CSE546 Machine Learning HW3

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A.1

a. [2 points] True or False: Given a data matrix $X \in R^{n \times d}$ where d is much smaller than n, if we project our data onto a k dimensional subspace using PCA where k = rank(X), our projection will have 0 reconstruction error (we find a perfect representation of our data, with no information loss).

Solution:
True: If k is rank(k), it means we have captured all variation from the data, and it can perfectly represent the data.

b. [2 points] True or False: The maximum margin decision boundaries that support vector machines construct have the lowest generalization error among all linear classifiers.

Solution:
False, SVM gives us a nice result, but it is not necessarily the lowest. It really depends on use cases and datasets. For example, the underlining true model need to be considered as well.

c. [2 points] True or False: An individual observation xi can occur multiple times in a single bootstrap sample from a dataset X, even if xi only occurs once in X.

Solution:
True: Bootstrap is done by draw sample with replacement.

d. [2 points] True or False: Suppose that the SVD of a square $n \times n$ matrix X is USV^T, where S is a diagonal $n \times n$ matrix. Then the rows of V are equal to the eigenvectors of $X^T X$.

Solution:
False, the columns are eigenvectors.

e. [2 points] True or False: Performing PCA to reduce the feature dimensionality and then applying the Lasso results in an interpretable linear model.

Solution:
False: When we use PCA, the data lost the interpretability, the data are reconstructed. Lasso can not make this model interpret-able.

f. [2 points] True or False: choosing k to minimize the k-means objective (see Equation (1) below) is a good way to find meaningful clusters.

Solution:
False, the bigger k we used, the less distance we will have, and this does not mean that our model gets better and better.

g. [2 points] Say you trained an SVM classifier with an RBF kernel $K(u, v) = exp(-\frac{||u-v||_2^2}{2\sigma^2})$. It seems to under-fit the training set: should you increase or decrease σ?

Solution:

We should decrease σ to increase some complexity of our model. When σ is big, the boundary tends to be pretty smooth, but when σ getting smaller, the boundary gets more strict.

A.2

Kernels and the Bootstrap

A2. *[5 points]* Suppose that our inputs x are one-dimensional and that our feature map is infinite-dimensional: $\phi(x)$ is a vector whose ith component is

$$\frac{1}{\sqrt{i!}} e^{-\frac{x^2}{2}} x^i$$

for all nonnegative integers i. (Thus, ϕ is an infinite-dimensional vector.) Show that $K(x, x') = e^{-\frac{(x-x')^2}{2}}$ is a kernel function for this feature map, i.e.,

$$\phi(x) \cdot \phi(x') = e^{-\frac{(x-x')^2}{2}}.$$

Hint: Use the Taylor expansion of e^z. (This is the one dimensional version of the Gaussian (RBF) kernel).

Solution:

From the question, we know that:

$$K(x, x') = \phi(x) \cdot \phi(x')$$

We also can get that:

$$\phi(x) = \frac{1}{\sqrt{i!}} e^{\frac{-x^2}{2}} x^i$$

$$\phi(x') = \frac{1}{\sqrt{i!}} e^{-\frac{1}{2}} * 1 = \frac{1}{\sqrt{i!}} \frac{1}{\sqrt{e}}$$

Then do the dot product:

$$K(x, x') = \phi(x) \cdot \phi(x')$$

$$\phi(x) \cdot \phi(x') = \sum_{i=0}^{\infty} \frac{1}{\sqrt{i!}} e^{\frac{-x^2}{2}} x^1 \frac{1}{\sqrt{i!}} \frac{1}{\sqrt{e}}$$

$$\phi(x) \cdot \phi(x') = \sum_{i=0}^{\infty} \frac{1}{i!} e^{\frac{-x^2}{2}} x^i \frac{1}{\sqrt{e}}$$

$$\phi(x) \cdot \phi(x') = \sum_{i=0}^{\infty} \frac{1}{i!} e^{-\frac{x^2+1}{2}} x^i$$

$$\phi(x) \cdot \phi(x') = e^{-\frac{x^2+1}{2}} \sum_{i=0}^{\infty} \frac{x^i}{i!}$$

After doing Taylor Expansion:

$$\phi(x) \cdot \phi(x') = e^{-\frac{x^2+1}{2}} e^x$$

$$\phi(x) \cdot \phi(x') = e^{-\frac{x^2-2x+1}{2}}$$

$$\phi(x) \cdot \phi(x') = e^{-\frac{(x-1)^2}{2}}$$

Here we know that $x' = 1$, then:

$$\phi(x) \cdot \phi(x') = e^{-\frac{(x-x')^2}{2}}$$

So,

$$K(x, x') = e^{-\frac{(x-x')^2}{2}}$$

A.3

a.

A3. This problem will get you familiar with kernel ridge regression using the polynomial and RBF kernels. First, let's generate some data. Let $n = 30$ and $f_*(x) = 4\sin(\pi x)\cos(6\pi x^2)$. For $i = 1, \ldots, n$ let each x_i be drawn uniformly at random on $[0, 1]$ and $y_i = f_*(x_i) + \epsilon_i$ where $\epsilon_i \sim \mathcal{N}(0, 1)$.
For any function f, the true error and the train error are respectively defined as

$$\mathcal{E}_{true}(f) = E_{XY}[(f(X) - Y)^2], \qquad \widehat{\mathcal{E}}_{train}(f) = \frac{1}{n}\sum_{i=1}^{n}(f(x_i) - y_i)^2.$$

Using kernel ridge regression, construct a predictor

$$\widehat{\alpha} = \arg\min_{\alpha} ||K\alpha - y||^2 + \lambda\alpha^T K\alpha \ , \qquad \widehat{f}(x) = \sum_{i=1}^{n}\widehat{\alpha}_i k(x_i, x)$$

where $K_{i,j} = k(x_i, x_j)$ is a kernel evaluation and λ is the regularization constant. Include any code you use for your experiments in your submission.

a. *[10 points]* Using leave-one-out cross validation, find a good λ and hyperparameter settings for the following kernels:

- $k_{poly}(x, z) = (1 + x^T z)^d$ where $d \in \mathbb{N}$ is a hyperparameter,
- $k_{rbf}(x, z) = \exp(-\gamma\|x - z\|^2)$ where $\gamma > 0$ is a hyperparameter[1].

Report the values of d, γ, and the λ values for both kernels.

Solution:

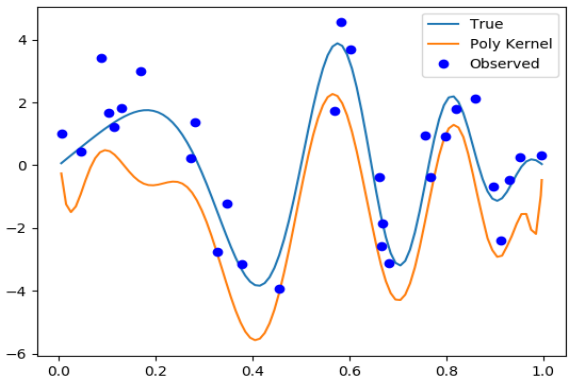
Best lamb for Poly kernel: 0.48828125.
Best d for Poly kernel: 44.

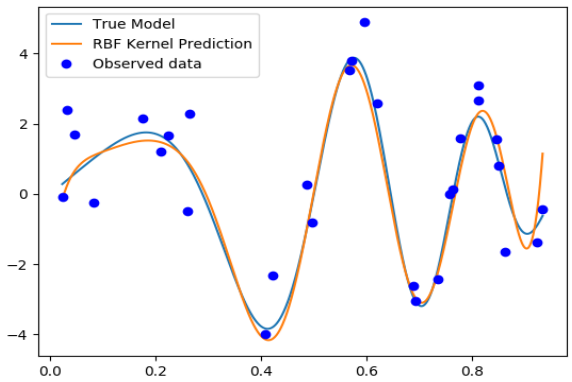
Best gamma for RBF kernel is : 8.175399541327897
Best Lambda for RBF kernel is : 9.313225746154785e-07

b.

b. *[10 points]* Let $\widehat{f}_{poly}(x)$ and $\widehat{f}_{rbf}(x)$ be the functions learned using the hyperparameters you found in part a. For a single plot per function $\widehat{f} \in \{\widehat{f}_{poly}(x), \widehat{f}_{rbf}(x)\}$, plot the original data $\{(x_i, y_i)\}_{i=1}^n$, the true $f(x)$, and $\widehat{f}(x)$ (i.e., define a fine grid on $[0, 1]$ to plot the functions).

Solution:





[1]

c.

c. *[5 points]* We wish to build bootstrap percentile confidence intervals for $\widehat{f}_{poly}(x)$ and $\widehat{f}_{rbf}(x)$ for all $x \in [0,1]$ from part b.[2] Use the non-parametric bootstrap with $B = 300$ bootstrap iterations to find 5% and 95% percentiles at each point x on a fine grid over $[0,1]$.

Specifically, for each bootstrap sample $b \in \{1,\ldots,B\}$, draw uniformly at randomly with replacement n samples from $\{(x_i,y_i)\}_{i=1}^n$, train an $\widehat{f}_b$ using the bth resampled dataset, compute $\widehat{f}_b(x)$ for each x in your fine grid; let the 5th percentile at point x be the largest value ν such that $\frac{1}{B}\sum_{b=1}^B \mathbf{1}\{\widehat{f}_b(x) \leq \nu\} \leq .05$, define the 95% analogously.

Plot the 5 and 95 percentile curves on the plots from part b.

