

CSE 446: Machine Learning Winter 2018

Assignment 2

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0 Policies

0.1 List of Collaborators

My collaborator was Edith Heiter (discussed Problem 2 and 4). The development of the answers though was completely independent and individually.

0.2 List of Acknowledgments

None.

0.3 Policies

I have read and understood these policies.

1 Perceptron Exercise

The evolution of the weight vector w are shown in figure 1 after the data was observed so the weights were already updated. In the same figure the maximum margin is shown since the perceptron didn't maximize the margin after the training set. To solve Problem 1.3 I will follow the proof according to [1].

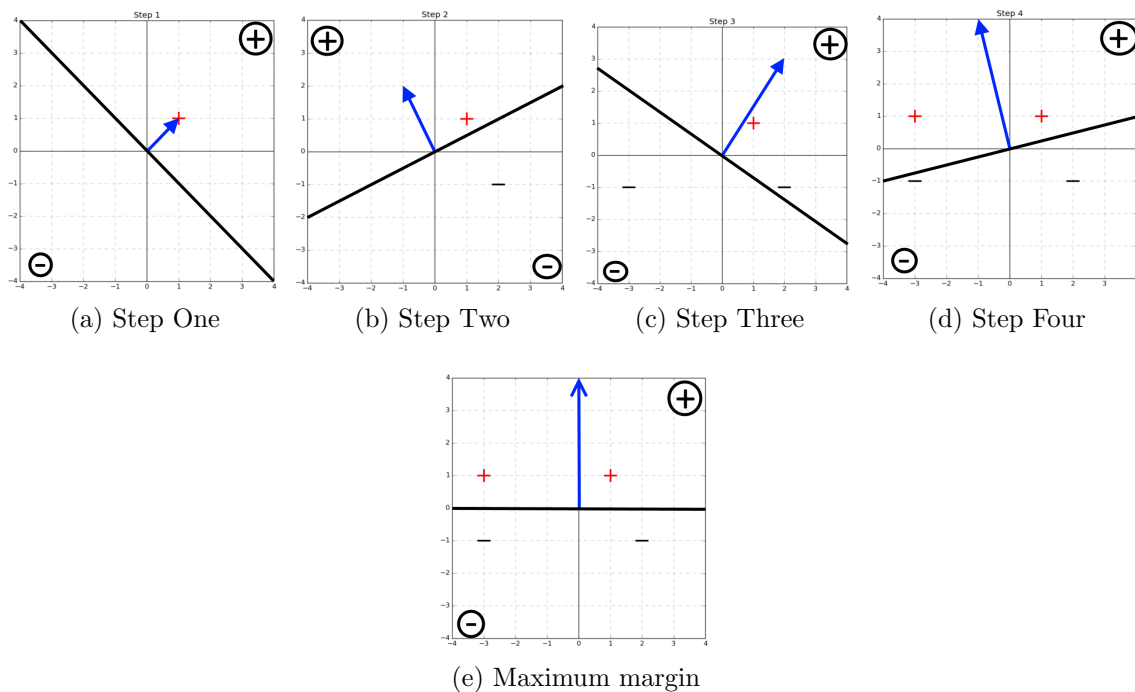


Figure 1: Visualization of the perceptron's decision boundary. The plots show the weight vector w in blue and the corresponding decision boundary (black) after they were updated. Plot (e) shows the maximum decision margin which is has the value 1 in this case.

Theorem 1.1. *If data D is linear separable with the geometric margin $\gamma^* = 0.5$ and has the maximum norm $\|x\| \leq 5 \forall x \in D$ then the algorithm will converge after at most $\frac{25}{\gamma^2}$ updates.*

Proof. Suppose x^* realizes $\gamma^* > 0$ and let $w^{(k)}$ be the k^{th} weight vector after k updates. We show in the following that the angle between w and w^* decreases such that the algorithm converges. That is when $w^* \cdot w$ increases faster than $\|w\|^2$. After the k^{th} update we find

$$w^* \cdot w^{(k)} = w^* (w^{(k-1)} + yx) = w^* \cdot w^{(k-1)} + yw^* \cdot x \geq w^* \cdot w^{(k-1)} + k\gamma$$

and

$$\|w^{(k)}\|^2 = \|w^{(k-1)} + yx\|^2 = \|w^{(k-1)}\|^2 + 2yw^{(k-1)} \cdot x + y^2 \cdot \|x\|^2 \geq \|w^{(k-1)}\|^2 + 5^2 + 0$$

