TP 5: Neural networks

Objectives

- **Coding 3-layer neural network**
- **Implementing backpropagation**

Entrée [1]:
```
# Import libraries

# math library
import numpy as np

# remove warning
import warnings
warnings.filterwarnings("ignore", category=RuntimeWarning)
warnings.filterwarnings("ignore", category=DeprecationWarning)

# computational time
import time

# import mat data
import scipy.io

# dynamic 3D rotations:
#%matplotlib notebook
# no 3D rotations but cleaner images:
%matplotlib inline
import matplotlib.pyplot as plt

# 3D visualization
import pylab
from mpl_toolkits.mplot3d import Axes3D
from matplotlib import pyplot

# high definition picture
from IPython.display import set_matplotlib_formats
set_matplotlib_formats('png2x','pdf')

# visualize 2D images
import scipy.ndimage

# import mat data
import scipy.io

# random number
import random

# colormap
import matplotlib.cm as cm

# for one-hot vector
from scipy.sparse import coo_matrix
```

1. Load training and test datasets

Entrée [2]:
```
X_train = np.load('data/nn_train_test_sets.npz')['X_train']
y_train = np.load('data/nn_train_test_sets.npz')['y_train']
X_test = np.load('data/nn_train_test_sets.npz')['X_test']
y_test = np.load('data/nn_train_test_sets.npz')['y_test']

print('Nb training data:',X_train.shape[1])
print('Nb test data:',X_test.shape[1])
print('Nb data features:',X_train.shape[0])

print(X_train.shape)
print(y_train.shape)
print(X_test.shape)
print(y_test.shape)
```

```
Nb training data: 1000
Nb test data: 4000
Nb data features: 400
(400, 1000)
(1000, 1)
(400, 4000)
(4000, 1)
```

2. Visualize the datasets

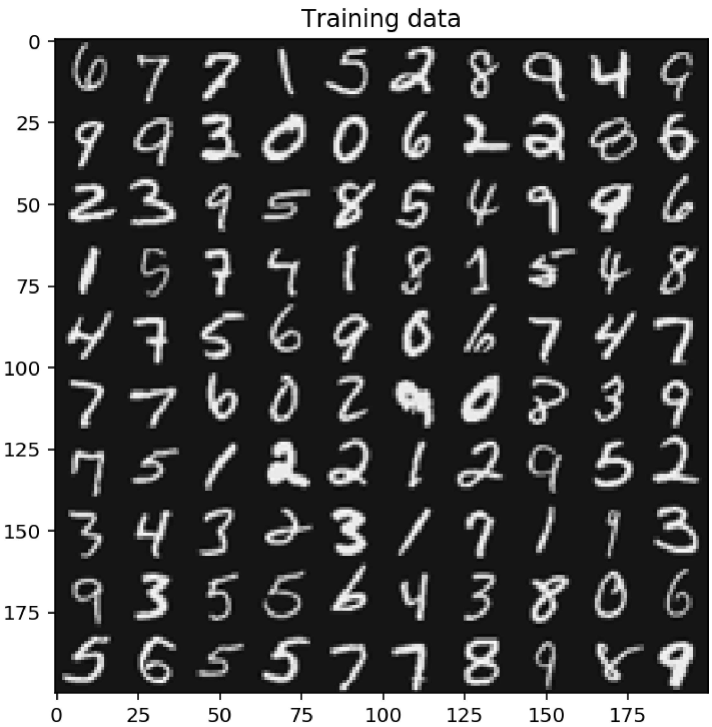
Hint: You may use function `display_data` .

