ORIE 3120: Practical Tools for OR, DS, and ML

Linear Regression

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April 9, 2020

Announcements

- submit recitation by 4:30pm ET Friday
- homework due 2:30pm ET Wednesday
- project milestone 1 due Sunday 4/18/2020 at noon

Outline

Introduction to Linear Models

Why use regression analysis? Linear models Estimation Data

Least squares

Python

Example: Electricity Usage I

Description

Electricity example

Statistical output

Multiple R Squared

Residual analysis

Checking for independence Checking for nonlinearity

Part 1: Linear Regression - Introduction

Regression can

- investigate how variables are related,
- predict future values of variables, and
- show how output variables will change if we change input variables.
- ... the last step can be useful for control!

Regression examples (from Kaggle)

kaggle

Sign Up About Kaggle Create a competition Competitions Forums Blog Careers

We're making data science a sport."

Participate in competitions

Kaggle is an arena where you can match your data science skills against a global cadre of experts in statistics, mathematics, and machine learning. Whether you're a world-class algorithm wizard competing for prize morey or a novice looking to learn from the best, here's your chance to jump in and geek out, for fame, fortune, or fun.

Create a competition

Kaggle is a platform for data prediction competitions that allows organizations to post their data and have it scrutinized by the world's best data scientists. In exchange for a prize, winning competitors provide the algorithms that beat all other methods of solving a data crunching problem. Most data problems can be framed as a competition.

Sign up as a competitor

See how it works

(Need convincing?

Featured Competitions Bro		Browse all »	Username	
	Heritage Health Prize	Ends 12 months		
	Identify patients who will be admitted to a hospital within the next year, using historical claims data.	905 teams	Sign in 📄 Remember me	
		🖞 \$3 million		
			Forgot your username/password?	
	The Hewlett Foundation: Automated	L Ends 33 days		
ASAP	Essay Scoring Develop an automated scoring algorithm for student-written essays.	2 94 teams	kepsie	
Automated Student Assessment Prize		Y \$100,000		
Phase One: Automated Essay Scoring			WE'RE	
			HIRING	

Regression for insurance claim predictions

Claim Prediction Challenge (Allstate)

Many factors contribute to the frequency and severity of car accidents including how, where and under what conditions people drive, as well as what they are driving.

Bodily Injury Liability Insurance covers other people's bodily injury or death for which the insured is responsible. The goal of this competition is to predict

Bodily Injury Liability Insurance claim payments based on the characteristics of the insured's vehicle.

Prize pool	Teams	Completed
\$10,000	107	5 months ago



Regression for finance

Benchmark Bond Trade Price Challenge

The Benchmark Bond Trade Price Challenge is a competition to predict the next price that a US corporate bond might trade at. Contestants are given information on the bond including current coupon, time to maturity and a reference price computed by **Benchmark Solutions**. Details of the previous 10 trades are also provided.





Regression for social network analysis



changed, though, is that they were increasingly failing to integrate into the Wikipedia community, and failing increasingly quickly. The Wikimedia community had become too hard to penetrate. For more information about these trends, please have a look at http://strategy.wikimedia.org/wiki/March.2011_Update

We want a quantitative answer to what factors predict future editing behavior, in order to ensure that the content of Wikipedia continues to grow both quantitively and qualitatively.

Regression setup

we want to predict output given inputs

▶ *p* input variables
$$X_1, \ldots, X_p \in \mathbf{R}$$

- also called "predictors", "independent variables", "covariates"
- output variable $Y \in \mathbf{R}$
 - also called "outcome", "response", "dependent variable", "label", "target" ...

In the Allstate example:

- Y is the cost of an insurance claim.
- X₁,..., X_p are the properties of the insured and his/her vehicle, e.g., credit score, age of the vehicle, ...

