Multiple Linear Regression

CD 530
Chapman
Spring 2021

Take Message for rest of course: Multiple Linear Regression

➤ Understand difference between mutli-variate & univariate models

➤ Encounter methods to decide which variables contribute to models

➤ See methods to deal with variable numbers of free parameters for different models

➤ Discuss situations that can be disruptive, or even destructive, when fitting models

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Multiple Linear Regression—Table of Contents

- > Simple vs. Multiple Linear Regression
- > Derivation of Multiple Linear Regression Model
- Multiple Linear Regression Model Diagnostics
- > Regression Example: Healthy Breakfast Dataset

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Simple vs. Multiple Linear Regression

We previously covered simple linear regression, where we tried to find relationship between single explanatory variable & response variable:

 $x \leftarrow$  explanatory variable

 $y \leftarrow$  response variable

Our simple linear regression model was

 $y = \beta_0 + \beta_1 x + \epsilon$ 

where

$$\begin{split} &\beta_0 \!\leftarrow \text{what we predict for } y \text{ when } x = 0 \\ &\beta_1 \!\leftarrow \text{amount } y \text{ changes per unit increase in } x \\ &\epsilon \leftarrow \text{error term, unexplained randomness (noise)} \end{split}$$

Simple vs. Multiple Linear Regression

What if we think the output, y, depends on more than one explanatory variable? We would use multiple linear regression. Our model now expands to

 $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \dots + \epsilon$ 

where

 $x_1 \leftarrow \text{the first explanatory variable}$ 

 $x_2 \leftarrow$  the second explanatory variable

 $x_3 \leftarrow$  the third explanatory variable

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## Simple vs. Multiple Linear Regression

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \dots + \epsilon$$

Each  $\beta_i$  represents the average effect on y caused by a unit increase in  $x_i$ , assuming all other x terms— $x_1...x_{i-1},x_{i+1},x_p$ —stay constant. This is not a trivial assumption.

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#### Simple vs. Multiple Linear Regression

With simple linear regression, the data points were on a 2-D plane, and we found a line of best fit

$$y = \hat{\beta}_0 + \hat{\beta}_1 x$$

where  $\hat{\beta}_0$  &  $\hat{\beta}_1$  were our coefficient estimates. We found this line by considering the residuals,  $\{e_i\}$ , which are the vertical differences between curve & data points.

 $e_i = (y_i - \hat{y}_i) \\ = (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)$ 

Simple vs. Multiple Linear Regression

We similarly find the hyperplane of

best fit by considering the residuals  $\{e_i\}$  that correspond with the distances along the y-axis between each point and the hyperplane

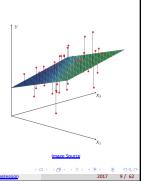
 $\begin{array}{l} e_i = \, (y_i - \hat{y}_i) \\ e_i = \, (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_{i1} - \hat{\beta}_2 x_{i2} - \cdots) \end{array}$ 

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Simple vs. Multiple Linear Regression

With multiple linear regression, if there are p explanatory variables and 1 response variable, the data points exist in (p+1)-dimensional space:  $(x_1, \dots, x_p, y)$ . The regression model is now a hyperplane in this (p+1)-dimensional space:

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



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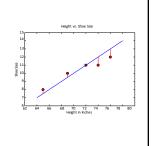
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# Simple vs. Multiple Linear Regression

To find line of best fit in simple linear regression, we found minimum of Residual Sum of Squares (RSS):

$$RSS = \sum_{i=1}^{p} (e_i)^{i}$$

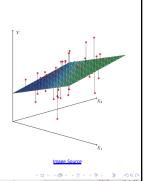
which, through some calculus & algebra, yielded tidy equations for coefficient estimates  $\hat{\beta}_0$  and  $\hat{\beta}_1$ .

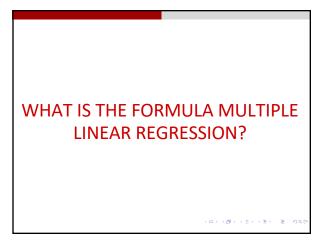


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To find hyperplane of best fit for multiple linear regression, we will similarly find minimum for RSS. This time, it will require some linear algebra too.





