

Homework 4

11 September 2006

1 Problem 2

The matrix S given in the file `signalsvd.txt` is in the form shown below

$$S = \begin{bmatrix} S(\lambda_1, t_1) & S(\lambda_2, t_1) & \cdots & S(\lambda_n, t_1) \\ S(\lambda_1, t_2) & S(\lambda_2, t_2) & \cdots & S(\lambda_n, t_2) \\ \cdots & & & \\ \cdots & & & \\ S(\lambda_1, t_k) & S(\lambda_2, t_k) & \cdots & S(\lambda_n, t_k) \end{bmatrix}$$

Signal due to each species can be written as

$$S_i = \sigma_i \begin{bmatrix} a_i(\lambda_1)x_i(t_1) & a_i(\lambda_2)x_i(t_1) & \cdots & a_i(\lambda_n)x_i(t_1) \\ a_i(\lambda_1)x_i(t_2) & a_i(\lambda_2)x_i(t_2) & \cdots & a_i(\lambda_n)x_i(t_2) \\ \cdots & & & \\ \cdots & & & \\ a_i(\lambda_1)x_i(t_n) & a_i(\lambda_2)x_i(t_n) & \cdots & a_i(\lambda_n)x_i(t_k) \end{bmatrix}$$

where a_i and x_i are the dimensionless signal strength and concentration of species i respectively. But the above array can be written as a product of two vectors as follows

$$S_i = \sigma_i \begin{bmatrix} x_i(t_1) \\ x_i(t_2) \\ \cdot \\ \cdot \\ \cdot \\ x_i(t_n) \end{bmatrix} \begin{bmatrix} a_i(\lambda_1) & a_i(\lambda_2) & \cdots & a_i(\lambda_k) \end{bmatrix}$$

The total signal measured due to all the species is

$$S = \sum S_i = \sum \sigma_i x_i a_i^T \quad (1)$$

The above expression for S looks very similar to the SVD of the matrix S . Thus let us perform the SVD of S and write it as

$$S = U\Sigma V^T = \sum \sigma_i u_i v_i^T \quad (2)$$

where

$$U = \begin{bmatrix} u_1 & u_2 & \cdots & u_n \end{bmatrix}$$

$$\Sigma = \begin{bmatrix} \sigma_1 & 0 & \cdots & 0 \\ 0 & \sigma_2 & \cdots & 0 \\ \cdot & & & \\ \cdot & & & \\ 0 & 0 & \cdots & \sigma_n \\ 0 & 0 & \cdots & 0 \\ \cdot & & & \\ \cdot & & & \\ 0 & 0 & \cdots & 0 \end{bmatrix}$$

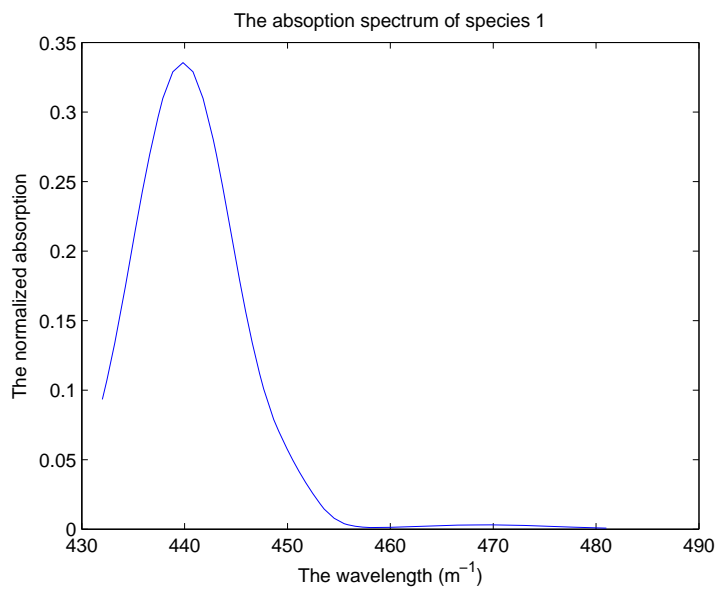
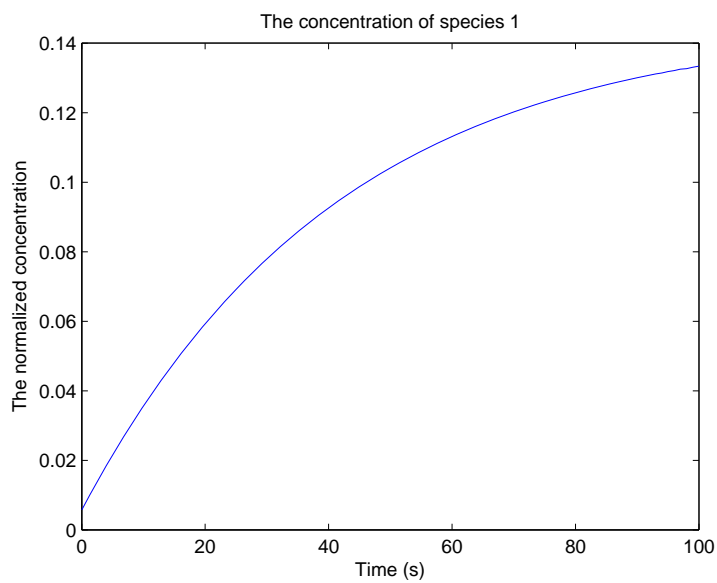
and

