In [1]:

```
%load_ext watermark
%watermark -a 'Sebastian Raschka' -u -d -v -p numpy,scipy,matplotlib
```

UsageError: unrecognized arguments: Raschka'

In [2]:

```
from IPython.display import Image
```

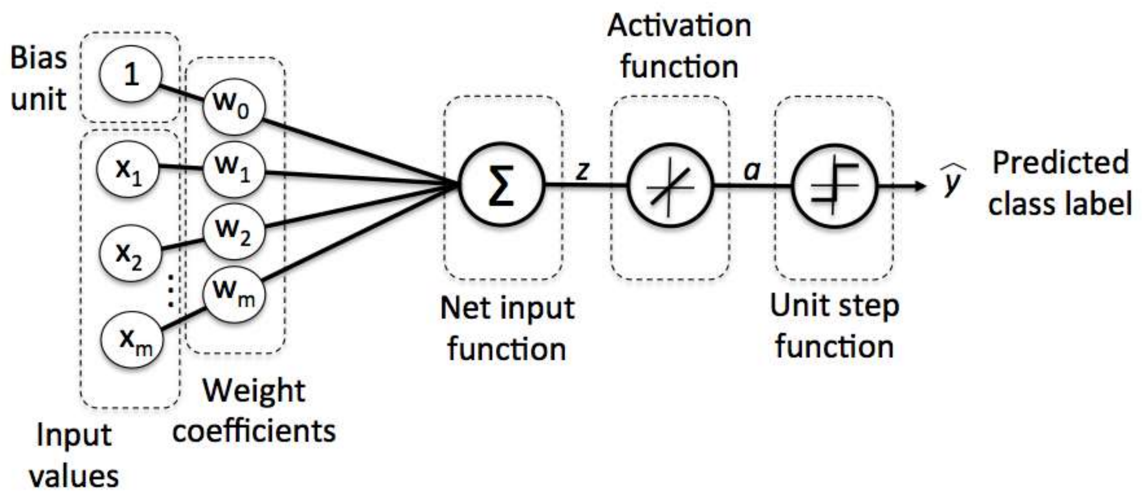
In [3]:

```
%matplotlib inline
```

In [4]:

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

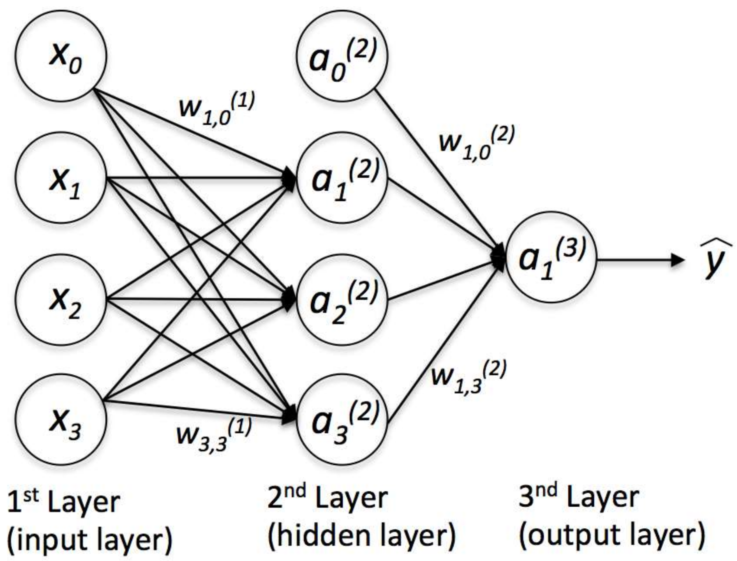
Out[4]:



In [5]:

```
Image(filename='12_02.png', width=400)
```

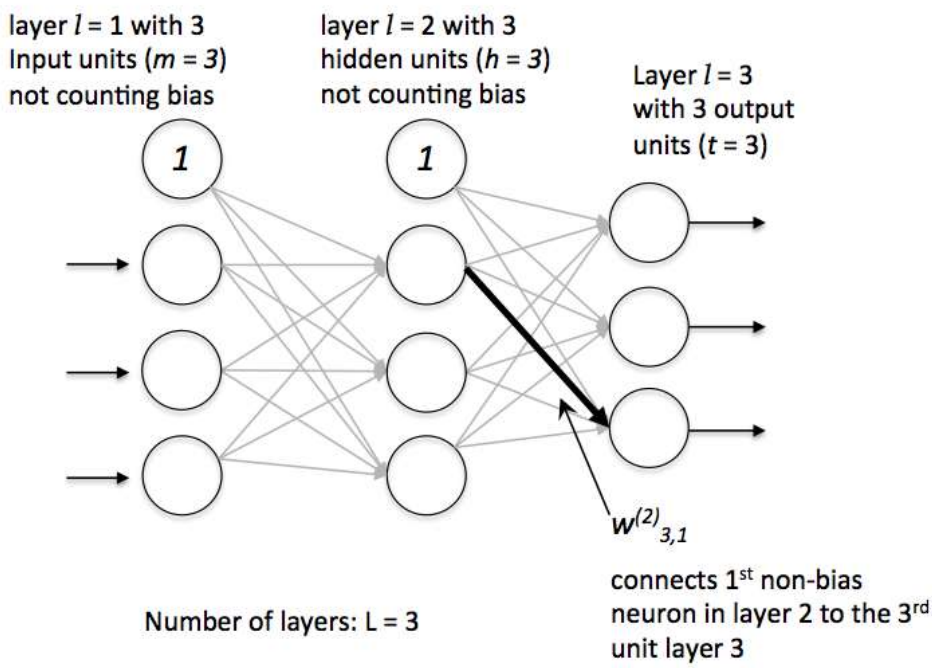
Out[5]:



