CSE 546 Homework #3

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May 29, 2020

Conceptual Questions

A.1

a. *[2 points]* False. Zero reconstruction error if k = rank(X) = d, so all error is due to missing components.

b. *[2 points]* False. The maximum margin hyperplane is often a reasonable choice but it is by no means optimal in all cases.

c. *[2 points]* True. An observation could be included several times in the sample or not at all

d. *[2 points]* False. The eigenvectors of $X^T X$ make up the columns of V , the eigenvectors of XX^T make up the columns of U.

e. *[2 points]* False. PCA sets all dimensions with small singular values to 0 at one time, while the remaining dimensions have a coefficient of 1. The essence of Lasso regression is a soft PCA regression. They can all improve the effect of linear regression by eliminating the multicollinearity of the data. They don't need to be used at the same time.

f. *[2 points]* False. If we know just little knowledge about the data, the k is hard to explainable.

g. *[2 points]* It would also be reasonable to try decreasing σ. From the defination of RBF kernel, σ is the denominator, decreasing σ will make the kernerl more sensitive.

Kernels and the Bootstrap

A.2 *[5 points]* The Taylor Series for e^x

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots$$

$$
\begin{aligned}
(x) \cdot (x') &= e^{-\frac{(x-x')^2}{2}} \\
&= e^{-\frac{1}{2}(x^2 - 2xx' + x'^2)} \\
&= e^{-\frac{1}{2}(x^2 + x'^2)}\left(1 + \frac{xx'}{1!} + \frac{(xx')^2}{2!} + \frac{(xx')^3}{3!} + \dots\right) \\
&= e^{-\frac{1}{2}(x^2 + x'^2)}\left(1 \cdot 1 + \frac{1}{\sqrt{1!}}x \cdot \frac{1}{\sqrt{1!}}x' + \frac{1}{\sqrt{2!}}x^2 \cdot \frac{1}{\sqrt{2!}}x'^2 + \frac{1}{\sqrt{3!}}x^3 \cdot \frac{1}{\sqrt{3!}}x'^3 + \dots\right) \\
&= e^{-\frac{x^2}{2}} \cdot e^{-\frac{x'^2}{2}} + \frac{1}{\sqrt{1!}}e^{-\frac{x^2}{2}}x \cdot \frac{1}{\sqrt{1!}}e^{-\frac{x'^2}{2}}x' + \frac{1}{\sqrt{2!}}e^{-\frac{x^2}{2}}x^2 \cdot \frac{1}{\sqrt{2!}}e^{-\frac{x'^2}{2}}x'^2 + \frac{1}{\sqrt{3!}}e^{-\frac{x^2}{2}}x^3 \cdot \frac{1}{\sqrt{3!}}e^{-\frac{x'^2}{2}}x'^3 + \dots
\end{aligned}
$$

Thus, $K(x, x') = e^{-\frac{(x-x')^2}{2}}$ is a kernel function for this feature map.

A.3

[1]:
```
"""
Created on Sun May 17 00:09:39 2020
HW3 A3 Kernels
@author: Leah
"""

import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
from sklearn import model_selection
loo = model_selection.LeaveOneOut()
```

[2]:
```
def create_data(n):
    ##x_i
    X = np.arange(1,n+1)/float(n)
    ##f(x_i)
    #fx = 4* np.sin(np.pi * X) * np.cos(6 * np.pi * X**2)
    ##y_i
    y = 4* np.sin(np.pi * X) * np.cos(6 * np.pi * X**2) + np.random.randn(n)
    return X,y
```

[3]:
```
def K_poly(X, d):
    K = np.zeros((X.shape[0],X.shape[0]))

    for i in np.arange(X.shape[0]):
        for j in np.arange(X.shape[0]):
            terms_to_eval = (1+np.dot(X[i].T,X[j]))
            K[i][j] = terms_to_eval**d
    return K

#    n = X.shape[0]
#    K = np.zeros((n,n))
#
```

```
#    for i in np.arange(n):
#        for j in np.arange(n):
#            K[i][j]  = (1 + np.dot(X[i].T,X[j]))**d
#    return K

def K_RBF(X, gamma):

    n = X.shape[0]
    K = np.zeros((n,n))

    for i in np.arange(n):
        for j in np.arange(n):
            K[i][j]  = np.exp(-gamma*(np.linalg.norm(X[i]-X[j])**2))
    return K

def alpha_hat_compute(K,lambda_val,y):
    #alpha = (k+lamda*I)^(-1)*y
    lhs = K + lambda_val*np.identity(np.shape(K)[0])
    alpha_hat = np.linalg.solve(lhs,y)

    return alpha_hat

def alpha_hat(K, lamda, y):
    obj = K + lamda*np.identity(np.shape(K)[0])
    alpha_hat = np.linalg.solve(obj, y)

    return alpha_hat


def to_kernel_poly(d, x1, x2):
    kernel_poly = []
    for i in np.arange(x2.shape[0]):
        eval_iter = float((1+np.dot(x1,x2[i]))**d)
        kernel_poly.append(eval_iter)

    return kernel_poly

def to_kernel_RBF(gamma, x1, x2):
    kernel_RBF = []
    for i in np.arange(x2.shape[0]):
        eval_iter = np.exp(-gamma*(np.linalg.norm(x1-x2[i])**2))
        kernel_RBF.append(eval_iter)

    return kernel_RBF

def cost_function(pre,real):
```

```
    cost = np.linalg.norm(pre-real)
    cost_total = np.sqrt(np.sum(cost))
    return cost_total

def LOO_poly(X, y, lamda_list,d_list):

    cost_history = np.zeros((lamda_list.shape[0],d_list.shape[0]))
    lambda_iter = 0

    for lamda in lamda_list:
        d_iter = 0

        for d in d_list:
            #print('lambda = {},d={}'.format(lamda,d))
            score_history = []
            for train_index, test_index in loo.split(X):
                X_train, X_test = X[train_index], X[test_index]
                y_train, y_test = y[train_index], y[test_index]
                K = K_poly(X_train, d)
                alpha__hat = alpha_hat_compute(K,lamda,y_train)
                eval_kernel = to_kernel_poly(d, X_test,X_train)
                f_hat = np.array([np.sum(alpha__hat.flatten()*eval_kernel)])␣
 ↪#f_hat
                cost = cost_function(f_hat,y_test)
                score_history.append(cost)

            cost_history[lambda_iter][d_iter] = np.mean(score_history)

            d_iter += 1

        lambda_iter += 1

    return cost_history

def LOO_RBF(X, y, lamda_list,gamma_list):

    cost_history = np.zeros((lamda_list.shape[0],gamma_list.shape[0]))
    lambda_iter = 0

    for lamda in lamda_list:
        gamma_iter = 0

        for gamma in gamma_list:
            #print('lambda = {},d={}'.format(lamda,d))
            score_history = []
            for train_index, test_index in loo.split(X):
                X_train, X_test = X[train_index], X[test_index]
```

```
                y_train, y_test = y[train_index], y[test_index]
                K = K_RBF(X_train, gamma)
                alpha__hat = alpha_hat_compute(K,lamda,y_train)
                eval_kernel = to_kernel_RBF(gamma, X_test,X_train)
                f_hat = np.array([np.sum(alpha__hat.flatten()*eval_kernel)])␣
↪#f_hat
                cost = cost_function(f_hat,y_test)
                score_history.append(cost)

            cost_history[lambda_iter][gamma_iter] = np.mean(score_history)

            gamma_iter += 1

        lambda_iter += 1

    return cost_history
```

[4]:
```
def plot_poly(X,y,xx,f_x,lamda,d):
    #plt.figure(dpi=600)
    K = K_poly(X, d)
    alpha__hat = alpha_hat_compute(K,lamda,y)
    f_hat = np.zeros((xx.shape))
    for i in np.arange(xx.shape[0]):
        eval_kernel = to_kernel_poly(d,float(xx[i]),X)
        y_pre = np.sum(alpha__hat.flatten()*np.array(eval_kernel))
        f_hat[i] = y_pre

    plt.figure()
    plt.plot(X,y,'o',label='original data')
    plt.plot(xx,f_x,label='true f(x)')
    plt.plot(xx,f_hat,label='$f^hat(x)$')
    plt.xlabel('x')
    plt.ylabel('f(x) or y')
    plt.title('Polynomial, lambda = {}, d = {}'.format(lamda,d))
    plt.legend()
    plt.ylim([-5,5])


def plot_RBF(X,y,xx,f_x,lamda,gamma):
    K = K_RBF(X, gamma)
    alpha__hat = alpha_hat_compute(K,lamda,y)
    f_hat = np.zeros((xx.shape))
    for i in np.arange(xx.shape[0]):
        eval_kernel = to_kernel_RBF(gamma,float(xx[i]),X)
        y_pre = np.sum(alpha__hat.flatten()*np.array(eval_kernel))
        f_hat[i] = y_pre
```

```
    plt.figure()
    plt.plot(X,y,'o',label='original data')
    plt.plot(xx,f_x,label='true f(x)')
    plt.plot(xx,f_hat,label='$f^hat(x)$')
    plt.xlabel('x')
    plt.ylabel('f(x) or y')
    plt.title('RBF, lambda = {}, gamma = {:.2f}'.format(lamda,gamma))
    plt.legend()
    plt.ylim([-5,5])
```

[5]:
```
def K_fold_poly(X, y, lamda_list,d_list,K):

    n = len(X)
    indices = np.arange(n).astype(int)
    k_folds = np.random.permutation(indices).reshape(K,int(n/K)) # Each row is a␣
 ↪k-fold.

    cost_history = np.zeros((lamda_list.shape[0],d_list.shape[0]))
    lambda_iter = 0

    for lamda in lamda_list:
        d_iter = 0

        for d in d_list:
            #print('lambda = {},d={}'.format(lamda,d))
            score_history = []
            for i, k_validation in enumerate(k_folds):
                train_index = list(set(indices ).difference(set(k_validation)))
                X_train, X_test = X[train_index], X[k_validation]
                y_train, y_test = y[train_index], y[k_validation]
                K = K_poly(X_train, d)
                alpha__hat = alpha_hat_compute(K,lamda,y_train)

                f_hat = np.zeros((X_test.shape))
                for i in np.arange(X_test.shape[0]):
                    eval_kernel = to_kernel_poly(d,float(X_test[i]),X_train)
                    y_pre = np.sum(alpha__hat.flatten()*np.array(eval_kernel))
                    f_hat[i] = y_pre

                cost = cost_function(f_hat,y_test)
                score_history.append(cost)

            cost_history[lambda_iter][d_iter] = np.mean(score_history)

            d_iter += 1

        lambda_iter += 1
```

```
    return cost_history

def K_fold_RBF(X, y, lamda_list,gamma_list,K):
    n = len(X)
    indices = np.arange(n).astype(int)
    k_folds = np.random.permutation(indices).reshape(K,int(n/K)) # Each row is a k-fold.
    cost_history = np.zeros((lamda_list.shape[0],gamma_list.shape[0]))
    lambda_iter = 0

    for lamda in lamda_list:
        gamma_iter = 0

        for gamma in gamma_list:
            #print('lambda = {},d={}'.format(lamda,d))
            score_history = []
            for i, k_validation in enumerate(k_folds):
                train_index = list(set(indices ).difference(set(k_validation)))
                X_train, X_test = X[train_index], X[k_validation]
                y_train, y_test = y[train_index], y[k_validation]
                K = K_RBF(X_train, gamma)
                alpha__hat = alpha_hat_compute(K,lamda,y_train)
                f_hat = np.zeros((X_test.shape))
                for i in np.arange(X_test.shape[0]):
                    eval_kernel = to_kernel_RBF(gamma,float(X_test[i]),X_train)
                    y_pre = np.sum(alpha__hat.flatten()*np.array(eval_kernel))
                    f_hat[i] = y_pre

                cost = cost_function(f_hat,y_test)
                score_history.append(cost)

            cost_history[lambda_iter][gamma_iter] = np.mean(score_history)

            gamma_iter += 1

        lambda_iter += 1

    return cost_history
```

