Linear Regression

Fittin' lines

Objectives

- Review Linear Regression
- Explain the difference between residuals and irreducible error
- Name some regression diagnostics
- Name model test statistics and when to use which
- State how we can deal with nonlinearity



- Goal: predict a continuous output variable (Y) from a set of predictor variables (X)
- Parametric model (vs. non-parametric models)
- Simple and interpretable
- Trying Linear Regression before trying more complicated models is often a good idea
- Example: predict house price based on # sqft and neighborhood

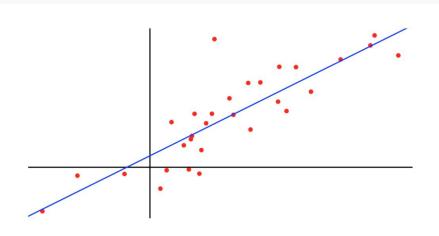
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With linear regression we "train" a model on some data.

Sometimes called learning, estimation, model fitting.

X data are generally called "features."

Sometimes called covariates, independent variables, inputs.



X	Y		
Stock Quote	Future Stock Price		
% of Diabetes	Mortality Rate		
Historic Web Logs	Page Views		
Airplane Flight Status	Arrival Time		
Anything!	Anything!		

Y data are generally called "targets."

Sometimes called labels, dependent variable, outputs.

$$Y=eta_0+eta_1X+\epsilon$$

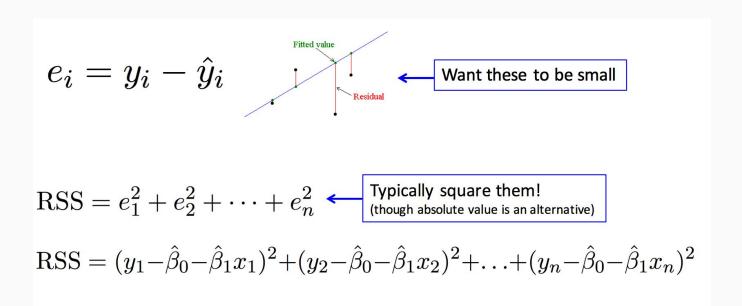
- $Y = \beta_0 + \beta_1 X + \epsilon = f(X) + \epsilon$
- $f(X) = \beta_0 + \beta_1 X$ is the true underlying dependency of Y on X
- ε is the irreducible error coming from factors that we have not or cannot measure
- $\hat{f}(X) = \hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X$ is out model's estimate for the true f(X)
- We try to minimize f(X) $f^{*}(X)$, this is called the reducible error
- We can never get rid of ε, unless we find new features that are correlated to them



- $Y = \beta_0 + \beta_1 X + \epsilon = f(X) + \epsilon$
- $\hat{y} = \hat{f}(X = x) = \hat{\beta}_0 + \hat{\beta}_1 x$ is your model's estimate for datapoint X=x
- $e_i = y_i \hat{y}_i$ is your model's error for datapoint \mathbf{x}_i
- e; contains the reducible and the irreducible error
- For the perfect model $e_i = \varepsilon_i$
- For linear regression we often use the residual sum of squares to assess the quality of the fit
- RSS = $e_1^2 + e_2^2 + ... + e_n^2$



Linear Regression is often called **Ordinary Least Squares (OLS) Regression** because the model simply finds coefficients that **minimize the sum total squared distance (residuals)** between each data point and the line.



Multiple Linear Regression (fitting hyperplanes)



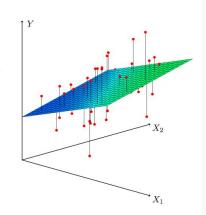
With Multiple Linear Regression we can combine many features into a single model.

Model

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

Fitted Value

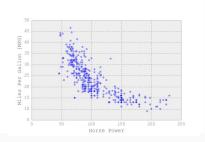
$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \dots + \hat{\beta}_p x_p$$



Residual Sum of Squares

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

= $\sum_{i=1}^{n} (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_{i1} - \hat{\beta}_2 x_{i2} - \dots - \hat{\beta}_p x_{ip})^2$



We can also have non-linear features, like X and X².

