- K近邻算法
- 1. Sklearn中的使用

```
from sklearn.neighbors import KNeighborsClassifier
from sklearn.model_selection import train_test_split
from sklearn.metrics import accuracy_score
from sklearn import datasets
iris = datasets.load_iris()
X = iris.data
y = iris.target
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=666, test_size=0.2)
knn_clf = KNeighborsClassifier(n_neighbors=5)
knn_clf.fit(X_train, y_train)
y_predict = knn_clf.predict(X_test)
knn_clf.score(X_test, y_test)
accuracy_score(y_test, y_predict)
```

2. 网格搜索与超参数

3. 数据归一化

```
最值归一化: 把所有数据映射到0-1之间
```

 $x_{scale} = rac{x - x_{min}}{x_{max} - x_{min}}$ (适用于分布有明显边界的情况)

均值方差归一化:将数据归一到均值为0方差为1的分布中

 $x_{scale} = \frac{x - x_{mean}}{e}$ (适用于数据分布没有明显的边界,有可能存在极端数据值)

注意: 对测试数据集进行归一化 $\frac{(x_{test}-mean_train)}{std_train}$

```
from sklearn.preprocessing import StandardScaler
standardScaler = StandardScaler()
standardScaler.fit(X_train)
standardScaler.mean_
standardScaler.scale_
X_train = standardScaler.transform(X_train)
X_test_standard = standardScaler.transform(X_test)
```

4. 总结

计算量大, m个样本, n个特征, 预测每一个新的数据, 需要O(m*n)

高度数据相关

预测结果不具有可解释性

• 线性回归算法

简单线性回归

- 1. 目标: 找到a和b,使得 $J(a,b) = \sum_{i=1}^m (y^{(i)} ax^{(i)} b)^2$ 尽可能小
- 2. 推导过程

$$\frac{\partial(a,b)}{\partial b} = 0, \frac{\partial(a,b)}{\partial a} = 0$$

$$a = rac{\sum_{i=1}^m (x^{(i)} - \overline{x})(y^{(i)} - \overline{y})}{\sum_{i=1}^m (x^{(i)} - \overline{x})^2}$$

$$b = \overline{y} - a\overline{x}$$

3. 向量化

$$\sum_{i=1}^{m} w^{(i)} \cdot v^{(i)}$$

$$w=(w^{(1)},w^{(2)},\cdots,w^{(m)})$$

$$v = (v^{(1)}, v^{(2)}, \cdots, v^{(m)})$$

$$\label{eq:alpha} a = (x_train-x_mean).dot(y_train_y_mean) / (x_train-x_mean).dot(x_train-x_mean)\\ b = y_mean - a * x_mean$$

4. 评价

MSE(均方误差)
$$\frac{1}{m}\sum_{i=1}^m(y_{test}^{(i)}-\hat{y}_{test}^{(i)})^2$$

RMSE(均方根误差)
$$\sqrt{\frac{1}{m}\sum_{i=1}^m(y_{test}^{(i)}-\hat{y}_{test}^{(i)})^2}$$

MAE(平均绝对误差) $\frac{1}{m}\sum_{i=1}^{m}|y_{test}^{(i)}-\hat{y}_{test}^{(i)}|$

$$R^2 = 1 - rac{\sum_i (\hat{y}^{(i)} - y^{(i)})^2}{\sum_i (ar{y} - y^{(i)})^2} = 1 - rac{\sum_i (\hat{y}^{(i)} - y^{(i)})^2/m}{\sum_i (ar{y} - y^{(i)})^2/m} = 1 - rac{MSE(\hat{y}, y)}{Var(y)}$$

 $R^2 \leq 1$,越大越好。当 $R^2 < 0$ 时,说明学习到的模型还不如基准模型,可能数据不存在线性关系。

5. Sklearn中的使用

多元线性回归

1. 公式

$$y = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_n x_n$$

$$\hat{y}^{(i)} = \theta_0 + \theta_1 X_1^{(i)} + \dots + \theta_n X_n^{(i)}$$

$$\theta = (\theta_0, \theta_1, \cdots, \theta_n)^T$$

$$X^{(i)} = (X_0^{(i)}, X_1^{(i)}, \cdots, X_n^{(i)}), X_0^{(i)} \equiv 1$$

$$\hat{y}^{(i)} = X^{(i)} \cdot \theta$$

$$X_b = \left(egin{array}{cccc} 1 & X_1^{(1)} & \cdots & X_n^{(1)} \ 1 & X_1^{(2)} & \cdots & X_n^{(2)} \ \cdots & & & & \ 1 & X_1^{(m)} & \cdots & X_n^{(m)} \end{array}
ight)$$

$$\hat{y} = X_b \cdot \theta$$

2. 目标: $\sum_{i=1}^{m} (y^{(i)} - \hat{y}^{(i)})^2$ 尽可能小

即使得 $(y - X_b \cdot \theta)^T (y - X_b \cdot \theta)$ 尽可能小

解得
$$\theta = (X_b^T X_b)^{-1} X_b^T y$$

3. Sklearn中的使用

```
from sklearn import datasets
from sklearn.model_selection import train_test_split
# 线性回归法解决回归问题
from sklearn.linear_model import LinearRegression
boston = datasets.load_boston()
X = boston_*data
y = boston.target
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=666)
lin_reg = LinearRegression()
lin_reg.fit(X_train, y_train)
lin_reg.coef_
lin_reg.intercept_
lin_reg.score(X_test, y_test)
# KNN解决回归问题
from sklearn neighbors import KNeighborsRegressor
knn_reg = KNeighborsRegressor()
lin_reg.fit(X_train, y_train)
lin_reg.score(X_test, y_test)
```

