

# Introduction to Linear Modeling

## Fundamental Techniques in Data Science with R



**Utrecht  
University**

Kyle M. Lang

Department of Methodology & Statistics  
Utrecht University

# Outline

---

## Simple Linear Regression

Model Fit

## Multiple Linear Regression

Model Comparison

## Categorical Predictors

Significance Testing for Dummy Codes

## Model-Based Prediction

Interval Estimates for Prediction

## Moderation

Categorical Moderators



# Visualizations of Simple Linear Regression

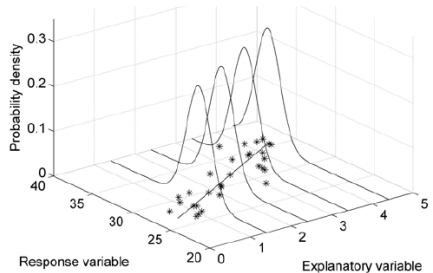
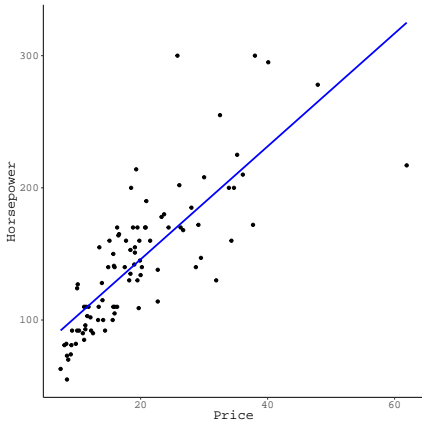


Image retrieved from:  
<http://www.seaturtle.org/mtn/archives/mtn122/mtn122p1.shtml>

# Simple Linear Regression Equation

---

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:

$$\begin{aligned} Y &= mX + b \\ &= \hat{\beta}_1 X + \hat{\beta}_0 \end{aligned}$$

$\hat{\beta}_0$  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  $X$ .

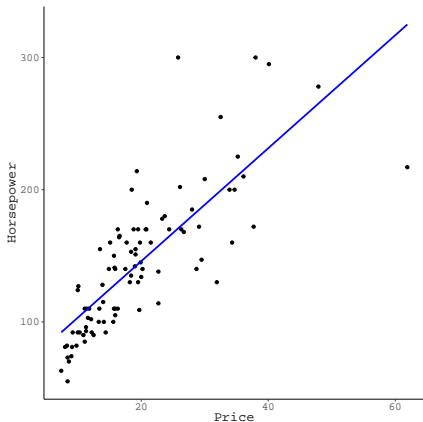


# Thinking about Error

---

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  $X$ .



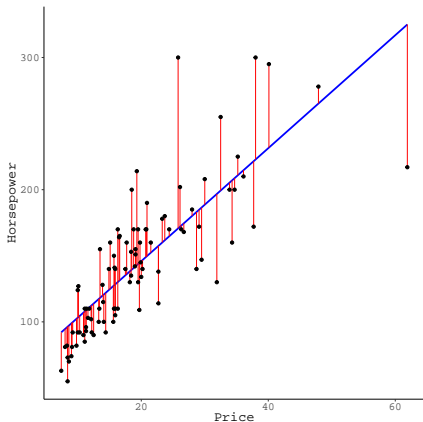
# Thinking about Error

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.
- $RSS = \sum_{n=1}^N \hat{\epsilon}_n^2$



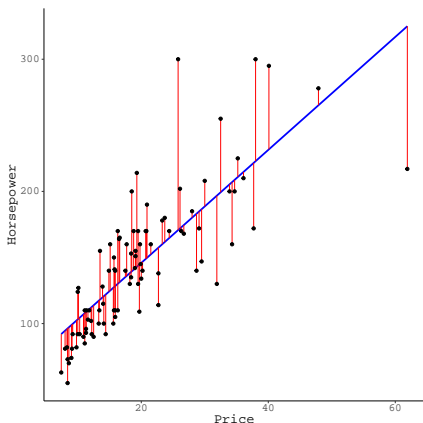
# Residuals as the Basis of Estimation

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

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

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

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





# Least Squares Example

Estimate the least squares coefficients for our example data:

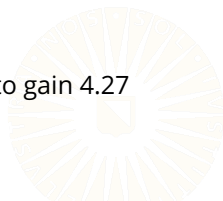
```
data(Cars93, package = "MASS")  
  
out1 <- lm(Horsepower ~ Price, data = Cars93)  
coef(out1)  
  
(Intercept)      Price  
  60.447578    4.273796
```

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

- A free car is expected to have 60.45 horsepower.

