**Materials Informatics – Fall 2017**

**Computer Final Project – Solutions**

**Due on: Dec 15 2017 11:59pm**

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1 Assignment

a)

|  |  |  |  |
| --- | --- | --- | --- |
|  | R2 | MSE | Coef |
| C | 0.006946233 | 167.4806988 | -16.20037641 |
| N | 0.034959498 | 162.7562002 | 20.0884865 |
| Ni | 0.497966097 | 84.66912027 | 2.33533817 |
| Fe | 0.405297187 | 100.2979356 | -1.44043074 |
| Mn | 0.008429205 | 167.2305924 | 0.34560156 |
| Si | 0.009027444 | 167.1296981 | -3.52081655 |
| Cr | 0.007253678 | 167.4288475 | 0.52131769 |

According to r2 value Ni is the best predictor of SRE



C



N



Ni



Fe



Mn



Si



Cr

The better r2 value will give us a better linear model, so the plot of points will be closer to the line that we drown in the graph, so Ni is the best graph.

2)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| exhaustive | R2 | Mse | Coef | ADR2 |  |
| Ni | 0.4979 | 84.669 | [2.33533817] | 0.4980 |  |
| N,Ni | 0.5535 | 75.300 | [ 25.38118739, 2.38869609] | 0.5513 |  |
| Fe,Mn,Cr | 0.5944 | 68.390 | [-2.3525984 , -1.41578646, -2.36709473] | 0.5905 |  |
| C,Fe,Mn,Cr | 0.6321 | 62.032 | [-41.60904346, -2.40349844, -1.11265247, -2.50073457] | 0.6268 |  |
| C,Fe,Mn,Si,Cr | 0.6621 | 56.97 | [-39.99242382, -2.44414191, -0.95862936, -6.71416018, -2.62653818] | 0.6555 |  |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| sequential | R2 | Mse | Coef | ADR2 |
| Ni | 0.4979 | 84.669 | [ 2.33533817] | 0.4979 |
| Ni,N | 0.5535 | 75.300 | [ 2.38869609, 25.38118739] | 0.5513 |
| Ni,N,Si | 0.5782 | 71.133 | [ 2.40089754, 29.27877211, -5.97779099] | 0.5741 |
| Ni,N,Si,C | 0.5920 | 68.799 | [ 2.42139354, 29.95825006, -5.32505189, -23.21994118] | 0.5861 |
| Ni,N,Si,C,Fe | 0.6000 | 67.448 | [ 1.92824932, 19.16906455, -5.52210355, -29.81984612, -0.45707106] | 0.5923 |

By comparing adjusted r2, exhaustive search will provide the best result. The result from this lab has a huge difference compare to lab 2. Because in lab 2 we have used exhaustive and sequential forward search for both 3NN and LDA model. So due to different method, the result may vary.

3)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | 50 | 30 | 15 | 7 | 3 |
| Lasso | -23.8941  17.8405  -1.80917  -4.03552  -3.00736  -7.36171  -4.03878 | -5.87233  6.95656  -1.57728  -3.79092  -2.66081  -6.58614  -3.70373 | 0  0  -0.577367  -2.84754  -1.71977  -4.52486  -2.77422 | 0  0  0.254709  -1.9607  -1.03157  0  -1.77636 | 0  0  1.46059  -0.660669  0  0  -0.115087 |
| Ridge | -25.5921  18.988  -1.8382  -4.06524  -3.04905  -7.44783  -4.07715 | -25.0109  18.8583  -1.8438  4.06952  -3.0543  -7.44719  -4.07877 | -23.212  18.3601  -1.86083  -4.08248  -3.06777  -7.44217  -4.08299 | -19.4332  16.8218  -1.89402  -4.10731  -3.08105  -7.4124  -4.08683 | -12.7535  12.4901  -1.92885  -4.12878  -3.04368  -7.24388  -4.0632 |
|  | 1 | 0.3 | 0.1 | 0.03 | 0.01 |
| Lasso | 0  0  0  1.46059  -0.660669  0  0.115087 | 0  0  1.22094  0.633447  0  0  0 | 0  0  0.679961  -0.654028  0  0  0 | 0  0  0  -0.529804  -0  -0  -0 | 0  0  0  0  0  0  0 |
| Ridge | -6.65414  6.97925  -1.85359  -4.04712  -2.88682  -6.70076  -3.93595 | -3.47978  3.66951  -1.60731  -3.80853  -2.63424  -5.77591  -3.67946 | -1.82206  1.86942  -1.17524  -3.39639  -2.26303  -4.50131  -3.26961 | -0.983493  0.965932  -0.618931  -2.86653  -1.80494  -3.16572  -2.75213 | -0.616655  0.583707  -0.164284  -2.43092  -1.4309  -2.25779  -2.32398 |



