

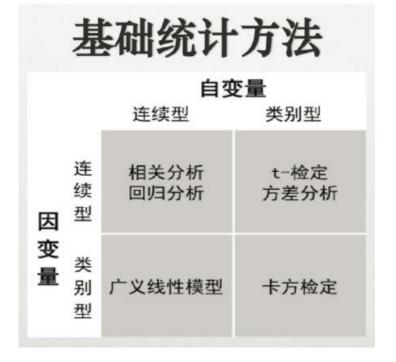
第六课(第16-18课时) 回归分析和基于模拟的分析

- 线性回归分析
- 点估计和区间估计
- 置换检验 (Permutation Test)
- 自助法(Bootstrap)

前情回顾



- > 如何检验一个变量的一组取值是否符合某种分布
 - 图形分析
 - 使用样本数字特征
 - 使用假设检验?
- > 如何检验两个变量之间的关系
 - 图形分析
 - 根据变量类型选择合适的分析方法
 - 如不相互独立,则进一步分析



载入数据:tips.csv

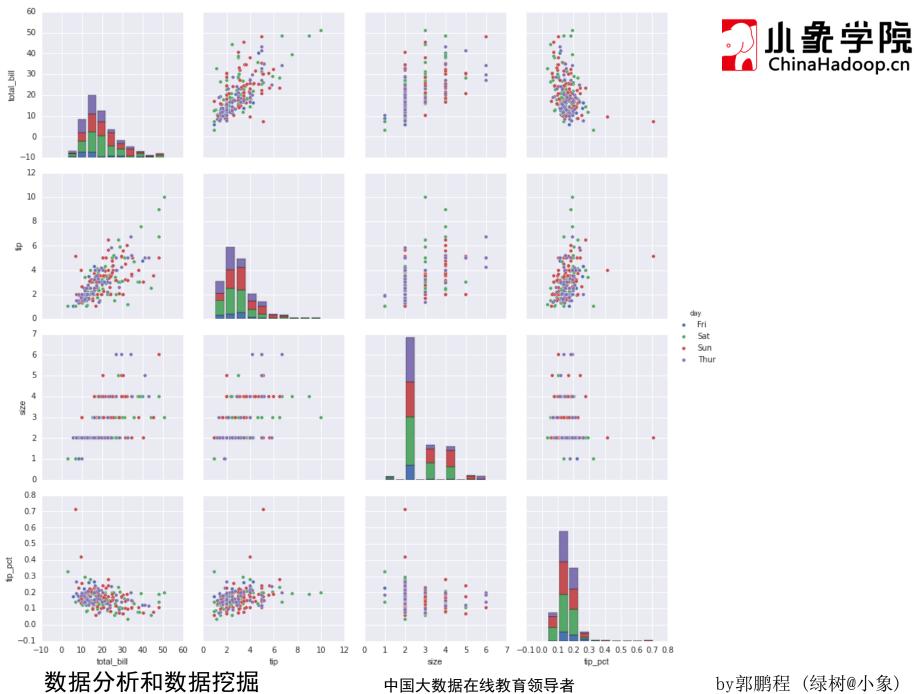


- > 载入常用库
 - import pandas as pd
 - import numpy as np
 - import matplotlib.pyplot as plt
- > 载入模块
 - from pandas import Series, DataFrame
 - from scipy import stats
- ▶ 数据:链接: http://pan.baidu.com/s/1bpKAd8V 密码: dw8g
 - tips.csv
- 读入数据(假设文件在工作目录路径下)
 - tips=pd.read_csv('tips.csv')
- > 加工数据:
 - tips['tip_pct']=tips['tip']/tips['total_bill']

可视化分析变量之间的关系



- import seaborn as sns
- sns.set()
- sns.pairplot(tips, hue="day")



by郭鹏程 (绿树@小象)

任务描述



- 通过回归分析,确定变量之间的关系,即"模型"
- 理解线性回归的原理,输出的含义
- > 掌握如何评价和选择回归模型
- 掌握基于重抽样(模拟)的分析方法:置换检验,和自助法



> 回归分析:

- 用一个或多个预测变量(自变量、解释变量)来预测响应变量(因变量、效标变量、结果变量)的方法
- 挑选与响应变量相关的解释变量
- 描述两者关系
- 通过解释变量预测响应变量
- 接近现实世界
- 交互式的,拟合一系列模型,选择"最佳"模型
- 难题:
 - 问题的提出,有用和可测的响应变量,合适的数据



