导入包、模块

```
# 基础
2 import os
3 | import zipfile
4 import numpy as np
5
   import pandas as pd
6 # 画图
7 import seaborn as sns
8
   import matplotlib.pyplot as plt
9 from matplotlib import font_manager as fm
10 | from matplotlib import cm
11 % matplotlib inline
12 plt.style.use('ggplot')
13
   # 中文图输出
14 from pylab import mpl
   mpl.rcParams['font.sans-serif'] = ['STZhongsong'] # 指定默认字体: 解决plot不
15
   能显示中文问题
   mpl.rcParams['axes.unicode_minus'] = False
                                                    #解决保存图像是负号'-'显示
16
   为方块的问题
   # 数据集归一化
17
   from sklearn import datasets
18
19 from sklearn import preprocessing
20 #切割训练数据和样本数据
   from sklearn.model_selection import train_test_split
   from sklearn.model_selection import cross_val_score
22
23
   from sklearn.model_selection import StratifiedKFold,cross_val_score
24
   # 模型
25 from sklearn.neighbors import KNeighborsClassifier
   from sklearn.neural_network import MLPClassifier
27
   from sklearn.ensemble import RandomForestClassifier
28
   from sklearn.svm import SVC
29 from sklearn.tree import DecisionTreeClassifier
30 from sklearn.linear_model import LogisticRegression
31
   # from sklearn.metrics import mean_squared_error
32 from sklearn.metrics import *
   # 导出决策树
33
34 | import graphviz
35 | import pydotplus
36 from sklearn.tree import export_graphviz
37 from sklearn.externals.six import StringIO
```

定义全局函数

```
1 # 定义一个路径引用的函数
2 def file_path(dir_path,dir_name):
3     con_path =
    "D:\\onedrive\\02_work\\01_ScienceResearch\\01_undergraduate_thesis\\01_data\\"
4     path = os.path.join(con_path,dir_path,dir_name)
     return path
```

对2010-2016年经济指标文件解压

```
# 对2010-2016年经济指标文件解压
2
   def unzip_file(path,zip_name):
3
       for file in os.listdir(path):
           file_path=os.path.join(path,file)
4
5
           if os.path.splitext(file_path)[1]==zip_name:
               fz=zipfile.ZipFile(file_path,'r')
6
7
               for zip_file in fz.namelist():
                   fz.extract(zip_file,path)
8
9
   unzip_file("D:\\onedrive\\02_work\\01_ScienceResearch\\01_undergraduate_thesi
   s\\01_data",".zip")
```

读入数据

```
1 # 去掉各个变量的标签
    pd.read_csv(file_path("01_rawdata", "ACS_10_5YR_DP02_with_ann.csv"))
    [1:].to_csv(file_path("02_output","ACS_10_5YR_DP02_with_ann.csv"),encoding="
    utf-8-sig")
    pd.read_csv(file_path("01_rawdata","ACS_11_5YR_DP02_with_ann.csv"))
    [1:].to_csv(file_path("02_output","ACS_11_5YR_DP02_with_ann.csv"),encoding="
    utf-8-sig")
    pd.read_csv(file_path("01_rawdata","ACS_12_5YR_DP02_with_ann.csv"))
    [1:].to_csv(file_path("02_output","ACS_12_5YR_DP02_with_ann.csv"),encoding="
    utf-8-sig")
    pd.read_csv(file_path("01_rawdata","ACS_13_5YR_DP02_with_ann.csv"))
    [1:].to_csv(file_path("02_output","ACS_13_5YR_DP02_with_ann.csv"),encoding="
    utf-8-sia")
    pd.read_csv(file_path("01_rawdata", "ACS_14_5YR_DP02_with_ann.csv"))
    [1:].to_csv(file_path("02_output","ACS_14_5YR_DP02_with_ann.csv"),encoding="
    utf-8-sig")
    pd.read_csv(file_path("01_rawdata", "ACS_15_5YR_DP02_with_ann.csv"))
    [1:].to_csv(file_path("02_output","ACS_15_5YR_DP02_with_ann.csv"),encoding="
    utf-8-sig")
    pd.read_csv(file_path("01_rawdata","ACS_16_5YR_DP02_with_ann.csv"))
    [1:].to_csv(file_path("02_output","ACS_16_5YR_DP02_with_ann.csv"),encoding="
    utf-8-sig")
    # 读入2010-2016年经济指标数据
9
10
    ACS_{10_5YR_DP02_with_ann} =
    pd.read_csv(file_path("02_output","ACS_10_5YR_DP02_with_ann.csv"),na_values=
    ["(X)","*****","***","-","+","N"])
    ACS_11_5YR_DP02_with_ann =
11
    pd.read_csv(file_path("02_output","ACS_11_5YR_DP02_with_ann.csv"),na_values=
    ["(X)","*****","***","-","+","N"])
12
    ACS_{12_{5YR_{DP02_{with_ann}}} =
    pd.read_csv(file_path("02_output","ACS_12_5YR_DP02_with_ann.csv"),na_values=
    ["(X)","*****","**","-","+","N"])
13
    ACS_13_5YR_DP02_with_ann =
    pd.read_csv(file_path("02_output","ACS_13_5YR_DP02_with_ann.csv"),na_values=
    ["(X)","*****","**","-","+","N"])
14
    ACS_14_5YR_DP02_with_ann =
    pd.read_csv(file_path("02_output","ACS_14_5YR_DP02_with_ann.csv"),na_values=
    ["(X)","*****","***","-","+","N"])
```

```
15 | ACS_15_5YR_DP02_with_ann =
    pd.read_csv(file_path("02_output","ACS_15_5YR_DP02_with_ann.csv"),na_values=
    ["(X)","*****","***","**","-","+","N"])
16
    ACS_16_5YR_DP02_with_ann =
    pd.read_csv(file_path("02_output","ACS_16_5YR_DP02_with_ann.csv"),na_values=
    ["(X)","*****","***","-","+","N"])
17
    # # 读入各个地区阿片类使用量数据
    MCM_NFLIS_Data=pd.read_excel(file_path("01_rawdata","MCM_NFLIS_Data.xlsx"),s
    heet_name=1
19
    # # 读入药物具体分类数据
   MCM_NFLIS_Medication=pd.read_csv(file_path("01_rawdata","class_medication.cs
20
    v"))
21
    # 读入变量标签数据
    ACS_10_5YR_DP02_metadata =
    pd.read_csv(file_path("01_rawdata","ACS_10_5YR_DP02_metadata.csv"),header=No
23
    ACS_{11_5YR_DP02_metadata} =
    pd.read_csv(file_path("01_rawdata","ACS_11_5YR_DP02_metadata.csv"),header=No
    ACS_12_5YR_DP02_metadata =
    pd.read_csv(file_path("01_rawdata","ACS_12_5YR_DP02_metadata.csv"),header=No
    ne)
25 ACS_13_5YR_DP02_metadata =
    pd.read_csv(file_path("01_rawdata","ACS_13_5YR_DP02_metadata.csv"),header=No
26 \quad ACS_14_5YR_DP02_metadata =
    pd.read_csv(file_path("01_rawdata","ACS_14_5YR_DP02_metadata.csv"),header=No
27 ACS_15_5YR_DP02_metadata =
    pd.read_csv(file_path("01_rawdata","ACS_15_5YR_DP02_metadata.csv"),header=No
28 \quad ACS_16_5YR_DP02_metadata =
    pd.read_csv(file_path("01_rawdata","ACS_16_5YR_DP02_metadata.csv"),header=No
```

