

法律声明

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人工智能之机器学习

回归算法

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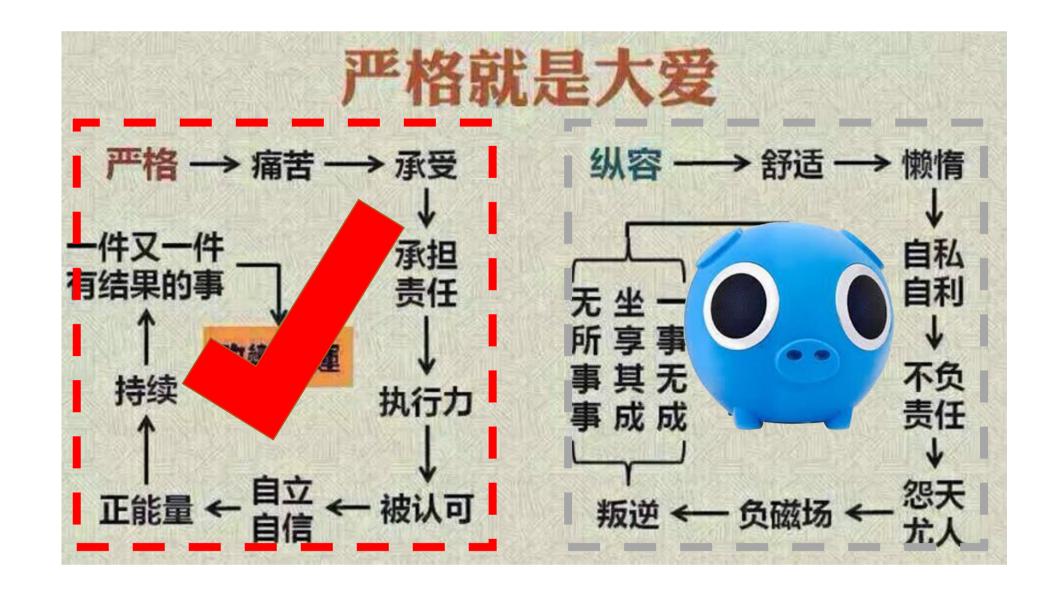


课程要求

- ■课上课下"九字"真言
 - ◆认真听,善摘录,勤思考
 - ◆多温故,乐实践,再发散
- ■四不原则
 - ◆不懒散惰性,不迟到早退
 - ◆不请假旷课,不拖延作业
- ■一点注意事项
 - ◆违反"四不原则",不包就业和推荐就业



严格是大爱





寄语



做别人不愿做的事,

做别人不敢做的事,

做别人做不到的事。



课程内容

- ■线性回归
- Logistic回归
- ■Softmax回归
- ■梯度下降
- ■特征抽取
- ■线性回归案例



什么是回归算法

- ■回归算法是一种比较常用的机器学习算法,用来建立"解释"变量和观测值之间的关系;从机器学习的角度来讲,用于构建一个算法模型(函数)来做属性与标签之间的映射关系,在算法的学习过程中,试图寻找一个函数_{h:R^d->R} 使得参数之间的关系拟合性最好。
- ■回归算法中算法(函数)的最终结果是一个**连续**的数据值,输入值(属性值)是一个d 维度的属性/数值向量



回归算法理性认知

■信用额度提升审批

属性/标签名称	值
年龄	30
年薪	320000
工作年限	8
最近三个月消费额	15623
当前额度	50000
可提高额度	15000

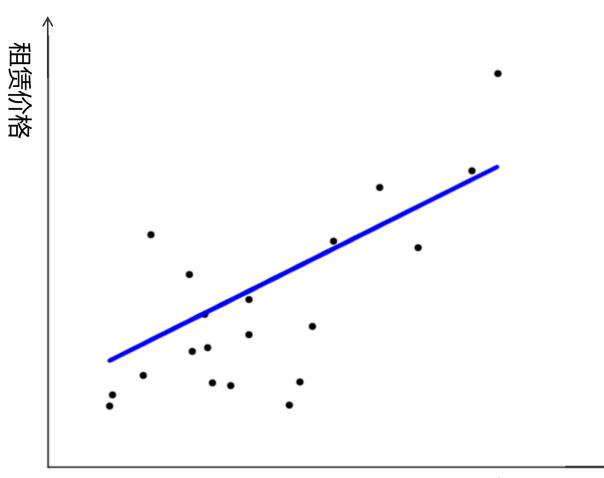
每个信用卡用户允许提高多少额度?



线性回归

y=ax+b

房屋面积(m^2)	租赁价格(1000¥)			
10	0.8			
15	1			
20	1.8			
30	2			
50	3.5			
60	3			
	•••••			



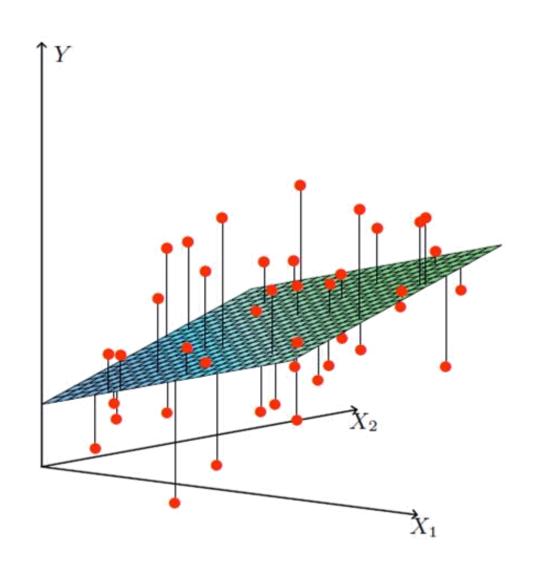




线性回归

$$\bullet h(x) = \theta_0 + \theta_1 X_1 + \theta_2 X_2 \qquad \uparrow^Y$$

房屋面积	房间数量	租赁价格		
10	1	0.8		
20	1	1.8		
30	1	2.2		
30	2	2.5		
70	3	5.5		
70	2	5.2		





线性回归

$$h_{\theta}(x) = \theta_0 + \theta_1 x_1 + \dots + \theta_n x_n$$

$$= \theta_0 1 + \theta_1 x_1 + \dots + \theta_n x_n$$

$$= \theta_0 x_0 + \theta_1 x_1 + \dots + \theta_n x_n$$

$$= \sum_{i=0}^n \theta_i x_i = \theta^T X$$

最终要求是计算出 θ 的值,并选择最优的 θ 值构成算法公式



线性回归、最大似然估计及二乘法

$$y^{(i)} = \theta^T x^{(i)} + \varepsilon^{(i)}$$

- ■误差 $\varepsilon^{(i)}(1 \le i \le n)$ 是独立同分布的,服从均值为0,方差为某定值 σ^2 的高斯分布。
 - ◆原因:**中心极限定理**
- ■实际问题中,很多随机现象可以看做**众多因素**的独立影响的综合反应,往往服从 正态分布



似然函数

$$y^{(i)} = \theta^T x^{(i)} + \varepsilon^{(i)}$$

$$p(\varepsilon^{(i)}) = \frac{1}{\sigma\sqrt{2\pi}}e^{\left(-\frac{\left(\varepsilon^{(i)}\right)^2}{2\sigma^2}\right)}$$

$$p(y^{(i)} \mid x^{(i)}; \theta) = \frac{1}{\sigma \sqrt{2\pi}} \exp\left(-\frac{\left(y^{(i)} - \theta^T x^{(i)}\right)^2}{2\sigma^2}\right)$$

$$L(\theta) = \prod_{i=1}^{m} p(y^{(i)} \mid x^{(i)}; \theta)$$

$$= \prod_{i=1}^{m} \frac{1}{\sigma \sqrt{2\pi}} \exp \left(-\frac{\left(y^{(i)} - \theta^{T} x^{(i)}\right)^{2}}{2\sigma^{2}}\right)$$

 $loss(y_j, \hat{y}_j) = J(\theta) = \frac{1}{2} \sum_{i=1}^{m} (h_{\theta}(x^{(i)}) - y^{(i)})^2$



对数似然、目标函数及最小二乘

$$\ell(\theta) = \log L(\theta)$$

$$= \log \prod_{i=1}^{m} \frac{1}{\sigma \sqrt{2\pi}} \exp \left(-\frac{\left(y^{(i)} - \theta^{T} x^{(i)}\right)^{2}}{2\sigma^{2}}\right)$$

$$= \sum_{i=1}^{m} \log \frac{1}{\sigma \sqrt{2\pi}} \exp \left(-\frac{\left(y^{(i)} - \theta^{T} x^{(i)}\right)^{2}}{2\sigma^{2}}\right)$$

$$= m \log \frac{1}{\sigma \sqrt{2\pi}} - \frac{1}{\sigma^2} \bullet \frac{1}{2} \sum_{i=1}^{m} \left(y^{(i)} - \theta^T x^{(i)} \right)^2$$

Ө的求解过程 $J(\theta) = \frac{1}{2} \sum_{i=1}^{m} (h_{\theta}(x^{(i)}) - y^{(i)})^2$

$$J(\theta) = \frac{1}{2} \sum_{i=1}^{m} \left(h_{\theta} \left(x^{(i)} \right) - y^{(i)} \right)^{2} = \frac{1}{2} (X\theta - Y)^{T} (X\theta - Y) \longrightarrow \min_{\theta} J(\theta)$$

$$\nabla_{\theta} J(\theta) = \nabla_{\theta} \left(\frac{1}{2} (X\theta - Y)^{T} (X\theta - Y) \right) = \nabla_{\theta} \left(\frac{1}{2} (\theta^{T} X^{T} - Y^{T}) (X\theta - Y) \right)$$

$$= \nabla_{\theta} \left(\frac{1}{2} \left(\theta^T X^T X \theta - \theta^T X^T Y - Y^T X \theta + Y^T Y \right) \right)$$

$$= \frac{1}{2} \left(2X^T X \theta - X^T Y - (Y^T X)^T \right)$$
$$= X^T X \theta - X^T Y$$

$$\theta = (X^T X)^{-1} X^T Y$$



最小二乘法的参数最优解

■参数解析式

$$\theta = (X^T X)^{-1} X^T Y$$

■最小二乘法的使用要求矩阵 X^TX 是可逆的;为了防止不可逆或者过拟合的问题存在,可以增加额外数据影响,导致最终的矩阵是可逆的:

$$\theta = (X^T X + \lambda I)^{-1} X^T y$$

■最小二乘法直接求解的难点:矩阵逆的求解是一个难处



普通最小二乘法线性回归案例

- 现有一批描述家庭用电情况的数据,对数据进行算法模型预测,并最终得到预测模型(每天各个时间段和功率之间的关系、功率与电流之间的关系等)
 - ◆数据来源: <u>Individual household electric power consumption Data Set</u>
 - ◆建议:使用python的sklearn库的linear_model中LinearRegression来获取算法

Individual household electric power consumption Data Set

Download: Data Folder, Data Set Description

Abstract: Measurements of electric power consumption in one household with a one-minute sampling rate over a period of almost 4 years. Different electrical quantities and some sub-metering values are available.