Linear models

linear model assumption: for some parameters $\beta_0, \ldots, \beta_p \in \mathbf{R}$,

$$E(Y|X_1,\ldots,X_p) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p$$

hence

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_p X_p + \epsilon$$

where ϵ is variation of Y about $E(Y|X_1, \ldots, X_p)$

β₀ is the intercept
 β₁,...,β_p are called regression coefficients
 also called "slopes" or "partial derivatives":

$$\beta_j = \frac{\partial}{\partial X_j} E(Y|X_1,\ldots,X_p)$$

ϵ is the unpredictable variation in Y
 i also called the "noise", "error", or "residual variation"

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Data

observe $(Y_{i}, X_{i,1}, ..., X_{i,p})$, for i = 1, ..., n

- n observations total
- i = index of "observation" = "subject" = "row in data spreadsheet"
- so the linear regression model can be rewritten as

$$Y_i = \beta_0 + \beta_1 X_{i,1} + \beta_2 X_{i,2} + \dots + \beta_p X_{i,p} + \epsilon_i$$

- notice that $\beta_0, \beta_1, \ldots, \beta_p$ do not depend on *i*
- the columns of the data spreadsheet are $Y_i, X_{i,1}, \ldots, X_{i,p}$

i	Y _i	$X_{i,1}$	<i>X</i> _{<i>i</i>,2}	 X _{i,p}
1	2.3	1.1	6.2	 5.9
2	12.7	2.4	5.4	 9.6
3	6.3	0.9	6.9	 1.5

Least squares estimation

What if we don't know the output Y_i for some subject *i*? Predict it!

Given estimates β̂₀,..., β̂_p for the regression coefficients, predict Y_i as

$$\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 X_{i,1} + \hat{\beta}_2 X_{i,2} + \dots + \hat{\beta}_p X_{i,p}$$

 Ŷ_i is an estimate of
 E(Y_i|X_{i,1},...,X_{i,p}) = β₀ + β₁X_{i,1} + β₂X_{i,2} + ··· + β_pX_{i,p}

 β̂₀, β̂₁,..., β̂_p find the "best" predictor by minimizing

$$\sum_{i=1}^n (Y_i - \hat{Y}_i)^2$$

Least squares estimation

What if we don't know the output Y_i for some subject *i*? Predict it!

Given estimates
 [^]
 [^]

$$\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 X_{i,1} + \hat{\beta}_2 X_{i,2} + \dots + \hat{\beta}_p X_{i,p}$$

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Q: Why minimize the square?

Residuals and Fitted Values

Fitted value:
$$\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 X_{i,1} + \hat{\beta}_2 X_{i,2} + \dots + \hat{\beta}_p X_{i,p}$$

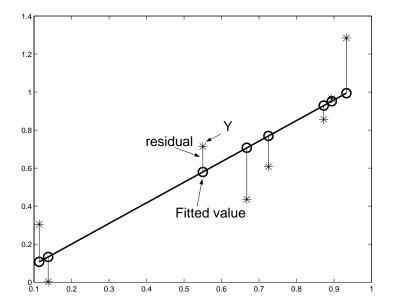
Residual: $\hat{\epsilon}_i = Y_i - \hat{Y}_i$ (estimates ϵ_i)

Least-squares: makes the sum of square residuals

$$\sum_{i=1}^{n} \hat{\epsilon}_i^2$$

as small as possible.

Least Squares, in pictures



When is a model linear?

Linear regression assumes

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_p X_p + \epsilon.$$

Definition: A model is **linear** if Y is linear in the **parameters** (linear in β_0, \ldots, β_p).

Key point: Covariates X_1, \ldots, X_p can be anything observable. They can be nonlinear functions of measured quantities.

- Nonlinear regression is covered in more advanced courses
- For this course, you only need to know a nonlinear model when you see it

Example:

$$Y = \beta_0 + \beta_1 \exp(\beta_2 X) + \epsilon$$

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Example:

$$Y = \beta_0 + \beta_1 \exp(\beta_2 X) + \epsilon$$

This model is nonlinear because Y is a nonlinear function of β_2 .

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Example:

$$Y = \beta_0 + \beta_1 \exp(\beta_2 X) + \epsilon$$

This model is nonlinear because Y is a nonlinear function of β_2 . Example:

$$Y = \beta_0 + \beta_1^3 \beta_2^4 \exp(X) + \epsilon$$

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Example:

$$Y = \beta_0 + \beta_1 \exp(\beta_2 X) + \epsilon$$

This model is nonlinear because Y is a nonlinear function of β_2 . Example:

$$Y = \beta_0 + \beta_1^3 \beta_2^4 \exp(X) + \epsilon$$

This model is nonlinear in the parameters, but can be rewritten as a linear model in $\beta_1'=\beta_1^3\beta_2^4$

$$Y = \beta_0 + \beta'_1 \exp(X) + \epsilon$$

Which of these models are linear in the parameters?

