# Introduction to Regression and Model Fit

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### Learning Objectives

### After this lesson, you should be able to:

- Define simple linear regression and multiple linear regression
- Build a linear regression model using a dataset that meets the linearity assumption
- Evaluate model fit
- Understand and identify multicollinearity in a multiple regression

### Outline

- Unit Project 2 due today (was extended)
- Unit 1 Review
- Unit 2 Overview
- Simple Linear Regression
- Variable Transformations
- How to fit a regression model to a dataset
- Common regression assumptions
- How to check modeling assumptions
- How to check normality assumption
- Inference and Fit and  $R^2$  (r-square)

- Multiple Linear Regression
- How to interpret the model's parameters
- Multicollinearity
- $\bar{R}^2$  (adjusted  $R^2$ )
- Lab
- Review
- In-flight
  - Final Project 1 (due in 1 week)
  - Unit Project 3 (due in 2.5 weeks)



# Pre-Work

### Pre-Work

### Before this lesson, you should already be able to:

- Understand the difference between vectors, matrices, pandas Series, and pandas DataFrames
- Understand the concepts of outliers and distance
- Effectively show correlations between an independent variable *X* and a dependent variable *Y*
- Be able to interpret t-values, p-values, and confidence intervals



## Unit 1 Review

## Unit 1 – Research Design and Data Analysis

Unit 1 – Research Design and Data Analysis	Research Design (session 2)	Data Visualization in Pandas (sessions 3–5)	Statistics (sessions 3 and 4)	Exploratory Data Analysis in Pandas (sessions 2–5)
Unit 2 – Foundations of Modeling	Linear Regression	Classification Models	Evaluating Model Fit	Presenting Insights from Data Models
Unit 3 – Data Science in the Real World	Decision Trees and Random Forest	Time Series Data	Natural Language Processing	Databases

### Unit 1 Review

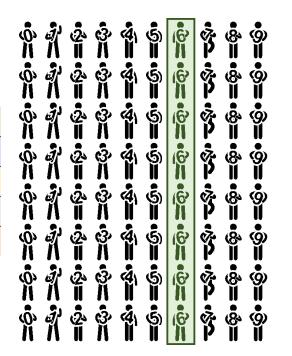
#### **1** IDENTIFY the Problem

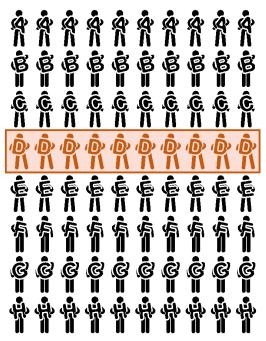
SMART Goals (session 2)

SPECIFIC	The dataset and key variables are clearly defined
MEASURABLE	The type of analysis and major assumptions are articulated
ATTAINABLE	The question you are asking is feasible for your dataset and is not likely to be biased
Reproducible	Another person (or you in 6 months!) can read your state and understand exactly how your analysis is performed
T <sub>IME-BOUND</sub>	You clearly state the time period and population for which this analysis will pertain

### **2** ACQUIRE the Data

Cross-sectional vs. Longitudinal Data (session 2)





Khoon Lay Gan © 123RF.com

#### PARSE the Data

### Data Dictionary (session 2)

#### VARIABLE DESCRIPTIONS: survival (0 = No; 1 = Yes)Passenger Class pclass (1 = 1st; 2 = 2nd; 3 = 3rd)name sex sibsp Number of Siblings/Spouses Aboard parch Number of Parents/Children Aboard ticket Ticket Number fare Passenger Fare cabin Cabin Port of Embarkation embarked (C = Cherbourg; Q = Queenstown; S = Southampton) SPECIAL NOTES: Pclass is a proxy for socio-economic status (SES) 1st ~ Upper; 2nd ~ Middle; 3rd ~ Lower Age is in Years; Fractional if Age less than One (1) If the Age is Estimated, it is in the form xx.5

With respect to the family relation variables (i.e. sibsp and parch) some relations were ignored. The following are the definitions used for sibsp and

Sibling: Brother, Sister, Stepbrother, or Stepsister of Passenger Aboard Titanic Spouse: Husband or Wife of Passenger Aboard

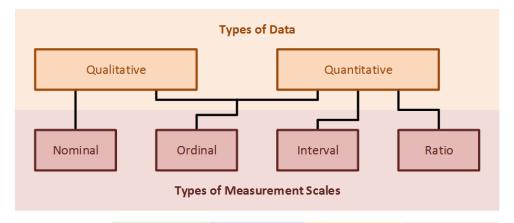
Titanic (Mistresses and Fiancés Ignored) Parent: Mother or Father of Passenger Aboard

Child: Son, Daughter, Stepson, or Stepdaughter of Passenger Aboard Titanic

Other family relatives excluded from this study include cousins, nephews/nieces, aunts/uncles, and in-laws. Some children travelled only with a nanny, therefore parch=0 for them. As well, some travelled with very close friends or neighbors in a village, however, the definitions do not support such relations.

