

Problem Set 3

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Late Day Policy All students will be given two no-questions-asked late periods, but only one late period can be used per homework and cannot be used for project deliverables. A late-period lasts 48 hours from the original deadline (so if an assignment is due on Thursday at 11:59 pm, the late period goes to the Saturday at 11:59pm Pacific Time).

Academic Integrity We take [academic integrity](#) extremely seriously. We strongly encourage students to form study groups. Students may discuss and work on homework problems in groups. However, each student must write down the solutions and the code independently. In addition, each student should write down the set of people whom they interacted with.

Discussion Group (People with whom you discussed ideas used in your answers):

On-line or hardcopy documents used as part of your answers:

I acknowledge and accept the Academic Integrity clause.

(Signed) _____

1 Dead Ends in PageRank Computations (25 points)

We learned about PageRank in lecture which is an algorithm for ranking webpages. In this problem, we are going to focus on dead ends and examine how they affect the PageRank computations.

Suppose we denote the matrix of the Internet as the n -by- n matrix M , where n is the number of webpages. Suppose there are k links out of the node (webpage) j , and

$$M_{ij} = \begin{cases} 1/k & \text{if there is a link from } j \text{ to } i \\ 0 & \text{otherwise} \end{cases}$$

For a webpage j that is a *dead end* (i.e., one having zero links out), the column j is all zeroes.

Let $\mathbf{r} = [r_1, r_2, \dots, r_n]^\top$ be *an estimate* of the PageRank vector. In one iteration of the PageRank algorithm, we compute the next estimate \mathbf{r}' of the PageRank as: $\mathbf{r}' = M\mathbf{r}$.

Given any PageRank estimate vector \mathbf{r} , define $w(\mathbf{r}) = \sum_{i=1}^n r_i$.

- (a) [6pts] Suppose the Web has no dead ends. Prove that $w(\mathbf{r}') = w(\mathbf{r})$.
- (b) [9pts] Suppose there are still no dead ends, but we use a teleportation probability (i.e., the probability of jumping to some random page) of $1 - \beta$, where $0 < \beta < 1$. The expression for the next estimate of r_i becomes $r'_i = \beta \sum_{j=1}^n M_{ij} r_j + (1 - \beta)/n$. Under what conditions will $w(\mathbf{r}') = w(\mathbf{r})$? Prove your conclusion.

Hint: The conditions required for the equality are related to $w(\mathbf{r})$.

- (c) [10pts] Now, let us assume a teleportation probability of $1 - \beta$ in addition to the fact that there are one or more dead ends. Call a node “dead” if it is a dead end and “live” if not. Assume $w(\mathbf{r}) = 1$. At each iteration, when not teleporting, each live node j distributes βr_j PageRank uniformly across each of the nodes it links to, and each dead node j distributes r_j/n PageRank to all the nodes.

Write the equation for r'_i in terms of β , M , \mathbf{r} , n , and D (where D is the set of dead nodes). Then, prove that $w(\mathbf{r}') = 1$.

What to submit

- (i) Proof [1(a)]
- (ii) Condition for $w(\mathbf{r}') = w(\mathbf{r})$ and Proof [1(b)]
- (iii) Equation for r'_i and Proof [1(c)]

2 The Louvain Algorithm for Community Detection (35 points)

Note: For this question, assume all graphs are undirected and weighted.

The Louvain Algorithm is commonly used for community detection in graphs which can be especially a good fit for graphs with a hierarchical structure. In this problem, we are going to understand how the Louvain algorithm works by following the steps of the algorithm. Furthermore, we are going to focus on how the algorithm works with the hierarchically structured graphs and how we can evaluate the quality of the communities we discover.