Ordinary Least Squares (OLS)

Minimize the RSS in terms of matrix algebra:

$$\mathbf{Y}_{n\times 1} = \mathbf{X}_{n\times p}\beta_{p\times 1} + \epsilon_{n\times 1}$$

$$\mathbf{X} = egin{bmatrix} X_{11} & X_{12} & \cdots & X_{1n} \ X_{21} & X_{22} & \cdots & X_{2n} \ dots & dots & \ddots & dots \ X_{m1} & X_{m2} & \cdots & X_{mn} \end{bmatrix}, \qquad oldsymbol{eta} = egin{bmatrix} eta_1 \ eta_2 \ dots \ eta_n \end{bmatrix}, \qquad \mathbf{y} = egin{bmatrix} y_1 \ y_2 \ dots \ eta_m \end{bmatrix}$$

X is called the "design" matrix, β is the parameter vector and \mathbf{y} the target vector

Ordinary Least Squares (OLS)

Minimize the RSS in terms of matrix algebra: $\mathbf{Y}_{n\times 1} = \mathbf{X}_{n\times p}\beta_{n\times 1} + \epsilon_{n\times 1}$

$$\mathbf{Y}_{n \times 1} = \mathbf{X}_{n \times p} \beta_{p \times 1} + \epsilon_{n \times 1}$$

Problem: find
$$\boldsymbol{\beta}$$
 such that $S(\boldsymbol{\beta}) = \sum_{i=1}^{m} |y_i - \sum_{j=1}^{n} X_{ij} \beta_j|^2 = \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2$ is minimized

Some matrix calculus yields:
$$\hat{oldsymbol{eta}} = (\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{y}$$

For 1D linear regression this yields

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

$$\hat{\beta}_1 = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2}$$

 $\hat{\beta}_1$ simply the covariance of x and y (normalized by variance of x)



Residual Sum of Squares

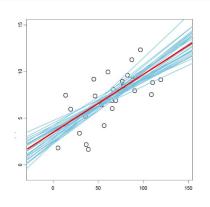
$$RSS = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$
 Not great...

R-Squared, or "Proportion of Variance Explained"

$$R^2 = \frac{TSS - RSS}{TSS} = 1 - \frac{RSS}{TSS}$$
 where $TSS = \sum_{i=1}^n (y_i - \bar{y})^2$ © Nice interpretation Independent of scale of y

Test statistics: t-test (Is this variable important?)





$$SE(\hat{\beta}_0)^2 = \sigma^2 \left[\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^n (x_i - \bar{x})^2} \right]$$

$$SE(\hat{\beta}_1)^2 = \frac{\sigma^2}{\sum_{i=1}^n (x_i - \bar{x})^2}$$

$$\sigma^2 = Var(\epsilon)$$

	Recall	Here		
Setup Hypothesis	H_0 : $\mu = 100$	$H_0: \beta_1 = 0$		
Sample Statistic	\bar{x}	\hat{eta}_1		
Test Statistic	$t = \frac{\overline{x} - \mu_0}{s / \sqrt{n}}$	$t = \frac{\hat{\beta}_1 - 0}{\text{SE}(\hat{\beta}_1)}$		
Confidence Interval	$(\overline{X} - t_{\alpha/2} \frac{S}{\sqrt{n}}, \overline{X} + t_{\alpha/2} \frac{S}{\sqrt{n}})$	$\left[\hat{\beta}_1 - 2 \cdot \operatorname{SE}(\hat{\beta}_1), \ \hat{\beta}_1 + 2 \cdot \operatorname{SE}(\hat{\beta}_1)\right]$		

Test if X has effect on Y

Test statistics: F-test (Is ANY variable important?)



F-test compares model with just a subset of m predictors to full model with p predictors (m<p)

Ex: predict MPG (Y) from set of variables:

Full model: Y =
$$\beta_0$$
 + β_{weight} + β_{height} + β_{model} + β_{year} + β_{color}

Reduced model:
$$Y = \beta_0 + \beta_{weight} + \beta_{year} + \beta_{color}$$

Calculate F-statistic (ratio of variance left unexplained by reduced model vs full model)

$$F = \frac{(RSS_{reduced} - RSS_{full})/(p_{full} - p_{reduced})}{RSS_{full}/(n - p_{full} - 1)}$$

where F has degrees of freedom (p_full - p_reduced), (n - p_full - 1)

Test statistics: F-test (Is ANY variable important?)



$$F = \frac{(RSS_{reduced} - RSS_{full})/(p_{full} - p_{reduced})}{RSS_{full}/(n - p_{full} - 1)}$$

where F has degrees of freedom (p_full - p_reduced), (n - p_full - 1)

If F is large, the dropped parameters are important

If you drop just one parameter and evaluate the p-value from the F-table you get back the p-value for the t-test for that parameter!