### **3** PARSE the Data (cont.)

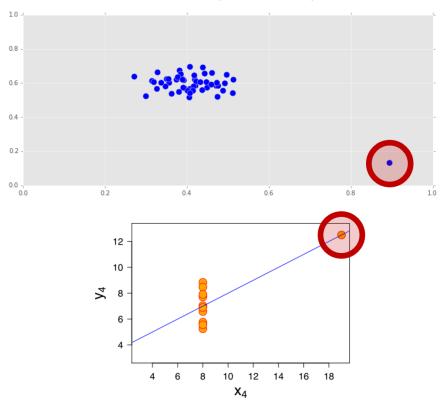
Types of Data/Measurement Scales (session 3)



	Nominal	Ordinal	Interval	Ratio
Categorize?	✓	✓	✓	✓
Rank-order?	×	✓	✓	✓
+; -?	×	×	✓	$\checkmark$
*; /?	×	×	×	✓

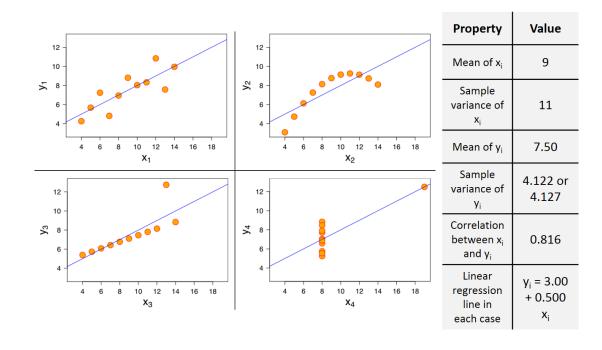
### **③** PARSE the Data (cont.)

Outliers (session 3)



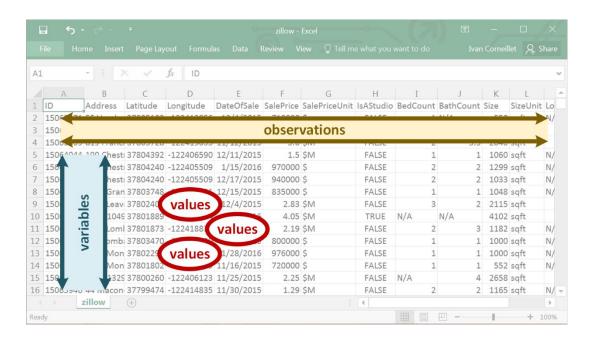
### **3** PARSE the Data (cont.)

Plot your Data! (session 3)



### **3** PARSE the Data / **4** MINE the Data

Tidy Data (session 3)

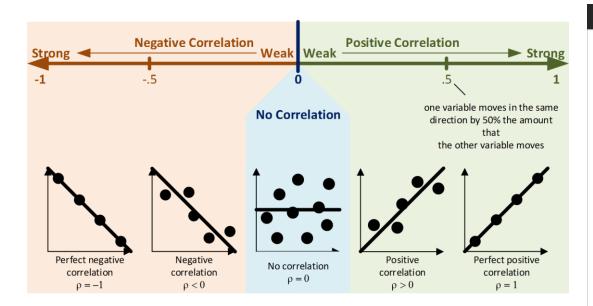


# **③ PARSE the Data / ④ MINE the Data**Tidy Data (cont.)

- Your tabular data will be easier to work with many data science tools if you follow these three rules:
  - Each observation is placed in its own row
  - Each variable in the dataset is placed in its own column
  - Each value is placed in its own cell

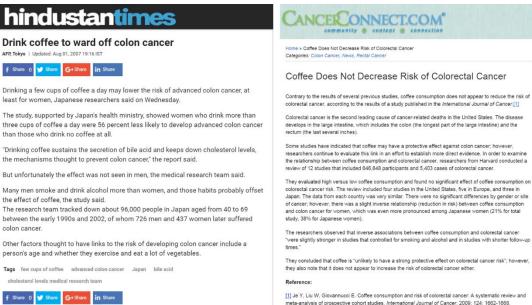
**3** PARSE the Data / **5** REFINE the Data (cont.)

Correlation (session 3)



### **3** PARSE the Data / **5** REFINE the Data (cont.)

Correlation does not imply causation (session 4)

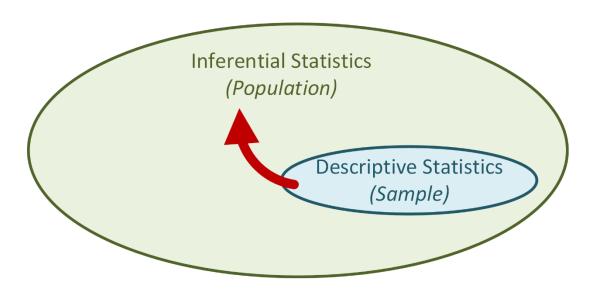


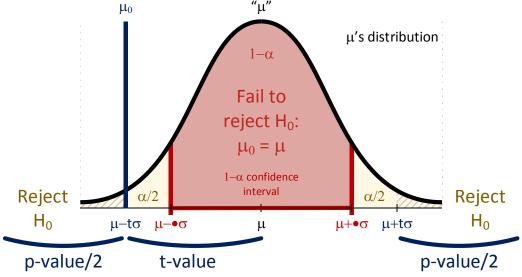
### **3** PARSE the Data / **5** REFINE the Data (cont.)

