1 Sparse Latent-Factor Models

If run the function `example_faces` it will load a set of face images under different lighting conditions. It will then fit a PCA model (with $k = 10$) and display 5 figures:

- Random faces taken from the dataset (Figure 1).
- The average face (Figure 2).
- The principal components (Figure 3).
- The original examples $x_i$ and the compressed variant $z_i$ (Figure 4).
- The same random faces, after reconstructing them from their corresponding $z_i$ (Figure 5).

The reconstructions tend to be reasonable given that they compress each 1024-pixel face down to just 10 numbers, although they often lack specific details and are less accurate for faces that do not look like the average face. In this model, some of the principal components are interpretable (e.g., they reflect different lighting conditions), but many of them are not. You can change the value of $k$ in this script to see the effect of including/excluding principal components, if you increase $k$ it will do a better job of reconstructing faces that do not look like the average face.

1.1 Uniqueness of Principal Components

If you re-run the script, you may get different principal components, even though all that changes between runs is the order of the training examples. What is the specific difference between the principal components that are obtained between different runs of the algorithm?
1.2 Non-Negative Matrix Factorization

If you replace the function `dimRedPCA` with `dimRedPCA_alternate`, then instead of using the SVD to compute the principal components it will compute them numerically by using a gradient method that alternates between updating $W$ and $Z$. Note that this returns different principal components because it doesn’t enforce any constraints on $W$, but (up to numerical accuracies) it will give an equivalent model. You would never actually use this method to fit a PCA model, but this optimization strategy generalizes to other models and it shows the learned principal components without the constraints. Below are the results obtained by `dimRedPCA_alternate` (right) with $k = 100$, and note that these look different from the usual PCA results because we aren’t enforcing constraints on $W$ (to make this plot, I initialized with samples from a standard normal divided by $10^{-5}$, but in the a5.zip it uses samples directly. This leads to poor results for PCA, that look like random noise, but makes a better initialization for other methods):

A disadvantage of PCA is that the principal components tend to be dense (they are all non-zero). One of the first models to address this is non-negative matrix factorization, where we use the PCA objective but add non-negative constraints on $W$. Using `dimRedPCA_alternate` as a template, write a function `dimRedNMF` that implements the non-negative matrix factorization (NMF) model. Hand in your code and hand in a plot of the latent factors (Figure 3) obtained when $k = 100$.

Hint: you need to make three changes. First, you need to change the initialization so that negative values of $W$ and $Z$ are set to 0. Second, you need to change the updates of $W$ and $Z$ to use an optimization method that includes the non-negativity constraint. You can use the function `findMinNN` minimizes a
smooth function subject to non-negative constraints. Finally, you need to update the compress function so that it finds the non-negative Z minimizing the objective with W fixed.

1.3 Sparse Matrix Factorization

While NMF leads to sparse values of W and Z, disallowing negative values leads to a much worse reconstruction error. In other words, ZW is a much worse approximation of X when using NMF than when using PCA. To explicitly trade off between the reconstruction error and the sparsity, we could instead use L1-regularization of W and Z. Write a function dimRedSPCA (for ‘sparse’ PCA) that uses dimRedPCA_alternate as a template but applies L1-regularization when estimate W and when estimating Z. Hand in your code and hand in a plot of the latent factors (Figure 3) obtained with k = 100 and $\lambda = \sqrt{nd}$.

2 Recommender Systems

If you run the function example_movies, it will load a dataset consisting of movie ratings for different users. The vector y contains the ratings, the first column of X contains the user numbers, and the second column of X contains the movie numbers. The script runs several simple baseline methods, and reports their performance on the validation set.

2.1 Latent-Factor Model

We have no features for the user/movies, we must predict the labels based on other labels (collaborative filtering). One way to improve on these methods is with a latent-factor model. Consider a model of the form

$$y_{um} = b_u + b_m + w_m^T z_u,$$

where the model has four parameters:

- $b_u$: a bias variable specific to user $u$.
- $b_m$: a bias variable specific to movie $m$.
- W: a matrix whose columns $w_j$ represent latent features for movie $m$.
- Z: a matrix whose rows $z_u$ represent latent features for user $u$.

Consider training this based on the squared loss function, which means that our error for a particular user $u$ and movie $m$ is given by

$$f(b_u, b_m, w_m, z_u) = \frac{1}{2}(y_{um} - (b_u + b_m + w_m^T z_u))^2.$$

Using the notation $r_{um} = (y_{um} - (b_u + b_m + w_m^T z_u))$, derive the partial derivative of this expression with respect to (i) $b_u$, (ii) $b_m$, (iii) ($w_m)_i$ for a particular element $i$ of $w_m$, and (iv) ($z_u)_i$ for a particular element $i$ of $z_u$.