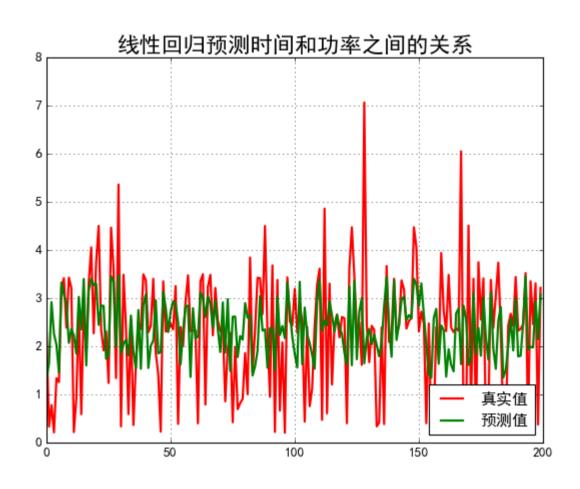
Data Set Characteristics:	Multivariate, Time-Series	Number of Instances:	2075259	Area:	Physical
Attribute Characteristics:	Real	Number of Attributes:	9	Date Donated	2012-08-30
Associated Tasks:	Regression, Clustering	Missing Values?	Yes	Number of Web Hits:	135342

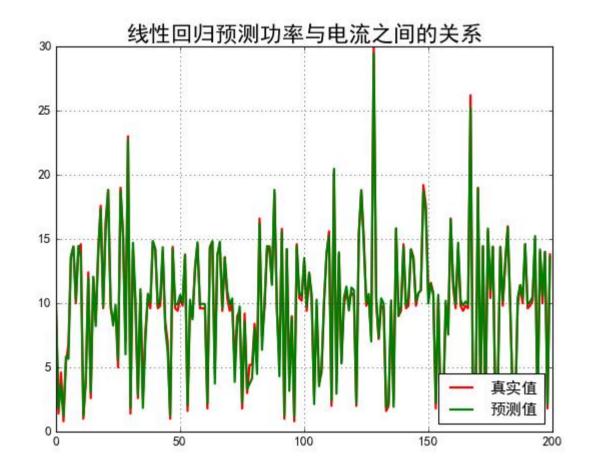
Attribute Information:

- 1.date: Date in format dd/mm/yyyy
- 2.time: time in format hh:mm:ss
- 3.global_active_power: household global minute-averaged active power (in kilowatt)
- 4. global reactive power: household global minute-averaged reactive power (in kilowatt)
- 5.voltage: minute-averaged voltage (in volt)
- 6.global_intensity: household global minute-averaged current intensity (in ampere)
- 7.sub_metering_1: energy sub-metering No. 1 (in watt-hour of active energy). It corresponds to the kitchen, containing mainly a dishwasher, an oven and a microwave (hot plates are not electric but gas powered).
- 8.sub_metering_2: energy sub-metering No. 2 (in watt-hour of active energy). It corresponds to the laundry room, containing a washing-machine, a tumble-drier, a refrigerator and a light.
- 9.sub_metering_3: energy sub-metering No. 3 (in watt-hour of active energy). It corresponds to an electric water-heater and an air-conditioner.



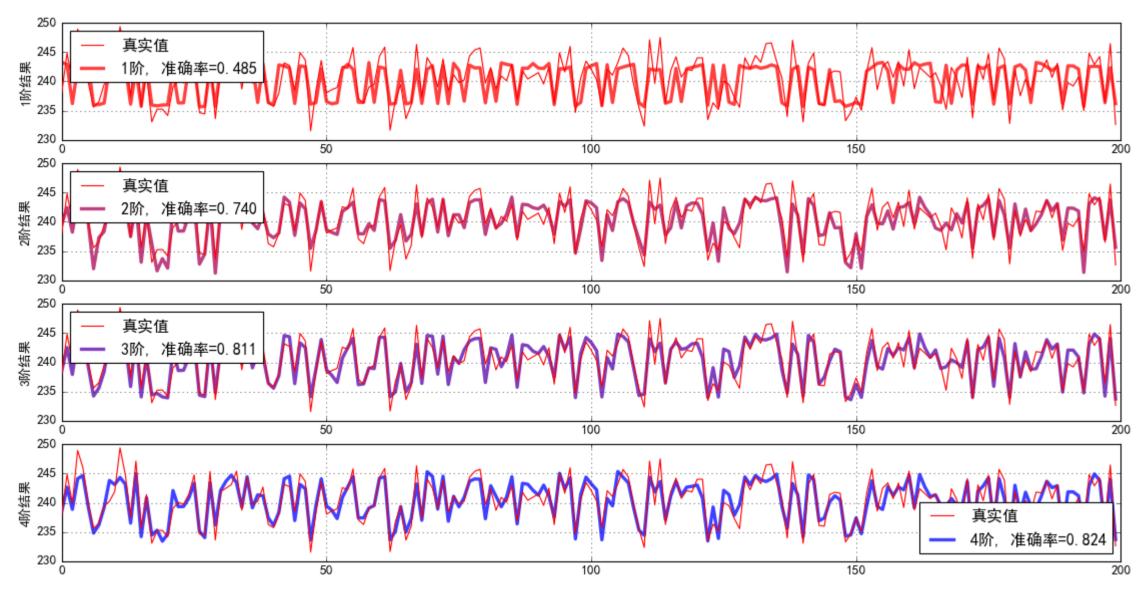
普通最小二乘法线性回归案例







普通最小二乘法线性回归案例





目标函数(loss/cost function)

■0-1损失函数
$$J(\theta) = \begin{cases} 1, Y \neq f(X) \\ 0, Y = f(X) \end{cases}$$

■感知损失函数
$$J(\theta) = \begin{cases} 1, |Y-f(X)| > t \\ 0, |Y-f(X)| \le t \end{cases}$$

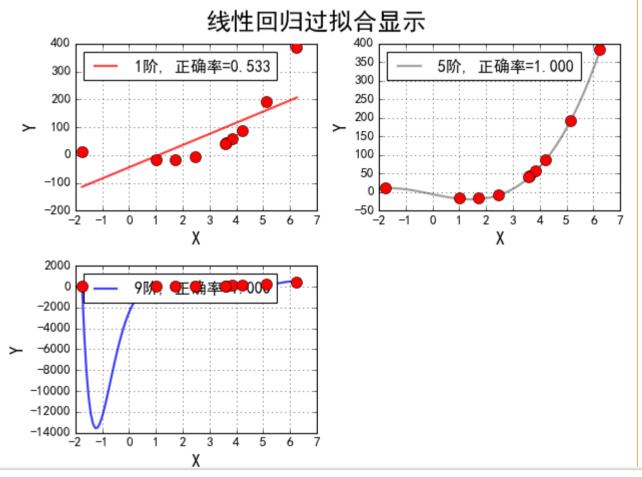
平方和损失函数
$$J(\theta) = \sum_{i=1}^{m} (h_{\theta}(x^{(i)}) - y^{(i)})^2$$

■绝对值损失函数
$$J(\theta) = \sum_{i=1}^{m} \left| h_{\theta}(x^{(i)}) - y^{(i)} \right|$$

■对数损失函数
$$J(\theta) = \sum_{i=1}^{m} (y^{(i)} \log h_{\theta}(x^{(i)}))$$



过拟合





1阶,系数为: [-44.14102611 40.05964256]

5阶,系数为: [-5.60899679-14.80109301 0.75014858 2.11170671 -0.07724668 0.00566633]

9阶,系数为: [-2465.58378507 6108.6381056 -5111.99327317 974.74973548 1078.89648247 -829.50276827 266.13230319 -45.71741527

4.11582735 -0.15281063]



线性回归的过拟合

- ■目标函数: $J(\theta) = \frac{1}{2} \sum_{i=1}^{m} (h_{\theta}(x^{(i)}) y^{(i)})^2$
- ■为了防止数据过拟合,也就是的θ值在样本空间中不能过大/过小,可以在目标函数之上增加一个平方和损失:

$$J(\theta) = \frac{1}{2} \sum_{i=1}^{m} (h_{\theta}(x^{(i)}) - y^{(i)}) + \lambda \sum_{i=1}^{n} \theta_{j}^{2}$$

■正则项(norm): $\lambda \sum_{j=1}^n \theta_j^2$; 这里这个正则项叫做L2-norm



过拟合和正则项

L2-norm:

$$J(\theta) = \frac{1}{2} \sum_{i=1}^{m} (h_{\theta}(x^{(i)}) - y^{(i)}) + \lambda \sum_{i=1}^{n} \theta_{j}^{2} \qquad \lambda > \mathbf{O}$$

