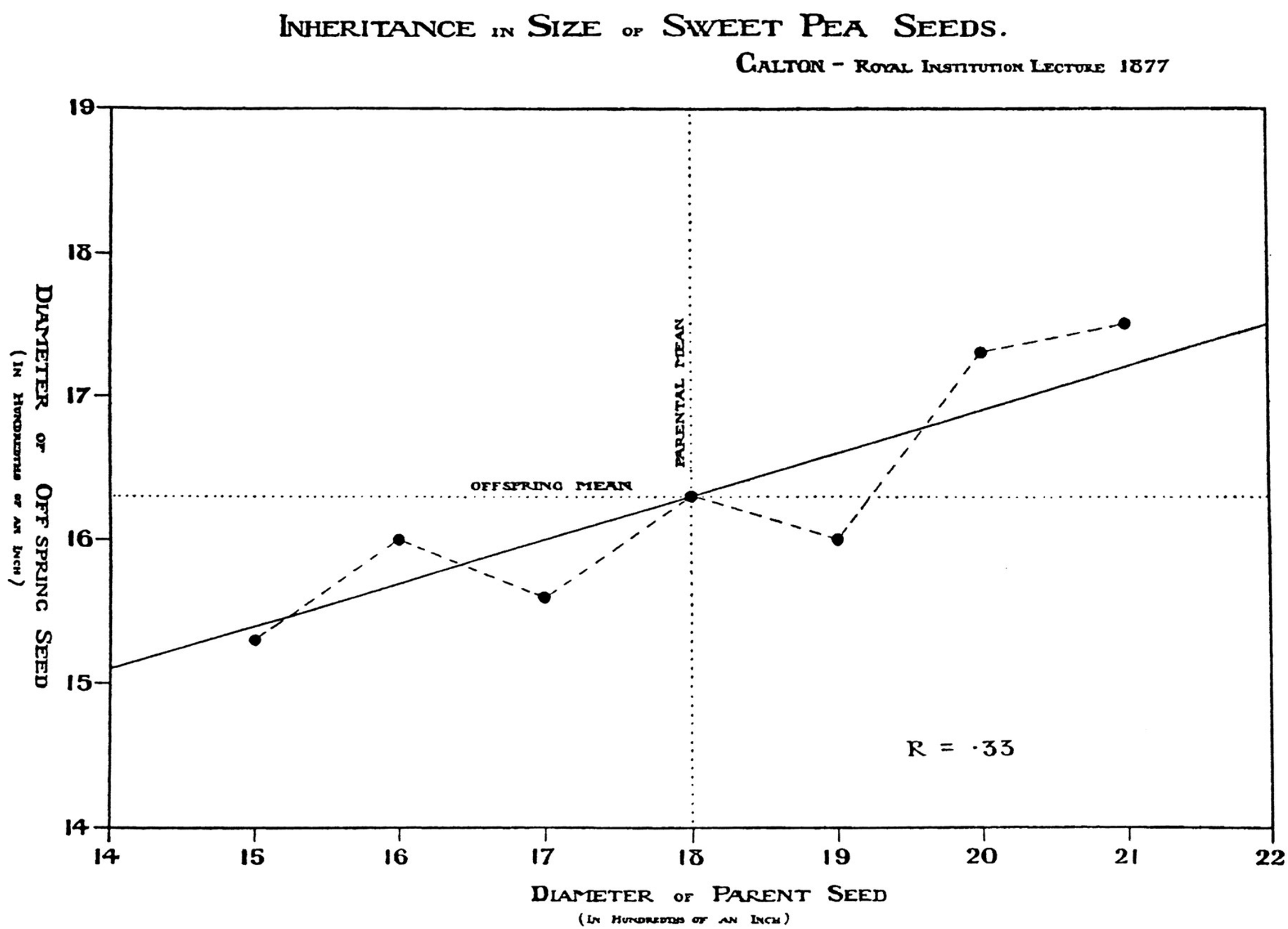
Linear and Logistic Regression

Thomas Schwarz, SJ

Linear Regression

- Sir Francis Galton : 16 Feb 1822 — Jan 17 1911
  - Cousin of Charles Darwin
    - Discovered "Regression towards Mediocrity":
      - Individuals with exceptional measurable traits have more normal progreny
  - If parent's trait is at $x\sigma$ from μ, then progeny has traits at $\rho x\sigma$ from μ
    - ρ is the *coefficient of correlation* between trait of parent and of progeny

Linear Regression



Statistical Aside

- Regression towards mediocrity **does not mean**
  - Differences in future generations are smoothed out
- It reflects a selection biases
  - Trait of parent is mean + inherited trait + error
    - The parents we look at have both inherited trait and error >>0
  - Progeny also has mean + inherited trait + error
    - But the error is now random, and on average ~ 0.

Statistical Aside

- Example:
  - You do exceptionally well in a chess tournament
    - Result is Skill + Luck
      - You probably will not do so well in the next one
        - Your skill might have increased, but you cannot expect your luck to stay the same
          - It might, and you might be even luckier, but the odds are against it

Aside: Regression to Normality

- Israeli fighter pilot training:
  - Proposes to criticize pilots in training severely
    - When pilots in training are reprimanded for a bad maneuver, then they are most likely to not do the same maneuver as badly the next time
    - When pilots in training are praised for a well-executed maneuver, then they are not likely to repeat the same maneuver as well

Aside: Regression to Normality

- Regression to Normality explanation:
  - The quality of a maneuver is a (statistically distributed) random variable
    - After a high-quality maneuver, the quality of the next maneuver is still distributed randomly
      - And therefore much more likely to be worse
    - After a low-quality maneuver, the quality of the next maneuver is still distributed randomly
      - And therefore much more likely to be better

Aside: Regression to Normality

- Regression to Normality
- Do not fall into the gambler's fallacy
  - A better than average maneuver is equally likely after a better than average maneuver as after a worse than average maneuver

Review of Statistics

- We have a population with traits
  - We are interested in only one trait
    - We need to make predictions based on a sample, a (random) collection of population members
    - We estimate the population mean by the sample mean
      - $$m = \frac{1}{N}\sum_{i=1}^{N} x_i$$
    - We estimate the population standard deviations by the (unbiased) sample standard deviation
      - $$s^2 = \frac{1}{N-1}\sum_{i=1}^{N} (x_i - \mu)^2$$

Unbiased ?

- Normally distributed variable with mean μ and st. dev. σ
  - Take sample $\{x_1, \ldots, x_N\}$
  - Calculate $s^2 = \frac{1}{N}\sum_{i=1}^{N}(x_i - \mu)^2$
- Turns out: expected value for s is less than σ
- Call $N - 1$ the *degree of freedom*

Forecasting

- Mean model
  - We have a sample
    - We predict the value of the next population member to be the sample mean
- What is the risk?
  - Measure the risk by the standard deviation

Forecasting

- Normally distributed variable with mean μ and st. dev. σ
    - Take sample $\{x_1, \ldots, x_N\}$
    - What is the expected squared difference of m and μ:
      $E((m-\mu)^2)$
- "*Standard error of the mean*"
    - $E((m-\mu)^2) = \frac{s}{\sqrt{N}}$

Forecasting

- Forecasting Error of : $x_{N+1} \leftarrow \frac{1}{N}\sum_{i=1}^{N} X_i$
- Two sources of error:
  - We estimate the standard deviation wrongly
    - x_{N+1} is on average one standard deviation away from the mean
- Expected error

$$= \sqrt{s^2 + (\frac{s}{\sqrt{N}})^2} = s\sqrt{1 + \frac{1}{N}}$$

model error parameter error

Forecasting

- There is still a *model risk*
  - We just might not have the right model
    - The underlying distribution is not normal

Confidence Intervals

- Assume that the model is correct
  - Simulate the model `run` times
  - The *x*-confidence interval then
    - contains *x%* of the runs contain the true value

Confidence Intervals

- Confidence intervals usually are
  $\pm t \times$ (standard error of forecast)
- Contained in t-tables and depend on sample size

Example

- Create a simulation that gives you a single figure of merit
- Create a batch of 50 simulations and get the average
- Repeat this 30 times
  - Because each of the 30 values is an average, it is more closely normally distributed

Example

- Values:

```
x = np.array([46.38324392, 48.32716522, 42.80399487,
    45.81826266, 43.23515335, 43.6001169 ,
47.49314264, 49.08597766, 42.95018079,
45.25707317, 45.43143526, 44.20980892,
44.86189782, 38.33234082, 44.17152394,
44.636054  , 46.95339903, 43.35623343,
44.08015344, 43.14105973, 46.28812561,
46.01398139, 46.25844065, 41.6666845 ,
45.42620433, 47.35499856, 42.46798488,
45.21081934, 43.64197297, 43.68351126])
```

Example

- Calculate sample mean and sample std deviation

```
loc = np.mean(x)

scale=np.std(x, ddof=1)/np.sqrt(len(x))
```

- Get confidence interval at $\alpha = 0.01$ using stats.t.interval

```
print(stats.t.interval(1-0.01,
                       len(x)-1,
                       loc = np.mean(x),
                       scale=np.std(x,
                      ddof=1)/np.sqrt(len(x))))
```

Result

- (38.752734290196 68, 50.723328447136645))
- (True value was 45)

