Introduction to Linear Modeling

Fundamental Techniques in Data Science with R



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Outline



Regression Problem

Some of the most ubiquitous and useful statistical models are *regression* models.

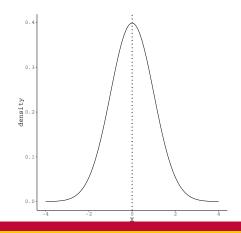
- Regression problems (as opposed to classification problems) involve modeling a quantitative response.
- The regression problem begins with a random outcome variable, Y.
- We hypothesize that the mean of Y is dependent on some set of fixed covariates, X.

Flavors of Probability Distribution

The distributions with which you're probably most familiar imply a constant mean.

- Each observation is expected to have the same value of Y, regardless of their individual characteristics.
- This type of distribution is called "marginal" or "unconditional."

```
Warning: Using 'size' aesthetic for lines was deprecated in ggplot2 3.4.0.
i Please use 'linewidth' instead.
```



Flavors of Probability Distribution

The distributions we consider in regression problems have conditional means.

- The value of Y that we expect for each observation is defined by the observations' individual characteristics.
- This type of distribution is called "conditional."

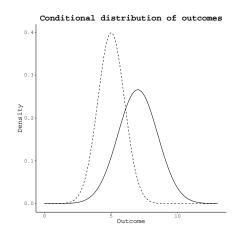
figures/conditional_density_figur

Image retrieved from: http://www.seaturtle.org/mtn/archives/mtn122/mtn122p1.shtml

Flavors of Probability Distribution

Even a simple comparison of means implies a conditional distribution.

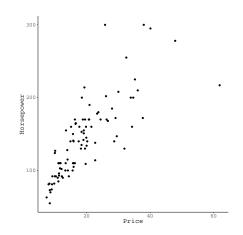
- The solid curve corresponds to outcome values for one group.
- The dashed curve represents outcomes from the other group.



Projecting a Distribution onto the Plane

In practice, we only interact with the X-Y plane of the previous 3D figure.

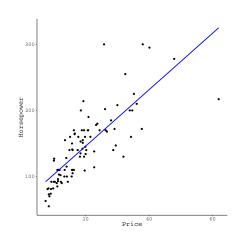
- On the Y-axis, we plot our outcome variable
- The X-axis represents the predictor variable upon which we condition the mean of Y.



Modeling the X-Y Relationship in the Plane

We want to explain the relationship between Y and X by finding the line that traverses the scatterplot as "closely" as possible to each point.

- · This is the "best fit line".
- For any given value of X the corresponding point on the best fit line is our best guess for the value of Y, given the model.



SIMPLE LINEAR REGRESSION



Simple Linear Regression

The best fit line is defined by a simple equation:

$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X$$

The above should look very familiar:

$$Y = mX + b$$
$$= \hat{\beta}_1 X + \hat{\beta}_0$$

 $\hat{\beta}_0$ is the *intercept*.

- The \hat{Y} value when X = 0.
- The expected value of Y when X = 0.

 $\hat{\beta}_1$ is the *slope*.

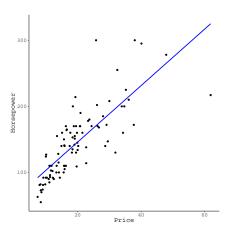
- The change in \hat{Y} for a unit change in X.
- The expected change in Y for a unit change in X.



Thinking about Error

The equation $\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X$ only describes the best fit line.

• It does not fully quantify the relationship between *Y* and *X*.



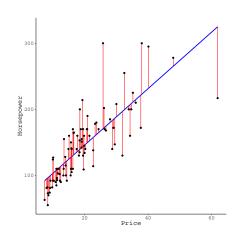
Thinking about Error

The equation $\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X$ only describes the best fit line.

• It does not fully quantify the relationship between *Y* and *X*.

We still need to account for the estimation error.

$$Y = \hat{\beta}_0 + \hat{\beta}_1 X + \hat{\varepsilon}$$



Estimating the Regression Coefficients

The purpose of regression analysis is to use a sample of N observed $\{Y_n, X_n\}$ pairs to find the best fit line defined by $\hat{\beta}_0$ and $\hat{\beta}_1$.

- The most popular method of finding the best fit line involves minimizing the sum of the squared residuals.
- $RSS = \sum_{n=1}^{N} \hat{\varepsilon}_n^2$



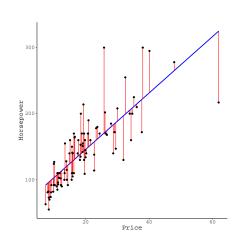
Residuals as the Basis of Estimation

The $\hat{\epsilon}_n$ are defined in terms of deviations between each observed Y_n value and the corresponding \hat{Y}_n .

$$\hat{\varepsilon}_n = Y_n - \hat{Y}_n = Y_n - \left(\hat{\beta}_0 + \hat{\beta}_1 X_n\right)$$

Each $\hat{\epsilon}_n$ is squared before summing to remove negative values.

$$RSS = \sum_{n=1}^{N} \hat{\varepsilon}_n^2 = \sum_{n=1}^{N} \left(Y_n - \hat{Y}_n \right)^2$$
$$= \sum_{n=1}^{N} \left(Y_n - \hat{\beta}_0 - \hat{\beta}_1 X_n \right)^2$$



Least Squares Example

Estimate the least squares coefficients for our example data:

The estimated intercept is $\hat{\beta}_0 = 60.45$.

• A free car is expected to have 60.45 horsepower.

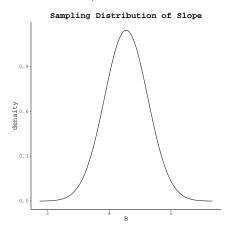
The estimated slope is: $\hat{\beta}_1 = 4.27$.

 For every additional \$1000 in price, a car is expected to gain 4.27 horsepower.

Sampling Distribution

Sampling distribution = Probability distribution of a parameter.

- The population is defined by an infinite sequence of repeated estimations.
 - The sampling distribution quantifies the possible values of the statistic over infinite repeated sampling.
- The area of a region under the curve represents the probability of observing a statistic within the corresponding interval.



