CS483: Big Data Mining Fall 2024

Homework 2

1 Singular Value Decomposition and Principal Component Analysis (20 points)

In this problem we will explore the relationship between two of the most popular dimensionality-reduction techniques, SVD and PCA, at a basic conceptual level. Before we proceed with the question itself, let us briefly recap the SVD and PCA techniques and a few important observations:

- First, recall that the eigenvalue decomposition of a *real*, *symmetric*, and *square matrix* B (of size $d \times d$) can be written as the following product:

$$B = Q\Lambda Q^{\mathrm{T}}$$

  where $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_d)$ contains the eigenvalues of B (which are always real) along its main diagonal and Q is an orthogonal matrix containing the eigenvectors of B as its columns.

- Principal Component Analysis (PCA): Given a data matrix M (of size $p \times q$), PCA involves the computation of the eigenvectors of MM^T or M^TM. The matrix of these eigenvectors can be thought of as a rigid rotation in a high dimensional space. When you apply this transformation to the original data, the axis corresponding to the principal eigenvector is the one along which the points are most "spread out." More precisely, this axis is the one along which the variance of the data is maximized. Put another way, the points can best be viewed as lying along this axis, with small deviations from this axis. Likewise, the axis corresponding to the second eigenvector (the eigenvector corresponding to the second-largest eigenvalue) is the axis along which the variance of distances from the first axis is greatest, and so on.

- Singular Value Decomposition (SVD): SVD involves the decomposition of a data matrix M (of size $p \times q$) into a product: $U\Sigma V^T$ where U (of size $p \times k$) and V (of size $q \times k$) are column-orthonormal matrices[1] and Σ (of size $k \times k$) is a diagonal matrix. The entries along the diagonal of Σ are referred to as singular values of M. The key to understanding what SVD offers is in viewing the r columns of U, Σ, and V as representing concepts that are hidden in the original matrix M.

For answering the questions below, let us define a real matrix M (of size $p \times q$) and let us assume this matrix corresponds to a dataset with p data points and q dimensions.

[1] A matrix $U \in \mathbb{R}^{p\times q}$ is column-orthonormal if and only if $U^TU = I$ where I denotes the identity matrix

(a) [3 points]

Are the matrices MM^T and M^TM symmetric, square and real? Explain.

(b) [5 points]

Prove that the nonzero eigenvalues of MM^T are the same as the nonzero eigenvalues of M^TM. You may ignore multiplicity of eigenvalues. Are their eigenvectors the same?

(c) [2 points]

Given that we now understand certain properties of M^TM, write an expression for M^TM in terms of Q, Q^T and Λ where $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_d)$ contains the eigenvalues of M^TM along its main diagonal and Q is an orthogonal matrix containing the eigenvectors of M^TM as its columns?
Hint: Check the definition of eigenvalue decomposition provided in the beginning of the question to see if it is applicable.

(d) [5 points]

SVD decomposes the matrix M into the product $U\Sigma V^T$ where U and V are column-orthonormal and Σ is a diagonal matrix. Given that $M = U\Sigma V^T$, write a simplified expression for M^TM in terms of V, V^T and Σ.

(e) [5 points]

In this question, let us experimentally test if SVD decomposition of M actually provides us the eigenvectors (PCA dimensions) of M^TM. We strongly recommend students to use Python and suggested functions for this exercise.[2] Initialize matrix M as follows:

$$M = \begin{bmatrix} 1 & 2 \\ 2 & 1 \\ 3 & 4 \\ 4 & 3 \end{bmatrix}$$

- Compute the SVD of M (*Use scipy.linalg.svd function in Python and set the argument* `full_matrices` *to False*). The function returns values corresponding to U, Σ and V^T. What are the values returned for U, Σ and V^T? *Note: Make sure that the first element of the returned array Σ has a greater value than the second element.*

[2] Other implementations of SVD and PCA might give slightly different results. Besides, you will just need fewer than five python commands to answer this entire question