数据处理

整理ACS_ALL_5YR_DP02数据

```
1 ## 处理无效数据
2
   # 2010
   # 删除类型异常的变量(NaN、(x))
   typedata = ACS_10_5YR_DP02_with_ann.dtypes.reset_index()
    nonnormal_var = typedata.loc[typedata.ix[:,1] == "object"]["index"]
    [2:].tolist()
    ACS_10_5YR_DP02_DropNorm =
6
    ACS\_10\_5YR\_DP02\_with\_ann.drop(nonnormal\_var,axis=1)
7
    # 删除全为空的变量(列)
    ACS_10_5YR_DP02_DropColumn=ACS_10_5YR_DP02_DropNorm.dropna(axis=1, how="all")
9
    # 用列均值填补缺失数据
   for column in
10
    list(ACS_10_5YR_DP02_DropColumn.columns[ACS_10_5YR_DP02_DropColumn.isnull().
    sum() > 0]):
11
        mean_val = ACS_10_5YR_DP02_DropColumn[column].mean()
12
       ACS_10_5YR_DP02_DropColumn[column].fillna(mean_val, inplace=True)
13
```

```
14 # 2011
15
    # 删除类型异常的变量(NaN、(x))
   typedata = ACS_11_5YR_DP02_with_ann.dtypes.reset_index()
16
    nonnormal_var = typedata.loc[typedata.ix[:,1] == "object"]["index"]
17
    [2:].tolist()
    ACS_11_5YR_DP02_DropNorm =
18
    ACS_11_5YR_DP02_with_ann.drop(nonnormal_var,axis=1)
19
    # 删除全为空的变量(列)
20 ACS_11_5YR_DP02_DropColumn=ACS_11_5YR_DP02_DropNorm.dropna(axis=1,how="all")
21
    # 用列均值填补缺失数据
22 | for column in
    list(ACS_11_5YR_DP02_DropColumn.columns[ACS_11_5YR_DP02_DropColumn.isnull().
    sum() > 0]):
       mean_val = ACS_11_5YR_DP02_DropColumn[column].mean()
23
24
        ACS_11_5YR_DP02_DropColumn[column].fillna(mean_val, inplace=True)
25
26 # 2012
    # 删除类型异常的变量(NaN、(x))
27
28
   typedata = ACS_12_5YR_DP02_with_ann.dtypes.reset_index()
    nonnormal_var = typedata.loc[typedata.ix[:,1] == "object"]["index"]
    [2:].tolist()
30
    ACS_12_5YR_DP02_DropNorm =
    ACS_12_5YR_DP02_with_ann.drop(nonnormal_var,axis=1)
31 # 删除全为空的变量(列)
    ACS_12_5YR_DP02_DropColumn=ACS_12_5YR_DP02_DropNorm.dropna(axis=1, how="all")
33
    # 用列均值填补缺失数据
34
   for column in
    list(ACS_12_5YR_DP02_DropColumn.columns[ACS_12_5YR_DP02_DropColumn.isnull().
    sum() > 0]):
35
        mean_val = ACS_12_5YR_DP02_DropColumn[column].mean()
36
        ACS_12_5YR_DP02_DropColumn[column].fillna(mean_val, inplace=True)
37
38 # 2013
39 # 删除类型异常的变量(NaN、(x))
   typedata = ACS_13_5YR_DP02_with_ann.dtypes.reset_index()
40
    nonnormal_var = typedata.loc[typedata.ix[:,1] == "object"]["index"]
    [2:].tolist()
42
    ACS_13_5YR_DP02_DropNorm =
    ACS_13_5YR_DP02_with_ann.drop(nonnormal_var,axis=1)
43
    # 删除全为空的变量(列)
    ACS_13_5YR_DP02_DropColumn=ACS_13_5YR_DP02_DropNorm.dropna(axis=1,how="all")
44
45
    # 用列均值填补缺失数据
46
   for column in
    list(ACS_13_5YR_DP02_DropColumn.columns[ACS_13_5YR_DP02_DropColumn.isnull().
    sum() > 0]):
47
       mean_val = ACS_13_5YR_DP02_DropColumn[column].mean()
48
        ACS_13_5YR_DP02_DropColumn[column].fillna(mean_val, inplace=True)
49
50 # 2013
51
    # 删除类型异常的变量(NaN、(x))
52
    typedata = ACS_14_5YR_DP02_with_ann.dtypes.reset_index()
    nonnormal_var = typedata.loc[typedata.ix[:,1] == "object"]["index"]
    [2:].tolist()
54
    ACS_14_5YR_DP02_DropNorm =
    ACS_14_5YR_DP02_with_ann.drop(nonnormal_var,axis=1)
55
    # 删除全为空的变量(列)
56
   ACS_14_5YR_DP02_DropColumn=ACS_14_5YR_DP02_DropNorm.dropna(axis=1,how="all")
57 # 用列均值填补缺失数据
```

```
58 | for column in
    list(ACS_14_5YR_DP02_DropColumn.columns[ACS_14_5YR_DP02_DropColumn.isnull().
    sum() > 0]):
59
        mean_val = ACS_14_5YR_DP02_DropColumn[column].mean()
60
        ACS_14_5YR_DP02_DropColumn[column].fillna(mean_val, inplace=True)
61
62
   # 2015
63
    # 删除类型异常的变量(NaN、(x))
   typedata = ACS_15_5YR_DP02_with_ann.dtypes.reset_index()
64
    nonnormal_var = typedata.loc[typedata.ix[:,1] == "object"]["index"]
    [2:].tolist()
    ACS_15_5YR_DP02_DropNorm =
66
    ACS_15_5YR_DP02_with_ann.drop(nonnormal_var,axis=1)
67
    # 删除全为空的变量(列)
    ACS_15_5YR_DP02_DropColumn=ACS_15_5YR_DP02_DropNorm.dropna(axis=1,how="all")
    # 用列均值填补缺失数据
69
70
   for column in
    list(ACS\_15\_5YR\_DP02\_DropColumn.columns[ACS\_15\_5YR\_DP02\_DropColumn.isnull().
    sum() > 0]):
71
        mean_val = ACS_15_5YR_DP02_DropColumn[column].mean()
       ACS_15_5YR_DP02_DropColumn[column].fillna(mean_val, inplace=True)
72
73
74
   # 2016
75
   # 删除类型异常的变量(NaN、(x))
76
   typedata = ACS_16_5YR_DP02_with_ann.dtypes.reset_index()
77
    nonnormal_var = typedata.loc[typedata.ix[:,1] == "object"]["index"]
    [2:].tolist()
    ACS_16_5YR_DP02_DropNorm =
78
    ACS_16_5YR_DP02_with_ann.drop(nonnormal_var,axis=1)
79
    # 删除全为空的变量(列)
80
   ACS_16_5YR_DP02_DropColumn=ACS_16_5YR_DP02_DropNorm.dropna(axis=1, how="all")
81
    # 用列均值填补缺失数据
   for column in
    list(ACS_16_5YR_DP02_DropColumn.columns[ACS_16_5YR_DP02_DropColumn.isnull().
    sum() > 0]):
83
       mean_val = ACS_16_5YR_DP02_DropColumn[column].mean()
        ACS_16_5YR_DP02_DropColumn[column].fillna(mean_val, inplace=True)
84
85
    # 纵向合并2010-2016年的数据到一个数据框中、# 删除第一行数据(变量标签)
86
87
    ACS_ALL_5YR_DP02=pd.concat([ACS_10_5YR_DP02_DropColumn,
88
                              ACS_11_5YR_DP02_DropColumn,
89
                              ACS_12_5YR_DP02_DropColumn,
90
                              ACS_13_5YR_DP02_DropColumn,
91
                              ACS_14_5YR_DP02_DropColumn,
92
                              ACS_15_5YR_DP02_DropColumn,
93
    ACS_16_5YR_DP02_DropColumn], axis=0, join="outer", keys=
    [2010,2011,2012,2013,2014,2015,2016]).reset_index().convert_objects(convert_
    numeric=True)
94
    # 用列均值填补缺失数据(合并各年份数据之后)
95
   for column in list(ACS_ALL_5YR_DP02.columns[ACS_ALL_5YR_DP02.isnull().sum()
    > 0]):
96
        mean_val = ACS_ALL_5YR_DP02[column].mean()
97
        ACS_ALL_5YR_DP02[column].fillna(mean_val, inplace=True)
   # 删除无效的变量(索引,中间产生变量、地理位置),重命名年份变量
98
    ACS_ALL_5YR_DP02_Clear = ACS_ALL_5YR_DP02.ix[:,:-2].drop(["GE0.display-
    label","level_1","GEO.id"],axis=1).rename(columns={"level_0":"YYYY"})
```

整理MCM NFLIS Data数据

```
# 对阿片类药物使用情况数据键值重命名
   MCM_NFLIS_Data_Rename=MCM_NFLIS_Data.rename(columns=
   {"FIPS_Combined":"GEO.id2"})
   # 删除2017相关数据
4 MCM_NFLIS_Data_Drop17=MCM_NFLIS_Data_Rename.loc[MCM_NFLIS_Data_Rename["YYYY"
   ] != 2017]
 5 # 匹配药物分类数据
   MCM_NFLIS_Class=pd.merge(MCM_NFLIS_Data_Drop17,MCM_NFLIS_Medication,how="lef
   t", on=["SubstanceName", "YYYY"])
   # 删除一些无效变量
   MCM_NFLIS_Class_Clear_Drop=MCM_NFLIS_Class.drop(["FIPS_State","FIPS_County",
   "SubstanceName", "code"], axis=1)
   # 按照中文名药物分类求和
   MCM_NFLIS_Class_Clear =
10
   MCM_NFLIS_Class_Clear_Drop.groupby(["YYYY","GEO.id2","State","COUNTY","Subst
   anceClass",
11
                                                          "SubstanceName_c"])
    ["DrugReports"].sum().reset_index()
```

整理ACS_AII_5YR_DP02_metadata数据

```
1
   # 纵向合并2010-2016年的数据到一个数据框中、# 删除第一行数据(变量标签)
   ACS_All_5YR_DP02_metadata=pd.concat([ACS_10_5YR_DP02_metadata,
 3
                              ACS_11_5YR_DP02_metadata,
4
                              ACS_12_5YR_DP02_metadata,
 5
                              ACS_13_5YR_DP02_metadata,
6
                              ACS_14_5YR_DP02_metadata,
7
                              ACS_15_5YR_DP02_metadata,
8
                              ACS_16_5YR_DP02_metadata],axis=0,join="outer",)
9 # 删除重复值
   ACS_A11_5YR_DP02_metadata_Dup =
10
   ACS_All_5YR_DP02_metadata.drop_duplicates(list(ACS_All_5YR_DP02_metadata.col
   umns)[0],keep="first")
11 ACS_All_5YR_DP02_metadata_Dup.columns = ["Var","Var_label"]
```

匹配阿片类药物使用情况

```
1 # 合并阿片类使用情况与相关经济指标
2 NFLIS_and_ACS_ALL=pd.merge(ACS_ALL_5YR_DP02_Clear,MCM_NFLIS_Class_Clear,how="right",on=["YYYY","GEO.id2"])
```

按照三类药物数据透视

```
columns=["YYYY"],values=
    ["DrugReports"])
    # 缺失值填补、转置
    NFLIS_and_ACS_ALL_Clear =
    NFLIS_and_ACS_ALL_Pivot[2:].fillna(0).stack().reset_index()
10
    # 合并
11
    NFLIS_and_ACS_ALL_Out = pd.merge(NFLIS_and_ACS_ALL_Clear,
12
                                    ACS_ALL_5YR_DP02_Clear,
13
                                    on=["GEO.id2","YYYY"],how="left")
14
    # 根据药物量分层
15
    NFLIS_and_ACS_ALL_Out["DrugReportsclass"] =
    np.where(NFLIS_and_ACS_ALL_Out["DrugReports"] >= 5000,"7、5000人以上",
16
    np.where(NFLIS_and_ACS_ALL_Out["DrugReports"] >= 1000,"6、1000-4999人",
17
     np.where(NFLIS_and_ACS_ALL_Out["DrugReports"] >= 500,"5、500-999人",
18
    np.where(NFLIS_and_ACS_ALL_Out["DrugReports"] >= 100,"4、100-499人",
19
     np.where(NFLIS_and_ACS_ALL_Out["DrugReports"] >= 10,"3、10-99人",
20
      np.where(NFLIS_and_ACS_ALL_Out["DrugReports"] >= 1,"2、1-9人","1、0
    人"))))))
```

统计描述

图1: 所有类阿片类药物构成饼图

整理数据为直接可用

```
1 # 提取画图数据"YYYY", "SubstanceName", "DrugReports", "State"
   NFLIS_Figure1_Data = MCM_NFLIS_Class_Clear.groupby(["SubstanceName_c"])
   ["DrugReports"].sum().reset_index().sort_values(by="DrugReports",ascending=T
   rue)
   #添加列:每种药物的百分占比
   NFLIS_Figure1_Data["Percent"] =
   NFLIS_Figure1_Data["DrugReports"]/(NFLIS_Figure1_Data["DrugReports"].sum())
   NFLIS_Figure1_Data["Label"] = NFLIS_Figure1_Data["SubstanceName_c"] +\
5
                                             ' + \
6
                                  NFLIS_Figure1_Data["Percent"].apply(lambda
7
   x: format(x, '.2%'))
8
   # 画图所用的数据
   Figure1_labels = NFLIS_Figure1_Data["Label"]
   Figure1_sizes = NFLIS_Figure1_Data["DrugReports"]
```

