

1. Illustrate:

这是崔连山和小伙伴们的机器学习拓展包，代有浓厚的社会主义开源分享精神，极富创造力和战斗力。在这里让我们为他们鼓掌 🙌

1.1 Spend

测试集数据位置: {Example}

配置如下:

	Windows	Windows	MacOS	Linux
型号	i7-9750H	i7-9750H	M1	E5-2640 V4
核心	6核心12线程	6核心12线程	8核心	20核心40线程
频率	2.67GHz	3.2GHz		2.40GHz

运行速度对比结果如下:

未集成	Windows1	Windows2	MacOS	Linux
ALL_FUNCTION	47.364	43.681	34.013	27.282
binary_ROC()	45.809	42.964	32.751	32.143
auto_model()	53.498	48.649	38.267	40.794
estimator_violion()	1.191	1.021	1.678	2.395

集成	Windows1	Windows2	MacOS	Linux
binary_ROC()	46.2 s	43.2 s	CPU times: user 4.82 s, sys: 365 ms, total: 5.18 s Wall time: 32.9s	CPU times: user 9.59 s, sys: 3.89 s, total: 13.5 s Wall time: 33.3 s
auto_model()	50.4 s	47.1 s	CPU times: user 9.75 s, sys: 247 ms, total: 10 s Wall time: 38.1 s	CPU times: user 15.1 s, sys: 1.68 s, total: 16.8 s Wall time: 41.1 s
estimator_violion()	1.16 s	Wall time: 1.01 s	CPU times: user 2.02 s, sys: 70.1 ms, total: 2.09 s Wall time: 1.69 s	CPU times: user 3.85 s, sys: 2.32 s, total: 6.17 s Wall time: 2.23 s

1.2 Request_install

可以参考学习当前目录下的环境备份：Auto_ML_C.yaml

主要是涉及到的软件如下：

Package	最低版本——待检测
python=3.8.10	
seaborn=0.11.2	
pandas=1.3.3	
matplotlib=3.4.2	
numpy=1.20.3	

2. Content:

该包是基于Sklearn，imblance等机器学习拓展包之上的Package，共计划分为两个部分，

- 分类任务
 1. binary_classification.py内部可用函数如下

函数名	功能	返回值
cal_add_1(num1,num2)👉	简单的欢迎函数	num1,num2
LogisticRegressionCV_mdoel(X, Y,cv)		
SGDClassifier_model(X,Y,cv)		
LinearDiscriminantAnalysis_model(X, Y,cv)		
LinearSVC_model(X, Y,cv)		
SVC_model(X, Y,cv)		
DecisionTreeClassifier_model(X,Y,cv)		
AdaBoostClassifier_model(X,Y,cv)		
BaggingClassifier_model(X, Y,cv)		
GradientBoostingClassifier_model(X, Y,cv)		
RandomForestClassifier_model(X, Y,cv)		
KNeighborsClassifier_model(X, Y,cv)		
BernoulliNB_model(X, Y,cv)		
GaussianNB_model(X,Y,cv)		
下面是总函数		
binary_ROC(X,Y,k,fig_name)	绘制标量超参数搜索下最佳的ROC	fig
auto_model(X, Y, k)	模型的标量超参数搜索结果	Auc_data, Acc_data, Recall_data, Precision_data
estimator_violion(df1,df2,fig_name)	为auto_model结果的Dataframe绘制小提琴图	fig