> 回归分析的类型

回归类型	用。途
简单线性	用一个量化的解释变量预测一个量化的响应变量
多项式	用一个量化的解释变量预测一个量化的响应变量,模型的关系是n阶多项式
多元线性	用两个或多个量化的解释变量预测一个量化的响应变量
多变量	用一个或多个解释变量预测多个响应变量
Logistic	用一个或多个解释变量预测一个类别型响应变量
泊松	用一个或多个解释变量预测一个代表频数的响应变量
Cox比例风险	用一个或多个解释变量预测一个事件(死亡、失败或旧病复发)发生的时间
时间序列	对误差项相关的时间序列数据建模
非线性	用一个或多个量化的解释变量预测一个量化的响应变量,不过模型是非线性的
非参数	用一个或多个量化的解释变量预测一个量化的响应变量,模型的形式源自数据形式,不事先设定
稳健	用一个或多个量化的解释变量预测一个量化的响应变量,能抵御强影响点的干扰



回归模型

- 对于机理尚不明确的变量建立模型

$$Y = f(X_1, X_2, ..., X_{p-1}) + \epsilon$$
 未考虑因素

- 利用观测数据确定f(Xi)和误差

> 线性回归

$$Y = \beta_0 + \beta_1 X_1 + \dots + \beta_{p-1} X_{p-1} + \epsilon$$

- 一般模型也可以转化为线性回归模型



> 线性回归:

- 对Y, X1,...Xp-1进行n (>=p) 次独立观测: (yi; xi1,...xi,p-1), i= 1, 2, ..., n

$$Y = \beta_0 + \beta_1 X_1 + \dots + \beta_{p-1} X_{p-1} + \epsilon$$

- 矩阵形式

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

$$Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, \quad X = \begin{bmatrix} 1 & x_{11} & \cdots & x_{1,p-1} \\ 1 & x_{21} & \cdots & x_{2,p-1} \\ \vdots & & \vdots & & \vdots \\ 1 & x_{n1} & \cdots & x_{n,p-1} \end{bmatrix}, \quad \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_{p-1} \end{bmatrix} \epsilon = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$



> 线性回归:



> 参数估计及其性质:

$$\beta$$
, σ^2



> 以R为例

```
> fit<-lm(weight~height, data=women)</p>
> summary(fit)
Call:
lm(formula = weight ~ height, data = women)
Residuals:
   Min 1Q Median 3Q Max
-1.7333 -1.1333 -0.3833 0.7417 3.1167
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) -87.51667 5.93694 -14.74 1.71e-09 ***
height
      3.45000 0.09114 37.85 1.09e-14 ***
Signif. codes: 0 \***' 0.001 \**' 0.01 \*' 0.05 \.' 0.1 \ ' 1
Residual standard error: 1.525 on 13 degrees of freedom
Multiple R-squared: 0.991, Adjusted R-squared: 0.9903
F-statistic: 1433 on 1 and 13 DF, p-value: 1.091e-14
```



> 以R为例

```
fitted(fit)
                                            160
112.5833 116.0333 119.4833 122.9333
                           15
                 14
153.9833 157.4333 160.8833
                                            150
> residuals(fit)
                                         women$weight
           1
 2.41666667 0.96666667
                            0.51666667
                                            140
          10
                        11
-1.63333333 -1.083333333 -0.533333333
> plot(women$height, women$weight)
                                            130
  abline(fit)
> coefficients(fit)
(Intercept) height
                                            120
  -87.51667
                  3.45000
                                                58
                                                     60
                                                          62
                                                               64
                                                                   66
                                                                        68
                                                                             70
                                                                                  72
```

women\$height



> stats.linregress

- from scipy import stats
- np.random.seed(12345678)
- x = np.random.random(10)
- y = np.random.random(10)
- slope, intercept, r_value, p_value, std_err = stats.linregress(x,y)

Examples

```
>>> from scipy import stats
>>> np. random. seed (12345678)
>>> x = np. random. random (10)
>>> y = np. random. random (10)
>>> slope, intercept, r_value, p_value, std_err = stats.linregress(x,y)
```

To get coefficient of determination (r_squared)

```
>>> print("r-squared:", r_value**2)
('r-squared:', 0.080402268539028335)
```

