Multiple Linear Regression
Fundamental Techniques in Data Science with R

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Outline

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  Model Comparison
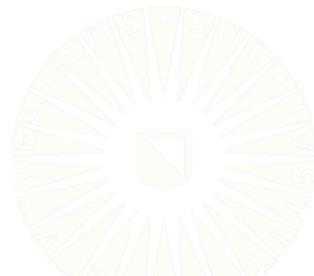
Categorical Predictors
  Significance Testing for Dummy Codes

Model-Based Prediction
 Interval Estimates for Prediction
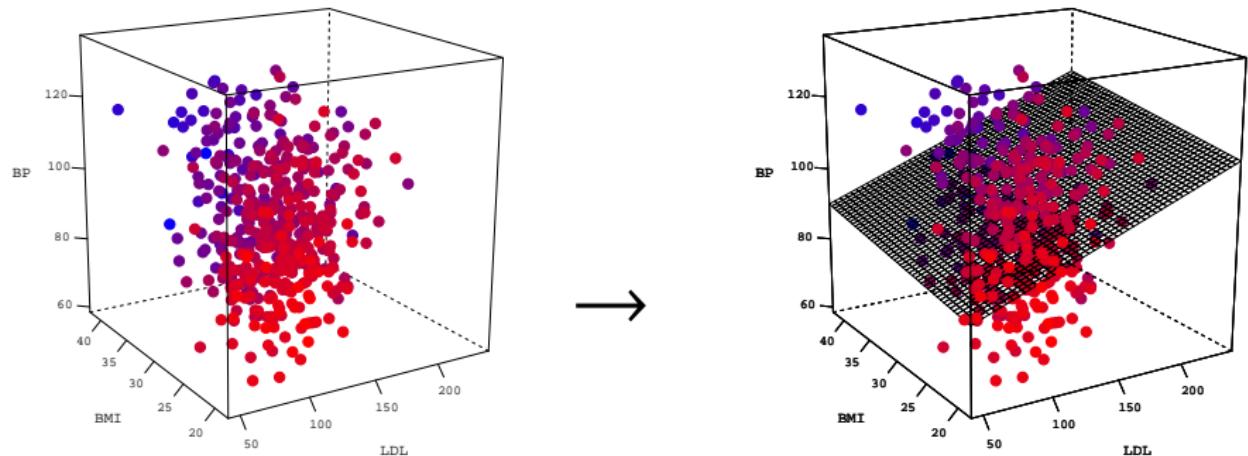
Moderation
  Categorical Moderators

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.
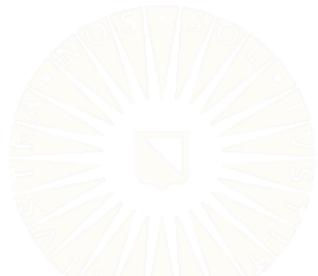
Partial Effects

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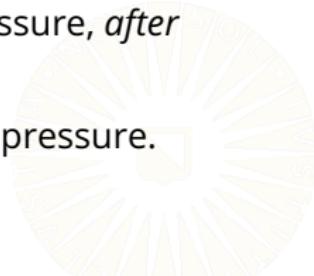
```r
## Read in the 'diabetes' dataset:
dDat <- readRDS(here::here("data", "diabetes.rds"))

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

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