The statsmodels F-statistic and p-value correspond to dropping all parameters (null model vs full model), it will tell you if at least one of the parameters of the full set is important

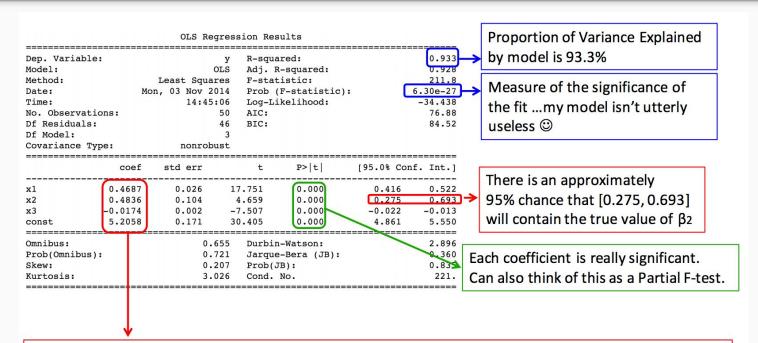
Model Interpretation (statsmodels)



OLS Regression Results								
Dep. Variable	:		y OLS	R-square	 ed: squared:			0.933
Method:		Least Squa	res	F-stati	stic:			211.8
Date:	Mo	on, 03 Nov 2	014	Prob (F	-statist	ic):	ij	6.30e−27 ←
Time:		14:45	:06	Log-Like	elihood:			-34.438
No. Observation	ons:		50	AIC:				76.88
Df Residuals:			46	BIC:				84.52
Df Model:			3					
Covariance Ty	pe:	nonrob	ust					
========				======		=======		======
	coef	std err		t	P> t	[95	.0% Con	f. Int.]
x1	0.4687	0.026	17	.751	0.000		0.416	0.522
x2	0.4836	0.104	4	.659	0.000		0.275	0.693
x 3	-0.0174	0.002	-7	.507	0.000	-1	0.022	-0.013
const	5.2058	0.171	30	.405	0.000		4.861	5.550
Omnibus:	=======	. 0	===== 655	Durbin-	====== Watson:	======		2.896
Prob(Omnibus)			721		Bera (JB):		0.360
Skew:	-		207	Prob(JB		, -		0.835
Kurtosis:			026	Cond. No				221.
			====	=======	 =======	=======	======	======

Model Interpretation (statsmodels)





"The average effect on Y of a one unit increase in X2, holding all other predictors (X1 & X3) fixed, is 0.4836"

- However, interpretations are generally pretty hazardous due to correlations among predictors.
- p-values for each coefficient ≈ 0, so might be okay here

Note: Magnitude of the Beta coefficients is NOT how to determine whether predictor contributes. Why?



- Linear relationship!
- Constant variance (homoscedasticity)
- Independence of errors
- Normality of errors
- Lack of multicollinearity

Non-linearity

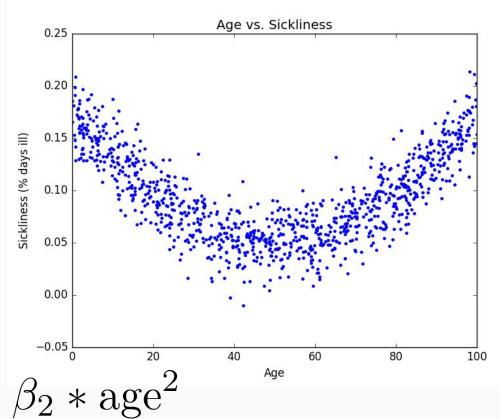
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We can make linear regression non-linear by inserting extra "interaction" features or higher-order features.

As you add more features, R^2 will only go up.