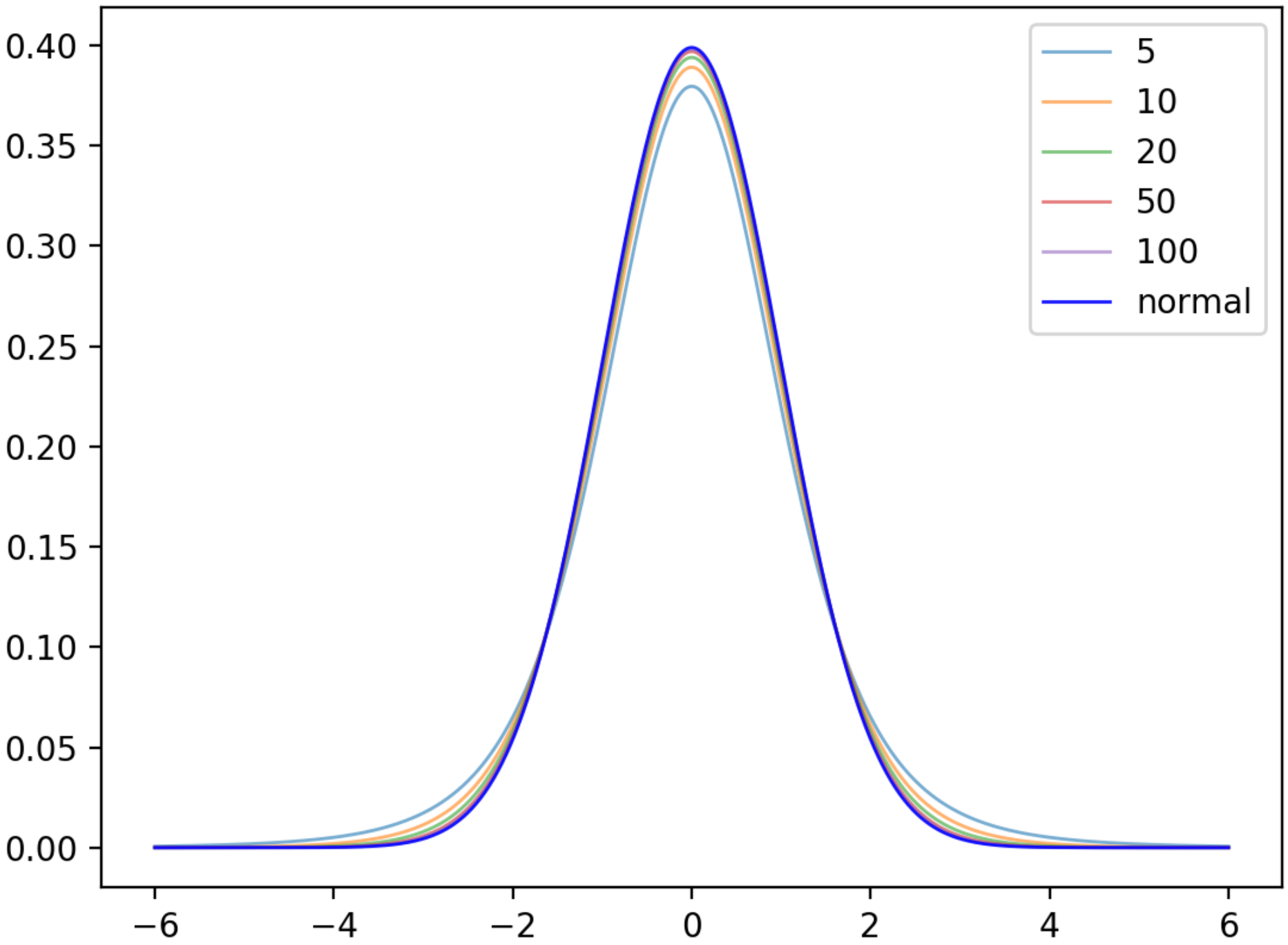
Student *t*-distribution

- Gossett (writing as "Student")
    - Distribution of

$$\frac{(m-\mu)}{s/\sqrt{N}}$$

    - With increasing N comes close to normal distribution

Student-*t* distribution



Example

- T-test for testing whether two means of two populations are different or not

$$t = \frac{\mu_X - \mu_Y}{\sqrt{\frac{\sigma_X^2}{n_X} + \frac{\sigma_Y^2}{n_Y}}}$$ with sample st. dev. σ_X and σ_Y

- Distributed according to degrees of freedom:
  - $n_X + n_Y - 2$

Example

- Blood pressure measurements for patients given a drug and a placebo

```
drug = [100, 110, 122, 109, 108, 111, 118,
105, 115, 119, 106]
placebo = [129, 125, 136, 129, 135, 134,
140, 128]
```

- Use scipy.stats.ttest_ind
  - Notice: there are many variants of t-tests:

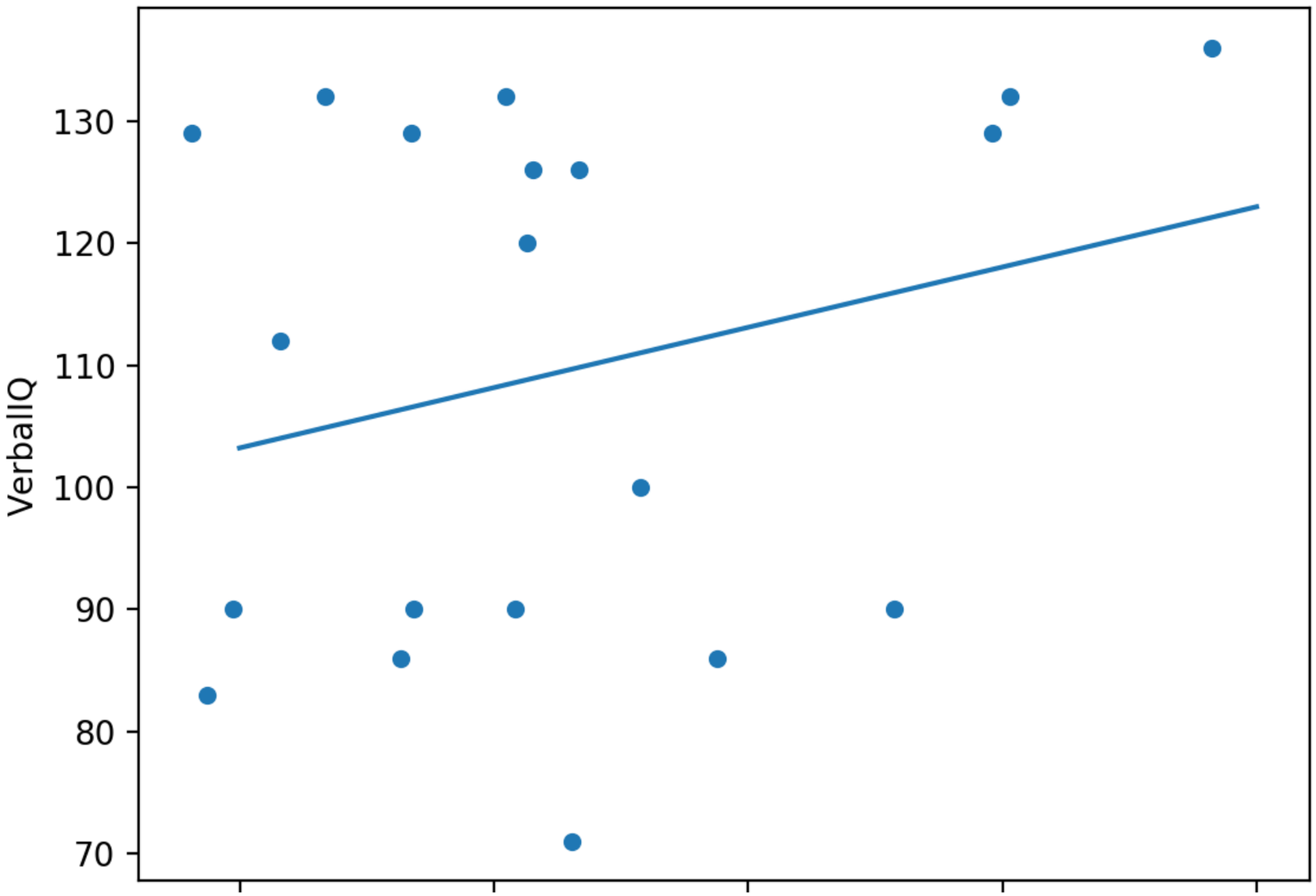
```
print(stats.ttest_ind(drug, placebo, equal_var=False))
```

Example

- Result is

```
Ttest_indResult(statistic=-7.761660781121691,
pvalue=5.591331997397221e-07)
```

- Since the p-value is so small
  - Conclude that the null hypothesis: "means are equal" is wrong



Linear Regression

Thomas Schwarz, SJ

Simple Linear Regression

- Linear regression uses straight lines for prediction
  - Model:
    - "Causal variable" x, "observed variable" y
    - Connection is linear (with or without a constant)
    - There is an additive "error" component
      - Subsuming "unknown" causes
      - With expected value of 0
      - Usually assumed to be normally distributed

Simple Linear Regression

- Model:

$$y = b_0 + b_1 x + \epsilon$$

Simple Linear Regression

- Assume $y = b_0 + b_1 x$

  Minimize $S = \sum_{i=1}^{n} (y_i - (b_0 + b_1 x_i))^2$

  Take the derivative with respect to b_0 and set it to zero:

$$\frac{\delta S}{\delta b_0} = \sum_{i=1}^{n} -2(y_i - b_0 - b_1 x_i) = 0$$

$$\Rightarrow \sum_{i=1}^{n} y_i = b_0 n + b_1 \sum_{i=1}^{n} x_i \Rightarrow \; b_0 = \frac{1}{n} \sum_{i=1}^{n} y_i - b_1 \frac{1}{n} \sum_{i=1}^{n} x_i$$

$$\Rightarrow b_0 = \bar{y} - b_1 \bar{x}$$

Simple Linear Regression

- Assume $y = b_0 + b_1 x$

$$\text{Minimize } S = \sum_{i=1}^{n} (y_i - \left(b_0 + b_1 x_i\right))^2$$

Take the derivative with respect to b_1 and set it to zero:

$$\frac{\delta S}{\delta b_1} = \sum_{i=1}^{n} - 2x_i(y_i - b_0 - b_1 x_i) = 0$$

$$\Rightarrow \sum_{i=1}^{n} x_i(y_i - b_0 - b_1 x_i) = \sum_{i=1}^{n} (x_i y_i - b_0 x_i - b_1 x_i^2) = 0$$

Simple Linear Regression

From previous, we know $b_0 = \bar{y} - b_1\bar{x}$

Our formula $\sum_{i=1}^{n}(x_i y_i - b_0 x_i - b_1 x_i^2) = 0$ becomes

$$\sum_{i=1}^{n}\left(x_i y_i - (\bar{y} - b_1\bar{x})x_i - b_1 x_i^2\right) = 0$$

$$\sum_{i=1}^{n}\left(x_i y_i - \bar{y}x_i\right) + b_1\sum_{i=1}^{n}\left(\bar{x}x_i - x_i^2\right) = 0$$

Simple Linear Regression

- This finally gives us a solution:

$$b_1 = \frac{\sum_{i=1}^{n}(x_i y_i - \bar{y} x_i)}{\sum_{i=1}^{n}(x_i^2 - \bar{x} x_i)}$$

$$b_0 = \bar{y} - b_1 \bar{x}$$

Simple Linear Regression

- Measuring fit:

Calculate the sum of squares $SS_{\text{tot}} = \sum_{i=1}^{n} (y_i - \bar{y})^2$

Residual sum of squares $SS_{res} = \sum_{i=1}^{n} (b_0 + b_1 x_i - y_i)^2$

Coefficient of determination $R^2 = 1 - \frac{SS_{res}}{SS_{tot}}$

Simple Linear Regression

- R^2 can be used as a goodness of fit
  - Value of 1: perfect fit
  - Value of 0: no fit
  - Negative values: wrong model was chosen

Simple Linear Regression

- Look at residuals:
  - Determine statistics on the residuals
  - Question: do they look normally distributed?

Simple Linear Regression

- Example 1: brain sizes versus IQ
  - A number of female students were given an IQ test
  - They were also given an MRI to measure the size of their brain
- Is there a relationship between brains size and IQ?

