Homework 5

11 September 2006

1 Problem 1

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

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

The total signal measured due to all the species is

$$S = \sum S_i = \sum \sigma_i x_i a_i^T \tag{1}$$

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

$$S = U\Sigma V^T = \sum \sigma_i u_i v_i^T \tag{2}$$

where

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

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

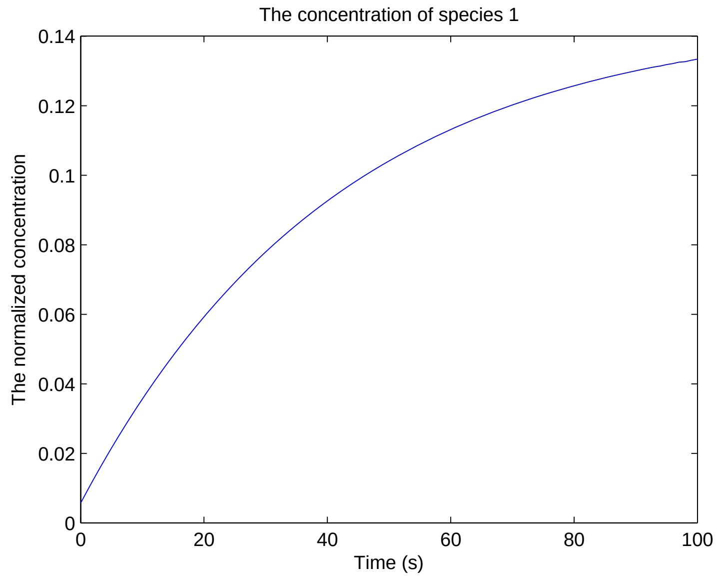
and

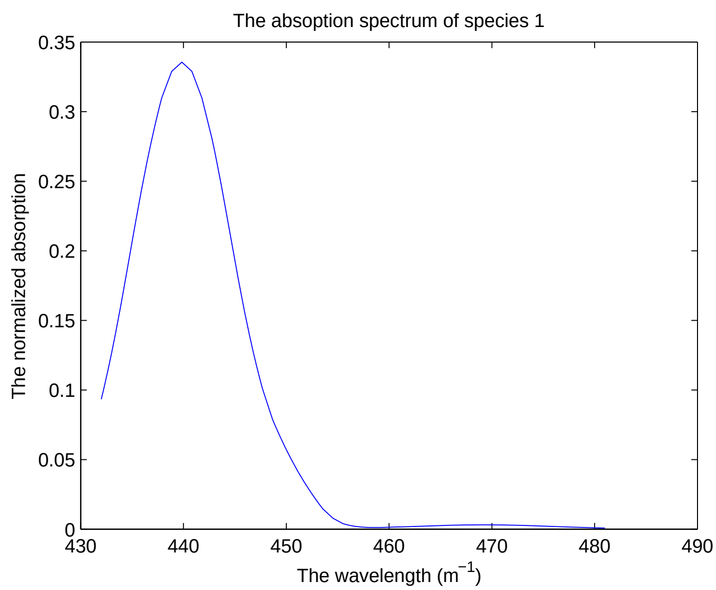
$$V = \begin{bmatrix} v_1 & v_2 & \cdots & v_k \end{bmatrix}$$

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.

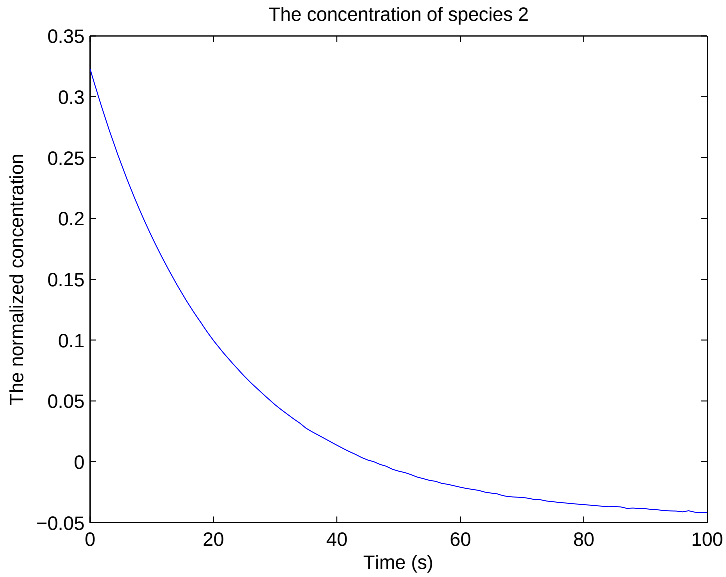
After we do the decomposition we find that $\sigma_1 = 16.3161$, $\sigma_2 = 1.9227$ and the rest of the σ values are less than equal to 0.0083. Thus this makes us think that there are only 2 species and the rest of it is just noise. Plots of concentration and signal strength for species 1, 2 and 3 are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