RSS for Multiple Linear Regression

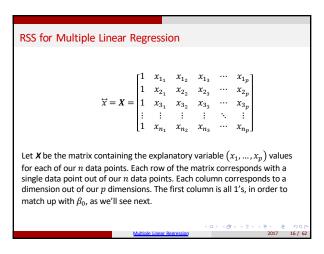
Suppose we have n data points and p explanatory variables  $(x_1,...,x_p)$ . Let  $\vec{y} = y$  be the column vector containing the response variable  $(y_i)$  value for each of our n observations.  $\vec{y} = y = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_n \end{bmatrix}$ 

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RSS for Multiple Linear Regression

Let  $m{\beta}$  be the column vector containing all the coefficients for our model. There are p explanatory variables  $(x_1,...,x_p)$ . So, including y-intercept  $(\beta_0)$ ,  $m{\beta}$  contains p+1 elements.  $\vec{\beta} = m{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \\ \vdots \\ \beta_p \end{bmatrix}$ 

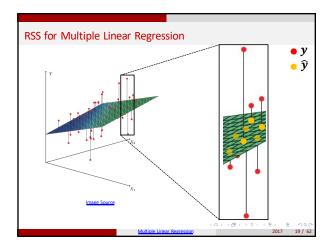
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 $\widehat{\mathbf{y}} = \mathbf{x} \boldsymbol{\beta} = \begin{bmatrix} 1 & x_{11} & x_{12} & x_{13} & \cdots & x_{1p} \\ 1 & x_{21} & x_{22} & x_{23} & \cdots & x_{2p} \\ 1 & x_{31} & x_{32} & x_{33} & \cdots & x_{np} \end{bmatrix} \cdot \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & x_{n3} & \cdots & x_{np} \end{bmatrix} \cdot \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \vdots \\ \beta_p \end{bmatrix}$   $\begin{bmatrix} \beta_0 + \beta_1 x_{11} + \beta_2 x_{12} + \cdots + \beta_p x_{1p} \\ \beta_0 + \beta_1 x_{21} + \beta_2 x_{22} + \cdots + \beta_p x_{2p} \\ \beta_0 + \beta_1 x_{31} + \beta_2 x_{32} + \cdots + \beta_p x_{3p} \\ \vdots \\ \beta_0 + \beta_1 x_{n1} + \beta_2 x_{n2} + \cdots + \beta_p x_{np} \end{bmatrix}$ The matrix product  $\mathbf{X} \boldsymbol{\beta}$  gives us a column vector of predicted values,  $\widehat{\mathbf{y}}$ . If we took the  $(x_1, \dots, x_p)$  values for each of our n data points and put them into our linear model, this is what it would return. This gives us the  $\mathbf{y}$ -values of the data points if they were projected onto our hyperplane.



# RSS for Multiple Linear Regression

As before with simple linear regression, we want to find values for our coefficient estimates,  $(\beta_0,\beta_1,...,\beta_p)$ , that minimize RSS, so that our hyperplane will be "as close as possible" to the data points. This will occur where the partial derivatives of RSS with respect to the coefficient estimates are equal to 0.

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# RSS for Multiple Linear Regression

Now, we'll take the derivative of RSS with respect to the  $\pmb{\beta}$  vector, set it equal to 0, and solve for  $\pmb{\beta}$ .

RSS = 
$$\mathbf{y}^T \mathbf{y} - 2\mathbf{\beta}^T \mathbf{X}^T \mathbf{y} + \mathbf{\beta}^T \mathbf{X}^T \mathbf{X}\mathbf{\beta}$$
  
 $\frac{\partial RSS}{\partial \mathbf{\beta}} = -2\mathbf{X}^T \mathbf{y} + 2\mathbf{X}^T \mathbf{X}\mathbf{\beta} = 0$   
 $\mathbf{X}^T \mathbf{X}\mathbf{\beta} = \mathbf{X}^T \mathbf{y}$ 

 $(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{X}\mathbf{B} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$ 

 $\widehat{\boldsymbol{\beta}} = (\boldsymbol{X}^T \boldsymbol{X})^{-1} \boldsymbol{X}^T \boldsymbol{y}$ 

Note: This is only valid if  $\boldsymbol{X}$  is a matrix of full rank, so that  $(\boldsymbol{X}^T\boldsymbol{X})$  is invertible.