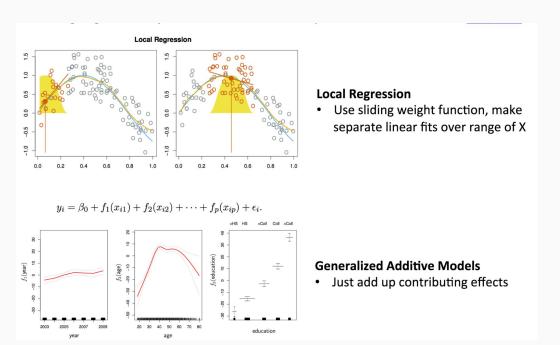
Example:

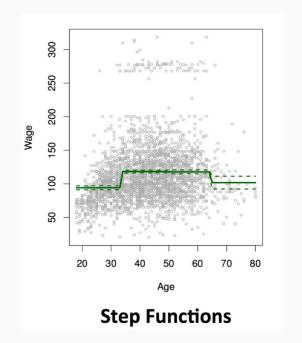
$$Y = \beta_0 + \beta_1 * age$$
 $Y = \beta_0 + \beta_1 * age + \beta_2 * age^2$





Many other methods for non-linear regression exist but will not be discussed ISLR and ESLR go into them in more detail: GAMs, local regression, splines etc





Multicollinearity



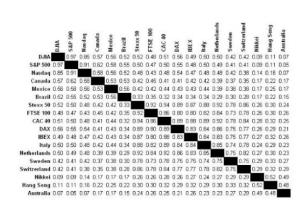
Multicollinearity occurs when two or more X features are correlated to each other.

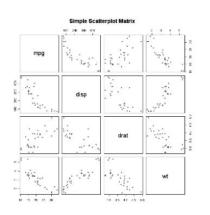
For example
$$x_2 = 2*x_1$$

What happens	What you do
 The uncertainty in the model coefficients becomes large. Does not affect the model accuracy, only the interpretability of the coefficients. 	 Use correlation matrix to look for pairwise correlations. Use VIF for more complicated relationships. Remove (but make note of) any predictor that is easily determined by the remaining predictors.

Multicollinearity diagnosis

Identification by correlation matrix and pairwise scatter plots





Downside is can only pick up pairwise effects ⊗

- Variance inflation factor (VIF) calculation:
 - o Run Linear regression for each predictor as target as function of all other predictors (p times)

$$X_1=lpha_2X_2+lpha_3X_3+\cdots+lpha_kX_k+c_0+e$$

$$ext{VIF}_{ ext{i}} = rac{1}{1-R_i^2}$$

• Rule of thumb: collinearity is high if $VIF(\hat{\beta}_i) > 10$

Inspecting residuals



$$e_i = y_i - \hat{y}_i$$

- They will be more useful if we standardize them:
- $r_i = e_i/\sigma$, with σ^2 the true population variance, which is unknown but can be estimated by the mean squared error (MSE)
- e_i/sqrt(MSE) is called the semi-studentized residual
- A better estimate of the real variance is $\widehat{V}(e_i) = MSE(1 h_{ii})$
- Which gives us the studentized residual: $r_i = \frac{e_i}{\sqrt{MSE(1-h_{ii})}}$

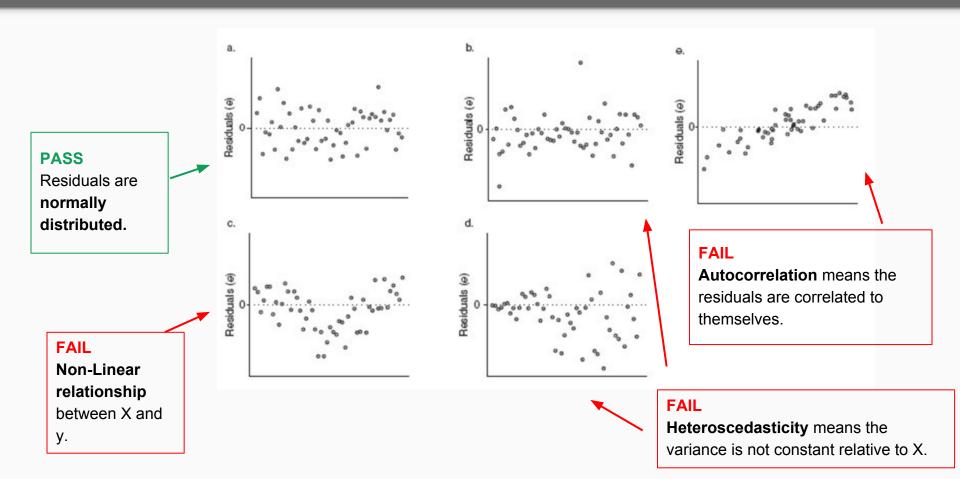
h_{ii} is called the "self-influence" and are diagonal elements of the "hat matrix" H (also "projection matrix")

