CMSC726 Machine Learning

Project 3

Unsupervised Learning

Angjoo Kanazawa, Ran Liu, and Austin Myers

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1 PCA and Kernel PCA

1.1 WU1

Depending exactly on your random data, one or more of these lines might not pass exactly through the data as we would like it to. Why not?

As shown in figure 1, the eigenvectors are actually what we would expect, with the first vector accounting for the axis of skew and the second vector orthogonal to the first. This is intuitive since the skew should be the primary source of variance, and the second eigenvector should simply be perpendicular to the first since it's a two dimensional projected space.

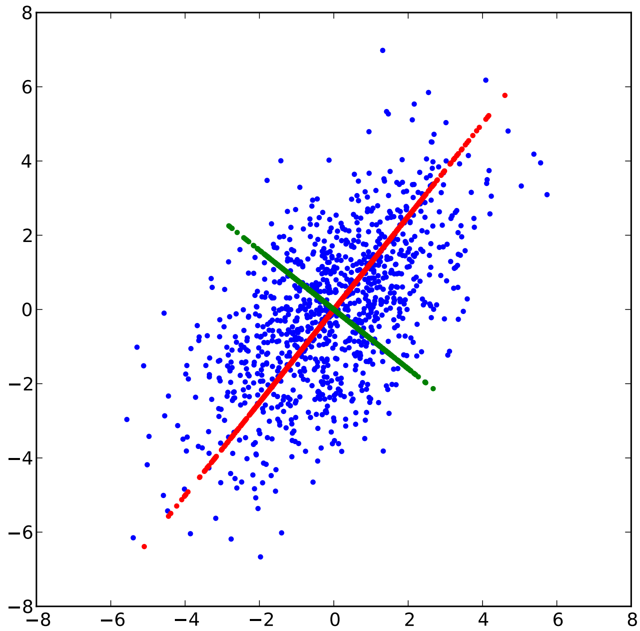


Figure 1: Eigenvectors and projected data

1.2 WU2

Plot the normalized eigenvalues (include the plot in your writeup). How many eigenvectors do you have to include before you've accounted for 90% of the variance? 95%? (Hint: see function cumsum.)

We need to include 81 eigenvectors to account for 90% of the variance and 135 eigenvectors to account for 95%. The eigenvalues are shown in figure 2 and the cumulative sum of the eigenvalues is shown in figure 3 with labels for the two points of interest.

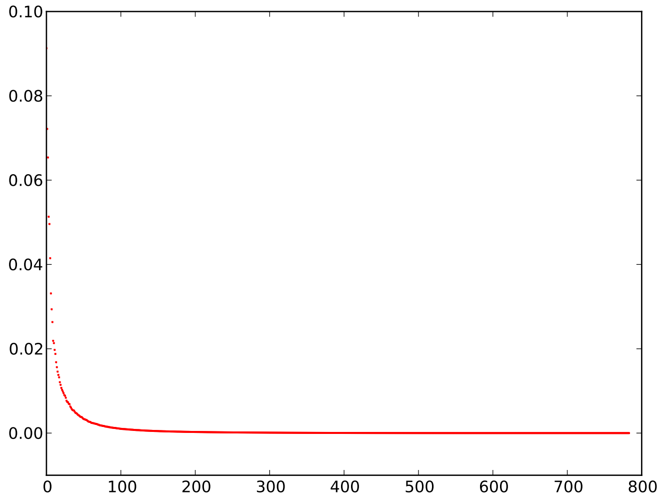


Figure 2: Plot of the normalized eigenvalues

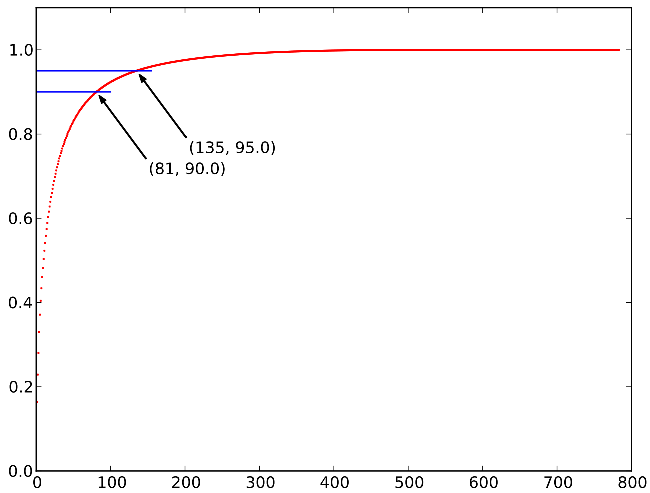


Figure 3: Plot of the normalized eigenvalues

1.3 WU3

Do these look like digits? Should they? Why or why not? (Include the plot in your write-up.)