[6]:
```
def bootstrap_poly(d,lamda,X,y,xx,B,n):
    '''
    draw B datasets each of size n with replacement from our training data
    '''
    f_hat_table = np.zeros((B, xx.shape[0]))
    inds = np.arange(n)
    for j in np.arange(B):
```

```python
        inds_choice = np.random.choice(inds,n) #
        x_samp = X[inds_choice]
        y_samp = y[inds_choice]

        f_hat = np.zeros((xx.shape))

        K = K_poly(x_samp,d)
        alpha_hat = alpha_hat_compute(K,lamda,y_samp)

        for i in np.arange(xx.shape[0]):
            eval_kernel = to_kernel_poly(d,float(xx[i]),x_samp)
            y_pre = np.sum(alpha_hat.flatten()*np.array(eval_kernel))
            #
            f_hat[i] = y_pre

        f_hat_table[j,:] = f_hat
    return f_hat_table


def plot_bootstrap_poly(X,y,xx,f_x,lamda,d,lower,upper):
    K = K_poly(X, d)
    alpha__hat = alpha_hat_compute(K,lamda,y)
    f_hat = np.zeros((xx.shape))
    for i in np.arange(xx.shape[0]):
        eval_kernel = to_kernel_poly(d,float(xx[i]),X)
        y_pre = np.sum(alpha__hat.flatten()*np.array(eval_kernel))
        f_hat[i] = y_pre

    plt.figure()
    plt.plot(X,y,'o',label='original data')
    plt.plot(xx,f_x,label='true f(x)')
    plt.plot(xx,f_hat,label='$f^hat(x)$')
    plt.fill_between(xx,lower,upper,alpha=0.3,label='95% confidence interval')
    plt.xlabel('x')
    plt.ylabel('f(x) or y')
    plt.title('Polynomial with 95% CI, lambda = {}, d = {}'.format(lamda,d))
    plt.legend()
    plt.ylim([-5,5])

def bootstrap_RBF(lamda,gamma,X,y,xx,B,n):
    '''
    draw B datasets each of size n with replacement from our training data
    '''
    f_hat_table = np.zeros((B, xx.shape[0]))
    inds = np.arange(n)
    for j in np.arange(B):
        inds_choice = np.random.choice(inds,n)
```

```
        x_samp = X[inds_choice]
        y_samp = y[inds_choice]

        f_hat = np.zeros((xx.shape))

        K = K_RBF(x_samp,gamma)
        alpha_hat = alpha_hat_compute(K,lamda,y_samp)

        for i in np.arange(xx.shape[0]):
            eval_kernel = to_kernel_RBF(gamma,float(xx[i]),x_samp)
            y_pre = np.sum(alpha_hat.flatten()*np.array(eval_kernel))
            #
            f_hat[i] = y_pre

        f_hat_table[j,:] = f_hat
    return f_hat_table


def plot_bootstrap_RBF(X,y,xx,f_x,lamda,gamma,lower,upper):
    K = K_RBF(X, gamma)
    alpha__hat = alpha_hat_compute(K,lamda,y)
    f_hat = np.zeros((xx.shape))
    for i in np.arange(xx.shape[0]):
        eval_kernel = to_kernel_RBF(gamma,float(xx[i]),X)
        y_pre = np.sum(alpha__hat.flatten()*np.array(eval_kernel))
        f_hat[i] = y_pre

    plt.figure()
    plt.plot(X,y,'o',label='original data')
    plt.plot(xx,f_x,label='true f(x)')
    plt.plot(xx,f_hat,label='$f^hat(x)$')
    plt.fill_between(xx,lower,upper,alpha=0.3,label='95% confidence interval')
    plt.xlabel('x')
    plt.ylabel('f(x) or y')
    plt.title('RBF with 95% CI, lambda = {}, gamma = {:.2f}'.format(lamda,gamma))
    plt.legend()
    plt.ylim([-5,5])
```

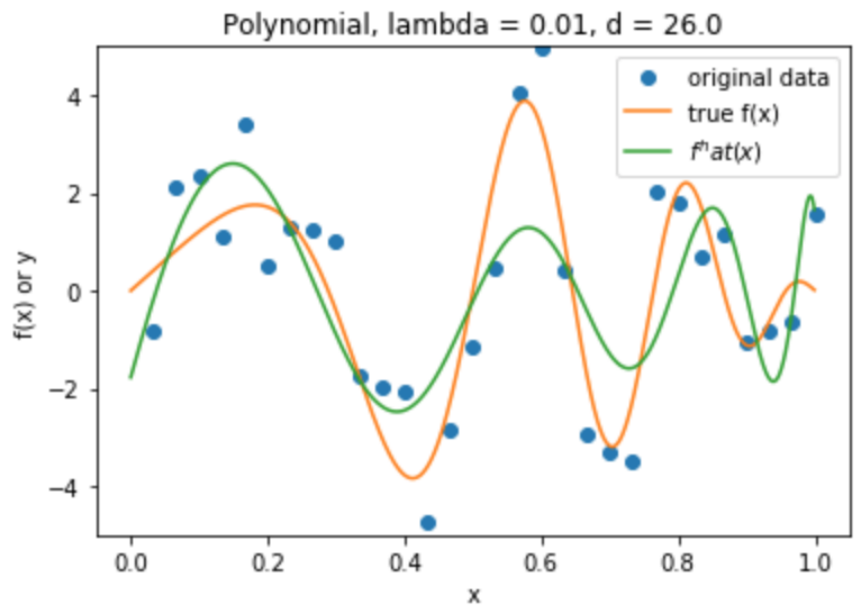
[7]:
```
def Poly_RBF(d,lamda_poly,lambda_RBF,gamma,X,y,xx,B,n):
    table = np.zeros((B, 1))
    inds = np.arange(n)
    for j in np.arange(B):
        inds_choice = np.random.choice(inds,n) #
        x_samp = X[inds_choice]
        y_samp = y[inds_choice]

        f_hat_poly = np.zeros((xx.shape))
```

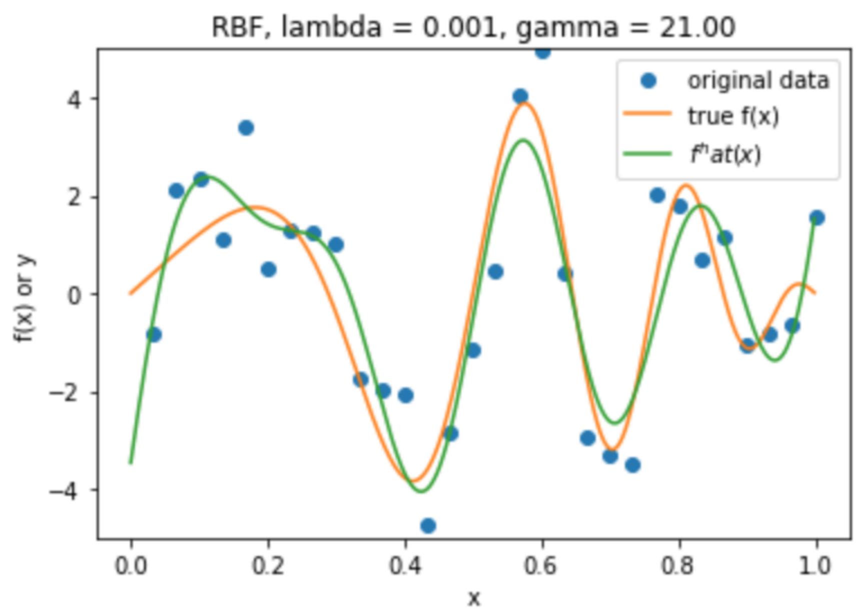
```
        f_hat_RBF = np.zeros((xx.shape))

        K__poly = K_poly(x_samp,d)
        alpha_hat_poly = alpha_hat_compute(K__poly,lamda_poly,y_samp)

        K__RBF = K_RBF(x_samp,gamma)
        alpha_hat_RBF = alpha_hat_compute(K__RBF,lambda_RBF,y_samp)

        for i in np.arange(xx.shape[0]):
            eval_kernel_poly = to_kernel_poly(d,float(xx[i]),x_samp)
            eval_kernel_RBF = to_kernel_RBF(gamma,float(xx[i]),x_samp)
            f_hat_poly[i] = np.sum(alpha_hat_poly.flatten()*np.
 ↪array(eval_kernel_poly))
            f_hat_RBF[i] = np.sum(alpha_hat_RBF.flatten()*np.
 ↪array(eval_kernel_RBF))

        diff = np.mean((y_samp - f_hat_poly )**2 -( y_samp-f_hat_RBF)**2)

        table[j,:] = diff
        #print(j)
    return table
```

[37]:
```
# ============================================================================
# part a
# ============================================================================
X,y = create_data(30)

#polynomial kernel
lamda_list = np.array([1e-5,1e-4,1e-3,1e-2,1e-1,1,10,100])
d_list = np.arange(1.0,50.0,5)

cost_history_poly = LOO_poly(X, y, lamda_list,d_list)
best_lambda_poly = lamda_list[int(np.floor(cost_history_poly.argmin() /
 ↪len(d_list)))]
best_d = d_list[int(np.ceil(cost_history_poly.argmin() /len(lamda_list)))]
print("For polynomial kernel, lambda = ", best_lambda_poly, " d = ",best_d)

#RBF kernel
gamma_list  = np.arange(1.0, 50.0, 5)

cost_history_RBF = LOO_RBF(X, y, lamda_list, gamma_list)
best_lambda_RBF = lamda_list[int(np.floor(cost_history_RBF.argmin() /
 ↪len(gamma_list)))]
best_gamma = gamma_list[int(np.ceil(cost_history_RBF.argmin() /len(lamda_list)))]
print("For RBF kernel, lambda = ", best_lambda_RBF, " gamma = ",best_gamma)
```

```
For polynomial kernel, lambda =  0.01  d =  26.0
For RBF kernel, lambda =  0.001  gamma =  21.0
```

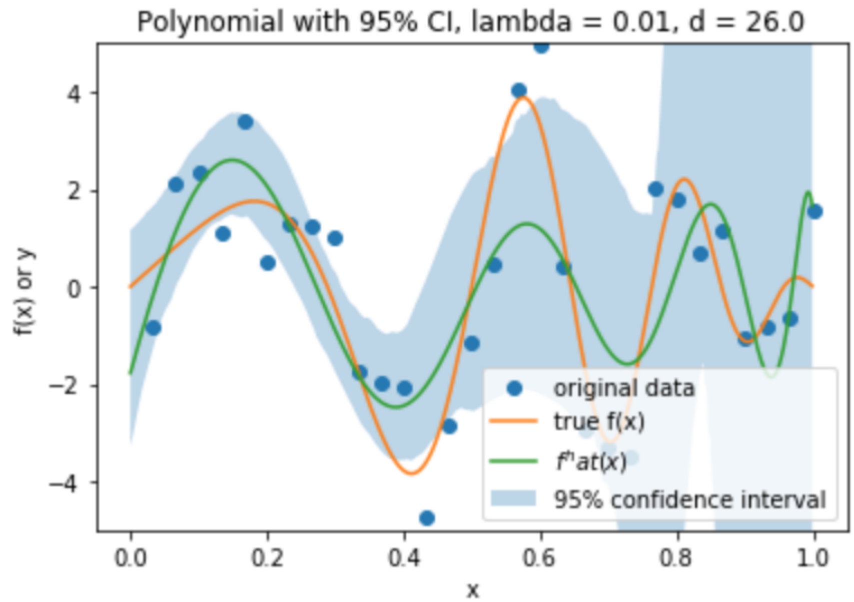
[38]:
```
# =============================================================================
# b plot
# =============================================================================

xx = np.arange(0,1,0.001)
f_x = 4*np.sin(np.pi*xx)*np.cos(6*np.pi*(xx**2))
#poly
plot_poly(X,y,xx,f_x,best_lambda_poly,best_d)
#RBF
plot_RBF(X,y,xx,f_x,best_lambda_RBF,best_gamma)
```