Descriptive and Inferential Statistics (sessions 3/4)

### **6** BUILD a Model

Two-Tail Hypothesis Testing (session 4)



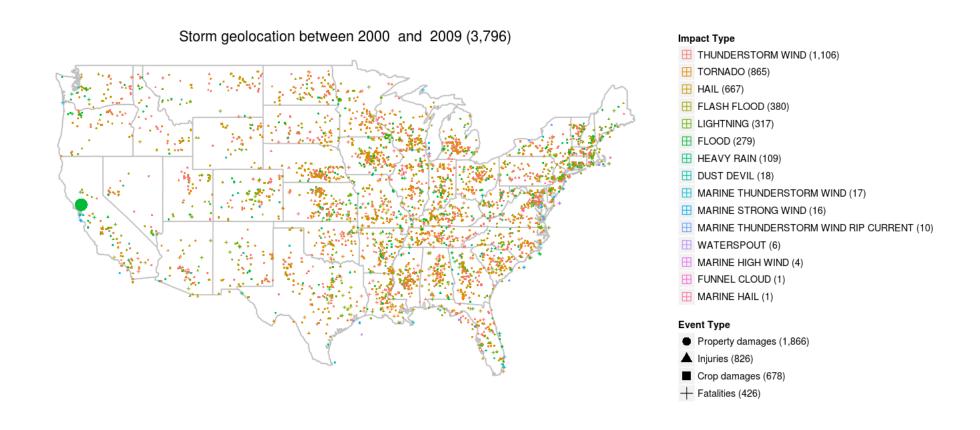


## pandas and Python (sessions 2-5)

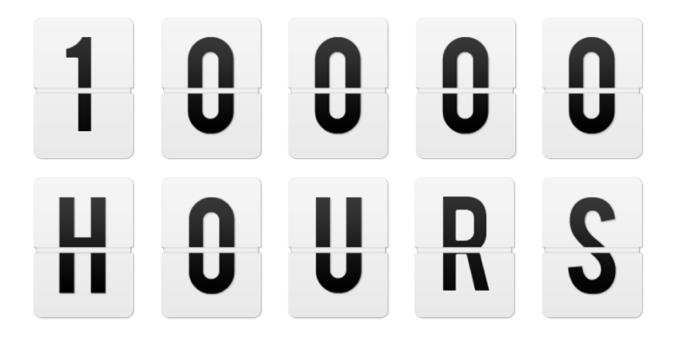
Measure of Centrality	.mean()	.median()	.mode()
Measure of Dispersion	.var(), .std()	<pre>.min(), .max()    .quantile()</pre>	
Summary	.desc	ribe()	
Graphical Methods		<pre>.plot(kind = 'box')</pre>	<pre>.plot(kind = 'hist')</pre>

Correlation Matrix	.corr()
Scatter plot	DataFrame.plot(kind = 'scatter', x = Series, y = Series)
Scatter matrix	<pre>pd.tools.plotting.scatter_matrix(DataFrame)</pre>

# There is much more you can do with the storm data, e.g.,



### Practice, Practice, and Practice...





Q&A

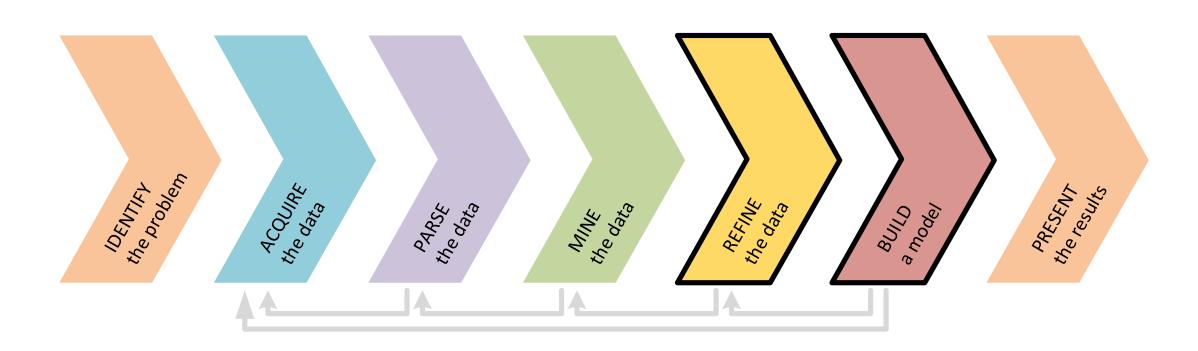


## Unit 2 Overview

## Unit 2 – Foundation of Modeling

Unit 3 – Data Science in the Real World	Decision Trees and Random Forest	Time Series Data	Natural Language Processing	Databases
Unit 2 – Foundations of Modeling	Linear Regression (session 6)	Classification Models (sessions 8 and 9)	Evaluating Model Fit (session 7)	Presenting Insights from Data Models (session 10)
Unit 1 – Research Design and Data Analysis	Research Design	Data Visualization in Pandas	Statistics	Exploratory Data Analysis in Pandas

### Unit 2 and the Data Science Workflow



### Unit 2 and the Data Science Workflow (cont.)

### **6** Refine the Data

- Identify trends and outliers(session 3)
- Apply descriptive (session 3) and inferential statistics (session 4)
- Document (session 2) andtransform data (units 2-3)