Although most of the images in figure 4 do not look like digits, a few do resemble simple primitives which some digits share. These eigenvectors likely contribute significantly to the basic structure of some digits, but most of the eigenvectors are encoding detail information which is not easily recognizable. We can show how only a few eignevectors encode some basic structure by taking the eigenvectors and the projected data and trying to reconstruct the original dataset. With 784 eigenvectors, the reconstructed data appears to be very accurate as shown in 5, but with only 5 we still see that some simple structures have been captured as shown in 6 which shows why some of the eignvectors in figure 4 may look like simple digit structures.

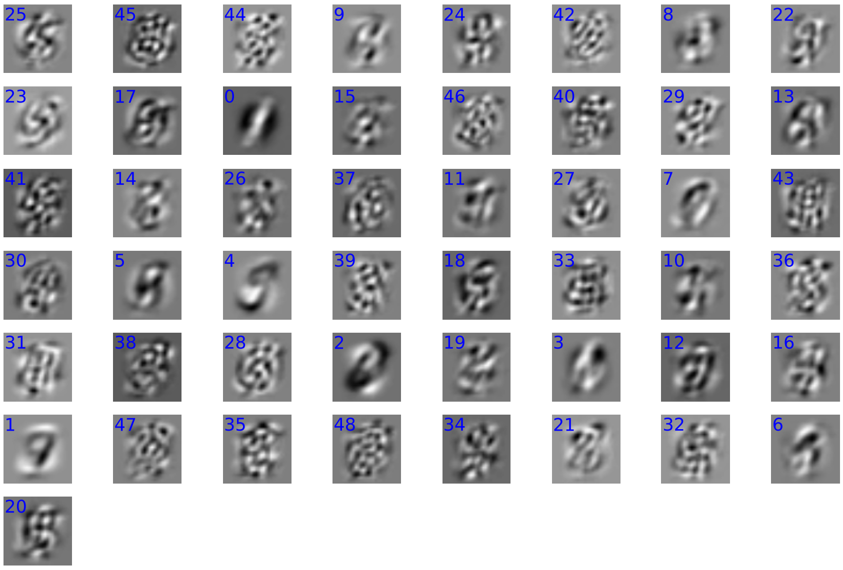


Figure 4: Plot of eigenvectors using vanilla pca

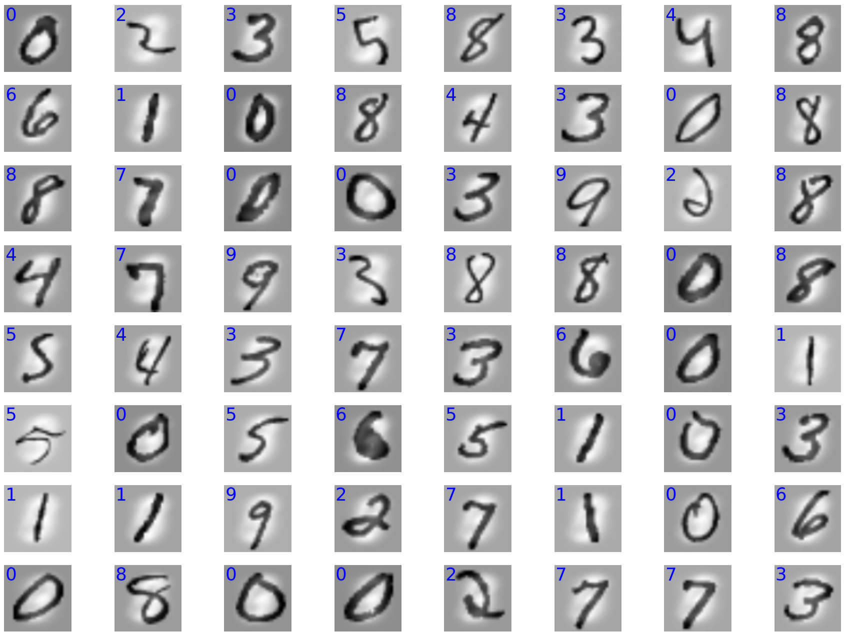


Figure 5: Reconstructed digit images using 784 eigenvectors

Figure 6: Reconstructed digit images using only 5 eigenvectors

1.4 WU4

Why does vanilla PCA find this data difficult? What is the significance of the relatively large value of the eigenvalues here?