总结

- 1. 典型的参数学习
- 2. 只能解决回归问题
- 3. 不需要数据归一化
- 梯度下降法
- 1. 线性回归中的梯度下降法

$$\theta = (\theta_0, \theta_1, \cdots, \theta_n)$$

$$-n\nabla J$$

$$\nabla J = (\frac{\partial J}{\partial \theta_0}, \frac{\partial J}{\partial \theta_1}, \cdots, \frac{\partial J}{\partial \theta_n})$$

$$J = \sum_{i=1}^m (y^{(i)} - \hat{y}^{(i)})^2$$

$$\hat{y}^{(i)}= heta_0+ heta_1X_1^{(i)}+\cdots+ heta_nX_n^{(i)}$$

目标:
$$\sum_{i=1}^m (y^{(i)} - heta_0 - heta_1 X_1^{(i)} - \dots - heta_n X_n^{(i)})^2$$
尽可能小

$$abla J(heta) = egin{pmatrix} \sum_{i=1}^m 2(y^{(i)} - X_b^{(i)} heta) \cdot (-1) \ \sum_{i=1}^m 2(y^{(i)} - X_b^{(i)} heta) \cdot (-X_1^{(i)}) \ & \cdots \ \sum_{i=1}^m 2(y^{(i)} - X_b^{(i)} heta) \cdot (-X_n^{(i)}) \end{pmatrix}$$

目标:
$$J = \frac{1}{m} \sum_{i=1}^m (y^{(i)} - \hat{y}^{(i)})^2$$
尽可能小

$$J(\theta) = MSE(y, \hat{y})$$

$$abla J(heta) = rac{2}{m} egin{pmatrix} \sum_{i=1}^m (X_b^{(i)} heta - y^{(i)}) \ \sum_{i=1}^m (X_b^{(i)} heta - y^{(i)}) \cdot X_1^{(i)} \ & \cdots \ \sum_{i=1}^m (X_b^{(i)} heta - y^{(i)}) \cdot X_n^{(i)} \end{pmatrix}$$

2. 向量化

$$\frac{\frac{2}{m} \cdot (x_b^{(1)}\theta - y^{(1)}, x_b^{(2)}\theta - y^{(2)}, \cdots, x_b^{(m)}\theta - y^{(m)}) \cdot \begin{pmatrix} 1 & X_1^{(1)} & \cdots & X_n^{(1)} \\ 1 & X_1^{(2)} & \cdots & X_n^{(2)} \\ \cdots & & & & \\ 1 & X_1^{(m)} & \cdots & X_n^{(m)} \end{pmatrix} = \frac{2}{m} \cdot (X_b\theta - y)^T \cdot X_b$$

$$abla J(heta) = rac{2}{m} \cdot X_b^T (X_b heta - y)$$

3. 实现线性回归中的梯度下降法(something wrong)

```
import numpy as np
x = 2 * np.random.random(size=100).reshape(-1, 1)
y = x * 3. + 4. + np.random.normal(size=100)
X_b = np.hstack([np.ones((len(x), 1)), x])
initial_theta = np.zeros(X_b.shape[1])
eta = 0.01
def J(theta, X_b, y):
        return np.sum((y - X_b.dot(theta))**2) / len(X_b)
    except:
        return float('inf')
def dJ(theta, X_b, y):
    return X_b.T.dot(X_b.dot(theta) - y) * 2. / len(X_b)
def gradient_descent(X_b, y, initial_theta, eta, n_iters = 1e4, epsilon=1e-8):
    theta = initial_theta
    print(theta)
    i_iter = 0
    while i_iter < n_iters:</pre>
        gradient = dJ(theta, X_b, y)
        last_theta = theta
        theta = theta - eta * gradient
        if abs(J(theta, X_b, y) - J(last_theta, X_b, y)) < epsilon:</pre>
            break
        i_iter += 1
    return theta
```

4. 随机梯度下降法

$$2egin{pmatrix} (X_b^{(i)} heta-y^{(i)})\ (X_b^{(i)} heta-y^{(i)})\cdot X_1^{(i)}\ & \dots\ (X_b^{(i)} heta-y^{(i)})\cdot X_n^{(i)} \end{pmatrix} = 2\cdot (X_b^{(i)})^T\cdot (X_b^{(i)} heta-y^{(i)})$$

 $\eta = rac{a}{i_iters+b}$ 经验取值a=5, b=50

```
from sklearn.linear_model import SGDRegressor
sgd_reg = SGDRegressor(n_iter=5)//默认值为5
sgd_reg.fit(X_train_standard,y_train)
sgd_reg.score(X_test_standard,y_test)
```

5. 梯度的调试

$$heta_0^+ = (heta_0 + arepsilon, heta_1, \cdots, heta_n)$$

$$\theta_0^- = (\theta_0 - \varepsilon, \theta_1, \cdots, \theta_n)$$

```
rac{\partial J}{\partial 	heta_0} = rac{J(	heta_0^+) - J(	heta_0^-)}{2arepsilon}
```

```
def dJ_debug(theta,x_b,y,epsilon=0.01):
    res = np.empty(len(theta))
    for i in range(len(theta)):
        theta_1 = theta.copy()
        theta_1[i] += epsilon
        theta_2 = theta.copy
        theta_2[i] -= epsilon
        res[i] = (J(theta_1,x_b,y)-J(theta_2,x_b,y))/(2*epsilon)
    return res
```

6. 总结

数据需要归一化

随机搜索

梯度上升法:最大化效用函数+ $\eta \frac{dJ}{d\theta}$

- 主成分分析法
- 1. 目标

$$egin{aligned} Var(X_{project}) &= rac{1}{m} \sum_{i=1}^m ||X_{project}^{(i)} - \overline{X}_{project}||^2$$
最大 demean处理, $rac{1}{m} \sum_{i=1}^m ||X_{project}^{(i)}||^2$ $w = (w_1, w_2)$ $X^{(i)} &= (X_1^{(i)}, X_2^{(i)})$ $rac{1}{m} \sum_{i=1}^m (X^{(i)} \cdot w)^2$ 拓展到n维: $rac{1}{m} \sum_{i=1}^m (X_1^{(i)} w_1 + X_2^2 w_2 + \dots + X_n^{(i)} w_n)^2$