Species 1

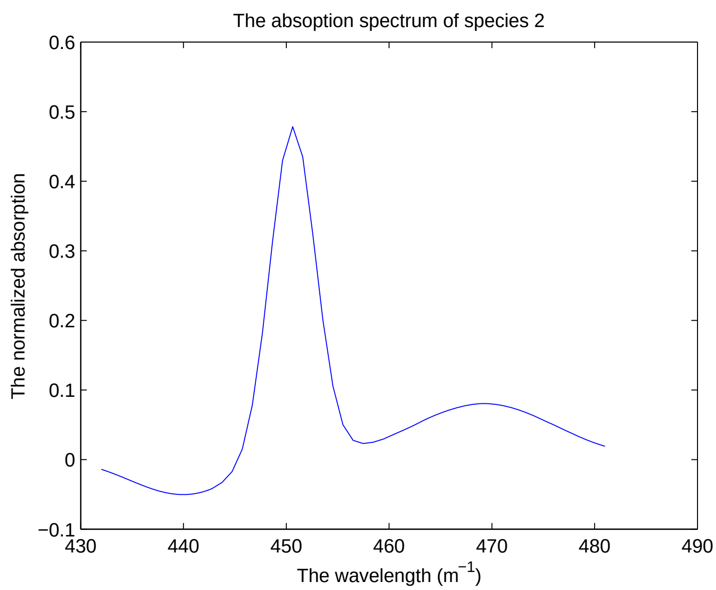

The concentration of species 1
The normalized concentration
Time (s)
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0
20
40
60
80
100


The absoption spectrum of species 1
The normalized absorption
The wavelength (m^{-1})
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
430
440
450
460
470
480
490

Species 2

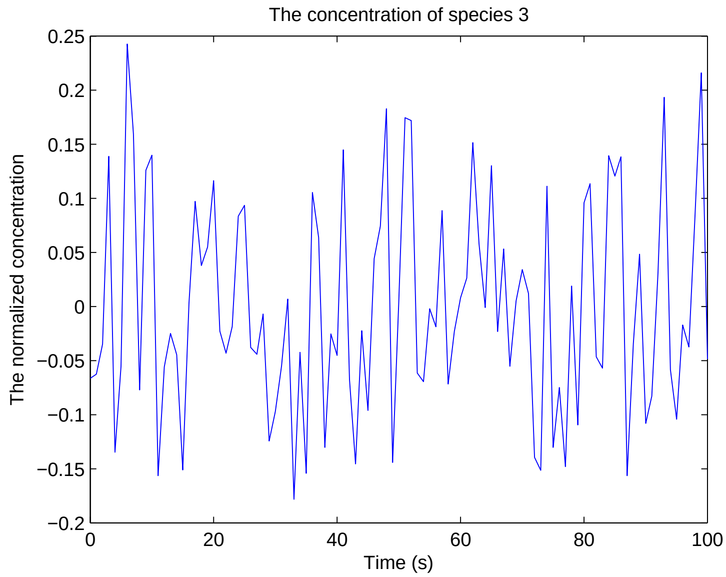


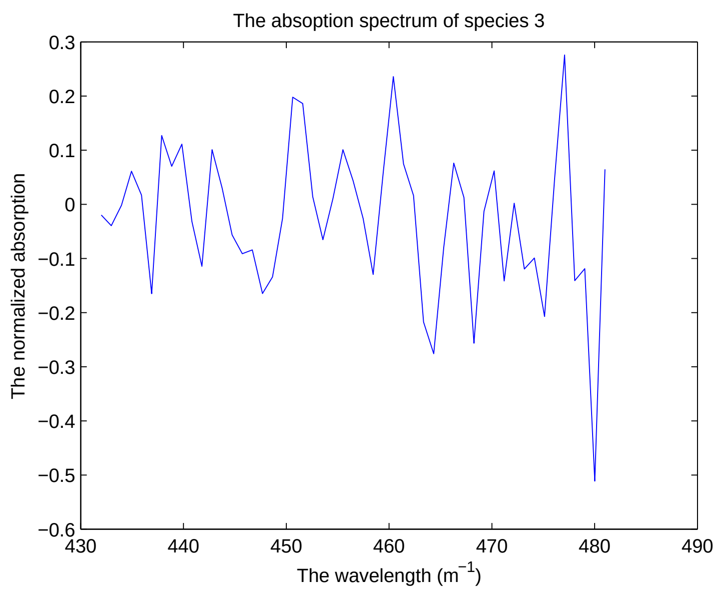
The concentration of species 2
The normalized concentration
Time (s)
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
−0.05
0
20
40
60
80
100



The absoption spectrum of species 2
The normalized absorption
The wavelength (m−1)
0.6
0.5
0.4
0.3
0.2
0.1
0
−0.1
430
440
450
460
470
480
490

Species 3


The concentration of species 3
The normalized concentration
0.25
0.2
0.15
0.1
0.05
0
−0.05
−0.1
−0.15
−0.2
0
20
40
60
80
100
Time (s)


The absoption spectrum of species 3
The normalized absorption
0.3
0.2
0.1
0
−0.1
−0.2
−0.3
−0.4
−0.5
−0.6
430
440
450
460
470
480
490
The wavelength (m−1)