The last line shows that $\|w^{(k)}\|$ increases by at least 25 every update. Therefore $\|w^{(k)}\|^2 \leq 25k$. So

$$\sqrt{25k} \geq \|w^{(k)}\| \geq w^* \cdot w^{(k)} \geq 5\gamma \Leftrightarrow k \leq \frac{25}{\gamma^2}$$

■

The maximum number of mistakes (updates) the perceptron has to make until it converges is given by $\frac{25}{\gamma^2} = \frac{25}{0.25} = 100$.

2 Implementation: Perceptron

See tables 1 and 2 for answers to questions 2 to 5. Some interesting plots concerning question 1 to 5 are shown in figures XXX.

When looking at data 6 to 8 we can see that the data is from the same source and not overlapping. In order to increase the precision on the test set (which is the same for 6 to 8) we merged the three training data sets combining now a total of 7000 observations to train the perceptron. The result can be seen in table 3 and figure ?? and 3.

3 Beat the Perceptron

4 PCA on Digits

4.1 Covariance matrix construction

Let $X \in \mathbb{R}^{n \times d}$ be the data matrix, $\vec{x}_i \in \mathbb{R}^{d \times 1}$ be the i^{th} element of X , $\vec{\mu} \in \mathbb{R}^{d \times 1}$ be the mean vector of all \vec{x}_i , $\vec{1}$ be a vector in $\mathbb{R}^{n \times 1}$ consisting of 1's, and $X_c = X - \vec{1}\vec{\mu}^T$ be the centered data matrix. Note that all vectors are considered as column vectors.

In figure 5 ten digits from the MNIST database are plotted, in figure 6 the mean image ($\vec{\mu}$) is plotted.

There are two methods to write down the covariance matrix:

- Vector based method:

$$\Sigma = \frac{1}{n} \sum_{i=1}^n (\vec{x}_i - \vec{\mu}) \cdot (\vec{x}_i - \vec{\mu})^T \quad (1)$$

- Matrix based method:

$$\Sigma = \frac{1}{n} (X_c^T \cdot X_c) \quad (2)$$

By considering the dimensions of the centered data matrix $X_c \in \mathbb{R}^{n \times d}$ we find for sigma $\Sigma \in \mathbb{R}^{d \times d}$.

By coding both methods (code attached to .tar.gz, as usual) we found for the vector method a runtime of roughly 191s and < 1 s for the matrix based method. This is an increase of over 19100% in runtime. By testing the average absolute difference between the two methods we found a very small value (9.78×10^{-16}), in the range of machine precision so the two results are equal. **NUMBER 4.1.6 IS MISSING!**

4.2 Eigen-Analysis

By using the SVD on the covariance matrix we find following eigenvalues:

- $\lambda_1 = 5.10819064381$
- $\lambda_2 = 3.70090586283$
- $\lambda_{10} = 1.24026412182$
- $\lambda_{30} = 0.362081056419$

