

# Statistics for Data Science

## Lecture 4

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# Plan for Lecture 4

- ① Last week's assignment
- ② OLS regression
  - Univariate regression
  - Multivariate regression
  - Regression with interactions
- ③ Regression diagnostics: beginner

# Before next time

## Assignment for next week

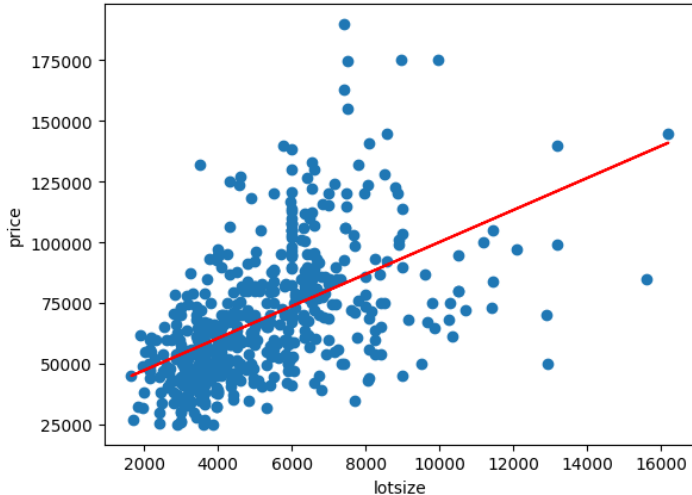
- Reread Chapter 2 & 3 (if needed)
- Read Chapter 4 (main material for next week)
- Reconsider/finish the in-class assignments
- Examples in book
- Small new programming assignment
  - Visualize the correlation between some (continuous) variables in the houseprice data using a scatter plot
  - Calculate the correlation
  - Perform a hypothesis test on this correlation (clearly formulate the hypotheses and the conclusion)
- Work on final assignment



# Univariate regression

# What can regression do?

- Data science is about exploring dependence across (multiple) variables
- The simplest model for dependence: linear relation (strong link with correlation)



# The setup of a regression

Can see “regression line” as

- Predicted value of price ( $y$ ) at certain value of lotsize ( $x$ )
- A fitted **model** that links  $y$  to  $x$

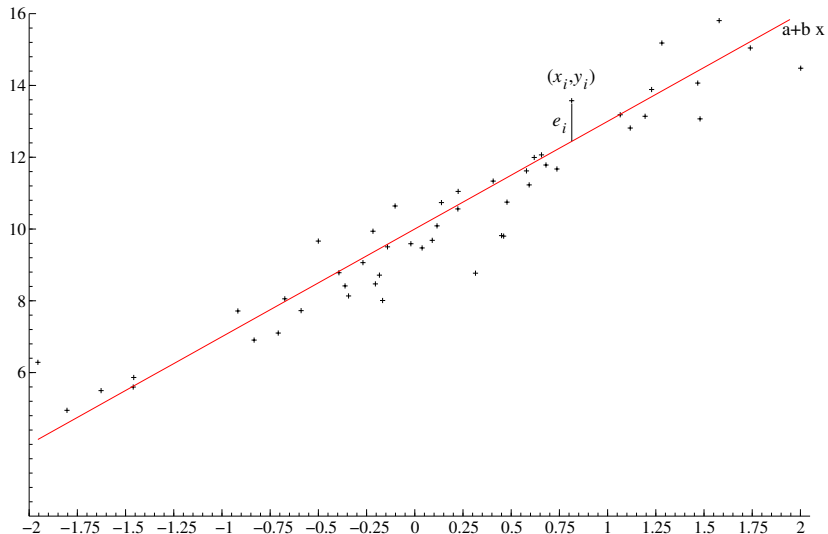
Mathematically,

$$y_i = a + bx_i + e_i$$

where

- $y_i$ : dependent variable (for observation  $i$ )
- $x_i$ : explanatory variable (for observation  $i$ )
- $a$  and  $b$ : estimated coefficients (apply to all observations)
- $e_i$ : residual, or prediction error (for observation  $i$ )