Ridge



Lasso

2 Assignment

a). convolution layer

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | Layer1 | Layer2 | Layer3 | Layer4 | Layer5 |
| Spheroidite,Network | 0.495 | 0.41 | 0.445 | 0.49 | 0.003 |
| Spheroidite,Pearlite | 0.5 | 0.49 | 0.49 | 0.5 | 0.035 |
| Spheroidite,Spheroidite+widmanstatten | 0.375 | 0.375 | 0.375 | 0.445 | 0.375 |
| Network,Pearlite | 0.5 | 0.41 | 0.445 | 0.5 | 0.035 |
| Network,Spheroidite+Widmanstatten | 0.375 | 0.375 | 0.375 | 0.375 | 0.012 |
| Pearlite,Spheroidite+widmanstatten | 0.375 | 0.375 | 0.445 | 0.375 | 0.112 |

By observing the result from part a, we can find that the layer 5 stall has the best result, but for spheroidite, spheroidite+widmanstatten, we can see the error is not being smaller at layer5, that is because spheroidite+widmanstatten has a part of feature of spheroidite.

b). One Vs One error

|  |  |
| --- | --- |
| spheroidite | 0.0401 |
| pearlite | 0 |
| network | 0.0982 |
| spheroidite+Widmanstatten | 0.4285 |

Pairwise Classifier error

|  |  |
| --- | --- |
| spheroidite | 0.0134 |
| pearlite | 0 |
| network | 0.0863 |
| spheroidite+Widmanstatten | 0.2063 |

By comparing two results, we can state that the pairwise classifier provide a better error than one vs one classifier.

c). Label for pearlite + spheroidite

|  |  |  |  |
| --- | --- | --- | --- |
| micrograph4.tif | spheroidite | micrograph779.tif | spheroidite |
| micrograph12.tif | spheroidite | micrograph808.tif | pearlite |
| micrograph15.tif | spheroidite | micrograph825.tif | spheroidite |
| micrograph62.tif | pearlite | micrograph866.tif | pearlite |
| micrograph71.tif | spheroidite | micrograph871.tif | spheroidite |
| micrograph109.tif | spheroidite | micrograph908.tif | pearlite |
| micrograph111.tif | spheroidite | micrograph910.tif | pearlite |
| micrograph119.tif | spheroidite | micrograph916.tif | spheroidite |
| micrograph131.tif | spheroidite | micrograph926.tif | spheroidite |
| micrograph137.tif | pearlite | micrograph994.tif | pearlite |
| micrograph166.tif | spheroidite | micrograph997.tif | spheroidite |
| micrograph186.tif | spheroidite | micrograph1033.tif | spheroidite |
| micrograph193.tif | spheroidite | micrograph1068.tif | spheroidite |
| micrograph201.tif | spheroidite | micrograph1168.tif | spheroidite |
| micrograph211.tif | spheroidite | micrograph1206.tif | spheroidite |
| micrograph224.tif | spheroidite | micrograph1226.tif | spheroidite |
| micrograph245.tif | spheroidite | micrograph1227.tif | spheroidite |
| micrograph288.tif | spheroidite | micrograph1241.tif | spheroidite |
| micrograph342.tif | spheroidite | micrograph1243.tif | spheroidite |
| micrograph380.tif | spheroidite | micrograph1247.tif | spheroidite |
| micrograph404.tif | spheroidite | micrograph1268.tif | spheroidite |
| micrograph431.tif | spheroidite | micrograph1271.tif | spheroidite |
| micrograph453.tif | spheroidite | micrograph1303.tif | spheroidite |
| micrograph466.tif | pearlite | micrograph1357.tif | spheroidite |
| micrograph481.tif | spheroidite | micrograph1366.tif | spheroidite |
| micrograph483.tif | spheroidite | micrograph1390.tif | pearlite |
| micrograph499.tif | spheroidite | micrograph1398.tif | pearlite |
| micrograph515.tif | spheroidite | micrograph1414.tif | spheroidite |
| micrograph522.tif | spheroidite | micrograph1432.tif | pearlite |
| micrograph532.tif | spheroidite | micrograph1433.tif | spheroidite |
| micrograph541.tif | spheroidite | micrograph1441.tif | spheroidite |
| micrograph544.tif | spheroidite | micrograph1450.tif | spheroidite |
| micrograph567.tif | spheroidite | micrograph1455.tif | spheroidite |
| micrograph572.tif | spheroidite | micrograph1458.tif | spheroidite |
| micrograph576.tif | spheroidite | micrograph1489.tif | pearlite |
| micrograph602.tif | spheroidite | micrograph1502.tif | pearlite |
| micrograph609.tif | spheroidite+widmanstatten | micrograph1503.tif | spheroidite |
| micrograph637.tif | spheroidite | micrograph1513.tif | spheroidite |
| micrograph644.tif | pearlite | micrograph1514.tif | pearlite |
| micrograph648.tif | spheroidite | micrograph1525.tif | spheroidite |
| micrograph656.tif | pearlite | micrograph1526.tif | pearlite |
| micrograph660.tif | spheroidite | micrograph1527.tif | spheroidite |
| micrograph672.tif | pearlite | micrograph1532.tif | spheroidite |
| micrograph676.tif | pearlite | micrograph1570.tif | pearlite |
| micrograph677.tif | spheroidite | micrograph1574.tif | spheroidite |
| micrograph704.tif | spheroidite | micrograph1582.tif | spheroidite |
| micrograph716.tif | spheroidite | micrograph1595.tif | pearlite |
| micrograph727.tif | spheroidite | micrograph1635.tif | spheroidite |
| micrograph742.tif | spheroidite | micrograph1643.tif | spheroidite |
| micrograph749.tif | spheroidite+widmanstatten | micrograph1644.tif | spheroidite |
| micrograph758.tif | spheroidite | micrograph1656.tif | pearlite |
| micrograph765.tif | pearlite | micrograph1657.tif | spheroidite |
| micrograph771.tif | spheroidite | micrograph1662.tif | spheroidite |
|  |  | micrograph1668.tif | network |

