CS246: Mining Massive Data Sets **Winter 2015**

Problem Set 2

Due 5:00pm February 5, 2015

Only one late period is allowed for this homework (2/10).

General Instructions

These questions require thought, but do not require long answers. Please be as concise as possible. Please fill the cover sheet and submit it as a front page with your answers. We will **subtract 2 points** for failing to include the cover sheet. Include the names of your collaborators (see the course website for the collaboration or honor code policy).

All students (Regular and SCPD) should submit their answers using Scoryst (see course website FAQ for further instructions). This submission should include the source code you used for the programming questions.

Additionally, all students (Regular and SCPD) should upload all code through a single text file per question using the url below. Please do not use .pdf, .zip or .doc files for your code upload.

Cover Sheet: http://cs246.stanford.edu/cover.pdf

Code (Snap) Upload: http://snap.stanford.edu/submit/

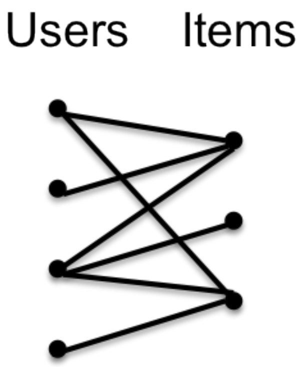
Assignment (Scoryst) Upload: https://scoryst.com/course/39/submit/

Questions

1 Recommendation Systems (25 points) [Clifford, Negar]

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 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 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.



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

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

Figure 1: User-Item bipartite graph.

(a) [**5 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. Recall that the cosine similarity of two vectors u and v is defined as $\frac{u \cdot v}{\|u\|\|v\|}$[1] Express S_I in terms of R, P and Q. Your answer should be a product of matrices, in particular you should not define each coefficient of S_I individually.

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.

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 $\frac{1}{2}$.)

(b) [**5 points**]

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

Similarly, the recommendation method using item-item collaborative filtering for user u can

[1] The definition of cosine simiarity we saw in class took the arc-cos of this expression. The definition we use here gives the same relative ordering, since the dot products are always positive in this case.

be described as follows: for all items s, compute $r_{u,s} = \Sigma_{x \in items} R_{ux} * \cos(x, s)$ and recommend the the top k items for which $r_{u,s}$ are 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 answer should show how you derived the expressions.

(c) [5 points]

Define the non-normalized user similarity matrix $T = R * R^T$. 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.).

(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.

Download the dataset[2] on `http://snap.stanford.edu/class/cs246-data/hw2-q1-dataset.zip`.

The ZIP file 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 500th user of the dataset. Let's call him Alex.

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 or not. 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.

[2]The original data is from Chris Volinksy's website at `http://www2.research.att.com/~volinsky/DataMining/Columbia2011/HW/HW6.html`.

- Using the formulas found in part (b), 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? What are their similarity score? In case of ties 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. Again, hand in the names of the shows and their similarity score.

Alex's original row is given in the file `alex.txt`. For a given number k, **the true positive rate at top-k** is defined as follows: using the matrix Γ computed previously, compute the top-k TV shows in S that are most similar to Alex (break ties as before). The true positive rate is the number of top-k TV shows that were watched by Alex in reality, divided by the total number of shows he watched in the held out 100 shows.

- Plot the **true positive rate at top-k** (defined above) as a function of k, for $k \in [1, 19]$, with predictions obtained by the user-user collaborative filtering.
- On the same figure, plot the true positive rate at top-k as a function of k, for $k \in [1, 19]$, with predictions obtained by the item-item collaborative filtering.
- Briefly comment on your results (one sentence is enough).

What to submit:

(a) Expression of S_I and S_U in terms of R, P and Q and accompanying explanation

(b) Expression of Γ in terms of R, P and Q and accompanying explanation

(c) Interpretation of T_{ii} and T_{ij}

(d) The answer to this question should include the followings:

- The five TV shows that have the highest similarity scores for Alex for the user-user collaborative filtering.
- The five TV shows that have the highest similarity scores for Alex for the item-item collaborative filtering.
- The graph of the true positive rate at top-k for both the user-user and the item-item collaborative filtering.
- A brief comment on this graph.
- Submit the source code via the SNAP electronic submission website and attach to your Scoryst submission as well.