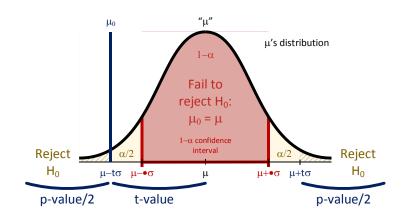
### 6 Build a Model

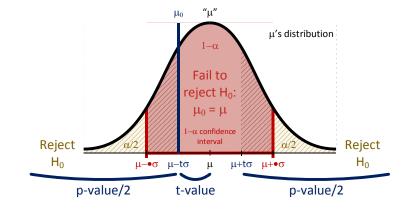
- Select appropriate model(units 2-3)
- Build model (units 2-3)
- Evaluate (session 4; units 2-3) and refine model (units 2-3)



# Two-Tail Hypothesis Testing Review

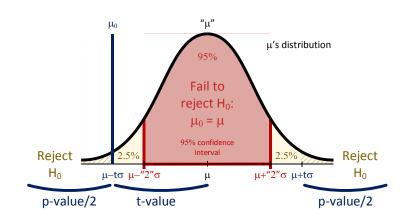
## Two-Tail Hypothesis Testing

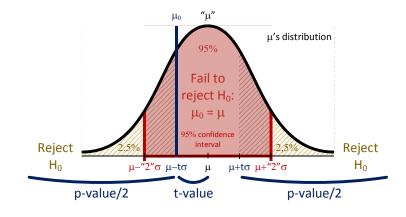




t-value	p-value	$1-\alpha$ Confidence Interval $([\mu_0-\cdot\sigma,\mu_0+\cdot\sigma])$	$H_0/H_a$	Conclusion
≥·	≤ <i>α</i>	$\mu_0$ is outside	Found evidence that $\mu \neq \mu_0$ : Reject $H_0$	$\mu \neq \mu_0$
<.	> α	$\mu_0$ is inside	Did not find that $\mu \neq \mu_0$ : Fail to reject $H_0$	$\mu = \mu_0$

## Two-Tail Hypothesis Testing ( $\alpha = .05$ ) (cont.)





t-value	p-value	$1-\alpha$ Confidence Interval $([\mu_0-2\sigma,\mu_0+2\sigma])$	$H_0/H_a$	Conclusion
$\geq$ " $\sim$ 2"(*) (check t-table)	≤ .025	$\mu_0$ is outside	Found evidence that $\mu \neq \mu_0$ : Reject $H_0$	$\mu \neq \mu_0$
< "~2"	> .025	$\mu_0$ is inside	Did not find that $\mu \neq \mu_0$ : Fail to reject $H_0$	$\mu=\mu_0$



# Simple Linear Regression

### Simple Linear Regression

The simple linear regression model captures a linear relationship between a single input variable *x* and a response variable *y* 

$$y = \beta_0 + \beta_1 \cdot x + \varepsilon$$

- y is the **response** variable (what we want to predict);
   also called *dependent* variable or *endogenous* variable
- *x* is the **explanatory** variable (what we use to train the model); also called *independent* variable, *exogenous* variable, *regressor*, or *feature*
- $\beta_0$  and  $\beta_1$  are the **regression's coefficients**; also called the model's parameters
  - $\beta_0$  is the line's intercept;  $\beta_1$  is the line's slope
- $ightharpoonup \varepsilon$  is the **error** term; also called the residual

## Simple Linear Regression (cont.)

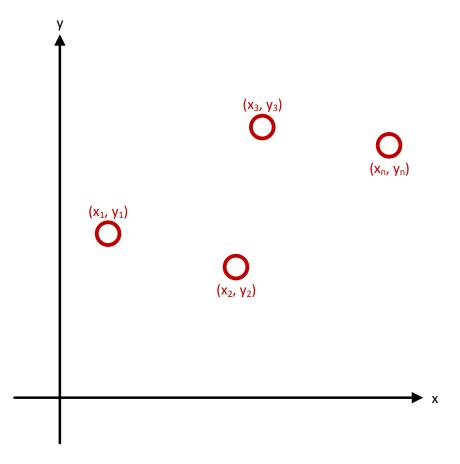
• Given  $x = (x_1, x_2, ..., x_n)$  and  $y = (y_1, y_2, ..., y_n)$ , we can formulate the linear model as

$$y_i = \beta_0 + \beta_1 \cdot x_i + \varepsilon_i$$

- In our Python environment, x and y represent pandas Series and  $x_i$  and  $y_i$  their values at row i-1 (index shifted by 1...)
- E.g. (Zillow),
  - x is the property's size (df.Size)
  - y is the property's sale price (df.SalePrice)

## Simple Linear Regression (cont.)

- In words, this equation says that for each observation i,  $y_i$  can be explained by  $\beta_0 + \beta_1 \cdot x_i$
- $\varepsilon_i$  is a "white noise" disturbance which <u>we do</u> not observe
  - $\epsilon_i$  models how the observations deviate from the exact slope-intercept relation
- We do not observe the constants  $\beta_0$  or  $\beta_1$  either, so we have to estimate them