2. 梯度上升法

$$abla f = rac{2}{m} egin{pmatrix} \sum_{i=1}^m (X^{(i)}w) X_1^{(i)} \ \sum_{i=1}^m (X^{(i)}w) X_2^{(i)} \ & \cdots \ \sum_{i=1}^m (X^{(i)}w) X_n^{(i)} \end{pmatrix} = rac{2}{m} X^T(Xw)$$

$$rac{2}{m} \cdot (X^{(1)}w, X^{(2)}w, \cdots, X^{(m)}w) \cdot egin{pmatrix} X_1^{(1)} & \cdots & X_n^{(1)} \ X_1^{(2)} & \cdots & X_n^{(2)} \ \cdots & & & \ X_1^{(m)} & \cdots & X_n^{(m)} \end{pmatrix} = rac{2}{m} \cdot (Xw)^T \cdot X$$

3. 实现主成分分析法

```
def f(w, X):
        return np.sum((X.dot(w) ** 2)) / len(X)
    def df(w, X):
        return X.T.dot(X.dot(w)) * 2. / len(X)
   def direction(w):
        return w / np.linalg.norm(w)
    def first_component(X, initial_w, eta=0.01, n_iters=1e4, epsilon=1e-8):
       w = direction(initial_w)
        cur_iter = 0
        while cur_iter < n_iters:</pre>
           gradient = df(w, X)
           last w = w
           w = w + eta * gradient
           w = direction(w) #将向量化为单位向量
           if (abs(f(w, X) - f(last_w, X)) < epsilon):
           cur_iter += 1
        return w
    X_pca = demean(X)
    self.components_ = np.empty(shape=(self.n_components, X.shape[1]))
    for i in range(self.n_components):
        initial_w = np.random.random(X_pca.shape[1]) #不能从0向量开始
        w = first_component(X_pca, initial_w, eta, n_iters)
        self.components_[i,:] = w
        X_pca = X_pca - X_pca.dot(w).reshape(-1, 1) * w
    return self
def transform(self, X):
    """将给定的X,映射到各个主成分分量中"""
    assert X.shape[1] == self.components_.shape[1]
    return X.dot(self.components_.T)
def inverse transform(self, X):
    """将给定的X,反向映射回原来的特征空间"""
    assert X.shape[1] == self.components_.shape[0]
    return X.dot(self.components_)
def __repr__(self):
    return "PCA(n_components=%d)" % self.n_components
```

注意:不能使用StandardScaler标准化数据

4. 高维数据向低维数据映射

$$X = egin{pmatrix} X_1^{(1)} & \cdots & X_n^{(1)} \ X_1^{(2)} & \cdots & X_n^{(2)} \ \cdots & & & & \ X_1^{(m)} & \cdots & X_n^{(m)} \end{pmatrix}$$
 $W_k = egin{pmatrix} W_1^{(1)} & \cdots & W_n^{(1)} \ W_1^{(2)} & \cdots & W_n^{(2)} \ \cdots & & & \ W_1^{(k)} & \cdots & W_n^{(k)} \end{pmatrix}$ 前体个主成分

 $X \cdot W_k^T = X_k$ 高维向低维映射

 $X_k \cdot W_k = X_m$ 低维恢复为高维, X_m 和X并不等同

5. Sklearn中的使用

```
from sklearn.decomposition import PCA
from sklearn import datasets
from sklearn.model_selection import train_test_split
from sklearn.neighbors import KNeighborsClassifier
digits = datasets.load_digits()
X = digits.data
```

```
y = digits.target
X_train, X_test, y_train, y_test = train_test_split(X, y)
pca = PCA(0.95) #解释95%的方差,还可以传入n_components
pca.fit(X_train)
X_train_reduction = pca.transform(X_train)
X_test_reduction = pca.transform(X_test)
knn_clf = KNeighborsClassifier()
knn_clf.fit(X_train_reduction, y_train)
print(knn_clf.score(X_test_reduction, y_test))
print(pca.explained_variance_ratio_)
print(pca.n_components_)
```

降到2维后的可视化

```
pca = PCA(n_components=2)
pca.fix(X)
X_reduction = pca.transform(X)
for i in range(10):
   plt.scatter(X_reduction[y==i,0], X_reduction[y==i,1], alpha=0.8)
plt.show()
```

6. PCA降噪应用-特征脸

```
import numpy as np
from sklearn.datasets import fetch_lfw_people
from sklearn.decomposition import PCA
faces = fetch_lfw_people()
random_indexes = np.random.permutation(len(faces.data))
X = faces.data[random_indexes]
pca = PCA(svd_solver="randomized")
pca.fit(X)
```

- 多项式回归与模型泛化
- 1. 引例

```
import numpy as np
import matplotlib.pyplot as plt
from sklearn.linear_model import LinearRegression
x = np.random.uniform(-3, 3, size=100)
X = x.reshape(-1, 1)
y = 0.5 * x**2 + x + 2 + np.random.normal(0, 1, size=100)
plt.scatter(x, y)
X2 = np.hstack([X, X**2])
lin_reg = LinearRegression()
lin_reg.fit(X2, y)
y_predict = lin_reg.predict(X2)
plt.plot(np.sort(x),y_predict[np.argsort(x)],color='r')
plt.show()
print(lin_reg.coef_)
print(lin_reg.intercept_)
```