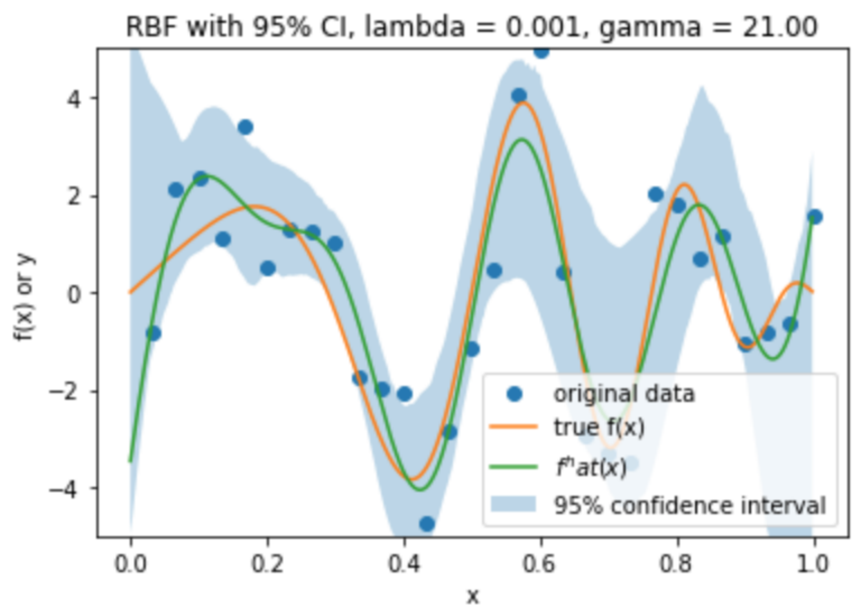




[39]:
```
# ==============================================================================
# c      bootstrap
# ==============================================================================
B = 300
n = 30
#poly
f_hat_table_poly = bootstrap_poly(best_d,best_lambda_poly,X,y,xx,B,n)
lower_poly,upper_poly = np.percentile(f_hat_table_poly,[2.5,97.5],axis=0)
plot_bootstrap_poly(X,y,xx,f_x,best_lambda_poly,best_d,lower_poly,upper_poly)
```

```
#RBF
f_hat_table_RBF = bootstrap_RBF(best_lambda_RBF,best_gamma,X,y,xx,B,n)
lower_RBF,upper_RBF= np.percentile(f_hat_table_RBF,[2.5,97.5],axis=0)
plot_bootstrap_RBF(X,y,xx,f_x,best_lambda_RBF,best_gamma,lower_RBF,upper_RBF)
```

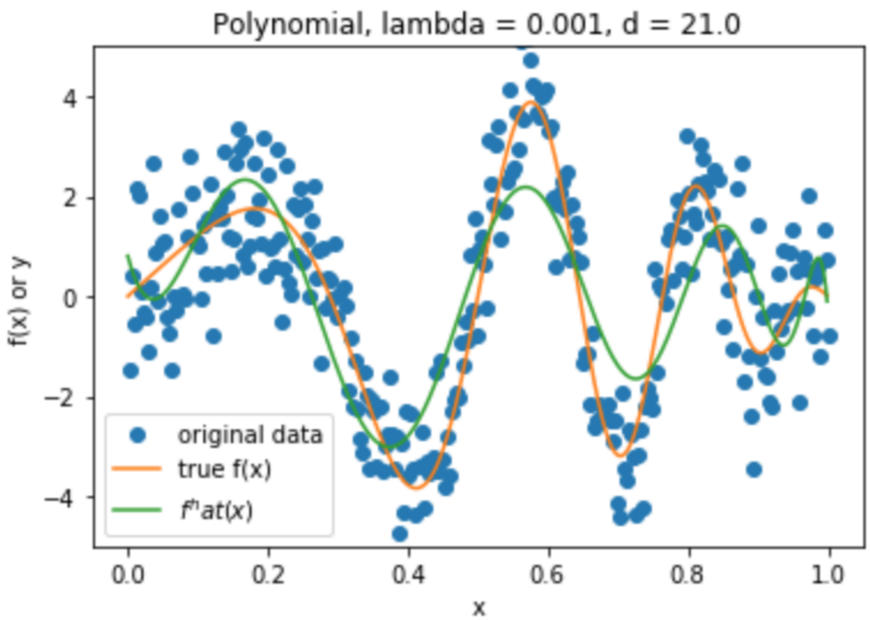


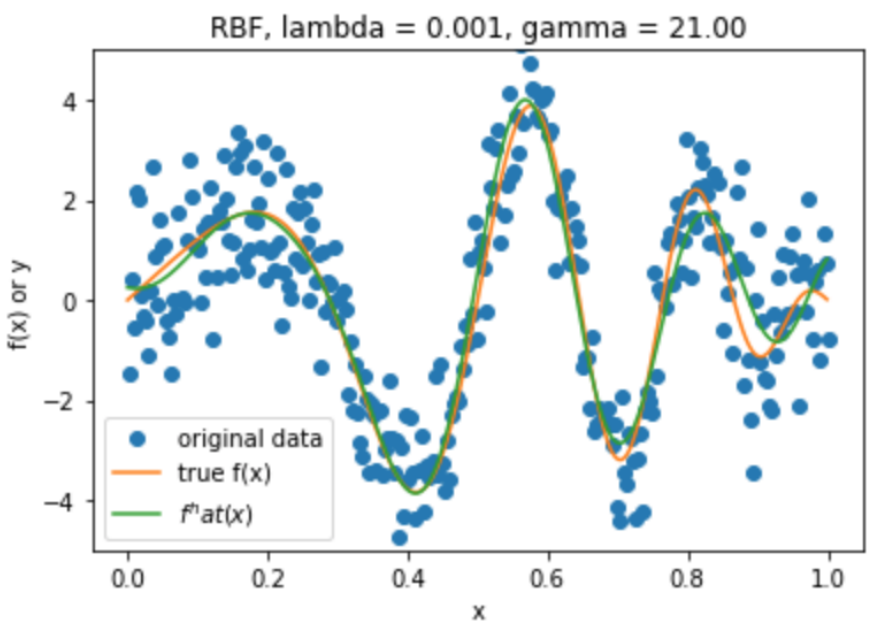


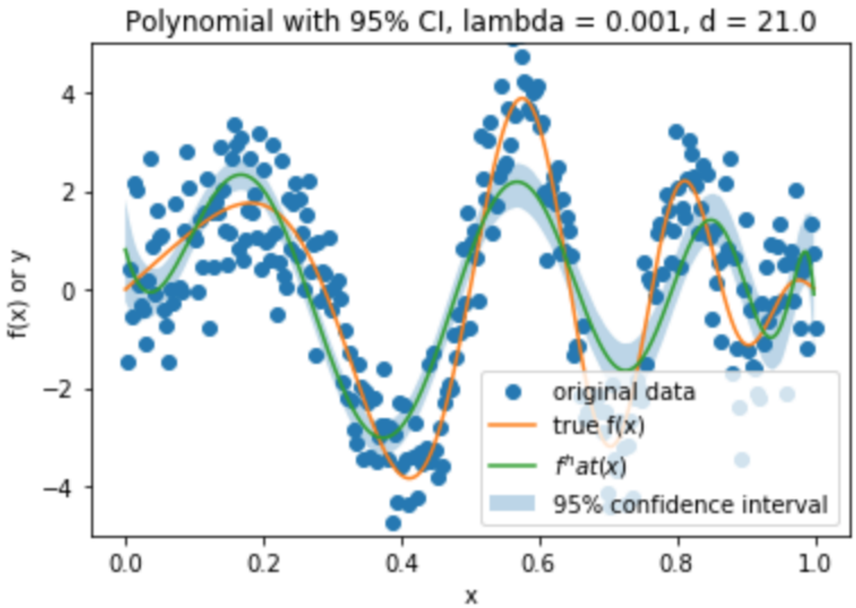
[40]:
```
# ==========================================================================
# d     repeat a,b,c with n = 300, 10-fold cv
# ==========================================================================
```

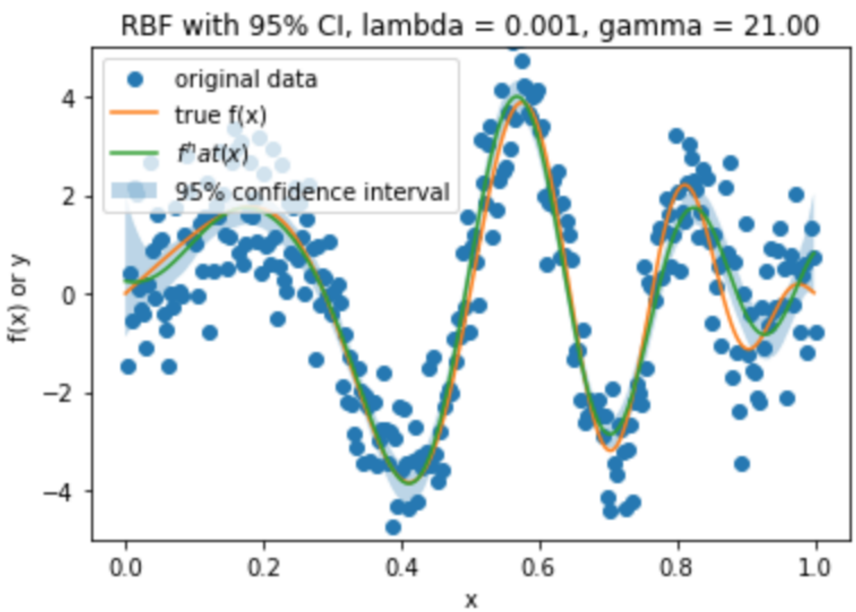
```python
X,y = create_data(300)
K = 10

cost_history_poly = K_fold_poly(X, y, lamda_list,d_list,K)
best_lambda_poly = lamda_list[int(np.floor(cost_history_poly.argmin() /
 ↪len(d_list)))]
best_d = d_list[int(np.ceil(cost_history_poly.argmin() /len(lamda_list)))]
print("For polynomial kernel, lambda = ", best_lambda_poly, " d = ",best_d)

#RBF kernel
gamma_list  = np.arange(1.0, 50.0, 5)

cost_history_RBF = K_fold_RBF(X, y, lamda_list, gamma_list,K)
best_lambda_RBF = lamda_list[int(np.floor(cost_history_RBF.argmin() /
 ↪len(gamma_list)))]
best_gamma = gamma_list[int(np.ceil(cost_history_RBF.argmin() /len(lamda_list)))]
print("For RBF kernel, lambda = ", best_lambda_RBF, " gamma = ",best_gamma)
# b plot
xx = np.arange(0,1,0.001)
f_x = 4*np.sin(np.pi*xx)*np.cos(6*np.pi*(xx**2))
#poly
plot_poly(X,y,xx,f_x,best_lambda_poly,best_d)
#RBF
plot_RBF(X,y,xx,f_x,best_lambda_RBF,best_gamma)


# c     bootstrap
B = 300
n = 300
#poly
f_hat_table_poly = bootstrap_poly(best_d,best_lambda_poly,X,y,xx,B,n)
lower_poly,upper_poly = np.percentile(f_hat_table_poly,[2.5,97.5],axis=0)
plot_bootstrap_poly(X,y,xx,f_x,best_lambda_poly,best_d,lower_poly,upper_poly)

#RBF
f_hat_table_RBF = bootstrap_RBF(best_lambda_RBF,best_gamma,X,y,xx,B,n)
lower_RBF,upper_RBF= np.percentile(f_hat_table_RBF,[2.5,97.5],axis=0)
plot_bootstrap_RBF(X,y,xx,f_x,best_lambda_RBF,best_gamma,lower_RBF,upper_RBF)
```

```
For polynomial kernel, lambda =  0.001  d =  21.0
For RBF kernel, lambda =  0.001  gamma =  21.0
```


Polynomial, lambda = 0.001, d = 21.0
f(x) or y
x
original data
true f(x)
f^at(x)


RBF, lambda = 0.001, gamma = 21.00
f(x) or y
x
original data
true f(x)
f^at(x)





[41]:
```
# ==============================================================================
# e
# ==============================================================================
#additional data
B = 300
m = 1000
n = m
add_X,add_y = create_data(m)
```

```
table =␣
 ↪Poly_RBF(best_d,best_lambda_poly,best_lambda_RBF,best_gamma,add_X,add_y,xx,B,n)
lower_RBF,upper_RBF= np.percentile(table,[2.5,97.5],axis=0)
print("For RBF kernel, the lower bound is  ", lower_RBF, " upper bound is␣
 ↪",upper_RBF)
```

```
For RBF kernel, the lower bound is   [-1.35258286]  upper bound is
[-0.81717693]
```

There is statistically significant evidence to suggest that $\hat{f}_{rbf}$ is better than $\hat{f}_{poly}$ at predicting Y from X, i.e. the confidence interval doesn't contain 0.