$$\hat{y} = X\hat{\beta} = X(X'X)^{-1}X'y = Hy,$$

$$e = y - \hat{y} = y - Hy = (I - H)y$$

Residual Plots Allow Us to Check Assumptions

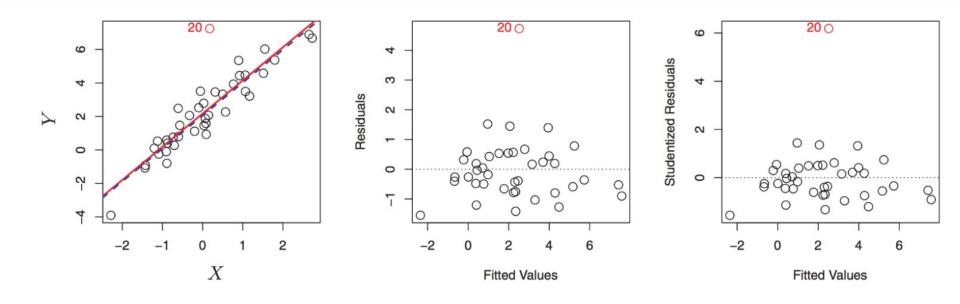




Outliers



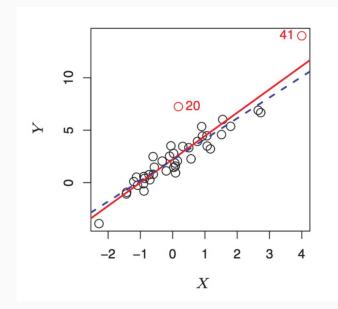
- Outliers are data points that are far from their predicted values
- Can be identified by inspecting residuals
- If studentized residual >> 2 or << -2, we consider them outliers

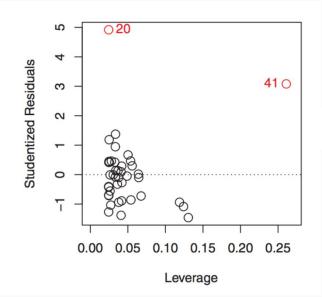


High leverage points



- Outliers are different from high leverage points
- A high leverage point has an extreme X value (far from the rest of the data)
- Commonly measured with the diagonal elements of the hat matrix H
- In the following dataset, 20 is an outlier, 41 is a leverage point AND outlier



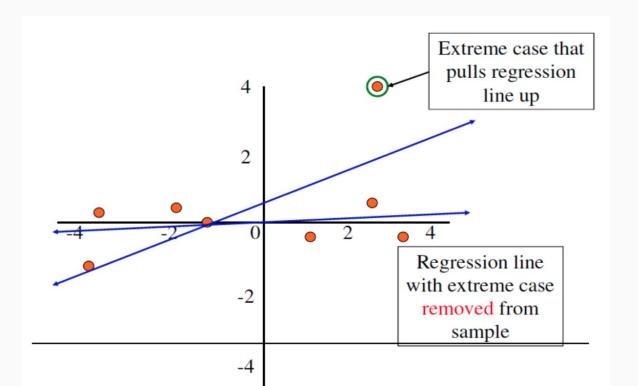


$$H = X(X^T X)^{-1} X^T$$

Influential points



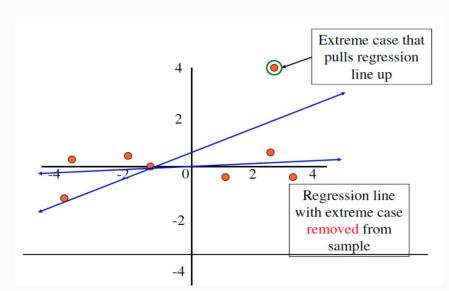
- Observations that are outliers and have high leverage tend to be influential
- Their removal from the data greatly affects the slope of the regression line