2. PolynomialFeatures

PolynomialFeatures(degree=3)

$$x_1, x_2 \begin{cases} 1, x_1, x_2 \\ x_1^2, x_2^2, x_1 x_2 \\ x_1^3, x_2^3, x_1^2 x_2, x_1 x_2^2 \end{cases}$$

```
import numpy as np
import matplotlib.pyplot as plt
from sklearn.linear_model import LinearRegression
x = np.random.uniform(-3, 3, size=100)
X = x.reshape(-1, 1)
```

```
y = 0.5 * x**2 + x + 2 + np.random.normal(0, 1, size=100)
from sklearn.preprocessing import PolynomialFeatures
poly = PolynomialFeatures(degree=2)
poly.fit(X)
X2 = poly.transform(X)
print(X2.shape)
lin_reg = LinearRegression()
lin_reg.fit(X2, y)
y_predict = lin_reg.predict(X2)
plt.scatter(x, y)
plt.plot(np.sort(x), y_predict[np.argsort(x)], color='r')
plt.show()
#PolynomialFeatures
import numpy as np
from sklearn.preprocessing import PolynomialFeatures
X = np.arange(1, 11).reshape(-1, 2)
poly = PolynomialFeatures(degree=2)
poly.fit(X)
X2 = poly.transform(X)
print(X2)
```

3. pipeline

4. 误差

```
from sklearn.metrics import mean_squared_error
print(mean_squared_error(y, y_predict))
```

5. 过拟合与欠拟合

欠拟合: 算法所训练的模型不能完整表述数据关系

过拟合: 算法训练的模型过多地表达了数据间的噪音关系

6. 学习曲线

```
from sklearn.metrics import mean_squared_error
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=666)
train_score = []
test_score = []
for i in range(1, 76):
    lin_reg = poly_reg
    lin_reg.fit(X_train[:i],y_train[:i])
    y_train_predict = lin_reg.predict(X_train[:i])
    train\_score.append(mean\_squared\_error(y\_train[:i], y\_train\_predict))
    y_test_predict = lin_reg.predict(X_test)
    test_score.append(mean_squared_error(y_test, y_test_predict))
plt.plot([i for i in range(1, 76)], np.sqrt(train_score), label="train")
plt.plot([i for i in range(1, 76)], np.sqrt(test_score), label="test")
plt.legend()
plt.show()
```

7. 验证数据集与交叉验证

数据划分

训练数据

验证数据

测试数据:不参与模型创建,作为衡量最终模型性能的数据集

交叉验证

训练数据化为A、B、C, BC训练A验证, AC训练B验证, AB训练C验证, k个模型均值为结果调参

```
import numpy as np
from sklearn import datasets
digits = datasets.load_digits()
X = digits.data
y = digits.target
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=666)
from sklearn.model_selection import cross_val_score
from sklearn.neighbors import KNeighborsClassifier
knn_clf = KNeighborsClassifier()
print(cross_val_score(knn_clf, X_train, y_train, cv=5)) #默认分成3份
```

k-folds交叉验证:把训练数据集分成k份,每次训练k个模型,相当于整体性能慢了k倍

留一法LOO-CV:将训练数据集分成m份(m个样本),Leave-One-Out Cross Validation,完全不受随机的影响,最接近模型真正的性能指标,但计算量巨大

8. 偏差与方差

偏差与方差

偏差(Bias):对问题本身假设不正确,欠拟合,如对非线性数据使用线性回归

方差(Variance):数据的一点点扰动都会较大地影响模型,通常原因在于使用的模型太复杂,过拟合,如高阶多项式回归

相关算法

天生高方差算法: KNN, 非参数学习通常都是高方差算法, 因为不对数据进行任何假设

天生高偏差算法:线性回归,参数学习通常都是高偏差的算法,因为对数据具有极强的假设

KNN中对k的调整: k越小,模型越复杂,偏差越小; k越大,模型越简单,方差越小。

线性回归中使用多项式回归, degree越小, 模型越简单, 偏差越大; degree越大, 模型越复杂, 方差越大。

解决高方差

- 降低模型复杂度
- 减少数据维度,降噪
- 增加样本数
- 使用验证集
- 模型正则化
- 9. 模型正则化

岭回归: 使
$$J(heta) = MSE(y,\hat{y}; heta) + lpha rac{1}{2} \sum_{i=1}^n heta_i^2$$
 尽可能小

LASSO回归: 使
$$J(heta) = MSE(y, \hat{y}; heta) + lpha \sum_{i=1}^n | heta_i|$$
尽可能小

LASSO趋向于使一部分theta值变为0,可作为特征选择用

弾性网:
$$\psi J(heta) = MSE(y,\hat{y}; heta) + rlpha \sum\limits_{i=1}^n | heta_i| + rac{1-r}{2}lpha \sum\limits_{i=1}^n heta_i^2$$
尽可能小

- 逻辑回归与分类评价
- 1. Sigmoid函数

$$\hat{p} = \sigma(heta^T \cdot x_b) = rac{1}{1 + e^{- heta^T \cdot x_b}}$$

$$\hat{y} = \begin{cases} 1 & \hat{y} \ge 0.5 \\ 0 & \hat{y} < 0.5 \end{cases}$$

2. 损失函数

$$cost = egin{cases} -log(\hat{p}) & y = 1 \ -log(1-\hat{p}) & y = 0 \end{cases}$$
 $cost = -ylog(\hat{p}) - (1-y)log(1-\hat{p})$

$$egin{aligned} J(heta) &= -rac{1}{m} \sum_{i=1}^m y^{(i)} log(\hat{p}^{(i)}) + (1-y^{(i)}) log(1-\hat{p}^{(i)}) \ J(heta) &= -rac{1}{m} \sum_{i=1}^m y^{(i)} log(\sigma(X_b^{(i)} heta)) + (1-y^{(i)}) log(1-\sigma(X_b^{(i)} heta)) \end{aligned}$$

3. 损失函数的梯度

$$rac{J(heta)}{ heta_j} = rac{1}{m} \sum_{i=1}^m (\sigma(X_b^{(i)} heta) - y^{(i)}) X_j^{(i)}$$

$$abla J(heta) = rac{1}{m} \left(egin{array}{c} \sum\limits_{i=1}^m (\hat{y}^{(i)} - y^{(i)}) \ \sum\limits_{i=1}^m (\hat{y}^{(i)} - y^{(i)}) \cdot X_1^{(i)} \ & \ddots \ \sum\limits_{i=1}^m (\hat{y}^{(i)} - y^{(i)}) \cdot X_n^{(i)} \end{array}
ight) = rac{1}{m} X_b^T \cdot (\sigma(X_b heta) - y)$$