■L1-norm:

$$J(\theta) = \frac{1}{2} \sum_{i=1}^{m} \left(h_{\theta} \left(x^{(i)} \right) - y^{(i)} \right) + \lambda \sum_{j=1}^{n} \left| \theta_{j} \right| \qquad \mathcal{A} > \mathbf{O}$$



Ridge回归

■使用L2正则的线性回归模型就称为Ridge回归(岭回归)

$$J(\theta) = \frac{1}{2} \sum_{i=1}^{m} (h_{\theta}(x^{(i)}) - y^{(i)}) + \lambda \sum_{i=1}^{n} \theta_{i}^{2} \qquad \mathcal{A} > \mathbf{O}$$



LASSO回归

■使用L1正则的线性回归模型就称为LASSO回归(Least Absolute Shrinkage and Selection Operator)

$$J(\theta) = \frac{1}{2} \sum_{i=1}^{m} \left(h_{\theta} \left(x^{(i)} \right) - y^{(i)} \right) + \lambda \sum_{j=1}^{n} \left| \theta_{j} \right| \quad \mathcal{A} > \mathbf{O}$$



Ridge(L1-norm)和LASSO(L2-norm)比较

- L2-norm中,由于对于各个维度的参数缩放是在一个圆内缩放的,不可能导致有维度参数变为0的情况,那么也就不会产生稀疏解;实际应用中,数据的维度中是存在噪音和冗余的,稀疏的解可以找到有用的维度并且减少冗余,提高回归预测的准确性和鲁棒性(减少了overfitting)(L2-norm可以达到最终解的稀疏性的要求)
- Ridge模型具有较高的准确性、鲁棒性以及稳定性;LASSO模型具有较高的求解速度。



Ridge(L1-norm)和LASSO(L2-norm)比较

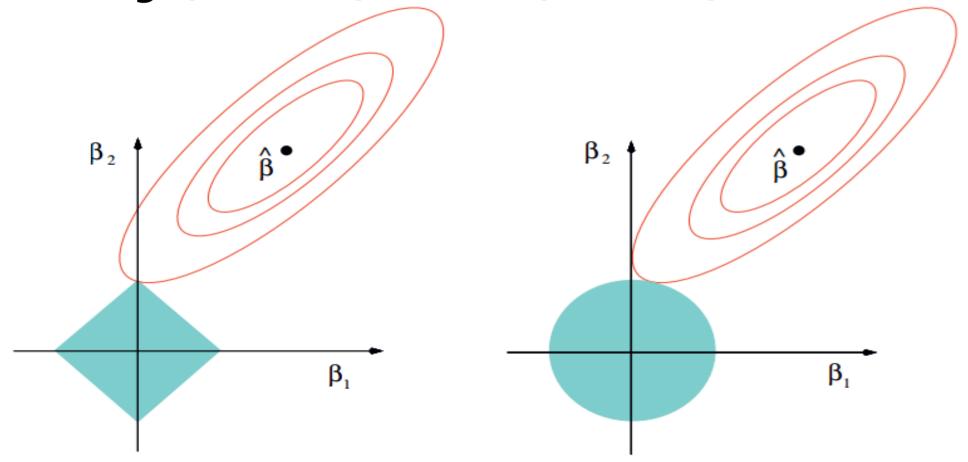


FIGURE 3.11. Estimation picture for the lasso (left) and ridge regression (right). Shown are contours of the error and constraint functions. The solid blue areas are the constraint regions $|\beta_1| + |\beta_2| \le t$ and $\beta_1^2 + \beta_2^2 \le t^2$, respectively, while the red ellipses are the contours of the least squares error function.



Elasitc Net

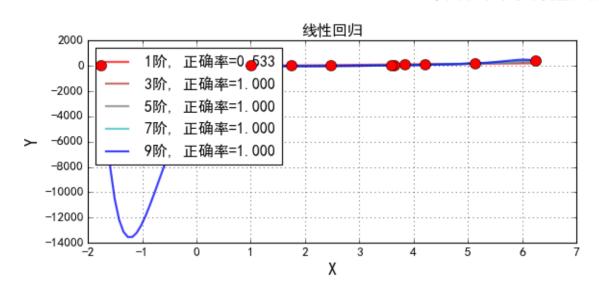
■同时使用L1正则和L2正则的线性回归模型就称为Elasitc Net算法(弹性网络算法)

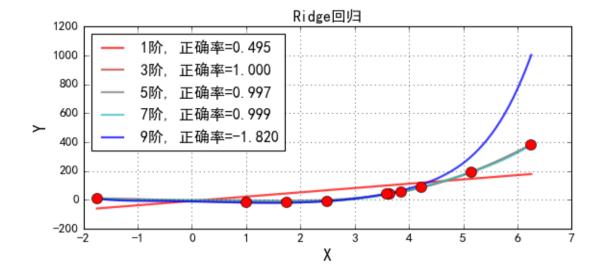
$$J(\theta) = \frac{1}{2} \sum_{i=1}^{m} \left(h_{\theta}(x^{(i)}) - y^{(i)} \right) + \lambda \left(p \sum_{j=1}^{n} \left| \theta_{j} \right| + (1-p) \sum_{j=1}^{n} \theta_{j}^{2} \right) \qquad \begin{cases} \lambda > 0 \\ p \in [0,1] \end{cases}$$

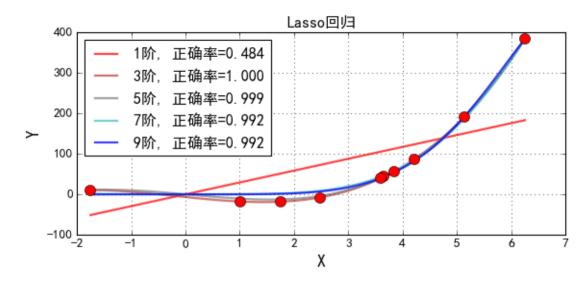


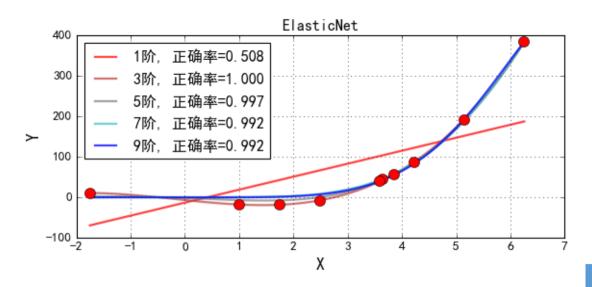
线性回归算法过拟合比较(一)

各种不同线性回归过拟合显示











线性回归算法过拟合比较(二)

```
线性回归:1阶,
            系数为:
                     [-44, 14102611
                                  40.059642561
线性回归:3阶,系数为:
                     [ -6.80525963 -13.743068
                                               0.93453895
                                                           1.798447911
线性回归:5阶,系数为:
                     [ -5,60899679 -14,80109301
                                               0.75014858
                                                           2.11170671 -0.07724668
                                                                                  -0.005666331
钱性回归:7阶,系数为:
                                  52, 38570529 -29, 56451338
                     [-41, 70721172
                                                         -7.66322829
                                                                      12,07162703
                                                                                 -3.86969096
                                                                                              0.53286096
                                                                                                         -0.027255361
                     [-2465, 58378507]
                                                                974, 74973548
                                                                             1078.89648247
                                    6108, 6381056 -5111, 99327317
                                                                                           -829, 50276827
                                                                                                          266, 13230319
                                                                                                                       -45,71741
527
       4, 11582735
                    -0.152810631
Ridge回归:1阶,系数为:
                       -6, 71593385
                                   29. 790900571
kidge回归:3阶,系数为:
                                 -13, 73679293
                      [-6.7819845]
                                                0.92827639
                                                            1, 799209541
kidge回归:5阶,系数为:
                      [-0.82920155 -1.07244754 -1.41803017 -0.93057536 0.88319116 -0.07073168]
kidge回归:7阶,系数为:
                      [-1,62586368 -2,18512108 -1,82690987 -2,27495708
                                                                  0.98685071 0.30551091 -0.10988434 0.008469081
                      0.80200162
                                                                       0.59148104 -0.23358235
                                                                                               0. 20297017
                                                                                                                       0.0132585
  -0.000721841
Lasso回归:1阶,系数为:
                                   29.27359177]
lasso回归:3阶,系数为:
                      -13.75928024
                                                0.93989323
                                                            1.797785981
lasso回归:5阶,系数为:
                                  -12.00109345
                                               -0.50746853
                                                            1,74395236
                                                                       0.07086952
                                                                                  -0.005836051
Lasso回归:7阶,系数为:
                                 ⊸.
                                            -0.
                                                       -0.08083315 0.19550746 0.03066137 -0.00020584 -0.000469281
Lasso回归:9阶,系数为
                                 -0.
                                            -0.
                                                                   0.04439727 0.05587113 0.00109023 -0.00021498 -0.00004479 -0.0000
                                                       ⊸0.
06741
ElasticNet:1阶,系数为:
                       [-13, 22089654
                                    32.083593381
ElasticNet:3阶,系数为:
                       -13.75928024
                                                 0.93989323
                                                             1, 797785981
ElasticNet:5阶,系数为:
                      [-1.65823671 -5.20271875 -1.26488859 0.94503683 0.2605984
                                                                              -0.01683786]
BlasticNet:7阶,系数为:
                                                        -0.15812511 0.22150166
                                                                              0.02955069 -0.00040066 -0.00046568]
                                  −0.
                                             −0.
flasticNet:9阶,系数为:
                                  ⊸.
                                             ⊸.
                                                        ⊸.
                                                                    0.05255118
                                                                              0.05364699 0.00111995 -0.00020596 -0.00004365 -0.000
006671
```