# Graphical interpretation



# Ordinary Least Squares [OLS]

How to find (estimate)  $a$  and  $b$  given data?

$$y_i = a + bx_i + e_i$$

**Idea:** Small values of  $e_i$  (close to zero) are preferred

→ Minimize sum of squared  $e_i$  (=OLS)

$$\min_{a,b} S(a, b) = \sum_i e_i^2 = \sum_{i=1}^n (y_i - a - bx_i)^2$$

Calculating the first derivatives and setting these to zero yields:

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

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

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# (Statistical) properties

## Properties OLS:

- + Easy calculation
- + Well-known statistical properties
- + Optimal under some assumptions
- Sensitive to outliers
- Not optimal if assumptions are *not* true

## Question

How to judge whether OLS is a good method?

Difficult! → Answer depends on the “true” relationship between  $y$  and  $x$

To analyze properties of OLS we need to

- define the true (unknown) relationship  
(also known as the data generating process [DGP])

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# Is OLS a good method? 6 assumptions to answer this

The “true” relationship between  $y$  and  $x$  (data generating process [DGP])

$$y_i = \alpha + \beta x_i + \varepsilon_i$$

where  $\alpha$  and  $\beta$  are unknown &  $\varepsilon_i$  is “pure” random variation (note the Greek letters)

## Formal assumptions:

A1 *Non-degeneration*:  $x_i$  are fixed (non-random) with  $\sum (x_i - \bar{x})^2 > 0$

A2 *Mean zero*:  $\varepsilon_i$  are random with  $E[\varepsilon_i] = 0$

A3 *Linearity*:  $y_i = \alpha + \beta x_i + \varepsilon_i$  holds exactly

A4 *Homoskedasticity*:  $E[\varepsilon_i^2] = \text{Var}(\varepsilon_i) = \sigma^2$

A5 *No autocorrelation*:  $E[\varepsilon_i \varepsilon_j] = 0$  for  $i \neq j$

A6 *Normality*:  $\varepsilon_i \sim N(0, \sigma^2)$

## Gauss-Markov theorem:

Under these assumptions one can show that OLS is “best” (= smallest uncertainty) 

→ not all assumptions are really necessary

# Summary

Linear regression (OLS):

- strong method
- often used
- building block for further analysis

Interpretation of coefficients:

Given the model  $y = \alpha + \beta x + \varepsilon$

- $\alpha$ : Expected value of  $y$  if  $x = 0$  (not always useful)
- $\beta$ : Increase in expected value if  $x$  increases by 1

# Linear model using Python

## Packages

- `import statsmodels.api as sm`
- `import statsmodels.formula.api as smf`

## Main function: `smf.ols()`

- `smf.ols(formula="y ~ x", data = yourframe)`: linear model with y explained by x (and a constant)
- Give the model a name, eg.: `m = smf.ols(formula="y ~ x", data = yourframe)`
- Estimate the parameters `res = m.fit()` and store the result

# Useful functions using `res`, the result of `.fit()`

- `res.summary()`: give a summary of the results
- `sm.graphics.abline_plot(model_results=res, color='red', ax=plt.gca())`: add a fitted (straight) line to an existing plot

Other properties and methods (will be useful later)



- `res.params`: give estimated coefficients
- `res.conf_int(alpha=..)`: provide confidence intervals
- `res.fittedvalues`: given in-sample fitted values
- `res.predict(exog={'x': [1,2,3]})`: give predicted values for new data

# Assignment

# In-class assignment 4.1

- Use housing data
- Explain price using lotsize using a linear model
- Reproduce scatter with fitted linear line
- Interpret the results of your final model

You will also need

-  `import pandas as pd`
-  `import matplotlib.pyplot as plt`

# Testing and model evaluation



# Evaluate goodness of fit

For a *good* model:

- All scatter points are close to the line
- All residuals  $e_i = y_i - a - bx_i$  are close to zero
- Fit is related to sum squared errors =  $SSE = \sum_i e_i^2$

Goodness of fit:

- Relate SSE to “scale of data” = Total sum of squares = SST or SSY

$$SSY = \sum_i (y_i - \bar{y})^2 = \sum_i y_i^2 - n\bar{y}^2$$

- Goodness of fit:  $R^2$

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

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Alternative definition of  $R^2$

$$R^2 = \frac{SSR}{SSY}$$

where  $SSR$  = “regression sum of squares” =  $\sum_i (\hat{y}_i - \bar{\hat{y}})^2$

Interpretation

- $R^2$  is squared correlation between  $x$  and  $y$
- $R^2$ : proportion of variation explained
- $R^2 = 0$ : nothing explained
- $R^2 = 1$ : everything explained

 `res.summary()` gives  $R^2$  as standard output  
(`res` is the result from  `smf.ols(...).fit()`)

# Estimating the variance of $\varepsilon_i$

**Question:** Which part of  $y$  can never be explained?

→ The error term:

$$\varepsilon_i = y_i - \alpha - \beta x_i$$

Denote the variance of  $\varepsilon_i$  by  $\sigma^2$

Estimation

- Estimate  $\varepsilon_i$  by  $e_i = y_i - a - bx_i$
- Estimate  $\sigma^2$  by  $s^2$

$$s^2 = \frac{\sum_i e_i^2}{n - k} = \frac{SSE}{n - k} \quad (\text{here: } k = 2)$$

- In general:  $k$ =number of parameters

# Estimation uncertainty

Note:

- We estimate  $\alpha$  and  $\beta$  (with  $a$  and  $b$ )
- There is estimation uncertainty!
- How large is this?
- Does  $x$  have a *significant* impact?  
→ Can we reject  $H_0 : \beta = 0$ ?

Quantifying the uncertainty

- Recall:  $a$  and  $b$  are a function of  $y$  (and  $x$ ) → a random variable
- In fact a linear function of  $y$  → can easily work out  $\text{Var}[a]$  and  $\text{Var}[b]$

$$\text{Var}[a] = \frac{\sigma^2 \bar{x}^2}{SSX}$$

$$\text{Var}[b] = \frac{\sigma^2}{\sum_i (x_i - \bar{x})^2} = \frac{\sigma^2}{SSX}$$

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# Variance/standard error of $b$

Estimate  $\sigma^2$  by  $s^2$ :

- Estimated variance of  $b$ :  $s^2/SSX$
- Estimated standard deviation = standard error of  $b = s/\sqrt{SSX}$

Small standard errors if

- small  $\sigma^2$  (find a good fitting model)
- large  $SSX$ :
  - many observations
  - large spread in  $x$

# Hypothesis testing

Interesting hypothesis

$$H_0 : \beta = 0$$

(note: formulated in terms of  $\beta$ , not  $b$ )

Using standard error, we can formulate a t-test (as before)

$$\text{t-stat}_b = \frac{b}{SE_b} \sim t_{n-k}$$

```
res = smf.ols(formula="y ~ x", data=df)  
res.summary()
```

Distribution is really  $t_{n-k}$  if:

→ all 6 assumptions are satisfied!