4. 决策边界

$$\theta^T \cdot x_b = 0$$

5. 多项式特征

正则化: $C \cdot J(\theta) + L_1/L_2$

```
import numpy as np
import matplotlib.pyplot as plt
np.random.seed(666)
X = np.random.normal(0,1,size=(200,2))
y = np.array(X[:,0]**2 + X[:,1] < 1.5,dtype='int')
for _ in range(20):
    y[np.random.randint(200)] = 1
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=666)
from sklearn.linear_model import LogisticRegression
from sklearn.preprocessing import PolynomialFeatures
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import StandardScaler
def PolynomialLogisticRegression(degree, C, penalty='l2'):
    return Pipeline([
        ('poly', PolynomialFeatures(degree=degree)),
        ('std_scaler', StandardScaler()),
        ('log_reg', LogisticRegression(C=C, penalty=penalty))
poly_log_reg = PolynomialLogisticRegression(degree=20, C=0.1,penalty='l1')
poly_log_reg.fit(X_train, y_train)
poly_log_reg.score(X_test, y_test)
```

6. OvR & OvO

OvR: n个类别进行n次分类

OvO: n个类别进行C(n,2)次分类

```
import numpy as np
import matplotlib.pyplot as plt
from sklearn import datasets
iris = datasets.load_iris()
X = iris.data
y = iris.target
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=666)
from sklearn.linear_model import LogisticRegression
log_reg = LogisticRegression(multi_class="multinomial",solver="newton-cg")#默认OvR, multinomial等价于
OvO
log_reg.fit(X_train, y_train)
log_reg.score(X_test, y_test)
```

```
from sklearn.multiclass import OneVsRestClassifier
from sklearn.multiclass import OneVsOneClassifier
ovr = OneVsRestClassifier(log_reg)
ovr.fit(X_train, y_train)
ovr.score(X_test, y_test)
```

7. 评价分类结果

混淆矩阵

真实\预测

0

1

0	预测negtive正确TN	预测positive错误FP	
1	预测negtive错误FN	预测positive正确TP	

精准率与召回率

精准率: $precision = \frac{TP}{TP+FP}$

召回率: $recall = \frac{TP}{TP+FN}$

```
import numpy as np
from sklearn import datasets
digits = datasets.load_digits()
X = digits.data
y = digits_target_copy()
y[digits target==9] = 1
y[digits.target!=9] = 0
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=666)
from sklearn.linear_model import LogisticRegression
log_reg = LogisticRegression()
log_reg.fit(X_train, y_train)
log_reg.score(X_test, y_test)
y_log_predict = log_reg.predict(X_test)
def TN(y_true, y_predict):
    assert len(y_true) == len(y_predict)
    return np.sum((y_true == 0) & (y_predict == 0))
def FP(y_true, y_predict):
    assert len(y_true) == len(y_predict)
    return np.sum((y\_true == 0) & (y\_predict == 1))
def FN(y_true, y_predict):
    assert len(y_true) == len(y_predict)
    return np.sum((y_true == 1) & (y_predict == 0))
def TP(y_true, y_predict):
```

```
assert len(y_true) == len(y_predict)
    return np.sum((y_true == 1) & (y_predict == 1))
def confusion_matrix(y_true, y_predict):
    return np.array([
        [TN(y_true, y_predict), FP(y_true, y_predict)],
        [FN(y_true, y_predict), TP(y_true, y_predict)]
    ])
def precision_score(y_true, y_predict):
    tp = TP(y_true, y_predict)
    fp = FP(y\_true, y\_predict)
        return tp / (tp + fp)
    except:
        return 0.0
def recall_score(y_true, y_predict):
    tp = TP(y\_true, y\_predict)
    fn = FN(y_true, y_predict)
    trv:
        return tp / (tp + fn)
    except:
        return 0.0
```

sklearn中的实现

```
from sklearn.metrics import confusion_matrix
from sklearn.metrics import precision_score
from sklearn.metrics import recall_score
confusion_matrix(y_test, y_log_predict)
precision_score(y_test, y_log_predict)
```

股票预测: 注重精准率 病人诊断: 注重召回率

F1 Score

 $F1 = \frac{2 \cdot precision \cdot recall}{precision + recall}$ (调和平均值)

调和平均值,有一个指标比较小,整体值也偏小

```
from sklearn.metrics import f1_score
print(f1_score(y_test, y_log_predict))
```

调整分类阈值

决策边界: $\theta^T \cdot x_b = threshold$ 默认为0

```
decision_scores = log_reg.decision_function(X_test)#(默认decision_scores=0)
y_log_predict2 = np.array(decision_scores >= 5, dtype='int')
```

提高阈值,往往会提高精准率,降低召回率。

精准率、召回率曲线

```
precisions = []
recalls = []
thresholds = np.arange(np.min(decision_scores), np.max(decision_scores), 0.1)
for threshold in thresholds:
    y_predict = np.array(decision_scores >= threshold, dtype='int')
    precisions.append(precision_score(y_test, y_predict))
    recalls.append(recall_score(y_test, y_predict))

plt.plot(thresholds, precisions)
plt.plot(thresholds, recalls)
plt.plot(precisions, recalls) #查看精准率、召回率制约曲线
plt.show()
```

sklearn中的封装

```
from sklearn.metrics import precision_recall_curve

precisions, recalls, thresholds = precision_recall_curve(y_test, decision_scores)

plt.plot(thresholds, precisions[:-1]) #thresholds比precision少一个数据

plt.plot(thresholds, recalls[:-1])

plt.show()
```