Intuition: http://onlinestatbook.com/stat_sim/sampling_dist/

Test Statistics

To "test" a slope coefficient, $\hat{\beta}$, we need a point of comparison.

• The *null-hypothesized* value of the slope, $H_0: \beta = \tilde{\beta}$.

Our hypothesis test is actually a test for the size of the difference: $\hat{eta} - \tilde{eta}$

• We define a *test statistic*, t, to quantify the size of this difference accounting for the precision with which we've estimated $\hat{\beta}$.

We can construct the test statistic for $\hat{\beta}$ as follows:

$$t = \frac{\hat{\beta} - \tilde{\beta}}{SE(\hat{\beta})} \stackrel{\tilde{\beta}=0}{\Longrightarrow} t = \frac{\hat{\beta} - 0}{SE(\hat{\beta})} = \frac{\hat{\beta}}{SE(\hat{\beta})}$$

For the slope in our example, we get a test statistic of:

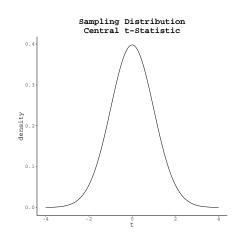
$$t = \frac{\hat{\beta}_1}{\text{SE}(\hat{\beta}_1)} = \frac{4.27}{0.35} = 12.2$$



Sampling Distribution of Test Statistic

The t-statistic also has a sampling distribution.

- Quantifies the possible values we could get if we repeatedly drew samples, of the <u>same size</u>, from the <u>same population</u> and re-computed a t-statistic each time.
- The distribution under the null hypothesis assumes a population wherein $\hat{\beta} = \tilde{\beta}$, and, consequently, t = 0.



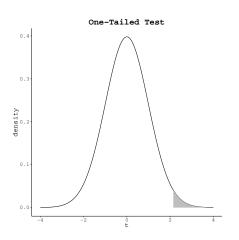
P-Values

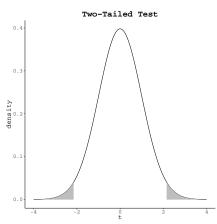
Once we compute our estimated test statistic, \hat{t} , we compare it to the appropriate null-hypothesized sampling distribution.

- By calculating the area in the null distribution that exceeds our estimated test statistic, we can compute the probability of observing the given test statistic, or one more extreme, if the null hypothesis were true.
 - In other words, we can compute the probability of having sampled the data we observed, or more unusual data, from a population wherein there is no true difference between $\hat{\beta}$ and $\tilde{\beta}$.
- This value is the infamous p-value.



P-Values





Interpreting P-Values

Consider the one-tailed test for our estimated test-statistic of $\hat{t}=2.15$ that produces a p-value of p=0.017.

- We <u>cannot</u> say that there is a 0.017 probability that the true mean difference is greater than zero.
- We <u>cannot</u> say that there is a 0.017 probability that the alternative hypothesis is true.
- We <u>cannot</u> say that there is a 0.017 probability that the null hypothesis is false.
- We <u>cannot</u> say that there is a 0.017 probability that the observed result is due to chance alone.
- We <u>cannot</u> say that there is a 0.017 probability of replicating the observed effect in future studies.

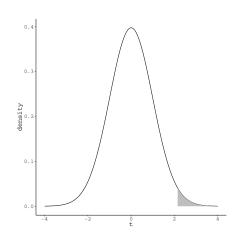
Interpreting P-Values

The p-value tells us $P(t \ge \hat{t}|H_0)$

• What we really want to know is $P(H_0|t \ge \hat{t})$.

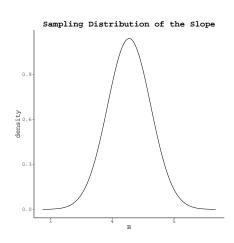
All that we <u>can</u> say is that there is a 0.017 probability of observing a test statistic at least as large as \hat{t} , if the null hypothesis is true.

 Our test uses the same logic as proof by contradiction.



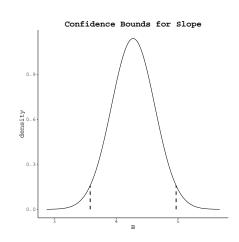
A sampling distribution quantifies the possible values of the statistic.

 We can use this distribution to estimate a plausible range for the population parameter.



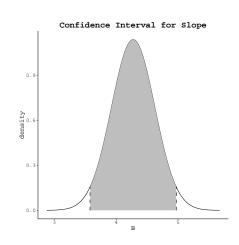
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 - 1. Exclude the tails of the distribution.



A sampling distribution quantifies the possible values of the statistic.

- We can use this distribution to estimate a plausible range for the population parameter.
 - Exclude the tails of the distribution.
 - The remaining values represent a good guess for plausible population values of the parameter.
- This range is known as the confidence interval.



We can construct confidence intervals by:

$$CI = \hat{\beta} \pm t_{crit} \times SE(\hat{\beta})$$

For our example slope, we get a 95% CI of:

$$CI_{95} = 4.27 \pm 1.99 \times 0.35 = [3.57; 4.97]$$

Which suggests that we can be 95% certain that the true value of β_1 is somewhere between 3.57 and 4.97.

• We are 95% certain in the sense that if we repeat this analysis an infinite number of times, 95% of the CIs that we calculate will surround the true value of β_1 .

Say we estimate a regression slope of $\hat{\beta}_1 = 0.5$ with an associated 95% confidence interval of CI = [0.25; 0.75].



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The true value of β_1 is fixed; it's a single quantity.

- β_1 is either in our estimated interval or it is not; there is no uncertainty.
- The probability that β_1 is within our estimated interval is either exactly 1 or exactly 0.

We don't talk about 95% probabilities when interpreting Cls; instead, we talk about 95% confidence.

- If we collected a new sample—of the same size—re-estimated our model, and re-computed the 95% CI for $\hat{\beta}_1$, we would get a different interval.
- Repeating this process an infinite number of times would give us a distribution of Cls.
- 95% of those CIs would surround the true value of β_1 .



