Python 数据科学 *速查表*
Scikit-learn

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Scikit-learn 是开源的 Python 库，通过统一的界面实现机器学习、预处理、交叉验证及可视化算法。

简例

```
>>> from sklearn import neighbors, datasets, preprocessing
>>> from sklearn.model_selection import train_test_split
>>> from sklearn.metrics import accuracy_score
>>> iris = datasets.load_iris()
>>> X, y = iris.data[:, :2], iris.target
>>> X_train, X_test, y_train, y_test= train_test_split(X, y, random_state=33)
>>> scaler = preprocessing.StandardScaler().fit(X_train)
>>> X_train = scaler.transform(X_train)
>>> X_test = scaler.transform(X_test)
>>> knn = neighbors.KNeighborsClassifier(n_neighbors=5)
>>> knn.fit(X_train, y_train)
>>> y_pred = knn.predict(X_test)
>>> accuracy_score(y_test, y_pred)
```

加载数据

参阅 NumPy 与 Pandas

Scikit-learn 处理的数据是存储为 NumPy 数组或 SciPy 稀疏矩阵的数字，还支持 Pandas 数据框等可转换为数字数组的其它数据类型。

```
>>> import numpy as np
>>> X = np.random.random((10,5))
>>> y = np.array(['M','M','F','F','M','F','M','M','F','F','F'])
>>> X[X < 0.7] = 0
```

训练集与测试集数据

```
>>> from sklearn.model_selection import train_test_split
>>> X_train, X_test, y_train, y_test = train_test_split(X,
                                                        y,
                                                        random_state=0)
```

数据预处理

标准化

```
>>> from sklearn.preprocessing import StandardScaler
>>> scaler = StandardScaler().fit(X_train)
>>> standardized_X = scaler.transform(X_train)
>>> standardized_X_test = scaler.transform(X_test)
```

归一化

```
>>> from sklearn.preprocessing import Normalizer
>>> scaler = Normalizer().fit(X_train)
>>> normalized_X = scaler.transform(X_train)
>>> normalized_X_test = scaler.transform(X_test)
```

二值化

```
>>> from sklearn.preprocessing import Binarizer
>>> binarizer = Binarizer(threshold=0.0).fit(X)
>>> binary_X = binarizer.transform(X)
```

编码分类特征

```
>>> from sklearn.preprocessing import LabelEncoder
>>> enc = LabelEncoder()
>>> y = enc.fit_transform(y)
```

输入缺失值

```
>>> from sklearn.preprocessing import Imputer
>>> imp = Imputer(missing_values=0, strategy='mean', axis=0)
>>> imp.fit_transform(X_train)
```

生成多项式特征

```
>>> from sklearn.preprocessing import PolynomialFeatures
>>> poly = PolynomialFeatures(5)
>>> poly.fit_transform(X)
```

创建模型

有监督学习评估器

线性回归

```
>>> from sklearn.linear_model import LinearRegression
>>> lr = LinearRegression(normalize=True)
```

支持向量机(SVM)

```
>>> from sklearn.svm import SVC
>>> svc = SVC(kernel='linear')
```

朴素贝叶斯

```
>>> from sklearn.naive_bayes import GaussianNB
>>> gnb = GaussianNB()
```

KNN

```
>>> from sklearn import neighbors
>>> knn = neighbors.KNeighborsClassifier(n_neighbors=5)
```

无监督学习评估器

主成分分析(PCA)

```
>>> from sklearn.decomposition import PCA
>>> pca = PCA(n_components=0.95)
```

K Means

```
>>> from sklearn.cluster import KMeans
>>> k_means = KMeans(n_clusters=3, random_state=0)
```

模型拟合

有监督学习

```
>>> lr.fit(X, y)                          拟合数据与模型
>>> knn.fit(X_train, y_train)
>>> svc.fit(X_train, y_train)
```

无监督学习

```
>>> k_means.fit(X_train)                  拟合数据与模型
>>> pca_model = pca.fit_transform(X_train) 拟合并转换数据
```

预测

有监督评估器

```
>>> y_pred = svc.predict(np.random.random((2,5)))   预测标签
>>> y_pred = lr.predict(X_test)                     预测标签
>>> y_pred = knn.predict_proba(X_test)              评估标签概率
```

无监督评估器

```
>>> y_pred = k_means.predict(X_test)      预测聚类算法里的标签
```

评估模型性能

分类指标

准确率

```
>>> knn.score(X_test, y_test)                          评估器评分法
>>> from sklearn.metrics import accuracy_score         指标评分函数
>>> accuracy_score(y_test, y_pred)
```

分类预估评价函数

```
>>> from sklearn.metrics import classification_report  精确度、召回率、F1
>>> print(classification_report(y_test, y_pred))       分数及支持率
```

混淆矩阵

```
>>> from sklearn.metrics import confusion_matrix
>>> print(confusion_matrix(y_test, y_pred))
```

回归指标

平均绝对误差

```
>>> from sklearn.metrics import
mean_absolute_error >>> y_true = [3, -0.5, 2]
>>> mean_absolute_error(y_true, y_pred)
```

均方误差

```
>>> from sklearn.metrics import mean_squared_error
>>> mean_squared_error(y_test, y_pred)
```

R^2 评分

```
>>> from sklearn.metrics import r2_score
>>> r2_score(y_true, y_pred)
```

群集指标

调整兰德系数

```
>>> from sklearn.metrics import adjusted_rand_score
>>> adjusted_rand_score(y_true, y_pred)
```

同质性

```
>>> from sklearn.metrics import homogeneity_score
>>> homogeneity_score(y_true, y_pred)
```

V-measure

```
>>> from sklearn.metrics import v_measure_score
>>> metrics.v_measure_score(y_true, y_pred)
```

交叉验证

```
>>> from sklearn.cross_validation import cross_val_score
>>> print(cross_val_score(knn, X_train, y_train, cv=4))
>>> print(cross_val_score(lr, X, y, cv=2))
```

模型调整

栅格搜索

```
>>> from sklearn.grid_search import GridSearchCV
>>> params = {"n_neighbors": np.arange(1,3),
              "metric": ["euclidean", "cityblock"]}
>>> grid = GridSearchCV(estimator=knn,
                        param_grid=params)
>>> grid.fit(X_train, y_train)
>>> print(grid.best_score_)
>>> print(grid.best_estimator_.n_neighbors)
```

随机参数优化

```
>>> from sklearn.grid_search import RandomizedSearchCV
>>> params = {"n_neighbors": range(1,5),
              "weights": ["uniform", "distance"]}
>>> rsearch = RandomizedSearchCV(estimator=knn,
                                 param_distributions=params,
                                 cv=4,
                                 n_iter=8,
                                 random_state=5)
>>> rsearch.fit(X_train, y_train)
>>> print(rsearch.best_score_)
```