模型效果判断

$$MSE = \frac{1}{m} \sum_{i=1}^{m} (y_i - \widehat{y}_i)^2$$

$$RMSE = \sqrt{MSE} = \sqrt{\frac{1}{m} \sum_{i=1}^{m} (y_i - \widehat{y}_i)^2}$$

$$R^{2} = 1 - \frac{RSS}{TSS} = 1 - \frac{\sum_{i=1}^{m} (y_{i} - \hat{y}_{i})^{2}}{\sum_{i=1}^{m} (y_{i} - \bar{y})^{2}} \qquad \bar{y} = \frac{1}{m} \sum_{i=1}^{m} y_{i}$$



模型效果判断

- ■MSE:误差平方和,越趋近于0表示模型越拟合训练数据。
- ■RMSE: MSE的平方根,作用同MSE
- R²:取值范围(负无穷,1],值越大表示模型越拟合训练数据;最优解是1;当模型 预测为随机值的时候,有可能为负;若预测值恒为样本期望,R²为0
- ■TSS:总平方和TSS(Total Sum of Squares),表示样本之间的差异情况,是伪方差的m倍
- ■RSS: 残差平方和RSS(Residual Sum of Squares),表示预测值和样本值之间的差异情况,是MSE的m倍



机器学习调参

- 在实际工作中,对于各种算法模型(线性回归)来讲,我们需要获取θ、λ、p的值;θ的求解其实就是算法模型的求解,一般不需要开发人员参与(算法已经实现),主要需要求解的是λ和p的值,这个过程就叫做调参(超参)
- ■交叉验证:将训练数据分为多份,其中一份进行数据验证并获取最优的超参:λ和p;比如:十折交叉验证、五折交叉验证(scikit-learn中默认)等

训练数据

测试数据



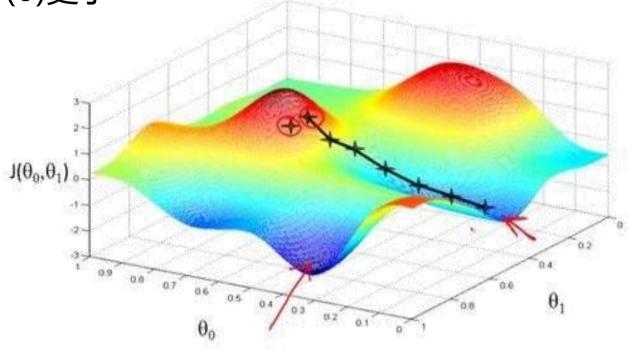
梯度下降算法

- ■目标函数θ求解 $J(\theta) = \frac{1}{2} \sum_{i=1}^{m} (h_{\theta}(x^{(i)}) y^{(i)})^2$
- ■初始化θ(随机初始化,可以初始为0)

■沿着负梯度方向迭代,更新后的θ使J(θ)更小

$$\theta = \theta - \alpha \bullet \frac{\partial J(\theta)}{\partial \theta}$$

◆α:学习率、步长



 $J(\theta) = \frac{1}{2} \sum_{i=1}^{m} (h_{\theta}(x^{(i)}) - y^{(i)})^{2}$



梯度方向

$$\frac{\partial}{\partial \theta_{j}} J(\theta) = \frac{\partial}{\partial \theta_{j}} \frac{1}{2} (h_{\theta}(x) - y)^{2}$$

$$= 2 \cdot \frac{1}{2} (h_{\theta}(x) - y) \cdot \frac{\partial}{\partial \theta_{j}} (h_{\theta}(x) - y)$$

$$= (h_{\theta}(x) - y) \frac{\partial}{\partial \theta} \left(\sum_{i=1}^{n} \theta_{i} x_{j} - y \right)$$

$$= (h_{\theta}(x) - y) x_{j}$$



批量梯度下降算法(BGD)

$$\frac{\partial}{\partial \theta_i} J(\theta) = (h_{\theta}(x) - y) x_j$$

$$\frac{\partial J(\theta)}{\partial \theta_{j}} = \sum_{i=1}^{m} \frac{\partial}{\partial \theta_{j}} = \sum_{i=1}^{m} \left(x_{j} \left(h_{\theta} \left(x^{(i)} \right) - y^{(i)} \right) \right) = \sum_{i=1}^{m} \left(h_{\theta} \left(x^{(i)} \right) - y^{(i)} \right) x_{j}^{(i)}$$

$$\theta_{j} = \theta_{j} + \alpha \sum_{i=1}^{m} \left(y^{(i)} - h_{\theta} \left(x^{(i)} \right) \right) x_{j}^{(i)}$$



随机梯度下降算法(SGD)

$$\frac{\partial}{\partial \theta_j} J(\theta) = (h_{\theta}(x) - y) x_j$$

for i= 1 to m,{

$$\theta_{j} = \theta_{j} + \alpha \left(y^{(i)} - h_{\theta} \left(x^{(i)} \right) \right) x_{j}^{(i)}$$

}



BGD和SGD算法比较

- ■SGD速度比BGD快(迭代次数少)
- ■SGD在某些情况下(全局存在多个相对最优解/J(θ)不是一个二次), SGD有可能跳出某些小的局部最优解,所以不会比BGD坏
- ■BGD一定能够得到一个局部最优解(在线性回归模型中一定是得到一个全局最优解),SGD由于随机性的存在可能导致最终结果比BGD的差
- ■注意:优先选择SGD



小批量梯度下降法(MBGD)

■如果即需要保证算法的训练过程比较快,又需要保证最终参数训练的准确率,而这正是小批量梯度下降法(Mini-batch Gradient Descent,简称MBGD)的初衷。MBGD中不是每拿一个样本就更新一次梯度,而且拿b个样本(b一般为10)的平均梯度作为更新方向。

for i= 1 to m/10, $\theta_j = \theta_j + \alpha \sum_{k=1}^{i+10} \left(y^{(k)} - h_\theta(x^{(k)}) \right) x_j^{(k)}$

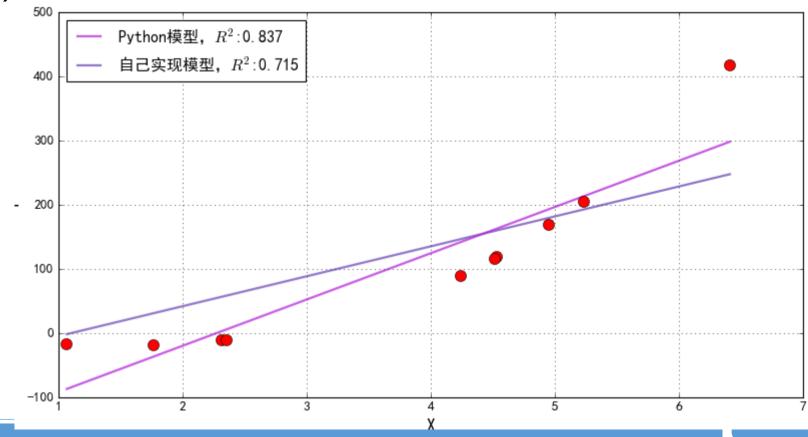


回归算法案例:基于梯度下降法实现线性回归算法

■基于梯度下降法编写程序实现回归算法,并自行使用模拟数据进行测试,同时对同样的模拟数据进行两种算法的比较(python sklearn LinearRegression和

自己实现的线性回归算法)