2. 多分类函数

等待

3. 特征筛选函数Feature_struction

4. waited

3. How to Use

3.1 Installation

```
1 # Method 1
2 # Create a new environment, here is conda as an example
3 conda create --name Auto_ML_C python=3.8.10
4
5 # Activate the newly created environment
6 conda activate Auto_ML_C
7
8 # Installation package
9 pip install Auto_ML_C==0.0.11
10 pip install imblearn
11
12 # Suggest the pipeline of Jupyter notebook [optional, recommended]
13 conda install jupyter notebook
14 conda install ipykernel
15 python -m ipykernel install --user --name Auto_ML_C --display-name
    "Auto_ML_C"
16 # Install sklearn 0.6. this will fixed next version
17 conda install -c conda-forge sklearn-contrib-lightning
18
19 # Method2
20 # Use the yaml environment file on the GitHub homepage to directly copy the
    current environment
21 conda env create -n Auto_ML_C -f Auto_ML_C.yaml
22
23 # Activate the newly created environment
24 conda activate
25
26 # Suggest the pipeline of Jupyter notebook [optional, recommended]
27 conda install jupyter notebook
28 conda install ipykernel
29 python -m ipykernel install --user --name Auto_ML_C --display-name
    "Auto_ML_C"
```

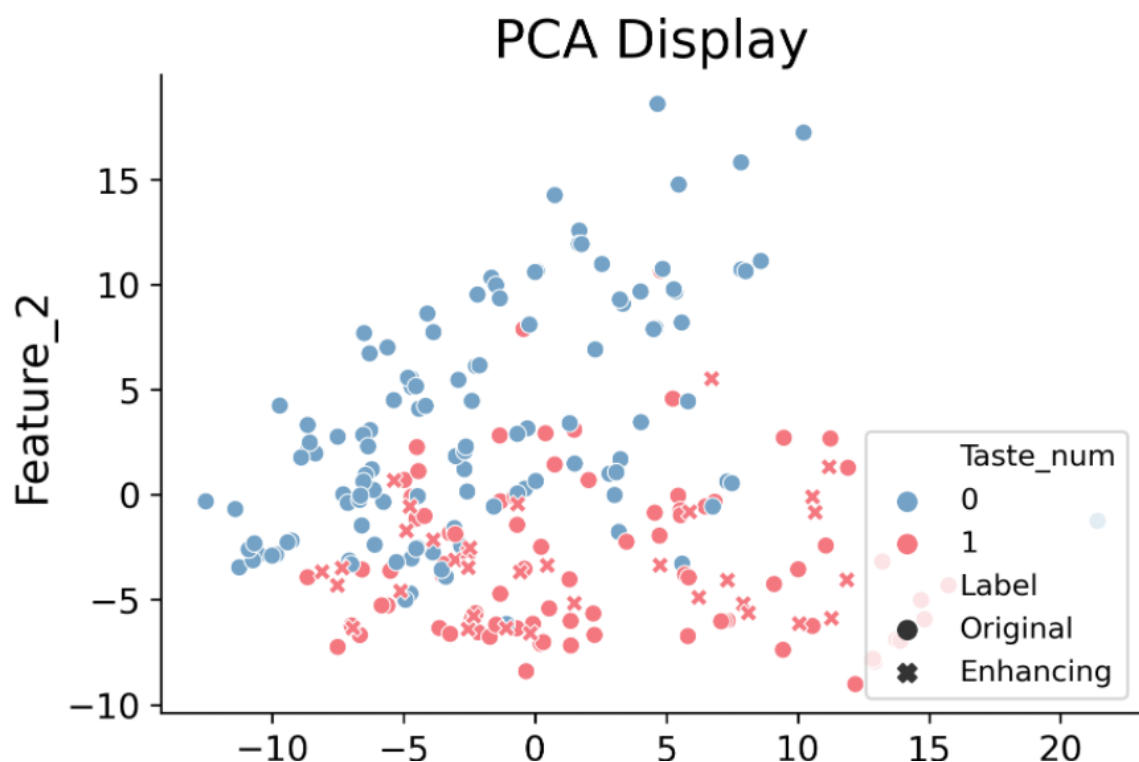
3.2 Feature_struction

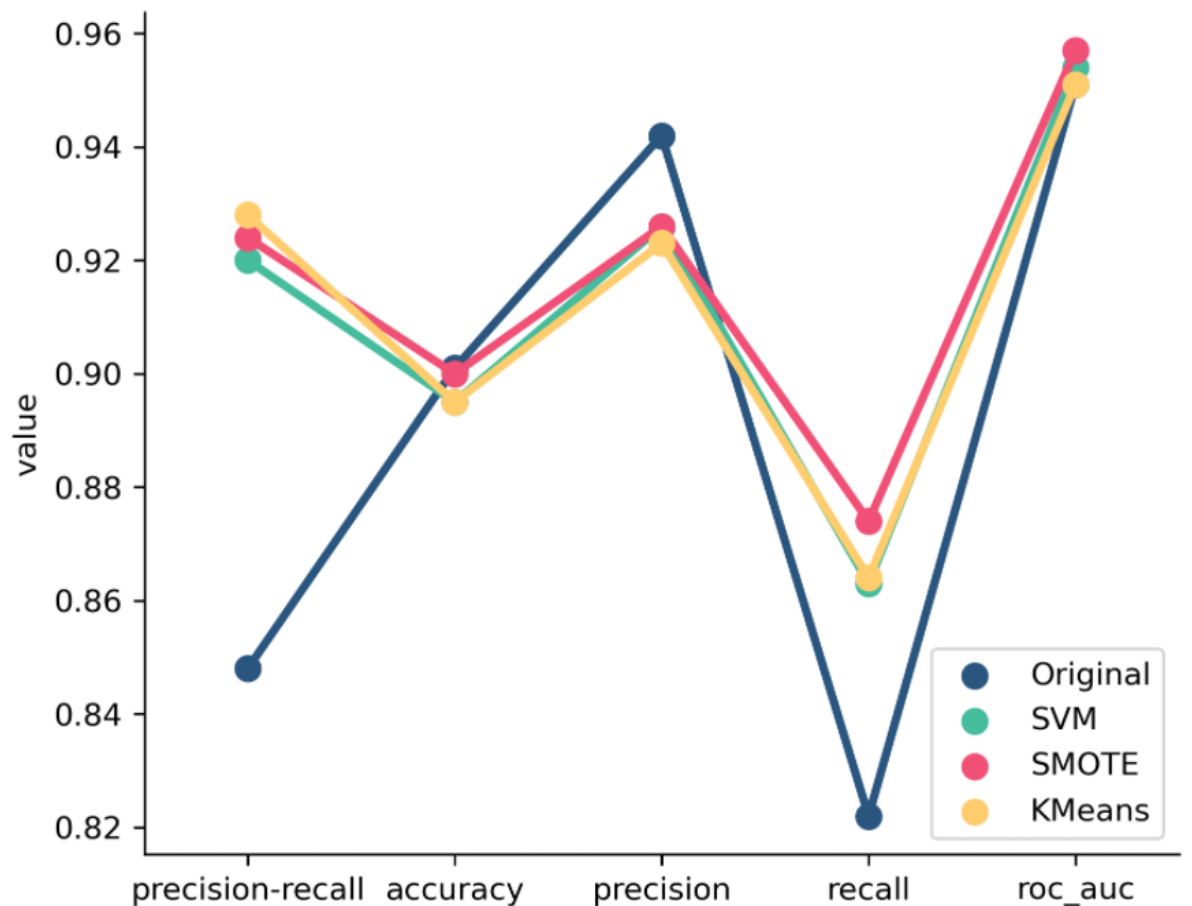
```
1 import auto_ml_c.Feature_structure as fs
2 import pandas as pd
3 df = pd.read_csv("1_23肽全部的构效数据.csv")
4 x = df.iloc[:,2:]
5 Y = df[["Taste"]]
6 Y["Taste_num"] = 10
7 for i in range(Y.shape[0]):
8     if Y["Taste"].iloc[i] == "Umami":
9         Y["Taste_num"].iloc[i] = 1
10    elif Y["Taste"].iloc[i] == "Bitter":
11        Y["Taste_num"].iloc[i] = 0
12
13 # Function 1: Use a variety of visualization methods to reduce
    dimensionality to visualize the data to be enhanced
```

```

14 # 函数1: 采用多种可视化方法进行降维可视化待增强数据
15 location = ""
16 tmp = fs.data_enhance_show(X,Y[["Taste_num"]],location,kind="SMOTE")
17 tmp
18
19 # Function 2: Using multiple indicators to evaluate the results of different
    enhancement methods
20 # 函数2: 采用多指标评价不同增强方法后的结果
21 tmp1 = fs.data_enhance(X.iloc[:, :-1],Y[["Taste_num"]])
22 tmp1
23
24 # Function 3: Visualize the return result of function 2
25 # 函数3: 可视化函数2的返回结果
26 location = ""
27 name="Test"
28 tmp2 = fs.data_enhance_compare(tmp1,location,name)
29 tmp2