A4

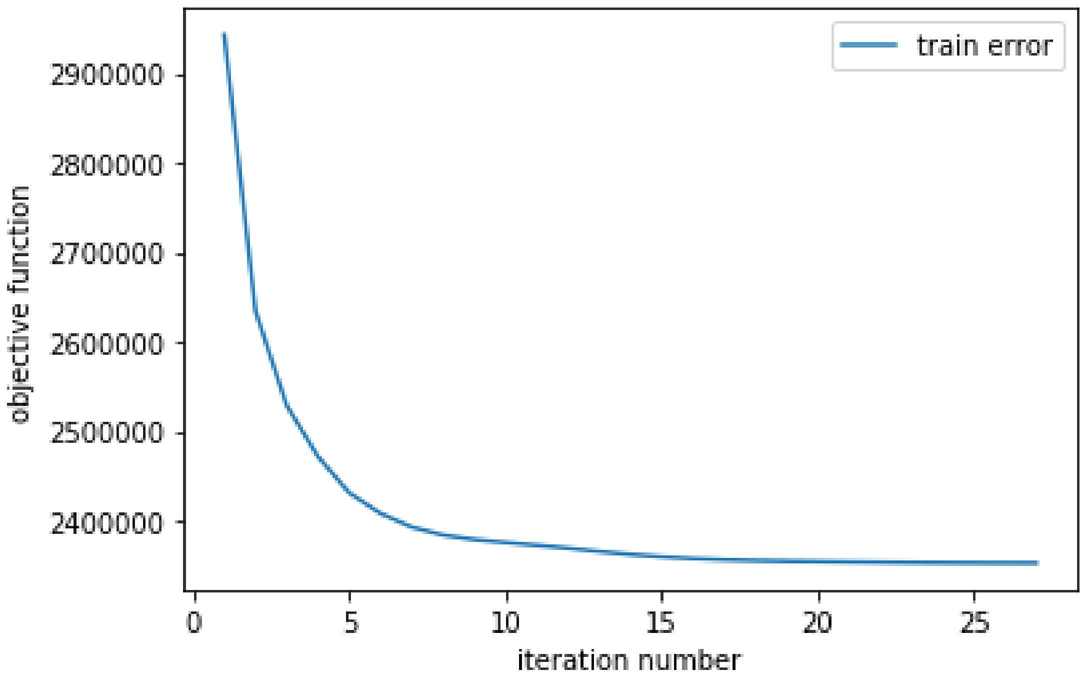
[1]:
```
"""
Created on Sun May 17 00:09:39 2020
HW3 A4 K-MEANS
@author: Leah
"""

import numpy as np
import matplotlib.pyplot as plt
from copy import deepcopy
from mnist import MNIST

# Number of clusters
K = 10

def load_dataset():
mndata = MNIST('./data/')
#mndata = MNIST('./dir_with_mnist_data_files')
X_train, labels_train = map(np.array, mndata.load_training())
X_test, labels_test = map(np.array, mndata.load_testing())
X_train = X_train/255.0
X_test = X_test/255.0
return X_train, labels_train, X_test, labels_test

def kmeans(X,K):
#X = X_train
# Number of training data
n = X.shape[0]
# Number of features in the data
c = X.shape[1]
###randomly pick K cluster centers(centroids).
mean = np.mean(X, axis = 0)
std = np.std(X, axis = 0)
centers = np.random.randn(K,c) *std + mean
centers_old = np.zeros(centers.shape) # to store old centers
```

```
centers_new = deepcopy(centers) # Store new centers
clusters = np.zeros(n)
distances = np.zeros((n,K))
error = np.linalg.norm(centers_new - centers_old)
iteration = 0
obj = list()
# When, after an update, the estimate of that center stays the same, exit ,!loop
while error > 0.1:
objective = 0
train_error = list()
# Measure the distance to every center
for i in range(K):
distances[:,i] = np.linalg.norm(X - centers_new[i], axis=1) # Assign all␣
,→training data to closest center
clusters = np.argmin(distances, axis = 1)
centers_old = deepcopy(centers_new) ###recompute centroids
for i in range(K):
centers_new[i] = np.mean(X[clusters == i], axis=0)
error = np.linalg.norm(centers_new - centers_old)
objective = objective + np.sum((X[clusters == i] - centers_new[i])**2)
train_error.append(np.sum((X - centers_new[i])**2))
iteration += 1
#objective = np.sum([np.sum(distances[clusters==c, c])/np.sum(clusters==c)
#                          if np.any(clusters==c) else 0 for c in range(K)])
obj.append((iteration, objective))
return centers_new, clusters ,obj, min(train_error)/len(X_train)

def kmeans_test(X_test,centers):
distances = np.zeros((X_test.shape[0],K))
objective = 0
test_error = list()
for i in range(K):
distances[:,i] = np.linalg.norm(X_test - centers[i], axis=1) # Assign all␣
,→training data to closest center
clusters = np.argmin(distances, axis = 1)
for i in range(K):
objective = objective + np.sum((X_test[clusters == i] - centers[i])**2)
test_error.append(np.sum((X_test - centers[i])**2))
return  objective , min(test_error)/len(X_test)
```

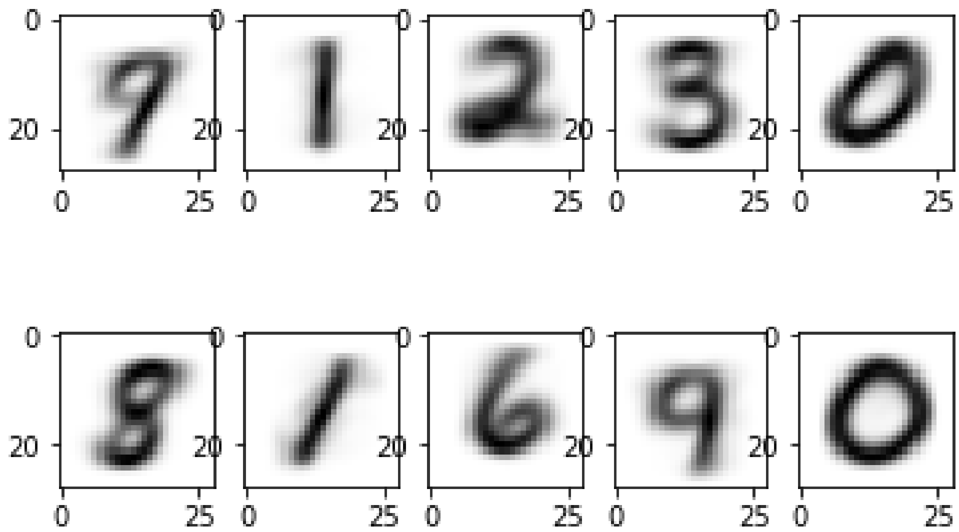
[2]:
```
X_train, labels_train, X_test, labels_test = load_dataset()

centers, clusters, obj, train_error = kmeans(X_train, K)

obj =  np.array(obj)
#plot
plt.figure()
```

```
plt.plot(obj[:,0],obj[:,1],label='train error')
plt.xlabel('iteration number')
plt.ylabel('objective function')
#plt.title('objective function versus iteration number')
plt.legend()
#plt.ylim([-5,5])
```

[2]: <matplotlib.legend.Legend at 0x125720d30>

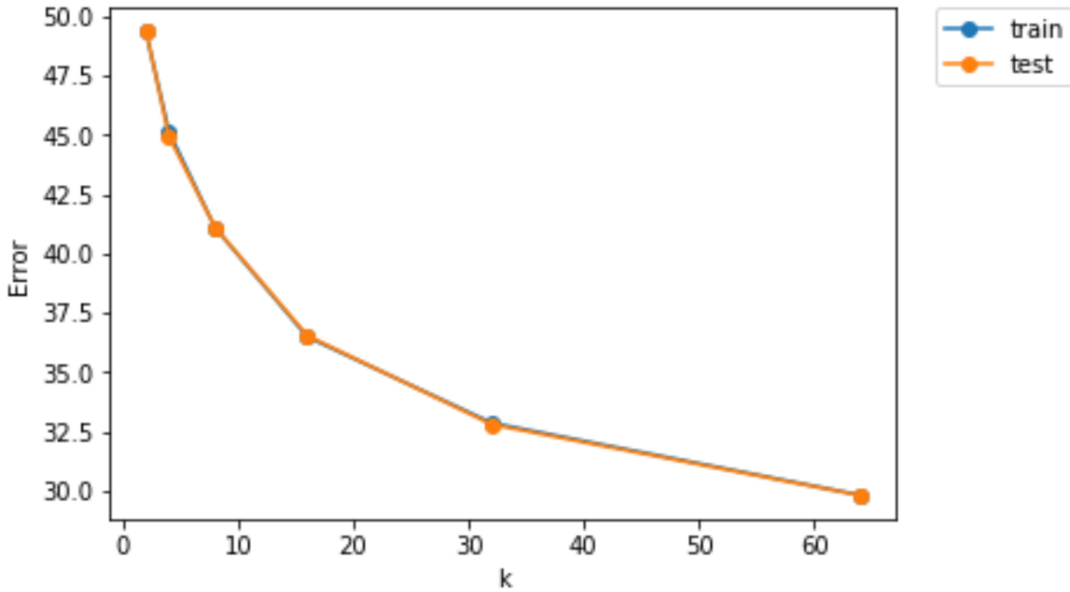


[3]:
```
fig, ax = plt.subplots(2,5)
for i, ax in enumerate(ax.flatten()):
    plottable_image = np.reshape(centers[i,:], (28, 28))
    ax.imshow(plottable_image, cmap='gray_r')
```



```
[4]: # ============================================================================
     # part c
     # ============================================================================
     K_list = np.array([2, 4, 8, 16, 32, 64])
     result = list()
     for k in K_list:
     centers, clusters, obj_train, train_error = kmeans(X_train, K)
     obj_test, test_error = kmeans_test(X_test, centers)
     result.append((k,train_error,test_error))

     result = np.array(result)
     #plot
     plt.figure()
     plt.plot(result[:,0],result[:,1],label='train')
     plt.plot(result[:,0],result[:,2],label='test')
     plt.xlabel('k')
     plt.ylabel('error')
     plt.legend()
```

```
[4]: <matplotlib.legend.Legend at 0x11d4b7e80>
```



