CH5440 HW5

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Problem 1

H is the pure component spectra obtained from NMF. P is the true pure component spectra.

	H(1,:)	H(2,:)	H(3,:)
P(1,:)	**0.5545729916**	-0.5707058235	0.1294911335
P(2,:)	0.2004820905	0.7188547893	-0.2450129603
P(3,:)	-0.4946498902	**0.821385503**	**0.4928965533**

Table 1: Correlation matrix obtained for the case where only the first of the 5 trials were taken. Here the 2nd and 3rd component of H are both related to 3rd component of P. This is inaccurate.

	H(1,:)	H(2,:)	H(3,:)
P(1,:)	**0.7586127475**	-0.0460677071	-0.6464171415
P(2,:)	-0.0912255659	0.056043019	**0.8390951193**
P(3,:)	-0.6833443025	**0.7950965931**	0.7335536387

Table 2: Correlation matrix obtained for the case where the mean of the 5 trials were taken. The mapping is uniquely obtained and the correlation is also better than the previous case.

The spectra are compared below for the mean data.

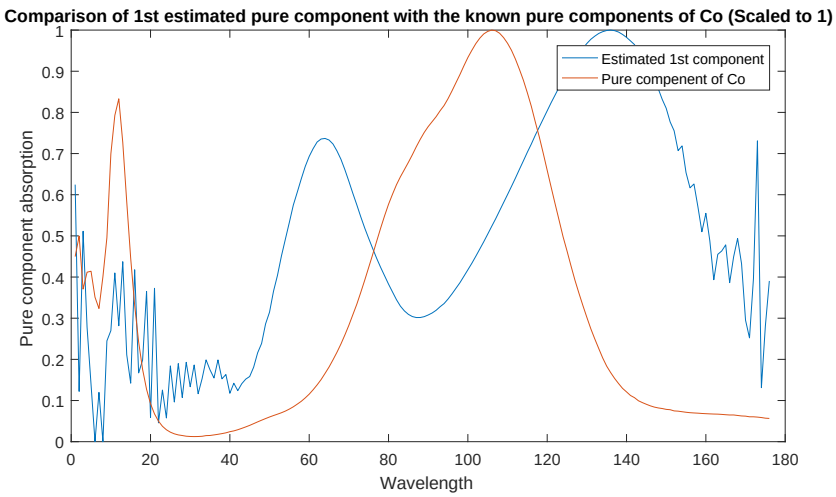

Figure 1: Pure spectra of Co

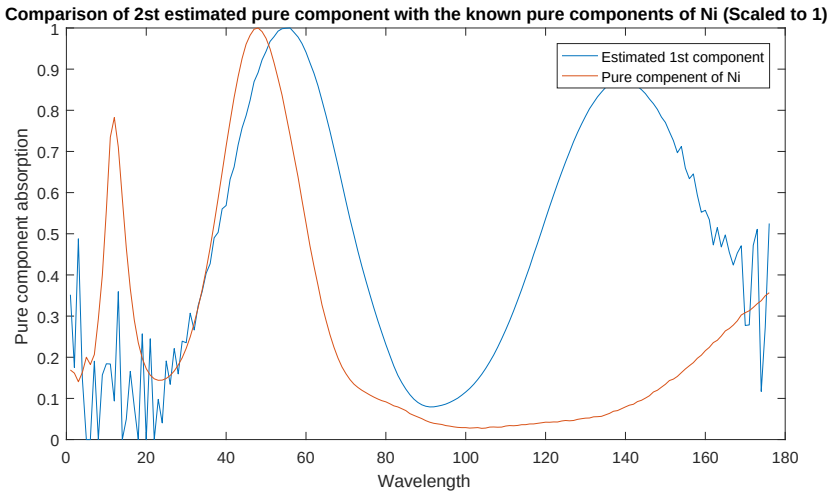

Figure 2: Pure spectra of Ni

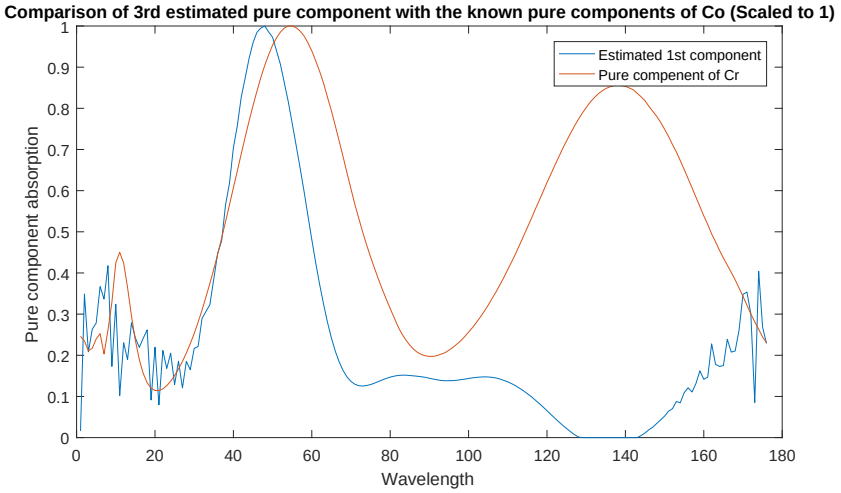

Figure 3: Pure spectra of Cr

Problem 2

Part a

E=measabs' (N variables xM samples) =(7x176)

Connectivity matrix A (NxL=7x3)

$$A = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{bmatrix}$$

Criterion 1: A must be full column rank

From matlab the rank was found to be 3. Hence this condition is satisfied.