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#### RSS for Multiple Linear Regression

To get a vector of residuals, we need the difference between our predicted and actual  $\boldsymbol{y}$  values:

$$e = y - \hat{y} = y - X\beta$$

To get the Residual Sum of Squares, we need the sum of the squares of the elements of this residual vector, which is the same as the dot product of this residual vector with itself

RSS = 
$$e \cdot e = (y - X\beta) \cdot (y - X\beta)$$
  
RSS =  $e^T e = (y - X\beta)^T (y - X\beta)$ 

where the  $\blacksquare^T$  indicates transpose of matrix  $\blacksquare$  (turns the columns into rows and vice-versa).

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### **RSS for Multiple Linear Regression**

Let's algebraically manipulate the expression for RSS first:

$$RSS = (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

$$= (\mathbf{y}^T - \boldsymbol{\beta}^T \mathbf{X}^T) (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

$$= \mathbf{y}^T \mathbf{y} - \boldsymbol{\beta}^T \mathbf{X}^T \mathbf{y} - \mathbf{y}^T \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\beta}^T \mathbf{X}^T \mathbf{X}\boldsymbol{\beta}$$

$$= \mathbf{y}^T \mathbf{y} - 2\boldsymbol{\beta}^T \mathbf{X}^T \mathbf{y} + \boldsymbol{\beta}^T \mathbf{X}^T \mathbf{X}\boldsymbol{\beta}$$

Note: we can combine terms in the last line because

$$\boldsymbol{\beta}^T \boldsymbol{X}^T \boldsymbol{y} = \boldsymbol{y}^T \boldsymbol{X} \boldsymbol{\beta}$$

as both terms are scalars, so (remember  $(AB)^T = B^TA^T$ )

$$\boldsymbol{\beta}^T \boldsymbol{X}^T \boldsymbol{y} = (\boldsymbol{\beta}^T \boldsymbol{X}^T \boldsymbol{y})^T = \boldsymbol{y}^T (\boldsymbol{\beta}^T \boldsymbol{X}^T)^T = \boldsymbol{y}^T \boldsymbol{X} \boldsymbol{\beta}$$

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## Multiple Linear Regression & Simple Linear Regression

Note the similarity between the expression for  $\widehat{m{\beta}}$  in multiple linear regression

$$\widehat{\boldsymbol{\beta}} = (\boldsymbol{X}^T \boldsymbol{X})^{-1} \boldsymbol{X}^T \boldsymbol{y}$$

and the expression for  $\hat{eta}_1$  in simple linear regression

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

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### RSS for Multiple Linear Regression

The coefficient estimates for multiple linear regression can thus be found with the equation:

$$\widehat{\boldsymbol{\beta}} = (\boldsymbol{X}^T \boldsymbol{X})^{-1} \boldsymbol{X}^T \boldsymbol{y}$$

But

- 1. How do we check the accuracy of this model and its coefficients?
- 2. How many variables should we include in our model?

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# Multiple Linear Regression: Model Diagnostics

When deciding how many variables to include in a model, consider the <u>Principle of Parsimony</u> (Occam's Razor):

If two models perform equally well, prefer the simpler model.

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# Multiple Linear Regression: Model Diagnostics

In somewhat similar way to simple linear regression, we can find an estimate of the SE of each  $\hat{\beta}_i$ . Using the SE, we can calculate a p-value for that  $\hat{\beta}_l$  being significantly different from 0. A sufficiently low p-value (e.g., less than 0.05) indicates that we can reject the null hypothesis that  $\hat{\beta}_l=0$  and say that  $\hat{\beta}_l$  is likely contributing to the model.

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## Multiple Linear Regression: Model Diagnostics

With simple linear regression, we used the Residual Standard Error (RSE) to help estimate  $\sigma^2$ , the variance of the error term  $\varepsilon$ . With multiple linear regression, we can also use the RSE, but the formula changes slightly:

$$\hat{\sigma} = \text{RSE} = \sqrt{\frac{\text{RSS}}{n - p - 1}}$$

where

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RSS←Residual Sum of Squares

 $n \leftarrow$ number of data points

 $p \leftarrow$ number of variables  $x_i$ 

We divide by  $\,n-p-1\,$  because we lose  $\,p+1\,$  degrees of freedom in our regression equation.