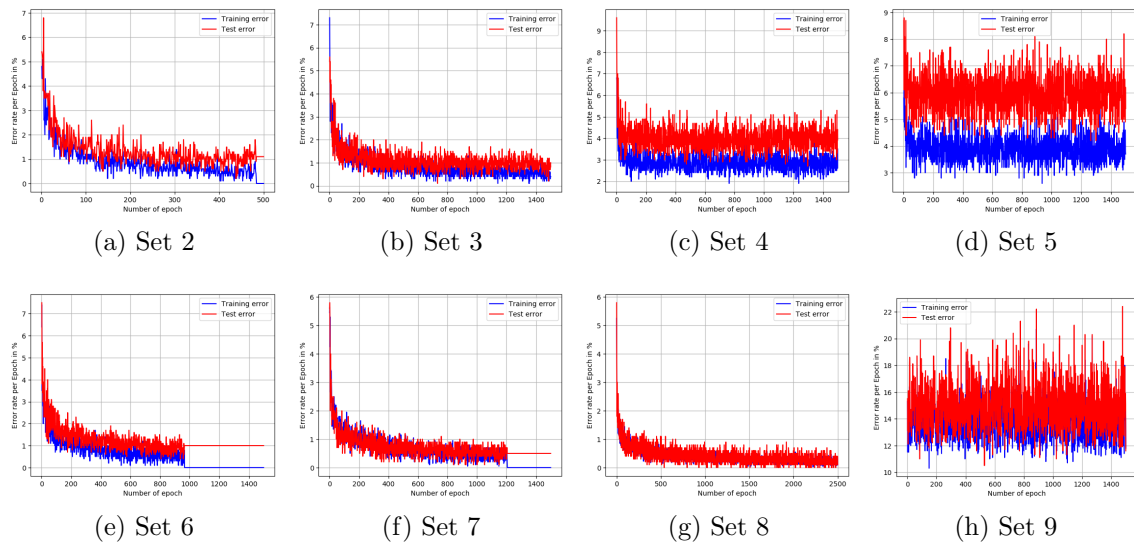


Figure 2: Visualization of the error rates of the different sets. In blue the training error rate and in red the test error rate.

dataset	question number			
	2	3	4	5
2	Is linear separable because error rate doesn't change after ≈ 380 epochs, the smallest margin found is ≈ 4 , see figure 2(a)	Does overfit slightly since test set error rises slowly for longer training times, see 2(a)	Weight of feature 9 is one to two orders of magnitude smaller than the others, might be noise	Tuned maximum number of iterations, set it to 94, got 10% training error, 19% test error, 5% development error
3	Is not linear separable because it does not converge and error rate rises a little after ≈ 1500 epochs	Does overfit a little Plot	Weight of feature 6 and 19 are one to two orders of magnitude smaller than the others, might be noise	Tuned maximum number of iterations, set it to 176, got 10% training error, 10% test error, 3% development error
4	Is not linear separable because it does not converge and error rate rises a little after ≈ 1500 epochs	Does overfit strongly Plot	No noise found	Tuned maximum number of iterations, set it to 815, got 20% training error, 46% test error, 7% development error (overall bad performance)
5	Is not linear separable because it does not converge and test error is steadily above training error rate	Does overfit Plot	No noise found	Tuned maximum number of iterations, set it to 632, got 17% training error, 31% test error, 8% development error (overall bad performance)

Table 1: Tabel with answers to questions of problem 2.

- $\lambda_{50} = 0.168298737356$

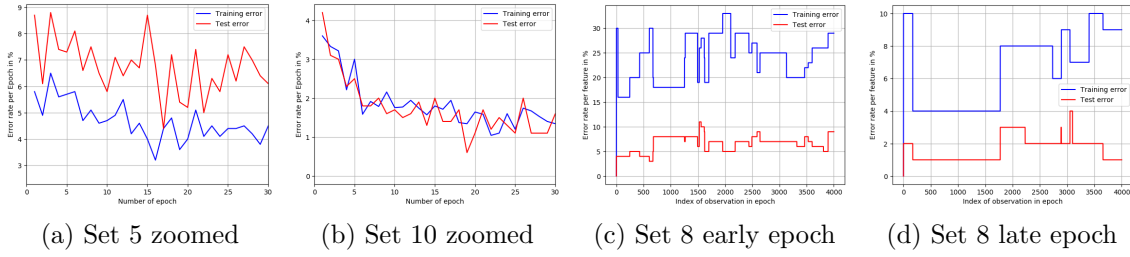


Figure 3: In (a) and (b) zoomed plots for early epochs for set 5 and 10 are shown. We can clearly see that set 5 starts with large discrepancy between the two error rates where set 10 has good performance on both training and test rate. Plot (c) and (d) show the error rate changing after encountering new observations for an early epoch (c) and a late epoch (d) in training set 8. We can see that in late epochs less mistakes are made as in earlier epochs.