Model-Based Prediction

In the social and behavioral sciences, regression modeling is often focused on inference about estimated model parameters.

- The association between the price of a car and its power.
- We model the system and scrutinize $\hat{\beta}_1$ to make inferences about the association between price and power.



Model-Based Prediction

In the social and behavioral sciences, regression modeling is often focused on inference about estimated model parameters.

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- We model the system and scrutinize $\hat{\beta}_1$ to make inferences about the association between price and power.

In data science applications, we're often more interested in predicting the outcome for new observations.

- After we estimate $\hat{\beta}_0$ and $\hat{\beta}_1$, we can plug in new predictor data and get a predicted outcome value for any new case.
- In our example, these predictions represent the projected horsepower ratings of cars with prices given by the new X_{price} values.

Inference vs. Prediction

When doing statistical inference, we focus on how certain variables relate to the outcome.

- Do men have higher job-satisfaction than women?
- Does increased spending on advertising correlate with more sales?
- Is there a relationship between the number of liquor stores in a neighborhood and the amount of crime?



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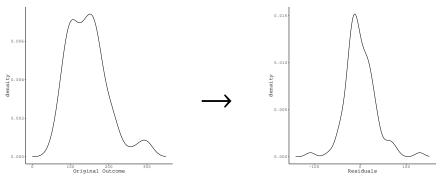
When doing prediction (or classification), we want to build a tool that can accurately guess future values.

- Will it rain tomorrow?
- How much will a company earn from investing in a certain research profile?
- What is a patient's risk of heart disease based on their medical history and test results?

Model Fit

We may also want to know how well our model explains the outcome.

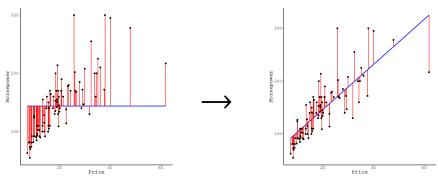
- Our model explains some proportion of the outcome's variability.
- The residual variance $\hat{\sigma}^2 = \text{Var}(\hat{\epsilon})$ will be less than Var(Y).



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Model Fit

We quantify the proportion of the outcome's variance that is explained by our model using the \mathbb{R}^2 statistic:

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

where

$$TSS = \sum_{n=1}^{N} (Y_n - \bar{Y})^2 = Var(Y) \times (N-1)$$

For our example problem, we get:

$$R^2 = 1 - \frac{95573}{252363} \approx 0.62$$

Indicating that car price explains 62% of the variability in horsepower.

Model Fit for Prediction

When assessing predictive performance, we will most often use the *mean squared error* (MSE) as our criterion.

$$MSE = \frac{1}{N} \sum_{n=1}^{N} (Y_n - \hat{Y}_n)^2$$

$$= \frac{1}{N} \sum_{n=1}^{N} (Y_n - \hat{\beta}_0 - \sum_{p=1}^{P} \hat{\beta}_p X_{np})^2$$

$$= \frac{RSS}{N}$$

For our example problem, we get:

$$MSE = \frac{95573}{93} \approx 1027.67$$



Interpreting MSE

The MSE quantifies the average squared prediction error.

Taking the square root improves interpretation.

$$RMSE = \sqrt{MSE}$$

The RMSE estimates the magnitude of the expected prediction error.

• For our example problem, we get:

RMSE =
$$\sqrt{\frac{95573}{93}} \approx 32.06$$

 When using price as the only predictor of horsepower, we expect prediction errors with magnitudes of 32.06 horsepower.

Information Criteria

We can use *information criteria* to quickly compare *non-nested* models while accounting for model complexity.

Akaike's Information Criterion (AIC)

$$AIC = 2K - 2\hat{\ell}(\theta|X)$$

Bayesian Information Criterion (BIC)

$$BIC = K \ln(N) - 2\hat{\ell}(\theta|X)$$



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Information criteria balance two competing forces.

- The optimized loglikelihood quantifies fit to the data.
- The penalty term corrects for model complexity.



Information Criteria

For our example, we get the following estimates of AIC and BIC:

$$AIC = 2(3) - 2(-454.44)$$

$$= 914.88$$

$$BIC = 3\ln(93) - 2(-454.44)$$

$$= 922.48$$

To compute the AIC/BIC from a fitted lm() object in R:

```
AIC(out1)
[1] 914.8821
BIC(out1)
[1] 922.4799
```

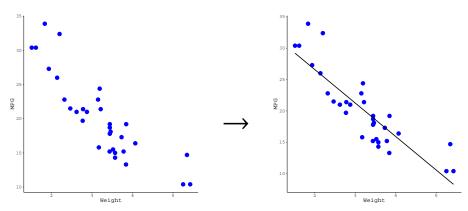
MULTIPLE LINEAR REGRESSION



Graphical Representations

A regression of two variables can be represented on a 2D scatterplot.

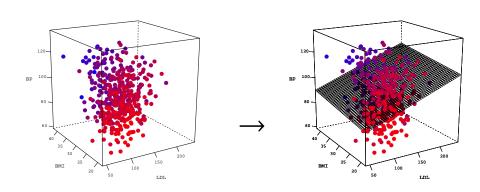
• Simple linear regression implies a 1D line in 2D space.



Graphical Representations

Adding an additional predictor leads to a 3D point cloud.

• A regression model with two IVs implies a 2D plane in 3D space.



Partial Effects

In MLR, we want to examine the *partial effects* of the predictors.

 What is the effect of a predictor after controlling for some other set of variables?

This approach is crucial to controlling confounds and adequately modeling real-world phenomena.



```
## Read in the 'diabetes' dataset:
dDat <- readRDS("../data/diabetes.rds")

## Simple regression with which we're familiar:
out1 <- lm(bp ~ age, data = dDat)</pre>
```

Asking: What is the effect of age on average blood pressure?



```
partSummary(out1, -1)
Residuals:
   Min 1Q Median 3Q Max
-31.188 -8.897 -1.209 8.612 39.952
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept) 77.47605 2.38132 32.535 < 2e-16
age 0.35391 0.04739 7.469 4.39e-13
Residual standard error: 13.04 on 440 degrees of freedom
Multiple R-squared: 0.1125, Adjusted R-squared: 0.1105
F-statistic: 55.78 on 1 and 440 DF, p-value: 4.393e-13
```

```
## Add in another predictor:
out2 <- lm(bp ~ age + bmi, data = dDat)</pre>
```

Asking: What is the effect of BMI on average blood pressure, after controlling for age?