- Compute the eigenvalue decomposition of $M^T M$ (*Use scipy.linalg.eigh function in Python*). The function returns two parameters: a list of eigenvalues (let us call this list $Evals$) and a matrix whose columns correspond to the eigenvectors of the respective eigenvalues (let us call this matrix $Evecs$). Sort the list $Evals$ in descending order such that the largest eigenvalue appears first in the list. Also, re-arrange the columns in $Evecs$ such that the eigenvector corresponding to the largest eigenvalue appears in the first column of $Evecs$. What are the values of $Evals$ and $Evecs$ (after the sorting and re-arranging process)?

- Based on the experiment and your derivations in part (c) and (d), do you see any correspondence between V produced by SVD and the matrix of eigenvectors $Evecs$ (after the sorting and re-arranging process) produced by eigenvalue decomposition? If so, what is it?
  Note: The function scipy.linalg.svd returns V^T (not V).

- Based on the experiment and the expressions obtained in part (c) and part (d) for $M^T M$, what is the relationship (if any) between the eigenvalues of $M^T M$ and the singular values of M? Explain.
  Note: The entries along the diagonal of Σ (part (e)) are referred to as singular values of M. The eigenvalues of $M^T M$ are captured by the diagonal elements in Λ (part (d))

What to submit:

(i) Written solutions to questions 1(a) to 1(e) with explanations wherever required

(ii) Upload the code via Gradescope [1(e)]

2 k-means on Spark (20 points)

Note: This problem should be implemented in Spark. You should **not** use the Spark MLlib clustering library for this problem. You may store the centroids in memory if you choose to do so.

* * *

This problem will help you understand the nitty gritty details of implementing clustering algorithms on Spark. In addition, this problem will also help you understand the impact of using various distance metrics and initialization strategies in practice. Let us say we have a set $\mathcal{X}$ of n data points in the d-dimensional space $\mathbb{R}^d$. Given the number of clusters k and the set of k centroids $\mathcal{C}$, we now proceed to define various distance metrics and the corresponding cost functions that they minimize.

Euclidean distance Given two points A and B in d dimensional space such that $A = [a_1, a_2 \cdots a_d]$ and $B = [b_1, b_2 \cdots b_d]$, the Euclidean distance between A and B is defined as:

$$||a - b|| = \sqrt{\sum_{i=1}^{d}(a_i - b_i)^2} \tag{1}$$

The corresponding cost function ϕ that is minimized when we assign points to clusters using the Euclidean distance metric is given by:

$$\phi = \sum_{x \in \mathcal{X}} \min_{c \in \mathcal{C}} ||x - c||^2 \tag{2}$$

Note, that in the cost function the distance value is squared. This is intentional, as it is the squared Euclidean distance the algorithm is guaranteed to minimize.

Manhattan distance Given two random points A and B in d dimensional space such that $A = [a_1, a_2 \cdots a_d]$ and $B = [b_1, b_2 \cdots b_d]$, the Manhattan distance between A and B is defined as:

$$|a - b| = \sum_{i=1}^{d} |a_i - b_i| \tag{3}$$

The corresponding cost function ψ that is minimized when we assign points to clusters using the Manhattan distance metric is given by:

$$\psi = \sum_{x \in \mathcal{X}} \min_{c \in \mathcal{C}} |x - c| \tag{4}$$

Iterative k-Means Algorithm: We learned the basic k-Means algorithm in class which is as follows: k centroids are initialized, each point is assigned to the nearest centroid and the centroids are recomputed based on the assignments of points to clusters. In practice, the above steps are run for several iterations. We present the resulting iterative version of k-Means in Algorithm 1.

Iterative k-Means clustering on Spark: Implement iterative k-means using Spark. Please use the dataset from `q2/data` within the bundle for this problem.