ROC曲线

```
TPR = \frac{TP}{TP+FN} 即召回率
```

```
FPR = \frac{FP}{TN + FP}
```

```
from sklearn.metrics import roc_curve
fprs, tprs, thresholds = roc_curve(y_test, decision_scores)
plt.plot(fprs, tprs)
plt.show()
from sklearn.metrics import roc_auc_score
roc_auc_score(y_test, decision_scores) //面积越大越好
```

ROC曲线对有偏数据不敏感

多分类问题的评价

多分类精准率

```
from sklearn.metrics import precision_score
precision_score(y_test, y_predict, average="micro") #average默认为binary
```

多分类混淆矩阵

#天然支持多分类混淆矩阵

from sklearn.metrics import confusion_matrix confusion_matrix(y_test, y_predict)

可视化混淆矩阵

```
from sklearn.metrics import confusion_matrix
cfm = confusion_matrix(y_test, y_predict)
row_sums = np.sum(cfm, axis=1)
err_matrix = cfm / row_sums
np.fill_diagonal(err_matrix, 0)
plt.matshow(err_matrix, cmap=plt.cm.gray)
plt.show()
```

- 支撑向量机
- 1. hard margin

直线方程 $w^T x + b = 0$

$$egin{cases} rac{w^Tx^{(i)}+b}{||w||d} \geq 1 \quad orall y^{(i)} = 1 \ rac{w^Tx^{(i)}+b}{||w||d} \leq -1 \quad orall y^{(i)} = -1 \end{cases}$$

$$||w|| = \sqrt{w_1^2 + w_2^2 + \dots + w_n^2}$$

$$y^{(i)}(w^Tx^{(i)}+b) > 1$$

有条件的最优化问题: $max: \frac{|w^Tx+b|}{||w||} \to min: \frac{1}{2}||w||^2 \text{ (st. } y^{(i)}(w^Tx^{(i)}+b) \geq 1 \text{)}$

2. soft margin与正则化

$$y^{(i)}(w^Tx^{(i)}+b)\geq 1-\zeta_i \quad \zeta_i\geq 0$$

$$min:rac{1}{2}{||w||}^2+C\sum\limits_{i=1}^{m}\zeta_i$$
 L1正则 (L2正则: $rac{1}{2}{||w||}^2+C\sum\limits_{i=1}^{m}\zeta_i^2)$

C越大,容错空间越小

3. Sklearn中的使用

使用核函数

4. 核函数

多项式核函数:

$$K(x,y) = (x \cdot y + 1)^2 = (\sum_{i=1}^n x_i y_i + 1)^2 = \sum_{i=1}^n (x_i^2)(y_i^2) + \sum_{i=2}^n \sum_{j=1}^{i-1} (\sqrt{2}x_i x_j)(\sqrt{2}y_i y_j) + \sum_{i=1}^n (\sqrt{2}x_i)(\sqrt{2}y_i) + 1 = x'y'$$

$$x' = (x_n^2, \dots, x_1^2, \sqrt{2}x_n x_{n-1}, \dots, \sqrt{2}x_n, \dots, \sqrt{2}x_1, 1)$$

拓展: $K(x,y) = (x \cdot y + c)^d$, 可以指定degree与coef

线性核函数:

$$K(x,y) = x \cdot y$$

高斯核函数:

K(x,y)表示x和y的点乘

 $K(x,y)=e^{-\gamma ||x-y||^2}$ 将每一个样本点映射到一个无穷维的特征空间

高斯函数
$$g(x) = rac{1}{\sigma\sqrt{2\pi}}e^{-rac{1}{2}(rac{x-\mu}{\sigma})^2}$$

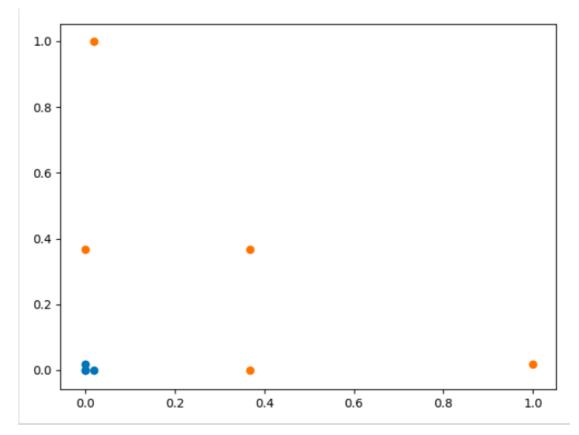
多项式特征: 依靠升维使原本线性不可分的点线性可分

以两个地标点l1,l2为例,对其可视化理解

$$x
ightarrow (e^{-\gamma ||x-l_1||^2}, e^{\gamma ||x-l_2||^2})$$



```
import numpy as np
import matplotlib.pyplot as plt
x = np.arange(-4, 5, 1)
y = np.array((x >= -2) & (x <= 2), dtype='int')
def gaussian(x, l):
    gamma = 1.0
    return np.exp(-gamma * (x-l)**2)
l1, l2 = -1, 1
X_new = np.empty((len(x), 2))
for i, data in enumerate(x):
    X_new[i, 0] = gaussian(data, l1)
    X_new[i, 1] = gaussian(data, l2)
plt.scatter(X_new[y==0,0], X_new[y==0,1])
plt.scatter(X_new[y==0,0], X_new[y==1,1])
plt.show()</pre>
```



m*n的数据映射成了m*m的数据

```
from sklearn.svm import SVC

def RBFKernelSVC(gamma=1.0):
    return Pipeline([
          ("std_scaler", StandardScaler()),
          ("svc", SVC(kernel="rbf", gamma=gamma))
])
```

gamma较大: 过拟合 gamma较小: 欠拟合

5. 解决回归问题

```
from sklearn import datasets
from sklearn.svm import LinearSVR
from sklearn.svm import SVR
from sklean.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler
from sklearn.pipeline import Pipeline
boston = datasets.load_boston()
X = boston.data
y = boston.target
X_train, X_test, y_train, y_test = train_test_split(X, y)
def StandardLinerSVR(epsilon=0.1):
    return Pipeline([
        ("std_scaler", StandardScaler()),
        ("linearSVR", LinearSVR(epsilon=epsilon))
   ])
svr = StandardLinerSVR()
svr.fit(X_test, y_test)
svr.score(X_test, y_test)
```