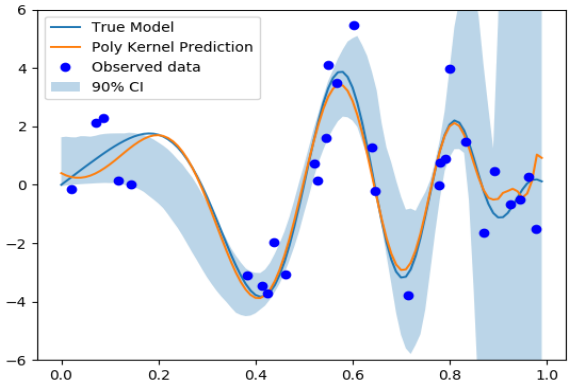
[1] Given a dataset $x_1,\ldots,x_n \in \mathbb{R}^d$, a heuristic for choosing a range of γ in the right ballpark is the inverse of the median of all $\binom{n}{2}$ squared distances $||x_i - x_j||_2^2$.

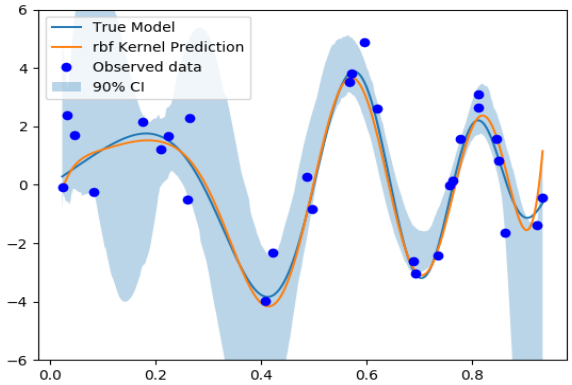
[2] See Hastie, Tibshirani, Friedman Ch. 8.2 for a review of the bootstrap procedure.

Solution:

In order to train a kernel model for each re-sampled bootstrap sample, we need to compute a new alpha and K each time, according to:

$$\hat{f}(x) = \sum_{i=1}^{n} \hat{\alpha}_i k(x_i, x)$$





Code for question a,b,c,

```
# b1 can also be used as part a's code
# A3.b1
import numpy as np
import matplotlib.pyplot as plt
```

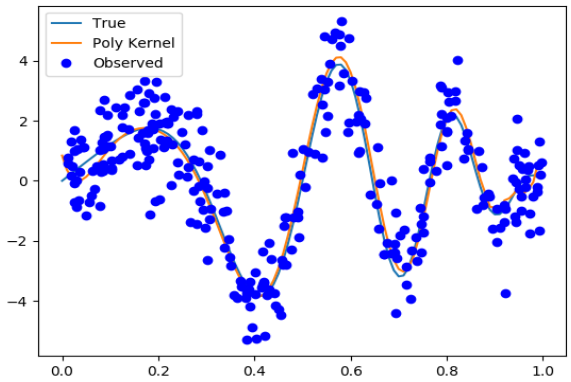
```

n = 30
# np.random.seed(1)
x = np.random.uniform(0,1,n)
x_mean = np.mean(x)
x_sd = np.std(x)
# x = (x-x_mean)  # x after standardization

y = 4*np.sin(np.pi*x)*np.cos(6*np.pi*(x**2)) + np.random.standard_normal(n)
# y = (y - x_mean) / x_sd
def k_poly(x, z, d):
  a = x @ z.T
  k = (1 + x @ z.T)**d
  return k

error_validation_list = []
lamb = 500
lamb_list = []
d_list = []
for lamb in list(500 * (1/2)**(np.arange(0,20))):
  for d in list(range(0, 51)):
    error_validation = 0
    print("Lam: ", lamb, ", d: ", d)
    for i in range(n):
      x_train = np.append(x[0:i], x[i+1:n])
      y_train = np.append(y[0:i], y[i+1:n])
      x_validation = x[i]
      y_validation = y[i]
      K = k_poly(x_train[:, np.newaxis], x_train[:, np.newaxis], d)
      alpha = np.linalg.pinv(K + lamb) @ y_train
      # in predicted y formula
      k_xi_x = (1 + x_validation * x_train[np.newaxis, :]) ** d   # use this when polynomial kernel
      # k_xi_x = np.exp(-gamma*np.linalg.norm(x_validation - x_train[np.newaxis, :], 2))
      y_predicted = alpha @ k_xi_x.T
      error_validation += (y_predicted - y_validation).T @ (y_predicted- y_validation)
      # error_validation = error_validation[0][0]
    error_validation /= n
    print("error_validation: ", error_validation)
    error_validation_list.append(error_validation)
    lamb_list.append(lamb)
    d_list.append(d)

min_error = min(error_validation_list)
index_boostrap_sample_min_error = error_validation_list.index(min(error_validation_list))
lamb_best_poly = lamb_list[index_boostrap_sample_min_error]
d_best = d_list[index_boostrap_sample_min_error]
print("Best lamb: ", lamb_best_poly, ", Best d: ", d_best)

# lamb_best_poly = 0.48828125
d_best = 30
# plots the comparaison
# np.random.seed(1)
x_fine = np.array(list(np.arange(min(x),max(x), 0.01))  )
n = len(x_fine)
y_fine_true = 4*np.sin(np.pi*x_fine)*np.cos(6*np.pi*(x_fine**2))
y_fine_grid = y_fine_true + np.random.standard_normal(n)
f_poly_predicted = []
for xi in x_fine:
```

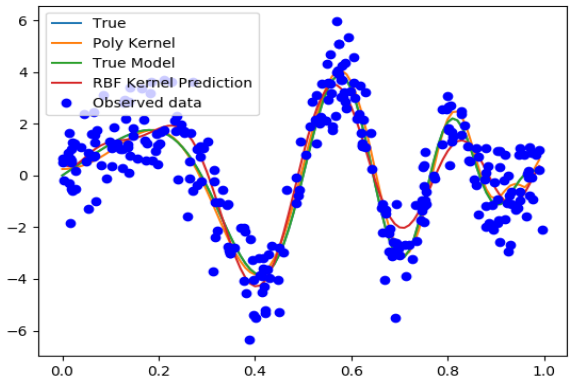
```
    K = k_poly(x_fine[:, np.newaxis], x_fine[:, np.newaxis], d_best)
    alpha = np.linalg.pinv(K + lamb_best_poly) @ y_fine_grid
    k_xi_x = (1 + xi * x_fine[np.newaxis, :]) ** d_best  # use this when polynomial kernel
    y_predicted = alpha @ k_xi_x.T
    f_poly_predicted.append(y_predicted)

plt.plot(x_fine, y_fine_true, label='True')
plt.plot(x_fine, f_poly_predicted, label='Poly Kernel')
plt.plot(x, y,'bo', label='Observed')
plt.xlabel("X")
plt.ylabel("Y")
plt.legend()
plt.savefig("/Users/yinruideng/Desktop/senior_spring/cse546/hw/hw3/latex/plots/A3b_1_test.png")
plt.show()


# A3.c1
B = 300
n = 30
n_fine = len(x_fine)
# np.random.seed(0)
boostrap_predicted_poly_matrix = []

for j in range(B):
    index_boostrap_sample = np.random.choice(n,n)
    x_training = x[index_boostrap_sample]
    y_training = y[index_boostrap_sample]
    K = k_poly(x_training[:,np.newaxis],x_training[:,np.newaxis], d_best)
    alpha = np.linalg.solve((K + lamb_best_poly*np.eye(n, n)), y_training)
    y_predicted_boostrap_ploy = []
    for xi in x_fine:
        y_predicted_boostrap_ploy.append(np.sum((1+xi*x_training[np.newaxis,:]) ** d_best @ alpha))
    boostrap_predicted_poly_matrix.append(y_predicted_boostrap_ploy)
boostrap_predicted_poly_matrix = np.array(boostrap_predicted_poly_matrix)

percent_5_list_poly = []
percent_95_list_poly = []
for i in range(n_fine):
    sorted_xi_from_300_B_sample = np.sort(boostrap_predicted_poly_matrix[:, i])
    x_percentile_5 = sorted_xi_from_300_B_sample[int(B * 0.05)]
    x_percentile_95 = sorted_xi_from_300_B_sample[int(B * 0.95)]
    percent_5_list_poly.append(x_percentile_5)
    percent_95_list_poly.append(x_percentile_95)

plt.plot(x_fine, y_fine_true, label = 'True Model')
plt.plot(x_fine, f_poly_predicted, label = 'Poly Kernel Prediction')
plt.plot(x, y,'bo', label ='Observed data')
plt.fill_between(x_fine, percent_5_list_poly, percent_95_list_poly, alpha=0.3, label="90% CI")
plt.ylim(-6, 6)
plt.legend()
plt.savefig("/Users/yinruideng/Desktop/senior_spring/cse546/hw/hw3/latex/plots/A3c_1_test.png")
plt.show()


#########################################################################################################
# A3.b2

def k_rbf(x, z, gamma):
```

```
  return np.exp(-gamma*(x-z)*(x-z))

n = 30
# np.random.seed(0)
# x = np.random.rand(n)
x = np.random.uniform(0,1,n)
y_true = 4*np.sin(np.pi*x)*np.cos(6*np.pi*(x**2))
y = y_true + np.random.randn(n)
error_validation_list = []
lamb_list = []
gamma_list = []
d_list =[]

lamb = 1
for lamb in list(500 * (1/2)**(np.arange(0,30))):
  for gamma in list(50 * (1/1.1)**(np.arange(0,30))):
    print("Lam: ", lamb, ", gamma: ", gamma)
    error_validation = 0
    for i in range(n):
      x_train = np.append(x[0:i], x[i+1:n])
      y_train = np.append(y[0:i], y[i+1:n])
      x_validation = x[i]
      y_validation = y[i]
      K = k_rbf(x_train[:,np.newaxis],x_train[np.newaxis,:], gamma)
      alpha = np.linalg.pinv(K + lamb) @ y_train
      k_xi_x = np.exp(-gamma*(x_validation-x_train[np.newaxis,:])**2)
      error_validation += (k_xi_x@alpha - y_validation).T@(k_xi_x@alpha - y_validation)
    error_validation_list.append(error_validation)
    print("error_validation: ", error_validation)
    lamb_list.append(lamb)
    gamma_list.append(gamma)

min_error = min(error_validation_list)
index_boostrap_sample_min_error = error_validation_list.index(min_error)
lamb_best_rbf = lamb_list[index_boostrap_sample_min_error]
gamma_best = gamma_list[index_boostrap_sample_min_error]
print('Best gamma for RBF kernel is : ', gamma_best)
print('Best Lambda for RBF kernel is :', lamb_best_rbf)


gamma_best= 10.175399541327897
lamb_best_rbf= 9.313225746154785e-07
# np.random.seed(10)

x_fine = np.arange(min(x),max(x),0.001)
n = len(x_fine)
y_fine_true = 4*np.sin(np.pi*x_fine)*np.cos(6*np.pi*(x_fine**2))
y_fine_grid = y_fine_true + np.random.standard_normal(n)

f_rbf_predicted = []
K_rbf = k_rbf(x_fine[:,np.newaxis],x_fine[np.newaxis,:], gamma_best)
alpha = np.linalg.solve((K_rbf + lamb_best_rbf*np.eye(n, n)), y_fine_grid)
for xi in x_fine:
  f_rbf_predicted.append(np.sum(alpha * np.exp(-gamma_best*(xi-x_fine)**2)))

plt.plot(x_fine, y_fine_true, label = 'True Model')
plt.plot(x_fine, f_rbf_predicted, label = 'RBF Kernel Prediction')
plt.plot(x, y,'bo', label ='Observed data')
```

```
plt.legend()
plt.savefig("/Users/yinruideng/Desktop/senior_spring/cse546/hw/hw3/latex/plots/A3b_2.png")
plt.show()

# A3.c2
B = 300
n=30
n_fine = len(x_fine)
# np.random.seed(0)
boostrap_predicted_rbf_matrix = []
# user x, y from previous
for j in range(B):
  index_boostrap_sample = np.random.choice(n,n)
  x_training = x[index_boostrap_sample]
  y_training = y[index_boostrap_sample]
  K_rbf = k_rbf(x_training[:, np.newaxis], x_training[np.newaxis, :], gamma_best)
  alpha = np.linalg.solve((K_rbf + lamb_best_rbf * np.eye(n, n)), y_training)

  y_predicted_boostrap_rbf = []
  for xi in x_fine:
    y_predicted_boostrap_rbf.append(np.sum(alpha * np.exp(-gamma_best*(xi-x_training)**2)))
boostrap_predicted_rbf_matrix.append(y_predicted_boostrap_rbf)
boostrap_predicted_rbf_matrix = np.array(boostrap_predicted_rbf_matrix)

percent_5_list_rbf = []
percent_95_list_rbf = []
for i in range(n_fine):
  sorted_xi_from_300_B_sample = np.sort(boostrap_predicted_rbf_matrix[:, i])
  x_percentile_5 = sorted_xi_from_300_B_sample[int(B * 0.05)]
  x_percentile_95 = sorted_xi_from_300_B_sample[int(B * 0.95)]
  percent_5_list_rbf.append(x_percentile_5)
  percent_95_list_rbf.append(x_percentile_95)


plt.plot(x_fine, y_fine_true, label = 'True Model')
plt.plot(x_fine, f_rbf_predicted, label = 'rbf Kernel Prediction')
plt.plot(x, y,'bo', label ='Observed data')
plt.fill_between(x_fine, percent_5_list_rbf, percent_95_list_rbf, alpha=0.3, label="90% CI")
plt.ylim(-6, 6)
plt.legend()
plt.savefig("/Users/yinruideng/Desktop/senior_spring/cse546/hw/hw3/latex/plots/A3c_2_test.png")
plt.show()
##########################################################################################################
```