The folder has 3 files:

1. `data.txt` contains the dataset which has 4601 rows and 58 columns. Each row is a document represented as a 58 dimensional vector of features. Each component in the vector represents the importance of a word in the document. The ID to download `data.txt` into a Colab is 1E-voIV2ctU4Brw022Na8RHVVRGOoNkO1

2. `c1.txt` contains k initial cluster centroids. These centroids were chosen by selecting $k = 10$ random points from the input data. The ID to download `c1.txt` into a Colab is 1yXNlZWMqUcAwDScBrkFChOHJwR1FZXmI

Algorithm 1 Iterative k-Means Algorithm

```
procedure ITERATIVE k-MEANS
    Select k points as initial centroids of the k clusters.
    for iterations := 1 to MAX_ITER do
        for each point p in the dataset do
            Assign point p to the cluster with the closest centroid
        end for
        Calculate the cost for this iteration.
        for each cluster c do
            Recompute the centroid of c as the mean of all the data points assigned to c
        end for
    end for
end procedure
```

3. `c2.txt` contains initial cluster centroids which are as far apart as possible, using Euclidean distance as the distance metric. (You can do this by choosing 1st centroid c1 randomly, and then finding the point c2 that is farthest from c1, then selecting c3 which is farthest from c1 and c2, and so on). The ID to download `c2.txt` into a Colab is 1vfovle9DgaeK0LnbQTH0j7kRaJjsvLtb

Tip: To download the datasets in Colab, you can follow the set-up instructions at the beginning of Colab2 and replace the ids correspondingly.

Set number of iterations (`MAX_ITER`) to 20 and number of clusters k to 10 for all the experiments carried out in this question. Your driver program should ensure that the correct amount of iterations are run.

When assigning points to centroids, if there are multiple equidistant centroids, choose the one that comes first in lexicographic order.

(a) Exploring initialization strategies with Euclidean distance [10 pts]

1. [**5 pts**] Using the Euclidean distance (refer to Equation 1) as the distance measure, compute the cost function $\phi(i)$ (refer to Equation 2) for every iteration i. This means that, for your first iteration, you'll be computing the cost function using the initial centroids located in one of the two text files. Run the k-means on `data.txt` using `c1.txt` and `c2.txt`. Generate a graph where you plot the cost function $\phi(i)$ as a function of the number of iterations i=1..20 for `c1.txt` and also for `c2.txt`. You may use a single plot or two different plots, whichever you think best answers the theoretical questions we're asking you about.

   (Hint: Note that you do not need to write a separate Spark job to compute $\phi(i)$. You should be able to calculate costs while partitioning points into clusters.)

2. [**5 pts**] What is the percentage change in cost after 10 iterations of the K-Means algorithm when the cluster centroids are initialized using `c1.txt` vs. `c2.txt` and the

distance metric being used is Euclidean distance? Is random initialization of k-means using `c1.txt` better than initialization using `c2.txt` in terms of cost $\phi(i)$? Explain your reasoning.

(Hint: to be clear, the percentage refers to (cost[0]-cost[10])/cost[0].)

(b) Exploring initialization strategies with Manhattan distance [10 pts]

1. [**5 pts**] Using the Manhattan distance metric (refer to Equation 3) as the distance measure, compute the cost function $\psi(i)$ (refer to Equation 4) for every iteration i. This means that, for your first iteration, you'll be computing the cost function using the initial centroids located in one of the two text files. Run the k-means on `data.txt` using `c1.txt` and `c2.txt`. Generate a graph where you plot the cost function $\psi(i)$ as a function of the number of iterations i=1..20 for `c1.txt` and also for `c2.txt`. You may use a single plot or two different plots, whichever you think best answers the theoretical questions we're asking you about.

   (Hint: This problem can be solved in a similar manner to that of part (a). Also note that It's possible that for Manhattan distance, the cost do not always decrease. K-means only ensures monotonic decrease of cost for squared Euclidean distance. Look up K-medians to learn more.)