饼图

```
1# 设置画布和子图2Figure1,axes = plt.subplots(figsize=(20,15),ncols=2)3Figure1_ax1,Figure1_ax2 = axes.ravel()4# 设置参数: 颜色盘-colormap; 间隙-与labels—对应,数值越大离中心区越远5explode = [x * 0.00325 for x in range(len(NFLIS_Figure1_Data))]6colors=cm.rainbow(np.arange(len(Figure1_sizes))/len(Figure1_sizes))7# 画饼图: 类别太多取消标签labels; 每个类别离中心的距离;
```

```
patches,texts =
    Figure1_ax1.pie(Figure1_sizes,labels=None,shadow=False,explode=explode,start
    angle=0,colors=colors)
# 子图: ax1-饼图、ax2-图例
Figure1_ax1.axis('equal')
Figure1_ax2.axis('off')
Figure1_ax2.legend(patches,Figure1_labels,loc="center left",fontsize="xx-large")
# 调整大小、读取图片
plt.tight_layout()
Figure1 = plt.gcf()
```

图2: 所有类阿片类药物数量条图

整理数据为直接可用

```
# 提取画图数据"YYYY","SubstanceName","DrugReports","State"; 排序;

NFLIS_Figure2_Data = MCM_NFLIS_Class_Clear.groupby(["SubstanceName_c"])
["DrugReports"].sum().reset_index().sort_values(by="DrugReports",ascending=True)

3
```

条图

```
1 # 设置画布
plt.figure(figsize=(16,10))
   # 设置参数: 颜色盘-colormap
4 color=cm.rainbow(np.arange(len(NFLIS_Figure2_Data))/len(NFLIS_Figure2_Data))
   # 从高到低排列,改变y轴刻度的排列顺序
6 plt.yticks(np.arange(len(NFLIS_Figure2_Data['SubstanceName_c'])),
   NFLIS_Figure2_Data['SubstanceName_c'])
   # 水平条图
 7
   plt.barh(np.arange(len(NFLIS_Figure2_Data['SubstanceName_c'])),
   NFLIS_Figure2_Data['DrugReports'], color=color)
9
   # 坐标轴标签
10 plt.ylabel("阿片类药物名")
11 plt.xlabel("报告量")
12 # 格式整理导出
13 | plt.tight_layout()
14 | Figure2 = plt.gcf()
```

图3: 五个州阿片类药物数量热力图

整理数据为直接可用

```
# 提取画图数据"YYYY", "SubstanceName", "DrugReports", "State"

NFLIS_Figure3_Clear1 =
MCM_NFLIS_Class_Clear.groupby(["State", "YYYY", "SubstanceName_c"])
["DrugReports"].sum().reset_index()

# 提取各个州的数据

NFLIS_Figure3_KY = NFLIS_Figure3_Clear1.loc[(NFLIS_Figure3_Clear1["State"])
== "KY")]

NFLIS_Figure3_OH = NFLIS_Figure3_Clear1.loc[(NFLIS_Figure3_Clear1["State"])
== "OH")]
```

```
NFLIS_Figure3_PA = NFLIS_Figure3_Clear1.loc[(NFLIS_Figure3_Clear1["State"]
    == "PA")]
   NFLIS_Figure3_VA = NFLIS_Figure3_Clear1.loc[(NFLIS_Figure3_Clear1["State"]
    == "VA")]
8 NFLIS_Figure3_WV = NFLIS_Figure3_Clear1.loc[(NFLIS_Figure3_Clear1["State"]
    == "WV")]
   # 匹配每种药物 (解决某年可能没有某种药)
   NFLIS_Figure3_KY_merge = pd.merge(NFLIS_Figure3_KY,MCM_NFLIS_Medication,how
10
    = "right", on = ["YYYY", "SubstanceName_c"])
11
    NFLIS_Figure3_OH_merge = pd.merge(NFLIS_Figure3_OH,MCM_NFLIS_Medication,how
    = "right",on = ["YYYY","SubstanceName_c"])
    NFLIS_Figure3_PA_merge = pd.merge(NFLIS_Figure3_PA,MCM_NFLIS_Medication,how
12
    = "right",on = ["YYYY","SubstanceName_c"])
    NFLIS_Figure3_VA_merge = pd.merge(NFLIS_Figure3_VA,MCM_NFLIS_Medication,how
13
    = "right", on = ["YYYY", "SubstanceName_c"])
    NFLIS_Figure3_WV_merge = pd.merge(NFLIS_Figure3_WV,MCM_NFLIS_Medication,how
14
    = "right",on = ["YYYY","SubstanceName_c"])
    # 将数据转置为dataframe矩阵
15
16
    NFLIS_Figure3_pivot_KY = NFLIS_Figure3_KY_merge.pivot_table(index =
    "SubstanceName_c", columns = "YYYY", values = "DrugReports")
    NFLIS_Figure3_pivot_OH = NFLIS_Figure3_OH_merge.pivot_table(index =
17
    "SubstanceName_c", columns = "YYYY", values = "DrugReports")
18
    NFLIS_Figure3_pivot_PA = NFLIS_Figure3_PA_merge.pivot_table(index =
    "SubstanceName_c", columns = "YYYY", values = "DrugReports")
    NFLIS_Figure3_pivot_VA = NFLIS_Figure3_VA_merge.pivot_table(index =
    "SubstanceName_c", columns = "YYYY", values = "DrugReports")
    NFLIS_Figure3_pivot_wV = NFLIS_Figure3_wV_merge.pivot_table(index =
    "SubstanceName_c",columns = "YYYY",values = "DrugReports")
```

热力图

```
1 # 设置画布大小
2 f, (Figure3_ax1, Figure3_ax2, Figure3_ax3, Figure3_ax4, Figure3_ax5) =
    plt.subplots(ncols=5, figsize=(30,10))
    # 设置连续调色板cubehelix_palette,as_camp传入matplotlib
4
   cmap=sns.cubehelix_palette(start=1,rot=3,gamma=0.8,as_cmap=True)
 5
    # KY州
    sns.heatmap(NFLIS_Figure3_pivot_KY,cmap=cmap,linewidths=0.05,ax=Figure3_ax1,
    cbar=False)
    Figure3_ax1.set_title("肯塔基州",fontsize=30)
    Figure3_ax1.set_xlabel('')
9
    Figure3_ax1.set_ylabel('阿片类药物名',fontsize=35)
10
   # OH州
11
    sns.heatmap(NFLIS_Figure3_pivot_OH,cmap=cmap,linewidths=0.05,ax=Figure3_ax2,
    cbar=False)
12
    Figure3_ax2.set_title("俄亥俄州",fontsize=30)
13
    Figure3_ax2.set_xlabel('')
14
    Figure3_ax2.set_ylabel(' ')
15
    Figure3_ax2.set_yticklabels([])
16
    # PA州
17
    sns.heatmap(NFLIS_Figure3_pivot_PA,cmap=cmap,linewidths=0.05,ax=Figure3_ax3,
    cbar=False)
    Figure3_ax3.set_title("宾夕法尼亚州",fontsize=30)
18
    Figure3_ax3.set_xlabel('年份',fontsize=35)
19
20
    Figure3_ax3.set_ylabel('')
    Figure3_ax3.set_yticklabels([])
21
22
    # VA州
```

```
sns.heatmap(NFLIS_Figure3_pivot_VA,cmap=cmap,linewidths=0.05,ax=Figure3_ax4,
    cbar=False)
24
    Figure3_ax4.set_title("弗吉尼亚州",fontsize=30)
25
    Figure3_ax4.set_xlabel('')
26
    Figure3_ax4.set_ylabel('')
27
    Figure3_ax4.set_yticklabels([])
28
    # WV州
29
   sns.heatmap(NFLIS_Figure3_pivot_wV,cmap=cmap,linewidths=0.05,ax=Figure3_ax5,
    cbar=True)
30
    Figure3_ax5.set_title("西弗吉尼亚州",fontsize=30)
31
    Figure3_ax5.set_xlabel('')
32
    Figure3_ax5.set_ylabel('')
33
    Figure3_ax5.set_yticklabels([])
34
35 plt.tight_layout()
36 Figure3 = plt.gcf()
```

图4: 五个州三类阿片药物量折线图

整理数据为直接可用

```
1 # 五个州的总量情况分组
2 NFLIS_Fugure3_Clear1 =
   MCM_NFLIS_Class_Clear.groupby(["YYYY","SubstanceClass"])
    ["DrugReports"].sum().reset_index()
   NFLIS_Fugure3_Class1_all =
   NFLIS_Fugure3_Clear1.loc[(NFLIS_Fugure3_Clear1["SubstanceClass"] == "半合成阿
   片类药物")]
   NFLIS_Fugure3_Class2_all =
   NFLIS_Fugure3_Clear1.loc[(NFLIS_Fugure3_Clear1["SubstanceClass"] == "合成阿片
   类药物")]
 5 NFLIS_Fugure3_Class3_all =
   NFLIS_Fugure3_Clear1.loc[(NFLIS_Fugure3_Clear1["SubstanceClass"] == "非合成阿
   片类药物")]
6 # 五个州的分别情况分组
   NFLIS_Fugure3_Class =
   MCM_NFLIS_Class_Clear.groupby(["YYYY","State","SubstanceClass"])
    ["DrugReports"].sum().reset_index()
   NFLIS_Fugure3_Class1 =
   NFLIS_Fugure3_Class.loc[(NFLIS_Fugure3_Class["SubstanceClass"] == "半合成阿片
   类药物")]
   NFLIS_Fugure3_Class2 =
   NFLIS_Fugure3_Class.loc[(NFLIS_Fugure3_Class["SubstanceClass"] == "合成阿片类
   药物")]
   NFLIS_Fugure3_Class3 =
   NFLIS_Fugure3_Class.loc[(NFLIS_Fugure3_Class["SubstanceClass"] == "非合成阿片
   类药物")]
11 # 对每个州进行汇合
   NFLIS_Figure2_Data_Class1 =
   NFLIS_Fugure3_Class1.pivot_table(index="YYYY",columns="State",values="DrugRe
   ports").reset_index()
13 | NFLIS_Figure2_Data_Class2 =
   NFLIS_Fugure3_Class2.pivot_table(index="YYYY",columns="State",values="DrugRe
   ports").reset_index()
14 NFLIS_Figure2_Data_Class3 =
   NFLIS_Fugure3_Class3.pivot_table(index="YYYY",columns="State",values="DrugRe
    ports").reset_index()
```