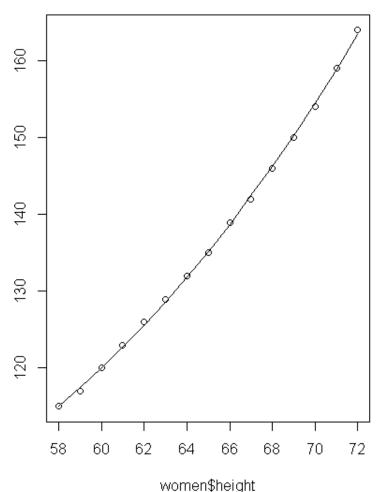


```
import matplotlib.pyplot as plt
import numpy as np
from sklearn import datasets, linear_model
# Load the diabetes dataset
diabetes = datasets.load diabetes()
# Use only one feature
diabetes_X = diabetes.data[:, np.newaxis, 2]
# Split the data into training/testing sets
diabetes X train = diabetes X[:-20]
diabetes_X_test = diabetes_X[-20:]
# Split the targets into training/testing sets
diabetes_y_train = diabetes.target[:-20]
diabetes_y_test = diabetes.target[-20:]
# Create Linear rearession object
regr = linear_model.LinearRegression()
# Train the model using the training sets
regr.fit(diabetes_X_train, diabetes_y_train)
# The coefficients
print('Coefficients: \n', regr.coef_)
# The mean square error
print("Residual sum of squares: %.2f"
      % np.mean((regr.predict(diabetes_X_test) - diabetes_y_test) ** 2))
# Explained variance score: 1 is perfect prediction
print('Variance score: %.2f' % regr.score(diabetes_X_test, diabetes_y_test))
# Plot outputs
plt.scatter(diabetes_X_test, diabetes_y_test, color='black')
plt.plot(diabetes_X_test, regr.predict(diabetes_X_test).color='blue'.
         linewidth=3)
plt.xticks(())
plt.yticks(())
```



> 多项式回归,以R为例

```
> fit2<-lm(weight~height+I(height^2), data=women)</p>
> summary(fit2)
Call:
lm(formula = weight ~ height + I(height^2), data = wome
Residuals:
                    Median
                                 30
     Min
               10
                                         Max
-0.50941 -0.29611 -0.00941 0.28615 0.59706
Coefficients:
                                                       women$weight
             Estimate Std. Error t value Pr(>|t|)
(Intercept) 261.87818
                        25.19677 10.393 2.36e-07 ***
height
             -7.34832 0.77769 -9.449 6.58e-07 ***
                         0.00598 13.891 9.32e-09 ***
I(height^2) 0.08306
                0 `***' 0.001 `**' 0.01 `*' 0.05 `.' 0.
Signif. codes:
Residual standard error: 0.3841 on 12 degrees of freedo
Multiple R-squared: 0.9995, Adjusted R-squared: 0.
F-statistic: 1.139e+04 on 2 and 12 DF, p-value: < 2.26
> plot(women$height, women$weight)
> lines(women$height,fitted(fit2))
```





> 多元线性回归,以R为例

```
> fit<-lm(Murder~Population+Illiteracy+Income+Frost,data=states)</p>
> summary(fit)
Call:
lm(formula = Murder ~ Population + Illiteracy + Income + Frost,
   data = states)
Residuals:
   Min 10 Median 30
                                  Max
-4.7960 -1.6495 -0.0811 1.4815 7.6210
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 1.235e+00 3.866e+00 0.319 0.7510
Population 2.237e-04 9.052e-05 2.471 0.0173 *
Illiteracy 4.143e+00 8.744e-01 4.738 2.19e-05 ***
Income 6.442e-05 6.837e-04 0.094 0.9253
Frost 5.813e-04 1.005e-02 0.058 0.9541
Signif. codes: 0 \*** 0.001 \** 0.01 \*/ 0.05 \./ 0.1 \ / 1
Residual standard error: 2.535 on 45 degrees of freedom
Multiple R-squared: 0.567, Adjusted R-squared: 0.5285
F-statistic: 14.73 on 4 and 45 DF, p-value: 9.133e-08
```



> 多元线性回归,以R为例

```
> fit<-lm(mpg~hp+wt+hp:wt,data=mtcars)</pre>
> summary(fit)
Call:
lm(formula = mpq ~ hp + wt + hp:wt, data = mtcars)
Residuals:
   Min 1Q Median 3Q Max
-3.0632 -1.6491 -0.7362 1.4211 4.5513
Coefficients:
          Estimate Std. Error t value Pr(>|t|)
(Intercept) 49.80842 3.60516 13.816 5.01e-14 ***
hp
   -8.21662 1.26971 -6.471 5.20e-07 ***
TITT.
      0.02785 0.00742 3.753 0.000811 ***
hp:wt
Signif. codes: 0 \***/ 0.001 \**/ 0.01 \*/ 0.05 \./ 0.1 \ / 1
Residual standard error: 2.153 on 28 degrees of freedom
Multiple R-squared: 0.8848, Adjusted R-squared: 0.8724
F-statistic: 71.66 on 3 and 28 DF, p-value: 2.981e-13
```