Label for pearlite + widmanstatten

|  |  |
| --- | --- |
| pearlite | micrograph346.tif |
| pearlite | micrograph490.tif |
| pearlite | micrograph496.tif |
| spheroidite | micrograph523.tif |
| spheroidite+widmanstatten | micrograph553.tif |
| pearlite | micrograph753.tif |
| spheroidite | micrograph836.tif |
| pearlite | micrograph857.tif |
| spheroidite | micrograph875.tif |
| spheroidite | micrograph882.tif |
| pearlite | micrograph911.tif |
| pearlite | micrograph932.tif |
| pearlite | micrograph1046.tif |
| spheroidite | micrograph1078.tif |
| spheroidite | micrograph1097.tif |
| pearlite | micrograph1104.tif |
| pearlite | micrograph1123.tif |
| pearlite | micrograph1204.tif |
| spheroidite | micrograph1214.tif |
| spheroidite+widmanstatten | micrograph1215.tif |
| pearlite | micrograph1255.tif |
| pearlite | micrograph1267.tif |
| pearlite | micrograph1287.tif |
| spheroidite+widmanstatten | micrograph1370.tif |
| pearlite | micrograph1395.tif |
| spheroidite | micrograph1417.tif |
| pearlite | micrograph1684.tif |

By obverting those two results, we can find that our one vs one classifier by using layer 5 is good enough to be a classifier

d).