Influential points



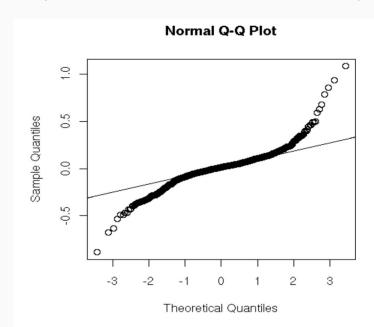
- An influential point may represent bad data, possibly the result of measurement error. If possible, check the validity of the data point.
- Compare the decisions that would be made based on regression equations defined with and without the influential point. If the equations lead to contrary decisions, use caution.



Normality of errors



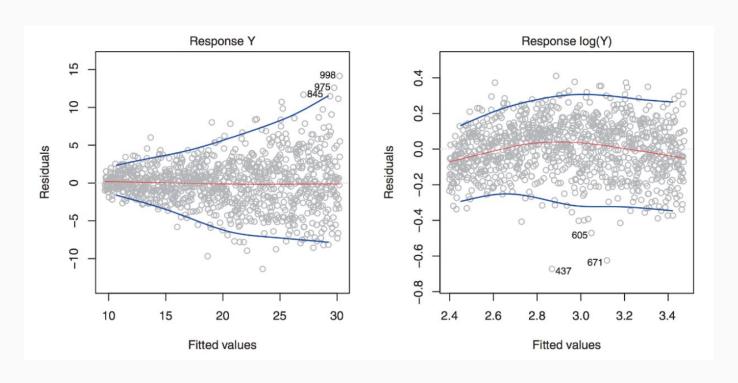
- Normality assumption allows us to do hypothesis testing (t-tests) on our parameters, and construct confidence intervals
- Ways to check: QQ-plots of residuals against normal distribution
- Ways to fix: transformation of Y (e.g. log(Y))



Heteroscedasticity of errors



- Variance changes depending on X
- Fix: transform Y (log(Y) or sqrt(Y) for example)



Linear Regression

Fittin' lines

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Afternoon

Categorical variables and interactions

Objectives

- State how to deal with categorical variables
- State how to include interactions into your model
- State why model validation is important and how it works



Categorical variables



- Independent variable might not be numerical
- Ex: using "gender" and "ethnicity" to predict credit card balances
- Solution: Create "dummy variable" that takes on value of 0 or 1

$$x_i = \begin{cases} 1 & \text{if } i \text{th person is female} \\ 0 & \text{if } i \text{th person is male} \end{cases}$$

$$y_i = \beta_0 + \beta_1 \underline{x_i} + \epsilon_i = \begin{cases} \beta_0 + \beta_1 + \epsilon_i & \text{if } i \text{th person is female} \\ \beta_0 + \epsilon_i & \text{if } i \text{th person is male.} \end{cases}$$

Categorical variables with more than 2 levels



Ethnicity has 3 levels: African-American, Asian, Caucasian

$$x_{i1} = \begin{cases} 1 & \text{if } i \text{th person is } \underline{\text{Asian}} \\ 0 & \text{if } i \text{th person is not Asian} \end{cases}$$

$$x_{i2} = \begin{cases} 1 & \text{if } i \text{th person is } \underline{\text{Caucasian}} \\ 0 & \text{if } i \text{th person is not Caucasian} \end{cases}$$

$$y_{i} = \beta_{0} + \beta_{1} \underline{x_{i1}} + \beta_{2} \underline{x_{i2}} + \epsilon_{i} = \begin{cases} \beta_{0} + \beta_{1} + \epsilon_{i} & \text{if } i \text{th person is Asian} \\ \beta_{0} + \beta_{2} + \epsilon_{i} & \text{if } i \text{th person is Caucasian} \\ \beta_{0} + \epsilon_{i} & \text{if } i \text{th person is AA.} \end{cases}$$