2 Singular Value Decomposition (25 points + 5 extra credit points) [Hristo, Peter]

In this problem we will explore SVD and its relationships to eigenvalue decomposition and linear regression and show that it gives an optimal low rank approximation to a matrix.

First, recall that the eigenvalue decomposition of a real, *symmetric*, and square matrix $B \in \mathbb{R}^{d \times d}$ decomposes it into the product

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

where $\Sigma = \operatorname{diag}(\lambda_1, \ldots, \lambda_d)$ 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. When B has rank $r < d$ we will often be concerned only with the non-zero eigenvalues (and corresponding eigenvectors). In this case we take the term "non-zero eigenvectors" to mean eigenvectors corresponding to non-zero eigenvalues.

We will start by showing how to compute the SVD of a matrix $A \in \mathbb{R}^{m \times n}$ via eigenvalue decomposition. This technique is particularly useful when one dimension of A is much larger than the other (i.e. $m \gg n$ or vice versa). For concreteness, we will assume that $m = 100$ and $n = 10,000$ (A is a wide matrix) and that it has rank $r \leq m$. Let $A = USV^{\mathrm{T}}$ be the SVD of A so that $U \in \mathbb{R}^{m \times r}$, $S = \operatorname{diag}(\sigma_1, \ldots, \sigma_r)$ contains the singular values of A, and $V \in \mathbb{R}^{n \times r}$. Note that both, U and V, have orthonormal columns so that $U^{\mathrm{T}}U = V^{\mathrm{T}}V = I_r$ but that the *rows* of these matrices are not necessarily orthonormal.

(a) [12 points]

Finding the SVD using AA^T or A^TA:

1. Show that the matrices $C = A^{\mathrm{T}}A$ and $K = AA^{\mathrm{T}}$ are symmetric, and express the non-zero eigenvalues and eigenvectors of these matrices in terms of U, S, V from the SVD of A.
2. Suppose that we are only interested in the singular values of A. It takes $O(d^3)$ operations to find the eigenvalues of a symmetric $d \times d$ matrix. Should we use C or K to find the singular values of A?
3. Show how to extract U *and* V using only the matrix A and the eigenvalue decomposition of C.
4. Show how to extract U *and* V using only the matrix A and the eigenvalue decomposition of K.

(b)[13 points]

Document similarity using SVD:

In this exercise, you will play around with the SVD on some real data. To complete the problem it will be the easiest to use Matlab. In Matlab the SVD of a matrix A can be retrieved as: `[U, S, V] = svd(A, 'econ');` If you do not have access to Matlab you can also use the open source "Matlab" implementation called Octave. You can also use any other software package/language.

First, download the input file http://snap.stanford.edu/class/cs246-data/hw2_q2-Data.zip [3] which is a normalized document-term incidence matrix X of various IMDb movie reviews. Here, each of the rows i can be considered to be a document d_i while the columns represent the occurrence of words within the corresponding document. Alongside X is a vector of binary labels y where $y_i = 1$ indicates that review i liked its movie and $y_i = -1$ indicates that review i disliked the movie.

Let $X = USV^T$ be the SVD of X and define $U(k)$ to be the k columns of U corresponding to the k largest singular values of X. The matrix $U(k)$ gives a k-dimensional representation of the reviews where $U(k)_i$, i.e. row i of $U(k)$, is a k-dimensional vector that corresponds to the i^{th} review. We want to figure out how well this decomposition performs when identifying positive and negative reviews as our feature representation increases in dimensionality. Define $w(k) = \sum_{i=41}^{640} y_i U(k)_i$ to be a simple classifier built on reviews 41 through 640 and let $r(k) = -\sum_{i=1}^{40} y_i U(k)_i^T w(k)$ be a measure of the agreement between the predicted and actual sentiment of the first 40 reviews, where lower is better. Compute $r(k)$ for $k = \{1, 21, 41, \dots, 601\}$ and plot a graph showing how r changes as k varies.

(c) Extra Credit [5 points]

This is a hard (but nice) problem. Only attempt it if you have extra time after you finished all other problems.