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

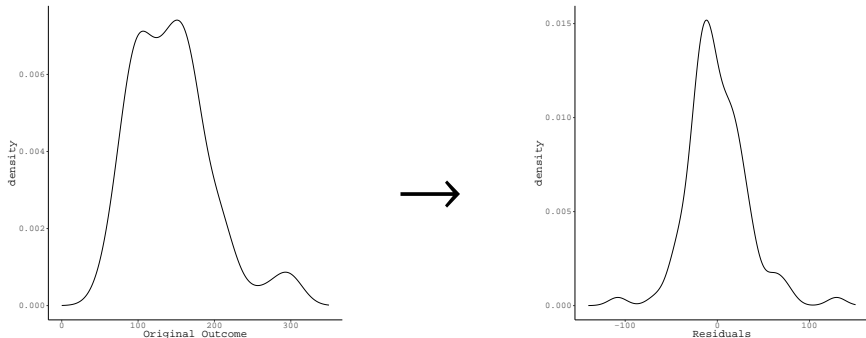
- For every additional \$1000 in price, a car is expected to gain 4.27 horsepower.



# Model Fit

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

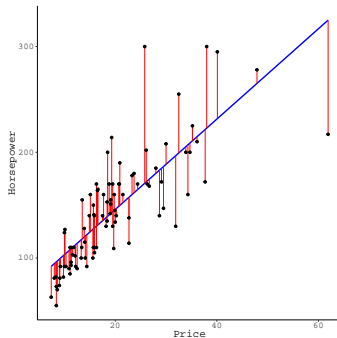
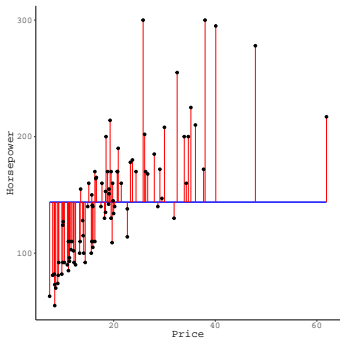
- Our model explains some proportion of the outcome's variability.
- The residual variance  $\hat{\sigma}^2 = \text{Var}(\hat{\varepsilon})$  will be less than  $\text{Var}(Y)$ .



# 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  $\hat{\sigma}^2 = \text{Var}(\hat{\varepsilon})$  will be less than  $\text{Var}(Y)$ .



# Model Fit

---

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

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

where

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

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.

$$\begin{aligned} \text{MSE} &= \frac{1}{N} \sum_{n=1}^N \left( Y_n - \hat{Y}_n \right)^2 \\ &= \frac{1}{N} \sum_{n=1}^N \left( Y_n - \hat{\beta}_0 - \sum_{p=1}^P \hat{\beta}_p X_{np} \right)^2 \\ &= \frac{\text{RSS}}{N} \end{aligned}$$

For our example problem, we get:

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



# Interpreting MSE

---

The MSE quantifies the average squared prediction error.

- Taking the square root improves interpretation.