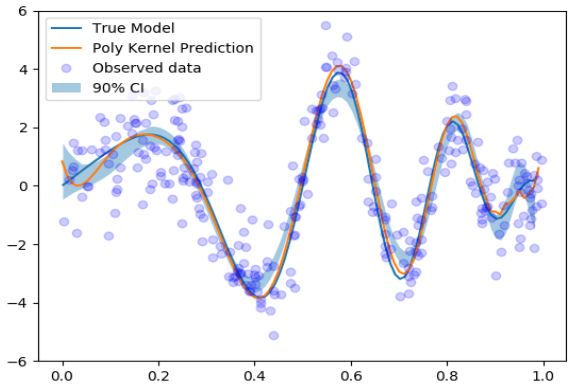
d.

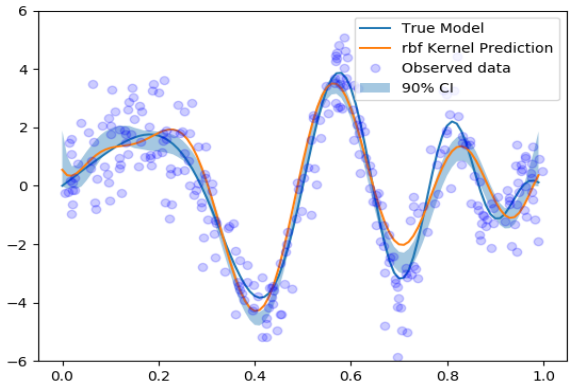




Best lamb: 0.003814697265625 , Best d: 33

Best gamma for RBF kernel is : 8.992939495460687
Best Lambda for RBF kernel is : 1.862645149230957e-06





e.

5%: -0.14401336443720553
95%: -0.0253960255137911
In my case, 0 is not included in the confidence interval. And since the 5% and 95% are negative, so it is suggesting that with 90% confidence that RBF kernel is better than Polynomial kernel regression.

Code for question d,e,

```
# A3.d - 1 ##########################################################################################
import numpy as np
import matplotlib.pyplot as plt

n = 300
# np.random.seed(1)

x = np.random.uniform(0,1,n)
y = 4*np.sin(np.pi*x)*np.cos(6*np.pi*(x**2)) + np.random.standard_normal(n)

def k_poly(x, z, d):
  a = x @ z.T
  k = (1 + x @ z.T)**d
  return k