|  |  |  |
| --- | --- | --- |
| spheroidite | micrograph4.tif | spheroidite |
| spheroidite | micrograph12.tif | spheroidite |
| spheroidite | micrograph15.tif | spheroidite |
| pearlite | micrograph62.tif | pearlite |
| spheroidite | micrograph71.tif | spheroidite |
| spheroidite | micrograph109.tif | spheroidite |
| spheroidite | micrograph111.tif | spheroidite |
| spheroidite | micrograph119.tif | spheroidite |
| spheroidite | micrograph131.tif | spheroidite |
| pearlite | micrograph137.tif | pearlite |
| spheroidite | micrograph166.tif | spheroidite |
| spheroidite | micrograph186.tif | spheroidite |
| spheroidite | micrograph193.tif | spheroidite |
| spheroidite | micrograph201.tif | spheroidite |
| spheroidite | micrograph211.tif | spheroidite |
| spheroidite | micrograph224.tif | spheroidite |
| spheroidite | micrograph245.tif | spheroidite |
| spheroidite | micrograph288.tif | spheroidite |
| spheroidite | micrograph342.tif | spheroidite |
| spheroidite | micrograph380.tif | spheroidite |
| spheroidite | micrograph404.tif | spheroidite |
| spheroidite | micrograph431.tif | spheroidite |
| spheroidite | micrograph453.tif | spheroidite |
| pearlite | micrograph466.tif | pearlite |
| spheroidite | micrograph481.tif | spheroidite |
| spheroidite | micrograph483.tif | spheroidite |
| spheroidite | micrograph499.tif | spheroidite |
| spheroidite | micrograph515.tif | spheroidite |
| spheroidite | micrograph522.tif | spheroidite |
| spheroidite | micrograph532.tif | spheroidite |
| spheroidite | micrograph541.tif | spheroidite |
| spheroidite | micrograph544.tif | spheroidite |
| spheroidite | micrograph567.tif | spheroidite |
| spheroidite | micrograph572.tif | spheroidite |
| spheroidite | micrograph576.tif | spheroidite |
| spheroidite | micrograph602.tif | spheroidite |
| spheroidite | micrograph609.tif | spheroidite+widmanstatten |
| spheroidite | micrograph637.tif | spheroidite |
| pearlite | micrograph644.tif | pearlite |
| spheroidite | micrograph648.tif | spheroidite |
| pearlite | micrograph656.tif | pearlite |
| spheroidite | micrograph660.tif | spheroidite |
| pearlite | micrograph672.tif | pearlite |
| pearlite | micrograph676.tif | pearlite |
| spheroidite | micrograph677.tif | spheroidite |
| spheroidite | micrograph704.tif | spheroidite |
| spheroidite | micrograph716.tif | spheroidite |
| spheroidite | micrograph727.tif | spheroidite |
| spheroidite | micrograph742.tif | spheroidite |
| spheroidite | micrograph749.tif | spheroidite+widmanstatten |
| spheroidite | micrograph758.tif | spheroidite |
| pearlite | micrograph765.tif | pearlite |
| spheroidite | micrograph771.tif | spheroidite |
| spheroidite | micrograph779.tif | spheroidite |
| pearlite | micrograph808.tif | pearlite |
| spheroidite | micrograph825.tif | spheroidite |
| pearlite | micrograph866.tif | pearlite |
| spheroidite | micrograph871.tif | spheroidite |
| pearlite | micrograph908.tif | pearlite |
| pearlite | micrograph910.tif | pearlite |
| spheroidite | micrograph916.tif | spheroidite |
| spheroidite | micrograph926.tif | spheroidite |
| pearlite | micrograph994.tif | pearlite |
| spheroidite | micrograph997.tif | spheroidite |
| spheroidite | micrograph1033.tif | spheroidite |
| spheroidite | micrograph1068.tif | spheroidite |
| spheroidite | micrograph1168.tif | spheroidite |
| spheroidite | micrograph1206.tif | spheroidite |
| spheroidite | micrograph1226.tif | spheroidite |
| spheroidite | micrograph1227.tif | spheroidite |
| spheroidite | micrograph1241.tif | spheroidite |
| spheroidite | micrograph1243.tif | spheroidite |
| spheroidite | micrograph1247.tif | spheroidite |
| spheroidite | micrograph1268.tif | spheroidite |
| spheroidite | micrograph1271.tif | spheroidite |
| spheroidite | micrograph1303.tif | spheroidite |
| spheroidite | micrograph1357.tif | spheroidite |
| spheroidite | micrograph1366.tif | spheroidite |
| pearlite | micrograph1390.tif | pearlite |
| pearlite | micrograph1398.tif | pearlite |
| spheroidite | micrograph1414.tif | spheroidite |
| pearlite | micrograph1432.tif | pearlite |
| spheroidite | micrograph1433.tif | spheroidite |
| spheroidite | micrograph1441.tif | spheroidite |
| spheroidite | micrograph1450.tif | spheroidite |
| spheroidite | micrograph1455.tif | spheroidite |
| spheroidite | micrograph1458.tif | spheroidite |
| pearlite | micrograph1489.tif | pearlite |
| pearlite | micrograph1502.tif | pearlite |
| spheroidite | micrograph1503.tif | spheroidite |
| spheroidite | micrograph1513.tif | spheroidite |
| pearlite | micrograph1514.tif | pearlite |
| spheroidite | micrograph1525.tif | spheroidite |
| pearlite | micrograph1526.tif | pearlite |
| spheroidite | micrograph1527.tif | spheroidite |
| spheroidite | micrograph1532.tif | spheroidite |
| pearlite | micrograph1570.tif | pearlite |
| spheroidite | micrograph1574.tif | spheroidite |
| spheroidite | micrograph1582.tif | spheroidite |
| pearlite | micrograph1595.tif | pearlite |
| spheroidite | micrograph1635.tif | spheroidite |
| spheroidite | micrograph1643.tif | spheroidite |
| spheroidite | micrograph1644.tif | spheroidite |
| pearlite | micrograph1656.tif | pearlite |
| spheroidite | micrograph1657.tif | spheroidite |
| spheroidite | micrograph1662.tif | spheroidite |
| spheroidite | micrograph1668.tif | network |

The left label is the result from part d and right label is the result from part c, there are totally three difference between part c and d which are micrograph1668, 749 and 609, because one vs one can classify data up to 4 label but pairwise can only do it for 2 label, but it is also mean those two classifiers are good enough.