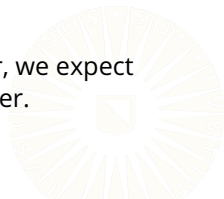
$$RMSE = \sqrt{MSE}$$

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)

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



# 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)

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

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:

$$\begin{aligned}AIC &= 2(3) - 2(-454.44) \\ &= 914.88\end{aligned}$$

$$\begin{aligned}BIC &= 3 \ln(93) - 2(-454.44) \\ &= 922.48\end{aligned}$$

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

```
AIC(out1)
```

```
[1] 914.8821
```

```
BIC(out1)
```

```
[1] 922.4799
```

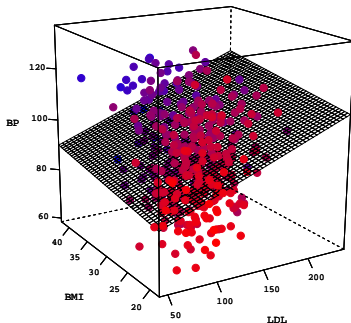
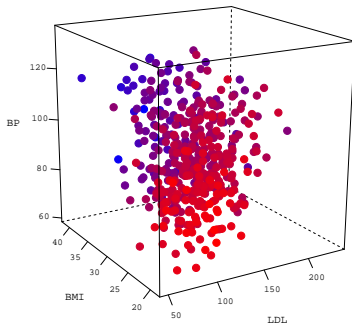
# MULTIPLE LINEAR REGRESSION



# Graphical Representations

Adding an additional predictor to a simple linear regression problem 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.



# Example

---

```
## Read in the 'diabetes' dataset:  
dDat <- readRDS("../data/diabetes.rds")  
  
## Simple regression with which we're familiar:  
out1 <- lm(bp ~ age, data = dDat)
```

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

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

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.

# Example

---

```
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
age	0.28651	0.04504	6.362	5.02e-10
bmi	1.08053	0.13363	8.086	6.06e-15

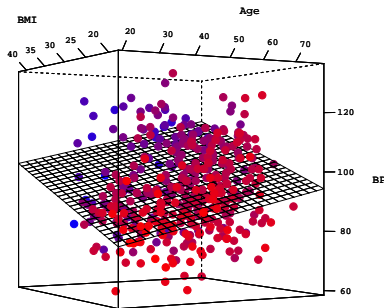
Residual standard error: 12.18 on 439 degrees of freedom

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 $R^2$

---

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

- Check the  $R^2$  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
```



# 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

# F-Statistic

---

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

      value      numdf      dendif
64.6647      2.0000 439.0000

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

      value
2.433518e-25
```

# Comparing Models

---

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

- Compute the  $\Delta R^2$

```
## Compute change in R^2:
```

```
r2.2 - r2.1
```

```
[1] 0.115049
```

# Significance Testing

How do we know if  $\Delta R^2$  represents a significantly greater degree of explained variation?

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

```
## Is that increase significantly greater than zero?  
anova(out1, out2)
```

Analysis of Variance Table

Model 1: bp ~ age

Model 2: bp ~ age + bmi

	Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
1	440	74873				
2	439	65167	1	9706.1	65.386	6.057e-15 ***

---

Signif. codes:

0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

# 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
```

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



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



# Example Dummy Codes

Now, a slightly more complex example:

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



# Using Dummy Codes

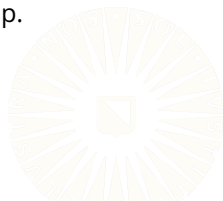
---

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.



# Example

```
## Load some data:
data(Cars93, package = "MASS")

## Use a nominal predictor:
out3 <- lm(Price ~ DriveTrain, data = Cars93)
partSummary(out3, -1)
```

Residuals:

Min	1Q	Median	3Q	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
DriveTrainFront	-0.09418	2.96008	-0.032	0.97469
DriveTrainRear	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.



# Example

---

Include two sets of dummy codes:

```
out4 <- lm(Price ~ Man.trans.avail + DriveTrain, data = Cars93)
partSummary(out4, -c(1, 2))
```

Coefficients:

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	21.7187	2.9222	7.432	6.25e-11
Man.trans.availYes	-5.8410	1.8223	-3.205	0.00187
DriveTrainFront	-0.2598	2.8189	-0.092	0.92677
DriveTrainRear	10.5169	3.3608	3.129	0.00237

Residual standard error: 8.314 on 89 degrees of freedom

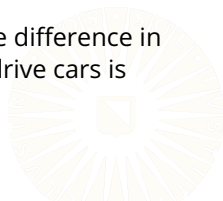
Multiple R-squared: 0.2834, Adjusted R-squared: 0.2592

F-statistic: 11.73 on 3 and 89 DF, p-value: 1.51e-06

# 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.



# Contrasts

---

All R factors have an associated *contrasts* attribute.