VerbalIQ	Brain Size
132	816.932
132	951.545
90	928.799
136	991.305
90	854.258
129	833.868
120	856.472
100	878.897
71	865.363
132	852.244
112	808.02
129	790.619
86	831.772
90	798.612
83	793.549
126	866.662
126	857.782
90	834.344
129	948.066
86	893.983

Simple Linear Regression

- First package: statsmodels
  - Linear Regression can use different models
    - Standard: Ordinary least squares OLS
      - Exogenous variables: variable determined outside the model (an independent variable)
      - Endogenous variables: variable determined from other variables according to the model (dependent variable)
- model is sm.OLS(endogenous_data, exogenous_data)
- result is model.fit

Simple Linear Regression

- Can use statsmodels

```
import statsmodels.api as sm

df = pd.read_csv('brain-size.txt', sep = '\t')
Y = df['VerbalIQ']
X = df['Brain Size']
X = sm.add_constant(X)

model = sm.OLS(Y,X).fit()
predictions = model.predict(X)
print(model.summary())
```

Add's a column of ones

Simple Linear Regression

- Gives a very detailed feed-back

OLS Regression Results

Dep. Variable:	VerbalIQ	R-squared:	0.065
Model:	OLS	Adj. R-squared:	0.013
Method:	Least Squares	F-statistic:	1.251
Date:	Thu, 02 Jul 2020	Prob (F-statistic):	0.278
Time:	16:22:00	Log-Likelihood:	-88.713
No. Observations:	20	AIC:	181.4
Df Residuals:	18	BIC:	183.4
Df Model:	1		
Covariance Type:	nonrobust		

	coef	std err	t	P>|t|	[0.025	0.975]
const	24.1835	76.382	0.317	0.755	-136.288	184.655
Brain Size	0.0988	0.088	1.119	0.278	-0.087	0.284

Omnibus:	5.812	Durbin-Watson:	2.260
Prob(Omnibus):	0.055	Jarque-Bera (JB):	1.819
Skew:	-0.259	Prob(JB):	0.403
Kurtosis:	1.616	Cond. No.	1.37e+04

Simple Linear Regression

- Interpreting the outcome:

Omnibus:	5.812	Durbin-Watson:	2.260
Prob(Omnibus):	0.055	Jarque-Bera (JB):	1.819
Skew:	-0.259	Prob(JB):	0.403
Kurtosis:	1.616	Cond. No.	1.37e+04

- Are the residuals normally distributed?
- Omnibus: test for skew and kurtosis
  - Should be zero
- In this case: Probability of this or worse is 0.055

Simple Linear Regression

- Interpreting the outcome:

Omnibus:	5.812	Durbin-Watson:	2.260
Prob(Omnibus):	0.055	Jarque-Bera (JB):	1.819
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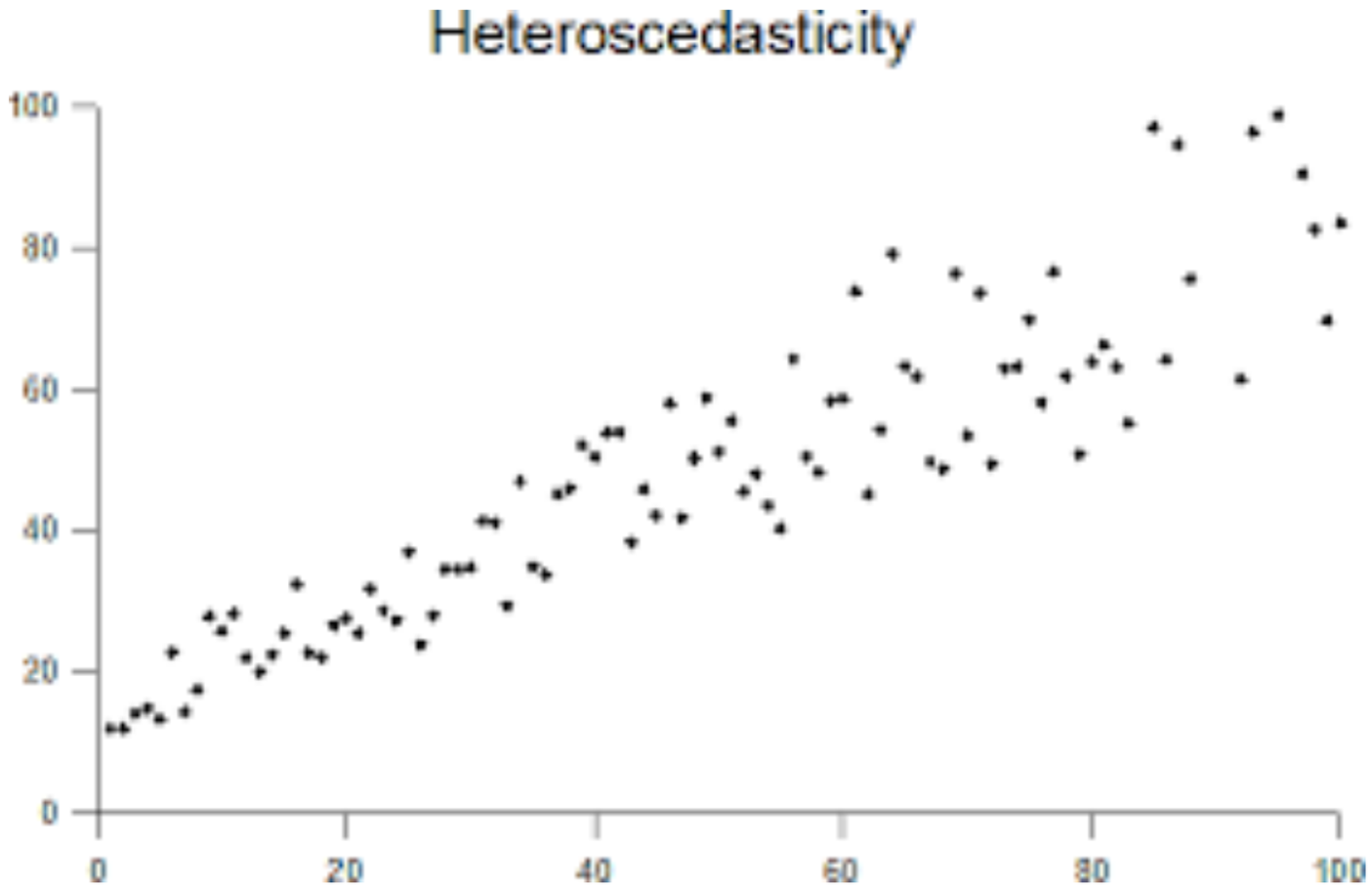
- Are the residuals normally distributed?
- Durbin-Watson: tests homoscedasticity
  - Is the Variance of the errors consistent

Simple Linear Regression

- Homoscedasticity
  - Observe that variance increases



Simple Linear Regression

- Durbin Watson statistics is between 0 and 4
- Value of 2.0 means no correlation
- Values close to 4.0 mean positive correlation
- Values close to 0 mean negative correlation

Simple Linear Regression

- Interpreting the outcome:

Omnibus:	5.812	Durbin-Watson:	2.260
Prob(Omnibus):	0.055	Jarque-Bera (JB):	1.819
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- Jarque-Bera:
  - Tests skew and kurtosis of residuals
  - Here acceptable probability

Simple Linear Regression

- Interpreting the outcome:

Omnibus:	5.812	Durbin-Watson:	2.260
Prob(Omnibus):	0.055	Jarque-Bera (JB):	1.819
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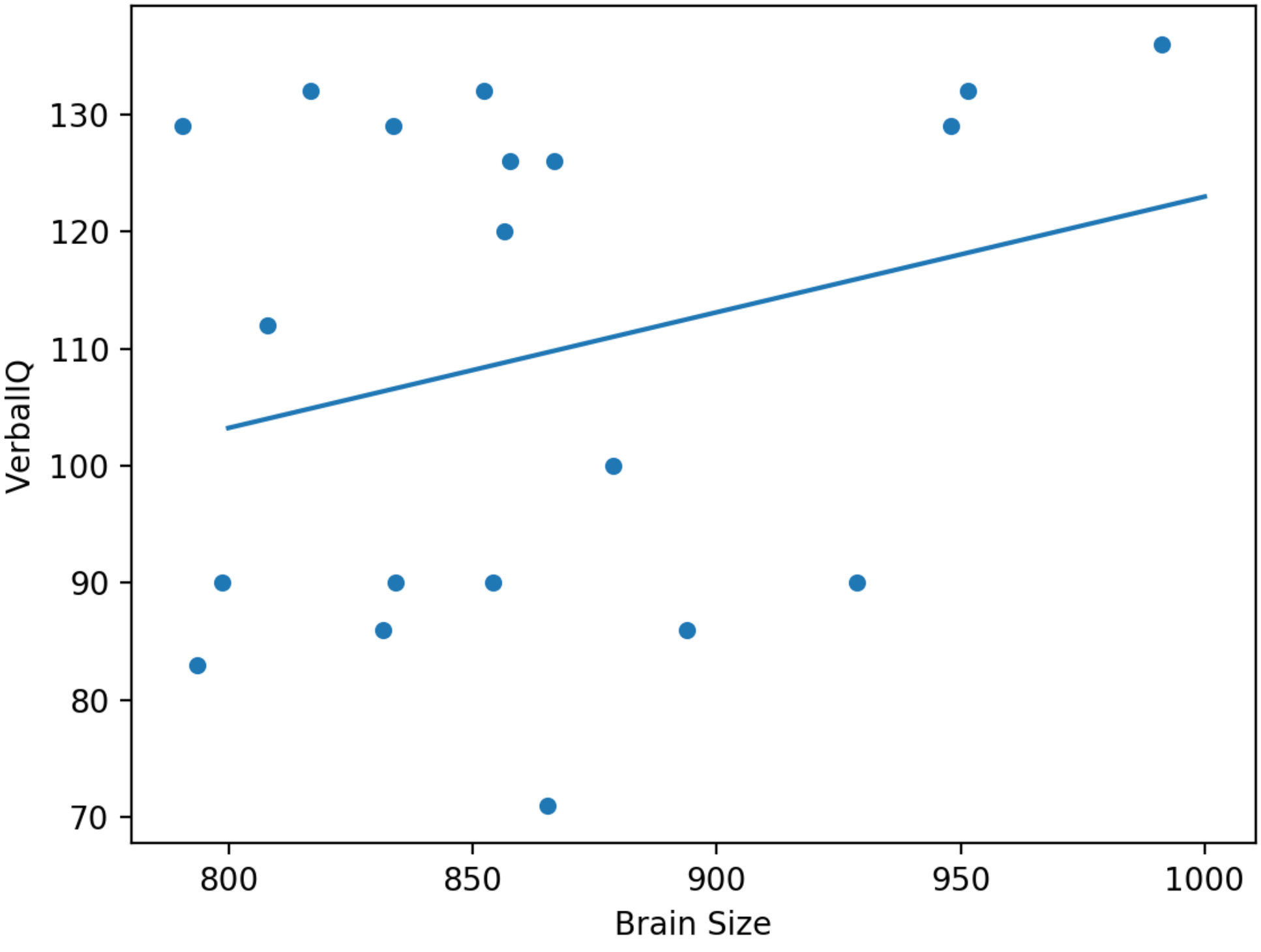
  - Condition number
    - Indicates either multicollinearity or numerical problems: small changes would have large effects
  - Multicollinearity: two or more explanatory variables are highly linearly related

Simple Linear Regression

- Plotting

```
my_ax = df.plot.scatter(x='Brain Size', y='VerbalIQ')

x=np.linspace(start=800,stop=1000)
my_ax.plot(x,24.1835+0.0988*x)
```