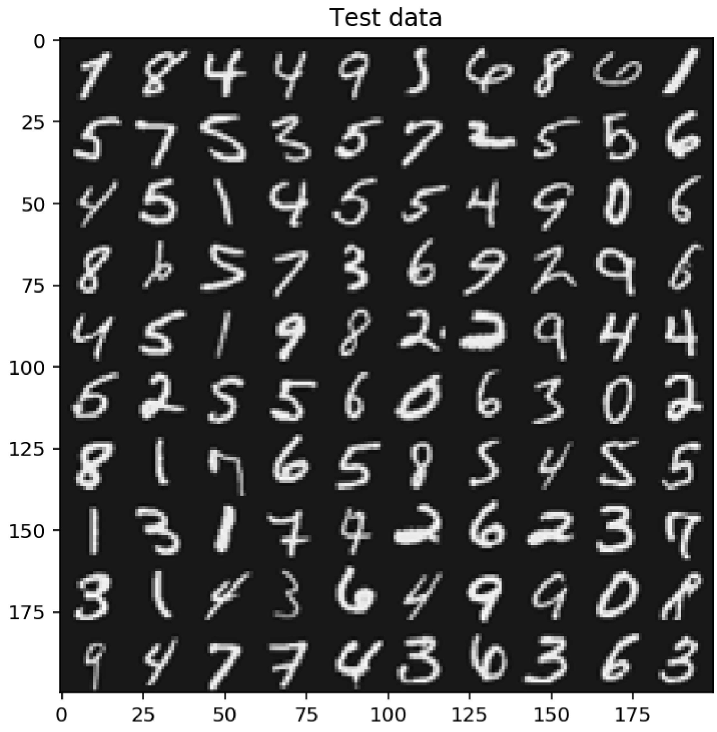
Entrée [3]:

```
def display_data(X,width,height,nrows,ncols,title):

    big_picture = np.zeros((height*nrows,width*ncols))
    indices_to_display = random.sample(range(X.shape[1]), nrows*ncols)
    irow, icol = 0, 0
    for idx in indices_to_display:
        if icol == ncols:
            irow += 1
            icol  = 0
        iimg = X[:,idx].reshape(width,height).T
        big_picture[irow*height:irow*height+iimg.shape[0],icol*width:icol*w
        icol += 1
    fig = plt.figure(figsize=(6,6))
    plt.title(title)
    plt.imshow(big_picture,cmap = cm.Greys_r)


#YOUR CODE HERE
display_data(X_train,20,20,10,10,'Training data')
display_data(X_test,20,20,10,10,'Test data')
```





3. Z-score the datasets

Entrée [4]:

```
#YOUR CODE HERE
X_train -= X_train.mean(axis=0)
X_train /= np.std(X_train,axis=0)

X_test -= X_test.mean(axis=0)
X_test /= np.std(X_test,axis=0)
```

4. Implement a 3-layer neural network classifier.

The input layer has $n_1 = d = 400$ neurons. The hidden layer has $n_2 = 25$ neurons. The output layer has $n_3 = K = 10$ neurons.

Entrée [5]:

```
K = 10 # number of classes
n = X_train.shape[1] # number of training data

n1 = 400
n2 = 25
n3 = K
```

4.1 Function definitions

Entrée [6]:
```
# one-hot transform function
def convert_to_one_hot(X,max_val=None):
    N = X.size
    data = np.ones(N,dtype=int)
    sparse_out = coo_matrix((data,(np.arange(N),X.ravel())), shape=(N,max_v
    return np.array(sparse_out.todense().T)

#Example:
a = np.array([3])
print(a)
print(convert_to_one_hot(a,10))


# sigmoid function
def sigmoid(z):
    sigmoid_f = 1 / (1 + np.exp(-z))
    return sigmoid_f


# derivate of the sigmoid function
def sigmoid_derivate(z):
    sigm = sigmoid(z)
    return sigm* (1-sigm)


# accuracy function
def compute_acc(y,ygt):
    diff = (y == ygt).astype('int')
    accuracy = 100* sum(diff)/ y.shape[0]
    return accuracy
```

```
[3]
[[0]
 [0]
 [0]
 [1]
 [0]
 [0]
 [0]
 [0]
 [0]
 [0]]
```

4.2 Convert the training label vector `y_train`, with values in $1, 2, \ldots, K$, to one-hot vector.

Hint: You may use function `convert_to_one_hot(y,K)` with `y` having values in $0, 1, \ldots, K-1$.

Entrée [7]:
```
#YOUR CODE HERE
Yhat = convert_to_one_hot(y_train-1,max_val=K)
print(Yhat.shape)
```

```
(10, 1000)
```

4.3 Initialize the weight matrices W^1 and W^2 with the formula

$$W^l = U\Big[-\frac{2}{\sqrt{n_l}}, \frac{2}{\sqrt{n_l}}\Big],$$

with U being the uniform distribution.