In [6]:

```
Image(filename='12_03.png', width=500)
```

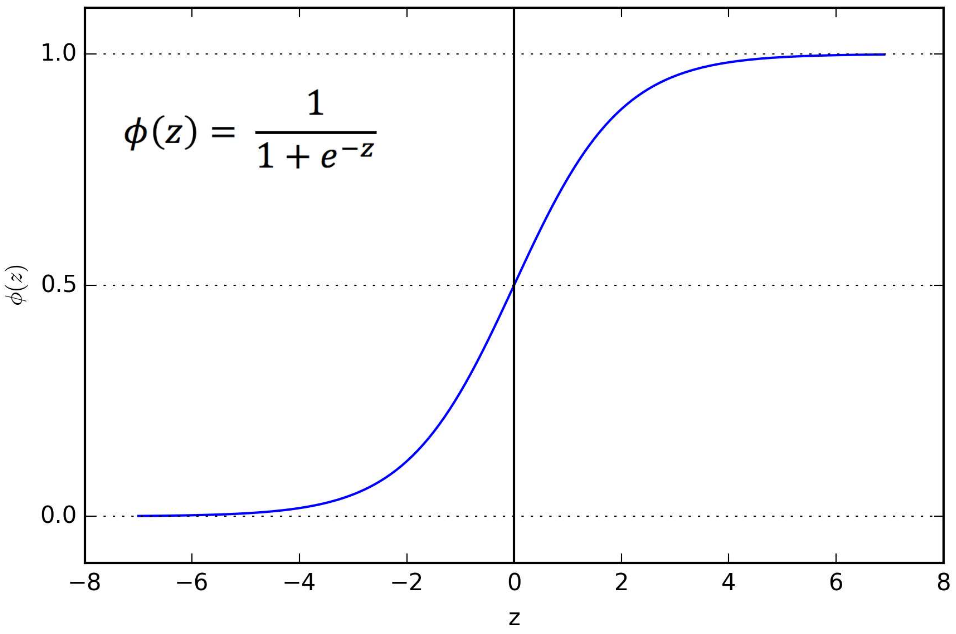
Out[6]:



In [7]:

```
Image(filename='12_04.png', width=500)
```

Out[7]:



In [8]:

```
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)

    return images, labels
```

In [9]:

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

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

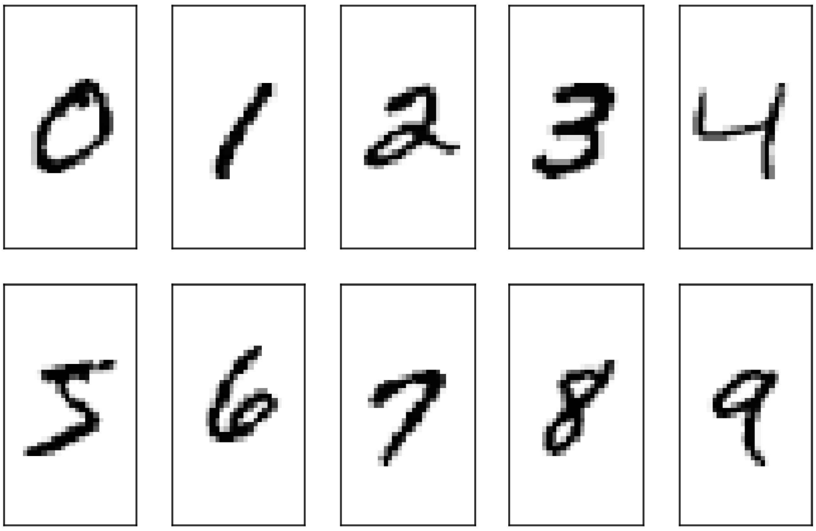
In [10]:

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

Rows: 10000, columns: 784

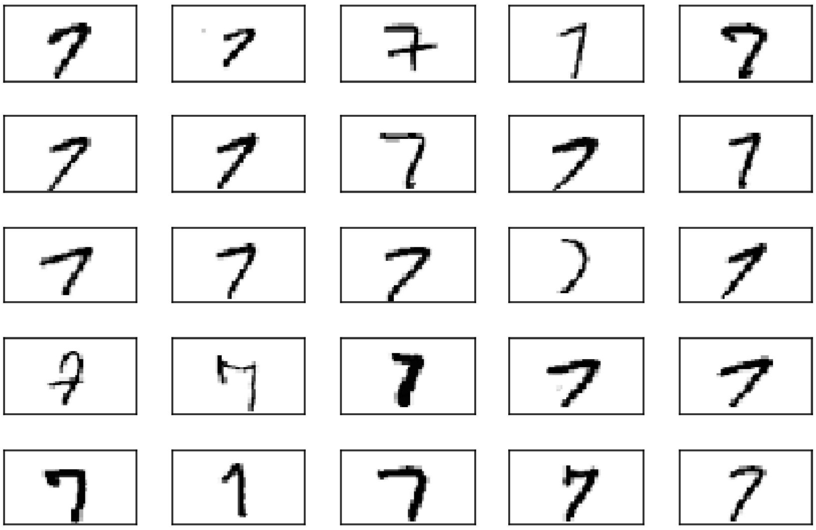
In [11]:

```
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', interpolation='nearest')

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



In [12]:

```
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', interpolation='nearest')

ax[0].set_xticks([])
ax[0].set_yticks([])
plt.tight_layout()
# plt.savefig('./figures/mnist_7.png', dpi=300)
plt.show()
```



In [13]:

```
# np.savetxt('train_img.csv', X_train, fmt='%i', delimiter=',')
# np.savetxt('train_labels.csv', y_train, fmt='%i', delimiter=',')
# X_train = np.genfromtxt('train_img.csv', dtype=int, delimiter=',')
# y_train = np.genfromtxt('train_labels.csv', dtype=int, delimiter=',')

# np.savetxt('test_img.csv', X_test, fmt='%i', delimiter=',')
# np.savetxt('test_labels.csv', y_test, fmt='%i', delimiter=',')
# X_test = np.genfromtxt('test_img.csv', dtype=int, delimiter=',')
# y_test = np.genfromtxt('test_labels.csv', dtype=int, delimiter=',')
```

In [14]:

```
import numpy as np
from scipy.special import expit
import sys


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

    Parameters
    ------------
    n_output : int
        Number of output units, should be equal to the
        number of unique class labels.
    n_features : int
        Number of features (dimensions) in the target dataset.
```

```
        Should be equal to the number of columns in the X array.
    n_hidden : int (default: 30)
        Number of hidden units.
    l1 : float (default: 0.0)
        Lambda value for L1-regularization.
        No regularization if l1=0.0 (default)
    l2 : float (default: 0.0)
        Lambda value for L2-regularization.
        No regularization if l2=0.0 (default)
    epochs : int (default: 500)
        Number of passes over the training set.
    eta : float (default: 0.001)
        Learning rate.
    alpha : float (default: 0.0)
        Momentum constant. Factor multiplied with the
        gradient of the previous epoch t-1 to improve
        learning speed
        w(t) := w(t) - (grad(t) + alpha*grad(t-1))
    decrease_const : float (default: 0.0)
        Decrease constant. Shrinks the learning rate
        after each epoch via eta / (1 + epoch*decrease_const)
    shuffle : bool (default: True)
        Shuffles training data every epoch if True to prevent circles.
    minibatches : int (default: 1)
        Divides training data into k minibatches for efficiency.
        Normal gradient descent learning if k=1 (default).
    random_state : int (default: None)
        Set random state for shuffling and initializing the weights.