Categorical variables with more than 2 levels



$$y_{i} = \beta_{0} + \beta_{1} \underline{x_{i1}} + \beta_{2} \underline{x_{i2}} + \epsilon_{i} = \begin{cases} \beta_{0} + \beta_{1} + \epsilon_{i} & \text{if } i \text{th person is Asian} \\ \beta_{0} + \beta_{2} + \epsilon_{i} & \text{if } i \text{th person is Caucasian} \\ \beta_{0} + \epsilon_{i} & \text{if } i \text{th person is AA.} \end{cases}$$

Data

<u>Ones</u>	<u>Ethnicity</u>		
1	AA		
1	Asian		
1	Asian		
1	Caucasian		
1	AA	-	
1	AA		
1	Asian		
1	Caucasian		
1	AA		

Recode Design Matrix

<u>Ones</u>	<u>Asian</u>	Caucasian
1	0	0
1	1	0
1	1	0
1	0	1
1	0	0
1	0	0
1	1	0
1	0	1
1	0	0

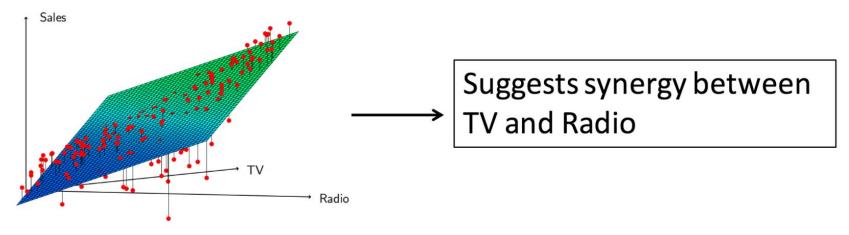
Categorical variables with more than 2 levels



$$y_{i} = \beta_{0} + \beta_{1} \underline{x_{i1}} + \beta_{2} \underline{x_{i2}} + \epsilon_{i} = \begin{cases} \beta_{0} + \beta_{1} + \epsilon_{i} & \text{if } i \text{th person is Asian} \\ \beta_{0} + \beta_{2} + \epsilon_{i} & \text{if } i \text{th person is Caucasian} \\ \beta_{0} + \epsilon_{i} & \text{if } i \text{th person is AA.} \end{cases}$$

- β_0 does not represent the general baseline anymore, but the baseline for group 0 (AA)
- β_1 represents the difference of the baseline of group 1 (Asian) to group 0 (AA)
- β_2 represents difference group 0 and group 2
- What does it mean if $\beta_1 = -20.3$?
- What do we do if we want to use Caucasians as the baseline?

$$\widehat{\mathtt{sales}} = \beta_0 + \beta_1 \times \mathtt{TV} + \beta_2 \times \mathtt{radio} + \beta_3 \times \mathtt{newspaper}$$



- Synergy between radio and TV means that spending 50K on both radio and TV is better for sales than spending 100K on only one of them
- How can we model this?

Interactions of quantitative variables



sales =
$$\beta_0 + \beta_1 \times \text{TV} + \beta_2 \times \text{radio} + \underline{\beta_3} \times (\text{radio} \times \text{TV}) + \epsilon$$

 = $\beta_0 + (\beta_1 + \beta_3 \times \text{radio}) \times \text{TV} + \beta_2 \times \text{radio} + \epsilon$.

Results:

	Coefficient	Std. Error	t-statistic	p-value	
Intercept	6.7502	0.248	27.23	< 0.0001	
TV	0.0191	0.002	12.70	< 0.0001	
radio	0.0289	0.009	3.24	0.0014	
${ t TV}{ imes { t radio}}$	0.0011	0.000	20.73	< 0.0001	← Improvemen

Changing radio will change the slope of TV!

