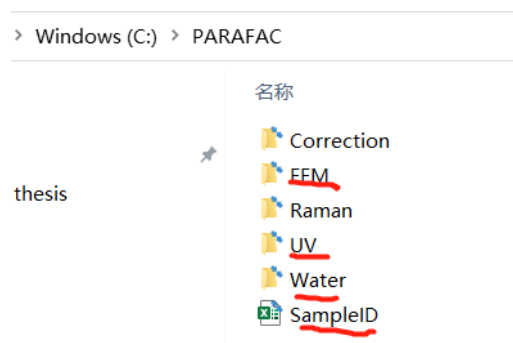
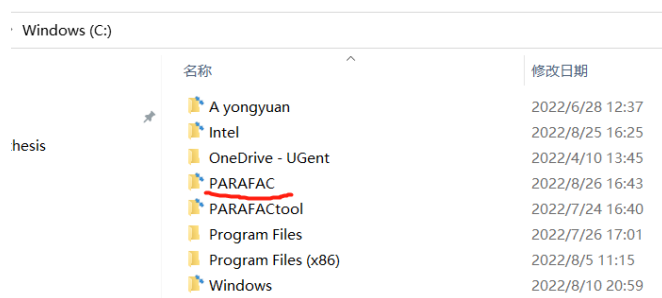


Manual of PARAFAC analysis using the PARAFAC.mlapp in MATLAB

Step 1: Prepare data files in demo PARAFAC, located in C disk.

%You need to replace/change the csv files of EEM, UV, Water and Sample ID based on your samples. But do not change the name and location of any folders.

If the location is change, for example you don't want to put the PARAFAC in C disk, the code of **PARAFAC.mlapp** should be adapted. You can use the MATLAB to open the **PARAFAC.mlapp** and adapt the code. %



Step 2: Load the **drEEM** folder into the path of your MATLAB:

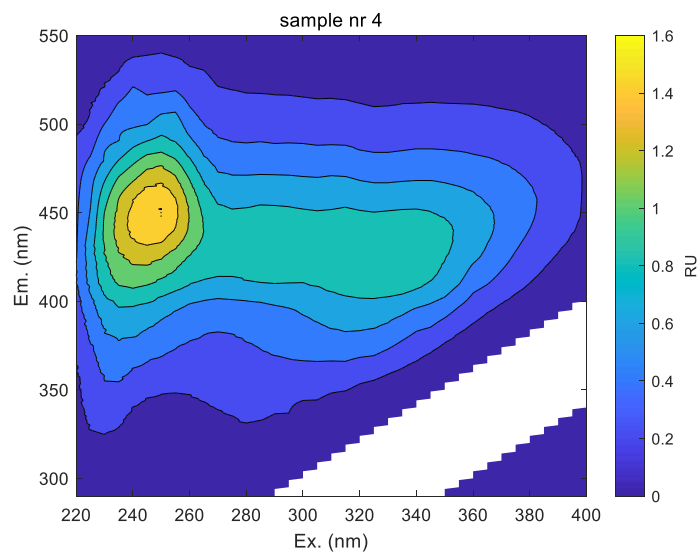
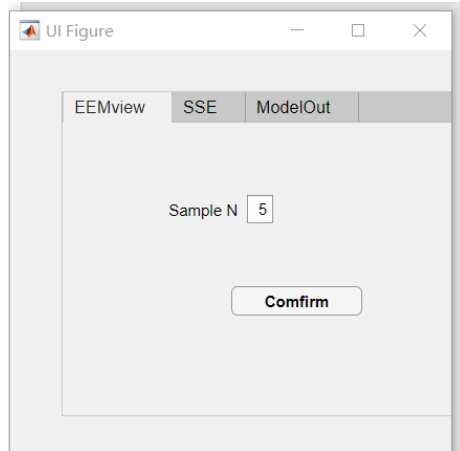
Step 3: Double click the PARAFAC.mlapp, which including the functions of **EEMview**, **SSE**, and **Modelout**.

% PARAFAC.mlapp is an APP (application) working on MATLAB. You can add more function or do the individualized design using the APP designer in MATLAB%

EEMview: Enter Sample N (e.g., 5) and **confirm**.

%Here we can obtain the EEM image of sample N with all necessary correction%

% It takes several mins, depending on the status of your laptop%.



SSE: Confirm.

%Here we are doing the PARAFAC modeling based on the component numbers from 3 to 7. You can get the output consists of a series of Figures. You can just look at **Figure 11** and determine which component number for modeling is suitable. As can be seen, the 3-component modeling appears high error, while 4 to 7 component modeling are comparable. Thus 4-component is suitable. More component modeling, e.g., 5 leading to a pair of components which could be highly correlated. %
% It takes several mins, depending on the status of your laptop%.