Communities, or clusters of densely linked nodes in a graph, are important elements of a graph's structure. Thus, discovering communities from an observed graph can help us summarize the overall structure of a graph and learn more about the underlying process. However, finding the "best" set of communities from data is often a difficult problem. One way to measure how well a network is partitioned into communities is to calculate the number of within-community edges relative to the number of between-community edges. This can be formalized using *modularity*, defined as:

$$Q = \frac{1}{2m} \sum_{1 \leq i, j \leq n} \left(\left[A_{ij} - \frac{d_i d_j}{2m} \right] \delta(c_i, c_j) \right)$$

Where A is the adjacency matrix of a graph G with n vertices and m edges, A_{ij} is the (i, j) -th entry of A , $2m = \sum_{i, j} A_{ij}$ is the sum of all entries in A , d_i is the degree of node i , δ is the Kronecker delta, i.e. $\delta(k, l) = 1$ when $k = l$, otherwise $\delta(k, l) = 0$, and c_i and c_j are the communities of i and j respectively. Here, we assume that communities are disjoint, i.e. each node can only belong to one community. The modularity of a graph lies in the range $[-1, 1]$.

Maximizing the modularity of a given graph is a computationally hard problem. The Louvain algorithm is a popular and efficient heuristic used to solve this problem. It is a greedy algorithm, meaning that at every step, it will take the path that provides the largest possible increase to the objective (modularity) at that step. Each pass of the algorithm has two phases:

- **Phase 1 (Modularity Optimization)** aims to group nodes in the graph G into communities in a way that maximizes the modularity of the graph. After the first pass, the input graph to this step is the graph produced by phase 2 in the previous pass (see below).
- **Phase 2 (Community Aggregation)** combines each community into a single node, producing a new graph H where each node represents a community of nodes in the graph G . This new graph H is fed into phase 1 in the next pass of the algorithm.

We repeat these two phases until we no longer increase modularity through one pass. The algorithm proceeds as follows:

Phase 1 (Modularity Optimization)

Input: a graph $G = (V, E)$ with a vertex set V and an edge set E . \triangleright The input changes in each pass of the algorithm; after pass 1 the input is the graph output by phase 2.

Output: a partition of G into communities.

```

1: Initialize each node  $i$  as its own community
2: for each node  $i \in V$  do
3:    $\mathcal{N}_i \leftarrow$  the set of neighbors of  $i$  in  $G$ 
4:   for each node  $j$  in  $\mathcal{N}_i$  do
5:      $\Delta Q_j \leftarrow$  the change in modularity when  $i$  is assigned to the community of  $j$ 
6:   end for
7:    $j^* \leftarrow$  the neighbor that gives the most positive change in modularity  $\Delta Q_{j^*}$ 
8:   if  $\Delta Q_{j^*} > 0$  then
9:     Assign node  $i$  to the community of  $j^*$ 
10:  else
11:    Keep node  $i$  in its current community
12:  end if
13: end for

```

Phase 2 (Community Aggregation)

Input: a graph $G = (V_G, E_G)$ with a vertex set V_G and an edge set E_G ; and the communities from Phase 1.

Output: a graph $H = (V_H, E_H)$ where each node now represents a community in the Phase 1 graph G .

```

1:  $V_H \leftarrow \emptyset$ 
2:  $E_H \leftarrow \emptyset$ 
3: for each community  $C$  do
4:    $V_H \leftarrow V_H \cup \{C\}$ 
5: end for
6: for each community  $C$  do
7:   for each community  $C'$  do
8:      $e \leftarrow \{C, C'\}$ 
9:     if  $e \notin E_H$  then
10:       $E_H \leftarrow E_H \cup \{e\}$  (including a self-edge if  $C = C'$ )
11:       $w_e \leftarrow \sum_{\substack{v \in C \\ u \in C'}} w_{v,u}$   $\triangleright w_e$  is the weight assigned to the edge  $e$  in the
        graph  $H$ . Initially,  $w_{v,u} = 1$  for all  $v$  and  $u$ .
12:     end if
13:   end for
14: end for

```

Again, we repeat phases 1 and 2 until no change in modularity occurs. We call each iteration of phases 1 and 2 one pass of the algorithm. Figure 1 below illustrates the Louvain algorithm.