## Multiple Linear Regression: Model Diagnostics

But we must first test for significance on the entire model—on all coefficients. We can perform the following hypothesis test:

$$H_0\colon \beta_1=\beta_2=\cdots=\beta_p=0$$

 $H_A$ :  $\beta_i \neq 0$  for at least one  $i \in \{1, ..., p\}$ 

In other words, the null hypothesis is that none of the model coefficients (except the intercept) are statistically significant—i.e., that the model does not fit the data at all. The alternative hypothesis is that at least one coefficient (besides the intercept) is nonzero.

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#### Multiple Linear Regression: Model Diagnostics

$$H_0\colon \beta_1=\beta_2=\cdots=\beta_p=0$$
  
 $H_A\colon \beta_i\neq 0$  for at least one  $i>0$ 

To check these hypotheses, we can calculate an F-statistic:

$$F = \frac{(\text{TSS} - \text{RSS})/p}{\text{RSS}/(n - p - 1)} = \frac{(\text{TSS} - \text{RSS})/p}{\hat{\sigma}}$$

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# Multiple Linear Regression: Model Fit

What if we want to check the overall goodness of fit of the model?

One measure of overall fit is the coefficient of determination  $\mathbb{R}^2$ , the same as that which we defined for simple linear regression:

$$R^2 = \frac{\text{TSS} - \text{RSS}}{\text{TSS}} = 1 - \frac{\text{RSS}}{\text{TSS}}.$$

Where.

RSS = Residual Sum of Squares = 
$$\sum_{i=1}^{n} (y_i - \hat{y})^2$$
TSS = Total Sum of Squares = 
$$\sum_{i=1}^{n} (y_i - y)^2$$

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# Multiple Linear Regression: Model Fit—Comparing Models

If Model A has more parameters than Model B, it typically fits better too. So,  $R_A^2 > R_B^2$  by default. How do we compare Models A & B?

One metric: The  $adjusted R^2$  statistic.

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#### Multiple Linear Regression: Model Diagnostics

$$H_0$$
:  $\beta_1=\beta_2=\cdots=\beta_p=0$   
 $H_A$ :  $\beta_i\neq 0$  for at least one  $i>0$ 

To check these hypotheses, we can calculate an F-statistic:  ${}_{1}H_{A,R}^{M}$ 

$$F = \frac{(TSS - RSS)/p}{RSS/(n - p - 1)} = \frac{(TSS - RSS)/p}{\hat{\sigma}}$$

If the model is strong, then we can expect a large F-statistic, and we can reject the null hypothesis. If the model is weak, the F-statistic will be close to 1, and we might fail to reject the null hypothesis. We check the associated p-value for significance of the F statistic.

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### Multiple Linear Regression: Model Fit

$$R^2 = \frac{\text{TSS} - \text{RSS}}{\text{TSS}} = 1 - \frac{\text{RSS}}{\text{TSS}}$$

As before with simple linear regression,  $R^2$  gives us a number between 0 and 1, where a higher  $R^2$  indicates a better model fit.  $R^2$  is the proportion of variance explained by the model.

This indicator can be problematic for multiple linear regression. Adding variables to our model usually improves fit and thus increases the value of  $\mathbb{R}^2$ . To compensate for that, there exists the *adjusted*  $\mathbb{R}^2$  measure.

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## Multiple Linear Regression: Model Fit—Comparing Models

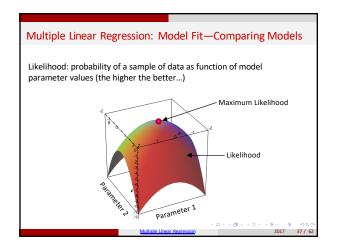
If Model A has more parameters than Model B, it typically fits better too. So,  $R_A^2>R_B^2$  by default. How do we compare Models A & B?

The adjusted  $\mathbb{R}^2$  statistic is

$$R_{\text{adj}}^2 = 1 - \frac{\text{RSS/}(n-p-1)}{\text{TSS/}(n-1)}$$

The *adjusted*  $R^2$  penalizes models for having more variables (a larger value of p) if those additional variables do not reduce the overall residual sum of squares (RSS). So, the *adjusted*  $R^2$  tends to favor more parsimonious models. This can help guard against overfitting.