```r
## 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
```
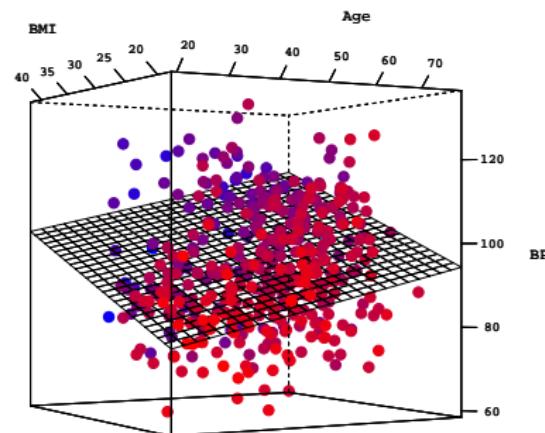
Interpretation

- 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    dendf
 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 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. $H_1 : \Delta R^2 > 0$

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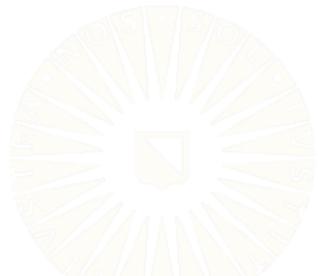
In this case, both the AIC and the BIC for the model with *BMI* included are smaller.

- We should prefer the larger model.
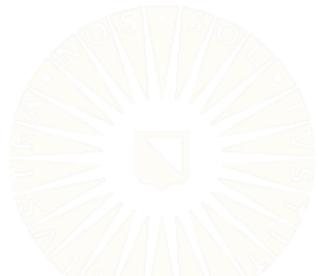
CATEGORICAL PREDICTORS

Dummy Coding

The most common way to code categorical predictors is *dummy coding*.
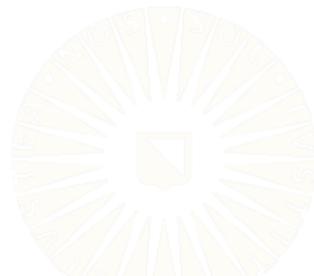
- A G-level factor must be converted into a set of $G - 1$ dummy codes.

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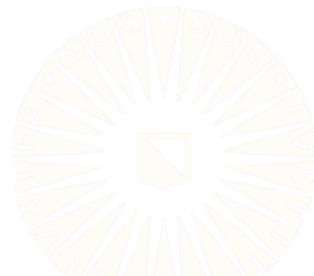
	sex	male
1	female	0
2	male	1
3	male	1
4	female	0
5	male	1
6	female	0
7	female	0
8	male	1
9	female	0
10	female	0

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.
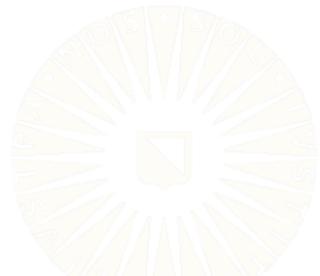
Example

```
## 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
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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
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```
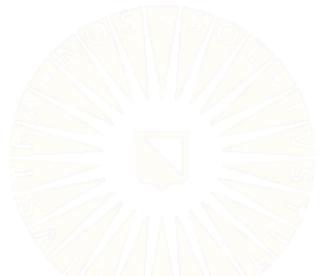
Model-Based Prediction
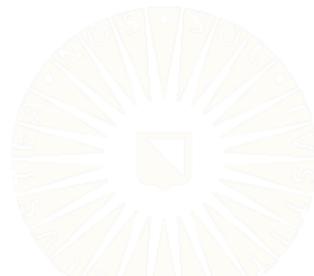
Prediction Example

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:

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

Prediction Example

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

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

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

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

Suppose a new patient presents with $BP = 121$, $gluc = 89$, and $BMI = 30.6$. We can predict their *LDL* score by:
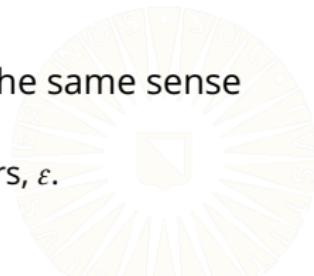
$$\hat{Y}_{LDL} = 22.135 + 0.089(121) + 0.498(89) + 1.48(30.6)$$
$$= 122.463$$