• We're partialing age out of the effect of BMI on blood pressure.



```
partSummary(out2, -1)
Residuals:
   Min 1Q Median 3Q Max
-29.287 -8.198 -0.178 8.413 41.026
Coefficients:
          Estimate Std. Error t value Pr(>|t|)
(Intercept) 52.24654 3.83168 13.635 < 2e-16
       0.28651 0.04504 6.362 5.02e-10
age
bmi 1.08053 0.13363 8.086 6.06e-15
Residual standard error: 12.18 on 439 degrees of freedom
Multiple R-squared: 0.2276, Adjusted R-squared: 0.224
F-statistic: 64.66 on 2 and 439 DF, p-value: < 2.2e-16
```

Interpretation

- The expected average blood pressure for an unborn patient with a negligible extent is 52.25.
- For each year older, average blood pressure is expected to increase by 0.29 points, after controlling for BMI.
- For each additional point of BMI, average blood pressure is expected to increase by 1.08 points, after controlling for age.

Multiple R²

How much variation in blood pressure is explained by the two models?

• Check the R² values.

```
## Extract R^2 values:
r2.1 <- summary(out1)$r.squared
r2.2 <- summary(out2)$r.squared
r2.1
[1] 0.1125117
r2.2
[1] 0.2275606</pre>
```

F-Statistic

How do we know if the R^2 values are significantly greater than zero?

• We use the F-statistic to test $H_0: R^2 = 0$ vs. $H_1: R^2 > 0$.

```
f1 <- summary(out1)$fstatistic
f1

   value   numdf   dendf
55.78116   1.00000 440.00000

pf(q = f1[1], df1 = f1[2], df2 = f1[3], lower.tail = FALSE)
   value
4.392569e-13</pre>
```

F-Statistic

```
f2 <- summary(out2)$fstatistic
f2

value   numdf   dendf
64.6647   2.0000   439.0000

pf(f2[1], f2[2], f2[3], lower.tail = FALSE)

   value
2.433518e-25</pre>
```

Comparing Models

How do we quantify the additional variation explained by BMI, above and beyond age?

• Compute the ΔR^2

```
## Compute change in R^2:
r2.2 - r2.1
[1] 0.115049
```

Significance Testing

How do we know if ΔR^2 represents a significantly greater degree of explained variation?

• Use an F-test for H_0 : $\Delta R^2 = 0$ vs. H_1 : $\Delta R^2 > 0$

Comparing Models

We can also compare models based on their prediction errors.

• For OLS regression, we usually compare MSE values.

```
mse1 <- MSE(y_pred = predict(out1), y_true = dDat$bp)
mse2 <- MSE(y_pred = predict(out2), y_true = dDat$bp)
mse1
[1] 169.3963
mse2
[1] 147.4367</pre>
```

In this case, the MSE for the model with *BMI* included is smaller.

• We should prefer the the larger model.

Comparing Models

Finally, we can compare models based on information criteria.

```
AIC(out1, out2)

df AIC
out1 3 3528.792
out2 4 3469.424

BIC(out1, out2)

df BIC
out1 3 3541.066
out2 4 3485.789
```

In this case, both the AIC and the BIC for the model with BMI included are smaller.

• We should prefer the the larger model.

CATEGORICAL PREDICTORS

Categorical Predictors

Most of the predictors we've considered thus far have been *quantitative*.

- Continuous variables that can take any real value in their range
- Interval or Ratio scaling

We often want to include grouping factors as predictors.

- These variables are qualitative.
 - Their values are simply labels.
 - There is no ordering of the categories.
 - Nominal scaling

How to Model Categorical Predictors

We need to be careful when we include categorical predictors into a regression model.

• The variables need to be coded before entering the model

Consider the following indicator of major:

$$X_{maj} = \{1 = Law, 2 = Economics, 3 = Data Science\}$$

 What would happen if we naïvely used this variable to predict program satisfaction?

How to Model Categorical Predictors

How to Model Categorical Predictors

```
partSummary(out1, -1)
Residuals:
  Min 10 Median 30 Max
-1.303 -0.313 -0.113 0.342 1.342
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept) -0.33200 0.12060 -2.753 0.00664
majN 2.04500 0.05582 36.632 < 2e-16
Residual standard error: 0.5582 on 148 degrees of freedom
Multiple R-squared: 0.9007, Adjusted R-squared: 0.9
F-statistic: 1342 on 1 and 148 DF, p-value: < 2.2e-16
```

Dummy Coding

The most common way to code categorical predictors is *dummy coding*.

- A G-level factor must be converted into a set of G-1 dummy codes.
- Each code is a variable on the dataset that equals 1 for observations corresponding to the code's group and equals 0, otherwise.
- The group without a code is called the reference group.



Example Dummy Code

Let's look at the simple example of coding biological sex:

	sex	male
1	male	1
2	male	1
3	female	0
4	male	1
5	female	0
6	male	1
7	male	1
8	female	0
9	male	1
10	female	0



Example Dummy Codes

Now, a slightly more complex example:

	drink	juice	tea
1	coffee	0	0
2	tea	0	1
3	coffee	0	0
4	coffee	0	0
5	coffee	0	0
6	coffee	0	0
7	juice	1	0
8	coffee	0	0
9	coffee	0	0
10	coffee	0	0



Using Dummy Codes

To use the dummy codes, we simply include the G-1 codes as G-1 predictor variables in our regression model.

$$Y = \beta_0 + \beta_1 X_{male} + \varepsilon$$

$$Y = \beta_0 + \beta_1 X_{juice} + \beta_2 X_{tea} + \varepsilon$$

- The intercept corresponds to the mean of Y for the reference group.
- Each slope represents the difference between the mean of Y in the coded group and the mean of Y in the reference group.