- > 线性回归:最小二乘法
 - 回归参数的最小二乘估计:误差项平方和最小

$$S(\beta) = \sum_{i=1}^{\infty} \epsilon_i^2$$

$$\hat{\beta} = (\hat{\beta}_0, \hat{\beta}_1, ..., \hat{\beta}_{p-1})^T = (X^T X)^{-1} X^T Y$$

> 经验回归方程(回归方程)

$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X_1 + \dots + \hat{\beta}_{p-1} X_{p-1}$$

- 可用来预测Y



- > 线性回归:误差方差的估计
 - 残差向量:

$$\hat{\epsilon} = Y - \hat{Y}$$

- 残差平方和

$$SSE = \sum_{i=1}^{n} \epsilon_i^2$$

- 无偏估计

$$\hat{\sigma}^2 = \frac{SSE}{n - p}$$



- > 线性回归:对参数的估计
- > 估计量的基本性质1

$$E(\hat{\beta}) = \beta$$

$$Cov(\hat{\beta}) = \sigma^{2}(X^{T}X)^{-1}$$

$$E(\hat{\sigma}^{2}) = \sigma^{2}$$



- > 线性回归:对参数的估计
- > 估计量的基本性质2

$$If \quad \epsilon \sim N(0, \sigma^2 I)$$

$$\hat{\beta} \sim N(\beta, \sigma^2 (X^T X)^{-1})$$

$$\frac{1}{\sigma^2} SSE = \frac{n-p}{\sigma^2} \hat{\sigma}^2 \sim \chi^2_{n-p}$$

$$\hat{\beta} \ and \ SSE(or\sigma^2) \$$
相互独立



- > 线性回归:对参数的估计
- > 估计量的基本性质3

If
$$\epsilon \sim N(0, \sigma^2 I)$$

$$E(\hat{\epsilon}) = 0$$
, $Cov(\hat{\epsilon}) = \sigma^2(I - H)$

$$\hat{\epsilon} \sim N(0, \sigma^2(I - H))$$



> 线性回归:拟合度

> 回归方程的显著性检验:因变量和自变量之间是否存在显著的线性关

系?

- 1. 总离差平方和

$$SST = \sum_{i=1}^{n} (y_i - \bar{y})^2$$

- 2. 残差(误差)平方和

$$SSE = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

- 3. 回归平方和

$$SSR = \sum_{i=1}^{n} (\hat{y}_i - \bar{y})^2$$

- 4. 复相关系数

$$R^2 = \frac{SSR}{SST} = 1 - \frac{SSE}{SST}$$



> 线性回归:线性回归关系的显著性检验:

$$H_0: \beta_1 = \beta_2 = \dots = \beta_{p-1} = 0 \longleftrightarrow H_1: \exists 1 \le i \le p-1 \ s.t. \ \beta_i \ne 0$$

$$F = \frac{SSR/(p-1)}{SSE/(n-p)} = \frac{MSR}{MSE}$$
$$F \sim F(p-1, n-p)$$



- > 线性回归:回归系数的统计推断
 - 若回归关系显著性H0被拒绝,仍需对每一自变量做显著性检验

$$H_{0k}: \beta_k = 0 \leftrightarrow H_{1k}: \beta_k \neq 0$$



> 多元线性回归,以R为例

```
> fit<-lm(mpg~hp+wt+hp:wt,data=mtcars)</pre>
> summary(fit)
Call:
lm(formula = mpq ~ hp + wt + hp:wt, data = mtcars)
Residuals:
   Min 1Q Median 3Q Max
-3.0632 -1.6491 -0.7362 1.4211 4.5513
Coefficients:
          Estimate Std. Error t value Pr(>|t|)
(Intercept) 49.80842 3.60516 13.816 5.01e-14 ***
hp
   -8.21662 1.26971 -6.471 5.20e-07 ***
TITT.
      0.02785 0.00742 3.753 0.000811 ***
hp:wt
Signif. codes: 0 \***/ 0.001 \**/ 0.01 \*/ 0.05 \./ 0.1 \ / 1
Residual standard error: 2.153 on 28 degrees of freedom
Multiple R-squared: 0.8848, Adjusted R-squared: 0.8724
F-statistic: 71.66 on 3 and 28 DF, p-value: 2.981e-13
```