# Non-linear models

# Non-linearity

The basic model specifies

$$y_i = \alpha + \beta x_i + \varepsilon_i, \varepsilon_i \sim N(0, \sigma^2)$$

→ Linear relation between  $x$  and  $y$

Alternatives:

- Also use transformations of  $x$  as explanatory variable
  - $x^2$
  - $\log(x)$
  - $\sqrt{x}$
  - $\frac{1}{x}$
  - etc.
  - (can also use multiple transformations at the same time)
- Transformations of  $y$ 
  - $\log(y)$  (most often used)
  - Simply write eg. `np.log(y)` inside the formula (🐍 using numpy as np)

Note: resulting models are still linear in the “econometric sense”



# Interpretation in most commonly used models

If

$$y_i = \alpha + \beta \log(x_i) + \varepsilon_i$$

→ increase  $x$  by 1%  $\implies y$  increases by  $\beta \log(1.01) \approx \beta/100$  units

If

$$\log(y_i) = \alpha + \beta \log(x_i) + \varepsilon_i$$

$$y_i = \exp(\alpha + \beta \log(x_i) + \varepsilon_i)$$

→ increase  $x$  by 1%  $\implies y$  increases by  $\beta\%$  (elasticity)

If

$$\log(y_i) = \alpha + \beta x_i + \varepsilon_i$$

$$y_i = \exp(\alpha + \beta x_i + \varepsilon_i)$$

→ increase  $x$  by 1 unit  $\implies y$  increases by  $100(\exp(\beta) - 1)\% \approx 100\beta\%$

# Assignment

## In-class assignment 4.2

- Consider the earlier regression model
- What is the  $R^2$ ? Does this model fit well?
- Use the output to perform a hypothesis test for no impact of lotsize
- Compare this result to the result of

```
from scipy import stats
stats.pearsonr(x,y)
```
- Also try a model for  $\log(\text{price})$  explained by  $\log(\text{lotsize})$ .
- How should the parameters in this model be interpreted?

Many more techniques are available

- Estimate a truly non-linear model  $y_i = \alpha + x_i^\beta + \varepsilon_i$
- Estimate with unknown/flexible functional form
  - Non-parametric estimation
  - General Additive Models
  - ...
- Estimate with multiple explanatory variables (next topic)
- Estimate with other types of dependent variables (later)

# Multiple regression

# Multiple explanatory variables

Why only 1 explanatory variable?

- Multiple factors influence  $y$
- These factors are often related!
- What is the true influence?

Important questions

- What do parameters mean in a model with multiple  $x$ ?
- What about interactions?
- Which variables to include? (later topic)

# Econometrics of multiple regression

Consider the model

$$y_i = \beta_1 + \beta_2 x_{i2} + \beta_3 x_{i3} + \dots + \beta_k x_{ik} + \varepsilon_i$$

(note there is no  $x_{i1}$ )

New *additional* assumptions:

- All variables show variation
- No *perfect* linear relations between variables

# Short-hand notation

If we introduce  $x_{i1} = 1$ , we can write

$$y_i = \sum_{j=1}^k \beta_j x_{ij} + \varepsilon_i$$

or with matrix/vector notation

$$y_i = (x_{i1}, x_{i2}, \dots, x_{ik}) \begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_k \end{pmatrix} + \varepsilon_i$$

which we summarize as

$$y_i = x_i' \beta + \varepsilon_i$$

( $x_i$  and  $\beta$  are both column vectors)



# Grouping all observations

Next we collect all observations  $i = 1, \dots, n$

$$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} x'_1 \\ x'_2 \\ \vdots \\ x'_n \end{pmatrix} \begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_k \end{pmatrix} + \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{pmatrix}$$

or

$$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} x_{11} & x_{12} & \dots & x_{1k} \\ x_{21} & x_{22} & \dots & x_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \dots & x_{nk} \end{pmatrix} \begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_k \end{pmatrix} + \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{pmatrix}$$

which we summarize as

$$y = X\beta + \varepsilon$$

→ extremely general notation!

# Estimating $\beta$

OLS can still be used to estimate  $\beta$

Define  $e_i = y_i - x_i' b$  and minimize

$$\text{SSE} = \sum_i e_i^2 = (e_1 \quad e_2 \quad \dots \quad e_n) \begin{pmatrix} e_1 \\ e_2 \\ \vdots \\ e_n \end{pmatrix} = e' e = (y - Xb)'(y - Xb)$$

with  $e = y - Xb$ .