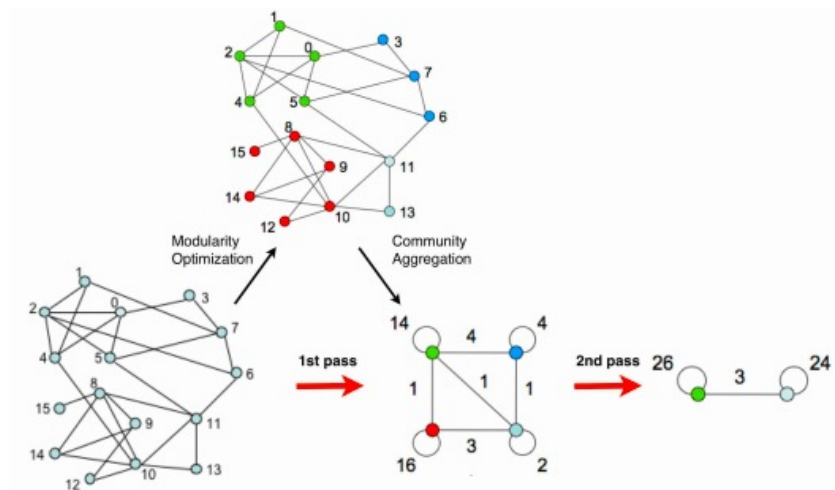


Figure 1: Example from Blondel et al. showing the two phases of the Louvain algorithm

(a) [9 points] Consider a node i that is in a community all by itself. Let C represent an existing community in the graph. Node i feels lonely and decides to move into the community C . This situation can be modeled by a graph (Figure 2) with C represented by a single node. We observe the following sums of weights:

- $\Sigma_{in} = \sum_{j,k \in C} w_{j,k}$ - the sum of the weights of edges within C .
- Σ_{tot} - the sum of the weights of the edges incident to a vertex in C .
- k_i - the sum of weights of edges incident to i (i.e., its weighted degree).
- $k_{i,in}/2$ - the sum of the weights of the edges between i and a vertex in C , i.e. the community of i and C are connected by an edge of weight $k_{i,in}/2$.
- As always, $2m = \sum_{i,j} A_{ij}$ is the sum of all entries in the adjacency matrix.

To begin with, C and i are in separate communities (colored green and red respectively). The third node represents the remainder of the graph.

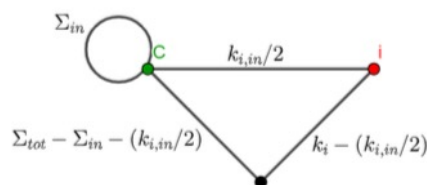


Figure 2: Before merging, i is an isolated node and C is a community. The rest of the graph is represented by a single node.

Prove that the modularity gain seen when i merges with C (i.e., the change in modularity

after they merge into one community) is given by:

$$\Delta Q = \left[\frac{\Sigma_{in} + k_{i,in}}{2m} - \left(\frac{\Sigma_{tot} + k_i}{2m} \right)^2 \right] - \left[\frac{\Sigma_{in}}{2m} - \left(\frac{\Sigma_{tot}}{2m} \right)^2 - \left(\frac{k_i}{2m} \right)^2 \right].$$

Note that this expression gives us a computationally efficient way to compute the modularity changes in phase 1.

Hint: Apply the community aggregation step of the Louvain algorithm to simplify the calculations.

- (b) **[12 points]** Consider the graph G in Figure 3, with 4 cliques of 4 nodes each, arranged in a ring. Assume all the edges have the same weight value 1. There exists exactly one edge between any two adjacent cliques. We will manually (by hand) inspect the results of the Louvain algorithm on this network.