## Simple Linear Regression (cont.)

• Given estimates for the model coefficients  $\widehat{\beta}_0$  ( $\beta_0$  hat) and  $\widehat{\beta}_1$ , we predict y using

$$\widehat{y} = \widehat{\beta_0} + \widehat{\beta_1} \cdot x$$

The hat symbol (^) denotes an estimated value

• E.g. (Zillow),

$$SalePrice = \widehat{\beta_0} + \widehat{\beta_1} \cdot Size$$



# Codealong – Part A1 Variable Transformations Simple Linear Regression

## SalePrice ~ Size (cont.)

SalePrice [\$M] = 
$$\underbrace{.155}_{\beta_0} + \underbrace{.750}_{\beta_1} \times Size$$
 [1,000 sqft]

(the slope is significant but not the intercept)



# Activity: Knowledge Check

## Activity: Knowledge Check



### ANSWER THE FOLLOWING QUESTIONS (5 minutes)

- 1. Using the table below,

  - a. How do you interpret the model's parameters? (intercept and slope)b. Replace all question marks (?) in the next slide with their number or answer

	coef	std err	t	P> t	[95.0% Conf. Int.]
Intercept	0.1551	0.084	1.842	0.066	-0.010 0.320
Size	0.7497	0.043	17.246	0.000	0.664 0.835

2. When finished, share your answers with your table

### **DELIVERABLE**

Answers to the above questions

## Activity: Knowledge Check (cont.)

$$Intercept(\beta_0) = .155$$

- Intercept = SalePrice [\$M] when Size = 0
- Intercept = \$0.155M = \$155k
- The simple linear regression predicts that a property of o sqft would sell for \$155k

$$Slope(\beta_1) = .750$$

$$Slope = \frac{SalePrice [\$M] - Intercept [\$M]}{Size[1,000 \ sqft]}$$

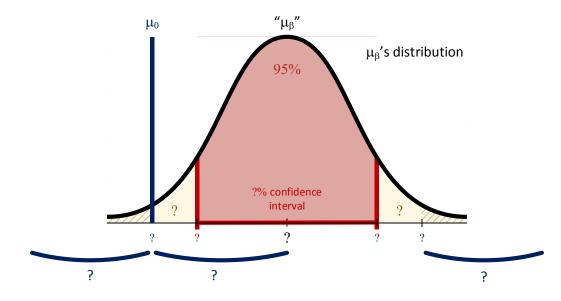
- Slope = .750 [\$M per 1,000 sqft] = \$750k/1,000 sqft
- The simple linear regression predicts that
   buyers would pay an \$750k for each 1,000 sqft

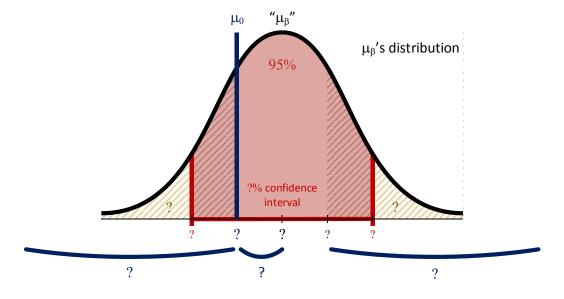
## Activity: Knowledge Check (cont.)

Intercept or Size?

Fail to reject  $H_0$ :  $\mu_{\beta_{Intercept/Size}} = \mu_0$  or reject  $H_0$ ? Intercept/Size significant or not significant? Fail to reject  $H_0$ :  $\mu_{\beta_{Intercept/Size}} = \mu_0$  or reject  $H_0$ ? Intercept/Size significant or not significant?

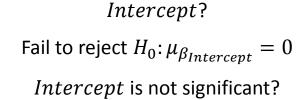
*Intercept* or *Size*?