A5

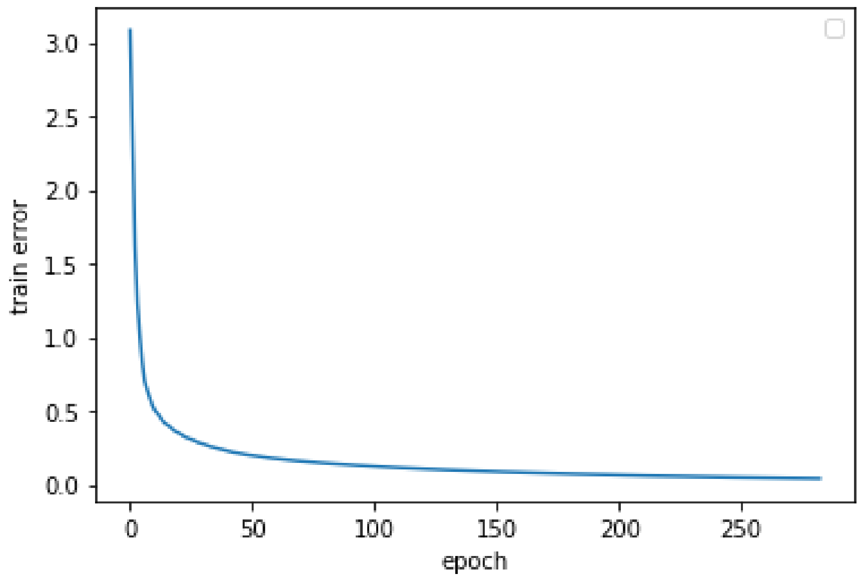
[1]:
```
#hw5_A5 NN

import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
from copy import deepcopy
from mnist import MNIST
import torch
import torch.nn as nn
import torch.nn.functional as F


def load_dataset():
    mndata = MNIST('./data/')
    #mndata = MNIST('./dir_with_mnist_data_files')
    X_train, labels_train = map(np.array, mndata.load_training())
    X_test, labels_test = map(np.array, mndata.load_testing())
    X_train = X_train/255.0
    X_test = X_test/255.0
    return X_train, labels_train, X_test, labels_test

def onehot(X):
    '''
    For each yi let yi be the one-hot encoding of yi (i.e., yi ∈ {0, 1}^k
    is a vector of all zeros aside from a 1 in the yith index).
    k = 10
    '''
```

```
    n_classes = 10
    ## transform labels_train(n-by-1) into n-by-k
    Y = np.zeros((len(X),n_classes))
    for i in range(0,len(Y)):
        Y[i,X[i]] = 1
    return Y
```

[2]:
```
#load data
X_train, labels_train, X_test, labels_test = load_dataset()
X_train = torch.tensor(X_train)
X_test = torch.tensor(X_test)
y_test = torch.tensor(labels_test)
y_train = torch.tensor(labels_train)
y_train = y_train.long()
y_test = y_test.long()

learning_rate = 0.01
accuracy = 0.99
```

[3]:
```
# ==============================================================================
# part a
# ==============================================================================
#Weight Initialization
h = 64  # # of hidden units
k = 10
d = 28*28
alpha = 1/np.sqrt(k)
W_0 = torch.tensor(np.random.uniform(-alpha, alpha, (h, d)),requires_grad=True)
W_1 = torch.tensor(np.random.uniform(-alpha, alpha, (k, h)),requires_grad=True)
b_0 = torch.tensor(np.random.uniform(-alpha, alpha, (h,1)),requires_grad=True)
b_1 = torch.tensor(np.random.uniform(-alpha, alpha, (1,k)),requires_grad=True)

#training NN
optim = torch.optim.Adam({W_0,W_1,b_0,b_1}, lr=learning_rate)
train_error = list()
accu = 0
iteration = 0
while accu < accuracy:
    y_hat = torch.matmul(F.relu(torch.matmul(W_0, X_train.T)+ b_0.
 ↪repeat(1,len(X_train))).T,W_1.T)+b_1.repeat(len(X_train),1)
    loss =  torch.nn.functional.cross_entropy(y_hat, y_train)
    optim.zero_grad()
    loss.backward()
    optim.step()
    train_error.append((iteration,loss.detach().numpy()))
    accu = sum(torch.argmax(y_hat,dim = 1) == y_train).numpy() / len(y_train)
    iteration += 1
```

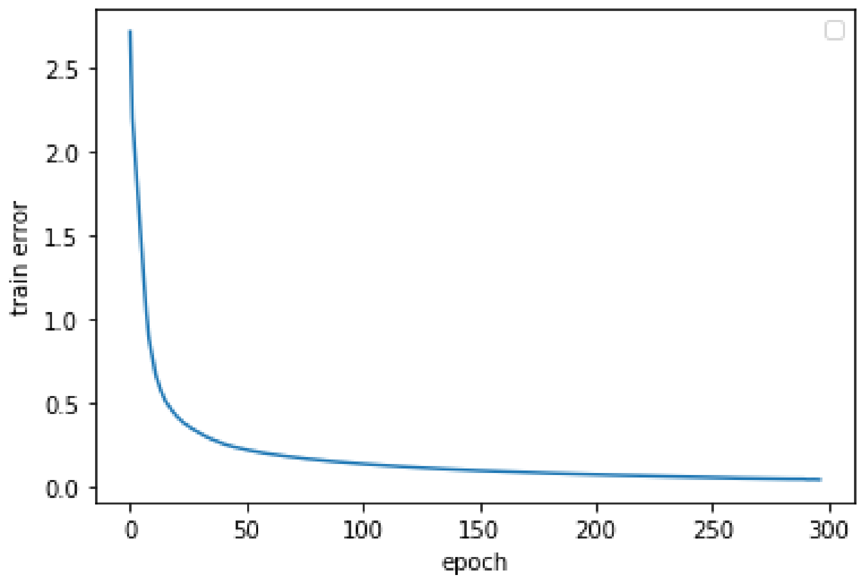
[4]:
```
#plot
train_error = np.array(train_error)
plt.figure()
plt.plot(train_error[:,0],train_error[:,1])
plt.xlabel('epoch')
plt.ylabel('train error')
plt.legend()
```



[13]:
```
for i in range(4):
    a = optim.param_groups[0]['params'][i].size()[0]
    b = optim.param_groups[0]['params'][i].size()[1]
    if a == h and b == d:
        W_0 = optim.param_groups[0]['params'][i]
    elif a == k and b == h:
        W_1 = optim.param_groups[0]['params'][i]
    elif b == 1:
        b_0 = optim.param_groups[0]['params'][i]
    else:
        b_1 = optim.param_groups[0]['params'][i]

#evaluate the model on the test data and report both the accuracy and the loss.
y_hat = torch.matmul(F.relu(torch.matmul(W_0, X_test.T)+ b_0.
 ↪repeat(1,len(X_test)))).T,W_1.T)+b_1.repeat(len(X_test),1)
test_loss =  torch.nn.functional.cross_entropy(y_hat, y_test)
test_accu = sum(torch.argmax(y_hat,dim = 1) == y_test).numpy() / len(y_test)
print("The accuracy of test data is {}, the error is {}".format(test_accu,␣
 ↪test_loss))
```

```
The accuracy of test data is 0.9696, the error is 0.10341335476065462
```

[14]:
```
# ==============================================================================
# part b a narrow but deeper network
# ==============================================================================
h_0 = h_1 = 32  # # of hidden units
k = 10
d = 28*28
alpha = 1/np.sqrt(k)
W_0 = torch.tensor(np.random.uniform(-alpha, alpha, (h_0, d)),requires_grad=True)
W_1 = torch.tensor(np.random.uniform(-alpha, alpha, (h_1,␣
 ↪h_0)),requires_grad=True)
W_2 = torch.tensor(np.random.uniform(-alpha, alpha, (k, h_1)),requires_grad=True)
b_0 = torch.tensor(np.random.uniform(-alpha, alpha, (h_0,1)),requires_grad=True)
b_1 = torch.tensor(np.random.uniform(-alpha, alpha, (1,h_1)),requires_grad=True)
b_2 = torch.tensor(np.random.uniform(-alpha, alpha, (1,k)),requires_grad=True)

optim = torch.optim.Adam({W_0,W_1,W_2,b_0,b_1,b_2}, lr=learning_rate)
train_error = list()
accu = 0
iteration = 0
while accu < accuracy:
    layer1 = torch.matmul(W_0, X_train.T)+ b_0.repeat(1,len(X_train))   #h_0 by n
    layer2 = torch.matmul(F.relu(layer1).T,W_1.T) + b_1.repeat(len(X_train),1)  ␣
 ↪# n by h_1
    y_hat = torch.matmul(W_2,F.relu(layer2).T).T + b_2.repeat(len(X_train),1)

    #y_hat = torch.matmul(W_2,F.relu(torch.matmul(F.relu(torch.matmul(W_0,␣
 ↪X_train.T)+ b_0.repeat(1,len(X_train))).T,W_1.T) + b_1.repeat(len(X_train),1)␣
 ↪).T).T + b_2.repeat(len(X_train),1)
    loss =  torch.nn.functional.cross_entropy(y_hat, y_train)
    optim.zero_grad()
    loss.backward()
    optim.step()
    train_error.append((iteration,loss.detach().numpy()))
    accu = sum(torch.argmax(y_hat,dim = 1) == y_train).numpy() / len(y_train)
    iteration += 1

train_error = np.array(train_error)
#plot
plt.figure()
plt.plot(train_error[:,0],train_error[:,1])
plt.xlabel('epoch')
plt.ylabel('train error')
plt.legend()
```



[14]:
```
for i in range(4):
    a = optim.param_groups[0]['params'][i].size()[0]
    b = optim.param_groups[0]['params'][i].size()[1]
    if a == h_0 and b == d:
        W_0 = optim.param_groups[0]['params'][i]
    if a == h_1 and b == h_0:
        W_1 = optim.param_groups[0]['params'][i]
    elif a == k and b == h_1:
        W_2 = optim.param_groups[0]['params'][i]
    elif b == 1:
        b_0 = optim.param_groups[0]['params'][i]
    elif a == 1 and b == h_1:
        b_1 = optim.param_groups[0]['params'][i]
    else:
        b_2 = optim.param_groups[0]['params'][i]

#evaluate the model on the test data and report both the accuracy and the loss.
layer1 = torch.matmul(W_0, X_test.T)+ b_0.repeat(1,len(X_test))   #h_0 by n
layer2 = torch.matmul(F.relu(layer1).T,W_1.T) + b_1.repeat(len(X_test),1)   # n␣
 ↪by h_1
y_hat = torch.matmul(W_2,F.relu(layer2).T).T + b_2.repeat(len(X_test),1)
test_accu = sum(torch.argmax(y_hat,dim = 1) == y_test).numpy() / len(y_test)
print("The accuracy of test data is {}, the error is {}".format(test_accu,␣
 ↪test_loss))
```

```
The accuracy of test data is 0.9632, the error is 0.10341335476065462
```

[15]:
```
print('the number of parameters for network 1 :',h*d+k*h+k+h)
print('the number of parameters for network 2 :', h_0*d+h_0*h_1 +
↪k*h_1+k+h_0+h_1)
```

```
the number of parameters for network 1 : 50890
the number of parameters for network 2 : 26506
```

[ ]:
```
# ==============================================================================
# part c comparision
# ==============================================================================
For wide, shallow network, there are 50890 parameters and the accuracy is 0.9696.
For narrow, deeper network, there are 26506 parameters which is larger than
↪another network and the accuracy is 0.9632 which is worse than the other one
↪but the difference is trival.
Intuitively, the narrow deeper network has a better performence due to less
↪parameters usually means lower memory usage and faster infrence.
```

A6

[15]:
```
"""
Created on Mon May 18 11:26:45 2020
HW3 A6 PCA
@author: Leah
"""

import numpy as np
import matplotlib.pyplot as plt
from mnist import MNIST

def load_dataset():
    mndata = MNIST('./data/')
    #mndata = MNIST('./dir_with_mnist_data_files')
    X_train, labels_train = map(np.array, mndata.load_training())
    X_test, labels_test = map(np.array, mndata.load_testing())
    X_train = X_train/255.0
    X_test = X_test/255.0
    return X_train, labels_train, X_test, labels_test

def topK(dataMat):
    meanVals = np.mean(dataMat, axis=0)
    meanRemoved = dataMat - meanVals
    eigVals,eigVects = np.linalg.eig(np.dot(meanRemoved.T,meanRemoved)/
↪len(X_train))
    idx = eigVals.argsort()[::-1]
    eig_vals = eigVals[idx]
    eig_vecs = eigVects[:,idx]

    return meanVals, eig_vals,eig_vecs
```

```
def mean_squared_error(U, V):
    error = np.mean((U - V)**2)
    return error
```

