# Math 420, Spring 2019
# Second Solo Homework:
# Introduction to the Threads

Due Tuesday, 12 February, 2019

**Exercise 1.** Compute $m_i$, $v_{ij}$, and $c_{ij}$ for each of the following groups of assets based on daily closing price data with uniform weights:

(i) VFINX, VBMFX, and VGSIX in 2018;
(ii) VFINX, VBMFX, and VGSIX in 2017 and 2018;
(iii) VFINX, VBMFX, VGSIX, VGTSX, VMVIX, and VTIBX in 2018;
(iv) VFINX, VBMFX, VGSIX, VGTSX, VMVIX, and VTIBX in 2017 and 2018.

a. Describe the assets VFINX, VBMFX, and VGSIX. Display $m_i$ as a 3-vector and $v_{ij}$ and $c_{ij}$ as $3 \times 3$-matrices for (i) and (ii). Explain the differences between these objects for groups (i) and (ii).
b. Compute a complete set of eigenpairs for the $3 \times 3$-matrices $v_{ij}$ for groups (i) and (ii). What conclusions do you draw from the eigenvalues about the dimensionality of these assets?
c. Describe the assets VGTSX, VMVIX, and VTIBX. Display $m_i$ as a 6-vector and $v_{ij}$ and $c_{ij}$ as $6 \times 6$-matrices for (iii) and (iv). Explain the differences between these objects for groups (iii) and (iv).
d. Compute a complete set of eigenpairs for the $6 \times 6$-matrices $v_{ij}$ for groups (iii) and (iv). What conclusions do you draw from the eigenvalues about the dimensionality of these assets?
e. Give explanations for the values of $c_{ij}$ you computed for groups (iii) and (iv).

**Exercise 2 on the next page.**

**Exercise 2.** Consider the database QM9 of chemical compounds from http://quantum-machine.org/datasets/ .

The datafile dsC7O2H10nsd_0001.xyz contains a geometric configuration of the 19-atom molecule $C_7O_2H_{10}$.

To answer the following questions you need to write a piece of Matlab code that loads relevant parts of the dsC7O2H10nsd_0001.xyz file and processes it correctly.

The file structure is the following:

Line 1: number of atoms [19]

Line 2: Various information (disregard for now) – 16 fields

Line 3-21: 5 fields : Atom X Y Z Q

Lines 22,23: Various information (disregard for now).

Your task is to write a Matlab code that loads lines 3 to $2+n$, where here $n = 19$ (the first field in the first line) and saves them into five vectors each of length $n = 19$. Call the first vector Atom. It is a string composed of letters chosen from $\{H, C, O, F, N\}$. The next four $n$-vectors should be called $X, Y, Z, Q$ respectively. For each atom $k$ between 1 and $n$, the triple $(X(k), Y(k), Z(k))$ represents the coordinates of that atom, while $Q(k)$ is an electric charge associated to that atom.

If you load the data correctly, the first elements of the five vectors should read $Atom(1) =' C'$, $X(1) = -1.8396130083$, $Y(1) = 0.5292955664$, $Z(1) = 3.1820679223$, $Q(1) = -0.414977$.

a. Write code that computes two $n \times n$ symmetric matrices $V, W$ whose main diagonals are 0 and off-diagonal elements $V_{k,l}, W_{k,l}$ are given by

$$V_{k,l} = \frac{Q(k)Q(l)}{\sqrt{(X(k) - X(l))^2 + (Y(k) - Y(l))^2 + (Z(k) - Z(l))^2}} \ , \ W_{k,l} = |V_{k,l}| \, .$$

b. Compute the weighted graph Laplacians $\Delta = D - W$ and $\Delta^V = D^V - V$, where $D = diag(W \cdot 1)$ and $D^V = diag(V \cdot 1)$. Detemine which matrix is positive semidefinite (i.e., nonnegative eigenvalues). Plot for each the ordered eigenvalues.

c. For the weighted graph Laplacian $\delta$, compute the normalized symmetric weighted graph Laplacian $\tilde{\Delta} = D^{-1/2}\Delta D^{-1/2}$ and the normalized asymmetric weighted graph Laplacian $L = D^{-1}\Delta$, where $D = diag(W \cdot 1)$. Compute their eigenvalues, order them ascendingly, and plot these eigenvalues in separate plots.

d. Plot the three projections of the 19-atom molecule into planes $(X, Y)$, $(X, Z)$, and $(Y, Z)$. This means, plot $(X(1:n), Y(1:n))$, $(X(1:n, z(1:n))$, and $(Y(1:n), Z(1:n))$, respectively.

e. Can you compute the normalized symmetric weighted graph Laplacian from $\Delta^V$? Why?