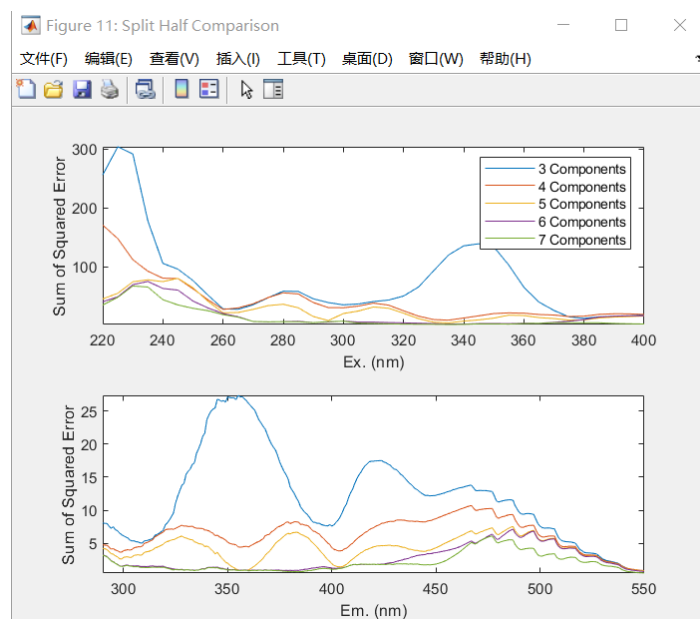
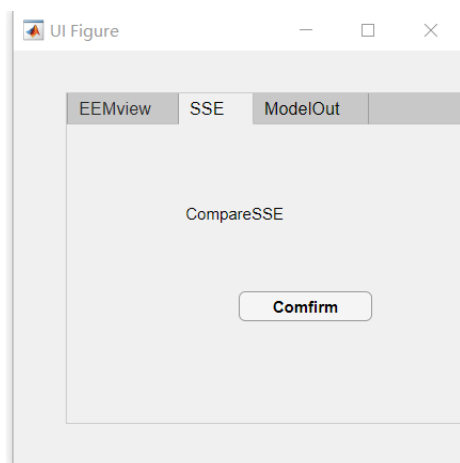
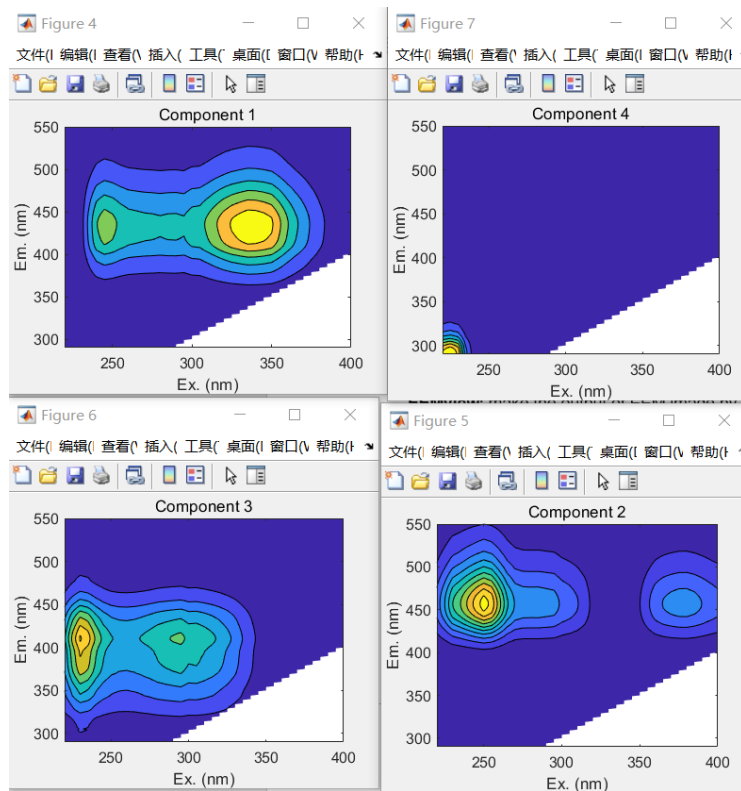
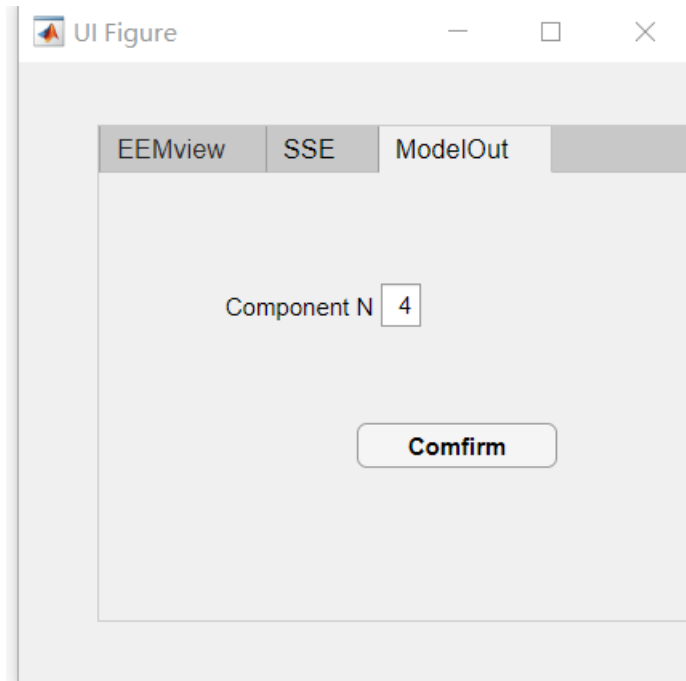