折线图

```
1 # 创建画布、6个子图
   plt.figure(figsize=(15,10))
   f4 = plt.figure(figsize=(20,15))
4 Figure_ax1 = f4.add_subplot(2, 3, 1)
5 Figure_ax2 = f4.add_subplot(2, 3, 2)
6
   Figure_ax3 = f4.add_subplot(2, 3, 3)
7
   Figure_ax4 = f4.add_subplot(2, 3, 4)
   Figure_ax5 = f4.add_subplot(2, 3, 5)
9
   Figure\_ax6 = f4.add\_subplot(2, 3, 6)
10
11
   # KY州不同类型药物的折线图
   Figure_ax1.plot(NFLIS_Figure2_Data_Class1["YYYY"],NFLIS_Figure2_Data_Class1
12
    ["KY"],label="半合成阿片类药物",linewidth=2)
   Figure_ax1.plot(NFLIS_Figure2_Data_Class2["YYYY"],NFLIS_Figure2_Data_Class2
13
    ["KY"],label="合成阿片类药物",linewidth=2)
14
   Figure_ax1.plot(NFLIS_Figure2_Data_Class3["YYYY"],NFLIS_Figure2_Data_Class3
    ["KY"],label="非合成阿片类药物",linewidth=2)
15
   | Figure_ax1.set_title("肯塔基州")
   Figure_ax1.legend(loc=2)
16
17
   Figure_ax1.grid(axis='x')
    #设置数字标签
18
19 for a.b in
    zip(NFLIS_Figure2_Data_Class1["YYYY"],NFLIS_Figure2_Data_Class1["KY"]):
20
        Figure_ax1.text(a, b+0.001, \frac{1}{5} b, ha=\frac{1}{5} center, va=
    'bottom', fontsize=11)
21 for a,b in
    zip(NFLIS_Figure2_Data_Class2["YYYY"],NFLIS_Figure2_Data_Class2["KY"]):
22
        Figure_ax1.text(a, b+0.001, '%s' % b, ha='center', va=
    'bottom', fontsize=11)
23
   for a,b in
    zip(NFLIS_Figure2_Data_Class3["YYYY"],NFLIS_Figure2_Data_Class3["KY"]):
24
        Figure_ax1.text(a, b+0.001, '%s' % b, ha='center', va=
    'bottom', fontsize=11)
25
26
    # OH州不同类型药物的折线图
27
    Figure_ax2.plot(NFLIS_Figure2_Data_Class1["YYYY"],NFLIS_Figure2_Data_Class1
    ["OH"], label="半合成阿片类药物", linewidth=2)
28
   Figure_ax2.plot(NFLIS_Figure2_Data_Class2["YYYY"],NFLIS_Figure2_Data_Class2
    ["OH"], label="合成阿片类药物", linewidth=2)
    Figure_ax2.plot(NFLIS_Figure2_Data_Class3["YYYY"], NFLIS_Figure2_Data_Class3
    ["OH"], label="非合成阿片类药物", linewidth=2)
30 Figure_ax2.set_title("俄亥俄州")
31
   Figure_ax2.legend(loc=2)
32
   Figure_ax2.grid(axis='x')
33
    #设置数字标签**
34
   for a,b in
    zip(NFLIS_Figure2_Data_Class1["YYYY"],NFLIS_Figure2_Data_Class1["OH"]):
35
        Figure_ax2.text(a, b+0.001, '%s' % b, ha='center', va=
    'bottom', fontsize=11)
36
   for a,b in
    zip(NFLIS_Figure2_Data_Class2["YYYY"],NFLIS_Figure2_Data_Class2["OH"]):
        Figure_ax2.text(a, b+0.001, '%s' % b, ha='center', va=
37
    'bottom',fontsize=11)
```

```
38 for a,b in
    zip(NFLIS_Figure2_Data_Class3["YYYY"],NFLIS_Figure2_Data_Class3["OH"]):
        Figure_ax2.text(a, b+0.001, '%s' % b, ha='center', va=
    'bottom',fontsize=11)
40
41
   # PA州不同类型药物的折线图
    Figure_ax3.plot(NFLIS_Figure2_Data_Class1["YYYY"],NFLIS_Figure2_Data_Class1
    ["PA"],label="半合成阿片类药物",linewidth=2)
   Figure_ax3.plot(NFLIS_Figure2_Data_Class2["YYYY"],NFLIS_Figure2_Data_Class2
    ["PA"],label="合成阿片类药物",linewidth=2)
   Figure_ax3.plot(NFLIS_Figure2_Data_Class3["YYYY"], NFLIS_Figure2_Data_Class3
44
    ["PA"], label="非合成阿片类药物", linewidth=2)
45
    Figure_ax3.set_title("宾夕法尼亚州")
46 | Figure_ax3.legend(loc=2)
   Figure_ax3.grid(axis='x')
    #设置数字标签**
48
49 for a,b in
    zip(NFLIS_Figure2_Data_Class1["YYYY"],NFLIS_Figure2_Data_Class1["PA"]):
        Figure_ax3.text(a, b+0.001, '%s' % b, ha='center', va=
50
    'bottom',fontsize=11)
51 | for a,b in
    zip(NFLIS_Figure2_Data_Class2["YYYY"],NFLIS_Figure2_Data_Class2["PA"]):
52
        Figure_ax3.text(a, b+0.001, '%s' % b, ha='center', va=
    'bottom', fontsize=11)
53 for a,b in
    zip(NFLIS_Figure2_Data_Class3["YYYY"],NFLIS_Figure2_Data_Class3["PA"]):
        Figure_ax3.text(a, b+0.001, '%s' \% b, ha='center', va=
54
    'bottom',fontsize=11)
55
    # VA州不同类型药物的折线图
    Figure_ax4.plot(NFLIS_Figure2_Data_Class1["YYYY"],NFLIS_Figure2_Data_Class1
    ["VA"], label="半合成阿片类药物", linewidth=2)
58
   Figure_ax4.plot(NFLIS_Figure2_Data_Class2["YYYY"],NFLIS_Figure2_Data_Class2
    ["VA"], label="合成阿片类药物", linewidth=2)
   Figure_ax4.plot(NFLIS_Figure2_Data_Class3["YYYY"],NFLIS_Figure2_Data_Class3
    ["VA"], label="非合成阿片类药物", linewidth=2)
60 Figure_ax4.set_title("弗吉尼亚州")
   Figure_ax4.grid(axis="x")
61
62
   Figure_ax4.legend(loc=2)
63
   for a,b in
    zip(NFLIS_Figure2_Data_Class1["YYYY"],NFLIS_Figure2_Data_Class1["VA"]):
        Figure_ax4.text(a, b+0.001, '%s' % b, ha='center', va=
    'bottom',fontsize=11)
   for a,b in
65
    zip(NFLIS_Figure2_Data_Class2["YYYY"],NFLIS_Figure2_Data_Class2["VA"]):
        Figure_ax4.text(a, b+0.001, '%s' % b, ha='center', va=
    'bottom',fontsize=11)
67
   for a,b in
    zip(NFLIS_Figure2_Data_Class3["YYYY"],NFLIS_Figure2_Data_Class3["VA"]):
68
        Figure_ax4.text(a, b+0.001, '%s' % b, ha='center', va=
   'bottom',fontsize=11)
    # WV州不同类型药物的折线图
70
    Figure_ax5.plot(NFLIS_Figure2_Data_Class1["YYYY"],NFLIS_Figure2_Data_Class1
71
    ["wv"],label="半合成阿片类药物",linewidth=2)
    Figure_ax5.plot(NFLIS_Figure2_Data_Class2["YYYY"],NFLIS_Figure2_Data_Class2
72
    ["wv"], label="合成阿片类药物", linewidth=2)
```

```
Figure_ax5.plot(NFLIS_Figure2_Data_Class3["YYYY"],NFLIS_Figure2_Data_Class3
     ["wv"], label="非合成阿片类药物", linewidth=2)
    Figure_ax5.set_title("西弗吉尼亚州")
75 | Figure_ax5.legend(loc=2)
76 Figure_ax5.grid(axis='x')
77
     #设置数字标签**
78 for a,b in
    zip(NFLIS_Figure2_Data_Class1["YYYY"],NFLIS_Figure2_Data_Class1["WV"]):
79
        Figure_ax5.text(a, b+0.001, '%s' % b, ha='center', va=
    'bottom',fontsize=11)
80
    for a,b in
    zip(NFLIS_Figure2_Data_Class2["YYYY"],NFLIS_Figure2_Data_Class2["WV"]):
        Figure_ax5.text(a, b+0.001, '%s' % b, ha='center', va=
81
     'bottom',fontsize=11)
82 for a,b in
    zip(NFLIS_Figure2_Data_Class3["YYYY"],NFLIS_Figure2_Data_Class3["WV"]):
83
        Figure_ax5.text(a, b+0.001, '%s' % b, ha='center', va=
     'bottom',fontsize=11)
84
    # 5个州总的不同类型药物的折线图
    Figure_ax6.plot(NFLIS_Fugure3_Class1_all["YYYY"],NFLIS_Fugure3_Class1_all["
    DrugReports"], label="半合成阿片类药物", linewidth=2)
87
    Figure_ax6.plot(NFLIS_Fugure3_Class2_all["YYYY"],NFLIS_Fugure3_Class2_all["
    DrugReports"], label="合成阿片类药物", linewidth=2)
    Figure_ax6.plot(NFLIS_Fugure3_Class3_all["YYYY"],NFLIS_Fugure3_Class3_all["
    DrugReports"], label="非合成阿片类药物", linewidth=2)
89 | Figure_ax6.set_title("总量")
    Figure_ax6.legend(loc=2)
90
91 | Figure_ax6.grid(axis='x')
92 for a,b in
    zip(NFLIS_Fugure3_Class1_all["YYYY"],NFLIS_Fugure3_Class1_all["DrugReports"
    ]):
93
        Figure_ax6.text(a, b+0.001, '%s' % b, ha='center', va=
    'bottom', fontsize=11)
94
   for a,b in
    zip(NFLIS_Fugure3_Class2_all["YYYY"], NFLIS_Fugure3_Class2_all["DrugReports"
    ]):
        Figure_ax6.text(a, b+0.001, '%s' \% b, ha='center', va=
95
     'bottom',fontsize=11)
96 for a,b in
    zip(NFLIS_Fugure3_Class3_all["YYYY"],NFLIS_Fugure3_Class3_all["DrugReports"
97
        Figure_ax6.text(a, b+0.001, '%s' % b, ha='center', va=
    'bottom',fontsize=11)
98
99 plt.tight_layout()
100 Figure4 = plt.gcf()
```