1. $Y = \beta_0 + \beta_1 \times (\text{CavityWidth}) + \beta_2 \times (\text{CavityWidth})^2$,

2. $Y = \beta_0 + \beta_1 \times (\text{CavityWidth}) + (\beta_2 \times \text{CavityWidth})^2$,

3. $Y = \beta_0 + \beta_1 \times (\text{CavityWidth}) + \exp(\beta_2 \times \text{CavityWidth}),$

- (yes) none of them
- (no) 1 only
- (up) 2 only
- (down) 3 only
- (coffee) more than one

Which of these can be rewritten as a linear model?

1. $Y = \beta_0 + \beta_1 \times (\text{CavityWidth}) + \beta_2 \times (\text{CavityWidth})^2$,

2. $Y = \beta_0 + \beta_1 \times (\text{CavityWidth}) + (\beta_2 \times \text{CavityWidth})^2$,

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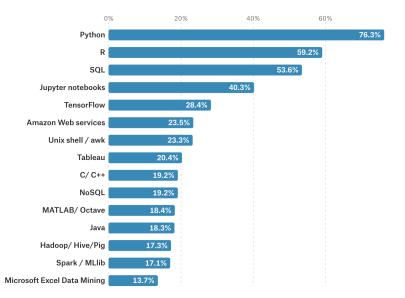
Statistical output

Multiple R Squared

Residual analysis

Checking for independence Checking for nonlinearity

Why python?



How to access python

two options to use python:

- install Anaconda python distribution on your computer
- use Google colab: no installation needed

see https://people.orie.cornell.edu/mru8/orie3120/
read/jupyter.pdf for details on using jupyter

A guide to python packages we use

- numpy (np): mathematical operations (esp. linear algebra)
- scipy: more mathematical operations (including statistics)
- pandas (pd): manipulate data tables (dataframes)
- matplotlib (plt): for plotting
- seaborn: for statistical plots
- sklearn: for machine learning (regression and beyond)
- statsmodels (sm): statistical models

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A guide to python packages we use

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- Q: why so many packages?

A: python is a lightweight, flexible language with a large developer community

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Example: Electricity Usage

- We are managing a large complex of apartments in the Northeast.
- We pay for the electricity used by our residents.
- We would like to predict electricity usage so that we can estimate how much money should be set aside.

Demo:

https://github.com/madeleineudell/orie3120-sp2020/ blob/master/demos/linear-regression.ipynb

Predictors (Independent Variables)

The following predictors were measured during data collection:

- year (1989 1994)
- ▶ month (1 12)
- usage (of electricity for month)
- temperature (average temperature for month)

We added two additional predictors:

- yearcts = year + (month 1)/12.
- tempsqr = temperature².

Here is python code for loading and plotting the data

```
usage = pd.read_csv('elec_usage.txt')
usage['tempsqr'] = usage['temperature']^2
usage['yearcts'] = usage['year'] + (usage['month']-1)/12
usage.plot.scatter(x='temperature', y='usage')
seaborn.pairplot(usage)
```

We fit this linear regression model

$$usage = \beta_0 + \beta_1 temp + \beta_2 temp^2 + \epsilon$$

Here

Y = usage
 X₁ = temp
 X₂ = temp²

Here's how we fit this linear regression model

Here's how to get Python to tell us the estimated regression coefficients

model.summary()

Output of model summary

OLS Regression Results						
Dep. Variable: Model: Method: Date: Time: No. Observations Df Residuals: Df Model: Covariance Type:	Sun, 0 :	st Squares 5 Apr 2020	Adj. R-squa F-statistic Prob (F-sta Log-Likelik AIC:	c: atistic):		0.785 0.768 45.76 .00e-16 -210.02 430.0 440.1
	coef	std err	t	P> t	[0.025	(
	-0.5207 -0.8402 -1.0414 -11.9054	0.792 0.785 8.117 97.321	-0.657	0.514 0.290 0.898 0.903	-2.112 -2.416 -17.344 -207.381	1
Omnibus: Prob(Omnibus): Skew:		0.794	Durbin-Watson: Jarque-Bera (JB): Prob(JB):		1.166 0.216 ₃ 10/- 8 98	

This command also provided other statistical analyses

- **>** Standard errors, p-values and t-values for each β_i
- Residual standard error
- Multiple R-squared and Adjusted R-squared
- F statistic and associated p-value

When are these statistical analyses appropriate?