$$V = \begin{bmatrix} v_1 & v_2 & \cdots & v_k \end{bmatrix}$$

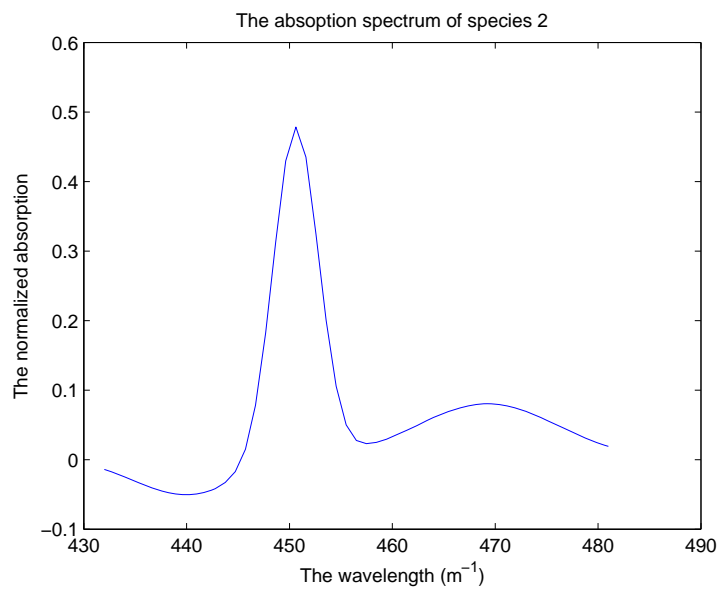
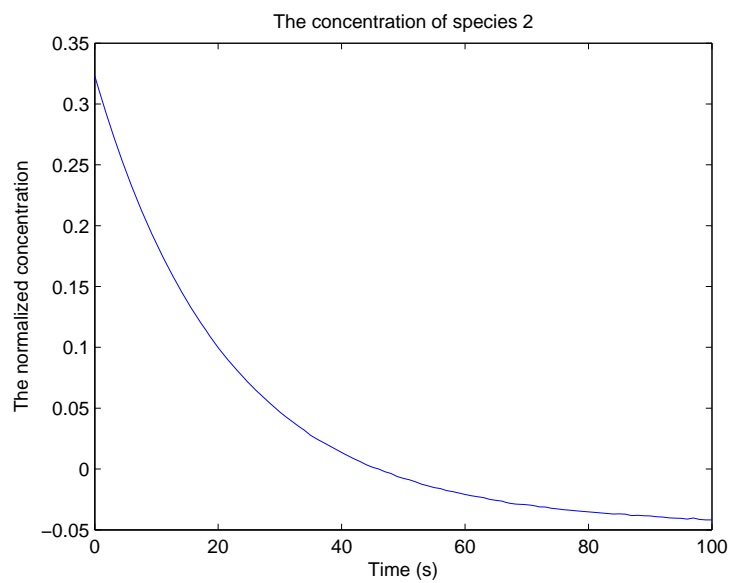
Comparing Equation 1 and Equation 2, we get the hint that the u corresponds to the concentration of species and v corresponds to the absorption spectrum of the species. The number of significant species are the number of non-zero or significantly different from 0 values of σ .

After we do the decomposition we find that $\sigma_1 = 16.3161$, $\sigma_2 = 1.9227$ and the rest of the σ values are less than equal to 0.0083. Thus this makes us think that there are only 2 species and the rest of it is just noise. Plots of concentration and signal strength for species 1, 2 and 3 are given below. It can be seen that the concentration and signal strength of species 3 is just random noise. Also it can be seen that concentration and absorption spectrum of species 2 has some negative numbers in it. This is unavoidable in a SVD analysis, because the columns of U and V must be orthonormal and hence some of the values in vector u and v will be negative.

Species 1



Species 2



Species 3