2. [**5 pts**] What is the percentage change in cost after 10 iterations of the K-Means algorithm when the cluster centroids are initialized using `c1.txt` vs. `c2.txt` and the distance metric being used is Manhattan distance? Is random initialization of k-means using `c1.txt` better than initialization using `c2.txt` in terms of cost $\psi(i)$? Explain why.

What to submit:

(i) Upload the code for 2(a) and 2(b) to Gradescope

(ii) A plot of cost vs. iteration for two initialization strategies [2(a)]

(iii) Percentage improvement values and your explanation [2(a)]

(iv) A plot of cost vs. iteration for two initialization strategies [2(b)]

(v) Percentage improvement values and your explanation [2(b)]

3 Latent Features for Recommendations (35 points)

Note: Please use native Python libraries like numpy/pandas/etc to solve this problem. Spark is not required. It usually takes several minutes to run, however, time may differ depending on the system you use.

* * *

The goal of this problem is to implement the *Stochastic Gradient Descent* algorithm to build a Latent Factor Recommendation system. We can use it to recommend movies to users. We encourage you to read the slides of the lecture "Recommender Systems 2" again before attempting the problem.

Suppose we are given a matrix R of ratings. The element R_{iu} of this matrix corresponds to the rating given by user u to item i. The size of R is $m \times n$, where m is the number of movies, and n the number of users.

Most of the elements of the matrix are unknown because each user can only rate a few movies.

Our goal is to find two matrices P and Q, such that $R \simeq QP^T$. The dimensions of Q are $m \times k$, and the dimensions of P are $n \times k$. k is a parameter of the algorithm.

We define the error as

$$E = \left(\sum_{(i,u) \in \text{ratings}} (R_{iu} - q_i \cdot p_u^T)^2 \right) + \lambda \left[\sum_u \|p_u\|_2^2 + \sum_i \|q_i\|_2^2 \right]. \tag{5}$$

The $\sum_{(i,u) \in \text{ratings}}$ means that we sum only on the pairs (user, item) for which the user has rated the item, *i.e.* the (i, u) entry of the matrix R is known. q_i denotes the i^{th} row of the matrix Q (corresponding to an item), and p_u the u^{th} row of the matrix P (corresponding to a user u). q_i and p_u are both row vectors of size k. λ is the regularization parameter. $\| \cdot \|_2$ is the L_2 norm and $\|p_u\|_2^2$ is square of the L_2 norm, *i.e.*, it is the sum of squares of elements of p_u.

(a) [10 points]

Let ε_{iu} denote the derivative of the error E with respect to R_{iu}. What is the expression for ε_{iu}? What are the update equations for q_i and p_u in the Stochastic Gradient Descent algorithm? Please show your derivation and use ε_{iu} in your final expression of q_i and p_u.

(b) [25 points]

Implement the algorithm. Read each entry of the matrix R from disk and update ε_{iu}, q_i and p_u for each entry.

To emphasize, you are not allowed to store the matrix R in memory. You have to read each element R_{iu} one at a time from disk and apply your update equations (to each element) each iteration. Each iteration of the algorithm will read the whole file.

Choose $k = 20$, $\lambda = 0.1$ and number of iterations $= 40$. Find a good value for the learning rate η, starting with $\eta = 0.1$. (You may not modify k or λ) The error E on the training set ratings.train.txt discussed below should be less than 65000 after 40 iterations; you should observe both q_i and p_u stop changing.

Based on values of η, you may encounter the following cases:

- If η is too big, the error function can converge to a high value or may not monotonically decrease. It can even diverge and make the components of vectors p and q equal to ∞.
- If η is too small, the error function doesn't have time to significantly decrease and reach convergence. So, it can monotonically decrease but not converge *i.e.* it could have a high value after 40 iterations because it has not converged yet.

Use the dataset at `q3/data` within the bundle for this problem. It contains the following files:

- `ratings.train.txt`: This is the matrix R. Each entry is made of a user id, a movie id, and a rating.

Plot the value of the objective function E (defined in equation 5) on the training set as a function of the number of iterations. What value of η did you find?