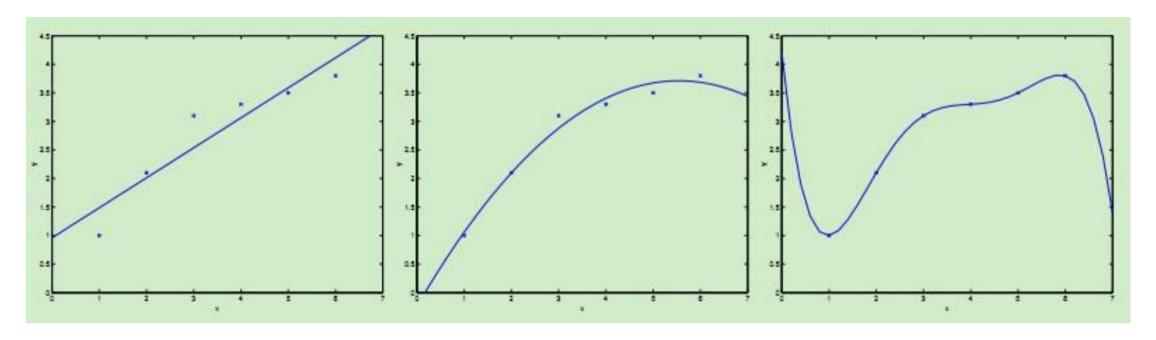
自定义的线性模型和模块中的线性模型比较





线性回归的扩展

- ■线性回归针对的是θ而言是一种,对于样本本身而言,样本可以是非线性的
- ■也就是说最终得到的函数f:x->y;函数f(x)可以是非线性的,比如:曲线等



$$y = \theta_0 + \theta_1 x$$

$$y = \theta_0 + \theta_1 x + \theta_2 x^2$$

$$y = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$$

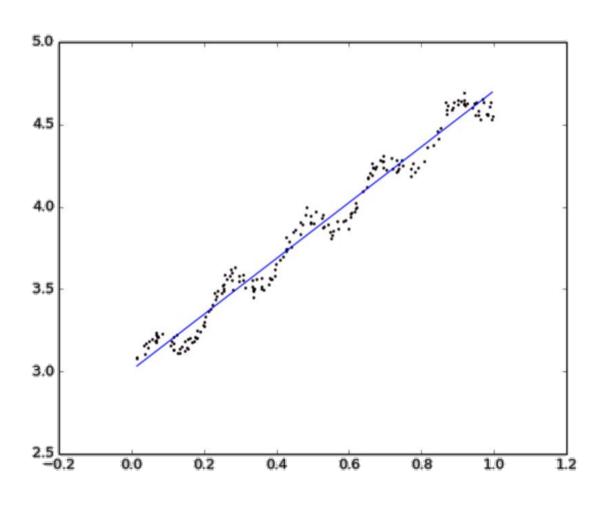


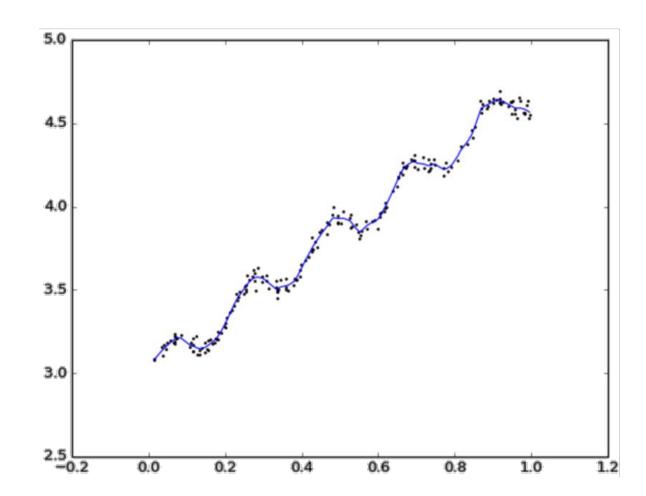
线性回归总结

- ■算法模型:线性回归(Linear)、岭回归(Ridge)、LASSO回归、Elastic Net
- ■正则化:L1-norm、L2-norm
- ■θ求解方式:最小二乘法(直接计算,目标函数是平方和损失函数)、梯度下降 (BGD\SGD\MBGD)



局部加权回归-直观理解







局部加权回归-损失函数

■普通线性回归损失函数:

$$J(\theta) = \sum_{i=1}^{m} \left(h_{\theta} \left(x^{(i)} \right) - y^{(i)} \right)^{2}$$

■局部加权回归损失函数:

$$J(\theta) = \sum_{i=1}^{m} w^{(i)} (h_{\theta}(x^{(i)}) - y^{(i)})^{2}$$



局部加权回归-权重值设置

■ w⁽ⁱ⁾是权重,它根据要预测的点与数据集中的点的距离来为数据集中的点赋权值。 当某点离要预测的点越远,其权重越小,否则越大。常用值选择公式为:

$$w^{(i)} = \exp\left(-\frac{(x^{(i)} - x)^2}{2k^2}\right)$$

- ■该函数称为指数衰减函数,其中k为波长参数,它控制了权值随距离下降的速率
- ■注意:使用该方式主要应用到样本之间的相似性考虑,主要内容在SVM中再考虑(核函数)

17, 40, 385, 05



回归算法综合案例(二):波士顿房屋租赁价格预测

■基于波士顿房屋租赁数据进行房屋租赁价格预测模型构建,分布使用Lasso回归、Ridge回两种回归算法构建模型,并分别构建1/2/3阶算法中的最优算法(参数),并比较这两种回归算法的效果;另外使用lasso回归算法做特征选择

0.31533

◆数据下载url: http://archive.ics.uci.edu/ml/datasets/Housing

Attribute Information:

```
0.52693
                                                                                                                                                                                   50.00
                                                                                              0.00
                                                                                                                        8.7250
                                                                                                                                 83, 00
                                                                                                                                                                             4, 63
1. CRIM: per capita crime rate by town
                                                                                   0.38214
                                                                                                                        8.0400
                                                                                                                                 86.50
                                                                                                                                                      307. 0 17. 40 387. 38
                                                                                                                                                                             3. 13
                                                                                                                                                                                   37.60
2. ZN: proportion of residential land zoned for lots over 25,000 sq.ft.
                                                                                   0.41238
                                                                                                                                                                                   31.60
                                                                                              0.00
                                                                                                                0.5040
                                                                                                                        7. 1630
                                                                                                                                                                             6.36
3. INDUS: proportion of non-retail business acres per town
                                                                                   0.29819
                                                                                                                0.5040
                                                                                                                        7,6860
                                                                                                                                         3, 3751
                                                                                              0.00
                                                                                                                                 17.00
                                                                                                                                                     307. 0 17. 40 377. 51
                                                                                                                                                                             3.92
                                                                                                                                                                                   46, 70
4. CHAS: Charles River dummy variable (= 1 if tract bounds river: 0 otherwise)
                                                                                   0.44178
                                                                                                                        6.5520
                                                                                                                0.5040
                                                                                                                                        3, 3751
                                                                                                                                                     307. 0 17. 40 380. 34
                                                                                                                                                                             3.76
                                                                                                                                                                                   31, 50
5. NOX: nitric oxides concentration (parts per 10 million)
                                                                                   0.53700
                                                                                                                                                                                   24, 30
                                                                                              0.00
                                                                                                                0.5040 5.9810
                                                                                                                                 68. 10 3. 6715
                                                                                                                                                      307. 0 17. 40 378. 35
                                                                                                                                                                            11, 65
6. RM: average number of rooms per dwelling
                                                                                   0.46296
                                                                                              0.00
                                                                                                                        7, 4120
                                                                                                                                        3, 6715
                                                                                                                                                                                   31, 70
                                                                                                                0.5040
                                                                                                                                 76, 90
                                                                                                                                                            17, 40, 376, 14
7. AGE: proportion of owner-occupied units built prior to 1940
                                                                                   0.57529
                                                                                                                        8, 3370
                                                                                                                                 73, 30
                                                                                                                                                                                   41, 70
                                                                                                                0.5070
                                                                                                                                                     307. 0 17. 40 385. 91
                                                                                                                                                                             2, 47
8. DIS: weighted distances to five Boston employment centres
                                                                                   0.33147
                                                                                              0.00
                                                                                                                        8.2470
                                                                                                                                                                             3.95
                                                                                                                                                                                   48.30
RAD: index of accessibility to radial highways
                                                                                   0.44791
                                                                                              0.00
                                                                                                                0.5070
                                                                                                                        6, 7260
                                                                                                                                 66, 50
                                                                                                                                         3, 6519
                                                                                                                                                            17, 40, 360, 20
                                                                                                                                                                             8, 05
                                                                                                                                                                                   29, 00
10. TAX: full-value property-tax rate per $10,000
                                                                                                                                        3.6519
                                                                                   0.33045
                                                                                              0.00
                                                                                                     6.200 0 0.5070
                                                                                                                        6.0860
                                                                                                                                 61.50
                                                                                                                                                     307. 0 17. 40 376. 75
                                                                                                                                                                            10.88
                                                                                                                                                                                   24.00
11. PTRATIO: pupil-teacher ratio by town
                                                                                                                                 76.50
                                                                                                                                                     307. 0 17. 40 388. 45
                                                                                                                                                                             9.54
                                                                                   0.52058
                                                                                              0.00
                                                                                                                0.5070
                                                                                                                        6.6310
                                                                                                                                        4. 1480
12. B: 1000(Bk - 0.63)<sup>2</sup> where Bk is the proportion of blacks by town
                                                                                   0.51183
                                                                                              0.00
                                                                                                                                                                                   31.50
13. LSTAT: % lower status of the population
                                                                                   0.08244
                                                                                                                                         6.1899
                                                                                                                                                                                   23.70
                                                                                             30.00
                                                                                                                                 18.50
                                                                                                                                                            16,60 379,41

    MEDV: Median value of owner-occupied homes in $1000's
```

0.00

0.5040

8, 2660

78. 30

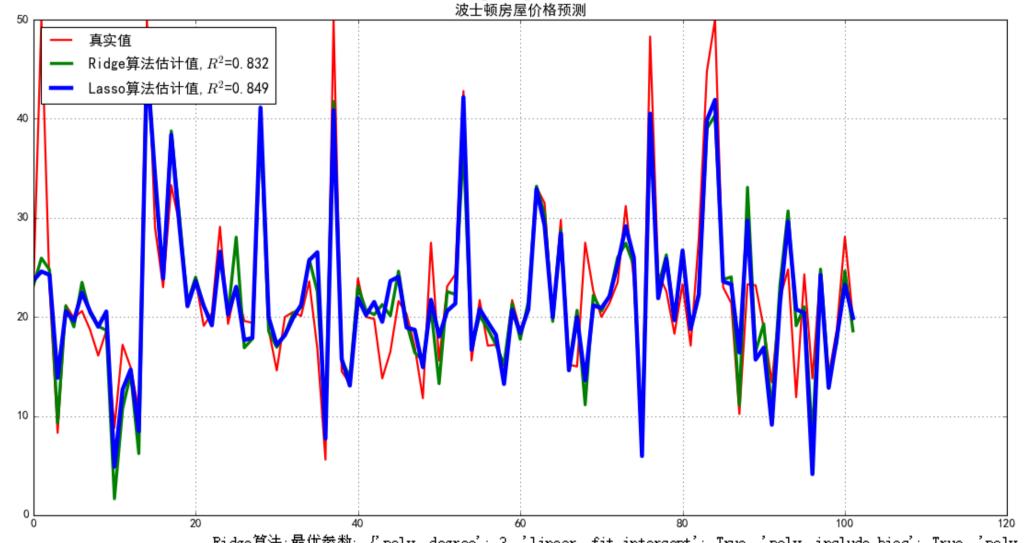
2, 8944

4, 14 44, 80



回归算法综合案例(二):波士顿房屋租赁价格预测





Ridge算法:最优参数:{'poly_degree': 3, 'linear_fit_intercept': True, 'poly_include_bias': True, 'poly_interaction_only': True}

Ridge算法:R值=0.832

Lasso算法:最优参数: {'poly_degree': 3, 'linear_fit_intercept': False, 'poly_include_bias': True, 'poly_interaction_only': True}