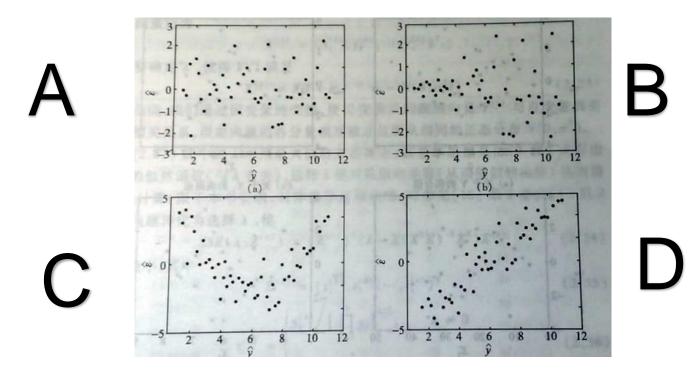
线性回归:分析结论的前提:数据满足统计假设

- 正态性:预测变量固定时,因变量正态分布

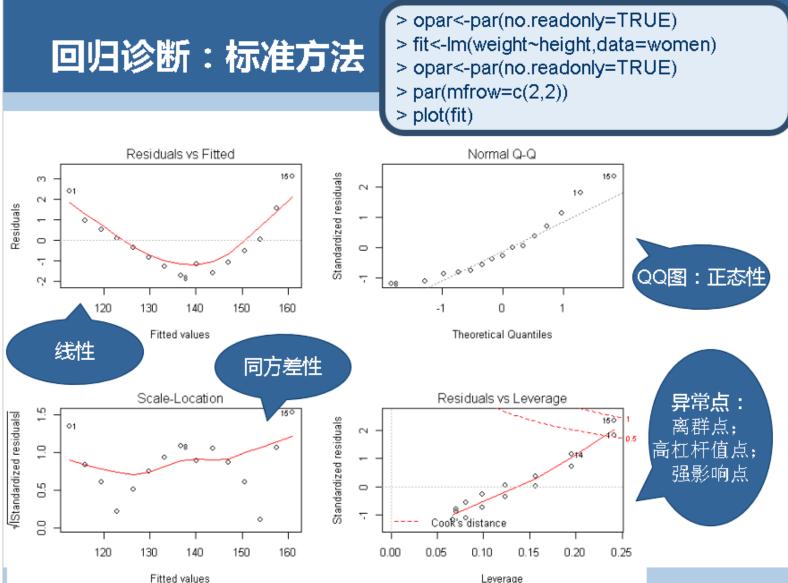
- 独立性:因变量互相独立

- 线性:因变量与自变量线性(残差白噪声)

- 同方差性:残差方差均匀







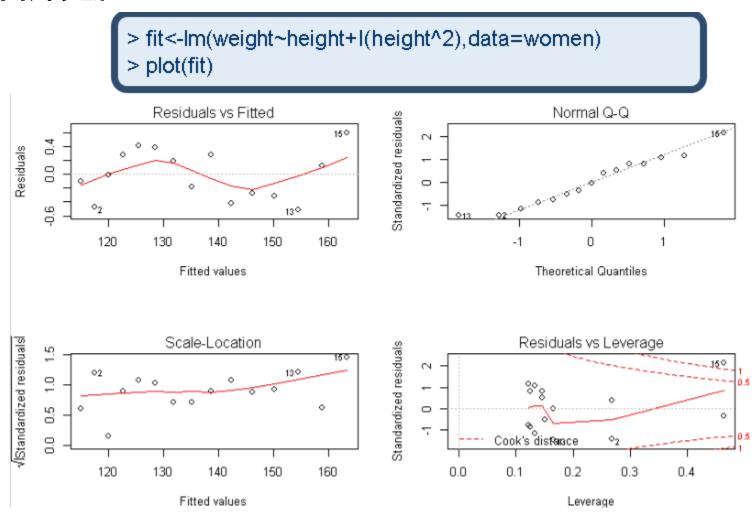
数据分析和数据挖掘

中国大数据在线教育领导者

by郭鹏程 (绿树@小象)