Simple Linear Regression



Simple Linear Regression

- scipy has a stats package

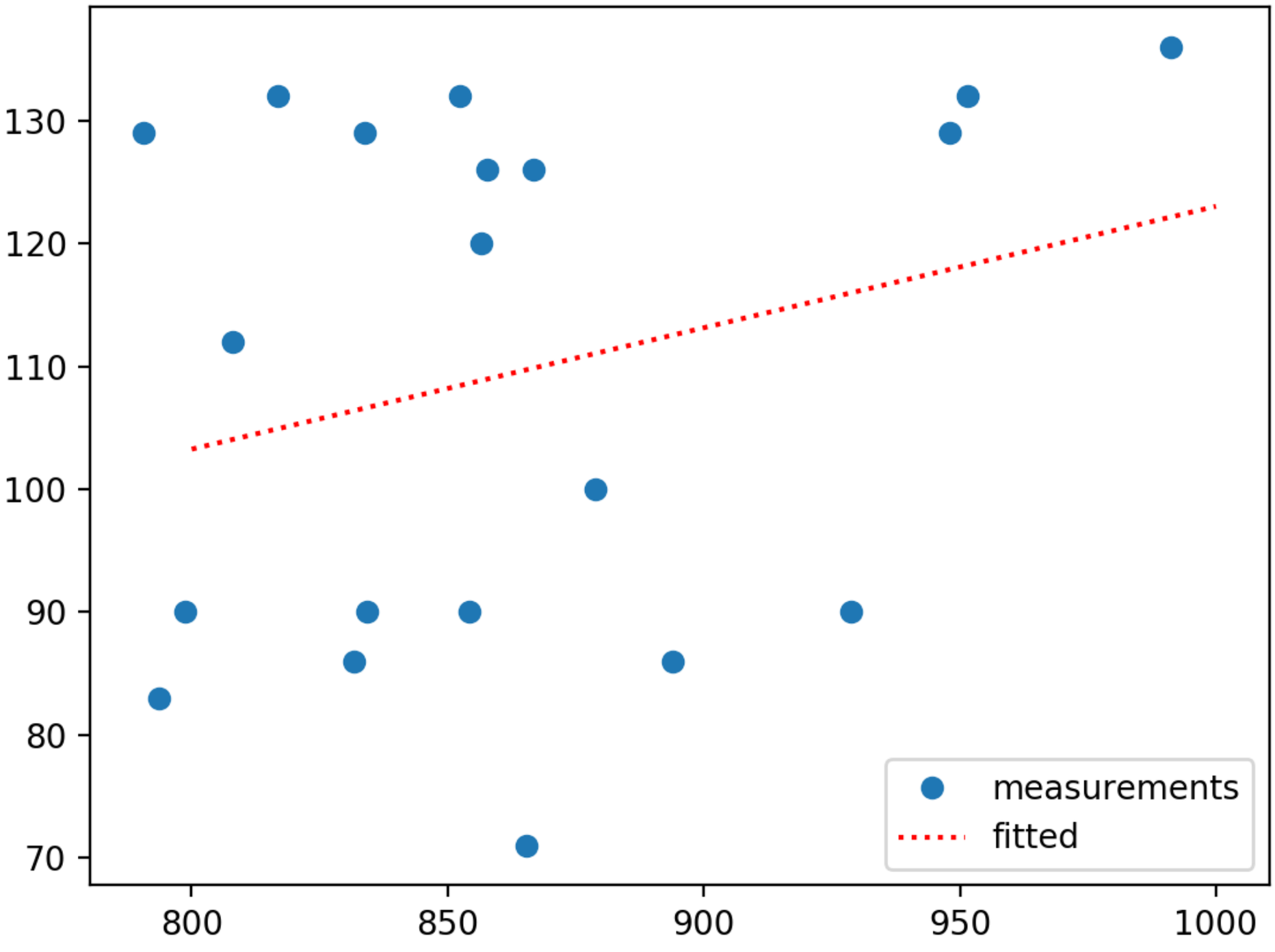
```
from scipy import stats
df = pd.read_csv('brain-size.txt', sep = '\t')
Y = df['VerbalIQ']
X = df['Brain Size']
x = np.linspace(800,1000)

slope, intercept, r_value, p_value, std_err =
stats.linregress(X, Y)
```

Simple Linear Regression

- plotting using plt

```
plt.plot(X, Y, 'o', label='measurements')
plt.plot(x, intercept+slope*x, 'r:', label='fitted')
plt.legend(loc='lower right')
print(slope, intercept, r_value, p_value)
plt.show()
```

Simple Linear Regression



Multiple Regression

- Assume now more explanatory variables
- $y = b_0 + b_1 x_1 + b_2 x_2 + \ldots + b_r x_r$

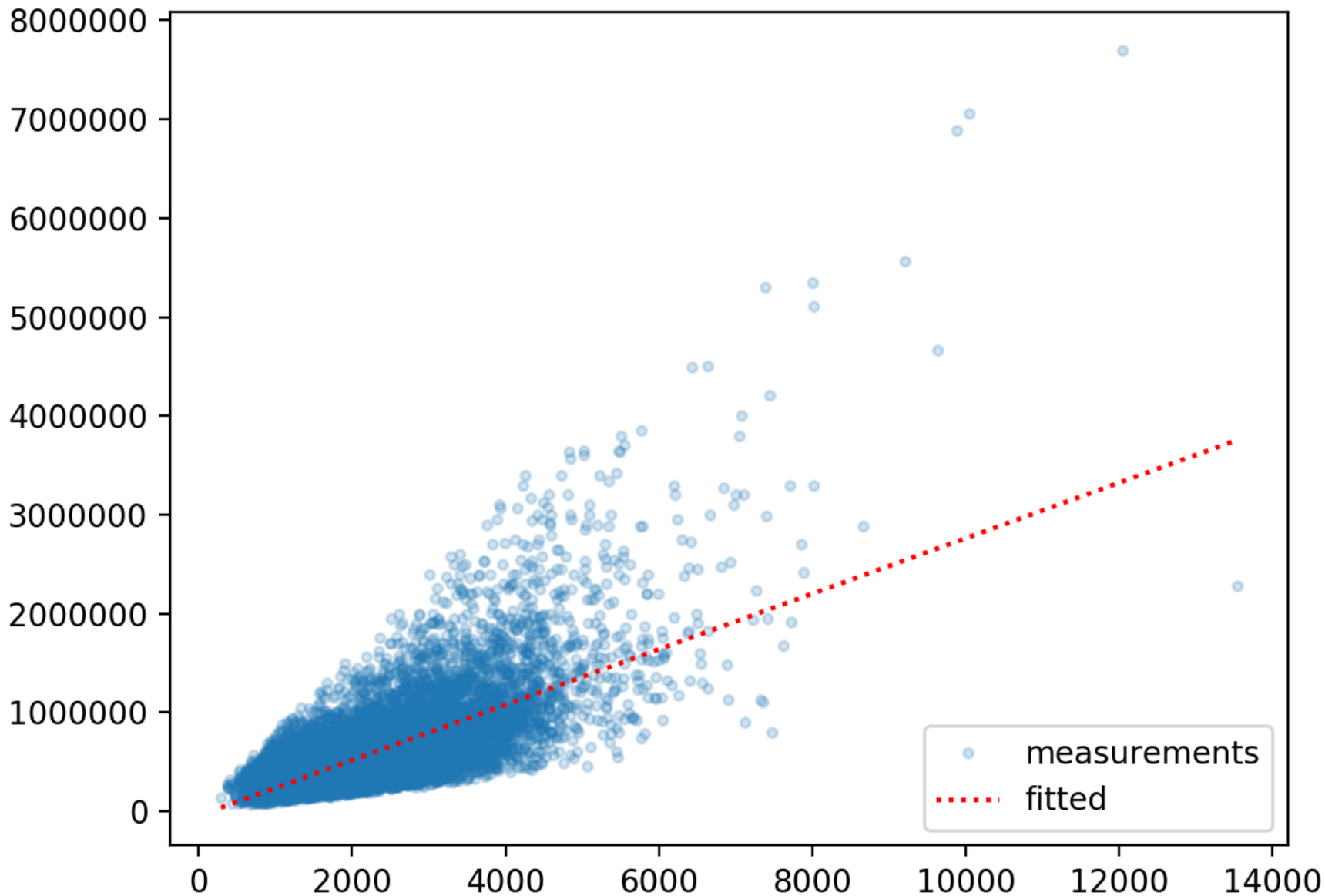
Multiple Regression

- Seattle Housing Market
  - Data from Kaggle

```
df = pd.read_csv('kc_house_data.csv')
df.dropna( inplace=True)
```

Multiple Regression

- Linear regression: price — grade



Multiple Regression

- Can use the same Pandas recipes

```
df = pd.read_csv('kc_house_data.csv')
df.dropna( inplace=True)
Y = df['price']
X = df[ ['sqft_living', 'bedrooms', 'condition',
'waterfront'] ]


model = sm.OLS(Y,X).fit()
predictions = model.predict(X)
print(model.summary())
```

OLS Regression Results

Dep. Variable:	price	R-squared (uncentered):	0.857
Model:	OLS	Adj. R-squared (uncentered):	0.857
Method:	Least Squares	F-statistic:	3.231e+04
Date:	Thu, 02 Jul 2020	Prob (F-statistic):	0.00
Time:	20:47:11	Log-Likelihood:	-2.9905e+05
No. Observations:	21613	AIC:	5.981e+05
Df Residuals:	21609	BIC:	5.981e+05
Df Model:	4		
Covariance Type:	nonrobust		

	coef	std err	t	P>|t|	[0.025	0.975]
sqft_living	303.8804	2.258	134.598	0.000	299.455	308.306
bedrooms	-5.919e+04	2062.324	-28.703	0.000	-6.32e+04	-5.52e+04
condition	3.04e+04	1527.531	19.901	0.000	2.74e+04	3.34e+04
waterfront	7.854e+05	1.96e+04	40.043	0.000	7.47e+05	8.24e+05

Omnibus:	13438.261	Durbin-Watson:	1.985
Prob(Omnibus):	0.000	Jarque-Bera (JB):	437567.612
Skew:	2.471	Prob(JB):	0.00
Kurtosis:	24.482	Cond. No.	2.65e+04

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
[2] The condition number is large, 2.65e+04. This might indicate that there are strong multicollinearity or other numerical problems.