Hint: You may use function `np.random.uniform`.

Entrée [8]:

```
#YOUR CODE HERE
a = 2/ np.sqrt(n1)
W1 = np.random.uniform(-a,a,[n2,n1+1])
a = 2/ np.sqrt(n2)
W2 = np.random.uniform(-a,a,[n3,n2+1])

print(W1.shape)
print(W2.shape)
```

```
(25, 401)
(10, 26)
```

4.4 Implement the backpropagation algorithm

Backpropagation algorithm

Step 1. Forward pass (compute all activations)

$$\begin{aligned} &\text{For } l = 1, 2, \ldots, L \\ &\qquad y^{l+1} = \sigma\left(W^l \begin{bmatrix} 1 \\ y^l \end{bmatrix}\right) \end{aligned}$$

Step 2. Backward pass (compute all gradients of weight parameters)

$$\delta^{l=L} = y^L - \hat{y}$$

$$\text{For } l = L-1, L-2, \ldots, 1$$

$$\nabla_{W^l} = \frac{1}{n}\delta^{l+1}\begin{bmatrix} 1 \\ y^l \end{bmatrix}^T$$

$$W^l \leftarrow W^l - \tau \nabla_{W^l}$$

$$\delta^l = (\bar{W}^l)^T \delta^{l+1} \,.\, \sigma'\left(y^l\right)$$

with

$$W^l = \begin{bmatrix} | & \\ W_0^l & \bar{W}^l \\ | & \end{bmatrix}$$

The learning rate is $\tau = 0.2$ and the number of iterations is 5000. Do not use any regularization at this moment $\lambda = 0$.

Note the accuracy of the train set and the test set for $n_2 = 25$ and $\lambda = 0$.

Entrée [9]:

```
tau = 0.2 # learning rate
lamb = 0  # regularization

# iterate
for iter in range(5000):

    # forward pass
    #YOUR CODE HERE
    Y1 = X_train
    Y1bias = np.insert(Y1,0,1,axis=0)
    Y2 = sigmoid(W1.dot(Y1bias))
    Y2bias = np.insert(Y2,0,1,axis=0)
    Y3 = sigmoid(W2.dot(Y2bias))

    # backward pass
    #YOUR CODE HERE
    Delta3 = Y3 - Yhat
    Grad2 = 1/n* Delta3.dot(Y2bias.T)
    Grad2 += 2* lamb* W2
    W2 = W2 - tau* Grad2
    W2bar = W2[:,1:n2+1]
    Delta2 = ( W2bar.T.dot(Delta3) ) * sigmoid_derivate(Y2)
    Grad1 = 1/n* Delta2.dot(Y1bias.T)
    Grad1 += 2* lamb* W1
    W1 = W1 - tau* Grad1

    # print intermediate result
    if not iter%500:

        # loss
        loss = -1/n* ( np.sum(Yhat* np.log(Y3+1e-10)) + \
                      np.sum((1-Yhat)* np.log((1-Y3)+1e-10)) ) + \
                lamb* ( np.sum(W1**2) + np.sum(W2**2) )

        # train accuracy
        Y3_classes = np.argmax(Y3,axis=0)
        Ygt = np.argmax(Yhat,axis=0)
        acc = compute_acc(Y3_classes,Ygt)

        # test accuracy (with forward pass on the test set)
        Y1_test = X_test
        Y1bias_test = np.insert(Y1_test,0,1,axis=0)
        Y2_test = sigmoid(W1.dot(Y1bias_test))
        Y2bias_test = np.insert(Y2_test,0,1,axis=0)
        Y3_test = sigmoid(W2.dot(Y2bias_test))
        Y3_classes_test = np.argmax(Y3_test,axis=0)
        Ygt_test = (y_test-1).squeeze()
        acc_test = compute_acc(Y3_classes_test,Ygt_test)

        # print
        print('iter:',iter,'loss:',loss,'train acc:',acc,'test acc:',acc_te


print('iter:',iter+1,'loss:',loss,'train acc:',acc,'test acc:',acc_test)
```

```
iter: 0 loss: 7.298046491651594 train acc: 9.7 test acc: 10.375
iter: 500 loss: 0.9617857257472444 train acc: 86.6 test acc: 82.775
iter: 1000 loss: 0.7915913606549568 train acc: 88.2 test acc: 83.075
iter: 1500 loss: 0.6768935222546129 train acc: 89.5 test acc: 83.025
iter: 2000 loss: 0.5976792596347217 train acc: 91.9 test acc: 82.9
iter: 2500 loss: 0.5379486965631015 train acc: 93.3 test acc: 82.925
iter: 3000 loss: 0.49107856610114486 train acc: 94.4 test acc: 83.225
iter: 3500 loss: 0.49080595502590496 train acc: 93.4 test acc: 83.5
iter: 4000 loss: 0.4774460009445754 train acc: 93.7 test acc: 83.125
iter: 4500 loss: 0.45070168537842387 train acc: 94.5 test acc: 83.0
iter: 5000 loss: 0.45070168537842387 train acc: 94.5 test acc: 83.0
```