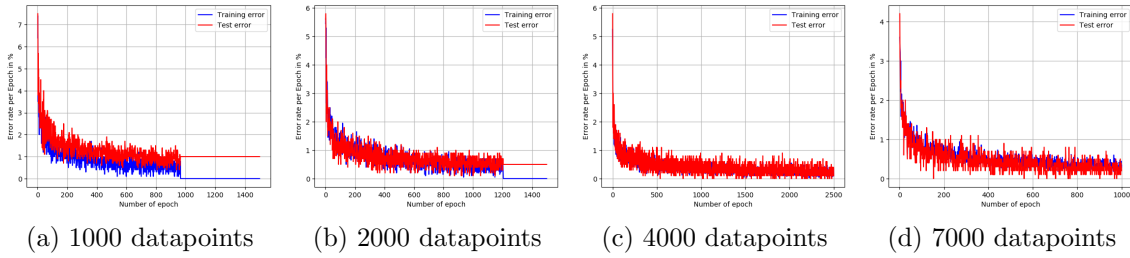


Figure 4: Visualization of the error rates of the sets from the same source with different sizes of training data. In blue the training error rate and in red the test error rate.

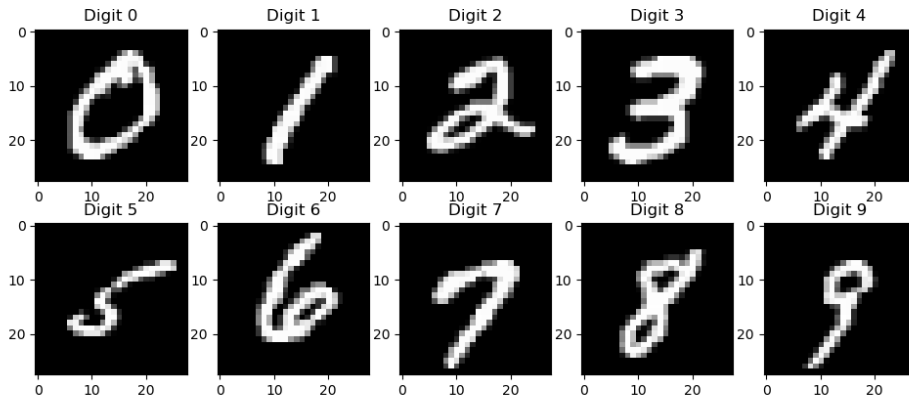


Figure 5: Grey scale plot of ten digits of the MNIST database

$$\bullet \sum_{i=1}^d \lambda_i = 52.4218857752$$

The fractional reconstruction error for the first $k = 100$ eigenvalues is plotted in figure 7.

The first 11 eigenvalues make up 50% of the total variance and the first 44 eigen-

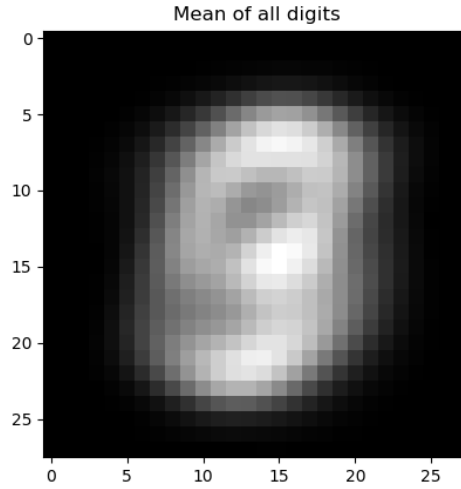


Figure 6: Grey scale plot of the mean image of the MNIST database

values make up 80% of the eigenvalues.

The first ten eigenvectors are shown in figure 8. They should represent the dimensions with the highest variance (biggest information) and therefore should carry essential information about the ten possible digits, zero to nine.

4.3 Pseudocode for Reconstruction

Goal: best reconstruction (squared error should be small) for dimensionality reduction from d to k dimensions.

1. Use the top k eigenvectors since they carry the largest variance (information) for the reconstruction. The actual number k is a hyperparameter which has to be optimized.
2. By using SVD on the covariance matrix Σ we get the k eigenvalues. The top k eigenvalues make up the matrix $\hat{U} \in \mathbb{R}^{d \times k}$. The reduced data matrix is then given by

$$\hat{X} = \left(X - \vec{1} \cdot \vec{\mu}^T \right) \cdot \hat{U} \quad (3)$$

3. The d -dimensional reconstruction is then given by

$$X_{\text{rec}} = \hat{X} \cdot \hat{U}^T + \vec{1} \cdot \vec{\mu} \quad (4)$$

4.4 Visualization and Reconstruction

For $k = 30$ it takes roughly 2s to reconstruct the data. The plots are shown for different k in figures 9 and 10. For low values of k ($k = 1, 3, 5$) we can see that the reconstruction is composed of one, three and five eigenvalues. The reconstruction itself is not useful for determining the original digit. For medium k ($k = 10, 25, 50$) the pictures get more and more blurry until for higher k ($k = 200, 500+$) one finally can estimate the digit.