SVD for rank reduction:

We will show that the SVD gives an optimal low rank approximation of a matrix $A \in \mathbb{R}^{m\times n}$. Along the way we will also explore its relationship to linear regression. In particular, we are interested in finding matrices $X \in \mathbb{R}^{m\times k}, W \in \mathbb{R}^{k\times n}$, where $k \leq \text{rank}(A)$ is given, that solve

$$\underset{X^{\mathrm{T}}X=I_k}{\text{minimize}} \|A - XW\|_F^2. \tag{1}$$

Here $\|\cdot\|_F^2$ extends the vector L_2-norm to matrices in that $\|A\|_F^2 = \sum_{i=1}^n \|\boldsymbol{a}_i\|_2^2$ where the $\boldsymbol{a}_i$ are the columns of A. Note that we require X to be orthogonal for convention[4].

[3] Original dataset received from Hristo Paskov

[4] Given a solution $(\hat{X}, \hat{W})$ that minimizes (1) in which X is not orthogonal, we can always come up with an orthogonal solution. If $\hat{X} = P\Sigma R^{\mathrm{T}}$ is the SVD of $\hat{X}$, we set $X = P$ and $W = \Sigma R^{\mathrm{T}}\hat{W}$ so that X is

Assuming that the SVD $A = USV^{\mathrm{T}}$ stores the singular values (and corresponding singular vectors) in *decreasing* order[5], we will show that if $\tilde{U}, \tilde{V}$ are the first k columns of U, V, respectively, and $\tilde{S} = \operatorname{diag}(\sigma_1, \dots, \sigma_k)$, then $(X = \tilde{U}, W = \tilde{S}\tilde{V}^{\mathrm{T}})$ are optimal for (1).

1. Given a vector $y \in \mathbb{R}^m$ and a matrix $Z \in \mathbb{R}^{m \times d}$ of features, linear regression finds a coefficient vector $w \in \mathbb{R}^d$ that approximates y linearly based on Z. The vector w minimizes $\|y - Zw\|_2^2$ and, assuming $\operatorname{rank}(Z) = d$, w can be expressed as

$$w = (Z^{\mathrm{T}}Z)^{-1}Z^{\mathrm{T}}y.$$

   Assuming X is fixed in equation (1), give a closed form expression for W in terms of A and X.

2. Suppose that we set $X = \tilde{U}$, which was defined as the first k columns of the SVD of X. Use your formula from above to give a simple expression for W in terms of $\tilde{S}$ and $\tilde{V}$.

3. We now turn to solving for X and no longer assume it is fixed. Use your solution to part 1 above to eliminate W from (1) and express it in the form $\min_{X^{\mathrm{T}}X=I_k} \|MA\|_F^2$ where M is a simple expression involving only product(s) and sum(s) of X. (Answers involving inverses will not get full credit.)

4. An alternative way to characterize the k largest eigenvectors[6] of a symmetric matrix $M \in \mathbb{R}^{m \times m}$ is via the problem $\max_{Q^{\mathrm{T}}Q=I_k} \operatorname{trace}(Q^{\mathrm{T}}MQ)$ where $Q \in \mathbb{R}^{m \times k}$. Using your expression from the previous question, show that problem (1) can be expressed as the eigenvalue problem $\max_{X^{\mathrm{T}}X=I_k} \operatorname{trace}(X^{\mathrm{T}}AA^{\mathrm{T}}X)$. You will need to use the fact that $\|M\|_F^2 = \operatorname{trace}(M^{\mathrm{T}}M)$ and the properties of the trace[7].

5. Finally, use what you have proved here and in part (a) to conclude that $X = \tilde{U}$ and $W = \tilde{S}\tilde{V}^{\mathrm{T}}$.

What to submit:

1. Part(a): Written solution to questions (1) to (4).

2. Part(b): The plot of r as a function of k and submit the source code via the electronic submission website.

3. Part(c): Written solution to questions (1) to (5).

orthogonal and $XW = \hat{X}\hat{W}$.

[5] i.e. $S = \operatorname{diag}(\sigma_1, \dots, \sigma_r)$ with $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r$.

[6] i.e. eigenvectors corresponding to the k largest eigenvalues.