Multiple Regression

- sklearn

```
from sklearn import linear_model

df = pd.read_csv('kc_house_data.csv')
df.dropna( inplace=True)
Y = df['price']
X = df[ ['sqft_living', 'bedrooms', 'condition',
'waterfront'] ]

regr = linear_model.LinearRegression()
regr.fit(X, Y)

print('Intercept: \n', regr.intercept_)
print('Coefficients: \n', regr.coef_)
```

Multiple Regression

- sklearn:
  - Score to get R^2 value:

```
regr = linear_model.LinearRegression()
regr.fit(X, Y)

print(regr.score(X, Y))
```

Multiple Regression

- statsmodel
  - ols takes the model as a string
    - Example:

```
model1 = ols("Y~Xsl+Xbr+Xco+Xwf", house).fit()
```

Multiple Regression

```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
from statsmodels.formula.api import ols
```

```
df = pd.read_csv('kc_house_data.csv')
y = df['price']
x1 = df['sqft_living']
x2 = df['grade']

model = ols("y ~ x1 + x2", df).fit()


print(model.summary())
```

Multiple Regression

- How can we access the ***importance*** of the different explanatory variables?
  - The size of the coefficient depends on the scale
    - Change sqft to square-meters and the coefficient will change by about 10

Multiple Regression

- How can we access the ***importance*** of the different explanatory variables?
  - Use the R^2 score differences
    - Example:
      - Waterside contributes 0.034
      - Bedrooms contribute 0.012
        - Notice that bedrooms correlates with square feet: correlation is 0.577

	R^2
All variables	0.548
All variables but waterside	0.514
All variables but bedrooms	0.536

```
house.sqft_living.corr(house.bedrooms)
```

Multiple Regression

- How can we access the ***<u>importance</u>*** of the different explanatory variables?
  - Depending on decision model (how do we penalize being wrong)
  - Sometimes use the square root of R^2, i.e. R

Multiple Regression

- How can we access the ***<u>importance</u>*** of the different explanatory variables?
  - Can use "standardized regression coefficient"
  - $\bar{b}_j = b_j \frac{S_{X_j}}{S_Y}$ with S_{X_j} std. dev. of X_j and S_Y std. dev of Y
- Example: `model1.params[1]*Xsl.std()/Y.std()`
  - square-feet: 0.765
  - bedroom: -0.134
  - condition: 0.082
  - waterfront: 0.185

Polynomial Regression

- What if the explanatory variables enter as powers?
- Can still apply multi-linear regression

$$y = b_0 + b_1 x_1 + b_2 x_2 + b_3 x_1^2 + b_4 x_1 x_2 + b_5 x_2^2$$

Logistic Regression

Categorical Data

- Outcomes can be categorical
  - Often, outcome is binary:
    - President gets re-elected or not
    - Customer is satisfied or not
- Often, explanatory variables are categorical as well
  - Person comes from an under-performing school
  - Order was made on a week-end
  - ...

Prediction Models for Binary Outcomes

- Famous example:
  - Taken an image of a pet, predict whether this is a cat or a dog

Prediction Models for Binary Outcomes

- Bayes: ***generative classifier***
    - Predicts indirectly $P(c \mid d)$
    - $\hat{c} =$ arg max$_{c \in C} P(d \mid c)P(c)$

```
                Likelihood Prior
```

- Evaluates product of likelihood and prior
    - Prior: Probability of a category c without looking at data
    - Likelihood: Probability of observing data if from a category c

Prediction Models for Binary Outcomes

- Regression is a ***discriminative classifier***
  - Tries to learn directly the classification from data
    - E.g.: All dog pictures have a collar
      - Collar present —> predict dog
      - Collar not present —> predict cat
- Computes directly $P(c \mid d)$

Prediction Models for Binary Outcomes

- Regression:
  - Supervised learning: Have a training set with classification provided
  - Input is given as vectors of numerical features
    - $\mathbf{x}^{(i)} = (x_{1,i}, x_{2,i}, \ldots, x_{n,i})$
  - Classification function that calculates the predicted class $\hat{y}(\mathbf{x})$
  - An objective function for learning: Measures the goodness of fit between true outcome and predicted outcome
  - An algorithm to optimize the objective function

Prediction Models for Binary Outcomes

- Linear Regression:
  - Classification function of type
    - $\hat{y}\left((x_1, x_2, \ldots, x_n)\right) = a_1 x_1 + a_2 x_2 + \ldots a_n x_n + b$
  - Objective function (a.k.a cost function)
    - Sum of squared differences between predicted and observed outcomes
      - E.g. Test Set $T = \{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \ldots \mathbf{x}^{(m)}\}$
      - Minimize cost function $\sum_{i=1}^{m} (y^{(i)} - \hat{y}^{(i)})^2$

Prediction Models for Binary Outcomes

- Linear regression can predict a numerical value
  - It can be made to predict a binary value
    - If the predictor is higher than a cut-off value: predict yes
    - Else predict no
- But there are better ways to generate a binary classifier

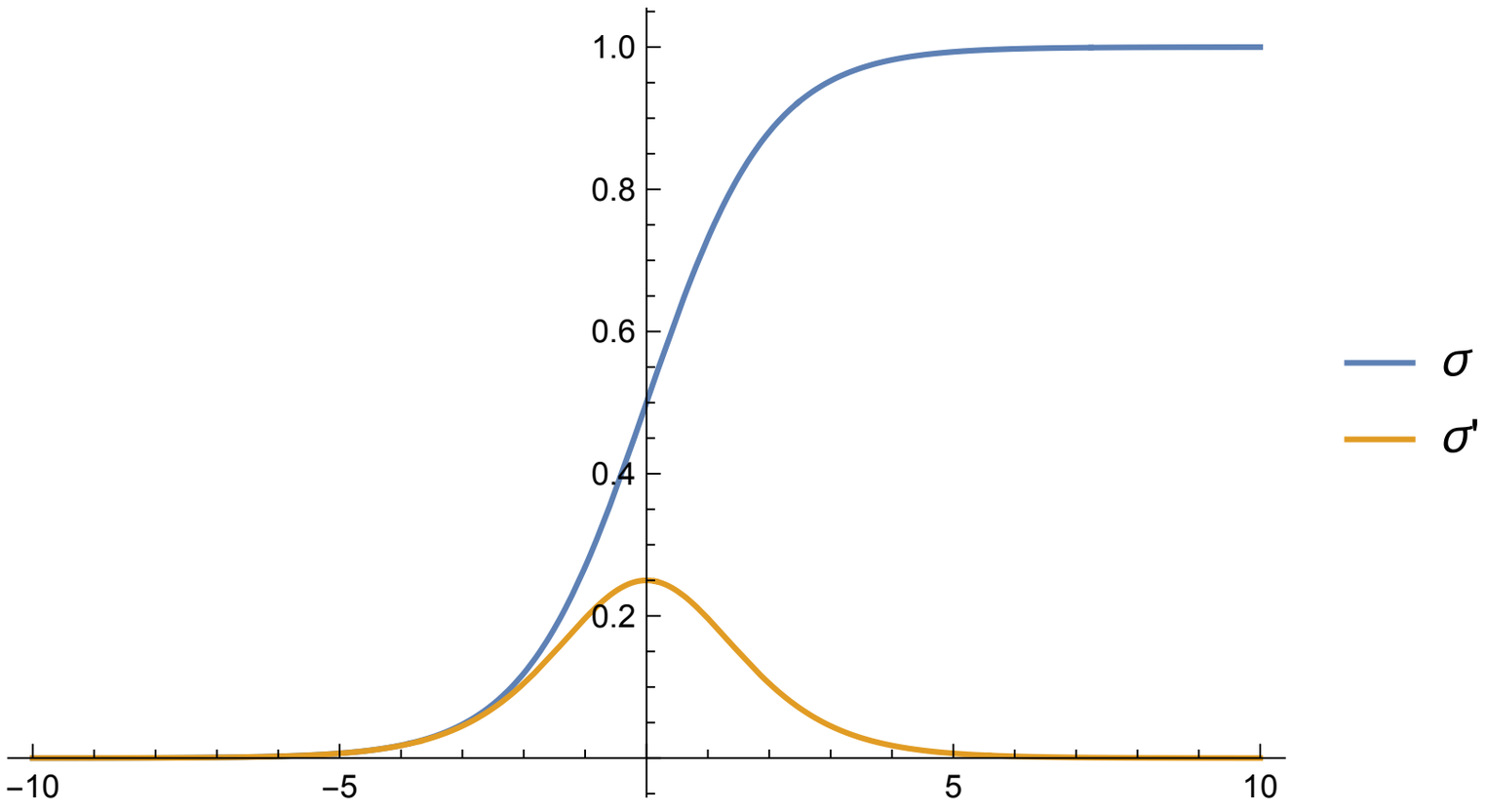
Prediction Models for Binary Outcomes

- Good binary classifier:
  - Since we want to predict the probability of a category based on the features:
    - Should look like a probability
  - Since we want to optimize:
    - Should be easy to differentiate
  - Best candidate classifier that has emerged:
    - Sigmoid classifier

Logistic Regression

- Use logistic function

$$\sigma(z) = \frac{1}{1 + \exp(-z)}$$



Logistic Regression

- Combine with linear regression to obtain logistic regression approach:
  - Learn best weights in
    - $\hat{y}\left((x_1, x_2, \ldots, x_n)\right) = \sigma(b + w_1 x_1 + w_2 x_2 + \ldots w_n x_n)$
  - We now interpret this as a probability for the positive outcome '+'
  - Set a ***decision boundary*** at 0.5
    - This is no restriction since we can adjust b and the weights

Logistic Regression

- We need to measure how far a prediction is from the true value
  - Our predictions $\hat{y}$ and the true value y can only be 0 or 1
    - If $y = 1$: Want to support $\hat{y} = 1$ and penalize $\hat{y} = 0$.
    - If $y = 0$: Want to support $\hat{y} = 0$ and penalize $\hat{y} = 1$.
- One successful approach:
  - $\text{Loss}(\hat{y}, y) = \hat{y}^y(1 - \hat{y})^{(1-y)}$

Logistic Regression

- Easier: Take the negative logarithm of the loss function
  - Cross Entropy Loss

$$L_{CE} = -y\log(\hat{y}) - (1-y)\log(1-\hat{y})$$

Logistic Regression

- This approach is successful, because we can use Gradient Descent
  - Training set of size m
    - Minimize $\sum_{i=1}^{m} L_{CE}(y^{(i)}, \hat{y}^{(i)})$
  - Turns out to be a convex function, so minimization is simple! (As far as those things go)
  - Recall:

$$\hat{y}\left((x_1, x_2, \ldots, x_n)\right) = \sigma(b + w_1x_1 + w_2x_2 + \ldots w_nx_n)$$

  - We minimize with respect to the weights and b

Logistic Regression

- Calculus:

$$\frac{\delta \mathsf{L}_{\mathsf{CE}}(w,b)}{\delta w_j} = \Big(\sigma(w_1x_1 + \ldots w_nx_n + b) - y\Big)\, x_j$$

$$= (\hat{y} - y)x_j$$

- Difference between true y and estimated outcome $\hat{y}$, multiplied by input coordinate

Logistic Regression

- Stochastic Gradient Descent
  - Until gradient is almost zero:
    - For each training point $x^{(i)}, y^{(i)}$:
      - Compute prediction $\hat{y}^{(i)}$
      - Compute loss
      - Compute gradient
      - Nudge weights in the opposite direction using a learning weight η
        - $(w_1, \ldots, w_n) \leftarrow (w_1, \ldots, w_n) - \eta \nabla \mathsf{L}_{\mathsf{CE}}$
      - Adjust η

Logistic Regression

- Stochastic gradient descent uses a single data point
  - Better results with random batches of points at the same time

Lasso and Ridge Regression

- If the feature vector is long, danger of overfitting is high
  - We learn the details of the training set
    - Want to limit the number of features with positive weight
- Dealt with by adding a regularization term to the cost function
  - Regularization term depends on the weights
    - Penalizes large weights

Lasso and Ridge Regression

- L2 regularization:
  - Use a quadratic function of the weights
    - Such as the euclidean norm of the weights
  - Called ***Ridge Regression***
    - Easier to optimize

Lasso and Ridge Regression

- L1 regularization
  - Regularization term is the sum of the absolute values of weights
  - Not differentiable, so optimization is more difficult
  - BUT: effective at lowering the number of non-zero weights
- Feature selection:
  - Restrict the number of features in a model
  - Usually gives better predictions