    Attributes
    -----------
    cost_ : list
      Sum of squared errors after each epoch.

    """
    def __init__(self, n_output, n_features, n_hidden=30,
                 l1=0.0, l2=0.0, epochs=500, eta=0.001,
                 alpha=0.0, decrease_const=0.0, shuffle=True,
                 minibatches=1, random_state=None):

        np.random.seed(random_state)
        self.n_output = n_output
        self.n_features = n_features
        self.n_hidden = n_hidden
        self.w1, self.w2 = self._initialize_weights()
        self.l1 = l1
        self.l2 = l2
        self.epochs = epochs
        self.eta = eta
        self.alpha = alpha
        self.decrease_const = decrease_const
        self.shuffle = shuffle
        self.minibatches = minibatches

    def _encode_labels(self, y, k):
        """Encode labels into one-hot representation

        Parameters
        ------------
        y : array, shape = [n_samples]
            Target values.
```

```
        Returns
        -----------
        onehot : array, shape = (n_labels, n_samples)

        """
        onehot = np.zeros((k, y.shape[0]))
        for idx, val in enumerate(y):
            onehot[val, idx] = 1.0
        return onehot

    def _initialize_weights(self):
        """Initialize weights with small random numbers."""
        w1 = np.random.uniform(-1.0, 1.0,
                               size=self.n_hidden*(self.n_features + 1))
        w1 = w1.reshape(self.n_hidden, self.n_features + 1)
        w2 = np.random.uniform(-1.0, 1.0,
                               size=self.n_output*(self.n_hidden + 1))
        w2 = w2.reshape(self.n_output, self.n_hidden + 1)
        return w1, w2

    def _sigmoid(self, z):
        """Compute logistic function (sigmoid)

        Uses scipy.special.expit to avoid overflow
        error for very small input values z.

        """
        # return 1.0 / (1.0 + np.exp(-z))
        return expit(z)

    def _sigmoid_gradient(self, z):
        """Compute gradient of the logistic function"""
        sg = self._sigmoid(z)
        return sg * (1.0 - sg)

    def _add_bias_unit(self, X, how='column'):
        """Add bias unit (column or row of 1s) to array at index 0"""
        if how == 'column':
            X_new = np.ones((X.shape[0], X.shape[1] + 1))
            X_new[:, 1:] = X
        elif how == 'row':
            X_new = np.ones((X.shape[0] + 1, X.shape[1]))
            X_new[1:, :] = X
        else:
            raise AttributeError('`how` must be `column` or `row`')
        return X_new

    def _feedforward(self, X, w1, w2):
        """Compute feedforward step

        Parameters
        -----------
        X : array, shape = [n_samples, n_features]
            Input layer with original features.
        w1 : array, shape = [n_hidden_units, n_features]
            Weight matrix for input layer -> hidden layer.
        w2 : array, shape = [n_output_units, n_hidden_units]
            Weight matrix for hidden layer -> output layer.

        Returns
```

```
        ----------
        a1 : array, shape = [n_samples, n_features+1]
            Input values with bias unit.
        z2 : array, shape = [n_hidden, n_samples]
            Net input of hidden layer.
        a2 : array, shape = [n_hidden+1, n_samples]
            Activation of hidden layer.
        z3 : array, shape = [n_output_units, n_samples]
            Net input of output layer.
        a3 : array, shape = [n_output_units, n_samples]
            Activation of output layer.

        """
        a1 = self._add_bias_unit(X, how='column')
        z2 = w1.dot(a1.T)
        a2 = self._sigmoid(z2)
        a2 = self._add_bias_unit(a2, how='row')
        z3 = w2.dot(a2)
        a3 = self._sigmoid(z3)
        return a1, z2, a2, z3, a3

    def _L2_reg(self, lambda_, w1, w2):
        """Compute L2-regularization cost"""
        return (lambda_/2.0) * (np.sum(w1[:, 1:] ** 2) +
                                np.sum(w2[:, 1:] ** 2))

    def _L1_reg(self, lambda_, w1, w2):
        """Compute L1-regularization cost"""
        return (lambda_/2.0) * (np.abs(w1[:, 1:]).sum() +
                                np.abs(w2[:, 1:]).sum())

    def _get_cost(self, y_enc, output, w1, w2):
        """Compute cost function.

        Parameters
        ----------
        y_enc : array, shape = (n_labels, n_samples)
            one-hot encoded class labels.
        output : array, shape = [n_output_units, n_samples]
            Activation of the output layer (feedforward)
        w1 : array, shape = [n_hidden_units, n_features]
            Weight matrix for input layer -> hidden layer.
        w2 : array, shape = [n_output_units, n_hidden_units]
            Weight matrix for hidden layer -> output layer.

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

        """
        term1 = -y_enc * (np.log(output))
        term2 = (1.0 - y_enc) * np.log(1.0 - output)
        cost = np.sum(term1 - term2)
        L1_term = self._L1_reg(self.l1, w1, w2)
        L2_term = self._L2_reg(self.l2, w1, w2)
        cost = cost + L1_term + L2_term
        return cost

    def _get_gradient(self, a1, a2, a3, z2, y_enc, w1, w2):
        """ Compute gradient step using backpropagation.
```

```
        Parameters
        ------------
        a1 : array, shape = [n_samples, n_features+1]
            Input values with bias unit.
        a2 : array, shape = [n_hidden+1, n_samples]
            Activation of hidden layer.
        a3 : array, shape = [n_output_units, n_samples]
            Activation of output layer.
        z2 : array, shape = [n_hidden, n_samples]
            Net input of hidden layer.
        y_enc : array, shape = (n_labels, n_samples)
            one-hot encoded class labels.
        w1 : array, shape = [n_hidden_units, n_features]
            Weight matrix for input layer -> hidden layer.
        w2 : array, shape = [n_output_units, n_hidden_units]
            Weight matrix for hidden layer -> output layer.

        Returns
        ---------
        grad1 : array, shape = [n_hidden_units, n_features]
            Gradient of the weight matrix w1.
        grad2 : array, shape = [n_output_units, n_hidden_units]
            Gradient of the weight matrix w2.