```

```
error_validation_list = []
lamb = 500
cv_size = int(n/10)
lamb_list = []
d_list = []
for lamb in list(500 * (1/2)**(np.arange(0, 20))):
  for d in list(range(0, 51)):
    error_validation = 0
    print("Lam: ", lamb, ", d: ", d)
    for i in range(0, n, cv_size):
      x_train = np.append(x[0:i], x[i+cv_size:n])
      y_train = np.append(y[0:i], y[i+cv_size:n])
      x_validation = x[i:i+cv_size]
      y_validation = y[i:i+cv_size]
      K = k_poly(x_train[:, np.newaxis], x_train[:, np.newaxis], d)
      alpha = np.linalg.pinv(K + lamb) @ y_train
      # in predicted y formula
      k_xi_x = (1 + np.multiply(x_validation, np.repeat(x_train[np.newaxis, :],
              cv_size).reshape(270,cv_size)))**d
      # y_predicted = alpha @ k_xi_x.T
      y_predicted = alpha[np.newaxis, :] @ k_xi_x
      error_validation += np.sum((y_predicted - y_validation).T @ (y_predicted- y_validation))
      # error_validation = error_validation[0][0]
      error_validation /= n
    print("error_validation: ", error_validation)
    error_validation_list.append(error_validation)
    lamb_list.append(lamb)
    d_list.append(d)

# min_error = min(error_validation_list)
index_boostrap_sample_min_error = error_validation_list.index(min(error_validation_list))
lamb_best_poly = lamb_list[index_boostrap_sample_min_error]
d_best = d_list[index_boostrap_sample_min_error]
print("Best lamb: ", lamb_best_poly, ", Best d: ", d_best)

# Best lamb:  0.003814697265625 , Best d:  40

# plots the comparaison
np.random.seed(1)
n = 100
x_fine = np.array(list(range(0, 100, 1))) / 100
y_fine_true = 4*np.sin(np.pi*x_fine)*np.cos(6*np.pi*(x_fine**2))
y_fine_grid = y_fine_true + np.random.standard_normal(n)
f_poly_predicted = []
for xi in x_fine:
  K = k_poly(x_fine[:, np.newaxis], x_fine[:, np.newaxis], d_best)
  alpha = np.linalg.pinv(K + lamb_best_poly) @ y_fine_grid
  k_xi_x = (1 + xi * x_fine[np.newaxis, :]) ** d_best  # use this when polynomial kernel
  y_predicted = alpha @ k_xi_x.T

  f_poly_predicted.append(y_predicted)

plt.plot(x_fine, y_fine_true, label='True')
plt.plot(x_fine, f_poly_predicted, label='Poly Kernel')
plt.plot(x, y,'bo', label='Observed')
plt.legend()
plt.savefig("/Users/yinruideng/Desktop/senior_spring/cse546/hw/hw3/latex/plots/A3d_1_test.png")
plt.show()
```

```
74
75  # ------------------------------- #
76
77  B = 300
78  n=300
79  m = 1000
80  x_fine = np.arange(min(x),max(x),0.01)
81  n_fine = len(x_fine)
82  # np.random.seed(10)
83  boostrap_predicted_poly_matrix = []
84  x = np.random.uniform(0,1,n)
85  y_true_sample = 4*np.sin(np.pi*x)*np.cos(6*np.pi*(x**2))
86  y_observed = y_true_sample + np.random.randn(n)
87
88  for j in range(B):
89    index_boostrap_sample = np.random.choice(n,n)
90    x_training = x[index_boostrap_sample]
91    y_training = y_observed[index_boostrap_sample]
92    K = k_poly(x_training[:,np.newaxis],x_training[:,np.newaxis], d_best)
93    alpha = np.linalg.solve((K + lamb_best_poly*np.eye(n, n)), y_training)
94    y_predicted_boostrap_ploy = []
95    # for xi in np.array(list(range(0, 100, 1))) / 100:
96    # test
97    K = k_poly(x_training[:,np.newaxis],x_training[:,np.newaxis], d_best)
98    alpha = np.linalg.solve((K + lamb_best_poly*np.eye(n, n)), y_training)
99
100   for xi in x_fine:
101     y_predicted_boostrap_ploy.append(np.sum((1+xi*x_training[np.newaxis,:]) ** d_best @ alpha))
102   boostrap_predicted_poly_matrix.append(y_predicted_boostrap_ploy)
103 boostrap_predicted_poly_matrix = np.array(boostrap_predicted_poly_matrix)
104
105 percent_5_list_poly = []
106 percent_95_list_poly = []
107 for i in range(n_fine):
108   sorted_xi_from_300_B_sample = np.sort(boostrap_predicted_poly_matrix[:, i])
109   x_percentile_5 = sorted_xi_from_300_B_sample[int(B * 0.05)]
110   x_percentile_95 = sorted_xi_from_300_B_sample[int(B * 0.95)]
111   percent_5_list_poly.append(x_percentile_5)
112   percent_95_list_poly.append(x_percentile_95)
113
114 # x_fine = np.array(list(range(0, 100, 1))) / 100
115 y_fine_true = 4*np.sin(np.pi*x_fine)*np.cos(6*np.pi*(x_fine**2))
116 plt.plot(x_fine, y_fine_true, label = 'True Model')
117 plt.plot(np.array(list(range(0, 100, 1))) / 100, f_poly_predicted, label = 'Poly Kernel Prediction')
118 plt.fill_between(x_fine, percent_5_list_poly, percent_95_list_poly, alpha=0.4, label="90% CI")
119 plt.plot(x, y_observed,'bo', alpha=0.2, label ='Observed data')
120 plt.ylim(-6, 6)
121 plt.legend()
122 plt.savefig("/Users/yinruideng/Desktop/senior_spring/cse546/hw/hw3/latex/plots/A3e_1_test.png")
123 plt.show()
124
125
126
127 ##########################################################################################################
128
129 # A3.d - 2
130
131 def k_rbf(x, z, gamma):
```

```
  return np.exp(-gamma*(x-z)*(x-z))

n = 300
np.random.seed(1)
cv_size = int(n/10)
x = np.random.uniform(0,1,n)
y_true = 4*np.sin(np.pi*x)*np.cos(6*np.pi*(x**2))
y = y_true + np.random.randn(n)
error_validation_list = []
lamb_list = []
gamma_list = []
d_list =[]

lamb = 1
for lamb in list(500 * (1/2)**(np.arange(0,30))):
  for gamma in list(50 * (1/1.1)**(np.arange(0,30))):
    print("Lam: ", lamb, ", gamma: ", gamma)
    error_validation = 0
    for i in range(0, n, cv_size):
      x_train = np.append(x[0:i], x[i+cv_size:n])
      y_train = np.append(y[0:i], y[i+cv_size:n])
      x_validation = x[i:i+cv_size]
      y_validation = y[i:i+cv_size]
      K = k_rbf(x_train[:,np.newaxis],x_train[np.newaxis,:], gamma)
      alpha = np.linalg.pinv(K + lamb) @ y_train
      k_xi_x = np.exp(-gamma*(x_validation - np.repeat(x_train[np.newaxis,:],
              cv_size).reshape((n-cv_size, cv_size)))**2)
      y_predicted = alpha[np.newaxis, :] @ k_xi_x
      error_validation += np.sum((y_predicted - y_validation).T @ (y_predicted- y_validation))
    error_validation /= n
    error_validation_list.append(error_validation)
    print("error_validation: ", error_validation)
    lamb_list.append(lamb)
    gamma_list.append(gamma)

min_error = min(error_validation_list)
index_boostrap_sample_min_error = error_validation_list.index(min_error)
lamb_best_rbf = lamb_list[index_boostrap_sample_min_error]
gamma_best = gamma_list[index_boostrap_sample_min_error]
print('Best gamma for RBF kernel is : ', gamma_best)
print('Best Lambda for RBF kernel is :', lamb_best_rbf)

# Best gamma for RBF kernel is :  8.992939495460687
# Best Lambda for RBF kernel is : 1.862645149230957e-06
# plots the comparaison
n = 100
np.random.seed(10)

x_fine = np.array(list(range(0, 100, 1))) / 100
y_fine_true = 4*np.sin(np.pi*x_fine)*np.cos(6*np.pi*(x_fine**2))
y_fine_grid = y_fine_true + np.random.standard_normal(n)

f_rbf_predicted = []
K_rbf = k_rbf(x_fine[:,np.newaxis],x_fine[np.newaxis,:], gamma_best)
alpha = np.linalg.solve((K_rbf + lamb_best_rbf*np.eye(n, n)), y_fine_grid)
for xi in x_fine:
  f_rbf_predicted.append(np.sum(alpha * np.exp(-gamma_best*(xi-x_fine)**2)))

```

```
plt.plot(x_fine, y_fine_true, label = 'True Model')
plt.plot(x_fine, f_rbf_predicted, label = 'RBF Kernel Prediction')
plt.plot(x, y,'bo', label ='Observed data')
plt.legend()
plt.savefig("/Users/yinruideng/Desktop/senior_spring/cse546/hw/hw3/latex/plots/A3d_2_test.png")
plt.show()


# A3.e2
B = 300
n=300
# m=1000
# n_fine = 100
np.random.seed(0)
boostrap_predicted_rbf_matrix = []
# x = np.array(list(range(0, 100, 1))) / 100
x = np.random.uniform(0,1,n)
y_true_sample = 4*np.sin(np.pi*x)*np.cos(6*np.pi*(x**2))
y_observed = y_true_sample + np.random.randn(n)

for j in range(B):
  index_boostrap_sample = np.random.choice(n,n)
  x_training = x[index_boostrap_sample]
  y_training = y_observed[index_boostrap_sample]
  K_rbf = k_rbf(x_training[:, np.newaxis], x_training[np.newaxis, :], gamma_best)
  alpha = np.linalg.solve((K_rbf + lamb_best_rbf * np.eye(n, n)), y_training)

  y_predicted_boostrap_rbf = []
  for xi in x_fine:
    # k_xi_x = np.exp(-gamma * (xi - x_training[np.newaxis, :]) ** 2)
    # predicted = k_xi_x@alpha
    y_predicted_boostrap_rbf.append(np.sum(alpha * np.exp(-gamma_best*(xi-x_training)**2)))
  boostrap_predicted_rbf_matrix.append(y_predicted_boostrap_rbf)
boostrap_predicted_rbf_matrix = np.array(boostrap_predicted_rbf_matrix)

percent_5_list_rbf = []
percent_95_list_rbf = []
for i in range(len(x_fine)):
  sorted_xi_from_300_B_sample = np.sort(boostrap_predicted_rbf_matrix[:, i])
  x_percentile_5 = sorted_xi_from_300_B_sample[int(B * 0.05)]
  x_percentile_95 = sorted_xi_from_300_B_sample[int(B * 0.95)]
  percent_5_list_rbf.append(x_percentile_5)
  percent_95_list_rbf.append(x_percentile_95)

x_fine = np.array(list(range(0, 100, 1))) / 100
y_fine_true = 4*np.sin(np.pi*x_fine)*np.cos(6*np.pi*(x_fine**2))
plt.plot(x_fine, y_fine_true, label = 'True Model')
plt.plot(x_fine, f_rbf_predicted, label = 'rbf Kernel Prediction')
plt.fill_between(x_fine, percent_5_list_rbf, percent_95_list_rbf, alpha=0.4, label="90% CI")
plt.plot(x, y_observed,'bo', alpha=0.2, label ='Observed data')
plt.ylim(-6, 6)
plt.legend()
plt.savefig("/Users/yinruideng/Desktop/senior_spring/cse546/hw/hw3/latex/plots/A3e_2_test.png")
plt.show()
```

```
248
249
250
251 ########################################## A3 e ##########################################
252 #
253 #                                          A3 e
254 #
255 ########################################## A3 e ##########################################
256 d_best=33
257
258 B = 300
259 n=300
260 m=1000
261 np.random.seed(4)
262 x = np.random.uniform(0,1,m+n)
263 y_true_sample = 4*np.sin(np.pi*x)*np.cos(6*np.pi*(x**2))
264 y_observed = y_true_sample + np.random.randn(m+n)
265 error_difference_list = np.zeros(B)
266
267 for j in range(B):
268   print("B: ", j)
269   index_boostrap_sample = np.random.choice(m+n,m)
270   x_training = x[index_boostrap_sample]
271   y_training = y_observed[index_boostrap_sample]
272   # comput poly kernel
273   K = k_poly(x_training[:, np.newaxis], x_training[:, np.newaxis], d_best)
274   alpha = np.linalg.pinv(K + lamb_best_poly) @ y_training
275   # compute rbf kernel
276   K_rbf = k_rbf(x_training[:, np.newaxis], x_training[np.newaxis, :], gamma_best)
277   alpha_rbf = np.linalg.solve((K_rbf + lamb_best_rbf * np.eye(m, m)), y_training)
278
279   error_difference = 0
280   for i in range(len(x_training)):
281     # poly predicted
282     k_xi_x = (1 + x_training[i] * x_training[np.newaxis, :]) ** d_best  # use this when polynomial k
283     y_predicted = alpha @ k_xi_x.T
284     # rbf predicted
285     y_predicted_rbf = np.sum(alpha_rbf * np.exp(-gamma_best*(x_training[i]-x_training)**2))
286     # error difference
287     error_difference += (y_training[i] - y_predicted)**2 - (y_training[i] - y_predicted_rbf)**2
288   error_difference /= len(x_training)
289   # error_difference_list.append(error_difference)
290   print("error_difference: ", error_difference)
291   error_difference_list[j] = error_difference
292   error_difference_list = np.sort(error_difference_list)
293
294 print("5%: ", error_difference_list[int(B * 0.05)])
295 print("95%: ", error_difference_list[int(B * 0.95)])
```

A.4

a.