Examples

- Example: quality.csv
  - Try to predict whether patient labeled care they received as poor or good

quality

MemberID	InpatientDays	ERVisits	OfficeVisits	Narcotics	DaysSinceLastERVisit	Pain	TotalVisits	ProviderCount	MedicalClaims	ClaimLines	StartedOnCombination	AcuteDrugGapSmall	PoorCare
1	0	0	18	1	731	10	18	21	93	222	FALSE	0	0
2	1	1	6	1	411	0	8	27	19	115	FALSE	1	0
3	0	0	5	3	731	10	5	16	27	148	FALSE	5	0
4	0	1	19	0	158	34	20	14	59	242	FALSE	0	0
5	8	2	19	3	449	10	29	24	51	204	FALSE	0	0
6	2	0	9	2	731	6	11	40	53	156	FALSE	4	1
7	16	1	8	1	173.9583333	4	25	19	40	261	FALSE	0	0
8	2	0	8	0	731	5	10	11	28	87	FALSE	0	0
9	2	1	4	3	45	5	7	28	20	98	FALSE	0	1
10	4	2	0	2	104	2	6	21	17	66	FALSE	0	0
11	6	5	20	2	156	9	31	19	43	126	FALSE	2	0
12	0	0	7	4	731	0	7	8	23	41	FALSE	2	0
13	0	1	3	1	389	23	4	13	18	70	FALSE	0	0
14	1	1	20	3	594.9583333	16	22	18	48	133	FALSE	0	0
15	6	2	31	3	640.9583333	70	39	28	101	233	FALSE	0	0
16	0	0	8	0	731	0	8	5	19	48	FALSE	0	0
17	2	0	9	0	731	29	11	22	39	120	FALSE	0	0
18	3	0	20	1	731	13	23	17	34	73	FALSE	3	1

Examples

- First column is an arbitrary patient ID
  - we make this the index
- One column is a Boolean, when imported into Python
  - so we change it to a numeric value

```
df = pd.read_csv('quality.csv', sep=',', index_col=0)
df.replace({False:0, True:1}, inplace=True)
```

Examples

- Farmington Heart Data Project:
  - https://framinghamheartstudy.org
  - Monitoring health data since 1948
  - 2002 enrolled grandchildren of first study

Examples

framingham

male	age	education	currentSmoker	cigsPerDay	BPMeds	prevalentStroke	prevalentHyp	diabetes	totChol	sysBP	diaBP	BMI	heartRate	glucose	TenYearCHD
1	39	4	0	0	0	0	0	0	195	106	70	26.97	80	77	0
0	46	2	0	0	0	0	0	0	250	121	81	28.73	95	76	0
1	48	1	1	20	0	0	0	0	245	127.5	80	25.34	75	70	0
0	61	3	1	30	0	0	1	0	225	150	95	28.58	65	103	1
0	46	3	1	23	0	0	0	0	285	130	84	23.1	85	85	0
0	43	2	0	0	0	0	1	0	228	180	110	30.3	77	99	0
0	63	1	0	0	0	0	0	0	205	138	71	33.11	60	85	1
0	45	2	1	20	0	0	0	0	313	100	71	21.68	79	78	0
1	52	1	0	0	0	0	1	0	260	141.5	89	26.36	76	79	0
1	43	1	1	30	0	0	1	0	225	162	107	23.61	93	88	0
0	50	1	0	0	0	0	0	0	254	133	76	22.91	75	76	0

Examples

- Contains a few NaN data
  - We just drop them

```
df = pd.read_csv('framingham.csv', sep=',')
df.dropna(inplace=True)
```

Logistic Regression in Stats-Models

- Import statsmodels.api

```
import statsmodels.api as sm
```

- Interactively select the columns that gives us high p-values

```
cols = [ 'Pain', 'TotalVisits',
         'ProviderCount',
         'MedicalClaims', 'ClaimLines',
         'StartedOnCombination',
         'AcuteDrugGapSmall',]
```

Logistic Regression in Stats-Models

- Create a logit model
  - Can do as we did for linear regression with a string
  - Can do using a dataframe syntax

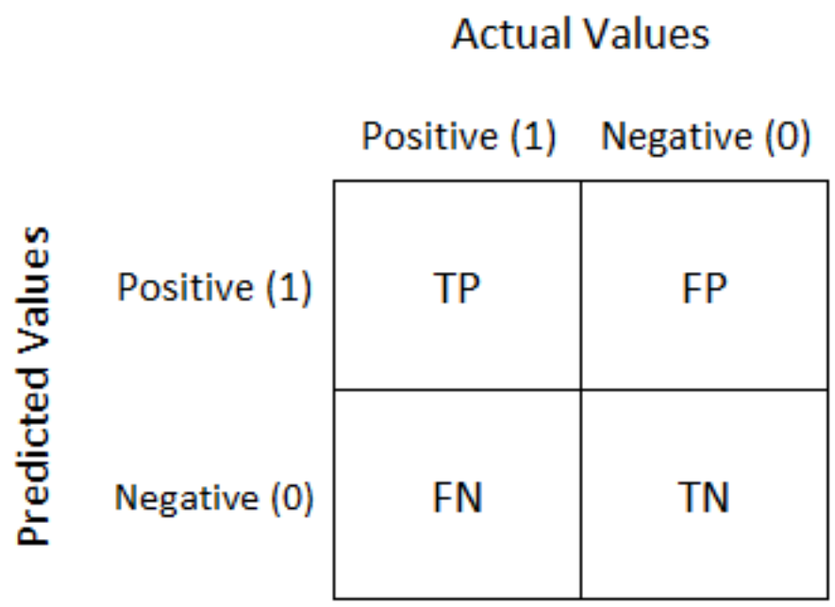
```
logit_model=sm.Logit(df.PoorCare,df[cols])
result=logit_model.fit()
```

- Print the summary pages

```
print(result.summary2())
```

Logistic Regression in Stats-Models

- Print the results
  - `print(result.pred_table())`
- This gives the "confusion matrix"
  - Coefficient [i,j] gives:
    - predicted i values
    - actual j values



Logistic Regression in Stats-Models

- Quality prediction:
  - ```
    [[91.  7.]
     [18. 15.]]
    ```
- 7 False negative and 18 false positives
    ```

Logistic Regression in Stats-Models

- Heart Event Prediction:
  - ```
    [[3075.   26.]
     [ 523.   34.]]
    ```
- 26 false negatives
- 523 false positives
    ```

Logistic Regression in Stats-Models

- Can try to improve using Lasso

```
result=logit_model.fit_regularized()
```

Logistic Regression in Stats-Models

- Can try to improve selecting only columns with high P-values

```
Optimization terminated successfully.
         Current function value: 0.423769
         Iterations 6
                          Results: Logit
==========================================================
Model:              Logit            Pseudo R-squared: 0.007
Dependent Variable: TenYearCHD       AIC:              3114.2927
Date:               2020-07-12 18:18 BIC:              3157.7254
No. Observations:   3658             Log-Likelihood:   -1550.1
Df Model:           6                LL-Null:          -1560.6
Df Residuals:       3651             LLR p-value:      0.0019166
Converged:          1.0000           Scale:            1.0000
No. Iterations:     6.0000
----------------------------------------------------------
                 Coef.  Std.Err.    z    P>|z|   [0.025  0.975]
----------------------------------------------------------
currentSmoker     0.0390   0.0908  0.4291 0.6679 -0.1391  0.2170
BPMeds            0.5145   0.2200  2.3388 0.0193  0.0833  0.9457
prevalentStroke   0.7716   0.4708  1.6390 0.1012 -0.1511  1.6944
prevalentHyp      0.8892   0.0983  9.0439 0.0000  0.6965  1.0818
diabetes          1.4746   0.2696  5.4688 0.0000  0.9461  2.0030
totChol          -0.0067   0.0007 -9.7668 0.0000 -0.0081 -0.0054
glucose          -0.0061   0.0019 -3.2113 0.0013 -0.0098 -0.0024
==========================================================
```

Logistic Regression in Stats-Models

- Select the columns
  - `cols = ['currentSmoker', 'BPMeds', 'prevalentStroke', 'prevalentHyp', 'diabetes', 'totChol','glucose']`
- Get a better (?) confusion matrix:
  - ```
    [[3086.   15.]
     [ 549.    8.]]
    ```
  - False negatives has gone down
  - False positives has gone up
    ```

Logistic Regression in Scikit-learn

- Import from sklearn

```
from sklearn.linear_model import LogisticRegression
from sklearn import metrics
from sklearn.metrics import confusion_matrix
from sklearn.model_selection import train_test_split
from sklearn.metrics import classification_report
```

Logistic Regression in Scikit-learn

- Create a logistic regression object and fit it on the data

```
logreg = LogisticRegression()
logreg.fit(X=df[cols], y = df.TenYearCHD)
y_pred = logreg.predict(df[cols])
confusion_matrix = confusion_matrix(df.TenYearCHD,
y_pred)
print(confusion_matrix)
```

Logistic Regression in Scikit-learn

- Scikit-learn uses a different algorithm
  - Confusion matrix on the whole set is
  -

```
[[3087   14]
 [ 535   22]]
```

Logistic Regression in Scikit-learn

- Can also divide the set in training and test set

```
X_train, X_test, y_train, y_test =
    train test split(df[cols],
                     df.TenYearCHD,
                     test_size=0.3,
                     random_state=0)
logreg.fit(X_train, y_train)
y_pred = logreg.predict(X_test)
confusion_matrix = confusion_matrix(y_test, y_pred)
print(confusion_matrix)
```

Logistic Regression in Scikit-learn

- Confusion matrix
  - ```
    [[915   1]
     [176   6]]
    ```
    ```

Measuring Success

	precision	recall	f1-score	support
0	0.84	1.00	0.91	916
1	0.86	0.03	0.06	182
accuracy			0.84	1098
macro avg	0.85	0.52	0.49	1098
weighted avg	0.84	0.84	0.77	1098

Measuring Success

- How can we measure accuracy?
  - accuracy = (fp+fn)/(tp+tn+fp+fn)
    - Unfortunately, because of skewed data sets, often very high
  - precision = tp/(tp+fp)
  - recall = tp/(tp+fn)
  - F measure = harmonic mean of precision and recall