变量选择

相关系数计算

计算各个年份相关系数

```
1 # 计算2010年相关系数
2 | df_corr_2010 =
    NFLIS_and_ACS_ALL_Out.loc[(NFLIS_and_ACS_ALL_Out["YYYY"]==2010)].corr().rese
    t_index()
3 df_corr_ext_2010 =
    df_corr_2010.loc[(df_corr_2010["index"].str.contains("HC"))]
4 df_corr_ext_2010_part =
    df_corr_ext_2010[["index","DrugReports"]].rename(columns=
    {"DrugReports":"2010年相关系数","index":"变量名"})
5 # 计算2011年相关系数
 6 | df_corr_2011 =
    NFLIS_and_ACS_ALL_Out.loc[(NFLIS_and_ACS_ALL_Out["YYYY"]==2011)].corr().rese
    t_index()
 7 df_corr_ext_2011 =
    df_corr_2011.loc[(df_corr_2011["index"].str.contains("HC"))]
   df_corr_ext_2011_part =
    df_corr_ext_2011[["index","DrugReports"]].rename(columns=
    {"DrugReports":"2011年相关系数","index":"变量名"})
    # 计算2012年相关系数
10 | df_corr_2012 =
    NFLIS_and_ACS_ALL_Out.loc[(NFLIS_and_ACS_ALL_Out["YYYY"]==2012)].corr().rese
    t_index()
11 | df_corr_ext_2012 =
    df_corr_2012.loc[(df_corr_2012["index"].str.contains("HC"))]
12
    df_corr_ext_2012_part =
    df_corr_ext_2012[["index","DrugReports"]].rename(columns=
    {"DrugReports":"2012年相关系数","index":"变量名"})
13
    # 计算2013年相关系数
   df corr 2013 =
    NFLIS_and_ACS_ALL_Out.loc[(NFLIS_and_ACS_ALL_Out["YYYY"]==2013)].corr().rese
    t_index()
15
   df_corr_ext_2013 =
    df_corr_2013.loc[(df_corr_2013["index"].str.contains("HC"))]
16 | df_corr_ext_2013_part =
    df_corr_ext_2013[["index","DrugReports"]].rename(columns=
    {"DrugReports":"2013年相关系数","index":"变量名"})
17
   # 计算2014年相关系数
18 | df_corr_2014 =
    NFLIS_and_ACS_ALL_Out.loc[(NFLIS_and_ACS_ALL_Out["YYYY"]==2014)].corr().rese
    t_index()
19 df_corr_ext_2014 =
    df_corr_2014.loc[(df_corr_2014["index"].str.contains("HC"))]
    df_corr_ext_2014_part =
    df_corr_ext_2014[["index","DrugReports"]].rename(columns=
    {"DrugReports":"2014年相关系数","index":"变量名"})
21
   # 计算2015年相关系数
   df_corr_2015 =
    NFLIS_and_ACS_ALL_Out.loc[(NFLIS_and_ACS_ALL_Out["YYYY"]==2015)].corr().rese
    t_index()
23 df_corr_ext_2015 =
    df_corr_2015.loc[(df_corr_2015["index"].str.contains("HC"))]
24 df_corr_ext_2015_part =
    df_corr_ext_2015[["index","DrugReports"]].rename(columns=
    {"DrugReports":"2015年相关系数","index":"变量名"})
25 # 计算2016年相关系数
```

```
df_corr_2016 =
NFLIS_and_ACS_ALL_Out.loc[(NFLIS_and_ACS_ALL_Out["YYYY"]==2016)].corr().rese
t_index()

df_corr_ext_2016 =
df_corr_2016.loc[(df_corr_2016["index"].str.contains("HC"))]

df_corr_ext_2016_part =
df_corr_ext_2016[["index","DrugReports"]].rename(columns=
{"DrugReports":"2016年相关系数","index":"变量名"})

# 计算全部数据的相关系数

df_corr_all = NFLIS_and_ACS_ALL_Out.corr().reset_index()

df_corr_ext_all = df_corr_all.loc[(df_corr_all["index"].str.contains("HC"))]

df_corr_ext_all_part =
df_corr_ext_all["index","DrugReports"]].rename(columns={"DrugReports":"合计相关系数","index":"变量名"})
```

合并各个年份的相关系数

```
1 # 合并各个年份的相关系数
   df_corr_merge_10_11 =
   pd.merge(df_corr_ext_2010_part,df_corr_ext_2011_part,on="变量名",how="outer")
   df_corr_merge_11_12 =
   pd.merge(df_corr_merge_10_11, df_corr_ext_2012_part, on="变量名", how="outer")
   df_corr_merge_12_13 =
   pd.merge(df_corr_merge_11_12,df_corr_ext_2013_part,on="变量名",how="outer")
   df_corr_merge_13_14 =
   pd.merge(df_corr_merge_12_13,df_corr_ext_2014_part,on="变量名",how="outer")
   df_corr_merge_14_15 =
   pd.merge(df_corr_merge_13_14,df_corr_ext_2015_part,on="变量名",how="outer")
   df_corr_merge_15_16 =
   pd.merge(df_corr_merge_14_15,df_corr_ext_2016_part,on="变量名",how="outer")
   df_corr_merge_all = pd.merge(df_corr_merge_15_16,df_corr_ext_all_part,on="变
   量名",how="outer")
9 # 计算平均数
   df_corr_merge_all["均值"] = df_corr_merge_all[["2010年相关系数","2011年相关系
   数","2012年相关系数",
                                               "2013年相关系数","2014年相关系
11
   数","2015年相关系数","2016年相关系数"]].mean(axis=1)
12 # 排序: 倒序
13 All_Corr = df_corr_merge_all.sort_values(by=["均
    值"],ascending=False).round(4)
```

选择相关系数大于0.5的变量

```
All_Corr_Condi = All_Corr[(abs(All_Corr["2010年相关系数"]) >= 0.5)
                                        & (abs(All_Corr["2011年相关系数"]) >=
   0.5)
3
                                        & (abs(All_Corr["2012年相关系数"]) >=
   0.5)
4
                                        & (abs(All_Corr["2013年相关系数"]) >=
   0.5)
5
                                        & (abs(All_Corr["2014年相关系数"]) >=
   0.5)
                                        & (abs(All_Corr["2015年相关系数"]) >=
6
   0.5)
                                        & (abs(All_Corr["2016年相关系数"]) >=
   0.5)
```

```
& (abs(All_Corr["合计相关系数"]) >=
8
    0.5)
9
                                          & (abs(All_Corr["均值"]) >= 0.5)]
10
   connames = []
11
    for conval in NFLIS_and_ACS_ALL_Out.columns.tolist():
12
       if "HC" not in conval:
13
            connames.append(conval)
14 NFLIS_and_ACS_All_Corr_Condi =
    NFLIS_and_ACS_ALL_Out.ix[:,list(NFLIS_and_ACS_ALL_Out[connames])+list(All_Co
    rr_Condi["变量名"])].dropna()
```

统计推断

归一化

```
data=NFLIS_and_ACS_All_Corr_Condi.ix[:,list(All_Corr_Condi["变量名"])]

NFLIS_and_ACS_All_Condi_Normal_CH = (data - data.mean())/data.std()

# 合并

NFLIS_and_ACS_All_Condi_Normal = pd.concat([NFLIS_and_ACS_All_Corr_Condi.ix[:,list(NFLIS_and_ACS_All_Corr_Condi.icconnames])],

NFLIS_and_ACS_All_Condi_Normal_CH],axis=1)
```

训练集与测试集

```
1 \mid \mathsf{Complex} =
    NFLIS_and_ACS_All_Condi_Normal.ix[NFLIS_and_ACS_All_Condi_Normal["SubstanceC
    lass"] == "合成阿片类药物"]
 2 Non_Complex =
    NFLIS_and_ACS_All_Condi_Normal.ix[NFLIS_and_ACS_All_Condi_Normal["SubstanceC
    lass"] == "非合成阿片类药物"]
    Semi_Complex =
    NFLIS_and_ACS_All_Condi_Normal.ix[NFLIS_and_ACS_All_Condi_Normal["SubstanceC
    lass"] == "半合成阿片类药物"]
4
    Complex_x_train,Complex_x_test,Complex_y_train,Complex_y_test =
 5
    train_test_split(Complex.ix[:,list(All_Corr_Condi["变量名"])],
 6
        Complex.ix[:,"DrugReportsclass"],
 7
        test_size=0.3,
 8
        random_state=1234 )
9
    Non_Complex_x_train, Non_Complex_x_test, Non_Complex_y_train, Non_Complex_y_tes
    t = train_test_split(Non_Complex.ix[:,list(All_Corr_Condi["变量名"])],
10
                        Non_Complex.ix[:,"DrugReportsclass"],
11
                        test_size=0.3,
12
                        random_state=1234 )
    Semi_Complex_x_train,Semi_Complex_x_test,Semi_Complex_y_train,Semi_Complex_y
13
    _test = train_test_split(Semi_Complex.ix[:,list(All_Corr_Condi["变量名"])],
```