You can use any programming language to implement this part, but Java, C/C++, and Python are recommended for speed. (In particular, Matlab can be rather slow reading from disk.) It should be possible to get a solution that takes on the order of minutes to run with these languages.

Hint: These hints will help you if you are not sure about how to proceed for certain steps of the algorithm, although you don't have to follow them if you have another method.

- *Initialization of P and Q: We would like q_i and p_u for all users u and items i such that $q_i \cdot p_u^T \in [0, 5]$. A good way to achieve that is to initialize all elements of P and Q to random values in $[0, \sqrt{5/k}]$.*
- *Update the equations: In each update, we update q_i using p_u and p_u using q_i. Compute the new values for q_i and p_u using the old values, and then update the vectors q_i and p_u.*
- *You should compute E at the end of a full iteration of training. Computing E in pieces during the iteration is incorrect since P and Q are still being updated.*

What to submit

(i) Equation for ε_{iu}. Update equations in the Stochastic Gradient Descent algorithm [3(a)]

(ii) Value of η. Plot of E vs. number of iterations. Make sure your graph has a y-axis so that we can read the value of E. Only one plot with your chosen η is required [3(b)]

(iii) Please upload all the code to Gradescope [3(b)]

4 Recommendation Systems (25 points)

Note: Please use native Python libraries like numpy/pandas/etc to solve this problem. Spark is not required. If you run into a memory error when doing large matrix operations, please make sure you are using 64-bit Python instead of 32-bit (which has a 4GB memory limit).

* * *

Consider a user-item bipartite graph where each edge in the graph between user U to item I, indicates that user U likes item I. We also represent the ratings matrix for this set of users and items as R, where each row in R corresponds to a user and each column corresponds to an item. If user i likes item j, then $R_{i,j} = 1$, otherwise $R_{i,j} = 0$. Also assume we have m users and n items, so matrix R is $m \times n$.

Let's define a matrix P, $m \times m$, as a diagonal matrix whose i-th diagonal element is the degree of user node i, *i.e.* the number of items that user i likes. Similarly, a matrix Q, $n \times n$, is a diagonal matrix whose i-th diagonal element is the degree of item node i or the number of users that liked item i. See figure below for an example.

(a) [4 points]

Define the non-normalized user similarity matrix $T = R * R^T$ (multiplication of R and transposed R). Explain the meaning of T_{ii} and T_{ij} $(i \neq j)$, in terms of bipartite graph structures (See Figure 1) (e.g. node degrees, path between nodes, etc.).

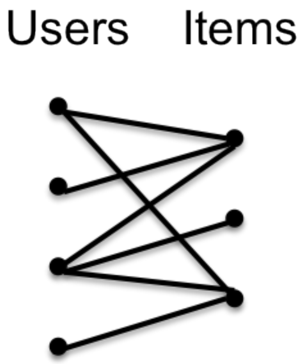
Cosine Similarity: Recall that the cosine similarity of two vectors u and v is defined as:

$$\textit{cos-sim(u,v)} = \frac{u \cdot v}{\|u\|\|v\|}$$

(b) [6 points]

Let's define the *item similarity matrix*, S_I, $n \times n$, such that the element in row i and column j is the cosine similarity of *item* i and *item* j which correspond to column i and column j of the matrix R. Show that $S_I = Q^{-1/2} R^T R Q^{-1/2}$, where $Q^{-1/2}$ is defined by $Q_{rc}^{-1/2} = 1/\sqrt{Q_{rc}}$ for all nonzero entries of the matrix, and 0 at all other positions.

Repeat the same question for *user similarity matrix*, S_U where the element in row i and column j is the cosine similarity of *user* i and *user* j which correspond to row i and row j of the matrix R. That is, your expression for S_U should also be in terms of some combination of R, P, and Q. Your answer should be an operation on the matrices, in particular you should not define each coefficient of S_U individually.



$$R=\begin{bmatrix} 1 & 0 & 1 \\ 1 & 0 & 0 \\ 1 & 1 & 1 \\ 0 & 0 & 1 \end{bmatrix}$$

$$P=\begin{bmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \quad Q=\begin{bmatrix} 3 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 3 \end{bmatrix}$$

Figure 1: User-Item bipartite graph.