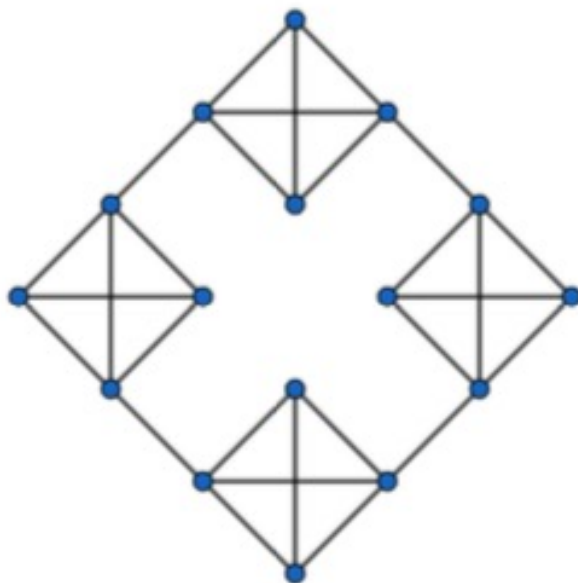


Figure 3: G is a subgraph. The whole graph has 16 nodes (4 cliques with 4 nodes per clique)

- [4 points]** The first phase of modularity optimization detects each clique as a single community, so there are 4 communities in total. Thus, the graph H output by the first pass of the Louvain algorithm is a graph with four nodes, each corresponding to one of the four cliques in G . What are the weights of each edge in the graph H ? Explain.
Hint: Note that the symmetry of the ring structure simplifies the calculation.
- [3 points]** Derive the modularity of the graph H after the first pass of the Louvain algorithm.

3. [5 points] Show mathematically that the modularity of H would not increase in the second pass of the algorithm, hence the algorithm terminates.

Hint: Due to the symmetry in H , you only need to calculate a single value of ΔQ . You may either calculate the modularity directly or extend the result of part (a).

- (c) [14 points] Modularity optimization often fails to identify communities smaller than a certain scale, which is known as the **resolution limit problem**. We illustrate this problem using a dataset with ground-truth communities; that is, we have labels for the “true” communities of the graph. We provide the following undirected YouTube social network. In the YouTube social network, users can form friendships with each other and users can create groups which other users can join. We consider such user-defined groups as ground-truth communities.

We are interested in quantifying how “good” the communities chosen by modularity by evaluating them via a goodness metric, which we present below. Here we compare 2 scoring functions: (1) *modularity* (higher is better) (2) *cut ratio* (lower is better): $f(S) = \frac{c_S}{n_S(n-n_S)}$, where c_S is the number of edges crossing the boundary of community S , n_S is the number of nodes in S and n is the number of nodes in the entire graph. Our goodness metric is *density* $g(S) = \frac{2m_S}{n_S(n_S-1)}$, where m_S is the number of edges within S .

Note that density favors small, highly connected communities; hence, we expect that scoring functions that do poorly with smaller communities will not perform well with respect to this metric, and that scoring functions that can accurately identify smaller communities will have strong performance with respect to this goodness metric. Thus, this creates a good test case for the resolution limit of *modularity*. From the definition, we could see cut ratio has already taken community size into account.

We run the following experiment: the file [youtube_community_top1000.txt](#) in the folder `louvain/data` contains the top 1000 ground-truth communities. For each community scoring function f , we rank the ground-truth communities by decreasing score of f . So, lower values of rank correspond to the “better” communities by each scoring function, whereas higher values of rank correspond to the “worse” communities under each scoring function. We measure the cumulative running average value of the goodness metric g of the top- k ground-truth communities under the ordering induced by f . Intuitively, a perfect community scoring function would rank the communities in decreasing order of the goodness metric, and thus the cumulative running average of the goodness metric would decrease monotonically with k .

You have been provided a skeleton in the file [PartitionQuality.py](#) in the folder `louvain/code`. Your task is to complete the functions `community_modularity`, `cut_ratio`, and `density`. Then, run the file, which executes the functions you have written and applies them to the YouTube dataset. Submit the plot [density.jpg](#) produced by the code as part of your write-up. Interpret the plot you produce. Which metric is performing better for this dataset? Using 2-3 sentences, explain why this might be the case.

Hint: For the first ground-truth community in `youtube_community_top1000.txt`, the modularity is approximately 2.15×10^{-5} , the cut ratio is approximately 1.39×10^{-4} , and the density is approximately 3.62×10^{-2} .