[16]:
```
# ============================================================================
# load data
# ============================================================================
d = 28*28
X_train, labels_train, X_test, labels_test = load_dataset()
```

[17]:
```
# ============================================================================
# part a
# ============================================================================
mu, eig_vals, eig_vecs = topK(X_train)
for i in [0,1,9,29,49]:
    print('\n {}th  Eigenvalues {}\n'.format(i+1, eig_vals[i]))
print('Sum of Eigenvalues : ', np.sum(eig_vals))
```

```

 1th  Eigenvalues 5.116787728342092



 2th  Eigenvalues 3.7413284788648316



 10th  Eigenvalues 1.2427293764173317



 30th  Eigenvalues 0.3642557202788918



 50th  Eigenvalues 0.16970842700672786

Sum of Eigenvalues :  52.725035495127
```

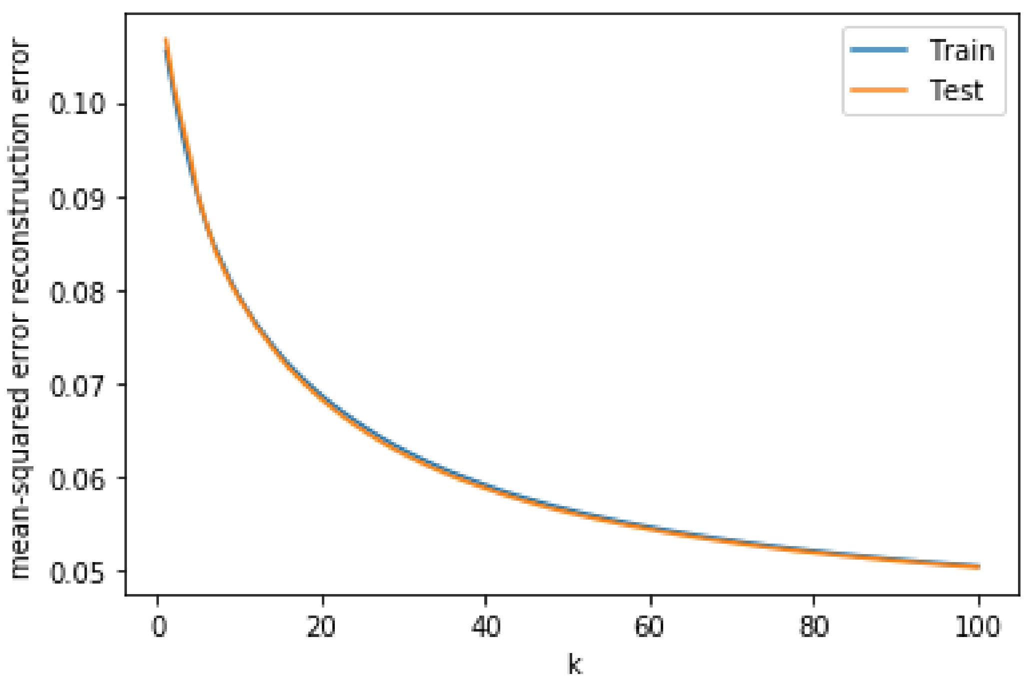
Part b: For any k, provide a formula for computing this approximation.
Let U denotes eignvectors, U_i corresponding to the i-th largest eigenvalue λ_i.

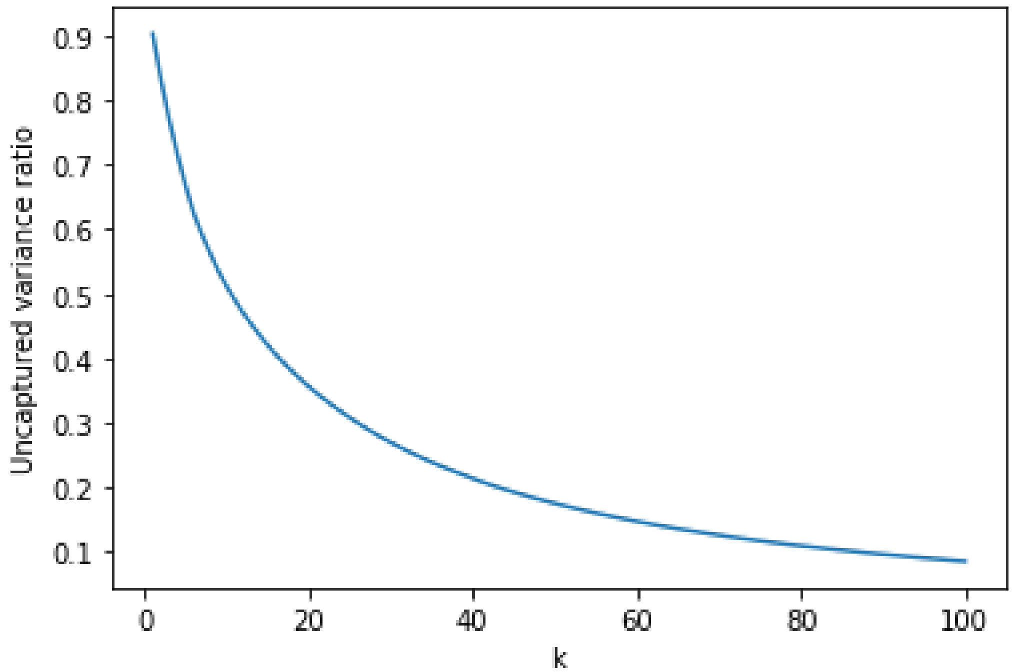
$$x' = \mu + [U_1 U_1^T(x-\mu), U_2 U_2^T(x-\mu), \ldots, U_k U_k^T(x-\mu)]^T$$

[18]:
```
# ============================================================================
# part c
# ============================================================================
#reconstruction error
mse_train = []
mse_test = []
ration_egivals = []
k_list = np.arange(1,101)
```

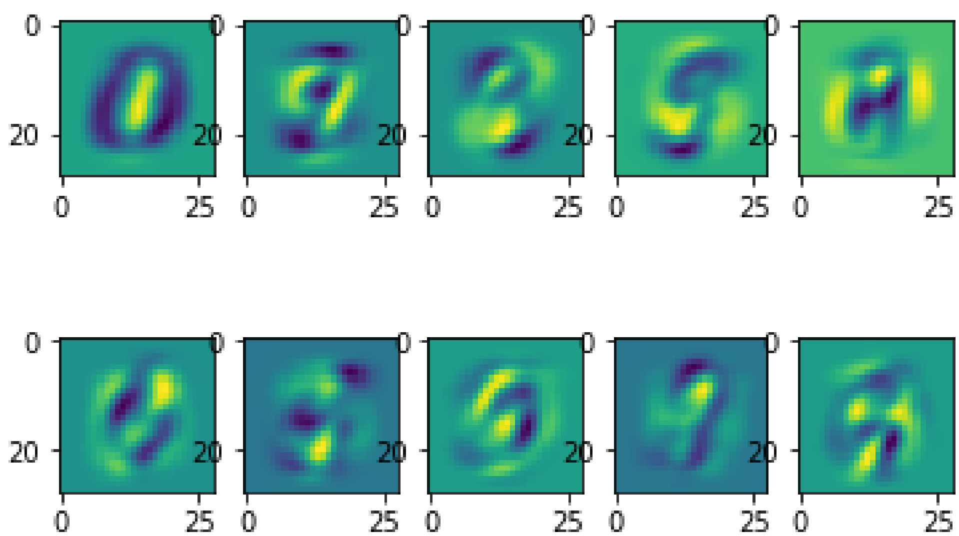
```
for k in k_list:
    EigenVectors = eig_vecs[:,0:k] #n by k
    Final_train = np.dot(np.dot(X_train - mu, EigenVectors),EigenVectors.T)
    Final_test = np.dot(np.dot(X_test - mu, EigenVectors),EigenVectors.T)
    mse_train.append(mean_squared_error(X_train, Final_train))
    mse_test.append(mean_squared_error(X_test, Final_test))
    ration_egivals.append(1-np.sum(eig_vals[0:k])/np.sum(eig_vals))

#plot1
plt.figure()
plt.plot(k_list,mse_train,label = 'Train')
plt.plot(k_list,mse_test,label = 'Test')
plt.xlabel('k')
plt.ylabel('mean-squared error reconstruction error')
plt.legend()

#plot2
plt.figure()
plt.plot(k_list,ration_egivals)
plt.xlabel('k')
plt.ylabel('Uncaptured variance ratio')
```

[18]:
```
Text(0, 0.5, 'Uncaptured variance ratio')
```



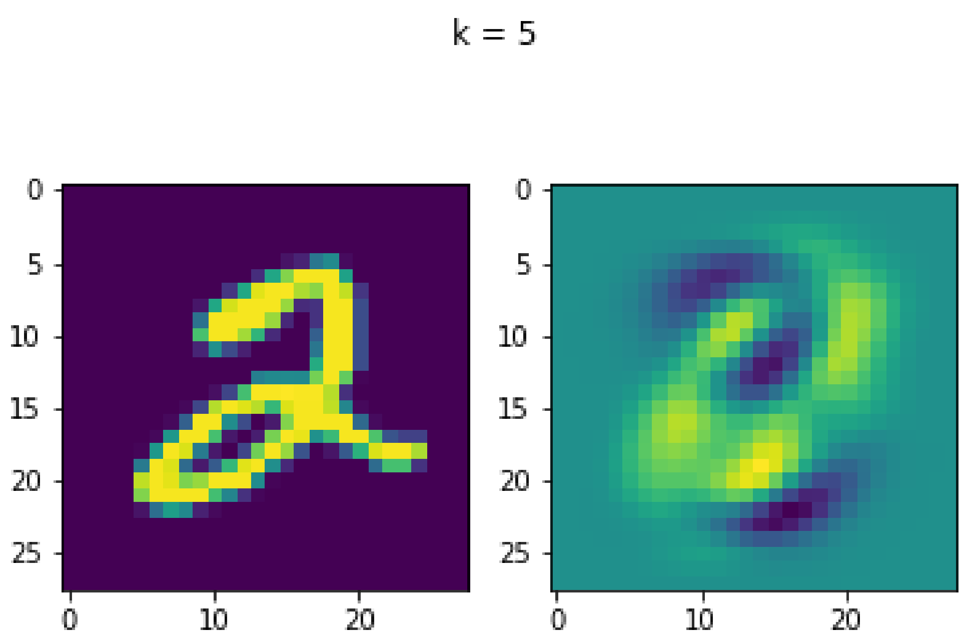


[19]:
```
# ==========================================================================
# part d Display first 10 egenvectors as image
# ==========================================================================
fig, ax = plt.subplots(2,5)
for i, ax in enumerate(ax.flatten()):
    plottable_image = np.reshape(eig_vecs[:,i], (28, 28))
    ax.imshow(plottable_image)
```

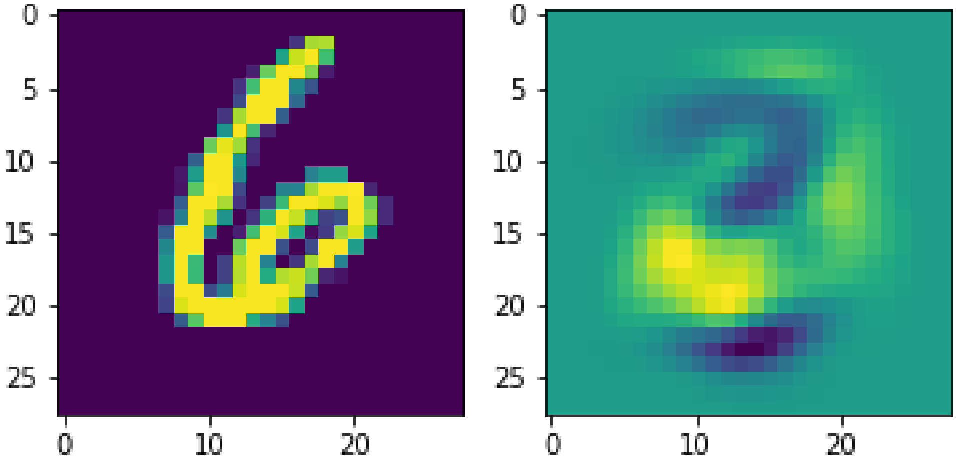


They capture the most common shape the mnist database provided. For example, the biggest eignvalue corresponding eignvector shows number '0'.