Interactions of categorical variables

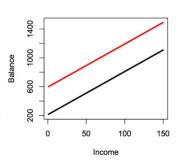


Interaction of student (categorical) and income (quantitative)

<u>No Interaction</u> $balance_i = \beta_0 + \beta_1 * income_i + \beta_2 * student_i$

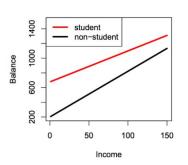
$$\begin{array}{ll} \mathbf{balance}_{i} & \approx & \beta_{0} + \beta_{1} \times \mathbf{income}_{i} + \begin{cases} \beta_{2} & \text{if } i \text{th person is a student} \\ 0 & \text{if } i \text{th person is not a student} \end{cases}$$

$$= & \underline{\beta_{1}} \times \mathbf{income}_{i} + \begin{cases} \underline{\beta_{0} + \beta_{2}} & \text{if } i \text{th person is a student} \\ \overline{\beta_{0}} & \text{if } i \text{th person is not a student} \end{cases}$$



<u>With Interaction</u> $balance_i = \beta_0 + \beta_1 * income_i + \beta_2 * student_i + \beta_3 * income_i * student_i$

$$\begin{array}{lll} \mathbf{balance}_i & \approx & \beta_0 + \beta_1 \times \mathbf{income}_i + \begin{cases} \beta_2 + \beta_3 \times \mathbf{income}_i & \text{if student} \\ 0 & \text{if not student} \end{cases} \\ & = & \begin{cases} \frac{(\beta_0 + \beta_2)}{\beta_0} + \frac{(\beta_1 + \beta_3)}{\beta_0} \times \mathbf{income}_i & \text{if student} \\ \frac{(\beta_0 + \beta_1)}{\beta_0} \times \mathbf{income}_i & \text{if not student} \end{cases} \end{array}$$

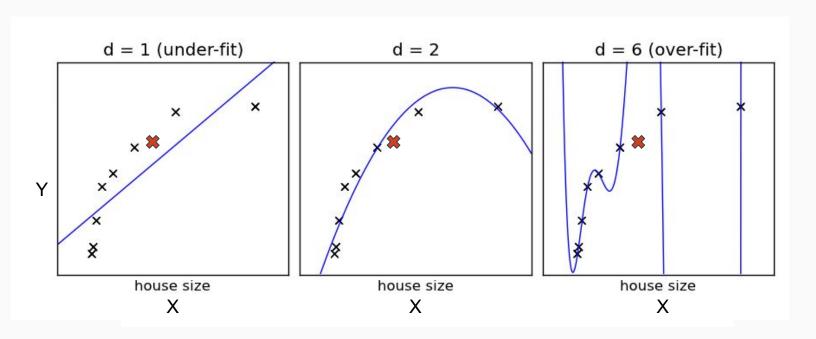


We *could* just keep inserting interaction features until $R^2 = 1$.

Boom. I <u>solved</u> data science. Here's my idea:

```
def train_super_awesome_perfect_model (X, y):
    while True:
        model = LinearRegression()
        model.fit(X, y)
        if calculate_r2(model, X, y) >= 0.999:
            return model
        else:
        X = insert_random_interaction_feature(X)
```

Why is this a bad idea?



What's bad about the <u>first</u> model?

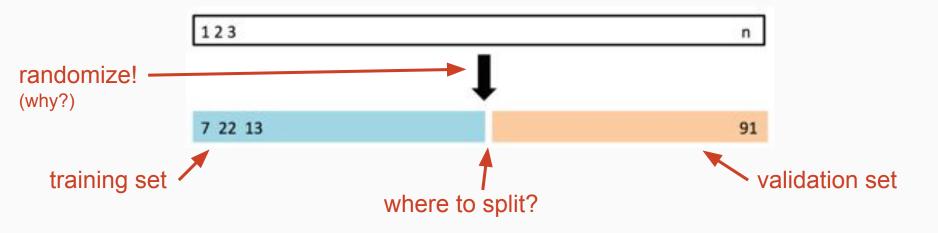
What's bad about the second model?

What's bad about the third model?



Main idea: Don't use all your data for training.

Instead: Split your data into a "training set" and a "validation set".



Validation techniques will be covered tomorrow!

Questions



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

- Name and explain all the elements of the above equation and its meaning
- How do we assess the quality of a model/fit
 - O How are the different measures related?
- How do you compare a submodel of a model to the model?
 - How does this relate to the t-statistic for individual parameter?
 - How does this relate to the standard F-statistic and p-value printed by statsmodels?
- How do we account for categorical variables?
 - o How do we change the baseline?
- What is an interaction/synergy?
 - O How do we account for it?

Afternoon

Categorical variables and interactions

Objectives

- State how to deal with categorical variables
- State how to include interactions into your model
- State why model validation is important and how it works