Probit Regression

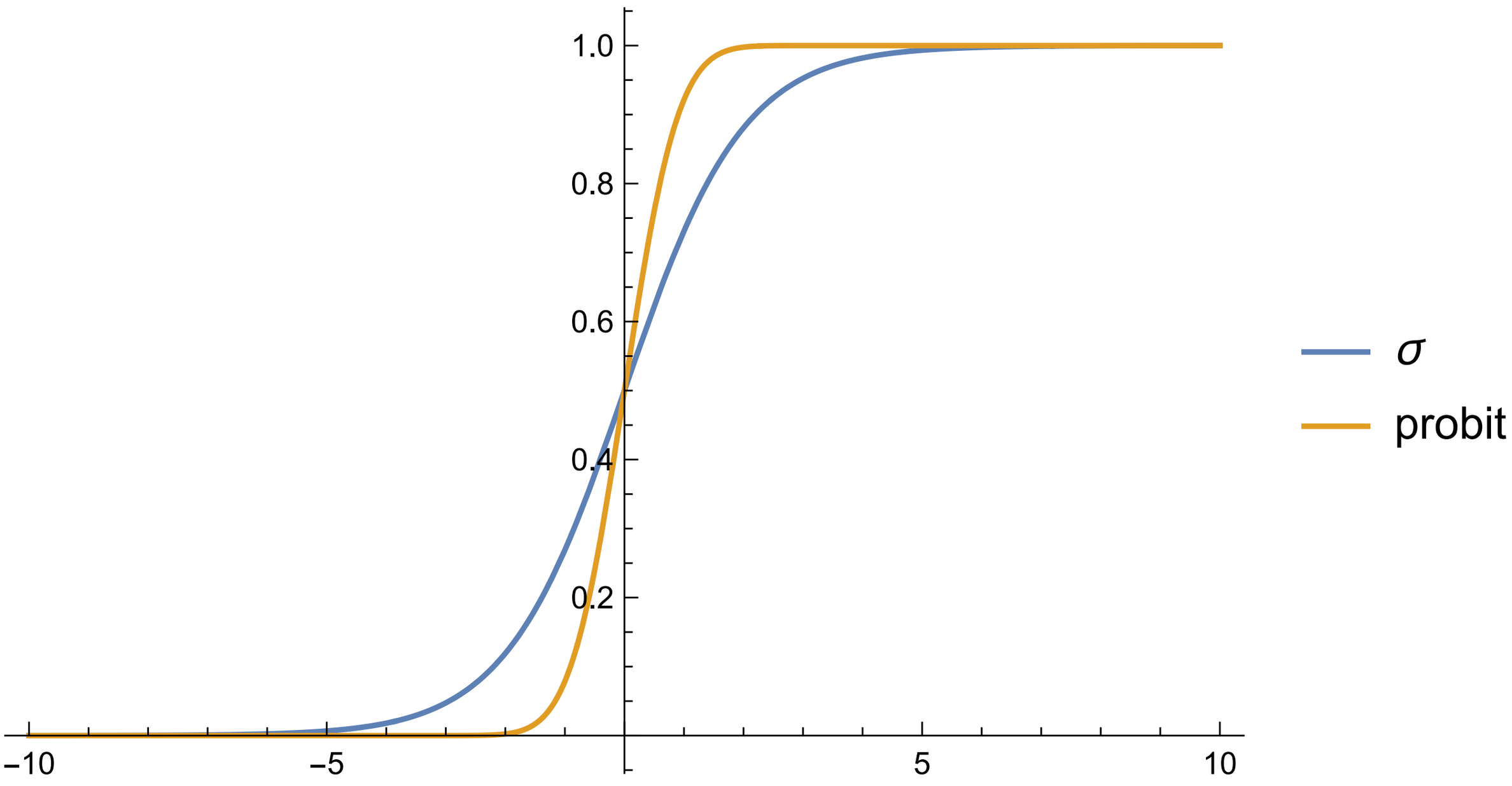
- Instead of using the logistic function σ, can also use the cumulative distribution function of the normal distribution

$$\text{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z \exp(-t^2) dt$$

- Predictor is then

$$\frac{1}{2}\left(1 + \text{erf}(b + w_1 x_1 + w_2 x_2 + \ldots + w_n x_n)\right)$$

Probit Regression



Probit Regression

- Calculations with probit are more involved
  - Statsmodels implements it
    - `from statsmodels.discrete.discrete_model import Probit`
  - Fit the probit model

```
probit_model=Probit(df.TenYearCHD,df[cols])
result=probit_model.fit()

print(result.summary())
print(result.pred_table())
for i in range(20):
   print(df.TenYearCHD.iloc[i],
result.predict(df[cols]).iloc[i])
```

Probit Regression

- Confusion matrix is now

```
[[3085.   16.]
 [ 547.   10.]]
```

- More false positives but less false negatives

Multinomial Logistic Regression

- Want to predict one of several categories based on feature vector
- Use the softmax function

$$\text{softmax}\left(z_1, z_2, \ldots, z_m\right) = \left(\frac{e^{z_1}}{\sum_{i=1}^{m} e^{z_i}}, \frac{e^{z_2}}{\sum_{i=1}^{m} e^{z_i}}, \ldots, \frac{e^{z_m}}{\sum_{i=1}^{m} e^{z_i}}\right)$$

Multinomial Logistic Regression

- Learning is still possible, but more complicated

Multinomial Logistic Regression

```
model1 = LogisticRegression(random_state=0,
                            multi_class='multinomial',
                            penalty='none',
                            solver='newton-cg').fit(X_train, y_train)
preds = model1.predict(X_test)
```

Final Example

- Spine data

Col1	Col2	Col3	Col4	Col5	Col6	Col7	Col8	Col9	Col10	Col11	Col12	Class_att						
63.0278175		22.55258597		39.60911701		40.47523153		98.67291675		-0.254399986	0.744503464	12.5661	14.5386	15.30468	-28.658501	43.5123	Abnormal	
39.05695098		10.06099147		25.01537822		28.99595951		114.4054254		4.564258645	0.415185678	12.8874	17.5323	16.78486	-25.530607	16.1102	Abnormal	
68.83202098		22.21848205		50.09219357		46.61353893		105.9851355		-3.530317314	0.474889164	26.8343	17.4861	16.65897	-29.031888	19.2221	Abnormal	Prediction is done by using binary classification.
69.29700807		24.65287791		44.31123813		44.64413017		101.8684951		11.21152344	0.369345264	23.5603	12.7074	11.42447	-30.470246	18.8329	Abnormal	
49.71285934		9.652074879		28.317406		40.06078446		108.1687249		7.918500615	0.543360472	35.494	15.9546	8.87237	-16.378376	24.9171	Abnormal	
40.25019968		13.92190658		25.1249496		26.32829311		130.3278713		2.230651729	0.789992856	29.323	12.0036	10.40462	-1.512209	9.6548	Abnormal	Attribute1 = pelvic_incidence (numeric)

- Use explanations to give column names
- Remove last column

Final Example

```
back_data = pd.read_csv("spine.csv")
del back_data['Unnamed: 13']
back_data.columns = ['pelvic_incidence','pelvic tilt',
                     'lumbar_lordosis_angle','sacral_slope',
                     'pelvic_radius','degree_spondylolisthesis',
                     'pelvic_slope','Direct_tilt','thoracic_slope',
                     'cervical tilt','sacrum angle','scoliosis slope',
                     'Status']
print(back_data.Status.describe())
```

Final Example

- Can also change the values of Status Column to 0 or 1

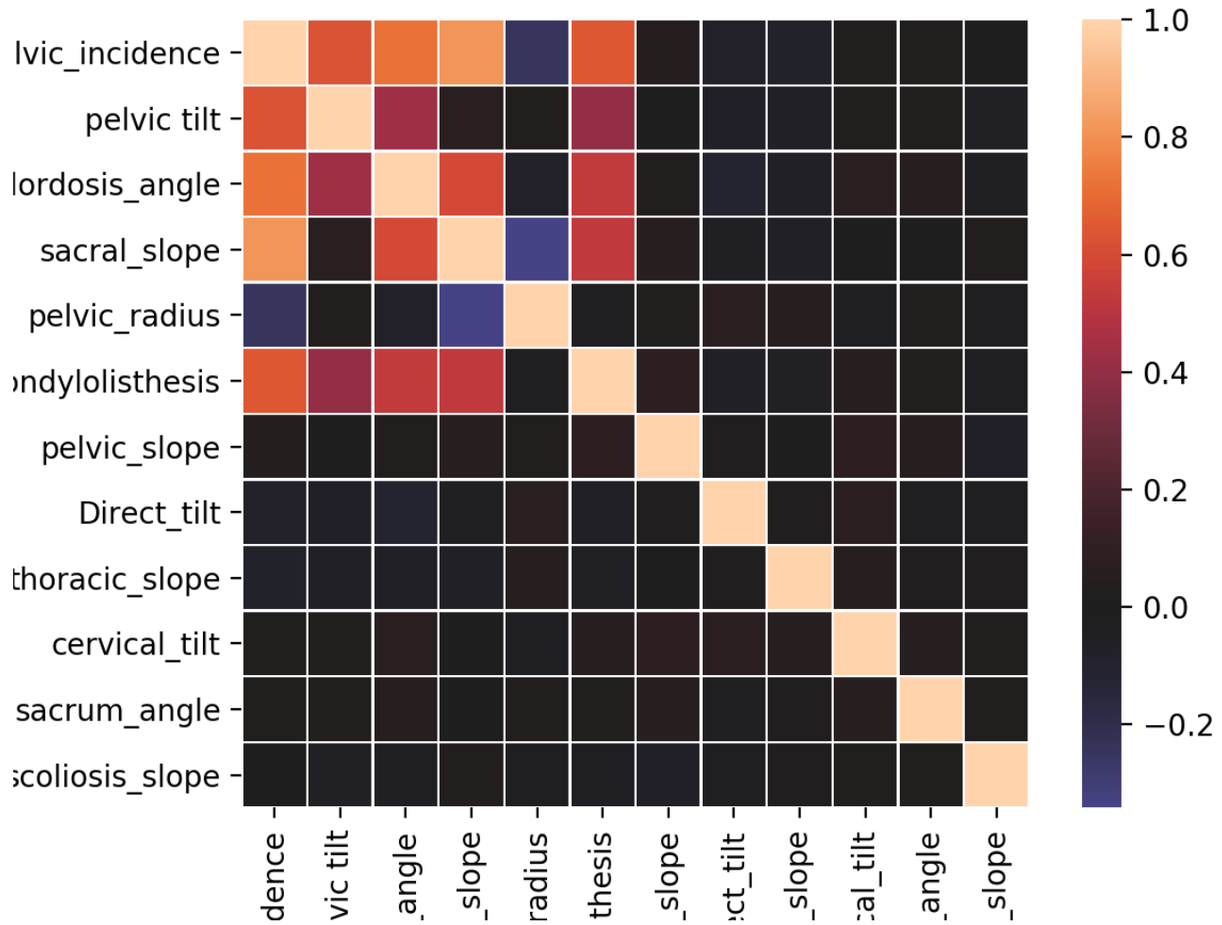
```
back_data.loc[back_data.Status=='Abnormal','Status'] = 1
back_data.loc[back_data.Status=='Normal','Status'] = 0
X = back_data.iloc[:, :12]
y = back_data.iloc[:, 12]
```

Final Example

- First task:
  - Are any of the columns strongly correlated?
    - Otherwise, model would have difficulties
    - Create a seaborn heatmap of the correlation

```
corr_back = back_data.corr()
sns.heatmap(corr_back, center=0, square=True,
linewidths=.5)
```

Final Example



Final Example

- We now see whether the values differ between normal and abnormal spines:

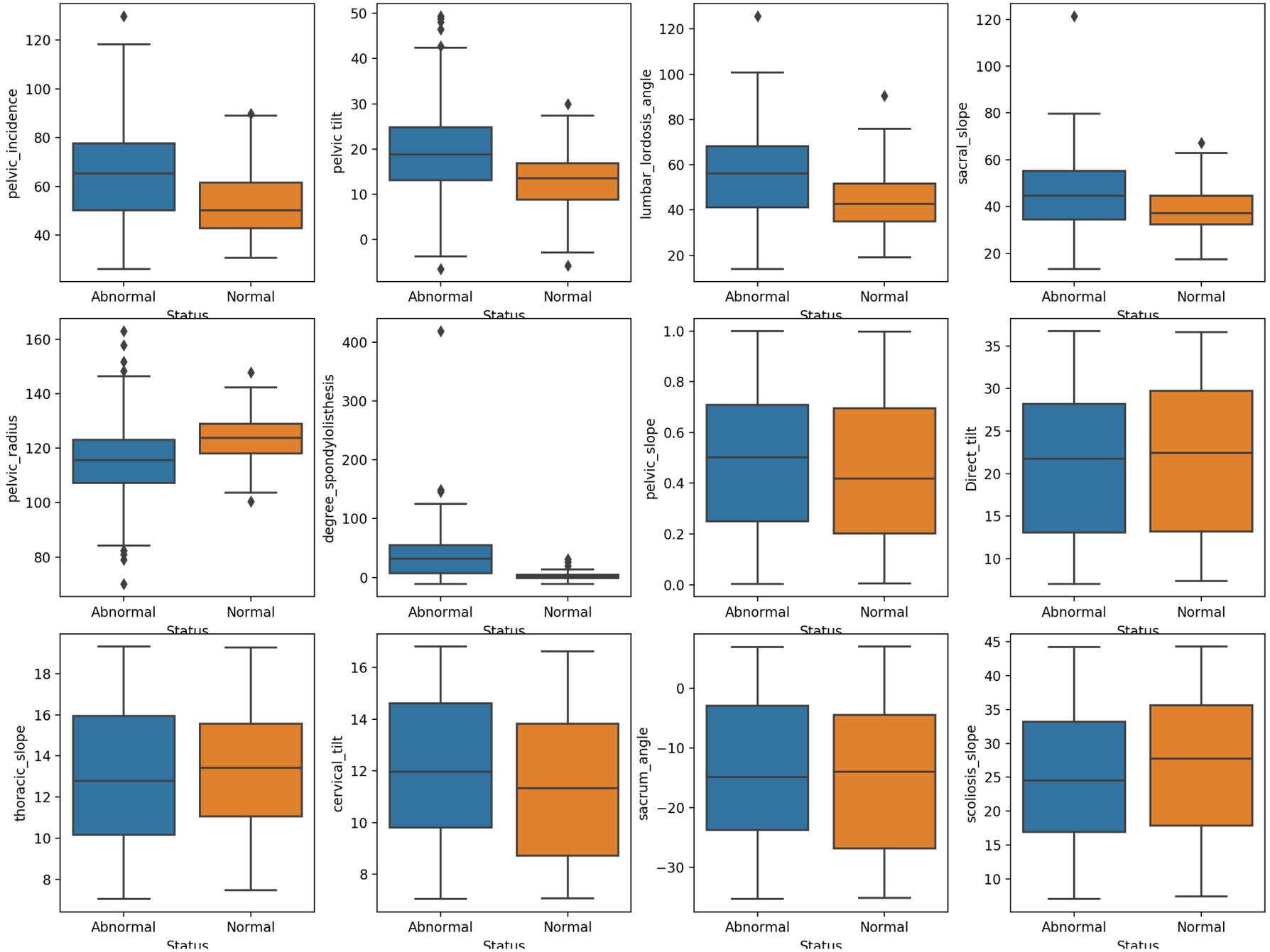
```
for x in back data.columns[:-1]:
   print(x, back_data.groupby('Status').mean()[x])
for x in back_data.columns[:-1]:
   print(x, back_data.groupby('Status').median()[x])
```

Final Example

- Can also use a box plot to see the difference

```
fig, axes = plt.subplots(3, 4, figsize = (15,15))
axes = axes.flatten()

for i in range(0,len(back_data.columns)-1):
    sns.boxplot(x="Status", y=back_data.iloc[:,i],
                data=back_data, orient='v', ax=axes[i])

plt.tight_layout()
plt.show()
```

Final Example



Final Example

- Need to create training set and test set
- Need to scale:
  - Mean is set to 0
  - StDev is set to 1
- Can be done with
  - sklearn.preprocessing.StandardScaler

Final Example

```
def data_preprocess(X,y):
    X_train, X_test, y_train,
        y_test = train_test_split(X, y.values.ravel(),
        test_size=0.3,
        random_state=0)
    from sklearn.preprocessing import StandardScaler
    scaler = StandardScaler(copy=True,
                            with_mean=True,
                            with_std=True)

    scaler.fit(X_train)

    train_scaled = scaler.transform(X_train)
    test_scaled = scaler.transform(X_test)
    return(train_scaled, test_scaled, y_train, y_test)
```

Final Example

- We use the logistic regression model from sklearn

```
from sklearn.linear_model import LogisticRegression
```

-

```
X_train_scaled, X_test_scaled, y_train, y_test =
data_preprocess(X,y)
logreg = LogisticRegression().fit(X_train_scaled,
y_train)

logreg_result = logistic_regression(X_train_scaled,
y_train)
    logreg = LogisticRegression().fit(x, y)
```

Final Example

- We can now read the results:

```
logreg result.score(X train scaled,y train)
Training set score: 0.876
logreg_result.score(X_test_scaled,y_test)
Test set score: 0.817
```

Final Example

- To see what influence variables have, we use statsmodels

```
X_train_scaled, X_test_scaled, y_train, y_test =
data_preprocess(X,y)

logit_model = sm.Logit(y_train, X_train_scaled)
result = logit_model.fit()
print(result.summary2())
```

Final Example

Results: Logit

Model:	Logit	Pseudo R-squared:	0.248
Dependent Variable:	y	AIC:	229.3058
Date:	2020-11-19 18:19	BIC:	269.8646
No. Observations:	217	Log-Likelihood:	-102.65
Df Model:	11	LL-Null:	-136.45
Df Residuals:	205	LLR p-value:	3.4943e-10
Converged:	0.0000	Scale:	1.0000
No. Iterations:	35.0000		

	Coef.	Std.Err.	z	P>|z|	[0.025	0.975]
x1	0.0814	11580039.8359	0.0000	1.0000	-22696460.9366	22696461.0993
x2	0.0765	6600560.9760	0.0000	1.0000	-12936861.7142	12936861.8673
x3	-0.2797	0.3142	-0.8904	0.3733	-0.8955	0.3361
x4	-0.5412	9111339.5243	-0.0000	1.0000	-17857897.8597	17857896.7773
x5	-1.1234	0.2351	-4.7773	0.0000	-1.5842	-0.6625
x6	2.3250	0.4401	5.2832	0.0000	1.4625	3.1875
x7	0.1711	0.1790	0.9561	0.3390	-0.1797	0.5220
x8	-0.2115	0.1770	-1.1950	0.2321	-0.5583	0.1354
x9	0.0724	0.1738	0.4166	0.6770	-0.2683	0.4131
x10	0.2003	0.1772	1.1301	0.2584	-0.1471	0.5476
x11	-0.1042	0.1804	-0.5778	0.5634	-0.4578	0.2493
x12	-0.2749	0.1764	-1.5579	0.1193	-0.6207	0.0709

Final Example

- There was no convergence, meaning that there was some high correlation between variables
- Pelvic Incidence column is sum of Pelvic Tilt and Sacral Slope
- Let’s remove these

```
cols_to_include = [cols for cols in X.columns
                   if cols not in
      ['pelvic_incidence', 'pelvic
tilt','sacral_slope']]
X = back_data[cols_to_include]
```

- And run again

Final Example

Optimization terminated successfully.
         Current function value: 0.481933
         Iterations 7

Results: Logit

Model:	Logit	Pseudo R-squared:	0.234
Dependent Variable:	y	AIC:	227.1591
Date:	2020-11-19 18:23	BIC:	257.5781
No. Observations:	217	Log-Likelihood:	-104.58
Df Model:	8	LL-Null:	-136.45
Df Residuals:	208	LLR p-value:	8.5613e-11
Converged:	1.0000	Scale:	1.0000
No. Iterations:	7.0000		

	Coef.	Std.Err.	z	P>|z|	[0.025	0.975]
x1	-0.5434	0.2568	-2.1158	**0.0344**	-1.0468	-0.0400
x2	-0.9642	0.2080	-4.6364	**0.0000**	-1.3719	-0.5566
x3	2.2963	0.4142	5.5443	**0.0000**	1.4846	3.1081
x4	0.1499	0.1771	0.8464	0.3974	-0.1972	0.4971
x5	-0.2442	0.1738	-1.4047	0.1601	-0.5849	0.0965
x6	0.0640	0.1732	0.3694	0.7118	-0.2754	0.4034
x7	0.2068	0.1747	1.1841	0.2364	-0.1355	0.5491
x8	-0.1183	0.1777	-0.6660	0.5054	-0.4666	0.2299
x9	-0.2872	0.1736	-1.6547	0.0980	-0.6274	0.0530

Final Example

- We concentrate on those variables with a low P-value:

	Coef.	Std.Err.	z	P>|z|	[0.025	0.975]
x1	-0.5434	0.2568	-2.1158	**0.0344**	-1.0468	-0.0400
x2	-0.9642	0.2080	-4.6364	**0.0000**	-1.3719	-0.5566
x3	2.2963	0.4142	5.5443	**0.0000**	1.4846	3.1081
x4	0.1499	0.1771	0.8464	0.3974	-0.1972	0.4971
x5	-0.2442	0.1738	-1.4047	0.1601	-0.5849	0.0965
x6	0.0640	0.1732	0.3694	0.7118	-0.2754	0.4034
x7	0.2068	0.1747	1.1841	0.2364	-0.1355	0.5491
x8	-0.1183	0.1777	-0.6660	0.5054	-0.4666	0.2299
x9	-0.2872	0.1736	-1.6547	0.0980	-0.6274	0.0530

Final Example

```
X_trim_1 = X.loc[:,['lumbar_lordosis_angle’,
                    'pelvic_radius',
                    'degree_spondylolisthesis']]

X_train_scaled, X_test_scaled, y_train, y_test =
data_preprocess(X_trim_1,y)
logit_model = sm.Logit(y_train, X_train_scaled)
result = logit_model.fit()
print(result.summary2())
```

Final Example

```
==========================================
Optimization terminated successfully.
         Current function value: 0.498420
         Iterations 7
                          Results: Logit
==========================================================================
Model:                  Logit               Pseudo R-squared:  0.207
Dependent Variable:     y                   AIC:               222.3145
Date:                   2020-11-19 18:30    BIC:               232.4542
No. Observations:       217                 Log-Likelihood:    -108.16
Df Model:               2                   LL-Null:           -136.45
Df Residuals:           214                 LLR p-value:       5.1622e-13
Converged:              1.0000              Scale:             1.0000
No. Iterations:         7.0000
--------------------------------------------------------------------------
       Coef.     Std.Err.        z        P>|z|       [0.025      0.975]
--------------------------------------------------------------------------
x1    -0.4688       0.2426    -1.9325     0.0533     -0.9443      0.0067
x2    -0.9188       0.2037    -4.5100     0.0000     -1.3181     -0.5195
x3     2.1897       0.3937     5.5626     0.0000      1.4182      2.9613
==========================================================================
```

Final Example

- Some improvement in scores:
-

```
Training set score: 0.857
Test set score: 0.774
```