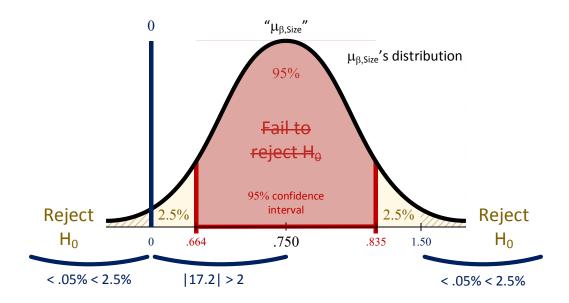


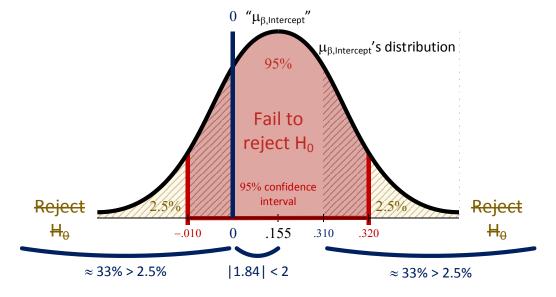


## Activity: Knowledge Check (cont.)

Size  $\mbox{Reject $H_0$: $\mu_{\beta_{Size}} = 0$}$  Size is significant









## Codealong – Part A2 Simple Linear Regression

#### SalePrice ~ 0 + Size (cont.)

SalePrice 
$$[\$M] = 0$$
.  $+.810 \times Size [1,000 sqft]$ 

#### SalePrice ~ Size (cont.)

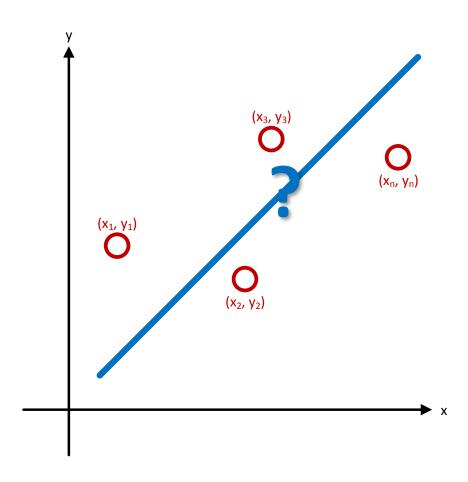
SalePrice 
$$[$M] = .708 + .278 \times Size [1,000 sqft]$$
  
(was .155) (was .750)

(both intercept and slope are now significant)

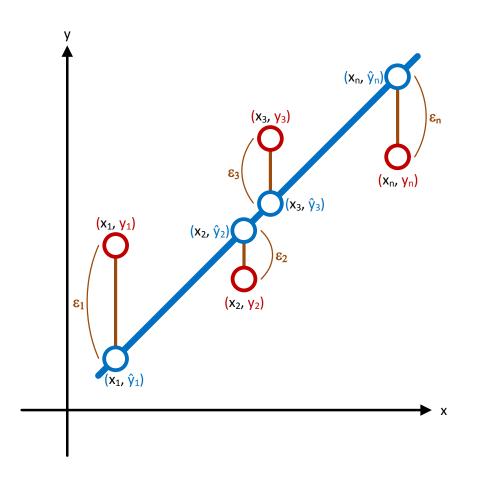


# How to fit a regression model to a dataset?

#### How do we estimate $\beta_0$ and $\beta_1$ ?



# We can estimate $\beta_0$ and $\beta_1$ with Ordinary Least Squares (OLS)



Minimize the sum of squared residuals

$$\min\left(\sum_{i=1}^{n} \varepsilon_i^2\right) = \min \|\varepsilon\|^2 = \min \|\beta_0 + \beta_1 \cdot x - y\|^2$$

statsmodels does this for you

$$sm.ols(formula = 'y \sim x', ...)$$

#### Common Regression Assumptions (part 1)

- The model is linear
  - $\rightarrow x$  significantly explains y
- $\epsilon \sim N(0, \cdot)$ 
  - Specifically, we expect  $\varepsilon$  to be 0 on average:  $\mu_{\varepsilon} = 0$
- x and  $\varepsilon$  are independent
  - $\rho(x,\varepsilon)=0$



## Codealong – Part B How to check modeling assumptions?



# How to check modeling assumptions?

## .plot\_regress\_exog() to check modeling assumptions with respect to a single regressor

- Scatterplot of observed values (y) compared to fitted values (ŷ) with confidence intervals against the regressor (x)
- .plot\_fit()

- "Residual Plot"
- Scatterplot of the model's residuals ( $\hat{\epsilon}$ ) against the regressor (x)

- "Partial Regression Plot" and "CCPR Plot (Component and Component-Plus-Residual)"
  - (useful for multiple regression) (more on this later)



# Codealong – Part C1 How to check normality assumption?



# How to check normality assumption?

#### .qqplot() to check normality assumption

- "Quantile-Quantile (q-q) Plot"
- Graphical technique for determining if two datasets come from populations with a common distribution
- Plot of the quantiles of the first dataset (vertically) against the quantiles of the second's (horizontally)
- If unspecified, the second dataset will default to N(0, 1)

- If the two datasets come from a population with the same distribution, the points should fall approximately along a 45-degree reference line
- The greater the departure from this reference line, the greater the evidence for the conclusion that the datasets have come from populations with different distributions