Can show that the solution is

$$b = (X'X)^{-1}X'y$$

→ Most important formula in econometrics

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# Estimation uncertainty and Goodness of fit

For multiple regression  $y = X\beta + \varepsilon$

- $b = (X'X)^{-1}X'y$  is an estimator of  $\beta$
- Possible to estimate the variance of  $b$ :  $SE_{b_j}$   $j = 1, 2, \dots, k$

Test hypothesis  $H_0 : \beta_j = 0$  for a given  $j$

- Test statistic

$$\text{t-stat}_{b_j} = \frac{b_j}{SE_{b_j}} \sim t_{n-k}$$

Test hypothesis  $H_0 : \beta_2 = \dots = \beta_k = 0$

- Apart from the “constant”, no variable in  $x$  explains the variation of  $y$
- Test statistic

$$F = \frac{\text{RegressionSS}/(k-1)}{\text{ErrorSS}/(n-k)} = \frac{\text{SSR}/(k-1)}{\text{SSE}/(n-k)} \sim F(k-1, n-k)$$

- If  $F$  is large, then reject the null

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# Multiple regression in R

Executing multiple regression is easy

Examples

- `formula=y ~ x2 + x3` inside the `smf.ols()` method
- a constant is always added automatically

→ Next use same functions as before

# Goodness of fit

For multiple regression

- $R^2$  same as before
- However: adding variables  $\rightarrow$  guaranteed increase in  $R^2$  (Q: why?)
- Adjusted  $R^2$

$$\text{Adj}R^2 = 1 - \frac{SSE/(n - k)}{SSY/(n - 1)}$$

includes penalty on additional variables

- Information criteria, eg. AIC
  - Balances fit vs. no. parameters
  - Lower numbers are better
  - Also counts variance as parameter
  - `res = model.fit()` and `res.aic`

# Parameter interpretation – ceteris paribus

Suppose an estimated model is

$$\log(\text{income}) = 7 + 0.01\text{age} + 0.025\text{educ} + e$$

with educ: number of years of education

How to interpret the coefficients?

- if age=educ=0  $\rightarrow \log(\text{income})=7 \rightarrow \text{income} \approx 1069$   
(does this mean anything?)
- if age=30, educ=12  $\rightarrow \log(\text{income})=7.6 \rightarrow \text{income} \approx 2000$
- if age +1  $\rightarrow \text{income} +1\%$  (holding educ constant!)
- if educ +1  $\rightarrow \text{income} +2.5\%$  (holding age constant!)

Important: all results are ceteris paribus! (keeping other things fixed)



# Interactions

# Regression with interaction

Consider the model

$$y = \alpha + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2 + \varepsilon$$

What's the point to add the interaction term ( $x_1 x_2$ )?

- Interaction effect: there is a “synergy” (or “anti-synergy”) regarding the impact of  $x_1$  and  $x_2$  on  $y$
- Moderation effect: the impact of  $x_1$  on  $y$  depends on  $x_2$  (or the other way around)

Typical mistakes in interpreting interaction regressions

- $\beta_1$  (or its estimate  $b_1$ ) is not the impact of  $x_1$  on  $y$ !
  - An insignificant  $b_1$  does not necessarily mean  $y_1$  and  $x$  are not related!
  - A significant  $b_1$  does not necessarily mean  $x_1$  and  $y$  are related either!

→ A significant  $b_3$  does mean that there is an interaction effect!

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# How to interpret regression with interaction?