What to submit

- (i) Proof of 2(a).
- (ii) Answers to the 3 subparts of 2(b).
- (iii) The plot `density.jpg` produced by your code and an interpretation thereof. [2(c)]
- (iv) Upload your completed implementation of `PartitionQuality.py` to Gradescope.

3 Spectral Clustering (40 points)

We saw in lecture several methods for partitioning different types of graphs. In this problem, we explore (yet another) such partitioning method called “spectral clustering”. The name derives from the fact that it uses the *spectrum of certain matrices* (that is, the eigenvalues and eigenvectors) derived from the graph and the key idea is to minimize cut. Mathematically, cut minimization is closely related to modularity maximization. We could also use the spectral clustering algorithm to solve the modularity maximization problem [1].

Our goals in this problem are to derive a simple algorithm for spectral clustering, apply it on a dataset, and interpret the clustering results.

Let us first fix the notation we’ll use in this problem.

- Let $G = (V, E)$ be a simple (that is, no self- or multi-edges), undirected, connected graph with $n = |V|$ and $m = |E|$.
- We use the notation $\{i, j\} \in E$ to denote that the nodes i and j are connected via an edge (note that since this is an undirected graph, we do not talk about the direction of the connection).
- Let A be the adjacency matrix of G : that is, $A_{ij} = \begin{cases} 1 & \text{if } \{i, j\} \in E \\ 0 & \text{otherwise} \end{cases}$.
- We use d_i to denote the degree of the i -th node; by definition of the adjacency matrix, $d_i = \sum_{j=1}^n A_{ij}$. We define the diagonal matrix D formed by placing the degrees of the nodes along its diagonal. That is, $D_{ii} = d_i$ for all $i = 1, 2, \dots, n$.
- We define the graph Laplacian as the $n \times n$ matrix $L = D - A$.
- We define a vector $e_i \in \mathbb{R}^n$ as zero on all coordinates *except* the i -th, at which it is 1. In this case, since $|V| = n$, the vector e_i is n -dimensional.
- Define the vector $e \in \mathbb{R}^n$ as the vector of all 1s. Again, e is an n -dimensional vector in this case.

For a set of nodes $S \subseteq V$, we associate two values that measure, in some sense, its quality as a cluster: the “cut” and the “volume”. We define these two values below.

The “cut” of a set S is defined as the number of edges that have one end point in the set S and the other in its complement, $\bar{S} = V \setminus S$:

$$\text{cut}(S) = \sum_{i \in S, j \in \bar{S}} A_{ij}. \quad (1)$$

Observe that by definition, $\text{cut}(S) = \text{cut}(\bar{S})$.

The “volume” of a set is defined as the sum of degrees of nodes in S :

$$\text{vol}(S) = \sum_{i \in S} d_i, \quad (2)$$

where d_i is the degree of node i .

In addition to the above measures associated with set S , we define the *normalized cut* of a graph (associated with a partitioning S) as

$$\text{NCUT}(S) = \frac{\text{cut}(S)}{\text{vol}(S)} + \frac{\text{cut}(\bar{S})}{\text{vol}(\bar{S})} \quad (3)$$

For a set S to have a small normalized cut value, it must have very few edges connecting the nodes inside S to the rest of the graph (making the numerators small), *as well as* roughly equal volumes of S and \bar{S} , so that neither denominator is too small.

We are now ready to start proving things. **Please be careful when reading expressions involving S and \bar{S} , since at a quick glance they may look the same.**

(a) Establishing Some Basics [18 points]

We first make some observations that will help us formulate the problem of minimizing normalized cut nicely in the next sub-problem.

Given a set of nodes S , we define a vector $x_S \in \mathbb{R}^n$, such that the i -th coordinate $x_S^{(i)}$ of x_S is defined as follows:

$$x_S^{(i)} = \begin{cases} \sqrt{\frac{\text{vol}(\bar{S})}{\text{vol}(S)}} & \text{if } i \in S \\ -\sqrt{\frac{\text{vol}(S)}{\text{vol}(\bar{S})}} & \text{otherwise} \end{cases} \quad (4)$$

To clarify (because the font may not be clear), in Equation 4, in the case $i \in \bar{S}$, the term in the denominator under the square root is $\text{vol}(\bar{S})$.