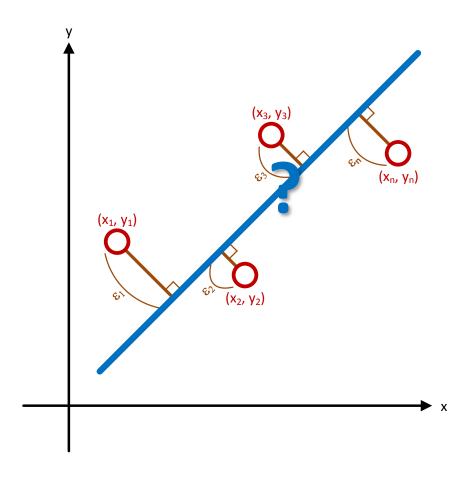


## Codealong – Part C2 How to check normality assumption?



# There are many ways to fit a line

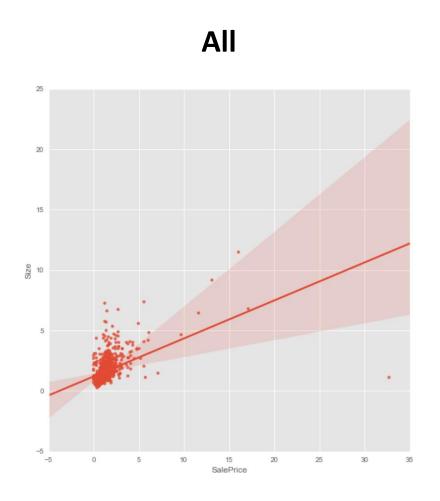
#### There are many ways to fit a line



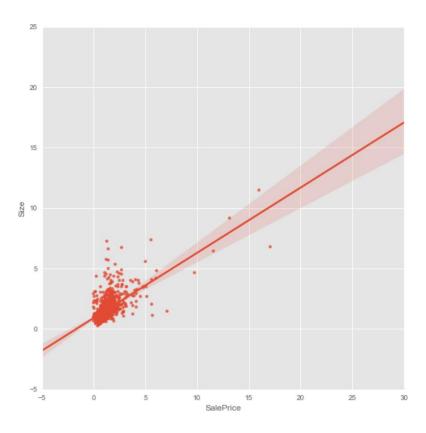


### Codealong — Part D Inference and Fit

# Effect of outliers on regression modeling (cont.)



#### "Top" Outlier Dropped

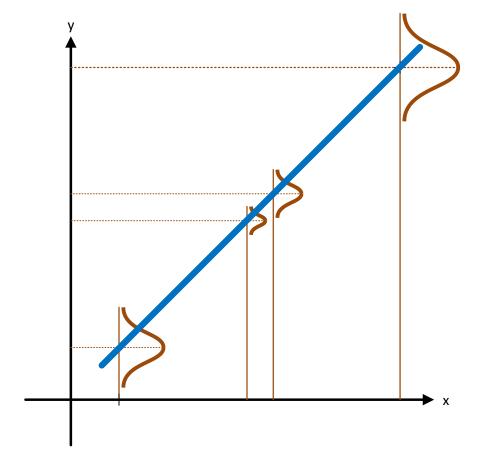




# Inference, Fit, and $R^2$ (r-square)

#### Inference and Fit

- The deviations of the data from the best fitting line are normally distributed about the line. Since  $\mu_{\varepsilon} = 0$ , we "expect" that on average, the line will be correct
- How confident we are about how well the relationship holds depends on  $\sigma_{\varepsilon}^2$



#### Measuring the fit of the line with $\mathbb{R}^2$

When a measure of how much of the total variation in y,  $\sigma_y^2 = \beta^2 \sigma_x^2 + \sigma_\varepsilon^2$ , is explained by the portion associated with the explanatory variable x; also called systematic variation

$$R^2 = \rho_{xy}^2 = \frac{\beta^2 \sigma_x^2}{\beta^2 \sigma_x^2 + \sigma_\varepsilon^2}$$

• 
$$0 \le R^2 \le 1$$
 (since  $-1 \le \rho_{xy} \le 1$ )

• 
$$1 - R^2 = \frac{\sigma_{\varepsilon}^2}{\beta^2 \sigma_{\chi}^2 + \sigma_{\varepsilon}^2}$$
 is the idiosyncratic variation

#### $R^2$ : Goodness of Fit

When x significantly explains y	When x does not significantly explains y
☐ The fit is <b>better</b>	☐ The fit is worse
☐ The <b>explained</b> systematic variation dominates	☐ The <b>unexplained</b> idiosyncratic variation dominates
$\square \beta^2 \sigma_{\chi}^2$ is high and/or $\sigma_{\varepsilon}^2$ is low	$\square$ $\beta^2 \sigma_{\chi}^2$ is low and/or $\sigma_{\varepsilon}^2$ is high
$\square R^2 = \frac{1}{1 + \underbrace{\frac{\sigma_{\mathcal{E}}^2}{\beta^2 \sigma_{\mathcal{X}}^2}}_{\cong 0}} $ is closer to 1	$\square R^2 = \frac{1}{1 + \underbrace{\frac{\sigma_{\varepsilon}^2}{\beta^2 \sigma_{\chi}^2}}_{\gg 1}} \text{ is closer to 0}$



# Codealong – Part E R 2



## Multiple Linear Regression

#### Multiple Linear Regression

- Simple linear regression with one variable can explain some variance, but using multiple variables can be much more powerful
- We can extend this model to several input variables, giving us the multiple linear regression model

$$y = \beta_0 + \beta_1 \cdot x_1 + \dots + \beta_k \cdot x_k + \varepsilon$$

• Given  $x_i = (x_{i,1}, x_{i,2}, ..., x_{i,n})$  and  $y = (y_1, y_2, ..., y_n)$ , we formulate the linear model as

$$y_i = \beta_0 + \beta_1 \cdot x_{1,i} + \dots + \beta_k \cdot x_{k,i} + \varepsilon_i$$

• Given estimates for the model coefficients  $\widehat{\beta}_i$ , we then predict y using

$$\widehat{y_i} = \widehat{\beta_0} + \widehat{\beta_1} \cdot x_1 + \dots + \widehat{\beta_k} \cdot x_k$$

#### Multiple Linear Regression (cont.)

• E.g. (Zillow),

$$SalePrice = \widehat{\beta_0} + \widehat{\beta_1} \cdot Size + \widehat{\beta_2} \cdot BedCount$$



## Codealong – Part F Multiple Linear Regression

#### Activity: Knowledge Check



#### ANSWER THE FOLLOWING QUESTIONS (5 minutes)

- Using the table below for SalePrice ~ Size + BedCount
  - a. How do you interpret the model's parameters? (units and values)