Rewrite the model!

$$y = \alpha + \beta_2 x_2 + (\beta_1 + \beta_3 x_2) x_1 + \varepsilon$$

- The intercept:  $\alpha + \beta_2 x_2$
- The slope for  $x_1$ :  $\beta_1 + \beta_3 x_2$
- Interpret in the context
  - choose a value for  $x_2$
  - calculate impact of  $x_1$  at that value of  $x_2$(or plot impact as a function of  $x_2$ )



→ Can of course also swap roles of  $x_1$  and  $x_2$

# Interaction regression in Python

## The model

$$y = \alpha + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2 + \varepsilon$$

## Estimate the model

- Easy, as if run a three variables regression
- Even easier, you do not have to construct  $x_1 x_2$ , Python does it for you  
 `.ols(formula = y ~ x1 + x2 + x1:x2, data=..)`
- A more convenient way:  `.ols(formula = y ~ x1*x2, data=..)`: It means “all individual and interaction effects based on  $x_1$  and  $x_2$ ”

Visualizing the interaction effects (useful for interpretation, but requires some work):

- 1 Create predictions varying one of the variables, keeping the other(s) fixed
- 2 Repeat for various values of “the other(s)”
- 3 Create plot



# Assignment

# In-class Assignment 4.3

- Use the Murder rate data (state.x77)

This standard R data file is available on Canvas as csv file.

```
import pandas as pd
```

```
statex77 = pd.read_csv("statex77.csv")
```

- Explain **Murder rate** by **Income**, **Population**
- Interpret the coefficients
- **Optional**
  - Add the interaction effect between Income and Population
  - Plot the interaction effect
  - Interpret the interaction
  - Question after the exercise *Do you have a story behind the result?*

# Preparing for diagnostics: Normality testing

# Normality tests

Many models/tests rely on normality of **error terms** (not the  $y$  or  $x$  variable!)

Can we **test** whether a **variable** is normally distributed?

- Yes, if variables are identically normal distributed under  $H_0$
- Not directly, if mean of variable depends on stuff that is not normally distributed (not iid)

Many tests exist, for example

- Shapiro-Wilk test

 `scipy.stats.shapiro(x)`

based on so-called order-statistics (*smallest, next-to-smallest, ..., largest* observation)

- Jarque-Bera test

 `scipy.stats.jarque_bera(x)`

based on skewness and kurtosis

- ...

Graphical procedures: **QQ-plots**



# QQ plots - more formal description

The idea of empirical distributions can be used to test for particular distributions.

→ Main idea: Compare **estimated** cdf versus **theoretical** cdf

Given  $n$  observations:

- If data is really normal: what would you expect the smallest observation to be?
- and the next-to-smallest?
- ...

## QQ plot

- Plot the observed quantiles vs. theoretical quantiles
- Should be nice straight line (intercept and slope depend on mean and variance, or are a least squares fit)

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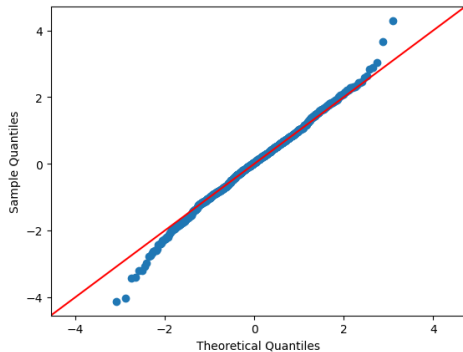
# Example QQ plot

## Options

- Using `scipy`  

```
fit = scipy.stats.fit(stats.norm,  
data, bounds)  
fit.plot(plottype='qq')
```
- Using `statsmodels.api.qqplot(x,  
line="45")`

→ Example: Data clearly not normal!





# Model diagnostics

# The assumptions

The Model (**data generating process** [DGP])

$$y = X\beta + \varepsilon$$

**Formal assumptions (omitting A1 and A2):**

**A3** *Linearity:*  $y_i = x_i\beta + \varepsilon_i$  holds exactly

**A4** *Homoskedasticity:*  $E[\varepsilon_i^2] = \text{Var}(\varepsilon_i) = \sigma^2$

**A5** *No autocorrelation:*  $E[\varepsilon_i\varepsilon_j] = 0$  for  $i \neq j$

**A6** *Normality:*  $\varepsilon_i \sim N(0, \sigma^2)$

Additional assumption in multivariate regression

**A7** No perfect linear relationship in  $X$

**Model diagnosis:** two key questions

- Are these assumptions valid?
- If an assumption fails, what to do?