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Multiple Linear Regression: Model Fit—Comparing Models Another measure of model fit is the Akaike Information Criterion (AIC):  $\mathsf{AIC} = 2p - 2\mathsf{ln}(L)$ where  $p \leftarrow$ number of explanatory variables  $L \leftarrow$  maximum value of likelihood function

Multiple Linear Regression: Model Fit—Comparing Models

 $BIC = p \cdot \ln(n) - 2\ln(L)$  where

Similarly to AIC, there is also the Bayesian Information Criterion (BIC):

 $p \leftarrow \! \mathsf{number} \; \mathsf{of} \; \mathsf{explanatory} \; \mathsf{variables}$ 

For  $n > e^2$  (so for  $n \ge 8$ ), BIC penalizes lack of simplicity more heavily

 $L \leftarrow$ maximum value of likelihood function

MULTICOLLINEARITY IN MULTIPLE

LINEAR REGRESSION

 $n \leftarrow \text{number of data points}$ 

than AIC. Again, lower values are better for BIC.

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Multiple Linear Regression: Model Fit—Comparing Models

 $AIC = 2p - 2\ln(L)$ 

The AIC came out of information theory. When a statistical model is used to represent the process that generated the data, some information will be lost by using the model. AIC estimates the relative amount of information lost by a given model: the less information a model loses, the higher the quality of that model.

It deals with tradeoff between goodness of fit (L) and simplicity (p)—or overfitting and underfitting. So, it rewards models that have a good fit, but penalizes models for having a large number of parameters. Generally, a lower AIC indicates a better model fit.

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Multiple Linear Regression: Model Fit—Comparing Models

Comparing AIC and BIC:

$$AIC = 2p - 2\ln(L)$$

$$\mathsf{BIC} = p \cdot \ln(n) - 2\ln(L)$$

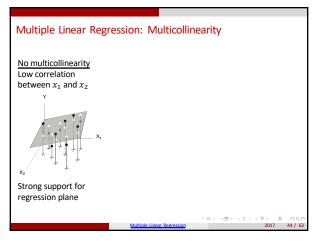
Practically, selecting models based on AIC and on BIC often results in the same selected model. When AIC and BIC support different models, some research suggests that AIC results should be preferred over BIC.

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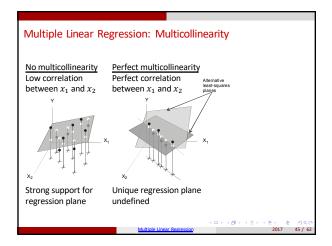
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# Multiple Linear Regression: Multicollinearity

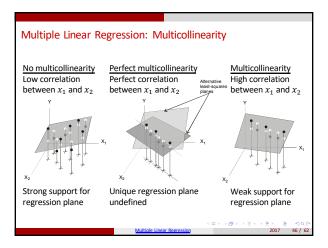
- Multicollinearity: two or more of the predictor variables  $(x_i \& x_j)$  are highly correlated (regressing one on other results in high  $R^{2}$ ).
- This is often bad because it affects our ability to determine which individual predictor variables are important for the overall model. Multicollinearity may "inflate" the variance for each of our coefficient estimates  $\hat{eta}_i$  .
- <u>Perfect multicollinearity</u>: one or more variables can be represented as a combination of one or more other variable
  - Example:  $x_i = cx_i + d$
- In perfect multicollinearity matrix  $\boldsymbol{X}$  is singular,  $(\boldsymbol{X}^T\boldsymbol{X})^{-1}$  does not exist, and multiple linear regression cannot be properly performed.