[7] i.e. $\operatorname{trace}(M) = \operatorname{trace}(M^{\mathrm{T}})$ for square M, $\operatorname{trace}(BCD) = \operatorname{trace}(DBC) = \operatorname{trace}(CDB)$, and $\operatorname{trace}(A + B) = \operatorname{trace}(A) + \operatorname{trace}(B)$.

3 Theory of k-means (20 points) [Clement, Jean-Yves]

In this problem, we study two different initialization methods for the k-means algorithm. First, let us set up the problem: we have a set $\mathcal{X}$ of n data points in the d-dimensional space $\mathbb{R}^d$. We are also given k, the number of clusters, and would like to choose a set of k centers $\mathcal{C}$ to minimize the cost function:

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

Then, the k-means algorithm for the above problem works as follows:

1. **Initialization**: Arbitrarily choose k initial centers $\mathcal{C} = \{c_1, c_2, \ldots, c_k\}$
2. $\forall\, i \in \{1, 2, \ldots, k\}$, set the cluster $C_i = \big\{x \in \mathcal{X} | \text{argmin}_{1 \le j \le k}\{||x - c_j||\} = i\big\}$
3. $\forall\, i \in \{1, 2, \ldots, k\}$, set c_i to be the center of mass of C_i, that is $c_i = \frac{1}{|C_i|} \sum_{x \in C_i} x$
4. Repeat steps 2 and 3 until $\mathcal{C}$ no longer changes.

We first prove some basic facts about this algorithm.

(a)[5 points]

Assume S is an arbitrary set of points (in $\mathbb{R}^d$) with center of mass $c(S)$, and assume z is an arbitrary point (not necessarily in S). The notation $|| \cdot ||$ denoting the L_2 norm, first prove that:

$$\sum_{x \in S} ||x - z||^2 - \sum_{x \in S} ||x - c(S)||^2 = |S| \cdot ||c(S) - z||^2.$$

(b)[5 points]

We denote by a superscript (t) the state of the k-means algorithm at the beginning of iteration t. Prove that, while $\mathcal{C}^{(t)}$ keeps changing, each iteration of the k-means algorithm decreases the cost, *i.e.* prove that for each iteration t (where $\phi^{(t)} = \sum_{x \in \mathcal{X}} \min_{c \in \mathcal{C}^{(t)}} ||x - c||^2$), we have $\phi^{(t)} \ge \phi^{(t+1)}$.

(c)[5 points]

Prove that when running k-means, the cost function ϕ converges to a finite value. (This claims holds independently from the dataset and the initial clusters.)

Finally, argue[8] that k-means converges, *i.e.* that the algorithm reaches a state where the centroids (or equivalently the assignments of points to clusters) do not change.

[8]For this part of the question, we expect more of a heuristic than a completely formal proof.

(d)[5 points]

With an example show that with a bad initialization, the k-means algorithm may converge to a clustering that has an unboundedly larger cost than the optimal clustering (*i.e.*, the one with the optimal cost). In other words, given an arbitrary number $r > 1$, give a situation where k-means converges to a clustering whose cost is at least r times larger than the cost of the optimal clustering. You may fix k.

(Note: A hard-coded example or the output of a coding example that behaves badly would not receive full credit. We are asking for a formal example that can work for any arbitrary number $r > 1$, and a formal analysis of the performance of the k-means algorithm.)

What to submit:

(a) Proof that $\sum_{x \in S} ||x - z||^2 - \sum_{x \in S} ||x - c(S)||^2 = |S| \cdot ||c(S) - z||^2$

(b) Proof that the cost of k-means decreases at each iteration

(c) Proof that the cost function always converges and argument that the cluster assignments also converge.

(d) Formal example that leads to non-optimal convergence and analysis

4 k-means on MapReduce (30 points) [Janice, James, Dima, Nat]

Automatic tagging and cross-linking of documents: Clustering algorithms are frequently used to automatically categorize documents by web services which receive a large number of new content items daily. As human intervention would be very expensive, these services need an automated way to find related items and to categorize and cross-link the documents. News-aggregation site feedly is an example service which processes and categorizes tens of thousands of new documents per day.

We will explore this use case in this problem.

