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1  #IMPORT MODULES
2  import numpy as np
3  import pandas as pd
4
5  #READING DATA
6  def read_data():
7      data = np.array(pd.read_csv(r'C:\Users\edwincaballero\Desktop\data.csv'))
8      return data
9
10 #MEAN CENTER THE DATA
11 def mean_centering(input_data):
12     for i in range(input_data.shape[0]):
13         output_data = []
14         input_data[i,:] -= input_data[i,:].mean()
15         output_data = input_data
16     return output_data
17
18 #CHOOSE REFERENCE DATA TRANSPOSED (intesities in rows)
19 def choosing_reference(input_data, reference = None):
20     #GET REFERENCE SPECTRUM. If not given, estimate it from the mean
21     if reference is None:
22         #CALCULATE MEAN
23         ref = np.mean(input_data, axis=0)
24     else:
25         ref = reference
26     return ref
27
28 #FIT AND CORRECT SPECTRAL DATA
29 def fit
30 inp_and_correct(input_data, ref):
31     fit = np.polyfit(ref, input_data, 1, full=True)
32     data_msc = (
33 ut_data - fit[0][1]) / fit[0][0]
34     return data_msc
35
36 #LOOP MSC
37 def loop_msc(input_data_grupal):
38     output_grupal = []
39     for input_data in input_data_grupal:
40         msc_data = fit_and_correct(input_data, ref)
41         output_grupal.append(msc_data)
42     return output_grupal
43
44 #SAVING DATA
45 def write_msc_output(ref):
46     msc_output_writer = r'C:\Users\edwincaballero\Desktop\msc_results.csv'
47     pd.DataFrame(ref).to_csv(msc_output_writer, index=False)
48     input_data = read_data()
49     output_data = mean_centering(input_data)
50     ref = choosing_reference(input_data, reference = None)
51     msc_data = loop_msc(input_data)
52     write_msc_output(msc_data)
53     count = len(msc_data)
54     print()
55     print('SUCCESS')
56     print(str(count)+ ' spectra transformed with MSC')

```