- 决策树
- 1. 信息墒

$$H = -\sum_{i=1}^{k} p_i log(p_i)$$

熵越大, 信息不确定性越大

2. 基尼系数

$$G=1-\sum_{i=1}^k p_i^2$$

基尼系数越大, 信息不确定性越大

3. 代码示例

```
import numpy as np
from sklearn.tree import DecisionTreeClassifier
from sklearn import datasets
from collections import Counter
from math import log
iris = datasets.load_iris()
X = iris.data[:,2:]
y = iris.target
#使用Sklearn
dt_clf = DecisionTreeClassifier(max_depth=2, criterion="entropy") #默认为基尼系数, 基尼系数稍快
dt_clf.fit(X, y)
#部分实现
def split(X, y, d, value):
    index_a = (X[:,d] \le value)
    index_b = (X[:,d] > value)
   return X[index_a], X[index_b], y[index_a], y[index_b]
def entropy(y):
   counter = Counter(y)
```

```
res = 0.0
    for num in counter.values():
        p = num / len(y)
        res += -p * log(p)
    return res
def gini(y):
    counter = Counter(y)
    res = 1.0
    for num in counter.values():
        p = num / len(y)
        res -= -p**2
    return res
def try_split(X, y):
    best_entropy = float('inf')
    best_d, best_v = -1, -1
    for d in range(X.shape[1]):
        sorted_index = np.argsort(X[:,d])
        for i in range(1, len(X)):
            if X[sorted_index[i-1], d] != X[sorted_index[i], d]:
                v = (X[sorted_index[i-1], d] + X[sorted_index[i], d]) / 2
                X_l, X_r, y_l, y_r = split(X, y, d, v)
                e = entropy(y_l) + entropy(y_r)
                \#e = gini(y_l) + gini(y_r)
                if e < best_entropy:</pre>
                    best_entropy, best_d, best_v = e, d, v
    return best_entropy, best_d, best_v
```

4. 常用超参数

```
max_depth: 2(越高越容易过拟合)
min_sample_split: 10(越高越不容易过拟合)
min_samples_leaf: 6(越高越不容易过拟合)
max_leaf_nodes: 4(越多越容易过拟合)
max_features
min_impurity_decrease 限制信息增益大小
class_weight
```

5. 绘制决策边界

```
def plot_decision_boundary(model,axis):
    x0, x1 = np.meshgrid(
        np.linspace(axis[0], axis[1], int((axis[1] - axis[0]) * 100)).reshape(-1, 1),
        np.linspace(axis[2], axis[3], int((axis[3] - axis[2]) * 100)).reshape(-1, 1)
    )
    x_new = np.c_[x0.ravel(), x1.ravel()]
    y_predict = model.predict(x_new)
    zz = y_predict.reshape(x0.shape)
    from matplotlib.colors import ListedColormap
    custom_cmap = ListedColormap(['# EF9A9A','#FFF59D','#90CAF9'])
    plt.contourf(x0, x1, zz, linewidth = 5, cmap = custom_cmap)
```

```
import numpy as np
import matplotlib.pyplot as plt
from sklearn.tree import DecisionTreeClassifier
from sklearn import datasets
X, y = datasets.make_moons(noise=0.25)
dt_clf = DecisionTreeClassifier(max_depth=2)

def plot_decision_boundary(model,axis):
    x0, x1 = np.meshgrid(
```

```
np.linspace(axis[0], axis[1], int((axis[1] - axis[0]) * 100)).reshape(-1, 1),
    np.linspace(axis[2], axis[3], int((axis[3] - axis[2]) * 100)).reshape(-1, 1)
)

x_new = np.c_[x0.ravel(), x1.ravel()]
y_predict = model.predict(x_new)
zz = y_predict.reshape(x0.shape)
from matplotlib.colors import ListedColormap
    custom_cmap = ListedColormap(['#EF9A9A','#FFF59D','#90CAF9'])
plt.contourf(x0, x1, zz, linewidth = 5, cmap = custom_cmap)

dt_clf.fit(X, y)
plot_decision_boundary(dt_clf, axis=[-1.5,2.5,-1.0,1.5])
plt.scatter(X[y==0,0],X[y==0,1])
plt.scatter(X[y==1,0],X[y==1,1])
plt.show()
```

6. 解决回归问题

```
from sklearn.tree import DecisionTreeRegressor
from sklearn import datasets
from sklearn.model_selection import train_test_split
boston = datasets.load_boston()
X = boston.data
y = boston.target
X_train, X_test, y_train, y_test = train_test_split(X, y)
dt_reg = DecisionTreeRegressor()
dt_reg.fit(X_train, y_train)
print(dt_reg.score(X_train, y_train))
print(dt_reg.score(X_test, y_test))
```