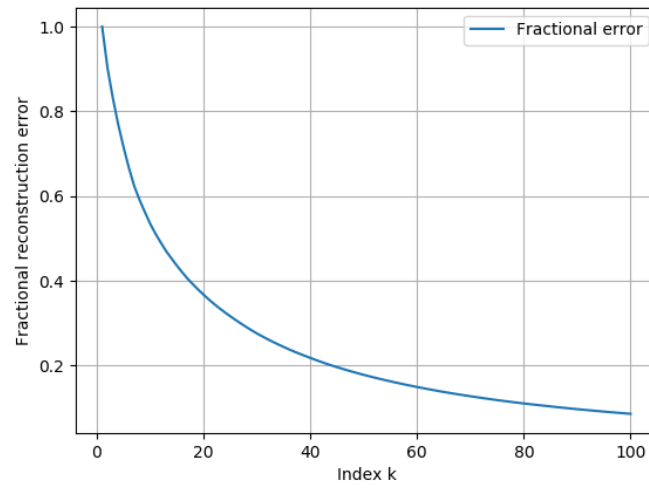


Figure 7: Fractional Reconstruction error for the first $k = 100$ eigenvalues

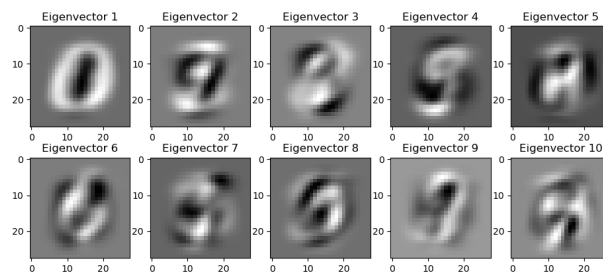


Figure 8: Plot of the first ten eigenvectors

5 Bayes Optimal Classifier

6 Bonus: Dimensionality Reduction

7 Bonus: The Bayes Optimal Hypothesis for Regression

*Bibliography

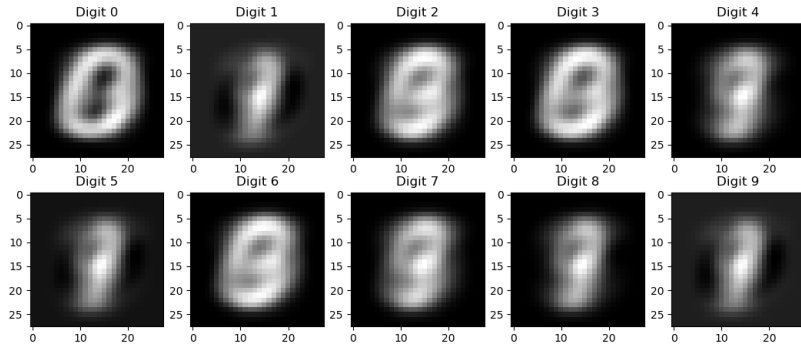
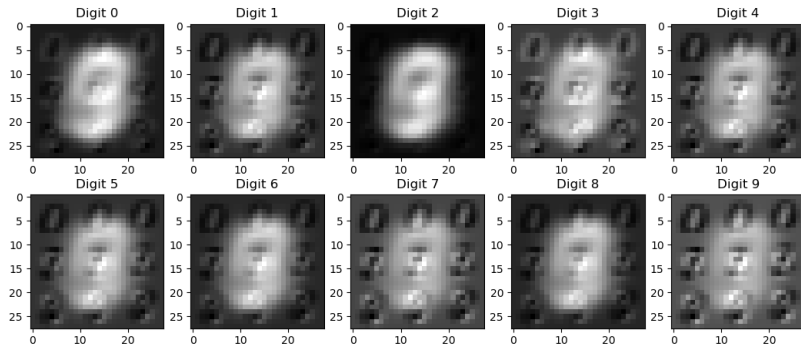
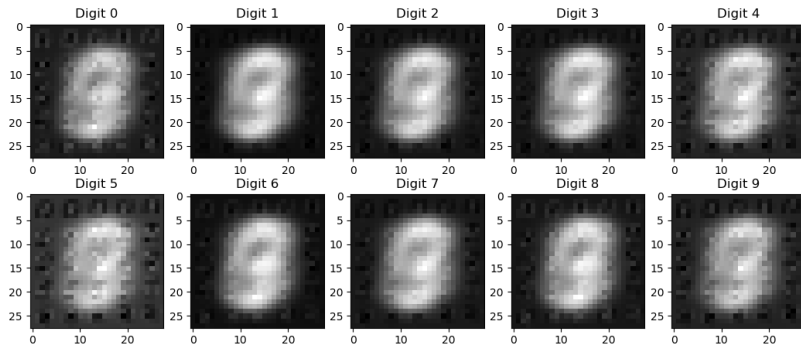
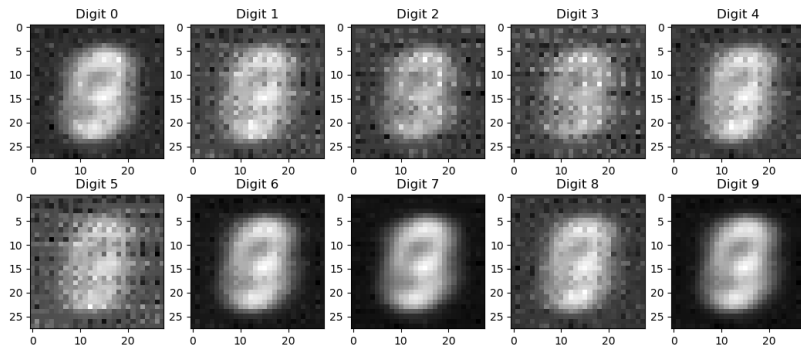
References

- [1] Hal Daume III. *A Course in Machine Learning*. Secondary printing, January 2017.

dataset	question number			
	2	3	4	5
6	The data is linear separable since the algorithm converges after roughly ≈ 950 epochs, the smallest margin is ≈ 4	Does overfit for larger epochs Plot	Feature 12 generates a weight which is 3 orders of magnitude smaller than the others, this might be noise	Tuned maximum number of iterations, set it to 68, got 13% training error, 28% test error, 4% development error
7	The data is linear separable since the algorithm converges after roughly ≈ 1207 epochs, the smallest margin is ≈ 30	Does not overfit for larger epochs Plot	Feature 10, 12 and 18 generate weights which are 3 to 4 orders of magnitude smaller than the others, this might be noise	Tuned maximum number of iterations, set it to 224, got 6% training error, 6% test error, 3% development error