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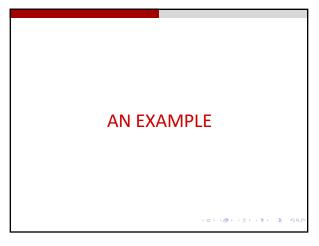
# Multiple Linear Regression: Multicollinearity

Several ways to detect multicollinearity

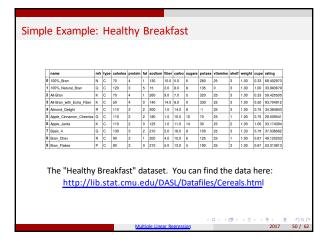
- 1. Adding or removing one predictor variable results in large changes in many regression coefficients
- 2. Group of variables with insignificant regression coefficients, but hypothesis that all variables are zero is rejected (using F-test)
- 3. Insignificant coefficient for specific variable while simple linear regression on that variable results in significant coefficient
- 4. Variance Inflation Factor (VIF) > 5 or 10

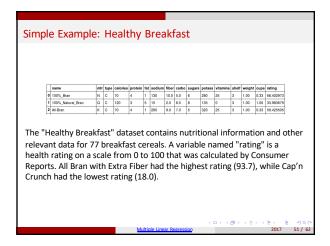
$$\text{VIF}(\beta_i) = \frac{1}{(1-R_i^2)'},$$
 where  $R_i^2$  is  $R^2$  when regressing  $x_i$  on all  $\left\{x_j\right\}_{j \neq i}$ 

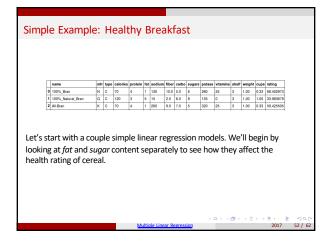
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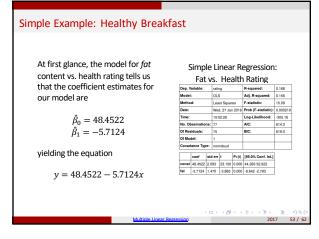


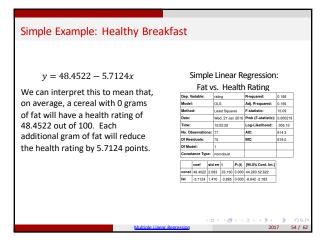


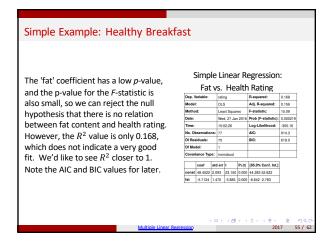


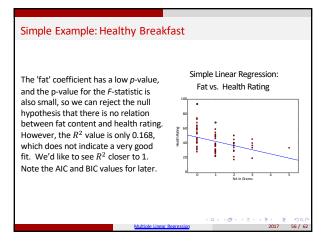






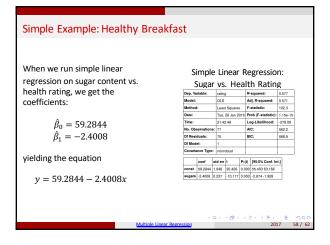






When plotted, we can see that there does appear to be a linear relation between fat content and health rating, but the data is still spread out in the *y*-direction, leading to significant variance in the residuals. This explains the relatively low  $R^2$  value.

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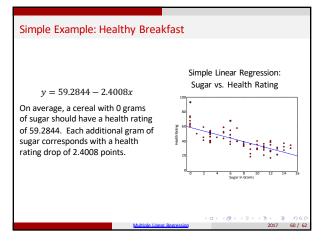
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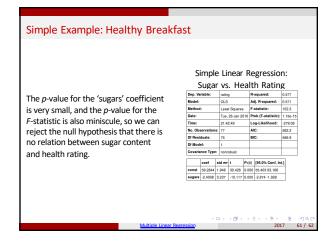
Python code (simple linear regression on sugar)

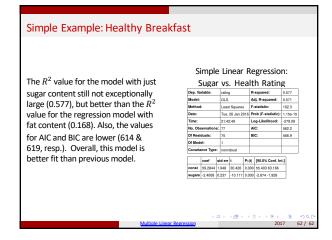
#simple linear regression on sugar
import textended:s api as en
import immory as np
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Simple Example: Healthy Breakfast

A plot of sugar content vs. health rating shows that the points fit closer to the line than when we plotted fat content vs. health rating. This is the reason the  $R^2$  value is higher and the AIC and BIC values are lower.

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Simple Example: Healthy Breakfast

What happens when we start adding more explanatory variables to our model? Will it necessarily improve the fit of the model? And how many explanatory variables is "too many"?