Statistical quantities in summary (standard errors, p-values, t-values, R squared, F statistic, ...) are computed assuming that $\epsilon_1, \ldots, \epsilon_n$

- 1. are mutually independent
- 2. are independent of $X_{i,j}$
- 3. are normally distributed
- 4. have a constant variance
- when these assumptions are true, we can use these quantities to lead us towards better models.
- if these assumptions are false, these statistics can be misleading.
- we can alter the data to make assumptions more true; sometimes improves model fit, too!

To check whether these assumptions are true, we must look at the residuals. We will show how to do this later.

Regression coefficients and standard errors

- Estimated regression coefficients: $\hat{\beta}_0, \ldots, \hat{\beta}_p$
- Std. Errors
 - the *j*th std. error is the standard deviation of $\hat{\beta}_i$
 - an approximate 95% confidence interval for β_j is Estimate ± (2)(Std. Error)
 - Used to quantify error in the estimates

Statistical tests

we may assess how well the model fits using a variety of statistical tests:

t value

- t value = Estimate $\hat{\beta}_j$ / Std. Error of $\hat{\beta}_j$
- how big is the coefficient's mean relative to its error?

p value

- the probability of a t value as large or larger than the one actually observed, if β_i = 0.
- If this probability is small, then β_j is probably not 0.
- Formally, we reject the hypothesis that β_j = 0 at the α = 0.05 significance level if p value < 0.05.</p>

More statistical tests

Residual std. error

- estimates the standard deviation of the ϵ_i
- F statistic
 - tests the hypothesis that β₁ = 0, β₂ = 0, ..., and β_p = 0 i.e., that Y is NOT related to ANY of the predictors
 - often it is obvious that this hypothesis is false
 - used occasionally for more sophisticated procedures built on top of linear regression.

Variance explained

Multiple R Squared

- A number between 0 and 1 that tells how well the data is explained by the linear model.
- Can be used to choose between different predictors.

Adjusted R Squared

- Like multiple R squared, but adjusted for the number of predictor variables.
- These are explained on the next few slides.

Multiple R Squared

 Multiple R Squared is the squared correlation between the observed and fitted values,

$$R^2 = \rho(Y, \hat{Y})^2$$

it is "multiple" because Ŷ uses all of the predictors
 ρ(Y, Ŷ) is the sample correlation

$$\rho(Y, \hat{Y}) = rac{\sum_i (Y_i - \operatorname{avg}(Y))(\hat{Y}_i - \operatorname{avg}(\hat{Y}))}{\sqrt{\sum_i (Y_i - \operatorname{avg}(Y))^2} \sqrt{\sum_i (\hat{Y}_i - \operatorname{avg}(\hat{Y}))^2}}$$

• The closer R^2 is to 1, the better \hat{Y}_i predicts Y_i .

Why use R^2 ?

 \triangleright R^2 can be used to determine which set of predictors is best.

- bigger R^2 is better
- problem: R^2 is biased in favor of more predictors
 - adding predictors increases R²
 - even if the additional predictors are not related to Y_i
- The bias of R^2 can be fixed by using

Adjusted
$$R^2 = 1 - (1 - R^2) \frac{n - 1}{n - p - 1}$$

(recall *n*=number of observations, *p*=number of covariates)
 ▶ Adjusted *R*² is preferred to *R*²

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Residual analysis

Checking for independence Checking for nonlinearity Statistics computed are valid if $\epsilon_1, \ldots, \epsilon_n$

- 1. independence I: are mutually independent
- 2. independence II: are independent of covariates
- 3. normality: are normally distributed
- 4. homoskedasticity: have a constant variance

To check whether these assumptions are true, we must look at the residuals

Residuals analysis: mutual independence

Let's look at each assumption and see how it can be checked.