Lasso 算法: R值=0.849



回归算法综合案例(二):波士顿房屋租赁价格预测

参数: [('CRIM', 22.600592809201991), ('ZN', -0.93534557687414488), ('INDUS', 1.0202352850146854), ('CHAS', -0.0), ('NOX', 0.594831384154614 9), ('RM', -1.8002644875942369), ('AGE', 2.5861907995357281), ('DIS', -0.064956108249539249), ('RAD', -2.8017533936656509), ('TAX', 1.934332 9692037559), ('PTRATIO', -1.7218677875512203), ('B', -2.2762334623842988), ('LSTAT', 0.70288003005515387)] 截距: 0.0

CHAS列的数据对于LassoCV模型而言无用,所以在 进行实际模型构建的时候,可以不考虑该特征



回归算法综合案例(三):葡萄酒质量预测

- ■基于葡萄酒数据进行葡萄酒质量预测模型构建,分布使用线性回归、Lasso回归、Ridge回归、Elasitc Net四类回归算法构建模型(并分别测试1/2/3阶),并比较这些回归算法的效果
 - ◆数据下载url: http://archive.ics.uci.edu/ml/datasets/Wine+Quality

Attribute Information:

For more information, read [Cortez et al., 2009]. Input variables (based on physicochemical tests):

- 1 fixed acidity
- 2 volatile acidity
- 3 citric acid
- 4 residual sugar
- 5 chlorides
- 6 free sulfur dioxide
- 7 total sulfur dioxide
- 8 density
- 9 pH
- 10 sulphates
- 11 alcohol

Output variable (based on sensory data):

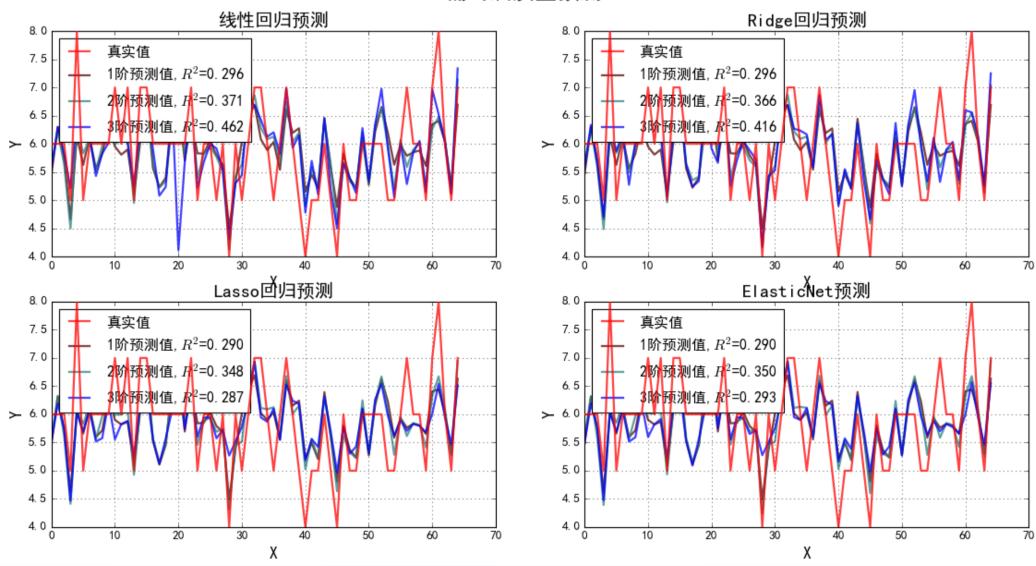
12 - quality (score between 0 and 10)

```
2 7.4; 0.7; 0; 1.9; 0.076; 11; 34; 0.9978; 3.51; 0.56; 9.4; 5
3 7.8; 0.88; 0; 2.6; 0.098; 25; 67; 0.9968; 3.2; 0.68; 9.8; 5
4 7.8; 0.76; 0.04; 2.3; 0.092; 15; 54; 0.997; 3.26; 0.65; 9.8; 5
5 11.2; 0.28; 0.56; 1.9; 0.075; 17; 60; 0.998; 3.16; 0.58; 9.8; 6
6 7.4; 0.7; 0; 1.9; 0.076; 11; 34; 0.9978; 3.51; 0.56; 9.4; 5
7 7.4; 0.66; 0; 1.8; 0.075; 13; 40; 0.9978; 3.51; 0.56; 9.4; 5
8 7.9; 0.6; 0.06; 1.6; 0.069; 15; 59; 0.9964; 3.3; 0.46; 9.4; 5
9 7.3; 0.65; 0; 1.2; 0.065; 15; 21; 0.9946; 3.39; 0.47; 10; 7
10 7.8; 0.58; 0.02; 2; 0.073; 9; 18; 0.9968; 3.36; 0.57; 9.5; 7
11 7.5; 0.5; 0.36; 6.1; 0.071; 17; 102; 0.9978; 3.35; 0.8; 10.5; 5
```



回归算法综合案例(三):葡萄酒质量预测

葡萄酒质量预测





Logistic回归

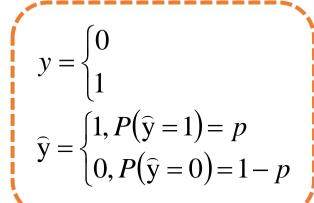
Logistic/sigmoid函数
$$p = h_{\theta}(x) = g(\theta^T x) = \frac{1}{1 + e^{-\theta^T x}}$$
 $y = \begin{cases} 0 \\ 1 \end{cases}$

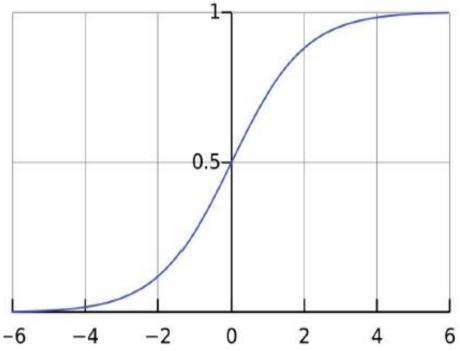
$$g(z) = \frac{1}{1 + e^{-z}}$$

$$g'(z) = \left(\frac{1}{1+e^{-z}}\right)' = \frac{e^{-z}}{\left(1+e^{-z}\right)^2}$$

$$= \frac{1}{1+e^{-z}} \cdot \frac{e^{-z}}{1+e^{-z}} = \frac{1}{1+e^{-z}} \cdot \left(1 - \frac{1}{1+e^{-z}}\right)$$

$$= g(z) \cdot (1 - g(z))$$







Logistic回归及似然函数

■假设: $P(y=1|x;\theta)=h_{\theta}(x)$ $P(y=0|x;\theta)=1-h_{\theta}(x)$

	y=1	y=0
p(y x)	θ	1-0

$$P(y \mid x; \theta) = (h_{\theta}(x))^{y} (1 - h_{\theta}(x))^{(1-y)}$$

■似然函数: $L(\theta) = p(\vec{y} \mid X; \theta) = \prod_{i=1}^{m} p(y^{(i)} \mid x^{(i)}; \theta)$ $= \prod_{i=1}^{m} (h_{\theta}(x^{(i)}))^{y^{(i)}} (1 - h_{\theta}(x^{(i)}))^{(1-y^{(i)})}$

■对数似然函数:
$$\ell(\theta) = \log L(\theta) = \sum_{i=1}^{m} \left(y^{(i)} \log h_{\theta}(x^{(i)}) + \left(1 - y^{(i)}\right) \log \left(1 - h_{\theta}(x^{(i)})\right) \right)$$



最大似然/极大似然函数的随机梯度

$$\frac{\partial \ell(\theta)}{\partial \theta_{j}} = \sum_{i=1}^{m} \left(\frac{y^{(i)}}{h_{\theta}(x^{(i)})} - \frac{1 - y^{(i)}}{1 - h_{\theta}(x^{(i)})} \right) \cdot \frac{\partial h_{\theta}(x^{(i)})}{\partial \theta_{j}}$$

$$= \sum_{i=1}^{m} \left(\frac{y^{(i)}}{g(\theta^{T} x^{(i)})} - \frac{1 - y^{(i)}}{1 - g(\theta^{T} x^{(i)})} \right) \cdot \frac{\partial g(\theta^{T} x^{(i)})}{\partial \theta_{j}}$$

$$= \sum_{i=1}^{m} \left(\frac{y^{(i)}}{g(\theta^{T} x^{(i)})} - \frac{1 - y^{(i)}}{1 - g(\theta^{T} x^{(i)})} \right) \cdot g(\theta^{T} x^{(i)}) \left(1 - g(\theta^{T} x^{(i)}) \right) \cdot \frac{\partial \theta^{T} x^{(i)}}{\partial \theta_{j}}$$

$$= \sum_{i=1}^{m} \left(y^{(i)} \left(1 - g \left(\theta^{T} x^{(i)} \right) \right) - \left(1 - y^{(i)} \right) g \left(\theta^{T} x^{(i)} \right) \right) \cdot x_{j}^{(i)} = \sum_{i=1}^{m} \left(y^{(i)} - g \left(\theta^{T} x^{(i)} \right) \right) \cdot x_{n}^{(i)}$$



θ参数求解

Logistic回归θ参数的求解过程为(类似梯度下降方法,往正梯度方向迭代):

$$\theta_{j} = \theta_{j} + \alpha \sum_{i=1}^{m} (y^{(i)} - h_{\theta}(x^{(i)})) x_{j}^{(i)}$$

$$\theta_j = \theta_j + \alpha \left(y^{(i)} - h_\theta(x^{(i)}) \right) x_j^{(i)}$$