Your answer should show how you derived the expressions.

(Note: To make the element-wise square root of a matrix, you may write it as matrix to the power of $\frac{1}{2}$.)

(c) [**5 points**]

The recommendation method using user-user collaborative filtering for user u, can be described as follows: for all items s, compute $r_{u,s} = \Sigma_{x \in users}\, \text{cos-sim}(x,u) * R_{xs}$ and recommend the k items for which $r_{u,s}$ is the largest.

Similarly, the recommendation method using item-item collaborative filtering for user u can be described as follows: for all items s, compute $r_{u,s} = \Sigma_{x \in items} R_{ux} * \text{cos-sim}(x,s)$ and recommend the k items for which $r_{u,s}$ is the largest.

Let's define the recommendation matrix, Γ, $m \times n$, such that $\Gamma(i,j) = r_{i,j}$. Find Γ for both item-item and user-user collaborative filtering approaches, in terms of R, P and Q. Your final answer should describe operations on matrix level, not specific terms of matrices.

Hint: For the item-item case, $\Gamma = RQ^{-1/2}R^T RQ^{-1/2}$.

Your answer should show how you derived the expressions (even for the item-item case, where we give you the final expression).

(d) [10 points]

In this question you will apply these methods to a real dataset. The data contains information about TV shows. More precisely, for 9985 users and 563 popular TV shows, we know if a given user watched a given show over a 3 month period.

Use the dataset from `q4/data` within the bundle for this problem.

The folder contains:

- `user-shows.txt` This is the ratings matrix R, where each row corresponds to a user and each column corresponds to a TV show. $R_{ij} = 1$ if user i watched the show j over a period of three months. The columns are separated by a space.
- `shows.txt` This is a file containing the titles of the TV shows, in the same order as the columns of R.

We will compare the user-user and item-item collaborative filtering recommendations for the 500$^{\text{th}}$ user of the dataset. Let's call him Alex. (i.e. with Python's 0-based indexing, Alex=users[499].)

In order to do so, we have erased the first 100 entries of Alex's row in the matrix, and replaced them by 0s. This means that we don't know which of the first 100 shows Alex has watched. Based on Alex's behaviour on the other shows, we will give Alex recommendations on the first 100 shows. We will then see if our recommendations match what Alex had in fact watched.

- Compute the matrices P and Q.
- Using the formulas found in part (c), compute Γ for the user-user collaborative filtering. Let S denote the set of the first 100 shows (the first 100 columns of the matrix). From all the TV shows in S, which are the five that have the highest similarity scores for Alex? In case of ties of similarity scores between two shows, choose the one with smaller index. Do not write the index of the TV shows, write their names using the file `shows.txt`.
- Compute the matrix Γ for the movie-movie collaborative filtering. From all the TV shows in S, which are the five that have the highest similarity scores for Alex? In case of ties between two shows, choose the one with smaller index.

For sanity check, your highest similarity score for user-user collaborative filtering should be above 900, and your highest similarity score for movie-movie filtering should be above 31.

What to submit:

(i) Interpretation of T_{ii} and T_{ij} [4(a)]

(ii) Expression of S_I and S_U in terms of R, P and Q and accompanying explanation [4(b)]

(iii) Expression of Γ in terms of R, P and Q and accompanying explanation [4(c)]

(iv) The answer to this question should include the followings: [4(d)]

- The **names** of five TV shows that have the highest similarity scores for Alex for the user-user collaborative filtering (no need to report the similarity scores)
- The **names** of five TV shows that have the highest similarity scores for Alex for the item-item collaborative filtering (no need to report the similarity scores)
- Upload the source code via Gradescope