7. 局限性

决策边界是横平竖直的

对个别数据敏感

8. 实战案例

```
from sklearn import tree
from sklearn.datasets import load_wine
from sklearn.model_selection import train_test_split
wine = load_wine()
import pandas as pd
pd.concat([pd.DataFrame(wine.data),pd.DataFrame(wine.target)],axis=1)
x_train,x_test,y_train,y_test = train_test_split(wine.data,wine.target,test_size=0.3)
clf = tree.DecisionTreeClassifier(criterion="entropy",random_state=30,splitter="random")#随机选择特
征,高维度随机性会表现更明显,splitter可以选择best
clf = clf.fit(x_train,y_train)
score = clf.score(x_test,y_test)
import graphviz
feature_name = ['酒精','苹果酸','灰','灰的碱性','镁','总酚','类黄酮','非黄烷类酚类','花青素','颜色强度','色
调','稀释葡萄酒','脯氨酸']
dot_data = tree.export_graphviz(clf,feature_names=feature_name,class_names=['琴酒','雪梨','贝尔摩
德'],filled=True,rounded=True)
graph = graphviz.Source(dot_data)
[*zip(feature_name,clf.feature_importances_)]
import matplotlib.pyplot as plt
test = []
for i in range(10):
   clf =
tree.DecisionTreeClassifier(max_depth=i+1,criterion="entropy",random_state=30,splitter="random")
```

```
clf = clf.fit(x_train,y_train)
    score = clf.score(x_test,y_test)
    test.append(score)
plt.plot(range(1,11),test,color="red",label="max_depth")
plt.legend()
plt.show()
```

```
from sklearn.datasets import load_boston
from sklearn.model_selection import cross_val_score
from sklearn.tree import DecisionTreeRegressor
boston = load_boston()
regressor = DecisionTreeRegressor(random_state=0)
cross_val_score(regressor,boston.data,boston.target,cv=10,scoring="neg_mean_squared_error") #默认返回
R^2
```

回归树拟合正弦曲线

```
import numpy as np
from sklearn.tree import DecisionTreeRegressor
import matplotlib.pyplot as plt
rng = np.random.RandomState(1)
x = np.sort(5*rng.rand(80,1),axis=0)
y = np.sin(x).ravel() #降维
y[::5] += 3*(0.5-rng.rand(16))
reg1 = DecisionTreeRegressor(max_depth=2)
reg2 = DecisionTreeRegressor(max_depth=5)
reg1.fit(x,y)
reg2.fit(x,y)
x_{\text{test}} = \text{np.arange}(0.0, 5.0, 0.01)[:, \text{np.newaxis}] ###
y_1 = reg1.predict(x_test)
y_2 = reg2.predict(x_test)
plt.figure()
plt.scatter(x,y,s=20,edgecolor="black",c="darkorange",label="data")
plt.plot(x_test,y_1,color="cornflowerblue",label="max_depth=2",linewidth=2)
plt.plot(x_test,y_2,color="yellowgreen",label="max_depth=5",linewidth=2)
plt.xlabel("data")
plt.ylabel("target")
plt.legend()
plt.show()
```

- 集成学习和随机森林
- 1. hard voting

```
from sklearn import datasets
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LogisticRegression
from sklearn.svm import SVC
from sklearn.tree import DecisionTreeClassifier
from sklearn.ensemble import VotingClassifier
X, y = datasets.make_moons(n_samples=500, noise=0.3)
X_train, X_test, y_train, y_test = train_test_split(X, y)
voting_clf = VotingClassifier(estimators=[
    ('log', LogisticRegression()),
    ('svm', SVC()),
    ('dt_clf', DecisionTreeClassifier())
], voting='hard')
voting_clf.fit(X_train, y_train)
print(voting_clf.score(X_test, y_test))
```

思想:根据分类概率加权

要求:模型能够估计概率

```
voting_clf = VotingClassifier(estimators=[
    ('log', LogisticRegression()),
    ('svm', SVC(probability=True)),
    ('dt_clf', DecisionTreeClassifier())
], voting='soft')
```

3. Bagging和Pasting

思想: 创建若干子模型,每个模型只看样本数据一部分,子模型不需要有很高准确度,但要有差异,

取样方式: 放回取样(Bagging)、不放回取样(Pasting)

4. 00B(Out of Bag)

思想: 放回取样可能导致一部分样本没有取到,可以不使用测试数据集,而是使用未被取到的样本测试,

5. 更多Bagging的探讨

思想: 针对特征随机采样(max_samples设置和n_estimators一致)

思想: 既针对样本, 又针对特征随机采样

6. 随机森林

决策树在节点划分上,在随机的特征子集上寻找最优划分特征

```
from sklearn.ensemble import RandomForestClassifier
rf_clf = RandomForestClassifier(n_estimators=500, oob_score=True)
```

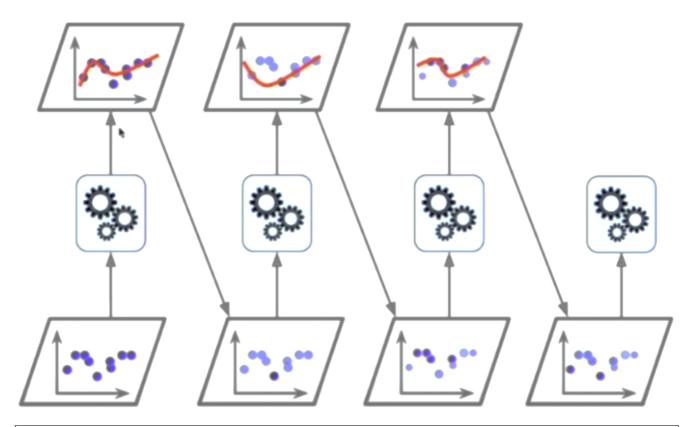
决策树在节点划分上,使用随机的特征和阈值

```
from sklearn.ensemble import ExtraTreesClassifier
```

集成学习也可以解决回归问题

7. Boosting

Ada Boostring



```
from sklearn.import datasets
from sklearn.imodel_selection import train_test_split
from sklearn.tree import DecisionTreeClassifier
X, y = datasets.make_moons(n_samples=500, noise=0.3)
X_train, X_test, y_train, y_test = train_test_split(X, y)
from sklearn.ensemble import AdaBoostClassifier
ada_clf = AdaBoostClassifier(DecisionTreeClassifier(max_depth=2),n_estimators=500)
ada_clf.fit(X_train, y_train)
```

gradient boosting

训练一个模型m1,产生错误e1

针对e1训练第二个模型m2,产生错误e2

针对e2训练第三个模型m3,产生错误e3

最终预测结果为m1+m2+m3

```
from sklearn.ensemble import GradientBoostingClassifier
gb_clf = GradientBoostingClassifier(max_depth=2, n_estimators=30) #默认基于决策树
```

8. Stacking