8	The data might be linear separable but the algorithm does not converge for 2500 iteration steps (might take longer since more data must be processed), the smallest margin can be guessed to the same margin as set 6, ≈ 4	Does not overfit, test error is nearly identical with training error	Feature 10, 12 and 18 still generate weights which are 3 to 4 orders of magnitude smaller than the others, this might be noise	Tuned maximum number of iterations, set it to 806, got 8% training error, 2% test error, 4% development error
9	Is not linear separable because it does not converge and error is nearly steady	Might not overfit since test error is steadily roughly two percent worse than training error rate	Weight of feature 1 and 20 are one to two orders of magnitude smaller than the others, might be noise	Tuned maximum number of iterations, set it to 409, got 80% training error, 154% test error, 27% development error (very bad performance, might not be a problem solvable by the perceptron.)

dataset	question number			
	2	3	4	5
Surpr.	Should be separable since it's from the same type of data as data 6, 7, and 8, so lower limit for the margin should be similar	Does not overfit, test error seems to perform equally good, maybe even better than training error	Feature 10, 12, 18, and 19 generate weights which are 3 to 4 orders of magnitude smaller than the others, this might be noise	Tuned maximum number of iterations, set it to 631, got 13% training error, 2% test error, 7% development error

Table 3: Surprising table with answers to the surprise problem.