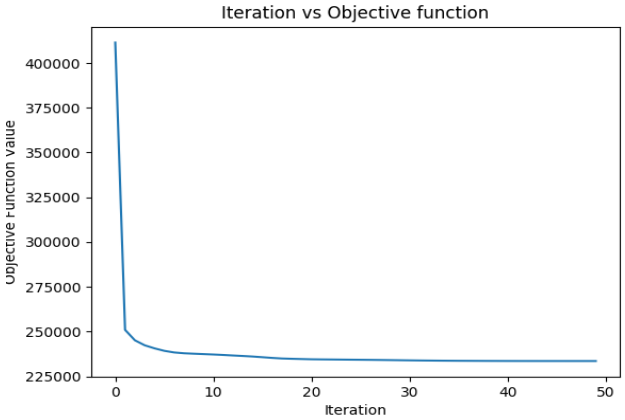
```
1 import numpy as np
2 import matplotlib.pyplot as plt
3 from mnist import MNIST
4 import random
5
```

```python
def load_data(size=1):
  print("Loading Date!")
  mndata = MNIST('python-mnist/data/')
  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

  if (size != 1):
    return X_train[:int(len(X_train)*size)], \
    labels_train[:int(len(labels_train)*size)], \
    X_test[:int(len(X_test)*size)], \
    labels_test[:int(len(labels_test)*size)]
  else:
    return X_train, labels_train, X_test, labels_test
X_train, y_train, X_test, y_test = load_data(size=0.1)
print("Load Data Compelete!")

def compute_cluster(X_train, centers, k):
  objective_value = 0
  clusters = [[] for i in range(k)]
  for i in np.arange(len(X_train)):
    distance_list = []
    for center in centers:
      norm = np.linalg.norm(X_train[i] - center)
      distance_list.append(norm)
    closesed_center_index = distance_list.index(min(distance_list))
    objective_value += min(distance_list)**2
    clusters[closesed_center_index].append(X_train[i])
  return clusters, objective_value

def compute_centers(classes):
  centers = []
  for i in range(len(classes)):
    centers.append(np.mean(classes[i], axis = 0))
  return centers

objective_value_list = []

k = 10
objs = []
iteration = 0
old_centers = random.sample(list(X_train), k)
new_centers = random.sample(list(X_train), k)
while not np.array_equal(old_centers, new_centers):
  iteration += 1
  print("Iteration: ", iteration)
  print("----------  Compute Clusters -----------")
  old_centers = new_centers
  clusters, objective_value = compute_cluster(X_train, new_centers, k)
  print("objective_value: ", objective_value)
  new_centers = compute_centers(clusters)
  objective_value_list.append(objective_value)
```

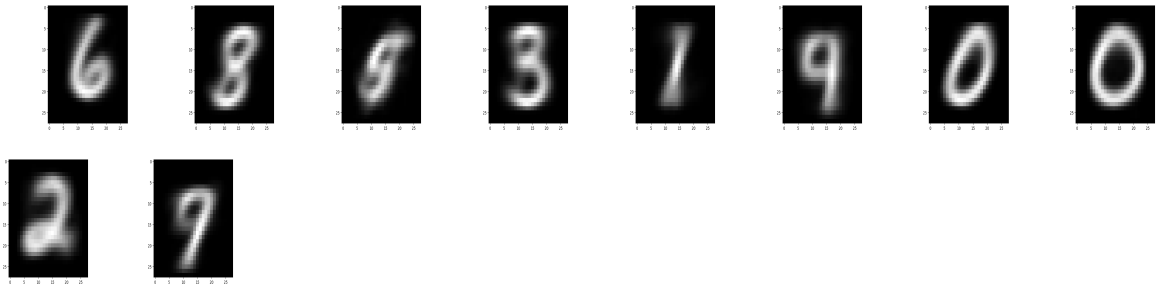
b.

```python
# plot center imgs
for i in range(k):
```

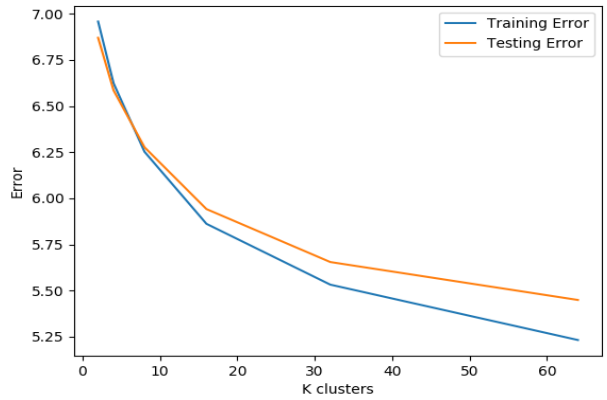
```
    plt.imshow(new_centers[i].reshape((28, 28)))
    plt.savefig("/Users/yinruideng/Desktop/senior_spring/cse546/hw/hw3/latex/plots/A4/A4b_"+
    str(i)+".png")
plt.show()
```



When K = 10, the centroids are:



c.




```
objective_value_list = []
training_error_list = []
testing_error_list = []
k_list = [2,4,8,16,32,64]

for k in k_list:
    objs = []
    iteration = 0
    old_centers = random.sample(list(X_train), k)
```

```
    new_centers = random.sample(list(X_train), k)
    while not np.array_equal(old_centers, new_centers):
      iteration += 1
      print("Iteration: ", iteration)
      print("----------  Compute Clusters -----------")
      old_centers = new_centers
      clusters, objective_value = compute_cluster(X_train, new_centers, k)
      print("objective_value: ", objective_value)
      new_centers = compute_centers(clusters)
      objective_value_list.append(objective_value)
    training_error = 0
    for x_i in X_train:
      distance_to_center = [np.linalg.norm(x_i - center) for center in new_centers]
      training_error += min(distance_to_center)
    training_error /= len(X_train)
    training_error_list.append(training_error)

    testing_error = 0
    for x_i in X_test:
      distance_to_center = [np.linalg.norm(x_i - center) for center in new_centers]
      testing_error += min(distance_to_center)
    testing_error /= len(X_test)
    testing_error_list.append(testing_error)

plt.plot(k_list, training_error_list, label="Training Error")
plt.plot(k_list, testing_error_list, label="Testing Error")
plt.ylabel("Error")
plt.xlabel("K clusters")
plt.legend()
plt.savefig("/Users/yinruideng/Desktop/senior_spring/cse546/hw/hw3/latex/plots/A4/A4c.png")
plt.show()
```

B.1

a.

From the hint, we get to know that:

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

Then based on for some $f_i \in \mathcal{F}$, we have $R(f_i) > \epsilon$,

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

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

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

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

$$e^{-\epsilon} - 1 \geq -R(f_i)$$

$$e^{-\epsilon} \geq 1 - R(f_i)$$

$$e^{-\epsilon} \geq 1 - E\left[\mathbb{1}\{f(x_1) \neq y_i\}\right]$$

$$e^{-\epsilon} \geq 1 - P\left[\hat{R}_n(f_i) \neq 0\right]$$

$$e^{-\epsilon} \geq P\left[\hat{R}_n(f_i) = 0\right]$$

$$(e^{-\epsilon})^n \geq (P\left[\hat{R}_n(f_i) = 0\right])^n$$

$$e^{-n\epsilon} \geq P\left[\hat{R}_n(f) = 0\right]$$

b.

Suppose there are k f_i satisfy the requirement and Let event:

$$A_i = \{R(f_i) > \epsilon \text{ and } \hat{R}_n(f) = 0\}$$

And from previous question we know that:

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

So this works as well,

$$Pr\big(\hat{R}_n(f) = 0\big) * Pr\big(R(f_i) > \epsilon\big) \leq e^{-n\epsilon}$$

$$Pr(A_i) \leq e^{-n\epsilon}$$

$$Pr(A_1 \cup A_2 \cup A_3 \cdots \cup A_n) \leq \sum_{i=1}^{i=k} A_i$$

$$Pr(A_1 \cup A_2 \cup A_3 \cdots \cup A_n) \leq \sum e^{-n\epsilon}$$

$$Pr(A_1 \cup A_2 \cup A_3 \cdots \cup A_n) \leq ke^{-n\epsilon}$$

So,

$$\prod Pr\big(R(f_i) > \epsilon \text{ and } \hat{R}_n(f) = 0\big) \leq |\mathcal{F}|e^{-n\epsilon}$$

$$Pr\big(\exists f \in \mathcal{F} s.t R(f) > \epsilon \text{ and } \hat{R}_n(f) = 0\big) \leq |\mathcal{F}|e^{-n\epsilon}$$

c.