Criterion 2: Each column of A must have atleast L-1=2 zeros which is satisfied.

Criterion 3: If E=AP, P must be a full row matrix. A necessary condition for this is L<M, or 3<176. This condition is satisfied.

Hence the given connectivity is NCA compliant

Part b

The rotation matrix M transforms the PCA estimated connectivity matrix to the real struture.

$$struc(M\hat{A^T}) = struc(A^T)$$

The second column of the connectivity matrix has 3 zeros. This makes it an overdetermined system of equations. Either only two equations can be used or the a least squares estimate can be obtained.

The least squares solution for the rotation matrix is as below:

$$M = \begin{bmatrix} 1 & 0.850658019 & 1.2257287588 \\ -0.0177462979 & 1 & 0.0029501312 \\ 0.3712629247 & -0.9856172775 & 1 \end{bmatrix}$$

A better rotation matrix that provided a near structure of A was obtained by using only the 2nd and 3rd zeros of the 2nd column.

$$M = \begin{bmatrix} 1 & 0.850658019 & 1.2257287588 \\ 0.4343763995 & 1 & -0.83980366252 \\ 0.3712629247 & -0.9856172775 & 1 \end{bmatrix}$$

The pure component spectra extracted and the true pure component spectra had a correlation of **0.7747.**

Part c

The NCA toolbox was used to obtain the pure component spectra. The problem solved is essentially, finding the pure component spectra matrix P_{3X176} having known the connectivity matrix A_{7X3} and the absorbance matrix, E_{7X176}, measured for 176 wavelengths.

$$E = AP$$

The correlation coefficient between the true pure component spectra and the measured pure component spetra is **0.9480.**

The spectra is shown below. The spectra match to a scale but has too much noise.

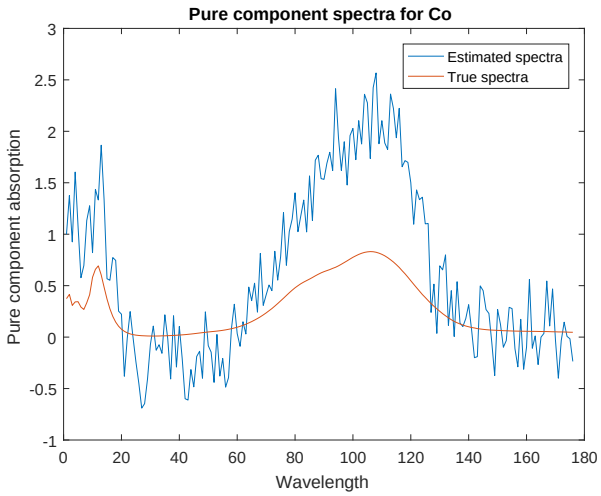

Figure 4: Pure spectra of Co

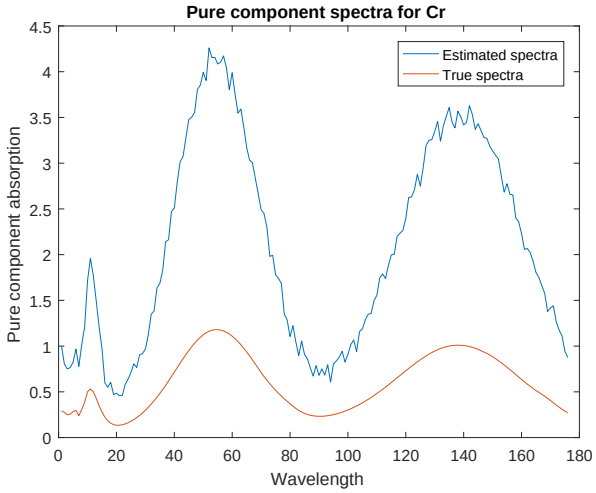

Figure 5: Pure spectra of Cr

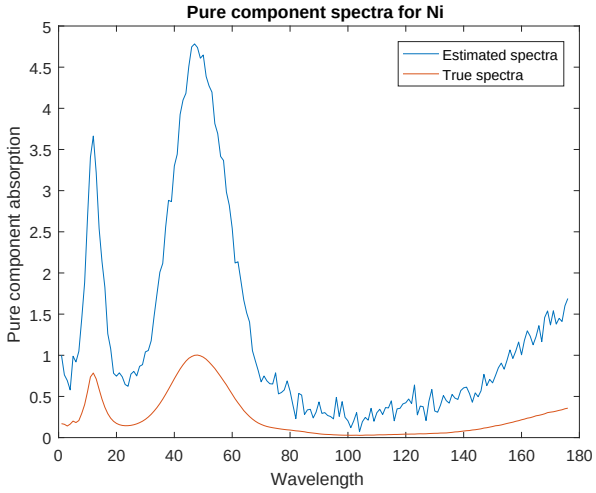

Figure 6: Pure spectra of Ni