KNN

```
Complex_KNN = KNeighborsClassifier()
    Complex_KNN.fit(Complex_x_train,Complex_y_train)
3
    Complex_KNN_Y_Predict = Complex_KNN.predict(Complex_x_test)
    Complex_KNN_train_score = Complex_KNN.score(Complex_x_train,
    Complex_y_train)
    Complex_KNN_test_score = Complex_KNN.score(Complex_x_test, Complex_y_test)
    Non_Complex_KNN = KNeighborsClassifier()
7
    Non_Complex_KNN.fit(Non_Complex_x_train,Non_Complex_y_train)
8
    Non_Complex_KNN_Y_Predict = Non_Complex_KNN.predict(Non_Complex_x_test)
    Non_Complex_KNN_train_score = Non_Complex_KNN.score(Non_Complex_x_train,
    Non_Complex_y_train)
    Non_Complex_KNN_test_score = Complex_KNN.score(Non_Complex_x_test,
10
    Non_Complex_y_test)
    Semi_Complex_KNN = KNeighborsClassifier()
11
    Semi_Complex_KNN.fit(Semi_Complex_x_train,Semi_Complex_y_train)
12
13
    Semi_Complex_KNN_Y_Predict = Semi_Complex_KNN.predict(Semi_Complex_x_test)
14
    Semi_Complex_KNN_train_score = Semi_Complex_KNN.score(Semi_Complex_x_train,
    Semi_Complex_y_train)
    Semi_Complex_KNN_test_score = Semi_Complex_KNN.score(Semi_Complex_x_test,
15
    Semi_Complex_y_test)
```

决策树

```
1 # 决策树
2 Complex_Decision = DecisionTreeClassifier()
3 Complex_Decision.fit(Complex_x_train,Complex_y_train)
    Complex_Decision_Y_Predict = Complex_Decision.predict(Complex_x_test)
    Complex_Decision_train_score = Complex_Decision.score(Complex_x_train,
    Complex_y_train)
    Complex_Decision_test_score = Complex_Decision.score(Complex_x_test,
    Complex_y_test)
    Non_Complex_Decision = DecisionTreeClassifier()
    Non_Complex_Decision.fit(Non_Complex_x_train,Non_Complex_y_train)
    Non_Complex_Decision_Y_Predict =
    Non_Complex_Decision.predict(Non_Complex_x_test)
10
    Non_Complex_Decision_train_score =
    Non_Complex_Decision.score(Non_Complex_x_train, Non_Complex_y_train)
11
    Non_Complex_Decision_test_score = Complex_Decision.score(Non_Complex_x_test,
    Non_Complex_y_test)
12
    Semi_Complex_Decision = DecisionTreeClassifier()
13
    Semi_Complex_Decision.fit(Semi_Complex_x_train,Semi_Complex_y_train)
14
    Semi_Complex_Decision_Y_Predict =
    Semi_Complex_Decision.predict(Semi_Complex_x_test)
    Semi_Complex_Decision_train_score =
    Semi_Complex_Decision.score(Semi_Complex_x_train, Semi_Complex_y_train)
```

```
Semi_Complex_Decision_test_score =
Semi_Complex_Decision.score(Semi_Complex_x_test, Semi_Complex_y_test)
```

随机森林

```
# 随机森林
    Complex_RFC = RandomForestClassifier()
   Complex_RFC.fit(Complex_x_train,Complex_y_train)
 3
    Complex_RFC_Y_Predict = Complex_RFC.predict(Complex_x_test)
    Complex_RFC_train_score = Complex_RFC.score(Complex_x_train,
    Complex_y_train)
    {\tt Complex\_RFC\_test\_score} = {\tt Complex\_RFC.score}({\tt Complex\_x\_test}, \ {\tt Complex\_y\_test})
 6
7
    Non_Complex_RFC = RandomForestClassifier()
8
    Non_Complex_RFC.fit(Non_Complex_x_train,Non_Complex_y_train)
    Non_Complex_RFC_Y_Predict = Non_Complex_RFC.predict(Non_Complex_x_test)
10
    Non_Complex_RFC_train_score = Non_Complex_RFC.score(Non_Complex_x_train,
    Non_Complex_y_train)
    Non_Complex_RFC_test_score = Complex_RFC.score(Non_Complex_x_test,
11
    Non_Complex_y_test)
    Semi_Complex_RFC = RandomForestClassifier()
12
13
    Semi_Complex_RFC.fit(Semi_Complex_x_train,Semi_Complex_y_train)
14
    Semi_Complex_RFC_Y_Predict = Semi_Complex_RFC.predict(Semi_Complex_x_test)
    Semi_Complex_RFC_train_score = Semi_Complex_RFC.score(Semi_Complex_x_train,
15
    Semi_Complex_y_train)
    Semi_Complex_RFC_test_score = Semi_Complex_RFC.score(Semi_Complex_x_test,
    Semi_Complex_y_test)
```

支持向量机

```
1 # SVM
    Complex_SVM = SVC()
    Complex_SVM.fit(Complex_x_train,Complex_y_train)
    Complex_SVM_Y_Predict = Complex_SVM.predict(Complex_x_test)
 5
    Complex_SVM_train_score = Complex_SVM.score(Complex_x_train,
    Complex_y_train)
6
    Complex_SVM_test_score = Complex_SVM.score(Complex_x_test, Complex_y_test)
 7
    Non\_Complex\_SVM = SVC()
    Non_Complex_SVM.fit(Non_Complex_x_train,Non_Complex_y_train)
9
    Non_Complex_SVM_Y_Predict = Non_Complex_SVM.predict(Non_Complex_x_test)
10
    Non_Complex_SVM_train_score = Non_Complex_SVM.score(Non_Complex_x_train,
    Non_Complex_y_train)
    Non_Complex_SVM_test_score = Complex_SVM.score(Non_Complex_x_test,
11
    Non_Complex_y_test)
12
    Semi_Complex_SVM = SVC()
13
    Semi_Complex_SVM.fit(Semi_Complex_x_train,Semi_Complex_y_train)
    Semi_Complex_SVM_Y_Predict = Semi_Complex_SVM.predict(Semi_Complex_x_test)
14
15
    Semi_Complex_SVM_train_score = Semi_Complex_SVM.score(Semi_Complex_x_train,
    Semi_Complex_y_train)
16
    Semi_Complex_SVM_test_score = Semi_Complex_SVM.score(Semi_Complex_x_test,
    Semi_Complex_y_test)
```

神经网络

```
# 神经网络
    Complex_MLP = MLPClassifier(solver='lbfgs', alpha=1e-5, hidden_layer_sizes=
    (5, 5), random_state=1)
    Complex_MLP.fit(Complex_x_train,Complex_y_train)
4
    Complex_MLP_Y_Predict = Complex_MLP.predict(Complex_x_test)
    Complex_MLP_train_score = Complex_MLP.score(Complex_x_train,
    Complex_y_train)
 6
    Complex_MLP_test_score = Complex_MLP.score(Complex_x_test, Complex_y_test)
    Non_Complex_MLP = MLPClassifier(solver='lbfgs', alpha=1e-
 7
    5, hidden_layer_sizes=(5, 5), random_state=1)
8
    Non_Complex_MLP.fit(Non_Complex_x_train,Non_Complex_y_train)
    Non_Complex_MLP_Y_Predict = Non_Complex_MLP.predict(Non_Complex_x_test)
10
    Non_Complex_MLP_train_score = Non_Complex_MLP.score(Non_Complex_x_train,
    Non_Complex_y_train)
    Non_Complex_MLP_test_score = Complex_MLP.score(Non_Complex_x_test,
11
    Non_Complex_y_test)
12
    Semi_Complex_MLP = MLPClassifier(solver='lbfgs', alpha=1e-
    5, hidden_layer_sizes=(5, 5), random_state=1)
13
    Semi_Complex_MLP.fit(Semi_Complex_x_train,Semi_Complex_y_train)
    Semi_Complex_MLP_Y_Predict = Semi_Complex_MLP.predict(Semi_Complex_x_test)
14
15
    Semi_Complex_MLP_train_score = Semi_Complex_MLP.score(Semi_Complex_x_train,
    Semi_Complex_y_train)
    Semi_Complex_MLP_test_score = Semi_Complex_MLP.score(Semi_Complex_x_test,
    Semi_Complex_y_test)
```

线性回归

```
1 # 线性回归
    Complex_LR = LogisticRegression()
    Complex_LR.fit(Complex_x_train,Complex_y_train)
    Complex_LR_Y_Predict = Complex_LR.predict(Complex_x_test)
4
5
    Complex_LR_train_score = Complex_LR.score(Complex_x_train, Complex_y_train)
6
    Complex_LR_test_score = Complex_LR.score(Complex_x_test, Complex_y_test)
7
    Non_Complex_LR = LogisticRegression()
8
    Non_Complex_LR.fit(Non_Complex_x_train,Non_Complex_y_train)
9
    Non_Complex_LR_Y_Predict = Non_Complex_LR.predict(Non_Complex_x_test)
10
    Non_Complex_LR_train_score = Non_Complex_LR.score(Non_Complex_x_train,
    Non_Complex_y_train)
11
    Non_Complex_LR_test_score = Complex_LR.score(Non_Complex_x_test,
    Non_Complex_y_test)
12
    Semi_Complex_LR = LogisticRegression()
13
    Semi_Complex_LR.fit(Semi_Complex_x_train, Semi_Complex_y_train)
    Semi_Complex_LR_Y_Predict = Semi_Complex_LR.predict(Semi_Complex_x_test)
14
15
    Semi_Complex_LR_train_score = Semi_Complex_LR.score(Semi_Complex_x_train,
    Semi_Complex_y_train)
16
    Semi_Complex_LR_test_score = Semi_Complex_LR.score(Semi_Complex_x_test,
    Semi_Complex_y_test)
```