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

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

$$-\epsilon n \leq log(\frac{\delta}{|\mathcal{F}|})$$

$$\epsilon n \geq log(\frac{|\mathcal{F}|}{\delta})$$

$$\epsilon \geq \frac{1}{n} log(\frac{|\mathcal{F}|}{\delta})$$

So,

$$\epsilon_{min} = \frac{1}{n} log(\frac{|\mathcal{F}|}{\delta})$$

d.

According to Chebyshev Inequality, for any random variable X and $\epsilon > 0$:

$$P(|X - E[X]| > \epsilon) \leq \frac{V[X]}{\epsilon^2}$$

$$P(|X - E[X]| \leq \epsilon) > \frac{V[X]}{\epsilon^2}$$

And here: X is $R(\hat{f})$,
From previous question we got:

$$\epsilon \geq \frac{1}{n} log(\frac{|\mathcal{F}|}{\delta})$$

So,

$$P\big(R(\hat{f}) - R(f^*) \leq \epsilon\big) \geq \frac{V[R(\hat{f})]}{\epsilon^2}$$

So now, we want to prove that:

$$\frac{V[R(\hat{f})]}{\epsilon^2} \geq 1 - \delta$$

So, here is what I will do, I will use the inequality from c:

$$\epsilon \geq \frac{1}{n} log(\frac{|\mathcal{F}|}{\delta})$$

$$(\epsilon)^2 \geq (\frac{1}{n} log(\frac{|\mathcal{F}|}{\delta}))^2$$

$$\frac{V[R(\hat{f})]}{\epsilon^2} \geq V[R(\hat{f})]/(\frac{1}{n} log(\frac{|\mathcal{F}|}{\delta}))^2$$

$$\frac{V[R(\hat{f})]}{\epsilon^2} \geq \frac{n^2 V[R(\hat{f})]}{(log(|\mathcal{F}|) - log(\delta))^2}$$

And the variance need to be noted, variance of distribution of the best function should be smaller than the variance of the original distribution, according to the variance of distribution of sample mean $\sigma_{\bar{x}}^2 = \frac{\sigma_{x_i}^2}{n}$, and same idea applies here. However, it is not nessesarily 1/n in this case, but I will just regard it this way and the inequality will still hold because we know that $V[R(f_i)]$ is bigger than $V[R(\hat{f})]$. And the reason I do this is because $V[R(\hat{f})]$ might be close to 0 and I don't want the numerator to risk to be 0, if the numerator is 0, then the proof failed. So, I will use the following:

$$V[R(\hat{f})] \approxeq \frac{V[R(f_i)]}{n}$$

So,

$$\frac{V}{\epsilon^2} \geq \frac{n^2 \frac{V[R(f_i)]}{n}}{(log(|\mathcal{F}|) - log(\delta))^2}$$

$$\frac{V}{\epsilon^2} \geq \frac{n V[R(f_i)]}{(log(|\mathcal{F}|) - log(\delta))^2}$$

Here, we know that $n > |\mathcal{F}|$ since $|\mathcal{F}|$ is finite, and n is infinity technically. And here $V[R(f_i)] \neq 0$. And since n is approximately infinity, and also the left hand side of the equation is positive, so:

$$n\frac{V[R(f_i)]}{(log(|\mathcal{F}|) - log(\delta))^2} \geq 1$$

$$n\frac{V[R(f_i)]}{(log(|\mathcal{F}|) - log(\delta))^2} \geq 1 - \delta$$

So, now we have proved that:

$$\frac{V[R(\hat{f})]}{\epsilon^2} \geq 1 - \delta$$

Then,

$$P\big(R(\hat{f}) - R(f^*) \leq \epsilon\big) \geq \frac{V[R(\hat{f})]}{\epsilon^2} \geq 1 - \delta$$

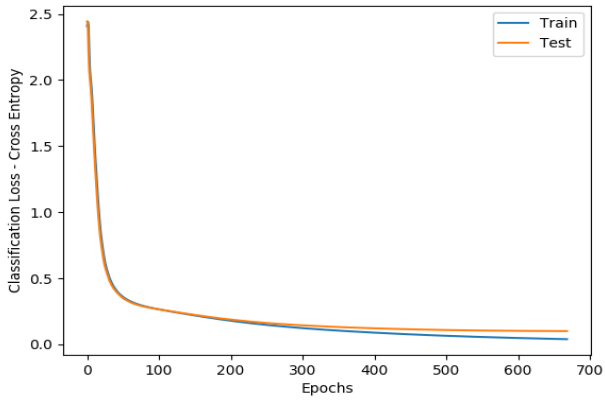
Then,

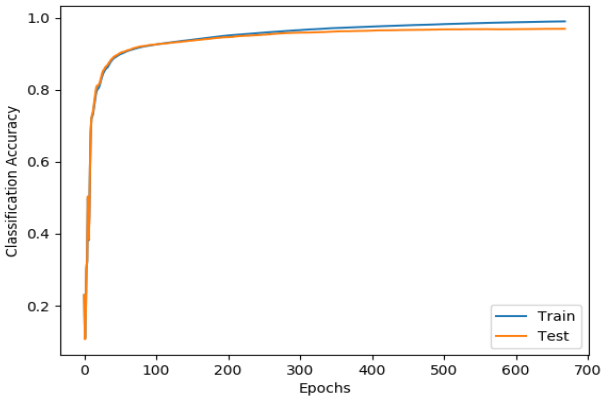
$$P\big(R(\hat{f}) - R(f^*) \leq \frac{log(|\mathcal{F}|/\delta)}{n}\big) \geq \frac{V[R(\hat{f})]}{\epsilon^2} \geq 1 - \delta$$

A.5

a.

This part used a simple nn:





Train Accuracy: 0.99
Test Accuracy: 0.9701
Train Loss: (0.0408)
Test Loss: (0.1029)

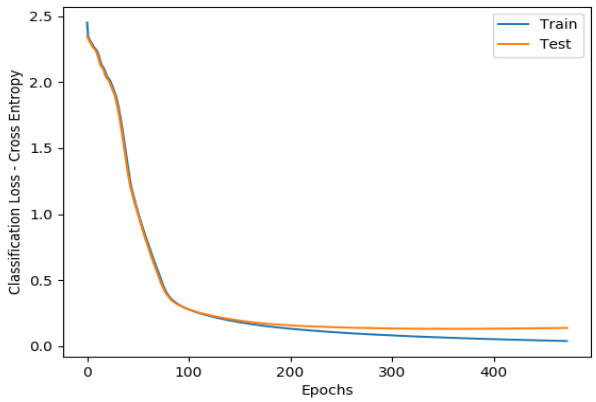
```
import numpy as np
import torch
import matplotlib.pyplot as plt
from mnist import MNIST

def load_data(size=1):
  print("Loading Date!")
  mndata = MNIST('python-mnist/data/')
  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

  if (size != 1):
    return X_train[:int(len(X_train)*size)], \
    labels_train[:int(len(labels_train)*size)], \
    X_test[:int(len(X_test)*size)], \
    labels_test[:int(len(labels_test)*size)]
  else:
    return X_train, labels_train, X_test, labels_test

# One hot encoding
def one_hot(y_train_, m):
  n = len(y_train_)
  reformed_tensor = torch.zeros(n, m)
  for i in range(n):
    index = y_train_[i]
    reformed_tensor[i][index] = 1
  return reformed_tensor

if __name__ == "__main__":
  X_train, y_train, X_test, y_test = load_data(size=1)
  print("Load Data Compelete!")
  # convert to tensor
```

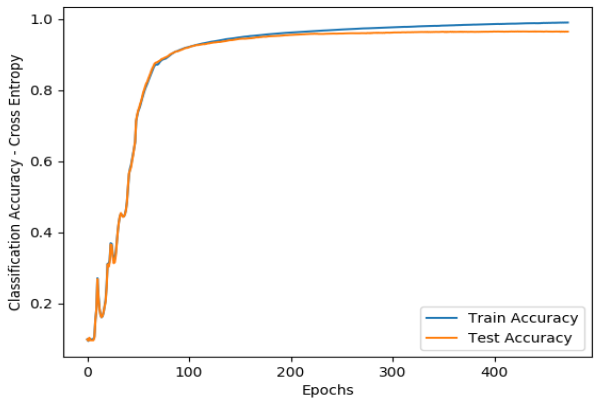
```
    dtype = torch.FloatTensor

    X_train_ = torch.tensor(X_train, dtype=torch.double).type(dtype)
    y_train_ = torch.tensor(y_train, dtype=torch.int64)

    X_test_ = torch.tensor(X_test, dtype=torch.double).type(dtype)
    y_test_ = torch.tensor(y_test, dtype=torch.int64)

    def ReLU(x):
      return abs(x) * (x > 0)

    def model(x, w0, w1, b0, b1):
      return (w1 @ ReLU(w0 @ x.T + b0) + b1).T

    def alpha(d):
    return 1 / np.sqrt(d)
    h = 64
    k = 10
    n_train, d_train = X_train.shape
    w0_data = (alpha(d_train) + alpha(d_train))*(torch.rand(h, d_train) -alpha(d_train)).type(dtype)
    w0 = torch.autograd.Variable(w0_data, requires_grad=True)
    b0_data = (alpha(d_train) + alpha(d_train))*(torch.rand(h, 1) -alpha(d_train)).type(dtype)
    b0 = torch.autograd.Variable(b0_data,requires_grad=True)
    w1_data = (alpha(d_train) + alpha(d_train))*(torch.rand(k, h) -alpha(d_train)).type(dtype)
    n_test, d_test = X_test.shape
    w1 = torch.autograd.Variable(w1_data,requires_grad=True)
    b1_data = (alpha(d_train) + alpha(d_train))*(torch.rand(k, 1) -alpha(d_train)).type(dtype)
    b1 = torch.autograd.Variable(b1_data, requires_grad=True)
    step_size = 0.001
    epochs = 150
    train_accuracy_list = []
    test_accuracy_list = []
    loss_train_list = []
    loss_test_list = []

    optim = torch.optim.Adam([w0, w1, b0, b1], lr=step_size)

    train_accu = 0
    test_accu = 0
    epochs_list = list(range(epochs))
    # for epoch in epochs_list:
    iter = 0
    while train_accu < 0.99:
      iter += 1
      # print("Epoch: ", epoch)
      optim.zero_grad()
      y_hat = model(X_train_, w0, w1, b0, b1)
      y_hat_index = torch.max(y_hat, dim=0).indices
      loss = torch.nn.functional.cross_entropy(y_hat, y_train_)
      loss.backward()
      optim.step()
      # Cross Entropy
      max_index_train = torch.max(model(X_train_, w0, w1, b0, b1), dim=1).indices.numpy()
      num_corrected_prediction_train = sum(max_index_train == y_train)
      train_accu = num_corrected_prediction_train / len(y_train)
      train_accuracy_list.append(train_accu)
      loss_train_list.append(loss)