PCA tries to find patterns in dataset that highlights the differences and similarities. Once we find such patterns, we can reduce the dimensionality of the data without losing too much information. Vanilla PCA will find this data difficult to characterize because the circular distribution of points cannot be represented using only two eigenvectors in two dimensions since this corresponds to linear combinations. Consequently, both of the eigenvalues are relatively similar because there is no one direction that maximizes the variance.

1.5 WU5

Did PCA do what we might want it to? Why or why not? Include the plot to justify your answer.

PCA did not do what we might want it to since we want the projected red data and the blue data points to be easily seperable or clustered. As shown in figure 7 the data has not been separated. Following from WU4, PCA does not work well because the circular distribution of points cannot be represented using linear combinations of two dimensional vectors.

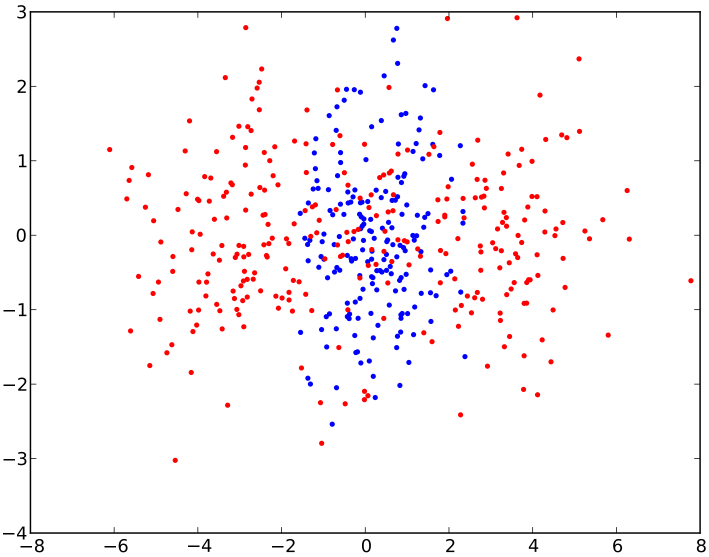


Figure 7: Projected data using eigenvectors found by vanilla PCA

1.6 WU6

How do the eigenvalues here compare to the linear case? What does this tell you? How does the plot look? How might this be useful for supervised learning?

Compared to the linear case, the eigenvalues are much smaller in magnitude $(0.08121919, 0.05313867)$, and the ratio of the first eigenvalue to the second eigenvalue is around 1.5, where the linear case exhibited a ratio that was closer to 1. This means that KPCA using rbf1 managed to...

As shown in figure 8, the projection clusters red datapoints into a small space, whereas blue datapoints a left dispersed but seperate from the red points by a small margin. This is useful for supervised learning because we can use KPCA projection to cluster the training data points that belong in the same class as much as possible, and feed that projected data to the classifier. Since we have the labels we can try different kernels and use the one that gives us the largest margin and is the easiest for our classifier to learn.

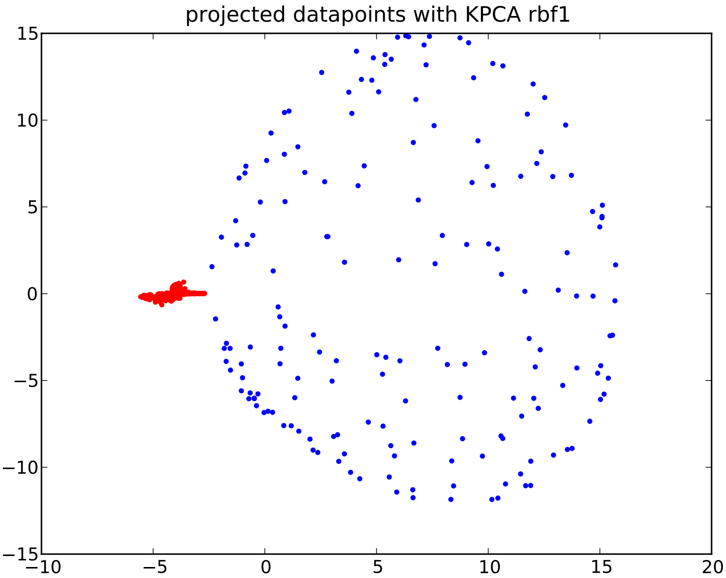
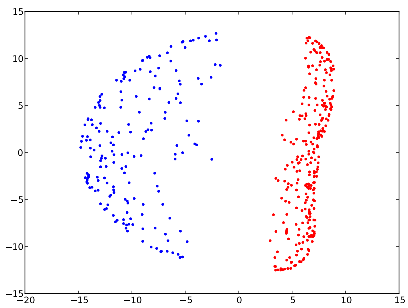