> 回归诊断

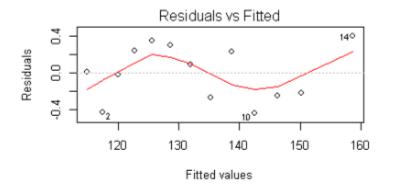


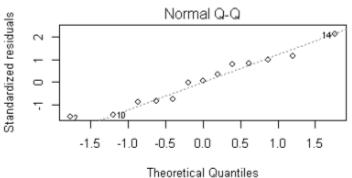


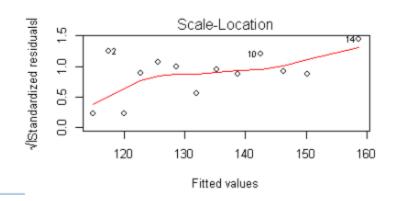
> 回归诊断:剔除数据

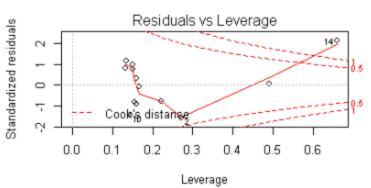
> fit<-lm(weight~height+I(height^2),data=women[-c(13,15),])

> plot(fit)







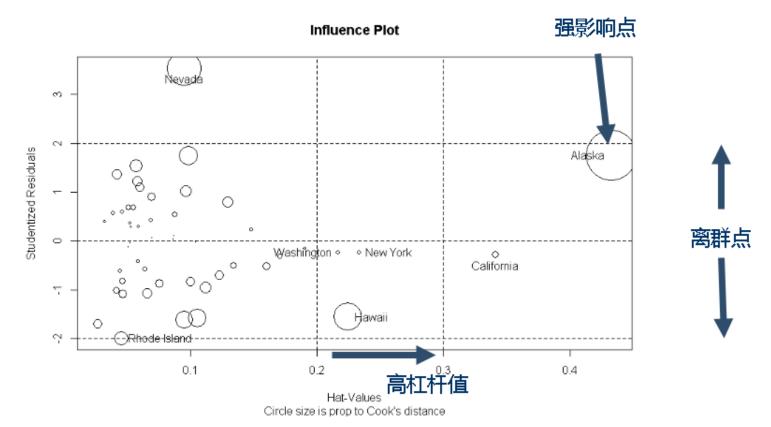




- > 回归诊断
- > 更多改进的方法
 - 正态性的诊断
 - 误差的独立性 Durbin-Watson自相关检验
 - 线性:成分残差图(偏残差图)
 - 同方差性
 - 多重共线性
 - 是指线性回归模型中的解释变量之间由于存在**精确相关关系或 高度相关关系**而使模型估计失真或难以估计准确
 - 导致模型参数的置信区间过大
 - 异常点观测值
 - 离群点、高杠杆值点、强影响点



- > 回归诊断
- > 异常点观测值
 - 离群点、高杠杆值点、强影响点





- 1. 总离差平方和
- 2. 残差(误差)平方和

 $R^2 = \frac{SSR}{SST} = 1 - \frac{SSE}{SST}$

- 3. 回归平方和
- 4. 复相关系数

$$SST = \sum_{i=1}^{n} (y_i - \bar{y})^2$$

$$SSE = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

$$SSR = \sum_{i=1}^{n} (\hat{y}_i - \bar{y})^2$$

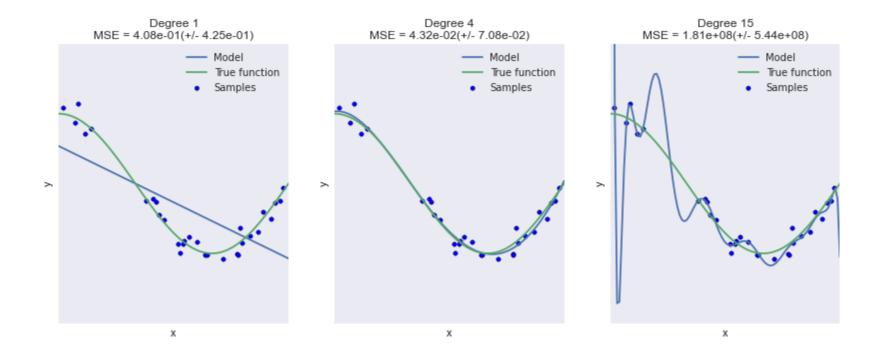
越大越显著
$$R_a^2(p) = 1 - (\frac{n-1}{n-p}) \frac{SSE_p}{SST} = 1 - \frac{MSE_p}{SST/(n-1)}$$