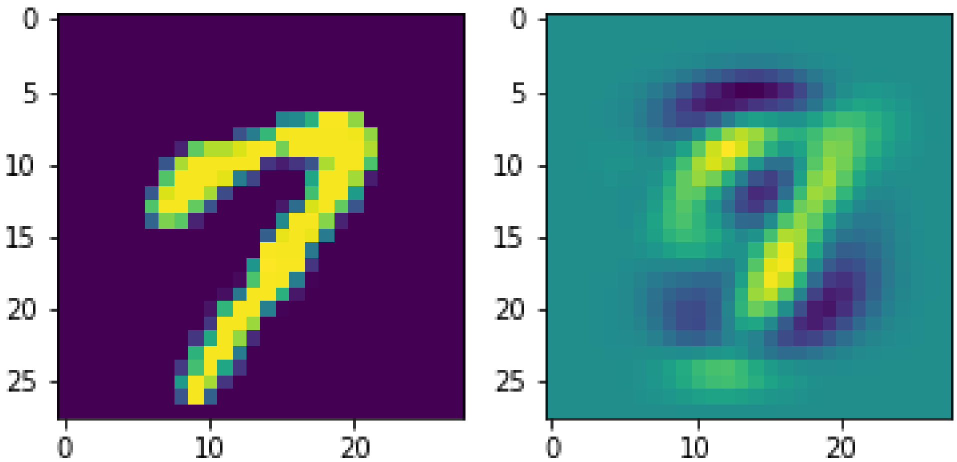
[20]:
```
# ============================================================================
# visualize a set of reconstructed digits
# from the training set for different values of k.
# ============================================================================
#choose an image from each digit arbitrarily
X_train_2 = X_train[labels_train == 2][0]
X_train_6 = X_train[labels_train == 6][0]
X_train_7 = X_train[labels_train == 7][0]
for k in [4,14,39,99]:
    for i in [2, 6, 7]:
        X_digit = X_train[labels_train == i][0]
        EigenVectors = eig_vecs[:,0:k]
        transform = np.dot(np.dot(X_digit - mu, EigenVectors),EigenVectors.T)

        #ploting
        fig, ax = plt.subplots(1,2)
        plottable_image = np.reshape(X_digit, (28, 28))
        ax[0].imshow(plottable_image)
        plottable_image = np.reshape(transform, (28, 28))
        ax[1].imshow(plottable_image)
        fig.suptitle('k = {}'.format(k+1))
```