5. Increase the learning capacity of the network by taking $n_2 = 100$.

Note the accuracy of the train set and the test set for $n_2 = 100$ and $\lambda = 0$.

Entrée [10]:

```
#YOUR CODE HERE
tau = 0.2 # learning rate
lamb = 0  # regularization

n2 = 100

a = 2/ np.sqrt(n1)
W1 = np.random.uniform(-a,a,[n2,n1+1])
a = 2/ np.sqrt(n2)
W2 = np.random.uniform(-a,a,[n3,n2+1])

print(W1.shape)
print(W2.shape)

# iterate
for iter in range(5000):

    # forward pass
    Y1 = X_train
    Y1bias = np.insert(Y1,0,1,axis=0)
    Y2 = sigmoid(W1.dot(Y1bias))
    Y2bias = np.insert(Y2,0,1,axis=0)
    Y3 = sigmoid(W2.dot(Y2bias))

    # backward pass
    Delta3 = Y3 - Yhat
    Grad2 = 1/n* Delta3.dot(Y2bias.T)
    Grad2 += 2* lamb* W2
    W2 = W2 - tau* Grad2
    W2bar = W2[:,1:n2+1]
    Delta2 = ( W2bar.T.dot(Delta3) ) * sigmoid_derivate(Y2)
    Grad1 = 1/n* Delta2.dot(Y1bias.T)
    Grad1 += 2* lamb* W1
    W1 = W1 - tau* Grad1

    # print intermediate result
    if not iter%500:

        # loss
        loss = -1/n* ( np.sum(Yhat* np.log(Y3+1e-10)) + \
                      np.sum((1-Yhat)* np.log((1-Y3)+1e-10)) ) + \
                lamb* ( np.sum(W1**2) + np.sum(W2**2) )

        # train accuracy
        Y3_classes = np.argmax(Y3,axis=0)
        Ygt = np.argmax(Yhat,axis=0)
        acc = compute_acc(Y3_classes,Ygt)

        # test accuracy (with forward pass on the test set)
        Y1_test = X_test
        Y1bias_test = np.insert(Y1_test,0,1,axis=0)
        Y2_test = sigmoid(W1.dot(Y1bias_test))
        Y2bias_test = np.insert(Y2_test,0,1,axis=0)
        Y3_test = sigmoid(W2.dot(Y2bias_test))
        Y3_classes_test = np.argmax(Y3_test,axis=0)
        Ygt_test = (y_test-1).squeeze()
        acc_test = compute_acc(Y3_classes_test,Ygt_test)

        # print
        print('iter:',iter,'loss:',loss,'train acc:',acc,'test acc:',acc_te
```

```
print('iter:',iter+1,'loss:',loss,'train acc:',acc,'test acc:',acc_test)

W1_no_regularization = W1 # for visualization
```

```
(100, 401)
(10, 101)
iter: 0 loss: 7.485882418952906 train acc: 11.4 test acc: 11.025
iter: 500 loss: 0.4652823081594802 train acc: 95.4 test acc: 88.3
iter: 1000 loss: 0.33083684903544036 train acc: 97.2 test acc: 88.175
iter: 1500 loss: 0.2768301930409436 train acc: 97.9 test acc: 88.05
iter: 2000 loss: 0.25041954988603193 train acc: 98.4 test acc: 87.45
iter: 2500 loss: 0.23881636534063938 train acc: 98.5 test acc: 86.85
iter: 3000 loss: 0.23261781870481094 train acc: 98.6 test acc: 86.625
iter: 3500 loss: 0.22557600079701925 train acc: 98.6 test acc: 86.675
iter: 4000 loss: 0.2159826439134632 train acc: 98.3 test acc: 86.825
iter: 4500 loss: 0.20045271104588352 train acc: 98.9 test acc: 86.725
iter: 5000 loss: 0.20045271104588352 train acc: 98.9 test acc: 86.725
```