e). martensite microstructure

|  |  |
| --- | --- |
| spheroidite | micrograph20.tif |
| network | micrograph41.tif |
| pearlite | micrograph44.tif |
| spheroidite | micrograph99.tif |
| spheroidite | micrograph114.tif |
| network | micrograph168.tif |
| spheroidite | micrograph345.tif |
| pearlite | micrograph366.tif |
| spheroidite | micrograph381.tif |
| spheroidite | micrograph459.tif |
| pearlite | micrograph492.tif |
| pearlite | micrograph502.tif |
| pearlite | micrograph785.tif |
| pearlite | micrograph951.tif |
| spheroidite | micrograph954.tif |
| pearlite | micrograph963.tif |
| spheroidite | micrograph984.tif |
| pearlite | micrograph1009.tif |
| spheroidite | micrograph1012.tif |
| pearlite | micrograph1030.tif |
| pearlite | micrograph1048.tif |
| spheroidite | micrograph1055.tif |
| spheroidite | micrograph1079.tif |
| pearlite | micrograph1174.tif |
| spheroidite | micrograph1177.tif |
| pearlite | micrograph1281.tif |
| pearlite | micrograph1316.tif |
| pearlite | micrograph1396.tif |
| spheroidite | micrograph1424.tif |
| spheroidite | micrograph1449.tif |
| pearlite | micrograph1531.tif |
| network | micrograph1552.tif |
| spheroidite | micrograph1599.tif |
| spheroidite | micrograph1697.tif |
| pearlite | micrograph1700.tif |
| spheroidite | micrograph1723.tif |

Code:

#!/usr/bin/env python3

# -\*- coding: utf-8 -\*-

"""

Created on Fri Dec 8 09:46:21 2017

@author: jianfengsong

"""

import xlrd as xl

import numpy as np

import matplotlib.pyplot as plt

import plotly.plotly as py

import plotly.figure\_factory as ff

import pandas as pd

import plotly

from sklearn import linear\_model

import operator

from itertools import combinations

from sklearn.linear\_model import LinearRegression as lnr

from sklearn.metrics import mean\_squared\_error, r2\_score

from sklearn.linear\_model import Ridge

class fun():

def excel\_data(n):

train\_rows\_value=list()

train\_cols\_value=list()

excel=xl.open\_workbook(n)

data\_table=excel.sheet\_by\_index(0)

rows=data\_table.nrows

cols=data\_table.ncols

for a in range(rows):

train\_rows\_value.append(data\_table.row\_values(a))

train\_row=np.asarray(train\_rows\_value)

data\_set=[[] for x in range(len(train\_row)-1)]

for a in range (1,len(train\_row),1):

for b in range(0,len(train\_row[a])):

data\_set[a-1].append(float(train\_row[a][b]))

return np.asarray(data\_set)

################################################################################

def get\_data():

data\_set=fun.excel\_data('SFE\_Dataset.xlsx')

data=data\_set.T

data\_1,data\_2=list(),list()

for a in range(len(data)):

num\_0=0

for b in range(len(data[a])):

if data[a][b]==0:

num\_0+=1

else:

num\_0=num\_0

pre\_0=num\_0/len(data[a])

if pre\_0<=0.4:

data\_1.append(data[a])

data\_1=np.asarray(data\_1).T

for a in range(len(data\_1)):

num\_0=0

for b in range(len(data\_1[a])):

if data\_1[a][b]==0:

num\_0+=1

if num\_0==0:

data\_2.append(data\_1[a])

data\_good=np.asarray(data\_2)

return data\_good

################################################################################

def data\_clas():

data\_set=fun.get\_data()

data\_no\_sfe=list()

data\_label=list()

for a in range(len(data\_set)):

b=len(data\_set[a])-1

if data\_set[a][b]<35:

data\_label.append(data\_set[a][b])

elif data\_set[a][b]>45:

data\_label.append(data\_set[a][b])

else:

data\_label.append(data\_set[a][b])

data\_set1=data\_set.T

for a in range(0,len(data\_set1)-1):

data\_no\_sfe.append(data\_set1[a])

data\_nosfe=np.asarray(data\_no\_sfe)

return data\_nosfe,data\_label

#################################################################################

def ehaustive(num):

selected\_feature\_set=list()

selected\_feature1=combinations(range(7),num)

selected\_feature=np.asarray(list(selected\_feature1))

return selected\_feature

#################################################################################

def linear(data,label):

data\_coef=list()

data\_mse=list()

data\_r2=list()

data\_list=list()

data\_pred\_list=list()

for a in (range(len(data))):

data\_var=data[a]

data\_var.shape=(211,1)

data\_lnr=lnr()

data\_lnr.fit(data\_var,label)

data\_pred=data\_lnr.predict(data\_var)

r2\_score=data\_lnr.score(data\_var,label)

data\_list.append(data\_var)

data\_pred\_list.append(data\_pred)

data\_r2.append(r2\_score)

data\_coef.append(data\_lnr.coef\_)