- The contrasts define a coding to represent the grouping information.
- Modeling functions code the factors using the rules defined by the contrasts.

```
contrasts(Cars93$Man.trans.avail)
```

	Yes
No	0
Yes	1

```
contrasts(Cars93$DriveTrain)
```

	Front	Rear
4WD	0	0
Front	1	0
Rear	0	1



# Significance Testing

---

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

```
out <- lm(Price ~ Man.trans.avail, data = Cars93)
partSummary(out, -c(1, 2))
```

Coefficients:

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	23.841	1.623	14.691	<2e-16
Man.trans.availYes	-6.603	2.004	-3.295	0.0014

Residual standard error: 9.18 on 91 degrees of freedom

Multiple R-squared: 0.1066, Adjusted R-squared: 0.09679

F-statistic: 10.86 on 1 and 91 DF, p-value: 0.001403

# Significance Testing

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

```
partSummary(out4, -c(1, 2))
```

Coefficients:

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	21.7187	2.9222	7.432	6.25e-11
Man.trans.availYes	-5.8410	1.8223	-3.205	0.00187
DriveTrainFront	-0.2598	2.8189	-0.092	0.92677
DriveTrainRear	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

# Significance Testing

```
summary(out4)$r.squared - summary(out)$r.squared
```

```
[1] 0.1767569
```

```
anova(out, out4)
```

Analysis of Variance Table

Model 1: Price ~ Man.trans.avail

Model 2: Price ~ Man.trans.avail + DriveTrain

	Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
1	91	7668.9				
2	89	6151.6	2	1517.3	10.976	5.488e-05 ***

---

Signif. codes:

0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

# Significance Testing

---

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

```
partSummary(out3, -c(1, 2))
```

Coefficients:

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	17.63000	2.76119	6.385	7.33e-09
DriveTrainFront	-0.09418	2.96008	-0.032	0.97469
DriveTrainRear	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

# MODEL-BASED PREDICTION



# Prediction Example

---

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

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

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

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



# Prediction Example

---

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

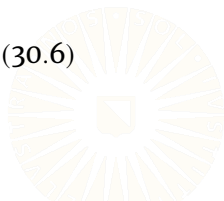
$$Y_{LDL} = \beta_0 + \beta_1 X_{BP} + \beta_2 X_{gluc} + \beta_3 X_{BMI} + \varepsilon$$

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

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

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

$$\begin{aligned}\hat{Y}_{LDL} &= 22.135 + 0.089(121) + 0.498(89) + 1.48(30.6) \\ &= 122.463\end{aligned}$$

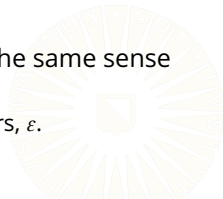


# Interval Estimates for Prediction

---

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  $m$ th 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  $m$ th outcome value.
  - Prediction intervals also account for the regression errors,  $\varepsilon$ .

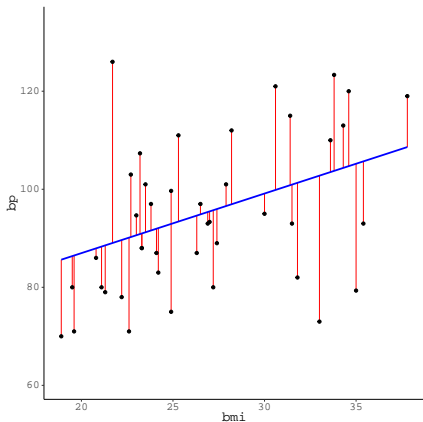




# Confidence vs. Prediction Intervals

Let's visualize the predictions from a simple model:

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

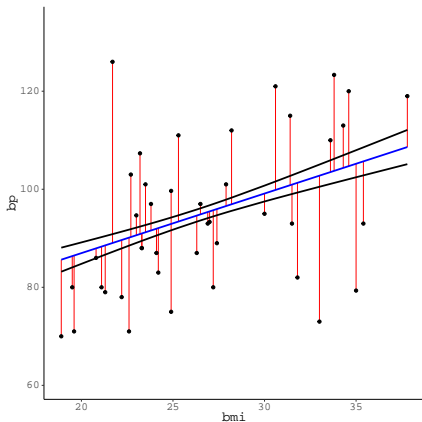


# Confidence vs. Prediction Intervals

Let's visualize the predictions from a simple model:

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

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

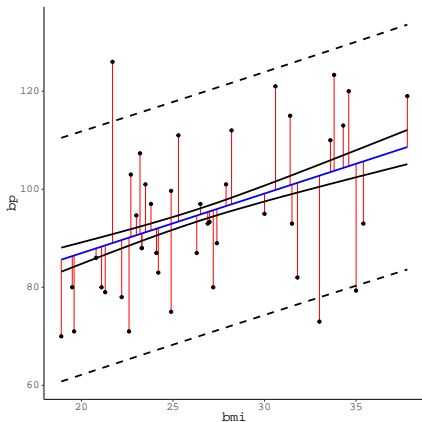


# Confidence vs. Prediction Intervals

Let's visualize the predictions from a simple model:

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

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



# Interval Estimates Example

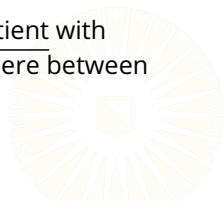
---

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.



# 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  $Z$ .



# Equations

---

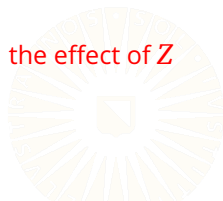
In additive MLR, we might have the following equation:

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

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

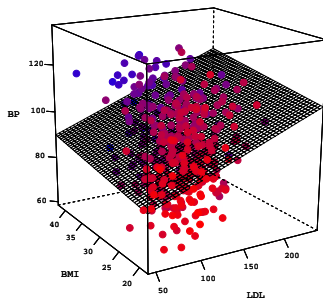
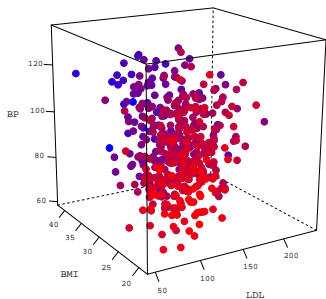
When  $X$  and  $Z$  are independent predictors, the following are true:

- $X$  and  $Z$  *can* be correlated.
- $\beta_1$  and  $\beta_2$  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

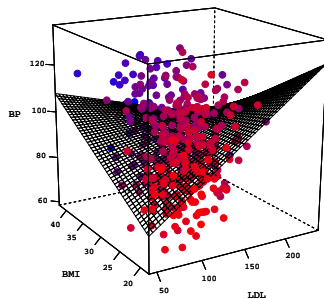
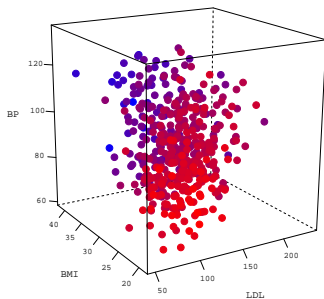
The effect of  $X$  on  $Y$  is the same at **all levels** of  $Z$ .





# Moderated Regression

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



# Equations

---

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:

$$Y = \beta_0 + f(Z)X + \beta_2Z + \varepsilon \quad (1)$$



# Equations

---

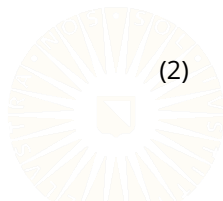
The following derivation is adapted from Hayes (2017).

- 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:

$$Y = \beta_0 + f(Z)X + \beta_2Z + \varepsilon \quad (1)$$

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

$$f(Z) = \beta_1 + \beta_3Z \quad (2)$$



# Equations

---

- Substituting Equation 2 into Equation 1 leads to:

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



# Equations

---

- Substituting Equation 2 into Equation 1 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.

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

- 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.