极大似然估计与Logistic回归损失函数

$$L(\theta) = \prod_{i=1}^{m} p(y^{(i)} \mid x^{(i)}; \theta) = \prod_{i=1}^{m} p_i^{y^{(i)}} (1 - p_i)^{1 - y^{(i)}} \qquad p_i = h_{\theta}(x^{(i)}) = \frac{1}{1 + e^{-\theta^T x^{(i)}}} = \frac{1}{1 + e^{-f_i}}$$

$$\ell(\theta) = \ln L(\theta) = \sum_{i=1}^{m} \ln \left[p_i^{y^{(i)}} (1 - p_i)^{1 - y^{(i)}} \right] = \sum_{i=1}^{m} \ln \left[\left(\frac{1}{1 + e^{-f_i}} \right)^{y^{(i)}} \left(\frac{1}{1 + e^{f_i}} \right)^{1 - y^{(i)}} \right]$$

$$loss(y^{(i)}, \hat{y}^{(i)}) = -\ell(\theta)$$

$$= \sum_{i=1}^{m} [y^{(i)} \ln(1 + e^{-f_i}) + (1 - y^{(i)}) \ln(1 + e^{f_i})]$$

$$= \begin{cases} \sum_{i=1}^{m} \ln(1 + e^{-f_i}), y^{(i)} = 1 \\ \sum_{i=1}^{m} \ln(1 + e^{f_i}), y^{(i)} = 0 \end{cases} \Rightarrow loss(y^{(i)}, \hat{y}^{(i)}) = \sum_{i=1}^{m} \ln(1 + e^{(1 - 2y^{(i)})\theta^{T}x^{(i)}}), y^{(i)} = \begin{cases} 1 \\ 0 \end{cases}$$



Logistic案例(一):乳腺癌分类

- ■基于<u>病理数据</u>进行乳腺癌预测(复发4/正常2),使用Logistic算法构建模型
 - ◆数据来源:

http://archive.ics.uci.edu/ml/datasets/Breast+Cancer+Wisconsin+%28Original%

29

#	Attribute	Domain
2. 3. 4. 5. 6. 7. 8. 9.	Sample code number Clump Thickness Uniformity of Cell Size Uniformity of Cell Shape Marginal Adhesion Single Epithelial Cell Size Bare Nuclei Bland Chromatin Normal Nucleoli Mitoses Class:	id number 1 - 10 1 - 10 1 - 10 1 - 10 1 - 10 1 - 10 1 - 10 1 - 10 1 - 10 1 - 10 1 - 10 1 - 10 1 - 10 1 - 10 1 - 10 1 - 10 1 - 10 1 - 10

```
1000025, 5, 1, 1, 1, 2, 1, 3, 1, 1, 2

1002945, 5, 4, 4, 5, 7, 10, 3, 2, 1, 2

1015425, 3, 1, 1, 1, 2, 2, 3, 1, 1, 2

1016277, 6, 8, 8, 1, 3, 4, 3, 7, 1, 2

1017023, 4, 1, 1, 3, 2, 1, 3, 1, 1, 2

1017122, 8, 10, 10, 8, 7, 10, 9, 7, 1, 4

1018099, 1, 1, 1, 1, 2, 10, 3, 1, 1, 2

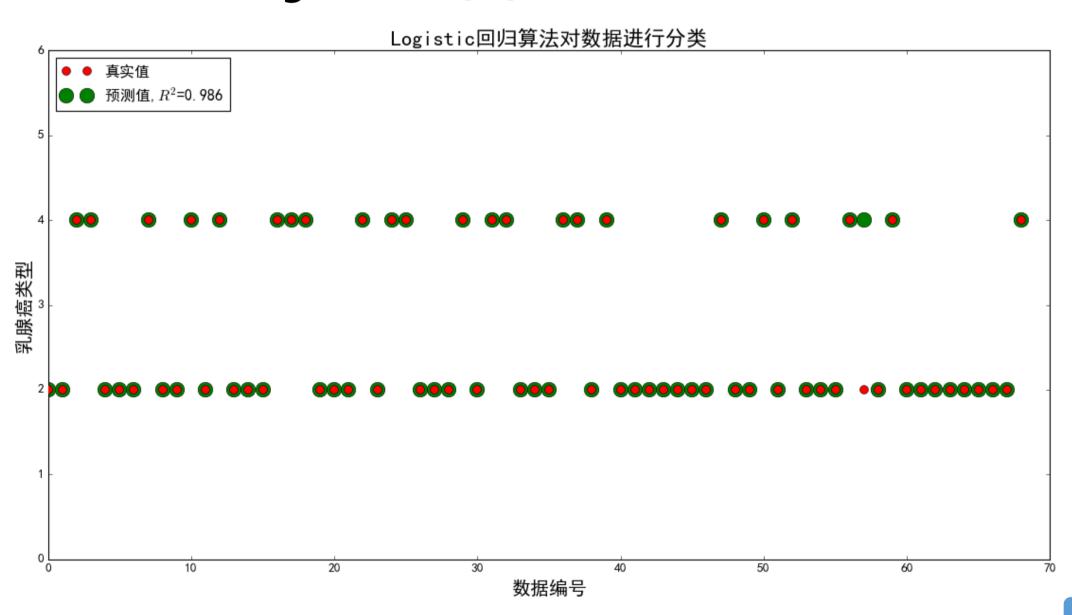
1018561, 2, 1, 2, 1, 2, 1, 3, 1, 1, 2

1033078, 2, 1, 1, 1, 2, 1, 1, 1, 5, 2

1035283, 1, 1, 1, 1, 1, 1, 1, 3, 1, 1, 2
```



Logistic案例(一):乳腺癌分类





Softmax回归

- softmax回归是logistic回归的一般化,适用于K分类的问题,第k类的参数为向量 θ_k ,组成的二维矩阵为 θ_{k*n} ;
- softmax函数的本质就是将一个K维的任意实数向量压缩(映射)成另一个K维的实数向量,其中向量中的每个元素取值都介于(0,1)之间。
- ■softmax回归概率函数为:

$$p(y = k \mid x; \theta) = \frac{e^{\theta_k^T x}}{\sum_{l=1}^K e^{\theta_l^T x}}, k = 1, 2 \dots, K$$

Softmax回归与似然估计

□似然函数 $L(\theta) = \prod_{i=1}^{m} \prod_{k=1}^{K} p(y = k \mid x^{(i)}; \theta)^{y_k^{(i)}} = \prod_{i=1}^{m} \prod_{k=1}^{K} \left(\frac{e^{\theta_k^T x^{(i)}}}{\sum_{i=1}^{K} e^{\theta_l^T x^{(i)}}} \right)^{y_k}$

■对数似然
$$\ell(\theta) = \ln L(\theta) = \sum_{i=1}^{m} \sum_{k=1}^{K} y_k^{(i)} \left(\theta_k^T x^{(i)} - \ln \sum_{l=1}^{K} e^{\theta_l^T x^{(i)}} \right)$$
$$\ell(\theta) = \sum_{k=1}^{K} y_k \left(\theta_k^T x - \ln \sum_{l=1}^{K} e^{\theta_l^T x} \right)$$

$$\ell(\theta) = \sum_{k=1}^{K} y_k \left(\theta_k^T x - \ln \sum_{l=1}^{K} e^{\theta_l^T x} \right)$$

■随机梯度

$$\frac{\partial \ell(\theta)}{\partial \theta_k} = y_k x - \frac{e^{\theta_k^T x}}{\sum_{l=1}^K e^{\theta_l^T x}} x = \left(y_k - \frac{e^{\theta_k^T x}}{\sum_{l=1}^K e^{\theta_l^T x}} \right) \cdot x = \left(y_k - p(y = k \mid x; \theta) \right) \cdot x$$



Softmax案例(一): 葡萄酒质量分类

- ■基于<u>葡萄酒数据</u>进行葡萄酒质量预测模型构建,使用Softmax算法构建模型, 并获取Softmax算法构建的模型效果(注意:分成11类)
 - ◆数据来源: http://archive.ics.uci.edu/ml/datasets/Wine+Quality

Attribute Information:

For more information, read [Cortez et al., 2009]. Input variables (based on physicochemical tests):

- 1 fixed acidity
- 2 volatile acidity
- 3 citric acid
- 4 residual sugar
- 5 chlorides
- 6 free sulfur dioxide
- 7 total sulfur dioxide
- 8 density
- 9 pH
- 10 sulphates
- 11 alcohol

Output variable (based on sensory data):

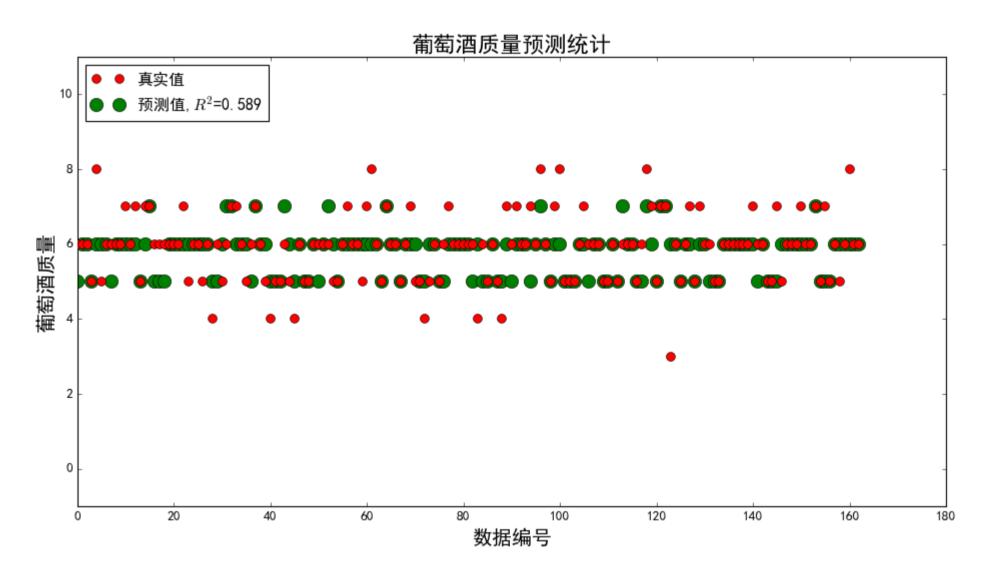
12 - quality (score between 0 and 10)

```
2 7.4;0.7;0;1.9;0.076;11;34;0.9978;3.51;0.56;9.4;5
3 7.8;0.88;0;2.6;0.098;25;67;0.9968;3.2;0.68;9.8;5
```

