AMSC 466. Spring 2020

Homework Assignment 4. Due Thursday March 5.

1. **(5 pts)** The transition rates between two low-energy configurations of the cluster of 38 rare gas atoms at a collection of temperature values have been measured by some sophisticated computations. (These two configurations are shown in Figure 1 here.) The data file `HW4Problem1data.txt` contains the results of these measurements. Its first column contains the absolute temperature values T_i while the second column contains the corresponding transition rates r_i. We want to fit these data to the Arrhenius law

$$r = Ce^{-V/T}, \tag{1}$$

where r is the rate, T is the absolute temperature, and C and V are constants. We would like to find estimates for the energetic barrier V and the constant C from this fit. First we take logarithms of both parts of (1) and get the following linear relationship between $\log r$ and $1/T$:

$$\log r = \log C - V/T. \tag{2}$$

Denoting $\log r$ by y, $1/T$ by x, and $\log C$ by c we get:

$$y = c - Vx. \tag{3}$$

Set up the least squares problem and write a program in any suitable language that finds C and V. Matlab is recommended.

2. **(5 pts)** Let A be an $n \times n$ matrix, and let $Q = [q_1, \dots, q_k]$ be an $n \times k$ matrix of rank k, where $1 \le k < n$. We say that $\text{span}(Q)$ is an invariant subspace of A if and only if for all vectors $v \in \text{span}(Q)$ we have $Av \in \text{span}(Q)$. Prove that $\text{span}(Q)$ is an invariant subspace of A if and only if

$$AQ = QC$$

for some $k \times k$ matrix C.

3. **(10 pts)**

   (a) Let A be a 3×3 matrix, and let T be its Schur form, i.e., there is a Hermitian matrix Q (i.e., $Q^*Q = QQ^* = I$ where Q^* denotes the transpose and complex conjugate of Q) such that

$$A = QTQ^*, \quad \text{where} \quad T = \begin{bmatrix} \lambda_1 & t_{12} & t_{13} \\ 0 & \lambda_2 & t_{23} \\ 0 & 0 & \lambda_3 \end{bmatrix}.$$

   i. Show that if v is an eigenvector of T then Qv is the eigenvector of A corresponding to the same eigenvalue.

   ii. Find eigenvectors of T. *Hint: Check that* $v_1 = [1, 0, 0]^\top$. *Look for* v_2 *of the form* $v_2 = [a, 1, 0]^\top$, *and then for* v_3 *of the form* $v_3 = [b, c, 1]^\top$, *where* a, b, c *are to be expressed via the entries of the matrix* T.

   iii. Write out eigenvectors of A in terms of the found eigenvectors of T and the columns of Q: $Q = [q_1, q_2, q_3]$.

(b) Let A be $n \times n$, and let T be its Schur form (an upper-triangular matrix with possibly complex entries), i.e., $A = QTQ^*$. Let $Q = [q_1, q_2, \ldots, q_n]$ where q_j denotes jth column of Q.

i. Let k be any integer $1 \le k \le n$. Show that the first k columns of Q span an invariant subspace of A. *Hint: write T in the block form with four blocks where the block at the upper left corner is $k \times k$. Write Q as two blocks $Q = [Q_k, Q_{n-k}]$ where Q_k is the matrix consisting of the first k columns of Q.*

ii. Let λ be an eigenvalue of T of multiplicity 1 located at the kth position along the main diagonal. Write T in the block-diagonal form

$$T = \left[\begin{array}{c|c|c} T_{11} & T_{12} & T_{13} \\ \hline 0 & \lambda & T_{23} \\ \hline 0 & 0 & T_{33} \end{array}\right],$$

where T_{11} is $(k-1) \times (k-1)$, λ is 1×1, and T_{33} is $(n-k) \times (n-k)$. Show that the eigenvector of T corresponding to the eigenvalue λ is

$$v_k = \begin{bmatrix} (\lambda I - T_{11})^{-1} T_{12} \\ 1 \\ 0 \end{bmatrix}.$$

iii. What is the eigenvector of A corresponding to λ?