



# Python 数据科学 速查表

## Scikit-learn

### Scikit-learn

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', '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)
```

### 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)
>>> knn.fit(X_train, y_train)
>>> svc.fit(X_train, y_train)
```

拟合数据与模型

#### 无监督学习

```
>>> k_means.fit(X_train)
>>> pca_model = pca.fit_transform(X_train)
```

拟合数据与模型  
拟合并转换数据

### 预测

#### 有监督评估器

```
>>> y_pred = svc.predict(np.random.random((2,5)))
>>> y_pred = lr.predict(X_test)
>>> y_pred = knn.predict_proba(X_test)
```

预测标签  
预测标签  
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)
>>> from sklearn.metrics import accuracy_score
>>> accuracy_score(y_test, y_pred)

分类预估评价函数
>>> from sklearn.metrics import classification_report
>>> print(classification_report(y_test, y_pred))

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

评估器评分法  
指标评分函数

精确度、召回率、F1  
分数及支持率

#### 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)

R² 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(1,5),
            "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_)
```

### 数据预处理

#### 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)
```

原作者

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