- 4 7.8; 0.76; 0.04; 2.3; 0.092; 15; 54; 0.997; 3.26; 0.65; 9.8; 5
- 5 11.2;0.28;0.56;1.9;0.075;17;60;0.998;3.16;0.58;9.8;6
- 6 7.4;0.7;0;1.9;0.076;11;34;0.9978;3.51;0.56;9.4;5
- 7 7.4;0.66;0;1.8;0.075;13;40;0.9978;3.51;0.56;9.4;5
- 8 7.9;0.6;0.06;1.6;0.069;15;59;0.9964;3.3;0.46;9.4;5
- 9 7.3;0.65;0;1.2;0.065;15;21;0.9946;3.39;0.47;10;7
- LO 7.8;0.58;0.02;2;0.073;9;18;0.9968;3.36;0.57;9.5;7
- 11 7.5;0.5;0.36;6.1;0.071;17;102;0.9978;3.35;0.8;10.5;5



Softmax案例(一): 葡萄酒质量分类





分类问题综合案例(一):信贷审批

- ■基于信贷数据进行用户信贷分类,使用Logistic算法和KNN算法构建模型,并 比较这两大类算法的效果
 - ◆数据来源: http://archive.ics.uci.edu/ml/datasets/Credit+Approval

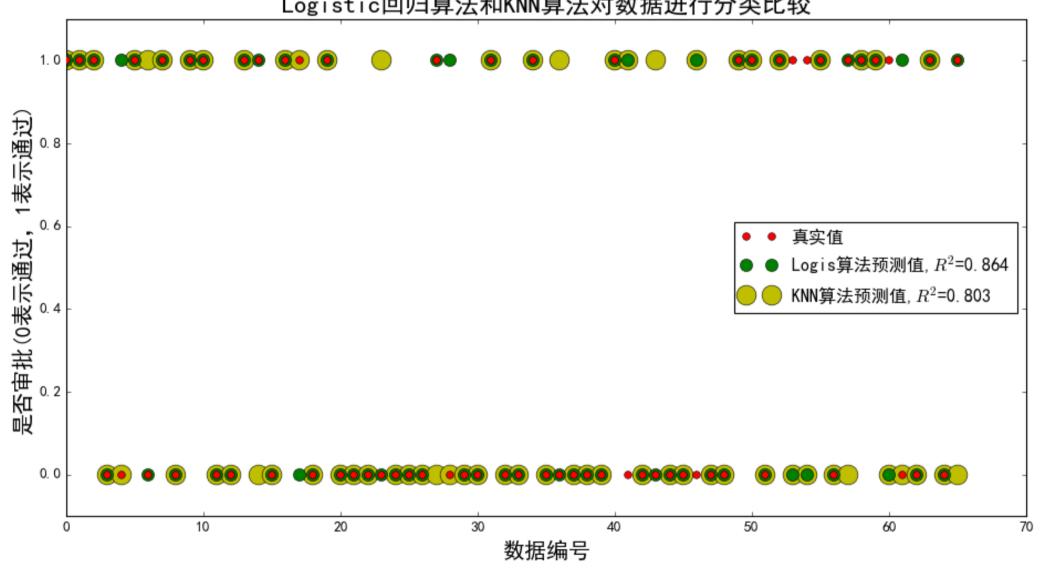
Attribute Information:

```
A1: b. a.
                                            a, 40, 83, 10, u, g, q, h, 1, 75, t, f, 0, f, g, 00029, 837, +
A2: continuous
A3: continuous
                                            b, 19.33, 9.5, u, g, q, v, 1, t, f, 0, t, g, 00060, 400, +
A4: u. v. l. t.
                                            a, 32, 33, 0, 54, u, g, cc, v, 0, 04, t, f, 0, f, g, 00440, 11177, +
A5: q, p, qq.
A6: c, d, cc, i, j, k, m, r, q, w, x, e, aa, ff.
                                            b, 36, 67, 3, 25, u, g, q, h, 9, t, f, 0, t, g, 00102, 639, +
A7: v, h, bb, j, n, z, dd, ff, o.
                                            b, 37. 50, 1. 125, y, p, d, v, 1. 5, f, f, 0, t, g, 00431, 0, +
A8: continuous.
A9: t, f.
                                            a, 25.08, 2.54, y, p, aa, v, 0.25, t, f, 0, t, g, 00370, 0, +
A10: t. f.
                                            b, 41.33, 0, u, g, c, bb, 15, t, f, 0, f, g, 00000, 0, +
A11: continuous.
A12: t. f.
                                            b, 56.00, 12.5, u, g, k, h, 8, t, f, 0, t, g, 00024, 2028, +
A13: g, p, s.
                                            a, 49.83, 13.585, u, g, k, h, 8.5, t, f, 0, t, g, 00000, 0, +
A14: continuous.
A15: continuous
A16: +,- (class attribute)
```



分类问题综合案例(一):信贷审批

Logistic回归算法和KNN算法对数据进行分类比较





分类问题综合案例(二): 鸢尾花数据分类

- 基于<u>鸢尾花数据</u>进行分类模型构建,使用logistics算法和KNN算法进行构建, 并计算两种算法的AOC值,以及画出对应的ORC曲线
 - ◆数据来源:http://archive.ics.uci.edu/ml/datasets/Iris

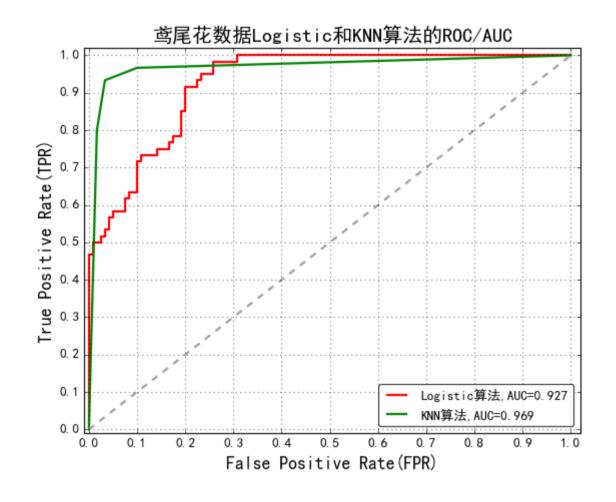
Data Set Characteristics:	Multivariate	Number of Instances:	150	Area:	Life
Attribute Characteristics:	Real	Number of Attributes:	4	Date Donated	1988-07-01
Associated Tasks:	Classification	Missing Values?	No	Number of Web Hits:	1319181

Attribute Information:

- 1. sepal length in cm
- 2. sepal width in cm
- 3. petal length in cm
- 4. petal width in cm
- 5. class:
- -- Iris Setosa
- -- Iris Versicolour
- -- Iris Virginica

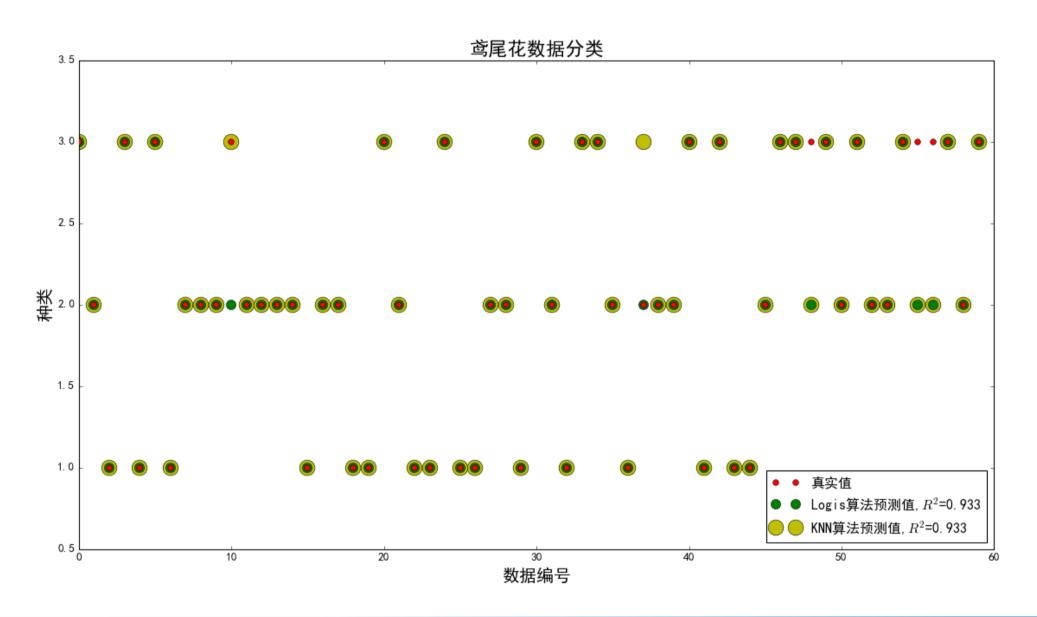


分类问题综合案例(二): 鸢尾花数据分类





分类问题综合案例(二): 鸢尾花数据分类





总结

- 线性模型一般用于回归问题, Logistic和Softmax模型一般用于分类问题
- 求θ的主要方式是梯度下降算法,梯度下降算法是参数优化的重要手段,主要是SGD,适用于在线学习以及跳出局部极小值
- Logistic/Softmax回归是实践中解决分类问题的最重要的方法
- 广义线性模型对样本要求不必要服从正态分布、只需要服从指数分布簇(二项分布、泊松分布、伯努利分布、指数分布等)即可;广义线性模型的自变量可以是连续的也可以是离散的。





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