First, an example with a single, binary dummy code:

```
## Read in some data:
cDat <- readRDS("../data/cars_data.rds")

## Fit and summarize the model:
out2 <- lm(price ~ mtOpt, data = cDat)</pre>
```

Interpretations

- The average price of a car without the option for a manual transmission is $\hat{\beta}_0 = 23.84$ thousand dollars.
- The average difference in price between cars that have manual transmissions as an option and those that do not is $\hat{\beta}_1 = -6.6$ thousand dollars.



Fit a more complex model:

```
out3 <- lm(price ~ front + rear, data = cDat)
partSummary(out3, -1)
Residuals:
   Min 10 Median
                          30
                                Max
-14.050 -6.250 -1.236 3.264 32.950
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept) 17.63000 2.76119 6.385 7.33e-09
front.
       -0.09418 2.96008 -0.032 0.97469
rear 11.32000 3.51984 3.216 0.00181
Residual standard error: 8.732 on 90 degrees of freedom
Multiple R-squared: 0.2006, Adjusted R-squared: 0.1829
F-statistic: 11.29 on 2 and 90 DF, p-value: 4.202e-05
```

Interpretations

- The average price of a four-wheel-drive car is $\hat{\beta}_0 = 17.63$ thousand dollars.
- The average difference in price between front-wheel-drive cars and four-wheel-drive cars is $\hat{\beta}_1 = -0.09$ thousand dollars.
- The average difference in price between rear-wheel-drive cars and four-wheel-drive cars is $\hat{\beta}_2 = 11.32$ thousand dollars.



Include two sets of dummy codes:

Interpretations

- The average price of a four-wheel-drive car that does not have a manual transmission option is $\hat{\beta}_0 = 21.72$ thousand dollars.
- After controlling for drive type, the average difference in price between cars that have manual transmissions as an option and those that do not is $\hat{\beta}_1 = -5.84$ thousand dollars.
- After controlling for transmission options, the average difference in price between front-wheel-drive cars and four-wheel-drive cars is $\hat{\beta}_2 = -0.26$ thousand dollars.
- After controlling for transmission options, the average difference in price between rear-wheel-drive cars and four-wheel-drive cars is $\hat{\beta}_3 = 10.52$ thousand dollars.

For variables with only two levels, we can test the overall factor's significance by evaluating the significance of a single dummy code.

For variables with more than two levels, we need to simultaneously evaluate the significance of each of the variable's dummy codes.

```
summary(out4)$r.squared - summary(out2)$r.squared
[1] 0.1767569
anova(out2, out4)
Analysis of Variance Table
Model 1: price ~ mtOpt
Model 2: price ~ mtOpt + front + rear
 Res.Df RSS Df Sum of Sq F Pr(>F)
 91 7668.9
 89 6151.6 2 1517.3 10.976 5.488e-05 ***
Signif. codes:
0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

For models with a single nominal factor is the only predictor, we use the omnibus F-test.

MODERATION



Moderation

So far we've been discussing additive models.

- Additive models allow us to examine the partial effects of several predictors on some outcome.
 - The effect of one predictor does not change based on the values of other predictors.

Now, we'll discuss moderation.

- Moderation allows us to ask when one variable, X, affects another variable, Y.
 - We're considering the conditional effects of X on Y given certain levels of a third variable Z.

In additive MLR, we might have the following equation:

$$Y = \beta_0 + \beta_1 X + \beta_2 Z + \varepsilon$$

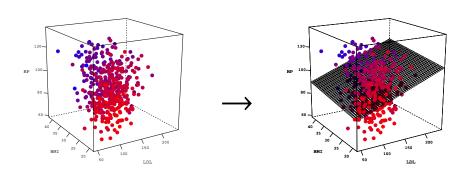
This additive equation assumes that X and Z are independent predictors of Y.

When X and Z are independent predictors, the following are true:

- X and Z can be correlated.
- β_1 and β_2 are *partial* regression coefficients.
- The effect of X on Y is the same at all levels of Z, and the effect of Z on Y is the same at all levels of X.

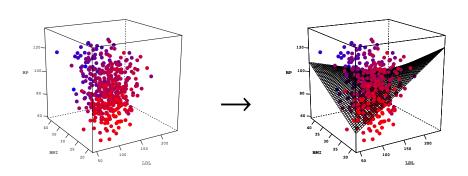
Additive Regression

The effect of *X* on *Y* is the same at **all levels** of *Z*.



Moderated Regression

The effect of *X* on *Y* varies **as a function** of *Z*.



The following derivation is adapted from hayes:2017.

- When testing moderation, we hypothesize that the effect of X on Y varies as a function of Z.
- We can represent this concept with the following equation:

$$Y = \beta_0 + f(Z)X + \beta_2 Z + \varepsilon \tag{1}$$



The following derivation is adapted from hayes:2017.

- When testing moderation, we hypothesize that the effect of X on Y varies as a function of Z.
- We can represent this concept with the following equation:

$$Y = \beta_0 + f(Z)X + \beta_2 Z + \varepsilon \tag{1}$$

• If we assume that *Z* linearly (and deterministically) affects the relationship between *X* and *Y*, then we can take:

$$f(Z) = \beta_1 + \beta_3 Z \tag{2}$$

• Substituting Equation ?? into Equation ?? leads to:

$$Y=\beta_0+(\beta_1+\beta_3Z)X+\beta_2Z+\varepsilon$$



Substituting Equation ?? into Equation ?? leads to:

$$Y = \beta_0 + (\beta_1 + \beta_3 Z)X + \beta_2 Z + \varepsilon$$

• Which, after distributing *X* and reordering terms, becomes:

$$Y = \beta_0 + \beta_1 X + \beta_2 Z + \beta_3 XZ + \varepsilon$$



Testing Moderation

Now, we have an estimable regression model that quantifies the linear moderation we hypothesized.

$$Y = \beta_0 + \beta_1 X + \beta_2 Z + \beta_3 X Z + \varepsilon$$

- To test for significant moderation, we simply need to test the significance of the interaction term, XZ.
 - Check if $\hat{\beta}_3$ is significantly different from zero.



Interpretation

Given the following equation:

$$Y = \hat{\beta}_0 + \hat{\beta}_1 X + \hat{\beta}_2 Z + \hat{\beta}_3 X Z + \hat{\varepsilon}$$

- $\hat{\beta}_3$ quantifies the effect of Z on the focal effect (the $X \to Y$ effect).
 - For a unit change in Z, $\hat{\beta}_3$ is the expected change in the effect of X on Y.
- $\hat{\beta}_1$ and $\hat{\beta}_2$ are conditional effects.
 - Interpreted where the other predictor is zero.
 - For a unit change in X, $\hat{\beta}_1$ is the expected change in Y, when Z = 0.
 - For a unit change in Z, $\hat{\beta}_2$ is the expected change in Y, when X = 0.

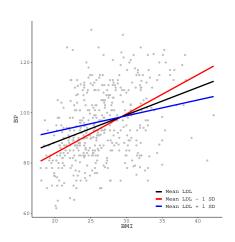
Still looking at the diabetes dataset.

- We suspect that patients' BMIs are predictive of their average blood pressure.
- We further suspect that this effect may be differentially expressed depending on the patients' LDL levels.



Visualizing the Interaction

We can get a better idea of the patterns of moderation by plotting the focal effect at conditional values of the moderator.



Categorical Moderators

Categorical moderators encode *group-specific* effects.

• E.g., if we include *sex* as a moderator, we are modeling separate focal effects for males and females.

Given a set of codes representing our moderator, we specify the interactions as before:

$$Y_{total} = \beta_0 + \beta_1 X_{inten} + \beta_2 Z_{male} + \beta_3 X_{inten} Z_{male} + \varepsilon$$

$$\begin{aligned} Y_{total} &= \beta_0 + \beta_1 X_{inten} + \beta_2 Z_{lo} + \beta_3 Z_{mid} + \beta_4 Z_{hi} \\ &+ \beta_5 X_{inten} Z_{lo} + \beta_6 X_{inten} Z_{mid} + \beta_7 X_{inten} Z_{hi} + \varepsilon \end{aligned}$$