Assumption 1. $\epsilon_1, \ldots, \epsilon_n$ are mutually independent

- this assumption might be violated if the observations are in time or spatial order
- check by: plotting $\hat{\epsilon}_i$ versus $\hat{\epsilon}_{i-1}$
 - should see no pattern

Residuals analysis – checking mutual independence with a scatterplot

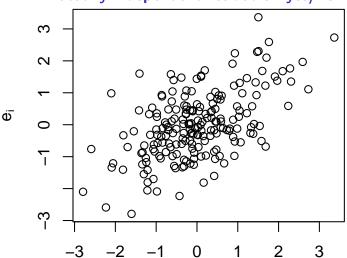
This code will show scatterplots from data with mutual independence.

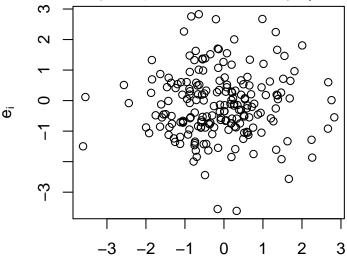
```
# generate data
n = 500 # number of observations
eps = randn(n) # independent normal(0,1)
x = 10*rand(n) # uniform(0,10)
y = x + eps
# form and fit model
model = sm.OLS(y, x).fit()
resid = model.resid
plt.scatter(resid[:-1], resid[1:])
```

Residuals analysis – checking mutual independence with a scatterplot

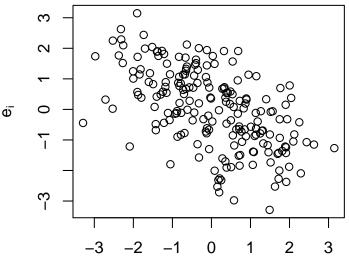
This code will show scatterplots from data **without** mutual independence.

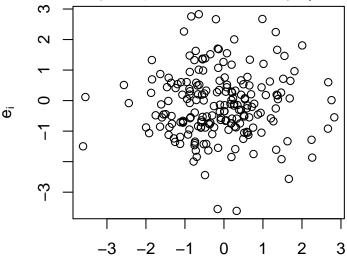
```
# generate data
   = 500 # number of observations
n
a = 1 # use this to control the correlation
w = randn(n+1) \# independent normal(0,1)
eps = w[:-1] + a*w[1:] # normal, not independent
x = 10*rand(n) \# uniform(0,10)
y = x + eps
# form and fit model
model = sm.OLS(y, x).fit()
resid = model.resid
plt.scatter(resid[:-1], resid[1:])
```





 e_{i-1}





 e_{i-1}

plot the autocorrelation function:

 $r(t) = \operatorname{corr}(\widehat{\epsilon}_i, \widehat{\epsilon}_{i-t})$

- ▶ r(t) should be 0 for all t > 0 (except for random variation)
- no (or only a few) autocorrelations should be outside the test bounds
- t is called the lag
- the scatterplots only looked at lag = 1
 - of course, we could have looked at other lags
 - but autocorrelations let us look at all lags simultaneously

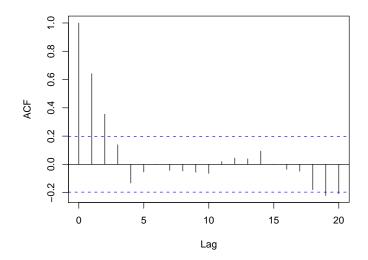
This code plots the autocorrelation for data with mutual independence.

```
n = 500 # number of observations
eps = randn(n) # independent normal(0,1)
x = 10*rand(n) # uniform(0,10)
y = x + eps
# form and fit model
model = sm.OLS(y, x).fit()
resid = model.resid
plt.acorr(resid)
```

This code plots the autocorrelation for data **without** mutual independence.

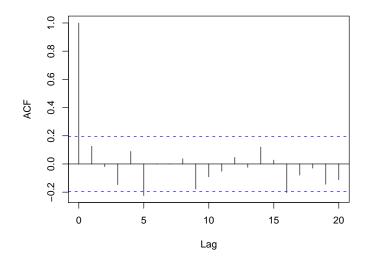
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= 500 # number of observations
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x = 10*rand(n) \# uniform(0,10)
y = x + eps
# form and fit model
model = sm.OLS(y, x).fit()
resid = model.resid
plt.acorr(resid)
```

ACF of Residuals



quick poll: (yes) independent (no) not independent

ACF of Residuals



quick poll: (yes) independent (no) not independent

Residuals analysis – linear in the predictors

Assumption 2. model is linear in the predictors (the $X_{i,j}$)

- equivalently, $\epsilon_1, \ldots, \epsilon_n$ are independent of all $X_{i,j}$
- Check by: plotting $\hat{\epsilon}_i$ versus $X_{i,j}$ for $j = 1, \dots, p$
- ▶ we should see that the average value of the *i* does not depend on X_{i,j}.
- if it does, then there is a problem

Plot residuals vs covariates to test linearity