        """
        # backpropagation
        sigma3 = a3 - y_enc
        z2 = self._add_bias_unit(z2, how='row')
        sigma2 = w2.T.dot(sigma3) * self._sigmoid_gradient(z2)
        sigma2 = sigma2[1:, :]
        grad1 = sigma2.dot(a1)
        grad2 = sigma3.dot(a2.T)

        # regularize
        grad1[:, 1:] += (w1[:, 1:] * (self.l1 + self.l2))
        grad2[:, 1:] += (w2[:, 1:] * (self.l1 + self.l2))

        return grad1, grad2

    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.

        """
        if len(X.shape) != 2:
            raise AttributeError('X must be a [n_samples, n_features] array.¥n'
                                 'Use X[:,None] for 1-feature classification,'
                                 '¥nor X[[i]] for 1-sample classification')

        a1, z2, a2, z3, a3 = self._feedforward(X, self.w1, self.w2)
        y_pred = np.argmax(z3, axis=0)
```

```
        return y_pred

    def fit(self, X, y, print_progress=False):
        """ Learn weights from training data.

        Parameters
        -----------
        X : array, shape = [n_samples, n_features]
            Input layer with original features.
        y : array, shape = [n_samples]
            Target class labels.
        print_progress : bool (default: False)
            Prints progress as the number of epochs
            to stderr.

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

        """
        self.cost_ = []
        X_data, y_data = X.copy(), y.copy()
        y_enc = self._encode_labels(y, self.n_output)

        delta_w1_prev = np.zeros(self.w1.shape)
        delta_w2_prev = np.zeros(self.w2.shape)

        for i in range(self.epochs):

            # adaptive learning rate
            self.eta /= (1 + self.decrease_const*i)

            if print_progress:
                sys.stderr.write('¥rEpoch: %d/%d' % (i+1, self.epochs))
                sys.stderr.flush()

            if self.shuffle:
                idx = np.random.permutation(y_data.shape[0])
                X_data, y_enc = X_data[idx], y_enc[:, idx]

            mini = np.array_split(range(y_data.shape[0]), self.minibatches)
            for idx in mini:

                # feedforward
                a1, z2, a2, z3, a3 = self._feedforward(X_data[idx],
                                                       self.w1,
                                                       self.w2)
                cost = self._get_cost(y_enc=y_enc[:, idx],
                                      output=a3,
                                      w1=self.w1,
                                      w2=self.w2)
                self.cost_.append(cost)

                # compute gradient via backpropagation
                grad1, grad2 = self._get_gradient(a1=a1, a2=a2,
                                                  a3=a3, z2=z2,
                                                  y_enc=y_enc[:, idx],
                                                  w1=self.w1,
                                                  w2=self.w2)

                delta_w1, delta_w2 = self.eta * grad1, self.eta * grad2
```

```
                self.w1 -= (delta_w1 + (self.alpha * delta_w1_prev))
                self.w2 -= (delta_w2 + (self.alpha * delta_w2_prev))
                delta_w1_prev, delta_w2_prev = delta_w1, delta_w2

        return self
```

In [15]:

```
nn = NeuralNetMLP(n_output=10,
                  n_features=X_train.shape[1],
                  n_hidden=50,
                  l2=0.1,
                  l1=0.0,
                  epochs=1000,
                  eta=0.001,
                  alpha=0.001,
                  decrease_const=0.00001,
                  minibatches=50,
                  shuffle=True,
                  random_state=1)
```

In [16]:

```
nn.fit(X_train, y_train, print_progress=True)
```

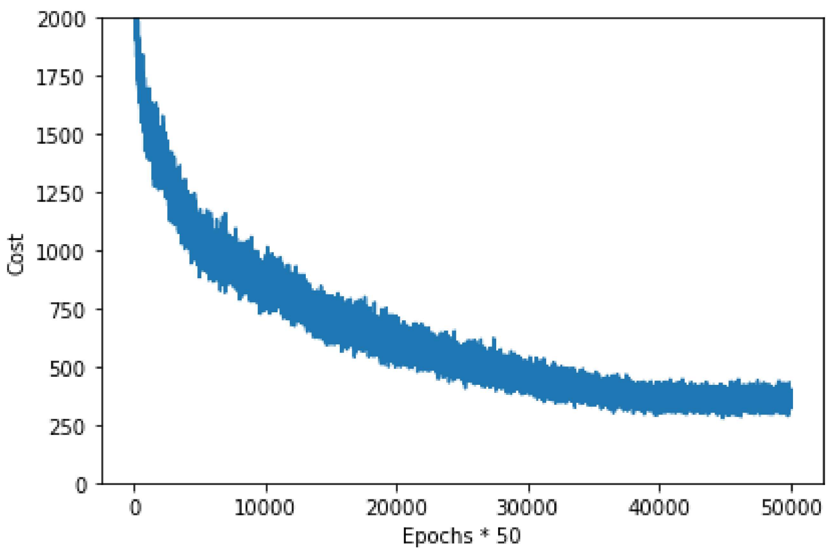
Epoch: 1000/1000

Out[16]:

<__main__.NeuralNetMLP at 0x18af0e11198>

In [17]:

```
import matplotlib.pyplot as plt

plt.plot(range(len(nn.cost_)), nn.cost_)
plt.ylim([0, 2000])
plt.ylabel('Cost')
plt.xlabel('Epochs * 50')
plt.tight_layout()
# plt.savefig('./figures/cost.png', dpi=300)
plt.show()
```

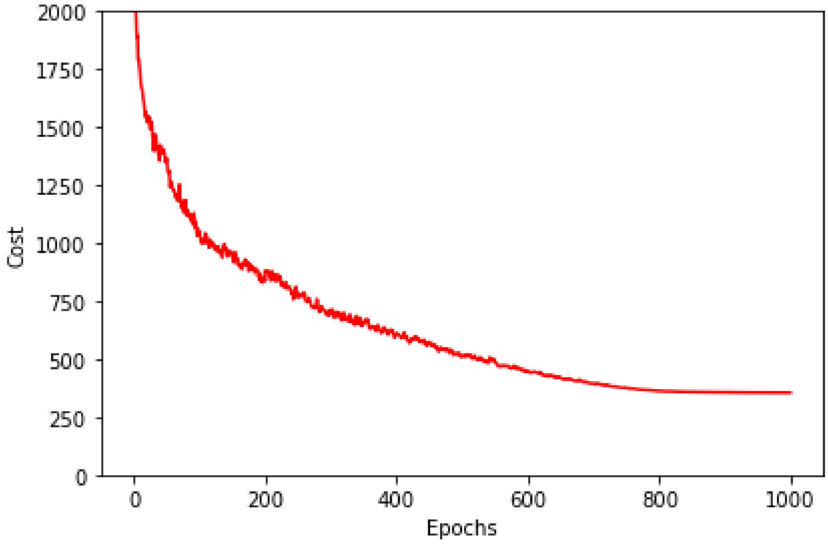


In [18]:

```
batches = np.array_split(range(len(nn.cost_)), 1000)
cost_ary = np.array(nn.cost_)
cost_avgs = [np.mean(cost_ary[i]) for i in batches]
```

In [19]:

```
plt.plot(range(len(cost_avgs)), cost_avgs, color='red')
plt.ylim([0, 2000])
plt.ylabel('Cost')
plt.xlabel('Epochs')
plt.tight_layout()
#plt.savefig('./figures/cost2.png', dpi=300)
plt.show()
```



In [20]:

```
y_train_pred = nn.predict(X_train)

if sys.version_info < (3, 0):
    acc = ((np.sum(y_train == y_train_pred, axis=0)).astype('float') /
           X_train.shape[0])
else:
    acc = np.sum(y_train == y_train_pred, axis=0) / X_train.shape[0]

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

Training accuracy: 97.69%

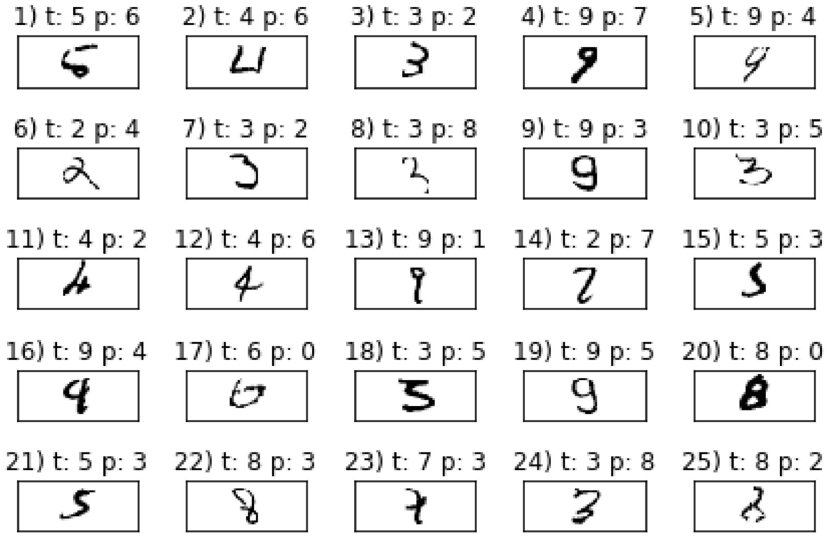
In [21]:

```
y_test_pred = nn.predict(X_test)

if sys.version_info < (3, 0):
    acc = ((np.sum(y_test == y_test_pred, axis=0)).astype('float') /
           X_test.shape[0])
else:
    acc = np.sum(y_test == y_test_pred, axis=0) / X_test.shape[0]

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

Test accuracy: 95.79%

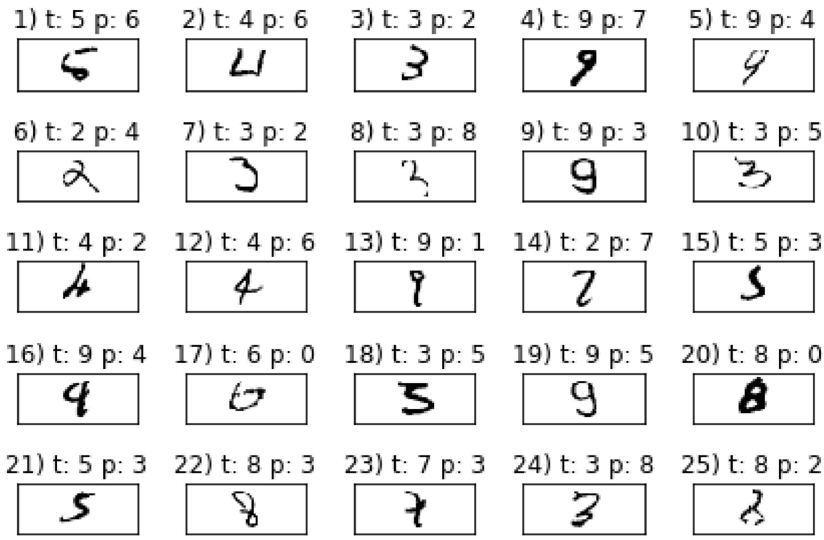
In [22]:

```
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('./figures/mnist_miscl.png', dpi=300)
plt.show()
```



In [23]:

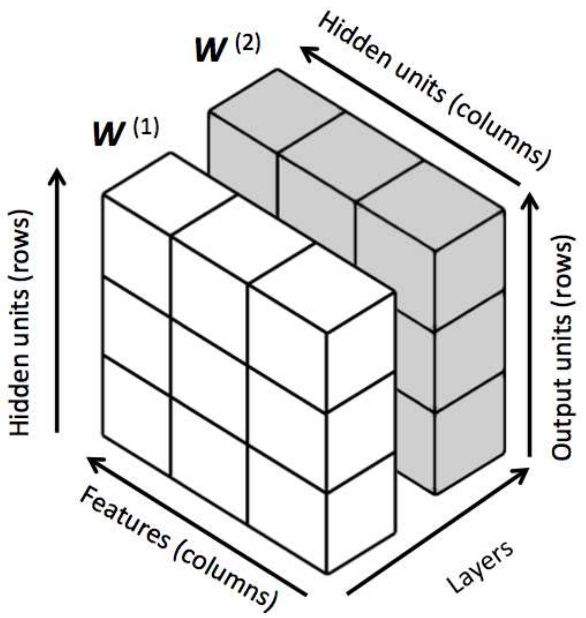
```
miscl_img = X_test[y_test != y_test_pred][:25]
correct_lab = y_test[y_test != y_test_pred][:25]
miscl_lab= y_test_pred[y_test != y_test_pred][:25]

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('./figures/mnist_miscl.png', dpi=300)
plt.show()
```



In [24]:

```
Image(filename='12_10.png', width=300)
```

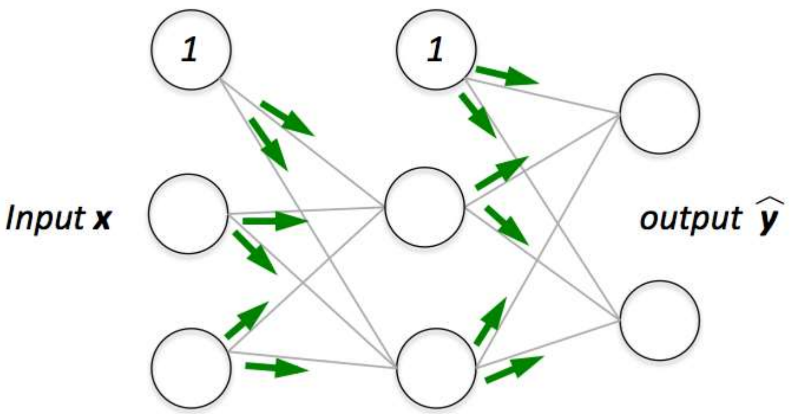
Out[24]:



In [25]:

```
Image(filename='12_11.png', width=400)
```

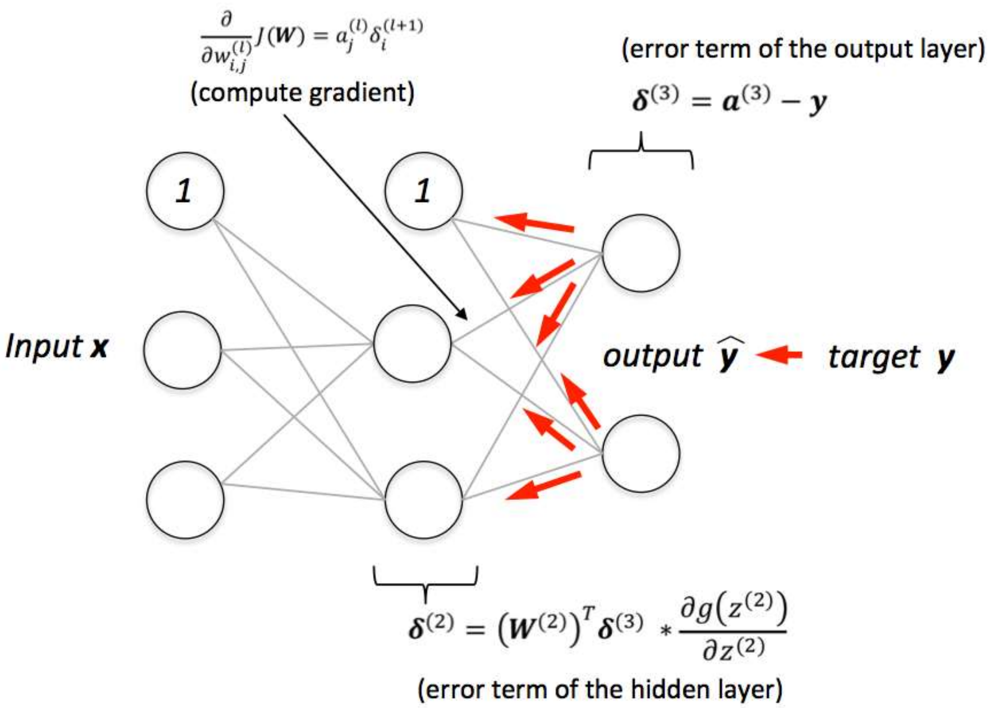
Out[25]:



In [26]:

```
Image(filename='12_12.png', width=500)
```

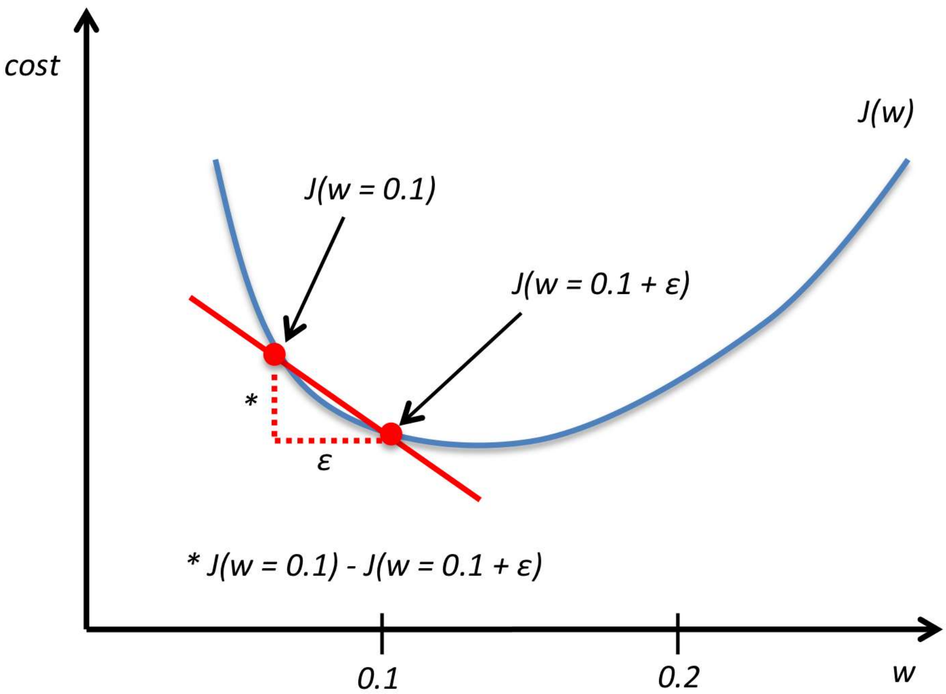
Out[26]:



In [27]:

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

Out[27]:



In [28]:

```
from scipy import __version__ as scipy_ver
from numpy import __version__ as numpy_ver

print('The following code requires NumPy >= 1.9.1. Your NumPy version is %s.' % (numpy_ver))
print('The following code requires SciPy >= 0.14.0. Your SciPy version is %s. ' % (scipy_ver))
```

```
The following code requires NumPy >= 1.9.1. Your NumPy version is 1.12.1.
The following code requires SciPy >= 0.14.0. Your SciPy version is 0.19.0.
```

In [29]:

```
import numpy as np
from scipy.special import expit
import sys


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

    Parameters
    ------------
    n_output : int
        Number of output units, should be equal to the
        number of unique class labels.
    n_features : int
        Number of features (dimensions) in the target dataset.
        Should be equal to the number of columns in the X array.
    n_hidden : int (default: 30)
        Number of hidden units.
    l1 : float (default: 0.0)
        Lambda value for L1-regularization.
        No regularization if l1=0.0 (default)
    l2 : float (default: 0.0)
        Lambda value for L2-regularization.
        No regularization if l2=0.0 (default)
    epochs : int (default: 500)
        Number of passes over the training set.
    eta : float (default: 0.001)
        Learning rate.
    alpha : float (default: 0.0)
        Momentum constant. Factor multiplied with the
        gradient of the previous epoch t-1 to improve
        learning speed
        w(t) := w(t) - (grad(t) + alpha*grad(t-1))
    decrease_const : float (default: 0.0)
        Decrease constant. Shrinks the learning rate
        after each epoch via eta / (1 + epoch*decrease_const)
    shuffle : bool (default: False)
        Shuffles training data every epoch if True to prevent circles.
    minibatches : int (default: 1)
        Divides training data into k minibatches for efficiency.
        Normal gradient descent learning if k=1 (default).
    random_state : int (default: None)
        Set random state for shuffling and initializing the weights.