• p增加时, SSEp减少, R^2_p增大, 因此需要修

儿針学院 ChinaHadoop.cn

> 线性回归:模型选择

> 欠拟合 vs 过拟合



```
25 import numpy as no
26 import matplotlib.pyplot as plt
27 from sklearn.pipeline import Pipeline
28 from sklearn.preprocessing import PolynomialFeatures
29 from sklearn.linear_model import LinearRegression
30 from sklearn import cross validation
31
32 np.random.seed(0)
33
34 \text{ n samples} = 30
35 degrees = [1, 4, 15]
36
37 true_fun = lambda X: np.cos(1.5 * np.pi * X)
38 X = np.sort(np.random.rand(n samples))
39 y = true fun(X) + np.random.randn(n samples) * 0.1
41 plt.figure(figsize=(14, 5))
42 for i in range(len(degrees)):
      ax = plt.subplot(1, len(degrees), i + 1)
43
      plt.setp(ax, xticks=(), yticks=())
44
45
      polynomial features = PolynomialFeatures(degree=degrees[i],
46
                                                 include bias=False)
47
      linear regression = LinearRegression()
48
      pipeline = Pipeline([("polynomial features", polynomial features),
49
50
                            ("linear regression", linear regression)])
      pipeline.fit(X[:, np.newaxis], y)
51
52
53
      # Evaluate the models using crossvalidation
54
      scores = cross validation.cross val score(pipeline,
55
          X[:, np.newaxis], y, scoring="mean squared error", cv=10)
56
      X_{\text{test}} = \text{np.linspace}(0, 1, 100)
57
      plt.plot(X test, pipeline.predict(X test[:, np.newaxis]), label="Model")
58
      plt.plot(X test, true fun(X test), label="True function")
59
      plt.scatter(X, y, label="Samples")
60
      plt.xlabel("x")
61
      plt.ylabel("y")
62
      plt.xlim((0, 1))
63
      plt.ylim((-2, 2))
64
65
      plt.legend(loc="best")
      plt.title("Degree {}\nMSE = {:.2e}(+/- {:.2e})".format(
66
          degrees[i], -scores.mean(), scores.std()))
67
68 plt.show()
『プヘッロファーバーリュラヘッロ・レッツ
                                                  工造八级加压级场目级可省
```



```
Python source code: plot underfitting overfitting.py
 print( doc )
 import numpy as np
 import matplotlib.pyplot as plt
 from sklearn.pipeline import Pipeline
 from sklearn.preprocessing import PolynomialFeatures
 from sklearn.linear model import LinearRegression
 from sklearn import cross validation
 np.random.seed(0)
 n samples = 30
 degrees = [1, 4, 15]
 true_fun = lambda X: np.cos(1.5 * np.pi * X)
 X = np.sort(np.random.rand(n samples))
 y = true fun(X) + np.random.randn(n samples) * 0.1
 plt.figure(figsize=(14, 5))
 for i in range(len(degrees)):
     ax = plt.subplot(1, len(degrees), i + 1)
     plt.setp(ax, xticks=(), yticks=())
     polynomial_features = PolynomialFeatures(degree=degrees[i],
                                              include bias=False)
     linear_regression = LinearRegression()
     pipeline = Pipeline([("polynomial_features", polynomial_features),
                          ("linear_regression", linear_regression)])
     pipeline.fit(X[:, np.newaxis], y)
     # Evaluate the models using crossvalidation
     scores = cross validation.cross val score(pipeline,
         X[:, np.newaxis], y, scoring="mean_squared_error", cv=10)
     X_{test} = np.linspace(0, 1, 100)
     plt.plot(X_test, pipeline.predict(X_test[:, np.newaxis]), label="Model")
     plt.plot(X_test, true_fun(X_test), label="True function")
     plt.scatter(X, y, label="Samples")
     plt.xlabel("x")
```



plt.title("Degree {}\nMSE = {:.2e}(+/- {:.2e})".format(
 degrees[i], -scores.mean(), scores.std()))

plt.ylabel("y")
plt.xlim((0, 1))
plt.ylim((-2, 2))
plt.legend(loc="best")

plt.show()

重抽样:基于模拟的分析方法



- 当数据抽样存在下列情况时,用什么方法?
 - 来自未知或混合分布
 - 样本量过小
 - 存在离群点
 - 基于理论分布设计合适的统计检验过于复杂
- > 置换检验
- > 自助法

重抽样:置换检验



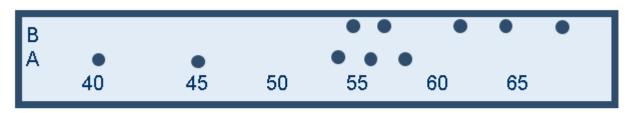
- > 举例:10个受试者随机分两组进行A或B实验,结果是否有不同?
- ➤ 假设检验:t-test
 - 假设数据抽样自等方差的正态分布
 - 独立分组的双尾t检验
 - 观测t值是否极端