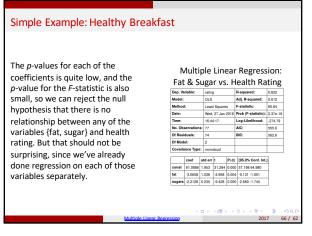
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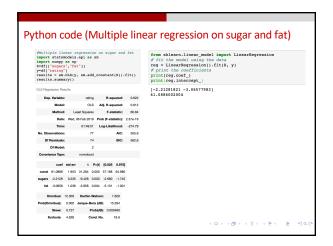
Simple Example: Healthy Breakfast

Let's start with multiple linear regression by considering the two explanatory variables we investigated so far: fat and sugar. We get the following model:  $y = 61.0886 - 3.0658x_1 - 2.2128x_2$ Where  $y \leftarrow \text{health rating}$   $x_1 \leftarrow \text{grams of fat}$   $x_2 \leftarrow \text{grams of sugar}$ Whilide I inour Regression:

Multiple Linear Regression:
Fat & Sugar vs. Health Rating  $\text{line of the sugar of t$ 

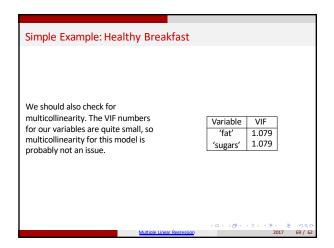
64



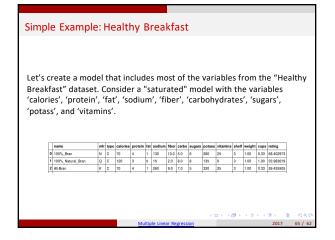


Simple Example: Healthy Breakfast The adjusted  $R^2$  for this model Multiple Linear Regression: (0.612) is only slightly higher than Fat & Sugar vs. Health Rating the adjusted  $R^2$  for the model with only sugar (0.571). Also, the AIC and BIC values are only slightly smaller for this model than for the model with just sugar. So this model, overall, is a slightly better fit than the previous simple linear regression model, but not by a wide margin.

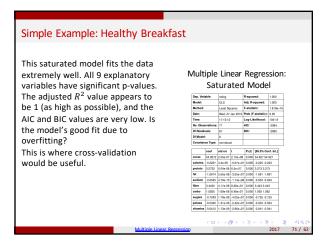
67



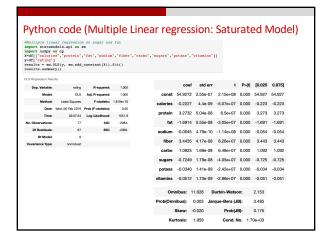
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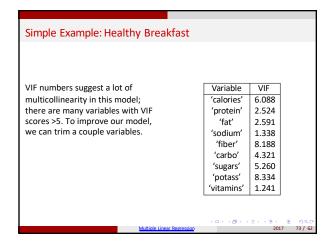


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Simple Example: Healthy Breakfast

For the 'pruned' model, we took the saturated model and removed two variables: calories and potassium.

All the variables in this model have significant p-values. The adjusted R² is 0.979, which is still really good. The AIC and BIC values are lower than what we had for the 2-variable model, but not as low as the full model. Overall, a good fit.

Multiple Linear Regression:

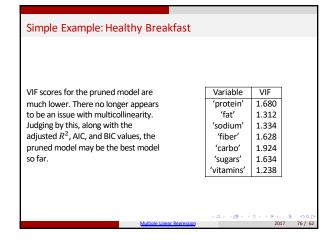
Pruned Model

Multiple Linear Regression:

Multiple Lin

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Conclusion: Simple Linear Regression

What is multiple linear regression? Extension of simple linear regression to multiple variables

The coefficient estimates for multiple linear regression can be found with the equation:  $\hat{\vec{\beta}} = (\vec{x}^T\vec{x})^{-1}\vec{x}^T\vec{y}$ We saw extensions of model diagnostics to multiple variables

Some variables might contribute to model, others not

We learned methods to quantify model fit:  $R^2$ ,  $R^2_{\text{adj}}$ , AIC, BIC

We saw the potential pitfalls of strong correlations between predictor variables—multicollinearity—and how to quantify it

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