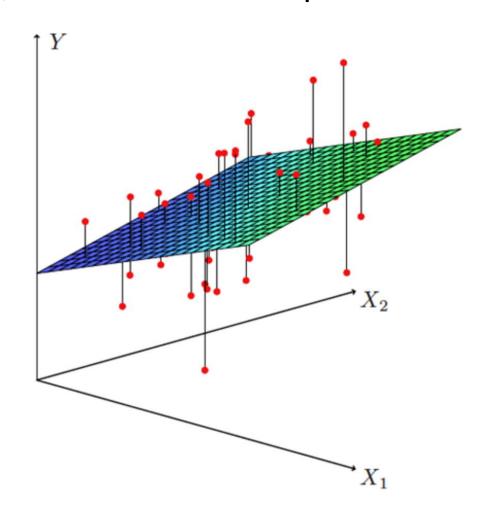
	coef	std err	t	P> t	[95.0% Conf. Int.]
Intercept	0.1968	0.068	2.883	0.004	0.063 0.331
Size	1.2470	0.045	27.531	0.000	1.158 1.336
BedCount	-0.3022	0.034	-8.839	0.000	-0.369 -0.235

2. When finished, share your answers with your table

#### **DELIVERABLE**

Answers to the above questions

We can still estimate  $\beta_i$  with Ordinary Least Squares (OLS); here a fitted plane when m=2



#### Common Regression Assumptions (part 2)

•  $x_i$  are independent from each other (low multicollinearity)

 Multicollinearity (or collinearity) is a phenomenon in which two or more predictors in a multiple regression model are highly correlated, meaning that one can be linearly predicted from the others with a substantial degree of accuracy

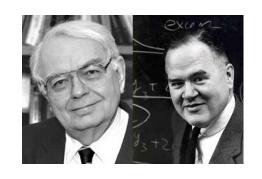
# The ideal scenario: when predictors are uncorrelated

- Each coefficient can be estimated and tested separately
- $\beta_i$  estimates the expected change in y per unit change in  $x_i$ , all other predictors held fixed
- However predictors usually change together

- Correlations amongst predictors cause problems
  - The variance of all coefficients tends to increase, sometimes dramatically
  - Interpretations become hazardous –
     when x<sub>i</sub> changes, everything else
     changes

# The woes of (interpreting) regression coefficients

 "The only way to find out what will happen when a complex system is distributed is to disturb the system, not merely to observe it passively" – Fred Mosteller and John Tukey





"Essentially, all models are wrong, but some are useful" –
 George Box

#### Common Regression Assumptions (part 3)

- Linear regression also works best when
  - the data is normally distributed (it doesn't have to be)
  - (if data is not normally distributed, we could introduce *bias*)

#### Activity: Variable Transformations



#### ANSWER THE FOLLOWING QUESTIONS (5 minutes)

1. We want to run the following regression with the following non-linear terms:

SalePrice 
$$\sim Size^2 + \sqrt{BedCount}$$

- a. How can we linearize it?
- 2. When finished, share your answers with your table

#### **DELIVERABLE**

Answers to the above questions



# Codealong – Part G Variable Transformations (cont.) Multicollinearity

#### .plot\_regress\_exog() (cont.)

- "Partial regression plot" (lower left)
- Partial regression for a single regressor
- The <u>full</u> model's  $\beta_i$  is the fitted line's slope
- The individual points can be used to assess the influence of points on the estimated coefficient
- .plot\_partregress()

- "CCPR plot" (lower right)
  - Component and Component-Plus-Residual
- Refined partial residual plot
- Judge the effect of one regressor on the response variable by taking into account the effects of the other independent variables
- Scatterplot of the <u>full</u> model's residuals  $(\hat{\varepsilon})$  plus  $\beta_i \cdot x_i$  against the regressor  $(x_i)$
- .plot\_ccpr()



# Codealong — Part H $\overline{R}^2$ (Adjusted $R^2$ )



 $\overline{R}^2$ 

#### $\bar{R}^2$

- R<sup>2</sup> increases as you add more variables in your model, even non-significant predictors; it's then tempting to add all the features from your dataset
- $\bar{R}^2$  attempts to adjust the explanatory power of regression models that contain different numbers of predictors so as to make comparisons possible

$$\bar{R}^2 = 1 - (1 - R^2) \cdot \frac{n - 1}{n - k - 1}$$

(n number of observations;k number of parameters)



## Lab



### Review

#### Linear Regression Review

- Linear regression is a simple approach to supervised learning. It assumes that the dependence of y (your response variable) on x (your input variables) is linear. Linear regressions are
- Highly interpretable and simple to explain
- Model training and prediction are fast
- No tuning is required (excluding regularization)
- (Input) Features don't need scaling
- Can perform well with a small number of observations
- Well-understood

#### Review

#### You should now be able to:

- Define simple linear regression and multiple linear regression
- Build a linear regression model using a dataset that meets the linearity assumption
- Evaluate model fit
- Understand and identify multicollinearity in a multiple regression



Q & A



#### Exit Ticket

Don't forget to fill out your exit ticket <a href="here">here</a>