(a) [10 pts]

k-Means clustering on Hadoop: Implement the k-means using Map Reduce where a single step of Map Reduce completes one iteration of the k-means algorithm. So, to run k-means for i iterations, you will have to run a sequence of i MapReduce jobs.

Run the k-Means algorithm on Hadoop to find the centroids for the dataset at: http://snap.stanford.edu/class/cs246-data/hw2-q4-kmeans.zip

The zip has 4 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.

2. `vocab.txt` contains the words used for generating the document vector. (For example the first word represents the first feature of the document vector. For document 2 (line 2 in `data.txt`), feature 3 "alkalemia" (line 3 in `vocab.txt`) has frequency `0.5`, so the third component of the document vector is `0.5`.)

3. `c1.txt` contains k initial cluster centroids. These centroids were chosen by selecting $k = 10$ random points from the input data.

4. `c2.txt` contains initial cluster centroids which are as far apart as possible. (You can do this by choosing 1^{st} 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).

Use Euclidean distance (ie, the $L2$ norm) as the distance measure. Set number of iterations to 20 and number of clusters to 10. Use points in `c1.txt` for initialization.

*Hint about **job chaining**:*

We need to run a sequence of Hadoop jobs where the output of one job will be the input for the next one. There are multiple ways to do this and you are free to use any method you are comfortable with. One simple way to handle a such a multistage job is to configure the output path of the first job to be the input path of the second and so on.

The following pseudo code demonstrates job chaining.

```
var inputDir
var outputDir
var centroidDir

for i in no-of-iterations (
     Configure job here with all params
     Set job input directory = inputDir
     Set job output directory = outputDir + i
     Run job
     centroidDir =  outputDir + i
)
```

You will also need to share the location of centroid file with the mapper. There are many ways to do this and you can use any method you find suitable. One way is to use the Hadoop Configuration object. You can set it as a property in the Configuration object and retrieve the property value in the Mapper setup function.

For more details see :

1. http://hadoop.apache.org/docs/r1.0.4/api/org/apache/hadoop/conf/Configuration.html#set(java.lang.String,java.lang.String)
2. http://hadoop.apache.org/docs/r1.0.4/api/org/apache/hadoop/conf/Configuration.html#get(java.lang.String)
3. http://hadoop.apache.org/docs/r1.0.4/api/org/apache/hadoop/mapreduce/Mapper.html#setup(org.apache.hadoop.mapreduce.Mapper.Context)

Cluster Initialization strategies: The output of k-Means algorithm depends on the initial points chosen. There are many ways of choosing the initial points. We will compare two of them: random selection, and selecting points as far apart as possible.

(b) [5 pts]

For every iteration, compute the cost function $\phi(i)$ (as defined at the beginning of question 3). This means that, for your first MapReduce job 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`.

(Hint: Note that you do not need to write a separate MapReduce job to do this. You can incorporate the computation of $\phi(i)$ into the Mapper/Reducer from part (a).)

(c) [5 pts]

Is random initialization of k-means using `c1.txt` better than initialization using `c2.txt` in terms of cost $\phi(i)$? Why? What is the percentage change in cost from using the initial centroids versus using those centroids obtained after 10 iterations of K-Means?

Automatically tagging documents: One way of tagging documents is to assign word tags to each cluster. To get the top `k` word tags for a cluster, sort the features for its centroid by their coordinate values in descending order, choose the top `k` features and use words from `vocab.txt` to get the word tags for these top `k` features.

For e.g. if the indexes of top 5 features of the centroid for cluster 1 are `[1, 2, 6, 7, 10]` then the tags for the documents in cluster 1 are `[activator, decay-corrected, softer, mitomycin, spc]` which are words at line `1, 2, 6, 7, 10` respectively in `vocab.txt`.

Use points in `c1.txt` for initialization.

(d) [10 pts]

Which 5 tags would you apply to the second document? *For verification, the 10th tag is* `alkalemia`.

What to submit:

(a) Code (both on your Scoryst submission and SNAP upload)

(b) Code (both on your Scoryst submission and SNAP upload), and graph for initialization strategies

(c) The answer should include percentage improvement values and your explanation.

(d) 5 best tags