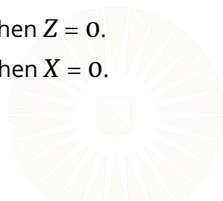
# Interpretation

---

Given the following equation:

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

- $\hat{\beta}_3$  quantifies the effect of  $Z$  on the focal effect (the  $X \rightarrow Y$  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  $X = 0$ .



# Example

---

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.





# Example

---

```
out <- lm(bp ~ bmi * ldl, data = dDat)
partSummary(out, -c(1, 2))
```

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

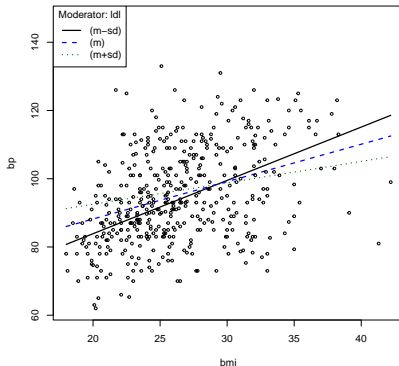
Multiple R-squared: 0.1834, Adjusted R-squared: 0.1778

F-statistic: 32.78 on 3 and 438 DF, p-value: < 2.2e-16

# 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.

```
library(rockchalk)
plotSlopes(out,
  plotx = "bmi",
  modx = "ldl",
  modxVals = "std.dev")
```



# Categorical Moderators

---

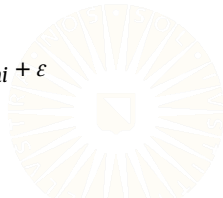
Categorical moderators encode *group-specific* effects.

- 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:

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

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



# Example

```
## Load data:  
socSup <- readRDS(paste0(dataDir, "social_support.rds"))
```

```
## Estimate the moderated regression model:  
out <- lm(bdi ~ tanSat * sex, data = socSup)  
partSummary(out, -c(1, 2))
```

Coefficients:

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	20.8478	6.2114	3.356	0.00115
tanSat	-0.5772	0.3614	-1.597	0.11372
sexmale	14.3667	12.2054	1.177	0.24223
tanSat:sexmale	-0.9482	0.7177	-1.321	0.18978

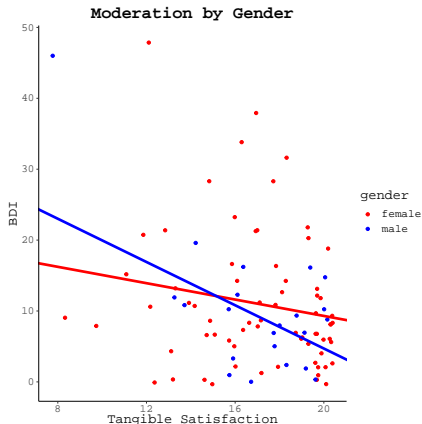
Residual standard error: 9.267 on 91 degrees of freedom

Multiple R-squared: 0.08955, Adjusted R-squared: 0.05954

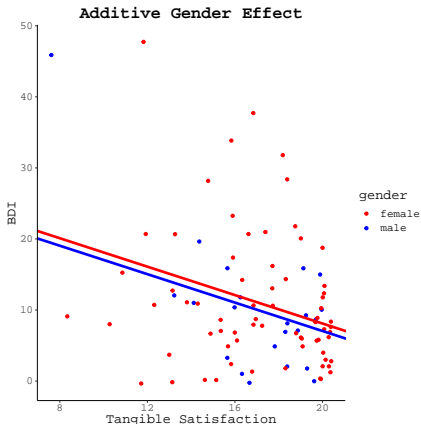
F-statistic: 2.984 on 3 and 91 DF, p-value: 0.03537

# Visualizing Categorical Moderation

$$\hat{Y}_{BDI} = 20.85 - 0.58X_{tsat} + 14.37Z_{male} - 0.95X_{tsat}Z_{male}$$



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



# References

---

Hayes, A. F. (2017). *Introduction to mediation, moderation, and conditional process analysis: A regression-based approach*. New York: Guilford Press.