```
## I.oa.d. d.a.t.a.:
socSup <- readRDS(paste0(dataDir, "social_support.rds"))</pre>
Error in pasteO(dataDir, "social_support.rds"): object 'dataDir' not found
## Focal effect:
out3 <- lm(bdi ~ tanSat, data = socSup)
Error in is.data.frame(data): object 'socSup' not found
partSummary(out3, -c(1, 2))
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept) 17.63000 2.76119 6.385 7.33e-09
front -0.09418 2.96008 -0.032 0.97469
rear 11.32000 3.51984 3.216 0.00181
Residual standard error: 8.732 on 90 degrees of freedom
Multiple R-squared: 0.2006, Adjusted R-squared: 0.1829
F-statistic: 11.29 on 2 and 90 DF, p-value: 4.202e-05
```

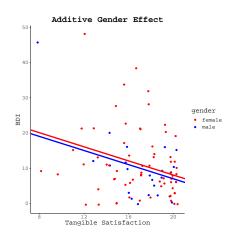
```
## Estimate the interaction:
out4 <- lm(bdi ~ tanSat * sex. data = socSup)
Error in is.data.frame(data): object 'socSup' not found
partSummary(out4, -c(1, 2))
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept) 21.7187 2.9222 7.432 6.25e-11
     -5.8410 1.8223 -3.205 0.00187
mt0pt
front -0.2598 2.8189 -0.092 0.92677
rear 10.5169 3.3608 3.129 0.00237
Residual standard error: 8.314 on 89 degrees of freedom
Multiple R-squared: 0.2834, Adjusted R-squared: 0.2592
F-statistic: 11.73 on 3 and 89 DF, p-value: 1.51e-06
```

Visualizing Categorical Moderation

$$\hat{Y}_{BDI} = 21.72 - 5.84X_{tsat} + -0.26Z_{male} \\ 10.52X_{tsat}Z_{male}$$

```
Error in relevel(socSup$sex, ref =
"male"): object 'socSup' not found
Error in is.data.frame(data): object
'socSup' not found
Error in coef(out5): object 'out5'
not found
```

$\hat{Y}_{BDI} = 28.10 - 1.00X_{tsat} - 1.05Z_{male}$



Let's walk through an example of the model-building process.

- We'll take $Y_{bp} = \beta_0 + \beta_1 X_{age.30} + \varepsilon$ as our baseline model.
- Next, we simultaneously add predictors of LDL and HDL cholesterol.

```
diabetes <- readRDS("../data/diabetes.rds")
## Center predictor variables:
diabetes <- mutate(diabetes,
                   1d1100 = 1d1 - 100.
                   hd160 = hd1 - 60,
                   age30 = age - 30)
Error in mutate(diabetes, ldl100 = ldl - 100, hdl60 = hdl - 60, age30 = age
-: could not find function "mutate"
## Baseline model:
out1 <- lm(bp ~ age30, data = diabetes)
Error in eval(predvars, data, env): object 'age30' not found
## Simultaneously add two predictors:
out2 \leftarrow lm(bp ~ age30 + ld1100 + hd160, data = diabetes)
 88 of 1
```

```
partSummary(out1, -1)
Residuals:
   Min 1Q Median
                          30
                                Max
-30.536 -8.508 -0.863 9.099 39.938
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept) 59.26577 3.91281 15.147 < 2e-16
        1.16567 0.14156 8.235 2.08e-15
bmi
ldl 0.04016 0.02056 1.953 0.0515
Residual standard error: 12.68 on 439 degrees of freedom
Multiple R-squared: 0.1636, Adjusted R-squared: 0.1598
F-statistic: 42.94 on 2 and 439 DF, p-value: < 2.2e-16
```