# Simple diagnosis in Python

- Fit the model:

```
model = smf.ols(formula=..., data=...).fit()
```

- Download `olsdiagnostics.py` from Canvas into working folder and

```
from olsdiagnostics import *
```

- Create OLSInfluence object (`from statsmodels.stats.outliers_influence`)

```
influence = OLSInfluence(model)
```

- Run `diagnosticplots(influence)`

→ creates four plots

# Checking assumptions using olsdiagnostics

4 diagnostic plots with: `olsdiagnostics`

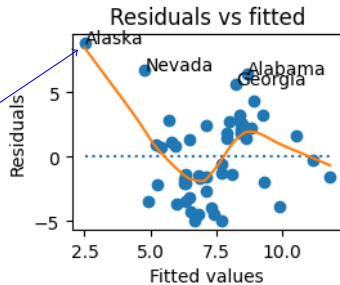
- 1 Plot of residuals vs. fitted values `residfitted(influence)`
  - Check for structure in mean of residuals (Linearity [A3])
  - Check for structure in absolute value of residuals (Heteroskedasticity [A4])
- 2 QQ plot of studentized residuals: Normality [A6] `qqresid(influence)`
  - Check for deviations from normality
- 3 Plot of  $\sqrt{|\text{stand. residual}|}$  vs fitted: Heteroskedasticity [A4]  
`scalelocation(influence)`
  - Check whether magnitude of residuals depends on fitted value
- 4 Leverage (high if “extreme in terms of x”) vs. standardized residual: Outliers  
`residleverage(influence)`
  - Does not correspond to one assumption, and is not very useful for outlier detection

(One missing assumption [A5])

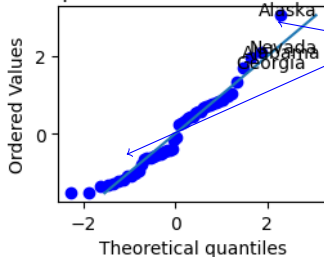


# Illustration on formula = "Murder ~ Population + Income"

Some structure in the residuals (due to Alaska)

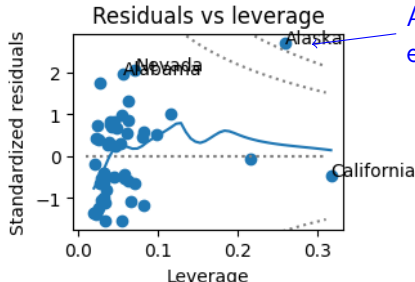
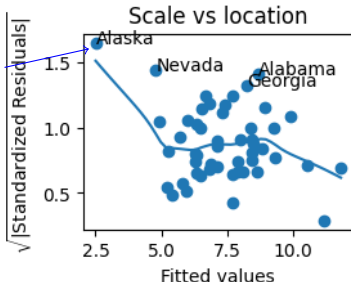


QQ plot of studentized residuals



Residuals do not look normal

No sign of heteroskedasticity (only Alaska deviates)



Alaska is extreme

# Take home assignment

- Use the Murder rate data (Murder as dependent variable)
- Start with four independent variables: Income, Population, Illiteracy, Frost
- Do some experimentation
  - If a variable is not significant, try to remove it
    - ▶ Does the  $R^2$  go up or go down? What about Adjusted  $R^2$ ?
    - ▶ What about AIC?
- Ultimate goal: find the best model (the lowest AIC)
- Finally: check the model assumptions using the diagnostics plot  
→ What do you conclude?

# Before next time

- Reread Chapter 4
- No new material for next week
- Reconsider/finish the in-class assignments
- Work on the take home assignment
- Final assignment (part 1 is due on Sunday)