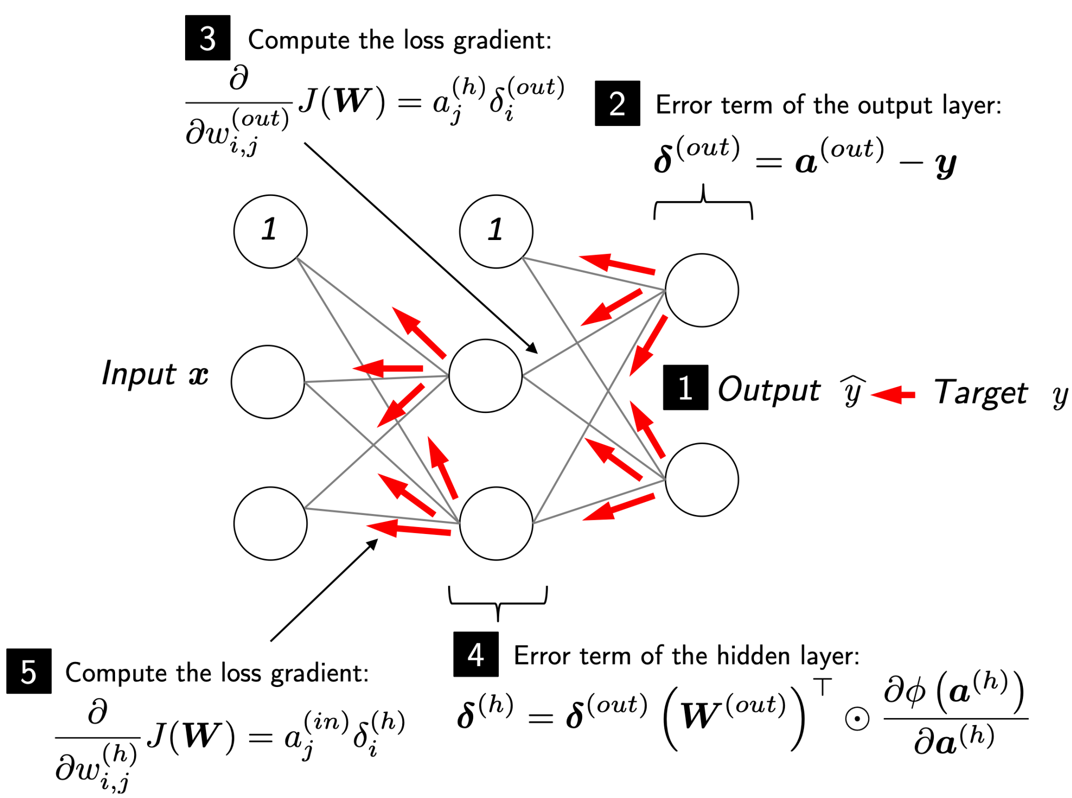
[26]:
```
Image(filename='./images/12_11.png', width=400)
```

[26]:




```
[27]: Image(filename='images/12_12.png', width=500)
```

[27]:

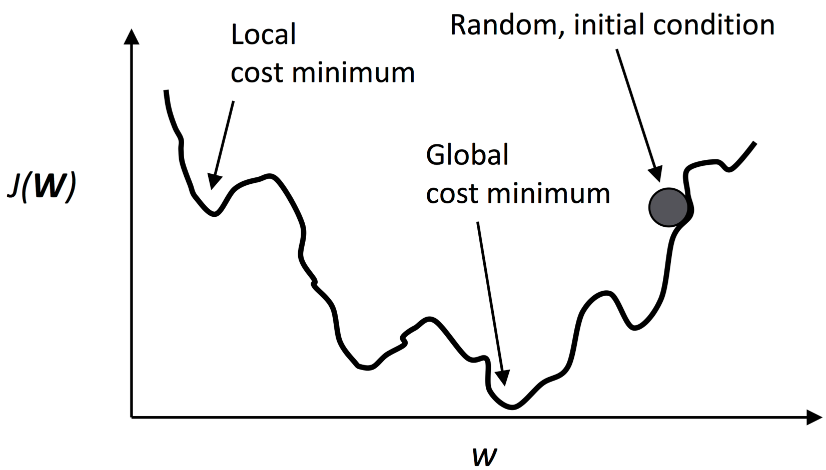


## 5 Convergence in neural networks

[28]:

```
Image(filename='images/12_13.png', width=500)
```

[28]:




...

## 6 Summary

...

---

Readers may ignore the next cell.

[29]:

```
! python ../.convert_notebook_to_script.py --input ch12.ipynb --output ch12.py
```

```
[NbConvertApp] Converting notebook ch12.ipynb to script
[NbConvertApp] Writing 19664 bytes to ch12.py
```