data\_mse.append(mean\_squared\_error(label,data\_pred))

return data\_r2,data\_coef,data\_mse,data\_pred\_list

################################################################################

def linear\_ex(data,label,num\_list):

data\_coef=list()

data\_mse=list()

data\_r2=list()

data\_list=list()

data\_pred\_list=list()

minr2=0

if len(num\_list)==7:

for a in num\_list:

data\_var=data[a,:]

data\_var.shape=(211,1)

data\_lnr=lnr()

data\_lnr.fit(data\_var,label)

data\_pred=data\_lnr.predict(data\_var)

r2\_score=data\_lnr.score(data\_var,label)

if minr2<r2\_score:

minr2=r2\_score

minfea=a

coef=data\_lnr.coef\_

mrss=mean\_squared\_error(label,data\_pred)

else:

for a in num\_list:

data\_var=data[a,:]

data\_var=data\_var.T

data\_lnr=lnr()

data\_lnr.fit(data\_var,label)

data\_pred=data\_lnr.predict(data\_var)

r2\_score=data\_lnr.score(data\_var,label)

if minr2<r2\_score:

minr2=r2\_score

minfea=a

coef=data\_lnr.coef\_

mrss=mean\_squared\_error(label,data\_pred)

return minr2,minfea,coef,mrss

################################################################################

def linear\_sf(data,label,num\_list):

data\_var=data[num\_list,:]

data\_var=data\_var.T

data\_lnr=lnr()

data\_lnr.fit(data\_var,label)

data\_pred=data\_lnr.predict(data\_var)

r2\_score=data\_lnr.score(data\_var,label)

coef=data\_lnr.coef\_

mrss=mean\_squared\_error(label,data\_pred)

return r2\_score,coef,mrss

#################################################################################

data,label=fun.data\_clas()

data\_r2,data\_coef,data\_mse,data\_pred=fun.linear(data,label)

for a in (range(len(data))):

plt.figure(a)

data\_var=data[a]

data\_var.shape=(211,1)

# plt.plot(data\_var,data\_pred[a])

# plt.plot(data\_var,label,'o')

####################### 2 ###################

minr2list=list()

minfealist=list()

coeflist=list()

mrsslist=list()

adr2list=list()

for a in range (1,6):

num\_list=fun.ehaustive(a)

minr2,minfea,coef,mrss=fun.linear\_ex(data,label,num\_list)

minr2list.append(minr2)

minfealist.append(minfea)

coeflist.append(coef)

mrsslist.append(mrss)

for r in range(len(minr2list)):

adr2=minr2list[r]-(len(minfealist[r])-1)/(211-len(minfealist[r]))\*(1-minr2list[r])

adr2list.append(adr2)

################

sfsr2,sfsr2in,sfs\_inlist,sfs\_r2=list(),list(),list(),list()

sfs\_coef,sfs\_mrss,sfsadr2list=list(),list(),list()

for a in range(7):

sfsr2.append(a)

for times in range(5):

sfr2=0

for a in sfsr2:

sfsr2in.append(a)

num\_list=np.asarray(sfsr2in)

r2,coef1,mrss1=fun.linear\_sf(data,label,num\_list)

if sfr2<r2:

minin=a

sfr2=r2

coef=coef1

mrss=mrss1

sfsr2in.remove(a)

sfsr2in.append(minin)

sfsr2.remove(minin)

sfs\_inlist.append(np.asarray(sfsr2in))

sfs\_r2.append(sfr2)

sfs\_coef.append(coef)

sfs\_mrss.append(mrss)

for h in range(len(sfs\_r2)):

sfsadr2=sfs\_r2[h]-(len(sfs\_inlist[h])-1)/(211-len(sfs\_inlist[h]))\*(1-sfs\_r2[h])

sfsadr2list.append(sfsadr2)

##################### 3 ###########################

alpha=[50, 30, 15, 7, 3, 1, 0.30, 0.10, 0.03, 0.01]

alpha1=[-0.1,-0.2,-0.3,-0.4,-0.5,-0.6,-0,7,-0.7,-0.8,-0.9]

clf\_list,lasso\_list=list(),list()

for a in alpha:

clf = Ridge(alpha=a)

clf.fit(data.T, label)

clf\_list.append(clf.coef\_)

for b in alpha:

lasso = linear\_model.Lasso(alpha=b)

lasso.fit(data.T,label)

lasso\_list.append(lasso.coef\_)

plt.figure(1)

plt.plot(alpha,clf\_list)

plt.figure(2)

plt.plot(-1\*np.log(alpha),lasso\_list)

#!/usr/bin/env python3

# -\*- coding: utf-8 -\*-

"""