    Attributes
    -----------
    cost_ : list
        Sum of squared errors after each epoch.
```

```
    """
    def __init__(self, n_output, n_features, n_hidden=30,
                 l1=0.0, l2=0.0, epochs=500, eta=0.001,
                 alpha=0.0, decrease_const=0.0, shuffle=True,
                 minibatches=1, random_state=None):

        np.random.seed(random_state)
        self.n_output = n_output
        self.n_features = n_features
        self.n_hidden = n_hidden
        self.w1, self.w2 = self._initialize_weights()
        self.l1 = l1
        self.l2 = l2
        self.epochs = epochs
        self.eta = eta
        self.alpha = alpha
        self.decrease_const = decrease_const
        self.shuffle = shuffle
        self.minibatches = minibatches

    def _encode_labels(self, y, k):
        """Encode labels into one-hot representation

        Parameters
        ------------
        y : array, shape = [n_samples]
            Target values.

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

        """
        onehot = np.zeros((k, y.shape[0]))
        for idx, val in enumerate(y):
            onehot[val, idx] = 1.0
        return onehot

    def _initialize_weights(self):
        """Initialize weights with small random numbers."""
        w1 = np.random.uniform(-1.0, 1.0,
                               size=self.n_hidden*(self.n_features + 1))
        w1 = w1.reshape(self.n_hidden, self.n_features + 1)
        w2 = np.random.uniform(-1.0, 1.0,
                               size=self.n_output*(self.n_hidden + 1))
        w2 = w2.reshape(self.n_output, self.n_hidden + 1)
        return w1, w2

    def _sigmoid(self, z):
        """Compute logistic function (sigmoid)

        Uses scipy.special.expit to avoid overflow
        error for very small input values z.

        """
        # return 1.0 / (1.0 + np.exp(-z))
        return expit(z)

    def _sigmoid_gradient(self, z):
        """Compute gradient of the logistic function"""
```

```
        sg = self._sigmoid(z)
        return sg * (1.0 - sg)

    def _add_bias_unit(self, X, how='column'):
        """Add bias unit (column or row of 1s) to array at index 0"""
        if how == 'column':
            X_new = np.ones((X.shape[0], X.shape[1] + 1))
            X_new[:, 1:] = X
        elif how == 'row':
            X_new = np.ones((X.shape[0]+1, X.shape[1]))
            X_new[1:, :] = X
        else:
            raise AttributeError('`how` must be `column` or `row`')
        return X_new

    def _feedforward(self, X, w1, w2):
        """Compute feedforward step

        Parameters
        -----------
        X : array, shape = [n_samples, n_features]
            Input layer with original features.
        w1 : array, shape = [n_hidden_units, n_features]
            Weight matrix for input layer -> hidden layer.
        w2 : array, shape = [n_output_units, n_hidden_units]
            Weight matrix for hidden layer -> output layer.

        Returns
        ----------
        a1 : array, shape = [n_samples, n_features+1]
            Input values with bias unit.
        z2 : array, shape = [n_hidden, n_samples]
            Net input of hidden layer.
        a2 : array, shape = [n_hidden+1, n_samples]
            Activation of hidden layer.
        z3 : array, shape = [n_output_units, n_samples]
            Net input of output layer.
        a3 : array, shape = [n_output_units, n_samples]
            Activation of output layer.

        """
        a1 = self._add_bias_unit(X, how='column')
        z2 = w1.dot(a1.T)
        a2 = self._sigmoid(z2)
        a2 = self._add_bias_unit(a2, how='row')
        z3 = w2.dot(a2)
        a3 = self._sigmoid(z3)
        return a1, z2, a2, z3, a3

    def _L2_reg(self, lambda_, w1, w2):
        """Compute L2-regularization cost"""
        return (lambda_/2.0) * (np.sum(w1[:, 1:] ** 2) +
                                np.sum(w2[:, 1:] ** 2))

    def _L1_reg(self, lambda_, w1, w2):
        """Compute L1-regularization cost"""
        return (lambda_/2.0) * (np.abs(w1[:, 1:]).sum() +
                                np.abs(w2[:, 1:]).sum())

    def _get_cost(self, y_enc, output, w1, w2):
        """Compute cost function.
```

```
        Parameters
        ----------
        y_enc : array, shape = (n_labels, n_samples)
            one-hot encoded class labels.
        output : array, shape = [n_output_units, n_samples]
            Activation of the output layer (feedforward)
        w1 : array, shape = [n_hidden_units, n_features]
            Weight matrix for input layer -> hidden layer.
        w2 : array, shape = [n_output_units, n_hidden_units]
            Weight matrix for hidden layer -> output layer.

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

        """
        term1 = -y_enc * (np.log(output))
        term2 = (1.0 - y_enc) * np.log(1.0 - output)
        cost = np.sum(term1 - term2)
        L1_term = self._L1_reg(self.l1, w1, w2)
        L2_term = self._L2_reg(self.l2, w1, w2)
        cost = cost + L1_term + L2_term
        return cost

    def _get_gradient(self, a1, a2, a3, z2, y_enc, w1, w2):
        """ Compute gradient step using backpropagation.

        Parameters
        ------------
        a1 : array, shape = [n_samples, n_features+1]
            Input values with bias unit.
        a2 : array, shape = [n_hidden+1, n_samples]
            Activation of hidden layer.
        a3 : array, shape = [n_output_units, n_samples]
            Activation of output layer.
        z2 : array, shape = [n_hidden, n_samples]
            Net input of hidden layer.
        y_enc : array, shape = (n_labels, n_samples)
            one-hot encoded class labels.
        w1 : array, shape = [n_hidden_units, n_features]
            Weight matrix for input layer -> hidden layer.
        w2 : array, shape = [n_output_units, n_hidden_units]
            Weight matrix for hidden layer -> output layer.

