HW4: Dimensionality Reduction, Ensemble Methods, Multiclass/Ranking

## 1 Written Exercises

- 1. Linear PCA does an eigen-decomposition of the  $D \times D$  covariance matrix of the data where D is the original dimensionality of the data. Kernel PCA (KPCA) which learns nonlinear projections is also based on doing an eigen-decomposition of the covariance matrix but this time the covariance matrix is defined in the feature space ( $\phi$ ) defined by the kernel. This feature space could even be infinite dimensional (e.g., if you use an RBF/Gaussian kernel). Explain how does KPCA get away with not computing this covariance matrix and doing its eigen-decomposition? What does it actually compute and does eigen-decomposition of? (10 points)
- 2. Dimensionality reduction methods take as input a set of points  $\{x_1, x_2, \ldots, x_N\}$  and learn a low-dimensional embedding (projection) of these points. Now suppose I give you a new point  $x_{N+1}$ . Of the various dimensionality reduction methods we have seen in the class (PCA, Kernel PCA, LLE, ISOMAP), which ones allow you to compute the low-dimensional projection of the new point  $x_{N+1}$  (for each, explain why or why not). This problem is known as the *out-of-sample problem*. Note that including  $x_{N+1}$  in the original data and re-running dimensionality reduction on the whole data is not an option. (10 points)
- 3. For multiclass classification, All-vs-All (AVA) seems more computationally intensive at training time than One-vs-All (OVA) because it trains  $\mathcal{O}(K^2)$  classifiers rather than  $\mathcal{O}(K)$  classifiers. However, all of the K-many OVA classifiers are on the full data set of N examples, while the  $\mathcal{O}(K^2)$  AVA classifiers are only on subsets of the data. Suppose that you have N data points, divided evenly into K classes (so that there are N/K examples per class).
  - (a) Suppose that the training time for your binary classifier is linear in the number of examples it receives. What is the complexity of training OVA and AVA, as a function of N and K?
  - (b) Suppose the training time is quadratic; then what is the complexity of AVA and OVA? (10 points)
- 4. One issue with multiclass classification based methods such as OVA and AVA is that the test time complexity grows linearly or quadratically with K, the total number of classes. Moreover the multiclass classification error also worsens as K grows (because basically we are using a collection of binary classifiers and their individual errors would just add up).
  - Now suppose we still want to construct a multiclass classification algorithm based on a set of binary classifiers but want to control the error such that it doesn't get worse than  $\mathcal{O}(\log_2 K)$ . How would you accomplish this (hint: what you want is minimizing the number of decisions you have to make at test time)? (10 points)
- 5. Define a ranking preference function  $\omega$  that penalizes mispredictions linearly up to a threshold K. In other words, for K=20, if I put the object that should be in position 5 in position 20, then I pay \$15; if I put it in position 30, I only pay \$20 because nothing costs more than K=\$20. (10 points)

## 2 Programming Exercises

1. Implement PCA, and Kernel PCA with RBF kernel. For the RBF kernel, there is a fairly decent heuristic for choosing the bandwidth parameter: compute the pairwise distances (Euclidean but don't square it) between all the points and take the *median* Euclidean distance as the bandwidth parameter.

The shell for both PCA and Kernel PCA are provided (PCA.m and KPCA.m) and you will need to fill in the TODO parts. Once you complete implementing these (they are independent), you can test them on the MNIST digits dataset (provided in mnist.mat).

The test scripts  $test\_pca.m$  and  $test\_kpca.m$  would test your implementations and will produce several plots, including the figures of reconstructed digits using the projected data. Observe (for both PCA and KPCA) how the reconstruct digits look like as you increase the number of dimensions d the data is projected on.

Submit the completed codes for PCA and KPCA, and all the plots. Also comment on your observations about the reconstruction accuracies of digits as d varies. (30 points)

2. In this task, we will implement AdaBoost. A shell for AdaBoost is in Boost.m. You will need to fill in the BoostTrain and BoostPredict functions. See the comments in Boost.m for a description of what each function should do and how it should store its outputs. Note that in order to do boosting properly, you need to have binary classification algorithms that can accept weighted data. I have provided an implmentation of Perceptron that does so in perceptron\_weighted.m (do not change that code! :) ). The data for this part is in data.mat. When you do load data.m, you would see trX,trY for the training data and teX,teY for the test data.

Once you are done implementing Boost.m, you can run test\_adaboost.m which will run a series of tests using different number of rounds for the boosting algorithm. To get a sense of whether your implementation is doing sensibly, here are some representative numbers: for boosting round 1, you should get about 62.5% training and 55.6% test accuracy; for round 3, you should get training accuracy of about 88.5% and 86.8% test accuracy. (20 points)