```
plt.subplot(2,1,1)
p = plt.scatter(x,y,marker='o',label="observed")
plt.scatter(x,yhat,marker="+",color="red",label="
plt.legend()
plt.subplot(2,1,2)
plt.scatter(x,resid)
plt.xlabel("x")
plt.ylabel("residual")
```

Residuals analysis – linear in the predictors

This code forms a model for which outcome is **not** linear in the predictor.

```
n = 500 # number of observations
eps = randn(n) # independent normal(0,1)
x = 10*rand(n) # uniform(0,10)
y = x + x**2 + eps
# form and fit model
model = sm.OLS(y, x).fit()
resid = model.resid
yhat = model.predict()
```

Residuals analysis – linear in the predictors

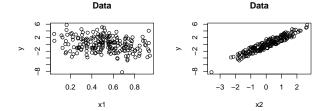
Here's how we fix the fit on the previous slide: use the square as a feature

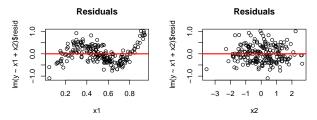
```
df = pd.DataFrame()
df['x'] = x
df['xsq'] = x**2
model = sm.OLS(y, df).fit()
```

Residuals detect nonlinearity better than raw data

In the next slide, data are simulated from:

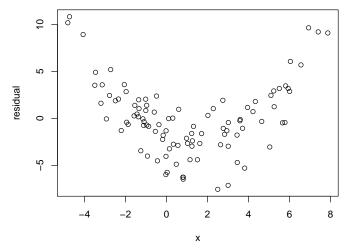
Residuals detect nonlinearity better than raw data





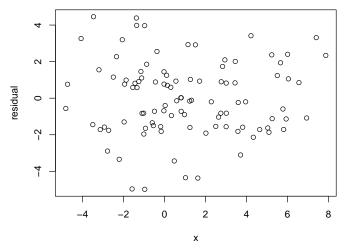
Raw data: Scatter due to X_2 obscures nonlinearity in X_1 Residuals: Scatter due to X_2 is removed and nonlinearity in X_1 is revealed

Checking for nonlinearity



quick poll: (yes) linear in x (no) not linear in x

Checking for nonlinearity



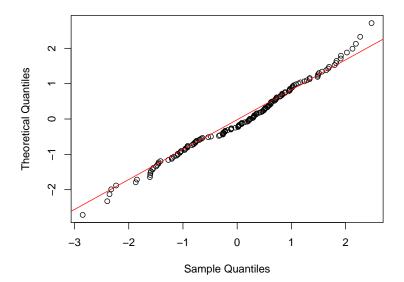
quick poll: (yes) linear in x (no) not linear in x

Residuals analysis – normal distribution

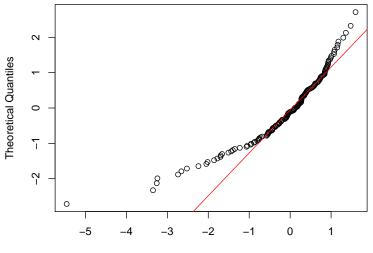
Assumption 3. $\epsilon_1, \ldots, \epsilon_n$ are normally distributed

- normal probability plot
- should see a straight line
- a pattern means skewness or heavy-tails

linear = normal

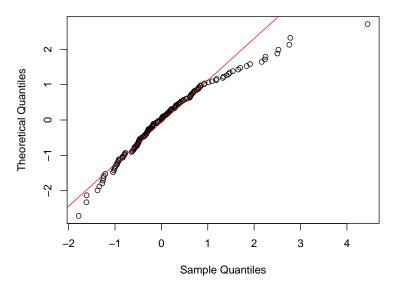


convex = left-skewed

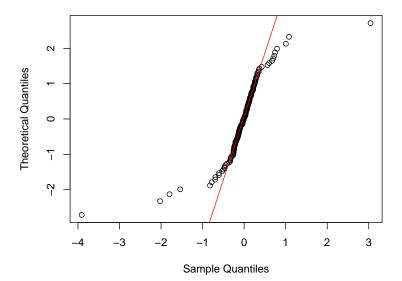


Sample Quantiles

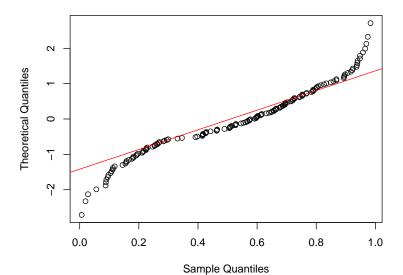
concave = right-skewed



convex-concave = heavy-tailed



concave-convex = light-tailed



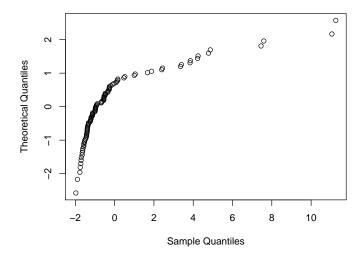
This code generates q-q plots for normal residuals:

```
n=500
eps = randn(n) # normal residuals
x = 10*rand(n)
y = x + eps
model = sm.OLS(y,x).fit()
sm.qqplot(model.resid, line='45');
```

This code generates q-q plots for residuals that are **not** normal:

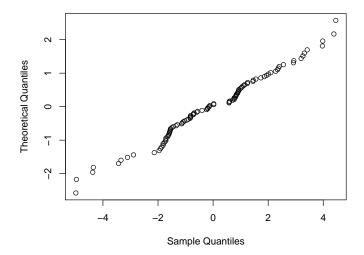
```
n=500
eps = exp(randn(n)) # not normal
x = 10*rand(n)
y = x + eps
model = sm.OLS(y,x).fit()
sm.qqplot(model.resid, line='45');
```

Normal Q-Q Plot



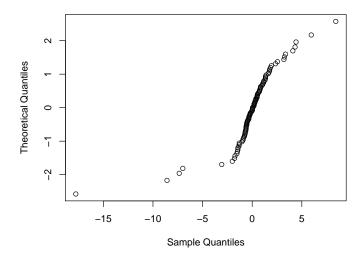
poll: (yes) residuals are normal (no) residuals are not normal

Normal Q-Q Plot



poll: (yes) residuals are normal (no) residuals are not normal

Normal Q-Q Plot



poll: (yes) residuals are normal (no) residuals are not normal

Residuals analysis – constant variance

Assumption 4. $\epsilon_1, \ldots, \epsilon_n$ have a constant variance

- plot absolute residuals against fitted values
- plot absolute residuals against X_{i,i} for each j
 - should see that the distribution does not depend on X_{i,j}
 - if it does, then the variance is not constant
- we call non-constant variance "heteroscedasticity"

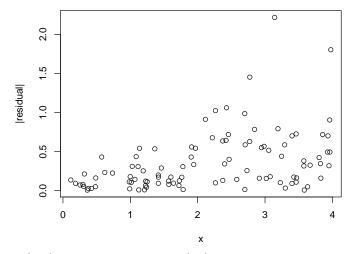
This code generates absolute residual plots for constant variance:

```
n=500
eps = randn(n)
x = 10*rand(n)
y = x + eps
model = sm.OLS(y,x).fit()
plt.scatter(x,np.abs(model.resid))
```

This code generates absolute residual plots for **non-constant** variance:

```
n=500
x = 10*rand(n)
eps = x*randn(n) # variance of noise depends on x
y = x + eps
model = sm.OLS(y,x).fit()
plt.scatter(x,np.abs(model.resid))
```

Checking for non-constant variance



poll: (yes) variance is constant (no) variance is not constant

Strategy for regression data analysis:

- 1. Decide: what problem(s) are you trying to solve?
 - keep the problem in mind while doing the remaining steps
- 2. Find (or collect) useful data
- 3. Find a useful model
 - all models are wrong (George Box)
 - some models are useful
- 4. Check model
 - how well does the model fit the data?
- 5. Modify model, if necessary
- 6. Use model to solve problem(s)