        Returns
        ---------
        grad1 : array, shape = [n_hidden_units, n_features]
            Gradient of the weight matrix w1.
        grad2 : array, shape = [n_output_units, n_hidden_units]
            Gradient of the weight matrix w2.

        """
        # backpropagation
        sigma3 = a3 - y_enc
        z2 = self._add_bias_unit(z2, how='row')
        sigma2 = w2.T.dot(sigma3) * self._sigmoid_gradient(z2)
        sigma2 = sigma2[1:, :]
        grad1 = sigma2.dot(a1)
        grad2 = sigma3.dot(a2.T)
```

```
        # regularize
        grad1[:, 1:] += (w1[:, 1:] * (self.l1 + self.l2))
        grad2[:, 1:] += (w2[:, 1:] * (self.l1 + self.l2))

        return grad1, grad2

    def _gradient_checking(self, X, y_enc, w1, w2, epsilon, grad1, grad2):
        """ Apply gradient checking (for debugging only)

        Returns
        ---------
        relative_error : float
          Relative error between the numerically
          approximated gradients and the backpropagated gradients.

        """
        num_grad1 = np.zeros(np.shape(w1))
        epsilon_ary1 = np.zeros(np.shape(w1))
        for i in range(w1.shape[0]):
            for j in range(w1.shape[1]):
                epsilon_ary1[i, j] = epsilon
                a1, z2, a2, z3, a3 = self._feedforward(X,
                                                       w1 - epsilon_ary1, w2)
                cost1 = self._get_cost(y_enc, a3, w1-epsilon_ary1, w2)
                a1, z2, a2, z3, a3 = self._feedforward(X,
                                                       w1 + epsilon_ary1, w2)
                cost2 = self._get_cost(y_enc, a3, w1 + epsilon_ary1, w2)
                num_grad1[i, j] = (cost2 - cost1) / (2.0 * epsilon)
                epsilon_ary1[i, j] = 0

        num_grad2 = np.zeros(np.shape(w2))
        epsilon_ary2 = np.zeros(np.shape(w2))
        for i in range(w2.shape[0]):
            for j in range(w2.shape[1]):
                epsilon_ary2[i, j] = epsilon
                a1, z2, a2, z3, a3 = self._feedforward(X, w1,
                                                       w2 - epsilon_ary2)
                cost1 = self._get_cost(y_enc, a3, w1, w2 - epsilon_ary2)
                a1, z2, a2, z3, a3 = self._feedforward(X, w1,
                                                       w2 + epsilon_ary2)
                cost2 = self._get_cost(y_enc, a3, w1, w2 + epsilon_ary2)
                num_grad2[i, j] = (cost2 - cost1) / (2.0 * epsilon)
                epsilon_ary2[i, j] = 0

        num_grad = np.hstack((num_grad1.flatten(), num_grad2.flatten()))
        grad = np.hstack((grad1.flatten(), grad2.flatten()))
        norm1 = np.linalg.norm(num_grad - grad)
        norm2 = np.linalg.norm(num_grad)
        norm3 = np.linalg.norm(grad)
        relative_error = norm1 / (norm2 + norm3)
        return relative_error

    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.

        """
        if len(X.shape) != 2:
            raise AttributeError('X must be a [n_samples, n_features] array.¥n'
                                 'Use X[:,None] for 1-feature classification,'
                                 '¥nor X[[i]] for 1-sample classification')

        a1, z2, a2, z3, a3 = self._feedforward(X, self.w1, self.w2)
        y_pred = np.argmax(z3, axis=0)
        return y_pred

    def fit(self, X, y, print_progress=False):
        """ Learn weights from training data.

        Parameters
        -----------
        X : array, shape = [n_samples, n_features]
            Input layer with original features.
        y : array, shape = [n_samples]
            Target class labels.
        print_progress : bool (default: False)
            Prints progress as the number of epochs
            to stderr.

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

        """
        self.cost_ = []
        X_data, y_data = X.copy(), y.copy()
        y_enc = self._encode_labels(y, self.n_output)

        delta_w1_prev = np.zeros(self.w1.shape)
        delta_w2_prev = np.zeros(self.w2.shape)

        for i in range(self.epochs):

            # adaptive learning rate
            self.eta /= (1 + self.decrease_const*i)

            if print_progress:
                sys.stderr.write('¥rEpoch: %d/%d' % (i+1, self.epochs))
                sys.stderr.flush()

            if self.shuffle:
                idx = np.random.permutation(y_data.shape[0])
                X_data, y_enc = X_data[idx], y_enc[idx]

            mini = np.array_split(range(y_data.shape[0]), self.minibatches)
            for idx in mini:

                # feedforward
                a1, z2, a2, z3, a3 = self._feedforward(X[idx],
                                                       self.w1,
                                                       self.w2)
                cost = self._get_cost(y_enc=y_enc[:, idx],
```

```
                                output=a3,
                                w1=self.w1,
                                w2=self.w2)
            self.cost_.append(cost)

            # compute gradient via backpropagation
            grad1, grad2 = self._get_gradient(a1=a1, a2=a2,
                                              a3=a3, z2=z2,
                                              y_enc=y_enc[:, idx],
                                              w1=self.w1,
                                              w2=self.w2)

            # start gradient checking
            grad_diff = self._gradient_checking(X=X_data[idx],
                                                y_enc=y_enc[:, idx],
                                                w1=self.w1,
                                                w2=self.w2,
                                                epsilon=1e-5,
                                                grad1=grad1,
                                                grad2=grad2)


            if grad_diff <= 1e-7:
                print('Ok: %s' % grad_diff)
            elif grad_diff <= 1e-4:
                print('Warning: %s' % grad_diff)
            else:
                print('PROBLEM: %s' % grad_diff)

            # update weights; [alpha * delta_w_prev] for momentum learning
            delta_w1, delta_w2 = self.eta * grad1, self.eta * grad2
            self.w1 -= (delta_w1 + (self.alpha * delta_w1_prev))
            self.w2 -= (delta_w2 + (self.alpha * delta_w2_prev))
            delta_w1_prev, delta_w2_prev = delta_w1, delta_w2

        return self
```

In [30]:

```
nn_check = MLPGradientCheck(n_output=10,
                            n_features=X_train.shape[1],
                            n_hidden=10,
                            l2=0.0,
                            l1=0.0,
                            epochs=10,
                            eta=0.001,
                            alpha=0.0,
                            decrease_const=0.0,
                            minibatches=1,
                            shuffle=False,
                            random_state=1)
```