模型评估

特征重要性

特征重要性计算

```
# 非合成类
 1
 2
    Non_Complex_Imp = 100.0*(Non_Complex_RFC.feature_importances_/
                                max(Non_Complex_RFC.feature_importances_))
    Non_Complex_Importance =
    pd.DataFrame(np.array([Non_Complex_x_test.columns,Non_Complex_Imp]).T,
5
                                         columns=["Var","非合成类重要度"])
    Non_Complex_Importance["非合成类重要度"].astype("float")
6
 7
    Non_Complex_Importance_Sort= Non_Complex_Importance.sort_values(by="非合成类重
    要度",ascending=False)
8
    # 合成类
9
    Complex_Imp = 100.0*(Complex_RFC.feature_importances_/
                                max(Complex_RFC.feature_importances_))
10
11
    Complex_Importance =
    pd.DataFrame(np.array([Complex_x_test.columns,Complex_Imp]).T,
12
                                     columns=["Var","合成类重要度"])
    Complex_Importance["合成类重要度"].astype("float")
13
14
    Complex_Importance_Sort= Complex_Importance.sort_values(by="合成类重要
    度",ascending=False)
    # 半合成类
15
16
    Semi_Complex_Imp = 100.0*(Semi_Complex_RFC.feature_importances_/
                                max(Semi_Complex_RFC.feature_importances_))
17
18
    Semi_Complex_Importance =
    pd.DataFrame(np.array([Semi_Complex_x_test.columns,Semi_Complex_Imp]).T,
                                              columns=["Var","半合成类重要度"])
19
20
    Semi_Complex_Importance["半合成类重要度"].astype("float")
    Semi_Complex_Importance_Sort= Semi_Complex_Importance.sort_values(by="半合成
    类重要度",ascending=False)
```

变量名匹配

```
Complex_Importance_Rename = pd.merge(Complex_Importance_Sort,
 2
                                           ACS_All_5YR_DP02_metadata_Dup,
 3
                                           on="Var",how="left")
    Non_Complex_Importance_Rename = pd.merge(Non_Complex_Importance_Sort,
 4
 5
                                           ACS_All_5YR_DP02_metadata_Dup,
                                           on="Var", how="left")
 6
 7
    Semi_Complex_Importance_Rename = pd.merge(Semi_Complex_Importance_Sort,
 8
                                           ACS_All_5YR_DP02_metadata_Dup,
 9
                                           on="Var", how="left")
    All_Importance_Rename = pd.concat([Complex_Importance_Rename,
10
11
                                       Non_Complex_Importance_Rename,
12
                                       Semi_Complex_Importance_Rename],
13
                                     axis=1, join="outer")
```

KFold验证

非合成类

```
strKFold = StratifiedKFold(n_splits=10, shuffle=False, random_state=1234)
 2
    Non_Complex_KNN_Kfold = cross_val_score(Non_Complex_KNN,
 3
                                 Non_Complex.ix[:,list(All_Corr_Condi["变量名"])],
 4
                                 Non_Complex.ix[:,"DrugReportsclass"],
 5
                                 scoring='accuracy',
 6
                                 cv=strKFold)
    Non_Complex_Decision_Kfold = cross_val_score(Non_Complex_Decision,
 8
                                 Non_Complex.ix[:,list(All_Corr_Condi["变量名"])],
                                 Non_Complex.ix[:,"DrugReportsclass"],
 9
10
                                 scoring='accuracy',
11
                                 cv=strKFold)
12
    Non_Complex_RFC_Kfold = cross_val_score(Non_Complex_RFC,
13
                                 Non_Complex.ix[:,list(All_Corr_Condi["变量名"])],
                                 Non_Complex.ix[:,"DrugReportsclass"],
14
15
                                 scoring='accuracy',
                                 cv=strKFold)
16
17
    Non_Complex_SVM_Kfold = cross_val_score(Non_Complex_SVM,
18
                                 Non_Complex.ix[:,list(All_Corr_Condi["变量名"])],
                                 Non_Complex.ix[:,"DrugReportsclass"],
19
20
                                 scoring='accuracy',
21
                                 cv=strKFold)
22
    Non_Complex_MLP_Kfold = cross_val_score(Non_Complex_MLP,
23
                                 Non_Complex.ix[:,list(All_Corr_Condi["变量名"])],
24
                                 Non_Complex.ix[:,"DrugReportsclass"],
25
                                 scoring='accuracy',
26
                                 cv=strKFold)
27
    Non_Complex_LR_Kfold = cross_val_score(Non_Complex_LR,
28
                                 Non_Complex.ix[:,list(All_Corr_Condi["变量名"])],
29
                                 Non_Complex.ix[:,"DrugReportsclass"],
30
                                 scoring='accuracy',
31
                                 cv=strKFold)
```

合成类

```
strKFold = StratifiedKFold(n_splits=10,shuffle=False,random_state=1234)
    Complex_KNN_Kfold = cross_val_score(Complex_KNN,
 2
 3
                                 Complex.ix[:,list(All_Corr_Condi["变量名"])],
4
                                Complex.ix[:,"DrugReportsclass"],
 5
                                 scoring='accuracy',
 6
                                 cv=strKFold)
    Complex_Decision_Kfold = cross_val_score(Complex_Decision,
 7
 8
                                 Complex.ix[:,list(All_Corr_Condi["变量名"])],
9
                                Complex.ix[:,"DrugReportsclass"],
10
                                 scoring='accuracy',
11
                                 cv=strKFold)
12
    Complex_RFC_Kfold = cross_val_score(Complex_RFC,
13
                                 Complex.ix[:,list(All_Corr_Condi["变量名"])],
14
                                Complex.ix[:,"DrugReportsclass"],
15
                                 scoring='accuracy',
16
                                 cv=strKFold)
17
    Complex_SVM_Kfold = cross_val_score(Complex_SVM,
18
                                 Complex.ix[:,list(All_Corr_Condi["变量名"])],
19
                                 Complex.ix[:,"DrugReportsclass"],
20
                                 scoring='accuracy',
```

```
21
                                 cv=strKFold)
22
    Complex_MLP_Kfold = cross_val_score(Complex_MLP,
23
                                 Complex.ix[:,list(All_Corr_Condi["变量名"])],
24
                                 Complex.ix[:,"DrugReportsclass"],
25
                                 scoring='accuracy',
26
                                 cv=strKFold)
27
    Complex_LR_Kfold = cross_val_score(Complex_LR,
                                 Complex.ix[:,list(All_Corr_Condi["变量名"])],
28
29
                                 Complex.ix[:,"DrugReportsclass"],
30
                                 scoring='accuracy',
                                 cv=strKFold)
31
```

半合成类

```
strKFold = StratifiedKFold(n_splits=10,shuffle=False,random_state=1234)
 2
    Semi_Complex_KNN_Kfold = cross_val_score(Semi_Complex_KNN,
 3
                                 Semi_Complex.ix[:,list(All_Corr_Condi["变量
    名"])],
4
                                 Semi_Complex.ix[:,"DrugReportsclass"],
 5
                                 scoring='accuracy',
 6
                                 cv=strKFold)
 7
    Semi_Complex_Decision_Kfold = cross_val_score(Semi_Complex_Decision,
                                 Semi_Complex.ix[:,list(All_Corr_Condi["变量
 8
    名"])],
9
                                 Semi_Complex.ix[:,"DrugReportsclass"],
10
                                 scoring='accuracy',
11
                                 cv=strKFold)
    Semi_Complex_RFC_Kfold = cross_val_score(Semi_Complex_RFC,
12
13
                                 Semi_Complex.ix[:,list(All_Corr_Condi["变量
    名"])],
                                 Semi_Complex.ix[:,"DrugReportsclass"],
14
15
                                 scoring='accuracy',
16
                                 cv=strKFold)
17
    Semi_Complex_SVM_Kfold = cross_val_score(Semi_Complex_SVM,
                                 Semi_Complex.ix[:,list(All_Corr_Condi["变量
18
    名"])],
19
                                 Semi_Complex.ix[:,"DrugReportsclass"],
                                 scoring='accuracy',
20
21
                                 cv=strKFold)
22
    Semi_Complex_MLP_Kfold = cross_val_score(Semi_Complex_MLP,
                                 Semi_Complex.ix[:,list(All_Corr_Condi["变量
23
    名"])],
                                 Semi_Complex.ix[:,"DrugReportsclass"],
24
25
                                 scoring='accuracy',
                                 cv=strKFold)
26
27
    Semi_Complex_LR_Kfold = cross_val_score(Semi_Complex_LR,
28
                                 Semi_Complex.ix[:,list(All_Corr_Condi["变量
    名"])],
29
                                 Semi_Complex.ix[:,"DrugReportsclass"],
                                 scoring='accuracy',
30
31
                                 cv=strKFold)
```

Kfold结果值

非合成类

```
Non_Complex_Kfold_Outdata = pd.DataFrame(np.array([Non_Complex_KNN_Kfold,
2
   Non_Complex_Decision_Kfold,
3
                                                    Non_Complex_RFC_Kfold,
                                                    Non_Complex_SVM_Kfold,
4
5
                                                    Non_Complex_MLP_Kfold,
6
   Non_Complex_LR_Kfold]).T.round(3),
                                           columns=["KNN","决策树","随机森林","支
  持向量机","神经网络","线性回归"])
  Non_Complex_Kfold_Box = Non_Complex_Kfold_Outdata.stack().reset_index()
9 Non_Complex_Kfold_Box = Non_Complex_Kfold_Box.rename(columns={"level_1":"各类
   机器学习算法","0":"Kfold值"})
```

合成类

```
Complex_Kfold_Outdata = pd.DataFrame(np.array([Complex_KNN_Kfold,
1
2
                                                    Complex_Decision_Kfold,
3
                                                    Complex_RFC_Kfold,
4
                                                    Complex_SVM_Kfold,
5
                                                    Complex_MLP_Kfold,
6
  Complex_LR_Kfold]).T.round(3),
                                           columns=["KNN","决策树","随机森林","支
  持向量机","神经网络","线性回归"])
  Complex_Kfold_Box = Complex_Kfold_Outdata.stack().reset_index()
  Complex_Kfold_Box = Complex_Kfold_Box.rename(columns={"level_1":"各类机器学习算
  法","0":"Kfold值"})
```

半合成类

```
1
  Semi_Complex_Kfold_Outdata = pd.DataFrame(np.array([Semi_Complex_KNN_Kfold,
   Semi_Complex_Decision_Kfold,
3
                                                     Semi_Complex_RFC_Kfold,
4
                                                     Semi_Complex_SVM_Kfold,
5
                                                     Semi_Complex_MLP_Kfold,
6
   Semi_Complex_LR_Kfold]).T.round(3),
                                           columns=["KNN","决策树","随机森林","支
7
  持向量机","神经网络","线性回归"])
  Semi_Complex_Kfold_Box = Semi_Complex_Kfold_Outdata.stack().reset_index()
  Semi_Complex_Kfold_Box = Semi_Complex_Kfold_Box.rename(columns={"level_1":"各
   类机器学习算法","0":"Kfold值"})
```