2.2 Stochastic Gradient

The function recommendSVD implements the model from the previous question, and trains it using gradient descent with a constant step size of .0001. Since there are nearly a million ratings, this is quite slow and the script only runs the method for 10 passes through the data (technically, it’s our Matlab implementation that
is slow as this dataset really isn’t that large). In cases like this where we have lots of data but are limited by time, we can often obtain better performance using stochastic gradient methods. Modify `recommendSVD` so it trains using a stochastic gradient method with a constant step-size, doing 10 ‘passes’ of nRatings stochastic gradient iterations (which takes the same time as 10 gradient descent iterations). Hand in your modified code, and report the validation error of the method using a larger step-size of .01 and \( k = 10 \).

Hint: since we are only changing the optimization method, you don’t need to change anything outside the ‘for iter = 1:maxIter’ loop. However, you will now need to compute the gradient with respect to a single randomly-chosen training example within the inner ‘for’ loop, and update the parameters based on the gradient with respect to this single example.

## 3 Multi-Dimensional Scaling

The function `example_MDS` loads the animals dataset and then shows (i) the raw data, (ii) the data projected onto the first two principal components, and (iii) the result of applying gradient descent to minimize the following multi-dimensional scaling (MDS) objective (starting from the PCA solution):

\[
\arg\min_{Z \in \mathbb{R}^{n \times k}} \frac{1}{2} \sum_{i=1}^{n} \sum_{j=i+1}^{n} (\|x_i - x_j\| - \|z_i - z_j\|)^2.
\]

(1)

As with PCA, it’s possible to minimize this objective with a singular value decomposition, but this code uses a gradient method since this generalizes to variations on the objective. The results of applying PCA and MDS are shown below on the left and right.

![PCA vs MDS](image)

We see that the crowding effect of PCA makes some non-sensical clusters (e.g., the cluster containing ‘spider monkey’, ‘polar bear’, and ‘hamster’). MDS is less crowded, but many of the results don’t make sense (‘persian cat’ and ‘siamise cat’ have ‘mouse’ and ‘chihuahua’ in between them, while ‘wolf’ and ‘grizzly bear’ are close to each other while ‘polar bear’ is on the opposite side of the scatterplot).

### 3.1 Samman Mapping

Make new function `visualizeSammon` that implements gradient descent for MDS Sammon mapping objective,

\[
\arg\min_{Z \in \mathbb{R}^{n \times k}} \frac{1}{2} \sum_{i=1}^{n} \sum_{j=i+1}^{n} \left( \frac{(\|x_i - x_j\| - \|z_i - z_j\|)^2}{\|x_i - x_j\|} \right).
\]

Hand in your code and the plot of the result.
3.2 ISOMAP

Euclidean distances between very different animals are unlikely to be particularly meaningful. However, since related animals tend to share similar traits we might expect the animals to live on a low-dimensional manifold. This suggests that ISOMAP may give a better visualization. Make a new function `visualizeISOMAP` that computes the approximate geodesic distance (shortest path through a graph where the edges are only between nodes that are $k$-nearest neighbour) between each pair of points, and then fits a standard MDS model (1) using gradient descent. Hand in your code and the plot of the result when using the 3-nearest neighbours.

Hint: the function `dijkstra` can be used to compute the shortest (weighted) distance between two points in a weighted graph. This function requires an $n$ by $n$ matrix giving the weights on each edge (use 0 as the weight for absent edges). Note that ISOMAP uses an undirected graph, while the $k$-nearest neighbour graph might be assymetric. One of the usual heuristics to turn this into a undirected graph is to include an edge $i$ to $j$ if $i$ is a KNN of $j$ or if $j$ is a KNN of $i$. (Another possibility is to include an edge only if $i$ and $j$ are mutually KNNs.)

3.3 ISOMAP with Disconnected Graph

An issue with measuring distances on graphs is that the graph may not be connected. For example, if you run your ISOMAP code with 2-nearest neighbours then some of the distances are infinite. One heuristic to address this is to set these infinite distances to the maximum distance in the graph (i.e., the geodesic distance), which will encourage non-connected points to be far apart. Modify your ISOMAP function to implement this heuristic. Hand in your code and the plot of the result when using the 2-nearest neighbours.

4 Visualizing a neural net for 1D regression

The file `example_nnet.m` contains a script to train a basic neural net. It is set up with a 1D example, i.e. where the neural net is used to learn a function mapping $\mathbb{R} \rightarrow \mathbb{R}$. When you run the script, you should be able to see training progress as the network begins to fit the data. However, in its current form it doesn’t fit the data very well. Try to improve the performance of the method by changing the structure of the network ($nHidden$ is a vector giving the number of hidden units in each layer) and the training procedure (e.g., change the sequence of step sizes, add momentum, or use `findMin` from the previous assignment). Hand in your plot after changing the code to have better performance, and list the changes you made.