Created on Wed Dec 13 20:31:51 2017

@author: jianfengsong

"""

import xlrd as xl

import numpy as np

import matplotlib.pyplot as plt

import plotly.plotly as py

import plotly.figure\_factory as ff

import pandas as pd

import plotly

import operator

from keras.applications.vgg16 import VGG16

from keras.preprocessing import image

from keras.applications.vgg16 import preprocess\_input

from keras.models import Model

from itertools import combinations

from sklearn.svm import SVC

from sklearn.multiclass import OneVsOneClassifier

class fun():

def excel\_data(n):

data=list()

excel=xl.open\_workbook(n)

data\_table=excel.sheet\_by\_index(0)

rows=data\_table.nrows

cols=data\_table.ncols

for a in range(rows):

data.append(data\_table.row\_values(a))

return data

################################################################################

def traindata():

data=fun.excel\_data('micrograph.xlsm')

label=['spheroidite','network','pearlite','spheroidite+widmanstatten']

data\_train=list()

# data\_sample=list()

index=list()

index.append(0)

for a in label:

times=0

if a is 'spheroidite+widmanstatten':

for b in range(1,len(data)):

if data[b][9] == a:

if times < 60:

data\_train.append(data[b])

index.append(b)

times+=1

else:

for b in range(1,len(data)):

if data[b][9]== a:

if times <100:

data\_train.append(data[b])

index.append(b)

times+=1

data\_sample=np.delete(data,index,axis=0)

return np.asarray(data\_train),np.asarray(data\_sample)

################################################################################

def isfloat(value):

try:

float(value)

return float(value)

except:

return value

################################################################################

def data():

datatrain,datasam=fun.traindata()

index=[0,2,4,7,8]

temp=list()

temptrain\_list=list()

tempsam\_list=list()

for a in range(len(datatrain.T)):

if a in index:

for b in range(len(datatrain.T[a])):

temp.append(fun.isfloat(datatrain.T[a][b]))

temptrain\_list.append(temp)

temp=list()

else:

temptrain\_list.append(datatrain.T[a])

for a in range(len(datasam.T)):

if a in index:

for b in range(len(datasam.T[a])):

temp.append(fun.isfloat(datasam.T[a][b]))

tempsam\_list.append(temp)

temp=list()

else:

tempsam\_list.append(datasam.T[a])

return tempsam\_list,temptrain\_list

################################################################################

def vg16(path):

img\_path = 'Micrograph/' + path

img = image.load\_img(img\_path)

img=img.crop((0,0,645,484))

x = image.img\_to\_array(img)

x = np.expand\_dims(x, axis=0)

x = preprocess\_input(x)

return x

################################################################################

def avg(matrix):

div=matrix.shape[1]\*matrix.shape[2]

matrix=np.sum(matrix,axis=1)

matrix=np.sum(matrix,axis=1)

matrix=np.divide(matrix,div)

matrix.shape=(matrix.shape[1],1)

return (matrix)

################################################################################

def diffea(train1,label,a):

sph,net,pea,sphw=[],[],[],[]

sphl,netl,peal,sphwl=[],[],[],[]

total,total\_lab=[],[]

svm,svmlab=[],[]

for x in range (0,99):

sph.append(train1[x])

sphl.append(label[x])

for x in range (100,199):

net.append(train1[x])

netl.append(label[x])

for x in range (200,299):

pea.append(train1[x])

peal.append(label[x])

for x in range (300,359):

sphw.append(train1[x])

sphwl.append(label[x])

total.append(sph);total.append(net);total.append(pea);total.append(sphw);

total\_lab.append(sph1);total\_lab.append(netl);total\_lab.append(peal);total\_lab.append(sphwl);

for b in total[a[0]]:

svm.append(b)

for b in total[a[1]]:

svm.append(b)

for b in total\_lab[a[0]]:

svmlab.append(b)

for b in total\_lab[a[1]]:

svmlab.append(b)

return svm,svmlab

################################################################################

datatest,datatrain=fun.data()

model=VGG16(include\_top=False,weights='imagenet',input\_tensor=None,input\_shape=(484,645,3),pooling=None)

model\_1= Model(inputs=model.input, outputs=model.get\_layer('block1\_pool').output)

model\_2= Model(inputs=model.input, outputs=model.get\_layer('block2\_pool').output)

model\_3= Model(inputs=model.input, outputs=model.get\_layer('block3\_pool').output)

model\_4= Model(inputs=model.input, outputs=model.get\_layer('block4\_pool').output)

train1\_fea,test1\_fea=list(),list()

train2\_fea,test2\_fea=list(),list()

train3\_fea,test3\_fea=list(),list()

train4\_fea,test4\_fea=list(),list()

train5\_fea,test5\_fea=list(),list()

train\_lab,test\_lab=list(),list()