6. Regularize the network with $\lambda = 0.005$

Note the accuracy of the train set and the test set.

Entrée [11]:
```
#YOUR CODE HERE
tau = 0.2 # learning rate
lamb = 0.005  # regularization

n2 = 100

a = 2/ np.sqrt(n1)
W1 = np.random.uniform(-a,a,[n2,n1+1])
a = 2/ np.sqrt(n2)
W2 = np.random.uniform(-a,a,[n3,n2+1])

print(W1.shape)
print(W2.shape)

# iterate
for iter in range(5000):

    # forward pass
    Y1 = X_train
    Y1bias = np.insert(Y1,0,1,axis=0)
    Y2 = sigmoid(W1.dot(Y1bias))
    Y2bias = np.insert(Y2,0,1,axis=0)
    Y3 = sigmoid(W2.dot(Y2bias))

    # backward pass
    Delta3 = Y3 - Yhat
    Grad2 = 1/n* Delta3.dot(Y2bias.T)
    Grad2 += 2* lamb* W2
    W2 = W2 - tau* Grad2
    W2bar = W2[:,1:n2+1]
    Delta2 = ( W2bar.T.dot(Delta3) ) * sigmoid_derivate(Y2)
    Grad1 = 1/n* Delta2.dot(Y1bias.T)
    Grad1 += 2* lamb* W1
    W1 = W1 - tau* Grad1

    # print intermediate result
    if not iter%500:

        # loss
        loss = -1/n* ( np.sum(Yhat* np.log(Y3+1e-10)) + \
                       np.sum((1-Yhat)* np.log((1-Y3)+1e-10)) ) + \
                lamb* ( np.sum(W1**2) + np.sum(W2**2) )

        # train accuracy
        Y3_classes = np.argmax(Y3,axis=0)
        Ygt = np.argmax(Yhat,axis=0)
        acc = compute_acc(Y3_classes,Ygt)

        # test accuracy (with forward pass on the test set)
        Y1_test = X_test
        Y1bias_test = np.insert(Y1_test,0,1,axis=0)
        Y2_test = sigmoid(W1.dot(Y1bias_test))
        Y2bias_test = np.insert(Y2_test,0,1,axis=0)
        Y3_test = sigmoid(W2.dot(Y2bias_test))
        Y3_classes_test = np.argmax(Y3_test,axis=0)
        Ygt_test = (y_test-1).squeeze()
        acc_test = compute_acc(Y3_classes_test,Ygt_test)

        # print
        print('iter:',iter,'loss:',loss,'train acc:',acc,'test acc:',acc_te
```