```



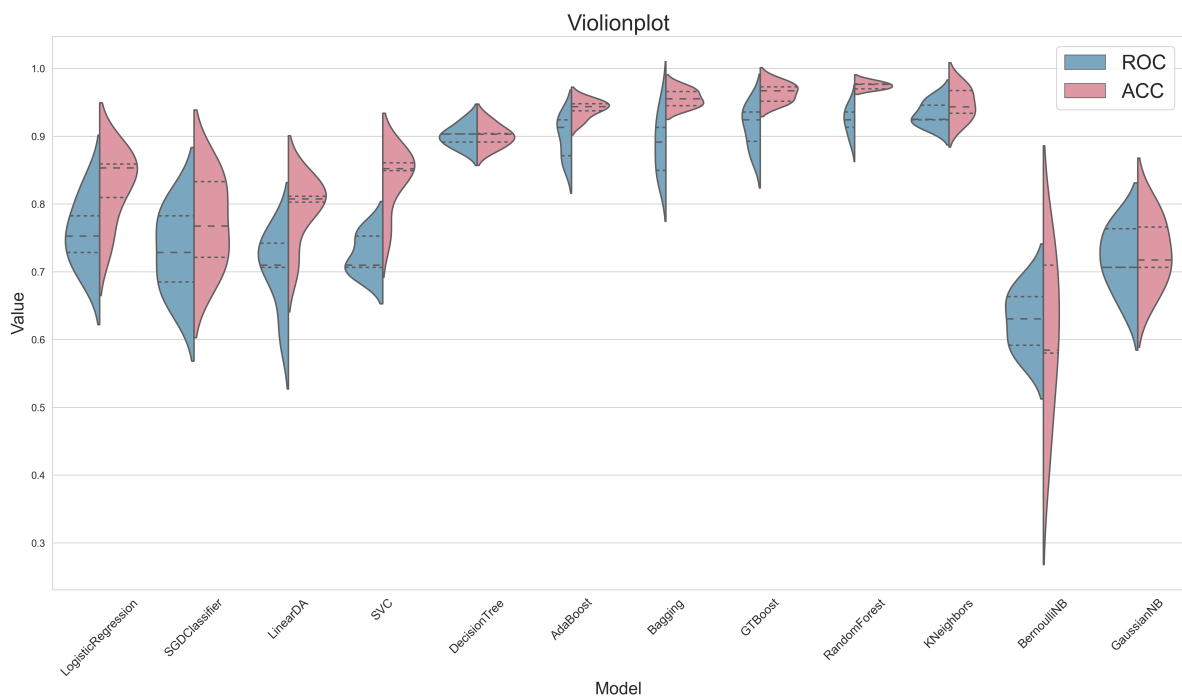
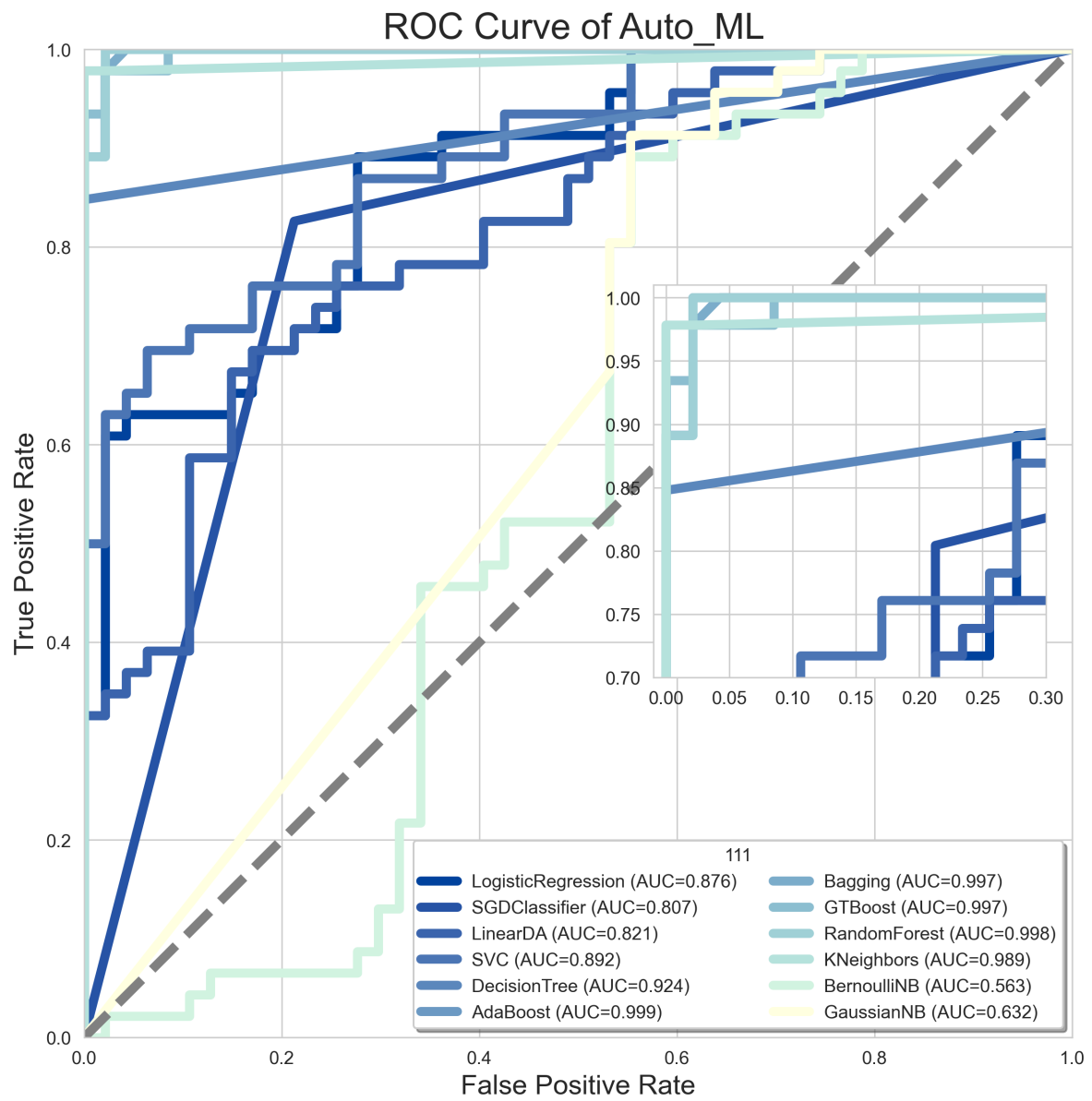


3.3 Binary Classification

```

1  # Here is an example of the function binary_classification_ws
2  # 这里以函数binary_classification_ws举例
3
4  # 开始加载环境
5  import pandas as pd
6  import numpy as np
7  import auto_ml_c.binary_classification as abc
8
9  # 读取测试数据
10 df = pd.read_csv("2_data_deal_smote.csv")
11 x = df.iloc[:, :-1]
12 y = df["label"]
13 score = 'accuracy'
14
15 # The first function, draw ROC image
16 tmp_a = abc.binary_ROC(X, Y, cv, "111", "accuracy")
17
18 # The second function, get Auc_data, Acc_data, Recall_data, Precision_data
19 tmp_b1, tmp_b2, tmp_b3, tmp_b4 = abc.auto_model(X, Y, cv, "accuracy")
20
21 # The third function, draw the evaluation graph obtained by function 2
22 auto_model
23 tmp_c = abc.estimator_violion(tmp_b1, tmp_b2, "violationplot")

```



4. ConTact

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