Figure 8: Projected data using KPCA and rbf1

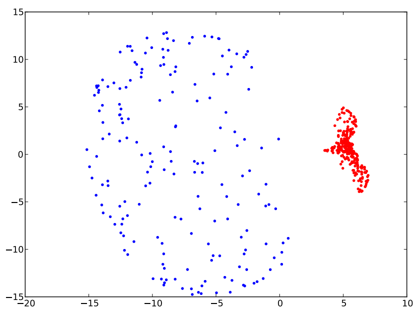
1.7 WU7

Experiment with different kernels, and perhaps interpolations of different kernels. Try to find a kernel that gets as much of the variance on the first two principle components as possible. Report your kernel and a plot of the data projected into 2d under that kernel.

The standalone kernel that seemed to perform the best were rbf0_2 and rbf0_5, as shown in figure 9a and figure 9b respectively. The former seemed to nicely separate the red and blue points, and the latter seemed to cluster the red points, so we tried to combine the two kernels multiplicatively. The result, shown in figure 10, was actually not much different than rbf0_5, but it seemed to be the best using combinations of the standard kernel functions. Finally, we tried to make our own function based on our knowledge of the data, yielding the function and result in figure 11. This function has reduced all the red data and blue data to separate points, however the function is probably not positive semi-definite, though this assertion has not been verified. Regardless, these are interesting examples of kernel function that might be useful if this type of data needed to be classified.