```

```
    max_index_test = torch.max(model(X_test_, w0, w1, b0, b1), dim=1).indices.numpy()
    num_corrected_prediction_test = sum(max_index_test == y_test)
    test_accu = num_corrected_prediction_test / len(y_test)
    test_accuracy_list.append(test_accu)
    loss_test_list.append(torch.nn.functional.cross_entropy(model(X_test_, w0, w1, b0, b1), y_test_)
    print("###################", iter, "###################")
    print("CROSS ENTROPY: Train Accuracy: ", train_accu)
    print("CROSS ENTROPY: Test Accuracy: ", test_accu)

  print("CROSS ENTROPY: Train Accuracy: ", train_accuracy_list[-1])
  print("CROSS ENTROPY: Test Accuracy: ", test_accuracy_list[-1])
  print("Train Loss: ", loss_train_list[-1])
  print("Test Loss: ", loss_test_list[-1])

  plt.plot(range(iter), train_accuracy_list, label="Train")
  plt.plot(range(iter), test_accuracy_list, label="Test")
  plt.xlabel("Epochs")
  plt.ylabel("Classification Accuracy - Cross Entropy")
  plt.legend()
  plt.savefig("/Users/yinruideng/Desktop/senior_spring/cse546/hw/hw3/latex/plots/A5a.png")
  plt.show()

  w0.shape[0] * w0.shape[1] + w1.shape[0] * w1.shape[1] + len(b0) + len(b1)
```

b.

This part used a little more complex nn than last part:





Train Accuracy: 0.99005
Test Accuracy: 0.9624
Train Loss: (0.0409)
Test Loss: (0.1531)

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


if __name__ == "__main__":
  X_train, y_train, X_test, y_test = load_data(size=1)
  print("Load Data Compelete!")
  # convert to tensor
```

```
    dtype = torch.FloatTensor

    X_train_ = torch.tensor(X_train, dtype=torch.double).type(dtype)
    y_train_ = torch.tensor(y_train, dtype=torch.int64)

    X_test_ = torch.tensor(X_test, dtype=torch.double).type(dtype)
    y_test_ = torch.tensor(y_test, dtype=torch.int64)

    def ReLU(x):
      return abs(x) * (x > 0)

    def model(x, w0, w1, b0, b1):
      return (w1 @ ReLU(w0 @ x.T + b0) + b1).T

    # In this question, use this 2 layers model.
    def model_2_layers(x, w0, w1, w2, b0, b1, b2):
      return (w2 @ ReLU(w1 @ ReLU(w0 @ x.T + b0) + b1) + b2).T

    def alpha(d):
      return 1 / np.sqrt(d)


    def get_n_params(model):
    pp = 0
    for p in list(model.parameters()):
    nn = 1
    for s in list(p.size()):
    nn = nn * s
    pp += nn
    return pp
    h0 = 32
    h1 = 32
    h2 = 32
    k = 10
    n_train, d_train = X_train.shape
    w0_data = (alpha(d_train) + alpha(d_train))*(torch.rand(h0, d_train) -alpha(d_train)).type(dtype)
    w0 = torch.autograd.Variable(w0_data, requires_grad=True)
    b0_data = (alpha(d_train) + alpha(d_train))*(torch.rand(h0, 1) -alpha(d_train)).type(dtype)
    b0 = torch.autograd.Variable(b0_data,requires_grad=True)
    w1_data = (alpha(d_train) + alpha(d_train))*(torch.rand(h1, h0) -alpha(d_train)).type(dtype)
    n_test, d_test = X_test.shape
    w1 = torch.autograd.Variable(w1_data,requires_grad=True)
    b1_data = (alpha(d_train) + alpha(d_train))*(torch.rand(h1, 1) -alpha(d_train)).type(dtype)
    b1 = torch.autograd.Variable(b1_data, requires_grad=True)

    w2_data = (alpha(d_train) + alpha(d_train))*(torch.rand(k, h2) -alpha(d_train)).type(dtype)
    n_test, d_test = X_test.shape
    w2 = torch.autograd.Variable(w2_data,requires_grad=True)
    b2_data = (alpha(d_train) + alpha(d_train))*(torch.rand(k, 1) -alpha(d_train)).type(dtype)
    b2 = torch.autograd.Variable(b2_data, requires_grad=True)

    step_size = 0.001
    epochs = 150
    train_accuracy_list = []
    test_accuracy_list = []

    optim = torch.optim.Adam([w0, w1, w2, b1, b0, b2], lr=step_size)

```

```
    train_accu = 0
    test_accu = 0
    epochs_list = list(range(epochs))
    loss_train_list = []
    loss_test_list = []
    # for epoch in epochs_list:
    iter = 0
    while train_accu < 0.99:
      iter += 1
      # print("Epoch: ", epoch)
      optim.zero_grad()
      y_hat = model_2_layers(X_train_, w0, w1, w2, b0, b1, b2)
      y_hat_index = torch.max(y_hat, dim=0).indices
      loss = torch.nn.functional.cross_entropy(y_hat, y_train_)
      loss.backward()
      optim.step()
      # Cross Entropy
      max_index_train = torch.max(model_2_layers(X_train_,
      w0, w1, w2, b0, b1, b2), dim=1).indices.numpy()
      num_corrected_prediction_train = sum(max_index_train == y_train)
      train_accu = num_corrected_prediction_train / len(y_train)
      train_accuracy_list.append(train_accu)
      loss_train_list.append(loss)

      max_index_test = torch.max(model_2_layers(X_test_,
      w0, w1, w2, b0, b1, b2), dim=1).indices.numpy()
      num_corrected_prediction_test = sum(max_index_test == y_test)
      test_accu = num_corrected_prediction_test / len(y_test)
      test_accuracy_list.append(test_accu)
      loss_test_list.append(torch.nn.functional.cross_entropy(model_2_layers(X_test_,
      w0, w1, w2, b0, b1, b2), y_test_))
      print("####################", iter, "####################")
      print("CROSS ENTROPY:
      Train Accuracy: ", train_accu)
      print("CROSS ENTROPY: Test Accuracy: ", test_accu)

    print("CROSS ENTROPY: Train Accuracy: ", train_accuracy_list[-1])
    print("CROSS ENTROPY: Test Accuracy: ", test_accuracy_list[-1])
    print("Train Loss: ", loss_train_list[-1])
    print("Test Loss: ", loss_test_list[-1])



    plt.plot(range(iter), train_accuracy_list, label="Train Accuracy")
    plt.plot(range(iter), test_accuracy_list, label="Test Accuracy")
    # plt.plot(range(iter), loss__train_list, label="Train Loss")
    # plt.plot(range(iter), loss__test_list, label="Test Loss")
    plt.xlabel("Epochs")
    plt.ylabel("Classification Accuracy - Cross Entropy")
    plt.legend()
    plt.savefig("/Users/yinruideng/Desktop/senior_spring/cse546/hw/hw3/latex/plots/A5b.png")
    plt.show()

    # w0.shape[0] * w0.shape[1] + w1.shape[0] * w1.shape[1] + w2.shape[0] * w2.shape[1] + len(b0) + le
```

c.

In this first model, we have 50890 parameters.
In the section model, I have 26506 parameters.

```
# one layer
w0.shape[0] * w0.shape[1] + w1.shape[0] * w1.shape[1] + len(b0) + len(b1)
# two layer
w0.shape[0] * w0.shape[1] + w1.shape[0] * w1.shape[1] +
  w2.shape[0] * w2.shape[1] + len(b0) + len(b1) + len(b2)
```

We can see that the one layer one has almost double the number of parameter. Interestingly they have similar accuracy. The two approach has similar results. One way to interpret this is that either more parameters or deeper network will give better fit to the data set. And in this case, we had similar accuracy because they are compensating each other. In this case, one has more parameter but shallower, on the other side, one has less parameters but deeper network.

A.6

a.

Solution:
Lambda 1: 5.116787728342091
Lambda 2: 3.7413284788648014
Lambda 10: 1.24272937641733
Lambda 30: 0.36425572027888947
Lambda 50: 0.16970842700672756
Sum of Lambdas: 52.72503549512679

$$\sum_{i=1}^{d} \lambda_i = 52.72$$

```
import torch
import numpy as np
import matplotlib.pyplot as plt
from mnist import MNIST
import random

def load_data(size=1):
  print("Loading Date!")
  mndata = MNIST('python-mnist/data/')
  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

  if (size != 1):
    return X_train[:int(len(X_train)*size)], \
    labels_train[:int(len(labels_train)*size)], \
    X_test[:int(len(X_test)*size)], \
    labels_test[:int(len(labels_test)*size)]
  else:
    return X_train, labels_train, X_test, labels_test
X_train, y_train, X_test, y_test = load_data(size=1)
print("Load Data Compelete!")