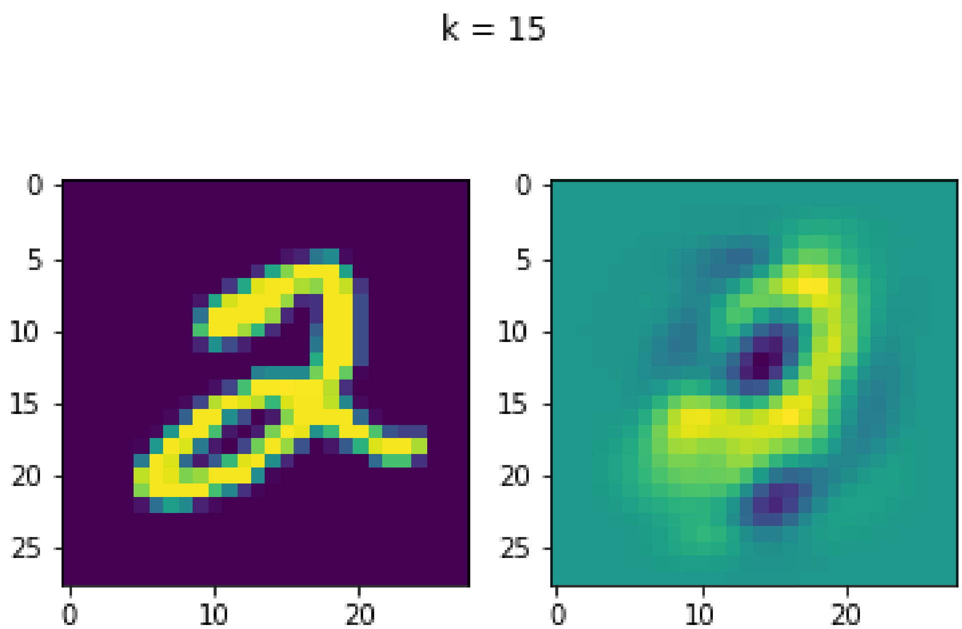


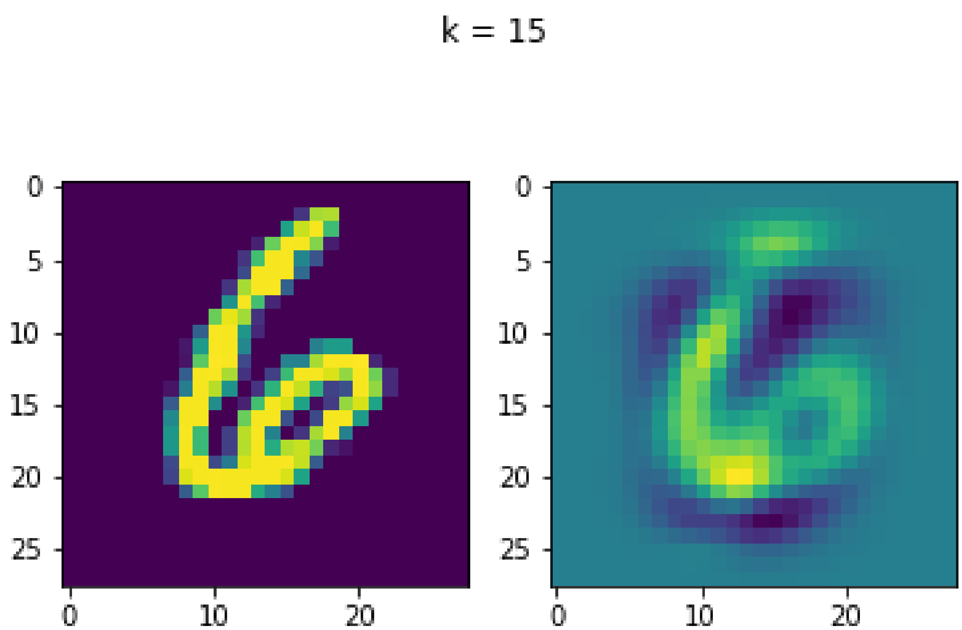
k = 5


0
5
10
15
20
25
0
10
20
0
5
10
15
20
25
0
10
20

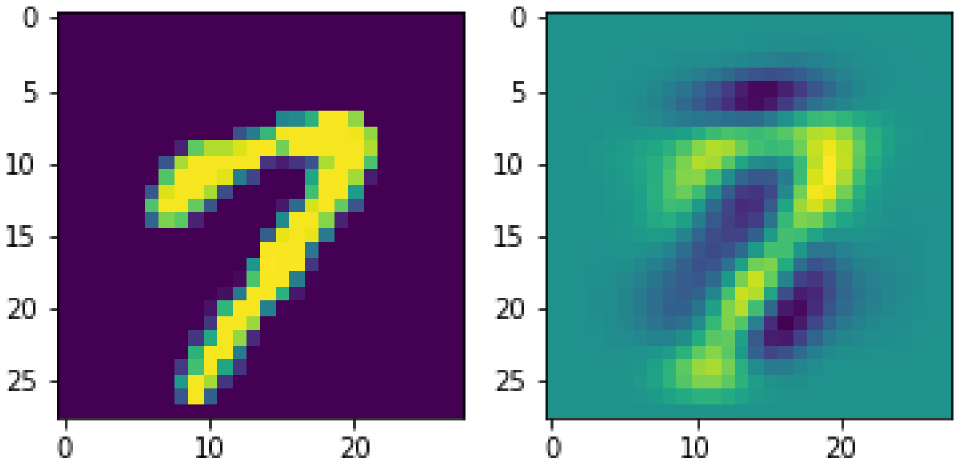
k = 5


0
5
10
15
20
25
0
10
20
0
5
10
15
20
25
0
10
20

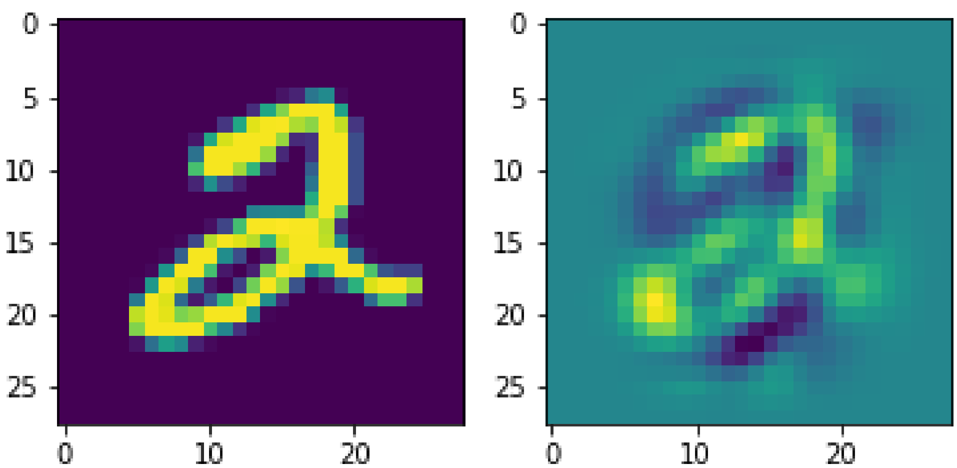

k = 15
0
5
10
15
20
25
0
10
20

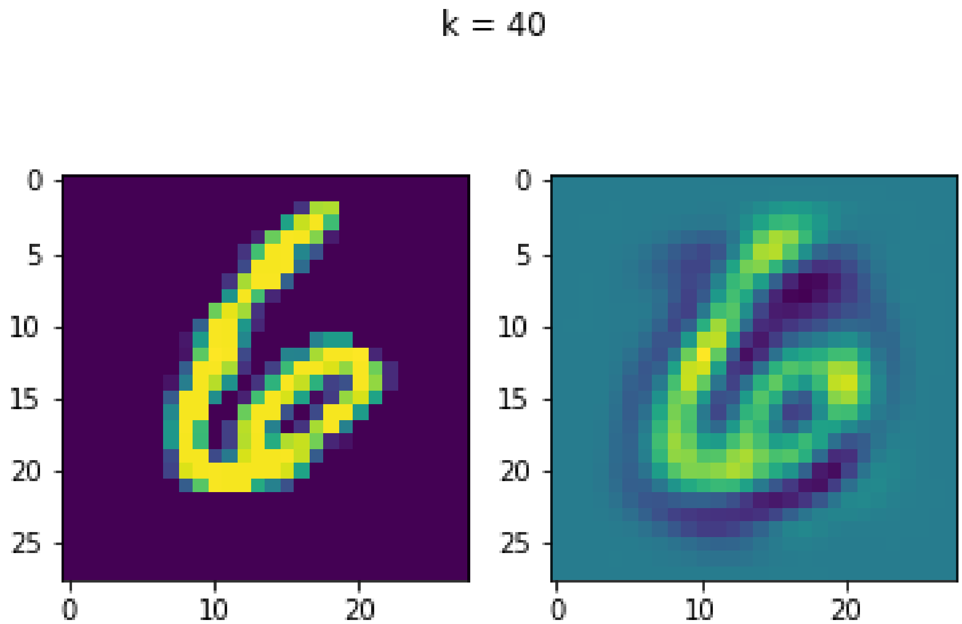

k = 15
0
5
10
15
20
25
0
10
20

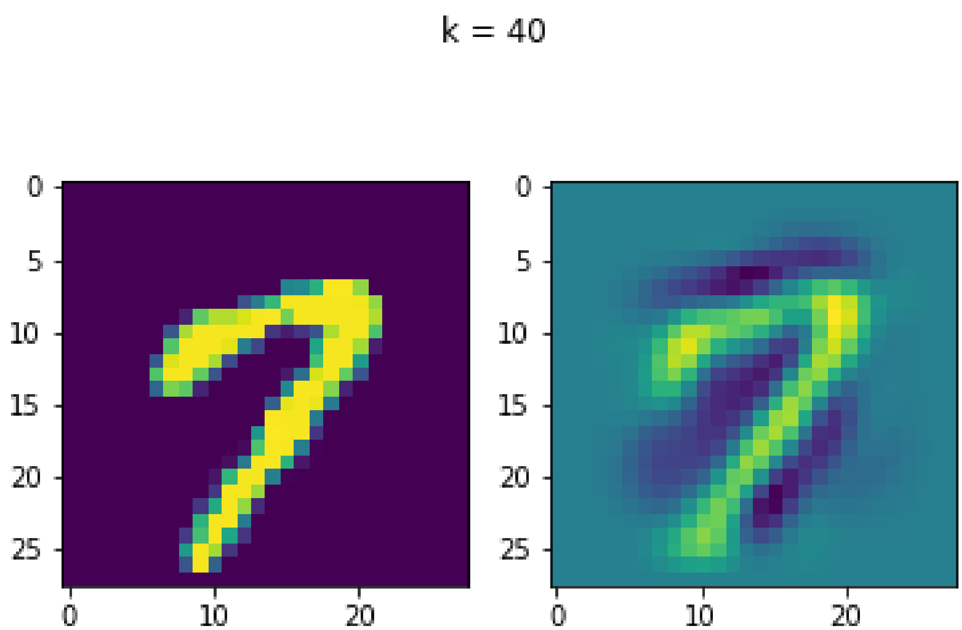
k = 15

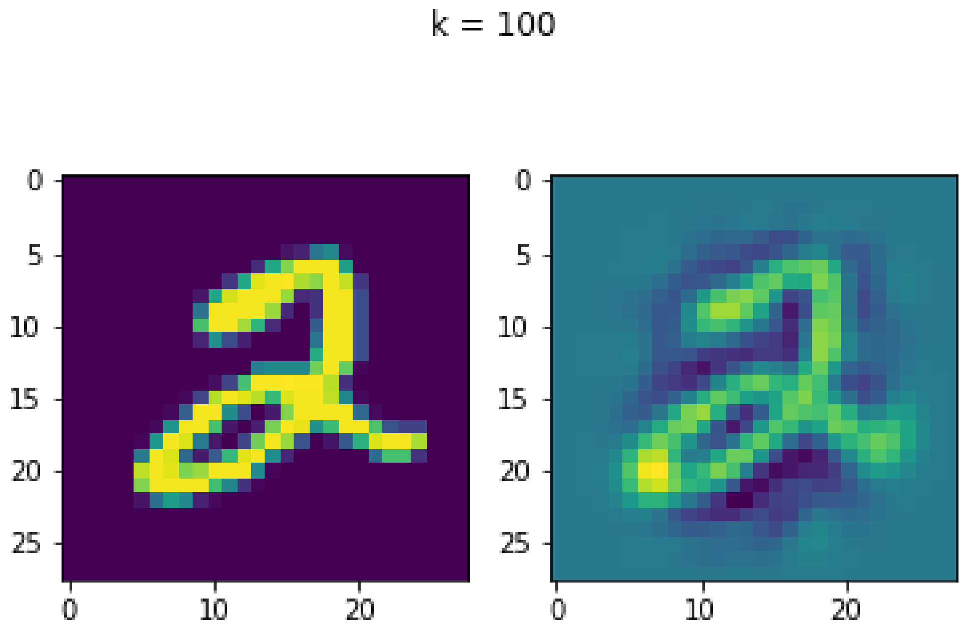


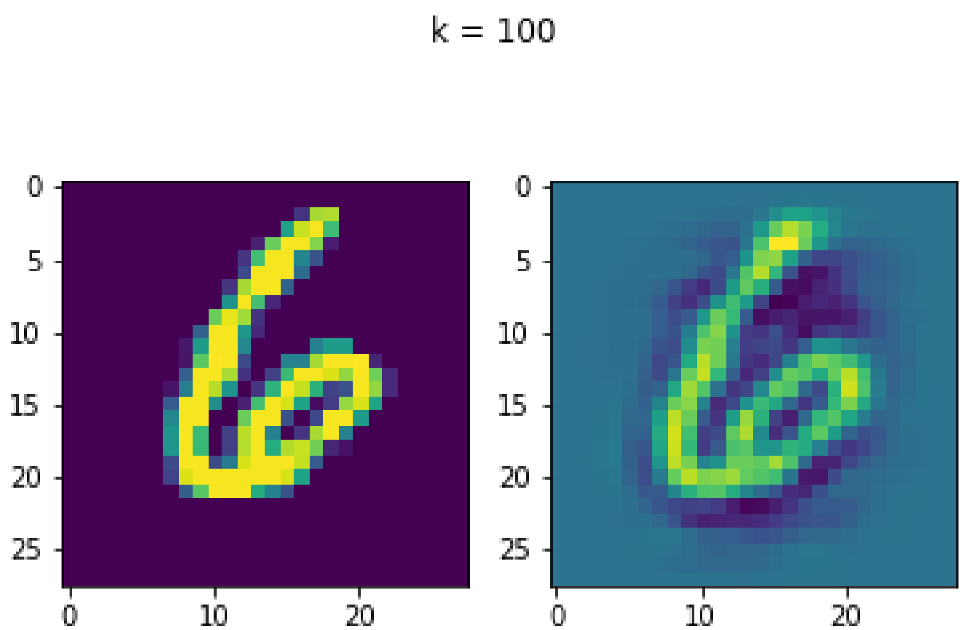
k = 40

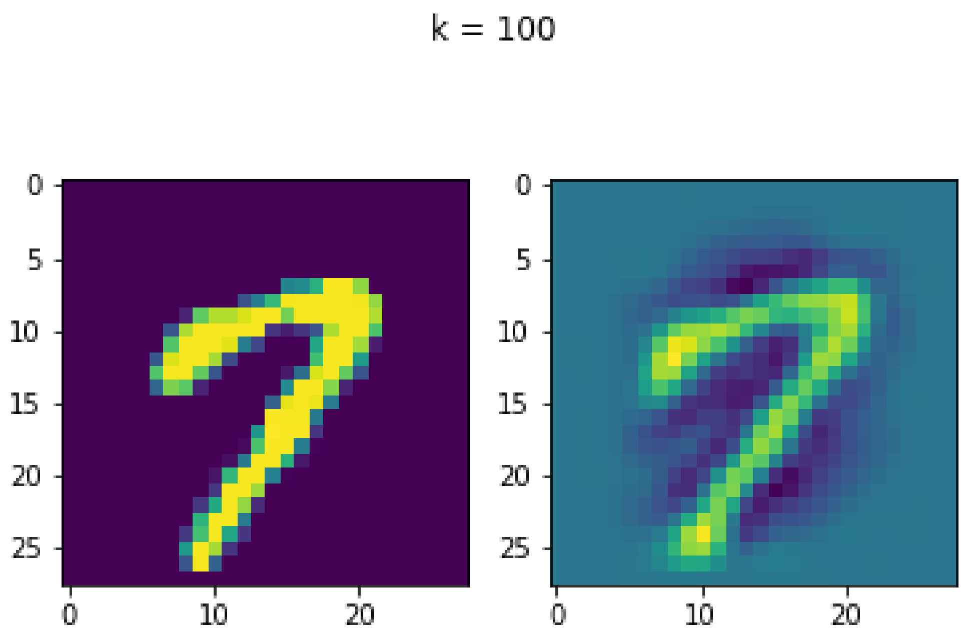



k = 40
0
5
10
15
20
25
0
10
20


k = 40
0
5
10
15
20
25
0
10
20


k = 100


k = 100



With the increasement of dimensionality(k), the reconstruction becomes more and more like the original image, i.e. the quality of these reconstructions become better. Because the more dimensionality, the more elements captured, less construction error.

B1.

a. *[2 points]*

$$1 - \epsilon \leq e^{-\epsilon}$$

$$1 - R(f) < 1 - \epsilon \leq e^{-\epsilon}$$

$$Pr(R(f) = 0) \leq e^{-\epsilon} \; since \; data \; drawn \; i.i.d$$

$$Pr(\hat{R_n}(f) = 0) = (Pr(R(f) = 0))^n \leq e^{-n\epsilon}$$

b. *[2 points]*

$$Pr(\exists f \in \mathbb{F} \; s.t.R(f) > \epsilon \; and \; \hat{R_n}(f) = 0)$$
$$= Pr(\exists f_1 \; s.t.R(f) > \epsilon \; and \; \hat{R_n}(f) = 0) \cdot Pr(\exists f_2 \; s.t.R(f) > \epsilon \; and \; \hat{R_n}(f) = 0) \ldots Pr(\exists f_n \; s.t.R(f) > \epsilon \; and \; \hat{R_n}($$
$$\leq \sum_{i=1}^{|\mathbb{F}|} Pr(\exists f_i \; s.t.R(f) > \epsilon \; and \; \hat{R_n}(f) = 0) \quad union \; bound$$
$$\leq |\mathbb{F}| e^{-n\epsilon} \quad according \; to \; part \; a$$

c. *[2 points]*

$$|\mathbb{F}| e^{-n\epsilon} \leq \delta$$

$$\epsilon \geq -\frac{log(\frac{\delta}{|\mathbb{F}|})}{n} = \frac{log(\frac{|\mathbb{F}|}{\delta})}{n}$$

So, the minimum $\epsilon = \frac{log(\frac{|\mathbb{F}|}{\delta})}{n}$

d. *[4 points]* Since $\hat{R}_n(f) \geq 0$ and $\hat{R}_n(\hat{f}) = 0$, then $\hat{f} \in arg\; min_{f \in \mathbb{F}} \hat{R}_n(f)$
From part b, we have

$$Pr(\exists \hat{f} \in arg\; min_{f \in \mathbb{F}} \hat{R}_n(f) \; s.t.R(\hat{f}) > \epsilon \; and \; \hat{R_n}(\hat{f}) = 0) \leq |\mathbb{F}| e^{-n\epsilon}$$

From part c, we have $\epsilon = \frac{log(\frac{|\mathbb{F}|}{\delta})}{n}$

$$Pr(\exists \hat{f} \in arg\; min_{f \in \mathbb{F}} \hat{R}_n(f) \; s.t.R(\hat{f}) > \frac{log(\frac{|\mathbb{F}|}{\delta})}{n} \; and \; \hat{R_n}(\hat{f}) = 0) \leq \delta$$

$$R(f) > \epsilon = \frac{log(\frac{|\mathbb{F}|}{\delta})}{n}$$

$$Pr(\hat{R_n}(f) = 0) \leq e^{-n\epsilon} = \delta / |\mathbb{F}|$$

Accoding to Hoeffding's inequality,

$$Pr[R(\hat{f}) - R(f^*) \geq \frac{log(|\mathbb{F}|/\delta|)}{n}] \leq \delta$$

Using inversion, we get that with probability at least $1 - \delta$:

$$R(\hat{f}) - R(f^*) \leq \frac{log(|\mathbb{F}|/\delta|)}{n}$$