In the following, we are using the notation established at the start of this problem and some set of node $S \subseteq V$. Prove the following statements:

1. $x_S^\top Lx_S = c \cdot \text{NCUT}(S)$ for some constant c that depends on the problem parameters. Note that you should specify this constant.

Hint: For any vector $x \in \mathbb{R}^n$, it holds that $x^\top Lx = \sum_{\{i,j\} \in E} (x_i - x_j)^2$. You can start the proof using this hint.

2. $x_S^\top De = 0$.

3. $x_S^\top Dx_S = 2m$.

(b) Normalized Cut Minimization [12 points]

Based on the facts we just proved about x chosen as per Equation 4, we can formulate the normalized cut minimization problem as follows:

$$\begin{aligned} & \underset{S \subset V}{\text{minimize}} && \frac{x_S^\top Lx_S}{x_S^\top Dx_S}, \\ & \text{subject to} && x_S^\top De = 0, \\ & && x_S^\top Dx_S = 2m. \end{aligned}$$

To be clear, we are minimizing over all (non-trivial) partitions (S, \bar{S}) , where the vectors x_S are defined as described in Equation 4. Note that the two constraints appearing in the optimization are trivially maintained due to the form x_S as we have shown in the previous sub-problem. However, constraining x to take the form of Equation 4 makes this optimization problem NP-Hard. We will instead relax the optimization problem, making it tractable, and then round the relaxed solution back to a feasible point of the *original* problem. The relaxation we choose eliminates the constraint on the form of x . This gives us the following *relaxed* optimization problem:

$$\begin{aligned} & \underset{x \in \mathbb{R}^n}{\text{minimize}} && \frac{x^\top Lx}{x^\top Dx}, \\ & \text{subject to} && x^\top De = 0, \\ & && x^\top Dx = 2m. \end{aligned} \tag{5}$$

We could show that a minimizer of the optimization problem 5 is

$$x^* = D^{-1/2}v,$$

where v is an eigenvector corresponding to the second smallest eigenvalue of the *normalized graph Laplacian* $\mathcal{L} = D^{-1/2}LD^{-1/2}$.

Let's prove this conclusion step by step.

1. Please prove that the smallest eigenvalue of L is 0 and the corresponding eigenvector is e .

2. Please prove the eigenvector corresponding to the smallest eigenvalue of \mathcal{L} (normalized graph Laplacian) is $D^{1/2}e$.

Hint: Use the conclusion from part 1.

3. Use the linear transformation $z = D^{1/2}x$ and $r = D^{1/2}e$. This is a valid operation because the graph is connected, and therefore all the degrees are positive. The optimization problem 5, in the transformed space, becomes:

$$\begin{aligned} & \underset{z \in \mathbb{R}^n}{\text{minimize}} && \frac{z^\top \mathcal{L} z}{z^\top z} \\ & \text{subject to} && z^\top r = 0 \\ & && z^\top z = 2m. \end{aligned}$$

Please prove the solution of this optimization problem is $z^* = v$ and $x^* = D^{-1/2}v$

Finally, to round the solution back to a feasible point in the original problem, we can take the nodes corresponding to the positive entries of the eigenvector to be in the set S and those corresponding to the negative entries to be in \bar{S} .

Hint 1: For a symmetric matrix P , we can write any vector z as $z = \sum_{i=1}^n w_i v_i$, where the v_i are orthonormal eigenvectors of P .

Hint 2: Use the conclusion from part 2.

(c) Programming [10 points]

Now that we have obtained the new transformed version of our normalized cut minimization problem and its solution, we will implement the spectral clustering algorithm for $k = 2$ clusters.

We have provided the dataset `songs.csv` in the folder `spectral_clustering/data`, which includes 10 features (e.g., `release`, `loudness`, `danceability`) for 1000 songs. The features are already normalized. In this question, you are going to implement spectral clustering and run it on the songs dataset to cluster these songs into two clusters. Then, you are going to investigate these inferred clusters and identify features that distinguish the two clusters.