Figure 11. Sum of Squared Errors for the PARAFAC modeling by different component number (3: 7).

ModelOut: enter **Component N** of modeling (based on SSE, here is 4) and **confirm**.

%Here we can get the results of 4-component modeling, including the component Figures, and data of Fmax (see EEMcomponents.xlsx in C:\PARAFAC). Fmax data at the column 1 (1:4) is the Fmax of component 1 (1:4) for all samples%
% It takes several mins, depending on the status of your laptop%.



lows (C:) > PARAFAC

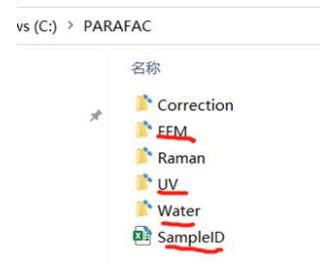
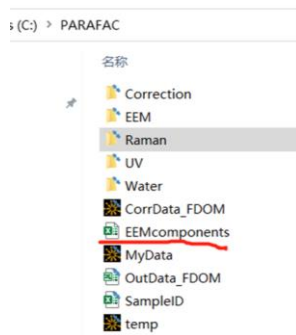
名称
 Correction
 EEM
 Raman
 UV
 Water
 CorrData_FDOM
 EEMcomponents
 MyData
 OutData_FDOM
 SampleID
 temp

	C1	C2	C3	C4	E	F
1	0.788562	1.005902	0.661956	0.030463		
2	0.704926	0.938182	0.545102	0.006774		
3	0.831684	0.963237	0.69182	0.132193		
4	0.814275	1.003416	0.697643	0.085158		
5	0.744082	0.955997	0.609195	0.043646		
6	0.824621	0.945019	0.697638	0.252035		
7	0.824494	0.989723	0.714103	0.120252		
8	0.734324	0.948232	0.606966	0.054439		
9	0.834657	0.908611	0.672188	0.215736		
10	0.814646	0.81774	0.62291	0.004076		
11	0.754715	0.811819	0.567949	0		
12	0.854801	0.741129	0.629811	0.109995		
13	0.744173	0.801744	0.619192	0.038588		
14	0.724568	0.74953	0.538039	0		
15	1.114208	1.17772	0.829452	0.009056		
16	1.004466	1.090985	0.702472	0.006028		
17	1.324795	1.141014	1.009211	0.092725		
18	1.244794	1.259343	0.951059	0.048188		
19	1.114776	1.235482	0.806785	0.014868		
20	1.164358	1.24672	0.916697	0.027755		
21	1.114339	1.228497	0.803902	0		
22	1.44488	1.219945	1.040832	0.021778		
23	1.114796	1.29568	0.876496	0.012342		
24	1.004495	1.302165	0.804866	0.001479		
25	1.114797	1.137494	0.942845	0.050311		
26	1.114736	1.367075	0.909332	0		
27	0.940335	1.212648	0.783561	0.052555		

Sheet1 FMax Em Loadings Ex Loadings

Cleaning the PARAFAC folder.

%After finish, it is suggested to clean the folder as follows%



Reference:

Murphy, K. R., Stedmon, C. A., Graeber, D., & Bro, R. (2013). Fluorescence spectroscopy and multi-way techniques. PARAFAC. Analytical Methods, 5(23), 6557-6566.