layer=[1,2,3,4,5]

for a in range(len(datatrain[1])):

vgg\_16=fun.vg16(datatrain[1][a])

train1\_fea.append(model\_1.predict(vgg\_16))

train2\_fea.append(model\_2.predict(vgg\_16))

train3\_fea.append(model\_3.predict(vgg\_16))

train4\_fea.append(model\_4.predict(vgg\_16))

train5\_fea.append(model.predict(vgg\_16))

train\_lab.append(datatrain[9][a])

for a in range(len(datatest[1])):

vgg\_16\_test=fun.vg16(datatest[1][a])

test1\_fea.append(model\_1.predict(vgg\_16\_test))

test2\_fea.append(model\_2.predict(vgg\_16\_test))

test3\_fea.append(model\_3.predict(vgg\_16\_test))

test4\_fea.append(model\_4.predict(vgg\_16\_test))

test5\_fea.append(model.predict(vgg\_16\_test))

test\_lab.append(datatest[9][a])

for a in range (len(train1\_fea)):

train1\_fea[a]=fun.avg(train1\_fea[a])

train2\_fea[a]=fun.avg(train2\_fea[a])

train3\_fea[a]=fun.avg(train3\_fea[a])

train4\_fea[a]=fun.avg(train4\_fea[a])

train5\_fea[a]=fun.avg(train5\_fea[a])

for a in range (len(test1\_fea)):

test1\_fea[a]=fun.avg(test1\_fea[a])

test2\_fea[a]=fun.avg(test2\_fea[a])

test3\_fea[a]=fun.avg(test3\_fea[a])

test4\_fea[a]=fun.avg(test4\_fea[a])

test5\_fea[a]=fun.avg(test5\_fea[a])

c42label=np.asarray(list(combinations(range(4),2)))

train,test=list(),list()

train.append((train1\_fea,train2\_fea,train3\_fea,train3\_fea,train4\_fea,train5\_fea))

test.append(test1\_fea,test2\_fea,test3\_fea,test4\_fea,test5\_fea)

score=[]

for a in train[0]:

for b in c42label:

svm,svmlab=fun.diffea(a,train\_lab,b)

svm=np.array(svm).reshape(len(svm),len(svm[0]))

clf=NuSVC()

scores=np.mean(cross\_val\_score(clf,svm,svmlab,cv=10))

score.append(1-scores)

train5\_fea=np.array(train5\_fea).reshape(len(train5\_fea),len(train5\_fea[0]))

lay5\_ovo= OneVsOneClassifier(NuSVC()).fit(train5\_fea,train\_lab)

#!/usr/bin/env python3

# -\*- coding: utf-8 -\*-

"""

Created on Fri Dec 15 22:17:34 2017

@author: jianfengsong

"""

import xlrd as xl

import numpy as np

import matplotlib.pyplot as plt

import plotly.plotly as py

import plotly.figure\_factory as ff

import pandas as pd

import plotly

import operator

from keras.applications.vgg16 import VGG16

from keras.preprocessing import image

from keras.applications.vgg16 import preprocess\_input

from keras.models import Model

from itertools import combinations

from sklearn.svm import SVC

from sklearn.multiclass import OneVsOneClassifier

train1\_fea,test1\_fea=list(),list()

train2\_fea,test2\_fea=list(),list()

train3\_fea,test3\_fea=list(),list()

train4\_fea,test4\_fea=list(),list()

train5\_fea,test5\_fea=list(),list()

train\_lab,test\_lab=list(),list()

mar=list();ps=list();pw=list()

ax =['spheroidite','network','pearlite','spheroidite+widmanstatten']

for a in ax:

# print(b[4].shape)

if a == 'spheroidite+widmanstatten':

for d in range(0,60):

train5\_fea.append(data\_features[a][d][5])

train\_lab.append(a)

else:

for d in range(0,100):

train5\_fea.append(data\_features[a][d][5])

train\_lab.append(a)

train5\_fea=np.array(train5\_fea).reshape(len(train5\_fea),512)

lay5\_ovo= OneVsOneClassifier(SVC()).fit(train5\_fea,train\_lab)

for d in range(0,36):

mar.append(data\_features\_rest['martensite'][d][5])

mar=np.array(mar).reshape(len(mar),512)

mar\_lab=lay5\_ovo.predict(mar)

for d in range(0,107):

ps.append(data\_features\_rest['pearlite+spheroidite'][d][5])

ps=np.array(ps).reshape(len(ps),512)

ps\_lab=lay5\_ovo.predict(ps)

for d in range(0,27):

pw.append(data\_features\_rest['pearlite+widmanstatten'][d][5])

pw=np.array(pw).reshape(len(pw),512)

pw\_lab=lay5\_ovo.predict(pw)

#

#

#

#

#