There are various methods for defining an adjacency matrix. For this question, we are going to generate a simple adjacency matrix where two songs i, j are connected (i.e., $A_{ij} = 1$) only if their Euclidean distance is smaller than 1. The adjacency matrix A for this dataset is defined as follows:

$$A_{ij} = \begin{cases} 1 & \text{if } \|x_i - x_j\| < 1 \\ 0 & \text{otherwise} \end{cases} \quad (6)$$

Note that here we are adopting a simple version of a general method called ϵ -neighbourhood graph which connects nodes (i.e., points) within ϵ distance of each other. Specifically, we are defining a 1-neighbourhood graph ($\epsilon = 1$) for our data matrix.

The algorithm for $k = 2$ clusters is as follows:

Algorithm 1 Spectral Clustering for $k = 2$

```

1: procedure SPECTRAL CLUSTERING
2:   Construct the adjacency matrix  $A \in \mathbb{R}^{n \times n}$ 
3:   Compute the degree matrix  $D$ 
4:   Compute the Laplacian  $L = D - A$  and the normalized Laplacian  $\mathcal{L} = D^{-1/2}LD^{-1/2}$ 
5:   Compute the eigenvector  $v$  corresponding to the second smallest eigenvalue of  $\mathcal{L}$  and compute  $x = D^{1/2}v$   $x = D^{-1/2}v \in \mathbb{R}^n$ 
6:   Let  $x_i$  be the  $i^{\text{th}}$  element of  $x$  for  $i = 1, \dots, n$ 
7:   for each  $x_i$  do
8:     Cluster  $x_i$  using the indicator function  $I$ , as defined in Equation 7, into clusters  $C_1, C_2$ 
9:   end for
10: end procedure

```

Most spectral clustering algorithms would use k-means algorithm in the last step. Here, for simplicity, we use an indicator function instead. The indicator function is defined as follows:

$$I(i) = \begin{cases} i \in C_1 & \text{if } x_i \geq 0 \\ i \in C_2 & \text{otherwise} \end{cases} \quad (7)$$

1. Please report the final cluster labels for the first 5 songs. For eigendecomposition, you may use library functions for obtaining the eigenvalues and eigenvectors of a matrix (e.g., `numpy.linalg.eig` in Python).

Hint: For sanity check, the clustering results for songs 6, 7, 8 are C_1, C_1, C_1 .

2. Now we start to explore the systematic differences between the two clusters. One simple way is to compare the mean difference of each of the 10 original features between the two clusters. In other words, for the two clusters you learned, calculate the mean feature values across all samples in that cluster. Once you have this mean representation for each cluster, calculate the difference between the mean features of the two clusters.

Please report the top 3 features with the highest absolute value of mean difference. Briefly explain (1-2 sentences) what these clusters might represent (any reasonable answer is correct).

3. Simply looking at the mean features for each cluster is useful yet quite limited. An alternative way of investigating the learned clusters is to run t-tests for each feature to see whether the differences between the two clusters are statistically significant.

For the 3 features you found in part 2, please run t-tests and report the p-values for each of the 3 features. If you apply a threshold of p-value=0.05, which of these 3 features are still significant? Briefly explain (1-2 sentences) why you think this is the case.

For running t-tests, please use the library function `scipy.stats.ttest_ind(equal_var = True)` in Python.

What to submit

- i. Proof of the 3 equalities in part 3(a).
- ii. Proof of the 3 conclusions in part 3(b).
- iii. The clustering result for the first 5 users [3(c)].
- iv. The top 3 features with the highest absolute value of mean difference and interpretation of the results [3(c)].
- v. The p-values for the 3 features, the list of significant features, and interpretation of the results [3(c)].
- vi. Upload your implementation of the spectral clustering algorithm to Gradescope.

References

- [1] NEWMAN, M. E. Spectral methods for community detection and graph partitioning. *Physical Review E* 88, 4 (2013), 042822.