```
partSummary(out2, -1)
Residuals:
   Min 1Q Median
                          3Q
                                 Max
-32.877 -8.427 -0.966 8.931 39.368
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept) 14.480616 14.291677 1.013 0.311514
bmi
           2.867825 0.541312 5.298 1.86e-07
ldl 0.448771 0.127160 3.529 0.000461
bmi:ldl -0.015352 0.004716 -3.255 0.001221
Residual standard error: 12.54 on 438 degrees of freedom
Multiple R-squared: 0.1834, Adjusted R-squared: 0.1778
F-statistic: 32.78 on 3 and 438 DF, p-value: < 2.2e-16
```

Interpretations

- The expected average blood pressure for a 30 year old patient with LDL = 100 and HDL = 60 is 14.48.
- For each additional year older, average blood pressure is expected to increase by NA, after controlling for LDL and HDL levels.
- For each additional unit of LDL level, average blood pressure is expected to increase by NA, after controlling for age and HDL.
- For each additional unit of HDL level, average blood pressure is expected to decrease by NA, after controlling for age and LDL.

Model Comparison

```
## Compute change in R^2:
summary(out2)$r.squared - summary(out1)$r.squared
[1] 0.01975773
## Significance test for change in R^2:
anova(out1, out2)
Analysis of Variance Table
Model 1: bp ~ bmi + ldl
Model 2: bp ~ bmi * ldl
 Res.Df RSS Df Sum of Sq F Pr(>F)
 439 70562
 438 68895 1 1666.9 10.597 0.001221 **
Signif. codes:
0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Model Comparison

```
(mse1 <- MSE(y_pred = predict(out1), y_true = diabetes$bp))</pre>
[1] 159.6421
(mse2 <- MSE(y_pred = predict(out2), y_true = diabetes$bp))</pre>
[1] 155.8709
AIC(out1, out2)
    df
        AIC
out.1 4 3504.579
out2 5 3496.012
BIC(out1, out2)
     df BTC
out1 4 3520,944
out2 5 3516,469
```

Interpretations

- Age, LDL, and HDL explain a combined 18.3% of the variation in blood pressure.
 - This proportion of variation explained is significantly greater than zero.
- Adding LDL and HDL produces a model that explains 2% more variation in blood pressure than a model with age as the only predictor.
 - This increase in variation explained is significantly greater than zero.
- Adding LDL and HDL produces a model with lower prediction error (i.e., MSE = 155.87 vs. MSE = 159.64).
- Both the AIC and the BIC also suggest that adding LDL and HDL produces a better model.

Continue Building the Model

So far we've established that age, LDL, and HDL are all significant predictors of average blood pressure.

 We've also established that adding LDL and HDL, together, explain significantly more variation than age alone.

Next, we'll add BMI to see what additional explanatory role it can play above and beyond age and cholesterol.

```
## Center BMI:
diabetes <- mutate(diabetes, bmi25 = bmi - 25)

Error in mutate(diabetes, bmi25 = bmi - 25): could not find function
"mutate"

## Now, add bmi:
out3 <- lm(bp ~ age30 + ldl100 + hdl60 + bmi25, data = diabetes)

Error in eval(predvars, data, env): object 'age30' not found</pre>
```

```
partSummary(out3, -1)
Residuals:
   Min 1Q Median
                          30
                                Max
-14.050 -6.250 -1.236 3.264 32.950
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept) 17.63000 2.76119 6.385 7.33e-09
front.
       -0.09418 2.96008 -0.032 0.97469
rear 11.32000 3.51984 3.216 0.00181
Residual standard error: 8.732 on 90 degrees of freedom
Multiple R-squared: 0.2006, Adjusted R-squared: 0.1829
F-statistic: 11.29 on 2 and 90 DF, p-value: 4.202e-05
```

Interpretations

BMI seems to have a pretty strong effect on average blood pressure, after controlling for age and cholesterol levels.

- After controlling for BMI, cholesterol levels no longer seem to be important predictors.
- Let's take a look at what happens to the cholesterol effects when we add BMI:

	LDL	HDL
Without BMI	0.449	-0.015
With BMI	11.320	11.320



How much additional variability in blood pressure is explained by BMI above and beyond age and cholesterol levels?

```
r2.3 <- summary(out3)$r.squared
r2.3 - r2.2
[1] 0.01726571</pre>
```



Is the additional 1.73% variation explained a significant increase?

```
anova(out2, out3)
Warning in anova.lmlist(object, ...): models with response '"price"'
removed because response differs from model 1
Analysis of Variance Table
Response: bp
          Df Sum Sq Mean Sq F value Pr(>F)
bmi
        1 13190 13190.5 83.8586 < 2.2e-16 ***
ldl 1 613 612.9 3.8968 0.049005 *
bmi:ldl 1 1667 1666.9 10.5971 0.001221 **
Residuals 438 68895 157.3
Signif. codes:
0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
mse3 <- MSE(y_pred = predict(out3), y_true = diabetes$bp)</pre>
Warning in y_true - y_pred: longer object length is not a multiple of
shorter object length
mse2
[1] 155.8709
mse3
[1] 5854.724
AIC(out2, out3)
Warning in AIC.default(out2, out3): models are not all fitted to the same
number of observations
     df
        AIC
out 2 5 3496,0121
out.3 4 671.9264
BIC(out2, out3)
 100 of 1
```

Model Modification

Maybe cholesterol levels are not important features once we've accounted for BMI.

