Math 420, Spring 2019
First Team Homework

due Tuesday, 26 February 2018

I. (3pts) Consider the undirected graph represented in Figure 1.

1. Find the number of vertices n, the number of edges m, and write down the list of vertices V and the list of edges E.
2. Compute the graph Laplacian Δ, the normalized graph Laplacian $\tilde{\Delta}$ and the normalized asymmetric Laplacian L.
3. Compute the set of eigenvalues and eigenvectors of the three matrices at part 2 (You can use Matlab)

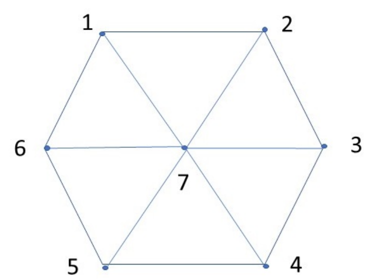

Figure 1: A Hexagonal Graph plus Star

Exercise II. (7pts) Use Matlab to do the folowing:

1. Load the dataset assigned to this homework, and extracts the vectors $X(1:n), Y(1:n), Z(1:n)$ and $Q(1:n)$ from lines $3:2+n$, columns 2,3,4 and 5, respectively. Here $n = 19$, the number of atoms in that molecule.
2. Compute the symmetric matrix F,

$$F_{k,l} = \frac{|Q(k)Q(l)|}{\sqrt{(X(k)-X(l))^2 + (Y(k)-Y(l))^2 + (Z(k)-Z(l))^2}} \ , \ 1 \leq k, l \leq n$$

3. Find a threshold $\tau > 0$ so that at least half of entries in matrix F are smaller than or equal to this threshold, and at least half of the entries are larger than or equal than this threshold.
4. Construct the weight matrix W by thresholding the entries in F by τ, i.e.,

$$W_{k,l} = \begin{cases} F_{k,l} & \text{if} \quad F_{k,l} \geq \tau \\ 0 & \text{if} \quad \text{otherwise} \end{cases}$$

5. Construct the graph Laplacian $\Delta = D - W$, with $D = diag(W \cdot 1)$ (as described in class).

6. Compute its eigenpairs and compute the 2D embedding in the real plane using the Graph Visualization Spectral Algorithm. Print out the coordinates of the $n = 19$ vectors.

7. Plot the graph using circles for vertices and edges between vertices where $W_{k,l} > 0$.