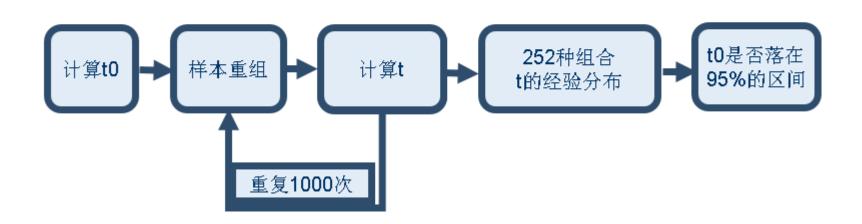
重抽样:置换检验



> 置换检验:生成零假设的p值

- 置换检验的思路:
 - 如果A,B两种方式真的等价,AB的结果应该是任意的

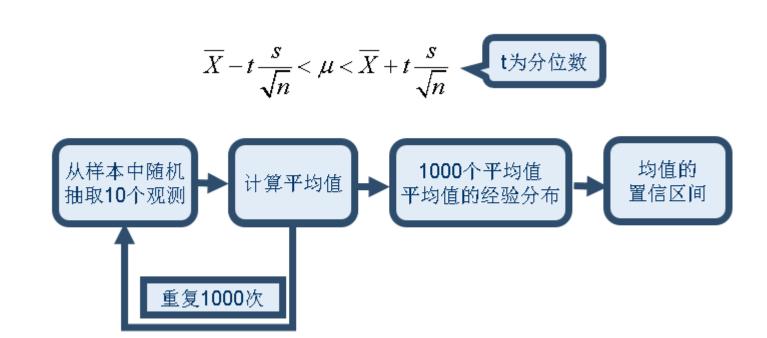




重抽样:自助法

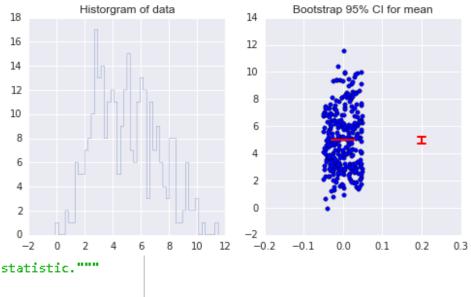


- 自助法:获取置信区间和估计测量精度
- 从初始样本重复随机替换抽样,生成待检验统计量的经验分布,生成统计量的置信区间
- > 例:



重抽样:自助法

```
14
                                                                   12
                                                                   10
                                                                    8
 1 # -*- coding: utf-8 -*-
                                                                    6
 Bimport numpy as np
                                                                    4
 4 import numpy.random as npr
                                                                    2
 5 import pylab
 7 def bootstrap(data, num samples, statistic, alpha):
       """Returns bootstrap estimate of 100.0*(1-alpha) CI for statistic.
       n = len(data)
      idx = npr.randint(0, n, (num_samples, n))
10
11
      samples = data[idx]
      stat = np.sort(statistic(samples, 1))
12
13
      return (stat[int((alpha/2.0)*num samples)],
14
               stat[int((1-alpha/2.0)*num samples)])
15
16
17# data of interest is bimodal and obviously not normal
18 \times = \text{np.concatenate}([\text{npr.normal}(3, 1, 100), \text{npr.normal}(6, 2, 200)])
19
20 # find mean 95% CI and 100,000 bootstrap samples
21 low, high = bootstrap(x, 100000, np.mean, 0.05)
23 # make plots
24 pylab.figure(figsize=(8,4))
25 pylab.subplot(121)
26 pylab.hist(x, 50, histtype='step')
27 pylab.title('Historgram of data')
28 pylab.subplot(122)
29 pylab.plot([-0.03,0.03], [np.mean(x), np.mean(x)], 'r', linewidth=2)
30 pylab.scatter(0.1*(npr.random(len(x))-0.5), x)
31 pylab.plot([0.19,0.21], [low, low], 'r', linewidth=2)
32 pylab.plot([0.19,0.21], [high, high], 'r', linewidth=2)
33 pylab.plot([0.2,0.2], [low, high], 'r', linewidth=2)
34 pylab.xlim([-0.2, 0.3])
35 pylab.title('Bootstrap 95% CI for mean')
```



by郭鹏程 (绿树@小象)

重抽样:基于模拟的分析



- ▶ 自助法:
 - 初始样本 20~30
 - 重复次数 >~ 1000

> 重抽样与自助法:

- 数据不满足标准的假设时
- 非万能:无法将烂数据转化为好数据



- > 练习
- > 回归分析:
 - tip~ total_bill+size



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