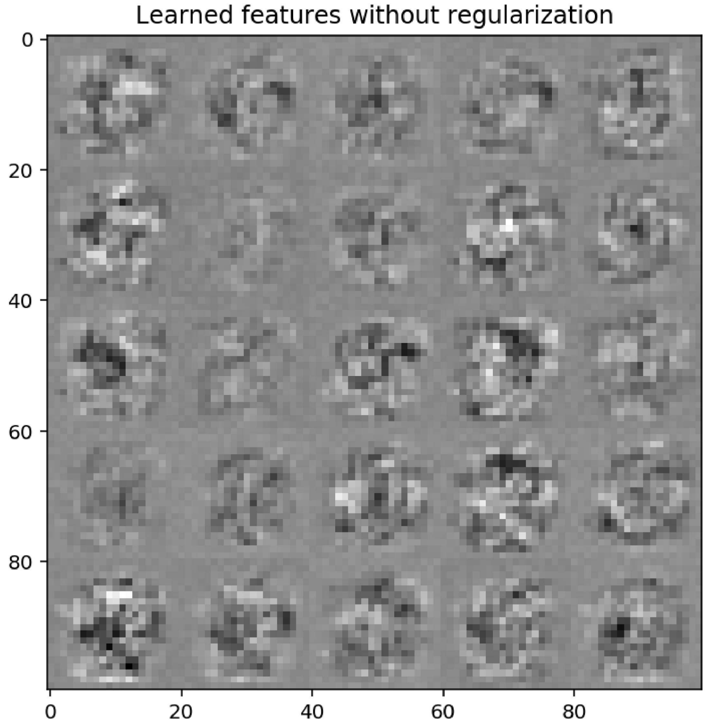
```
print('iter:',iter+1,'loss:',loss,'train acc:',acc,'test acc:',acc_test)
```

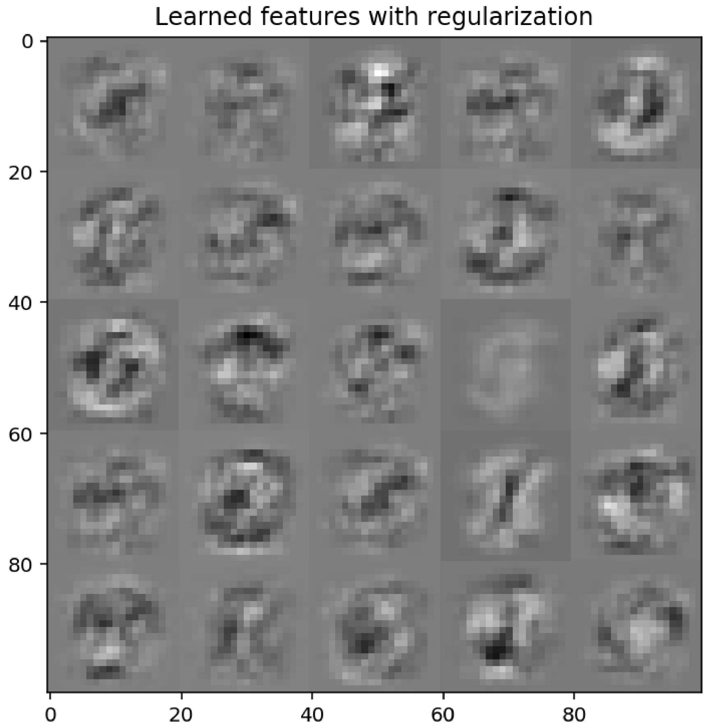
```
(100, 401)
(10, 101)
iter: 0 loss: 9.050493744351638 train acc: 10.0 test acc: 9.825
iter: 500 loss: 1.6193461153892361 train acc: 94.1 test acc: 88.25
iter: 1000 loss: 1.5677028405314224 train acc: 95.4 test acc: 88.575
iter: 1500 loss: 1.5586180950418038 train acc: 95.8 test acc: 88.6
iter: 2000 loss: 1.5564315019944528 train acc: 95.8 test acc: 88.8
iter: 2500 loss: 1.5467862913658994 train acc: 95.9 test acc: 88.85
iter: 3000 loss: 1.5486380630901047 train acc: 95.6 test acc: 88.625
iter: 3500 loss: 1.5547137529007462 train acc: 95.7 test acc: 88.8
iter: 4000 loss: 1.5636580363152672 train acc: 96.0 test acc: 88.625
iter: 4500 loss: 1.5716333351535627 train acc: 95.8 test acc: 88.475
iter: 5000 loss: 1.5716333351535627 train acc: 95.8 test acc: 88.475
```

7. Visualize the learned features [Bonus]

Entrée [12]:
```
W1bar = W1_no_regularization[:,1:].T
display_data(W1bar,20,20,5,5,'Learned features without regularization')

W1bar = W1[:,1:].T
display_data(W1bar,20,20,5,5,'Learned features with regularization')
```





Entrée [ ]:
```

```