CH5440 – Multivariate Data Analysis

1. Code:

```
clear
load Inorfull.mat
% Converting all negative absorbance values to 0
DATA = DATA - mean(DATA);
for i = 1 : size(DATA,1)
    for j = 1 : size(DATA,2)
        if DATA(i,j) < 0
            DATA(i,j) = 0;
        end
    end
end
% Pure SPectra
pure = [PureCo;PureCr;PureNi];
%% 1(a)
% Selecting data from the first replicate
data = [];
for i = 1 : 26
    data = [data;DATA(5*i-4,:)];
end
correl_repl = nmf_calc(data,pure);
tr_repl = trace(abs(correl_repl));
%% 1(b)
%Finding the average of the five replicates and repeating the above
%procedure,
data = [];
for i = 1:26
    data = [data;mean(DATA(5*i-4:5*i,:))];
end
correl_avg = nmf_calc(data,pure);
tr_avg = trace(abs(correl_avg));

%% Defiing a function to determine the correlation matrix
function correl_actual = nmf_calc(data,pure)
[u, s, v] = svd(data);
% Initial values of W and H from svd
Winit = abs(u(:,1:3));
Hinit = abs(v(:,1:3)');
[W, H] = nmf(data,Winit,Hinit,.0001,100,100);
% Permutations of the pure spectra
a = perms(1:3);
pureperm = H(a',:);
correl = [];
tr = [];
% Finding the correlation matrix and trace for eeach permutation
for i = 1:6
    correl = [correl;corr(pure',pureperm(3*i-2:3*i,:)')];
    tr = [tr;trace(abs(corr(pure',pureperm(3*i-2:3*i,:)')))];
end
%Finding the minimum trace and index corresponding to the minimimum trace
%and using it to find the correct permutation of the pure spectra.
[~, minindex] = min(tr);
pure_calc = H(a(minindex,:)',:);
```

```
correl_actual = corr(pure_calc',pure');

end
```

Correlation matrices for both cases are as follows:

For taking one replicate measurement:

Correlation matrix =

0.542943595313384	-0.0447816256064593	-0.602140299445024
-0.0175730490331306	-0.388475004894639	0.166216457078140
-0.574064688396812	0.561736732176967	0.885700010491079

Trace = 1.8171

For average measurements:

Correlation matrix =

0.594342506733202	0.0380248569527269	-0.688690705475994
0.0705452283122574	-0.501355215415244	0.0962396694588635
-0.596511964102904	0.479253080948714	0.916322157182470

Trace = 2.0120

Here correlation matrix is found in the order of the pure spectra Co, Cr and Ni.

We notice that in the correlation matrix, the diagonal elements are closer to 1 in the case of average measurements. Out of the 3 samples, we also observe that Ni has a very good correlation when compared to the other 2 elements.

2. Code

```
clear
load flowdata3
Astruct = Atrue;
[nconst,nvar] = size(Atrue);
nfact = nvar - nconst;

%% 2(b)
[u,s,v] = svd(Fmeas);
[eigvec,~,~] = svd(Fmeas');
for i = nfact +1 :nvar
    Aconst_PCA(i-nfact,:) = eigvec(:,i)';
end
E = u(:,nfact+1:end)*s(nfact+1:end,nfact+1:end)*v(:,nfact+1:end)';

[Aconst_NCA, ~] = fastNCA(E',Astruct',nconst);
```


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(a) Atrue =

1	1	-1	0	0
0	0	1	-1	0
0	-1	0	1	-1

We notice that the number of zeroes in each row = 2
Number of constraints = m = 3.
As the number of zeroes = m -1, the matrix is NCA compliant.

(b) maxdiff_PCA = 0.0460

theta_PCA = 1.2122

maxdiff_NCA = 0.0613

theta_NCA = 1.3505

Withput scaling, PCA gives a better constraint matrix than

(c)maxdiff_MLNCA = 0.0172

theta_MLNCA = 0.4196

maxdiff_MLPCA = 0.0146

theta_MLPCA = 0.6205

We can see that MLNCA is better than MLPCA in determining the correct constraint matrix.

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