(a) rbf0_2



(b) rbf0_5

Figure 9: Projected data using KPCA and standard kernels

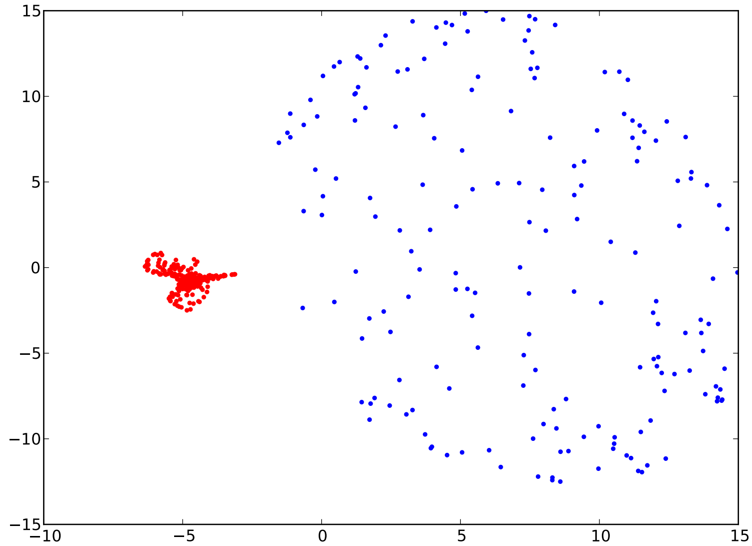


Figure 10: Projected data using KPCA and rbf0_2 and rbf0_5 combined

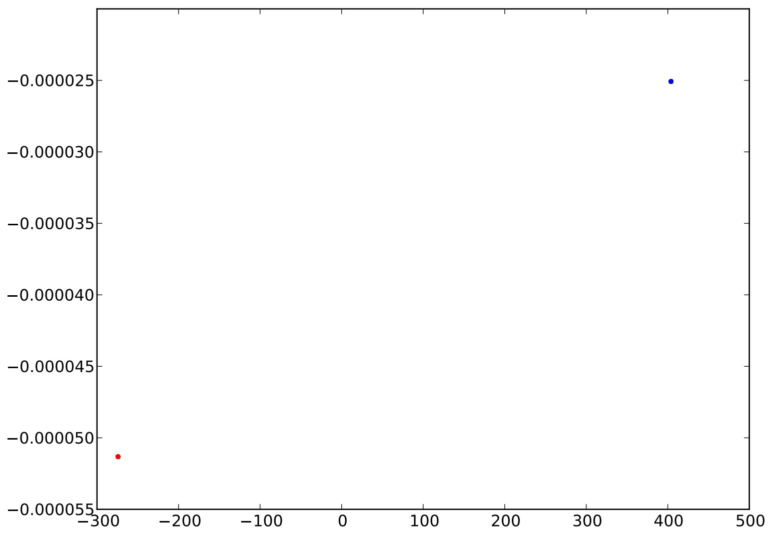


Figure 11: Projected data using KPCA and the custom function

$$\frac{1000}{1 + e^{-1000\sqrt{(x\cdot x)-2.75}} + e^{-1000\sqrt{(z\cdot z)-2.75}}}$$

2 HMMs:Viterbi

2.1 WU8

Find two different observation sequences of length four that differ only in one place, but differ in more than one place in the guessed output.

One example of this effect can be found with observation sequences [0,1,1,1] and [0,1,2,1] which differ only in the third observed emission, but which yield predictions of [0,0,0,0] and [0,0,1,1] respectively. Thus, the predictions differ in two states where the observations only differ in one.

3 HMMs:Forward-backward

3.1 WU9

Why does EM settle in this configuration? What is it saying? What happens when you use three states instead of two? What's the resulting probability of the data? What about four states? What happens and why?

EM settles in this configuration because it has found a local minima. The $\hat{\pi} = [1, 0, 0]$ means that we always start at state 0. We also get $P(X_t = 0|X_{t-1} = 0) = 0$, i.e. when we transition we always go to a different state. All together the results say that the most likely state sequence is the one where states alternate every step.

If we use three states instead of two, similar behavior happens with $\hat{\pi}$. One state has a probability of 1 and the rest gets 0. But in the transition probability, we do get a single state that has positive probabilities for more than one states.

When we increase the states to four, the behavior is still similar in a way that we have very high probabilities for specific transitions and emissions, but the probability of transition is more distributed.

This is because the way we produce the intial HMM is random. When there are only two states, the only way for the final probabilities to be well distributed is if initial transition from state 0 to state 0 and state 0 to state 1 is close i.e. 1/2, 1/2. If anything, it's very easy for EM to exaggerate the probability of the bigger one.

But as the number of states increases, the likelihood of uniformly distributin the initial HMM probabilities increases. So we get more reasonable (unskewed) results for EM.

3.2 WU10

Run EM on this data using two states. Run it a few times until you get a final log probability at least -9250. (It should happen in two or three trials. This will take a few minutes to run.) When you do this, it will print out the resulting initial state probabilities, transition probabilities and emission probabilities. What has it learned? Include all of this output in your write-up.

It has learned the probability of spaces and vowels vs the probability of consonants! State 0 emits all spaces or vowels and state 1 emits consonants. It also makes sense that the transition from state 0 to state 0 is lower than that of state 1, because it's more likely that consonants are followed by consonants than that vowels are followed by vowels.

The output of EM om this data is:

```
Initial state probabilities:
state(0): 7.4252e-202
state(1): 1

Transition probabilities:
FROM\TO
0  1
0  0.245207  0.754793
1  0.720637  0.279363

Emission probabilities:
State 0:
_  0.362509
e  0.232741
a  0.125778
o  0.120613
i  0.104855
u  0.04369
y  0.00345083
t  0.00258696
k  0.0019353
q  0.00121219
g  0.000467752
s  0.000115461
c  2.34141e-05
p  1.62641e-05
l  3.6812e-06
d  1.16317e-06
b  1.69503e-07
h  1.26829e-08
```

```
w  8.21573e-12
r  1.47438e-14
f  5.26943e-15
m  4.67596e-15
j  2.11457e-16
n  2.45545e-17
x  4.24731e-29
v  3.78819e-34
z  3.08129e-51
State 1:
t  0.141537
r  0.102944
n  0.0971604
s  0.0970502
h  0.094847
d  0.0670858
l  0.0636134
c  0.0479795
m  0.0439535
f  0.0347001
y  0.0337207
p  0.0329496
w  0.0306518
b  0.0260249
g  0.0244221
v  0.0202417
k  0.0166601
_  0.0155547
a  0.00316851
x  0.00173501
j  0.00173501
u  0.00168636
z  0.000578336
o  2.52571e-07
e  6.20806e-09
i  2.8181e-11
q  1.18265e-17
```