# A6.a
n, d = X_train.shape
```

```
mu = np.zeros(d)
for i in range(d):
  mu[i] = np.mean(X_train[:, i])

demean_X_train = X_train[:]
for row in range(X_train.shape[0]):
  demean_X_train[row] = X_train[row] - mu
demean_X_test = X_test[:]
for row in range(X_test.shape[0]):
  demean_X_test[row] = X_test[row] - mu

sigma = (demean_X_train.T @ demean_X_train) / 60000


U, S, V = np.linalg.svd(demean_X_train / np.sqrt(60000), False)
eigenvalues = S**2
print("Lambda 1: ", eigenvalues[0])
print("Lambda 2: ", eigenvalues[1])
print("Lambda 10: ", eigenvalues[9])
print("Lambda 30: ", eigenvalues[29])
print("Lambda 50: ", eigenvalues[49])
print("Sum of Lambdas: ", sum(eigenvalues))
```

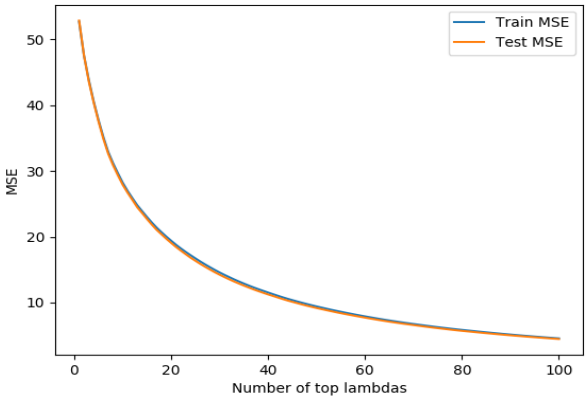
b.

Solution:
Reconstruct:
V_k is top k eigenvectors.

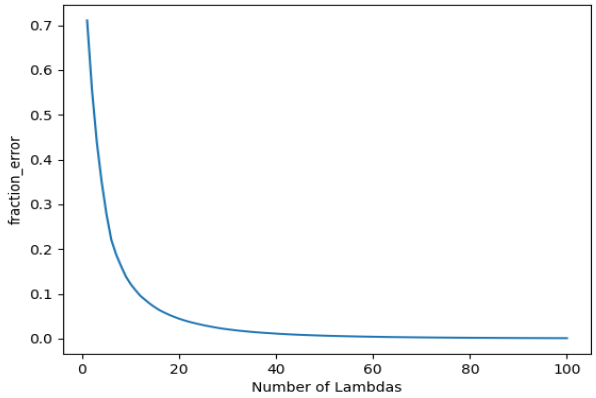
$$V_k V_k^T (x - \mu) + \mu$$

c.

Solution:
For reconstruction error (Mean Squared Error):
For k = 1 to 100, d = 784, plot $\frac{1}{n}\sum_{i=1}^{n}(\hat{X}_i - X_i)^2$



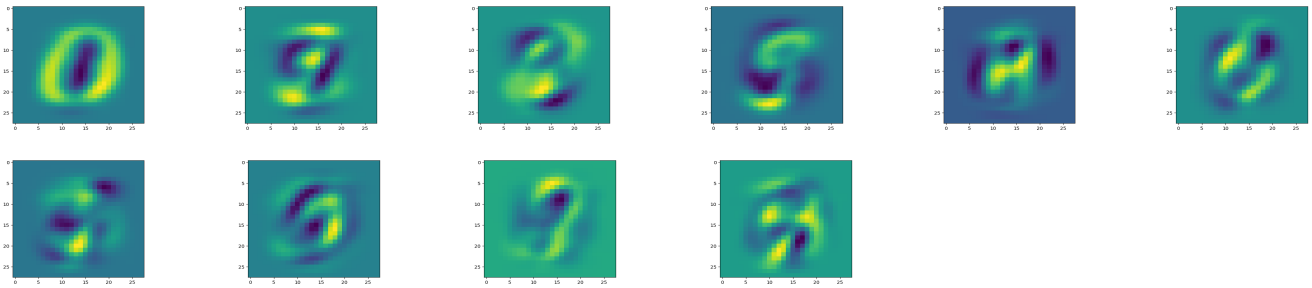
For fractional error:
For k = 1 to 100, d = 784, plot $1 - \frac{\sum_{i=1}^{k}\lambda_i}{\sum_{i=1}^{d}\lambda_i}$




```python
# plot mse
mean_squared_error_list_train = []
mean_squared_error_list_test = []
for k in range(0, 100):
  print("K: ", k)
  reconstructed = np.dot(V[:k, :].T.dot(V[:k, :]), demean_X_train[:, :].T).T
  MSE_train = np.sum((reconstructed - demean_X_train) ** 2) / demean_X_train.shape[0]
  mean_squared_error_list_train.append(MSE_train)

  reconstructed_test = np.dot(V[:k, :].T.dot(V[:k, :]), demean_X_test[:, :].T).T
  MSE_test = np.sum((reconstructed_test - demean_X_test) ** 2) / demean_X_test.shape[0]
  mean_squared_error_list_test.append(MSE_test)

plt.plot(range(1, 101), mean_squared_error_list_train, label="Train MSE")
plt.plot(range(1, 101), mean_squared_error_list_test, label="Test MSE")
plt.xlabel("Number of top lambdas")
plt.ylabel("MSE")
plt.legend()
plt.savefig("/Users/yinruideng/Desktop/senior_spring/cse546/hw/hw3/latex/plots/A6c_1.png")
plt.show()


# plot construction error
eigenvalues_sum = sum(eigenvalues)
fraction_error_list = []
for k in range(0,100):
  fraction_error = 1 - np.sum(eigenvalues[:(k+1)]) / eigenvalues_sum
  fraction_error_list.append(fraction_error)

plt.plot(range(1, 101), fraction_error_list)
plt.xlabel("Number of Lambdas")
plt.ylabel("fraction_error")
plt.savefig("/Users/yinruideng/Desktop/senior_spring/cse546/hw/hw3/latex/plots/A6c_2.png")
plt.show()
```

d.

Solution:



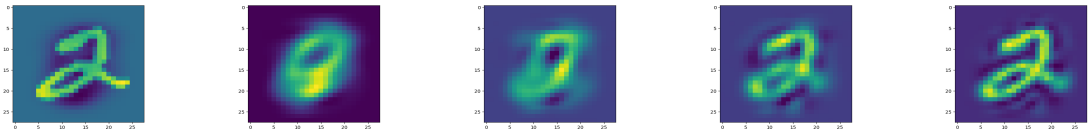
Interpretation:
Each of the image represent a PCA direction. It is a feature space with the highest variation. We can capture most of the variation and information through the top directions and thus we can reconstruct fairly close data.

```
# ======================== A6d ========================
for k in range(10):
  plt.imshow(V[k,:].reshape((28,28)))
  plt.savefig("/Users/yinruideng/Desktop/senior_spring/cse546/hw/hw3/latex/plots/A6d/A6d_"+
              str(k)+".png")
  plt.show()
```

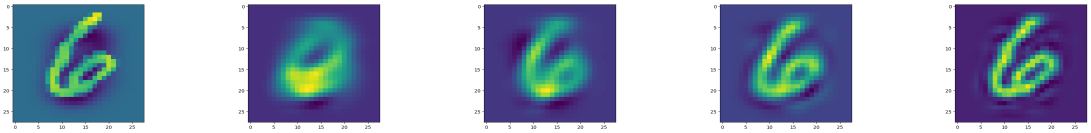
e.

Solution:

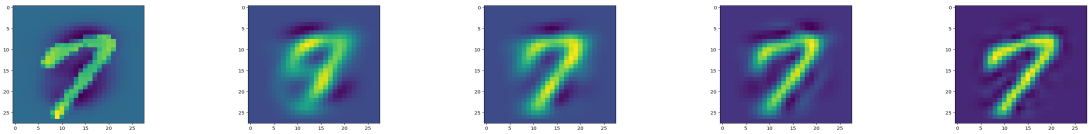
Plot the comparison between different number of top eigenvalues for [5, 15, 40, 100]:
For y = 2:



For y = 6:



For y = 7:



Interpretation:
For this reconstruction process, we used 5, 15, 40, 100 top lambdas to reconstruct the image, and we can see that with more dimensionality we got better representation of the original image. So basically, more dimensionality we used, we could capture more variation in the data.

```
# ======================== A6e ========================
y_train[5] # =2
y_train[13] # =6
y_train[15] # =7

```

```
for y in [5, 13, 15]:  # this is the index of y in the X_train
  plt.imshow(X_train[y,:].reshape((28,28)))
  plt.savefig("/Users/yinruideng/Desktop/senior_spring/cse546/hw/hw3/latex/plots/A6e/A6e_"+
  str(y)+".png")
  plt.show()

  for k in [5, 15, 40, 100]:
    plt.imshow(np.dot(V[:k, :].T.dot(V[:k, :]), X_train[:, :].T).T[y].reshape((28, 28)))
    plt.savefig("/Users/yinruideng/Desktop/senior_spring/cse546/hw/hw3/latex/plots/A6e/A6e_" +
    str(y) + "_"+str(k)+".png")
    plt.show()

# test case
plt.imshow(np.dot(V[:k, :].T.dot(V[:k, :]), X_train[:, :].T).T[y].reshape((28, 28)))
plt.show()
```