(a) Reconstruction for $k = 1$ (b) Reconstruction for $k = 3$ (c) Reconstruction for $k = 5$ (d) Reconstruction for $k = 10$ Figure 9: Reconstruction of the ten digits used in Problem part 4.1 for different k .

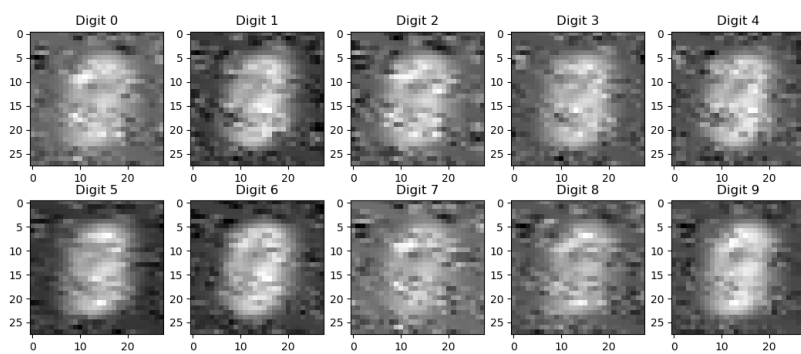
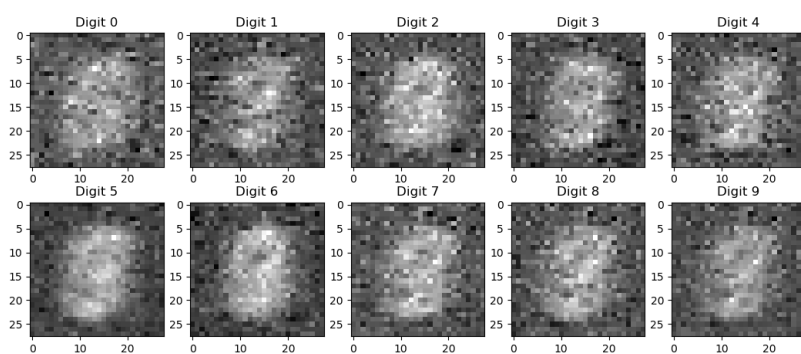
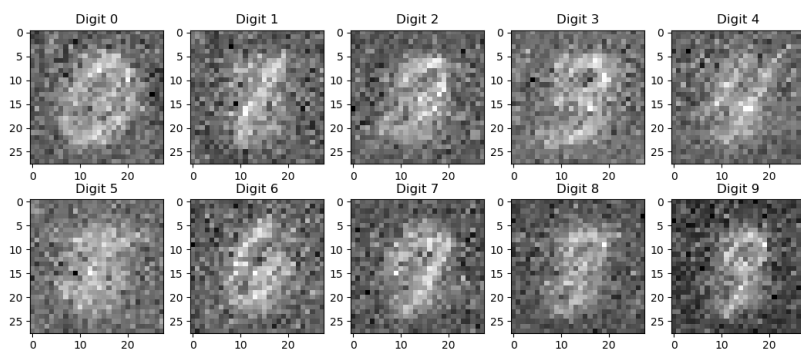
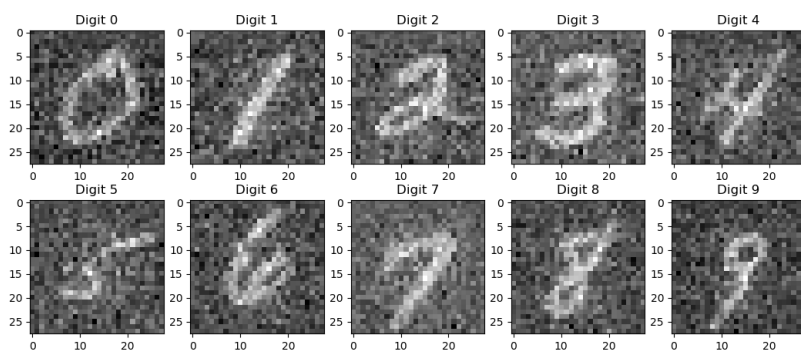
(a) Reconstruction for $k = 25$ (b) Reconstruction for $k = 50$ (c) Reconstruction for $k = 200$ (d) Reconstruction for $k = 500$

Figure 10: Reconstruction of the ten digits used in Problem part 4.1 for different k . Continuation from previous page.