• Let's try a model including BMI but excluding cholesterol levels.

```
## Take out the cholesterol variables:
out4 <- lm(bp ~ age30 + bmi25, data = diabetes)
Error in eval(predvars, data, env): object 'age30' not found</pre>
```



Model-Building Example

```
partSummary(out4, -1)
Residuals:
   Min
         1Q Median
                                Max
                          30
-17.336 -5.559 -2.218 4.082 29.664
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept) 21.7187
                      2.9222 7.432 6.25e-11
mt0pt
     -5.8410 1.8223 -3.205 0.00187
front
         -0.2598
                      2.8189 -0.092 0.92677
       10.5169
                      3.3608 3.129 0.00237
rear
Residual standard error: 8.314 on 89 degrees of freedom
Multiple R-squared: 0.2834, Adjusted R-squared: 0.2592
F-statistic: 11.73 on 3 and 89 DF, p-value: 1.51e-06
```

How much explained variation did we loose by removing the LDL and HDL variables?

```
r2.4 <- summary(out4)$r.squared
r2.3 - r2.4
[1] -0.08272339</pre>
```



Is this -8.27% loss in explained variance significant?

```
anova(out4, out3)

Analysis of Variance Table

Model 1: price ~ mtOpt + front + rear

Model 2: price ~ front + rear

Res.Df RSS Df Sum of Sq F Pr(>F)

1 89 6151.6

2 90 6861.7 -1 -710.1 10.274 0.001874 **
---

Signif. codes:
0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
mse4 <- MSE(y_pred = predict(out4), y_true = diabetes$bp)</pre>
Warning in y_true - y_pred: longer object length is not a multiple of
shorter object length
mse3
[1] 5854.724
mse4
[1] 5851.933
AIC(out3, out4)
    df
        AIC
out3 4 671,9264
out.4 5 663,7668
BIC(out3, out4)
     df
         BIC
out3 4 682.0568
out4 5 676.4208
```

MODEL-BASED PREDICTION



Prediction

So far, we've focused mostly on inferences about the estimated regression coefficients.

Asking questions about how X is related to Y.

We can also use linear regression for prediction.

• Given a new observation, X_m , what outcome value, \hat{Y}_m , does our model attribute to the mth observation?

Prediction

Train a model to predict psychological well-being from diet-related and exercise-related features.

 Plug-in new feature values corresponding to an experimental wellness program to see the expected well-being for a hypothetical patient treated with the new program.

Predict future gasoline prices based on geo-political events in oil-producing countries.

 If conflict escalates in the Middle East, adjust the appropriate features and project likely changes in gasoline prices.

Prediction Example

To fix ideas, let's reconsider the *diabetes* data and the following model:

$$Y_{LDL} = \beta_0 + \beta_1 X_{BP} + \beta_2 X_{qluc} + \beta_3 X_{BMI} + \varepsilon$$

Training this model on the first N=400 patients' data produces the following fitted model:

$$\hat{Y}_{LDL} = 22.135 + 0.089 X_{BP} + 0.498 X_{gluc} + 1.48 X_{BMI}$$



Prediction Example

To fix ideas, let's reconsider the *diabetes* data and the following model:

$$Y_{LDL} = \beta_0 + \beta_1 X_{BP} + \beta_2 X_{qluc} + \beta_3 X_{BMI} + \varepsilon$$

Training this model on the first N=400 patients' data produces the following fitted model:

$$\hat{Y}_{LDL} = 22.135 + 0.089 X_{BP} + 0.498 X_{gluc} + 1.48 X_{BMI}$$

Suppose a new patient presents with BP = 121, gluc = 89, and BMI = 30.6. We can predict their LDL score by:

$$\hat{Y}_{LDL} = 22.135 + 0.089(121) + 0.498(89) + 1.48(30.6)$$

= 122.463

Interval Estimates for Prediction

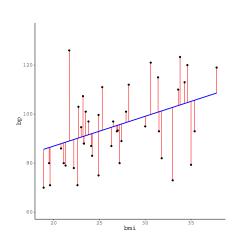
To quantify uncertainty in our predictions, we want to use an appropriate interval estimate.

- Two flavors of interval are applicable to predictions:
 - 1. Confidence intervals for \hat{Y}_m
 - 2. Prediction intervals for a specific observation, Y_m
- The CI for \hat{Y}_m gives a likely range (in the sense of coverage probability and "confidence") for the mth value of the true conditional mean.
 - CIs only account for uncertainty in the estimated regression coefficients, $\{\hat{\beta}_0, \hat{\beta}_p\}$.
- The prediction interval for Y_m gives a likely range (in the same sense as CIs) for the mth outcome value.
 - Prediction intervals also account for the regression errors, ε .

Confidence vs. Prediction Intervals

Let's visualize the predictions from a simple model:

$$Y_{BP} = \hat{\beta}_0 + \hat{\beta}_1 X_{BMI} + \hat{\varepsilon}$$

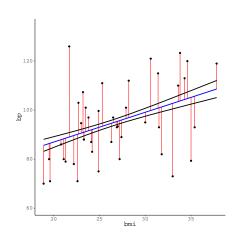


Confidence vs. Prediction Intervals

Let's visualize the predictions from a simple model:

$$Y_{BP} = \hat{\beta}_0 + \hat{\beta}_1 X_{BMI} + \hat{\varepsilon}$$

- Cls for \hat{Y} ignore the errors, ε .
 - They only care about the best-fit line, $\beta_0 + \beta_1 X_{BMI}$.

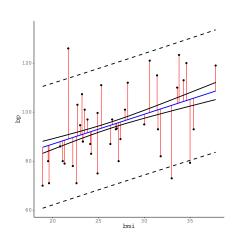


Confidence vs. Prediction Intervals

Let's visualize the predictions from a simple model:

$$Y_{BP} = \hat{\beta}_0 + \hat{\beta}_1 X_{BMI} + \hat{\epsilon}$$

- Cls for \hat{Y} ignore the errors, ε .
 - They only care about the best-fit line, $\beta_0 + \beta_1 X_{BMI}$.
- Prediction intervals are wider than Cls.
 - They account for the additional uncertainty contributed by ε .



Interval Estimates Example

Going back to our hypothetical "new" patient, we get the following 95% interval estimates:

95%
$$CI_{\hat{Y}} = [115.6; 129.33]$$

95% $PI = [66.56; 178.37]$

- We can be 95% confident that the average LDL of patients with Glucose = 89, BP = 121, and BMI = 30.6 will be somewhere between 115.6 and 129.33.
- We can be 95% confident that the *LDL* of a specific patient with *Glucose* = 89, *BP* = 121, and *BMI* = 30.6 will be somewhere between 66.56 and 178.37.