Kfold箱式图

```
f, (Complex_Box1, Non_Complex_Box2, Semi_Complex_Box3) =
    plt.subplots(nrows=3, figsize=(15,15))
2
 3
    sns.boxplot(x = "各类机器学习算法", y = Complex_Kfold_Box.ix[:,-1],
4
                data=Complex_Kfold_Box,ax=Complex_Box1)
 5
    Complex_Box1.set_xlabel('')
6
    Complex_Box1.set_ylabel('合成类')
 7
    sns.boxplot(x = "各类机器学习算法", y = Non_Complex_Kfold_Box.ix[:,-1],
8
9
                data=Non_Complex_Kfold_Box,ax=Non_Complex_Box2)
10
    Non_Complex_Box2.set_xlabel('')
    Non_Complex_Box2.set_ylabel('非合成类')
11
12
13
    sns.boxplot(x = "各类机器学习算法", y = Semi_Complex_Kfold_Box.ix[:,-1],
                data=Semi_Complex_Kfold_Box,ax=Semi_Complex_Box3)
14
15
    Semi_Complex_Box3.set_xlabel('')
    Semi_Complex_Box3.set_ylabel('半合成类')
16
17
18
    plt.tight_layout()
   All_Box = plt.gcf()
19
```

导出结果

数据清洗结果

```
# 整理后的ACS_ALL
   ACS_ALL_5YR_DP02.to_csv(file_path("02_output","ACS_ALL_5YR_DP02.csv"),encodi
   ng="utf-8-sig")
   # 整理后的MCM_NFLIS
   MCM_NFLIS_Class_Clear.to_csv(file_path("02_output","MCM_NFLIS_Class_Clear.cs
   v"), encoding="utf-8-sig")
   # 整理后的ACS_A11_5YR_DP02_metadata
   ACS_All_5YR_DP02_metadata_Dup.to_csv(file_path("02_output","ACS_All_5YR_DP02
    _metadata_Dup.csv"),encoding="utf-8-sig")
7
   # 按照三类药物数据合并
   NFLIS_and_ACS_ALL_Out.to_csv(file_path("02_output", "NFLIS_and_ACS_ALL_Out.cs
   v"), encoding="utf-8-sig")
   # 相关系数大于0.5的变量
9
   All_Corr_Condi.to_csv(file_path("02_output","All_Corr_Condi.csv"),encoding="
10
   utf-8-sig")
   # 相关系数大于0.5的变量的社会经济数据表
11
   NFLIS_and_ACS_All_Corr_Condi.to_csv(file_path("02_output","NFLIS_and_ACS_All
   _Corr_Condi.csv"),encoding="utf-8-sig")
   # 归一化后相关系数大于0.5的变量的社会经济数据表
13
14
   NFLIS_and_ACS_All_Condi_Normal.to_csv(file_path("02_output","NFLIS_and_ACS_A
   11_Condi_Normal.csv"),encoding="utf-8-sig")
```

统计描述结果

```
NFLIS_Figure2_Data_Class1.to_csv(file_path("02_output","NFLIS_Figure2_Data_Class1.csv"), encoding="utf-8-sig")
NFLIS_Figure2_Data_Class2.to_csv(file_path("02_output","NFLIS_Figure2_Data_Class2.csv"), encoding="utf-8-sig")
NFLIS_Figure2_Data_Class3.to_csv(file_path("02_output","NFLIS_Figure2_Data_Class3.csv"), encoding="utf-8-sig")

Figure1.savefig(file_path("02_output","Figure1_Pie.jpg"), dpi=500)
Figure2.savefig(file_path("02_output","Figure2_Bar.jpg"), dpi=500)
Figure3.savefig(file_path("02_output","Figure3_HeatMap.jpg"), dpi=500)
Figure4.savefig(file_path("02_output","Figure4_Plot.jpg"), dpi=500)
```

模型评估结果

5

```
1 # Kfold箱式图
2 All_Box.savefig(file_path("02_output","All_Box.jpg"),dpi=500)
3 # 三类药物特征重要度
4 All_Importance_Rename.to_csv(file_path("02_output","All_Importance_Rename.csv
"),encoding="utf-8-sig")
5 # K折验证
6 Complex_Kfold_Outdata.to_csv(file_path("02_output","Complex_Kfold_Outdata.csv
"),encoding="utf-8-sig")
7 Semi_Complex_Kfold_Outdata.to_csv(file_path("02_output","Semi_Complex_Kfold_O
utdata.csv"),encoding="utf-8-sig")
8 Non_Complex_Kfold_Outdata.to_csv(file_path("02_output","Non_Complex_Kfold_Out
data.csv"),encoding="utf-8-sig")
```

模型的混淆矩阵

```
1
   print('KNN合成类混淆矩阵为:', confusion_matrix(Complex_y_test,
   Complex_KNN_Y_Predict), sep='\n')
   print('KNN半合成类混淆矩阵为: ', confusion_matrix(Semi_Complex_y_test,
   Semi_Complex_KNN_Y_Predict), sep='\n')
   print('KNN非合成类混淆矩阵为: ', confusion_matrix(Non_Complex_y_test,
   Non_Complex_KNN_Y_Predict), sep='\n')
 6
   print('Decision合成类混淆矩阵为: ', confusion_matrix(Complex_y_test,
   Complex_Decision_Y_Predict), sep='\n')
7
   print('Decision半合成类混淆矩阵为: ', confusion_matrix(Semi_Complex_y_test,
   Semi_Complex_Decision_Y_Predict), sep='\n')
    print('Decision非合成类混淆矩阵为: ', confusion_matrix(Non_Complex_y_test,
   Non_Complex_Decision_Y_Predict), sep='\n')
9
10
   print('RFC合成类混淆矩阵为: ', confusion_matrix(Complex_y_test,
   Complex_RFC_Y_Predict), sep='\n')
   print('RFC半合成类混淆矩阵为: ', confusion_matrix(Semi_Complex_y_test,
   Semi_Complex_RFC_Y_Predict), sep='\n')
   print('RFC非合成类混淆矩阵为:', confusion_matrix(Non_Complex_y_test,
12
   Non_Complex_RFC_Y_Predict), sep='\n')
13
```

```
print('SVM合成类混淆矩阵为: ', confusion_matrix(Complex_y_test,
   Complex_SVM_Y_Predict), sep='\n')
   print('SVM半合成类混淆矩阵为: ', confusion_matrix(Semi_Complex_y_test,
15
   Semi_Complex_SVM_Y_Predict), sep='\n')
16
   print('SVM非合成类混淆矩阵为:', confusion_matrix(Non_Complex_y_test,
   Non_Complex_SVM_Y_Predict), sep='\n')
17
18
   print('MLP合成类混淆矩阵为:', confusion_matrix(Complex_y_test,
   Complex_MLP_Y_Predict), sep='\n')
19
    print('MLP半合成类混淆矩阵为:', confusion_matrix(Semi_Complex_y_test,
   Semi_Complex_MLP_Y_Predict), sep='\n')
20
   print('MLP非合成类混淆矩阵为: ', confusion_matrix(Non_Complex_y_test,
   Non_Complex_MLP_Y_Predict), sep='\n')
21
   print('LR合成类混淆矩阵为: ', confusion_matrix(Complex_y_test,
   Complex_LR_Y_Predict(), sep='\n')
   print('LR半合成类混淆矩阵为: ', confusion_matrix(Semi_Complex_y_test,
    Semi_Complex_LR_Y_Predict), sep='\n')
   print('LR非合成类混淆矩阵为: ', confusion_matrix(Non_Complex_y_test,
   Non_Complex_LR_Y_Predict), sep='\n')
25
```

模型的评估报告

```
print("最近邻法合成阿片类:")
   print(classification_report(Complex_KNN_Y_Predict,Complex_y_test))
   print("最近邻法非合成阿片类:")
   print(classification_report(Non_Complex_KNN_Y_Predict,Non_Complex_y_test))
   print("最近邻法半合成阿片类:")
6
   print(classification_report(Semi_Complex_KNN_Y_Predict,Semi_Complex_y_test))
8
   print("决策树合成阿片类:")
9
   print(classification_report(Complex_Decision_Y_Predict,Complex_y_test))
   print("决策树非合成阿片类:")
10
11
   print(classification_report(Non_Complex_Decision_Y_Predict,Non_Complex_y_tes
   t))
12
   print("决策树半合成阿片类:")
   print(classification_report(Semi_Complex_Decision_Y_Predict,Semi_Complex_y_t
13
   est))
14
   print("随机森林合成阿片类:")
15
   print(classification_report(Complex_RFC_Y_Predict,Complex_y_test))
16
17
   print("随机森林非合成阿片类:")
18
   print(classification_report(Non_Complex_RFC_Y_Predict, Non_Complex_y_test))
   print("随机森林半合成阿片类:")
19
20
   print(classification_report(Semi_Complex_RFC_Y_Predict,Semi_Complex_y_test))
21
22
   print("支持向量机合成阿片类:")
23
   print(classification_report(Complex_SVM_Y_Predict,Complex_y_test))
24
   print("支持向量机非合成阿片类:")
25
   print(classification_report(Non_Complex_SVM_Y_Predict,Non_Complex_y_test))
26
   print("支持向量机半合成阿片类:")
27
   print(classification_report(Semi_Complex_SVM_Y_Predict,Semi_Complex_y_test))
28
29
   print("神经网络合成阿片类:")
   \label{eq:print} {\tt print}({\tt classification\_report}({\tt Complex\_MLP\_Y\_Predict}, {\tt Complex\_y\_test}))
30
31 print("神经网络非合成阿片类:")
```

```
32
   print(classification_report(Non_Complex_MLP_Y_Predict,Non_Complex_y_test))
33
   print("神经网络半合成阿片类:")
   print(classification_report(Semi_Complex_MLP_Y_Predict,Semi_Complex_y_test))
34
35
   print("线性回归合成阿片类:")
36
   print(classification_report(Complex_LR_Y_Predict,Complex_y_test))
37
   print("线性回归非合成阿片类:")
38
39
   print(classification_report(Non_Complex_LR_Y_Predict,Non_Complex_y_test))
40 print("线性回归半合成阿片类:")
41
   print(classification_report(Semi_Complex_LR_Y_Predict,Semi_Complex_y_test))
42
```