Interval Estimates for Prediction

To quantify uncertainty in our predictions, we want to use an appropriate interval estimate.
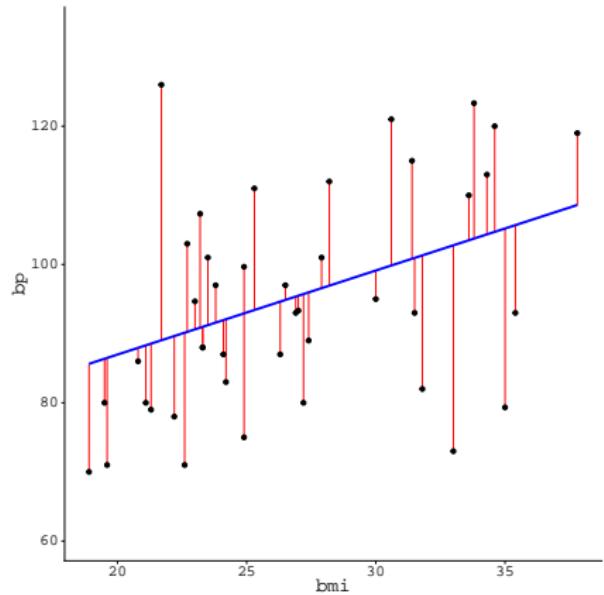
- Two flavors of interval are applicable to predictions:
    1. Confidence intervals for $\hat{Y}_m$
    2. Prediction intervals for a specific observation, Y_m

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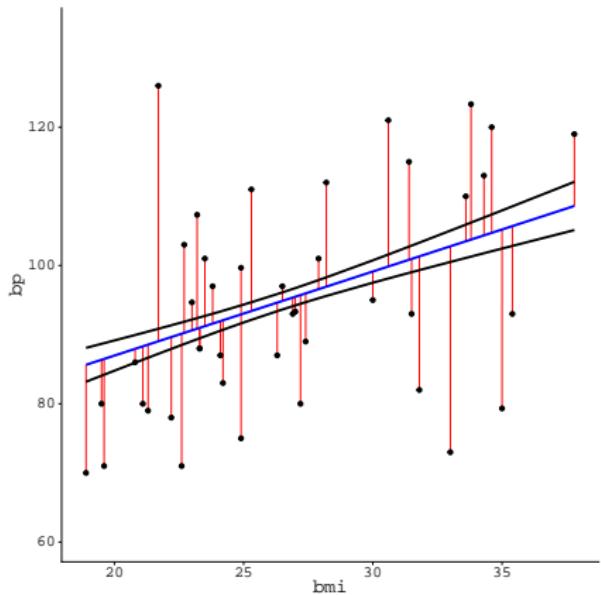
$$Y_{BP} = \hat{\beta}_0 + \hat{\beta}_1 X_{BMI} + \hat{\varepsilon}$$

Confidence vs. Prediction Intervals

Let's visualize the predictions from a simple model:

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

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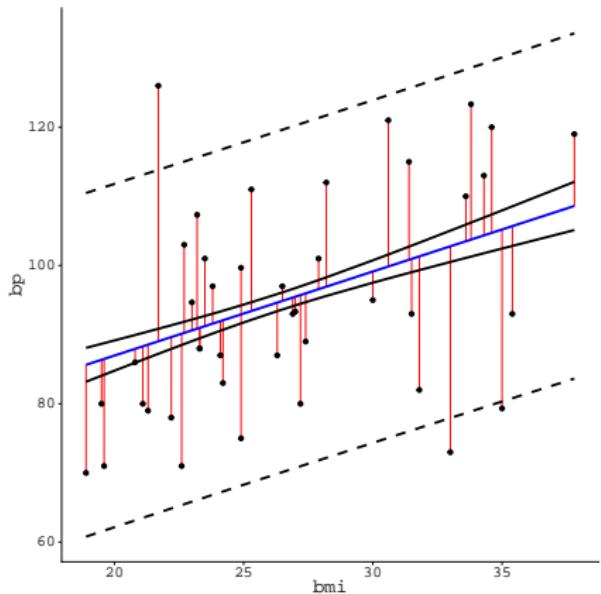
Confidence vs. Prediction Intervals

Let's visualize the predictions from a simple model:

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

- CIs 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 CIs.
 - 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:
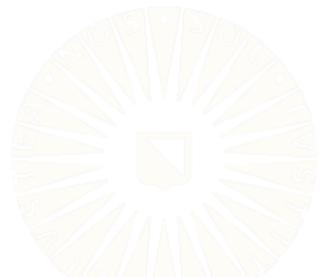
$$95\% \ CI_{\hat{Y}} = [115.6; 129.33]$$

$$95\% \ PI = [66.56; 178.37]$$

- 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.

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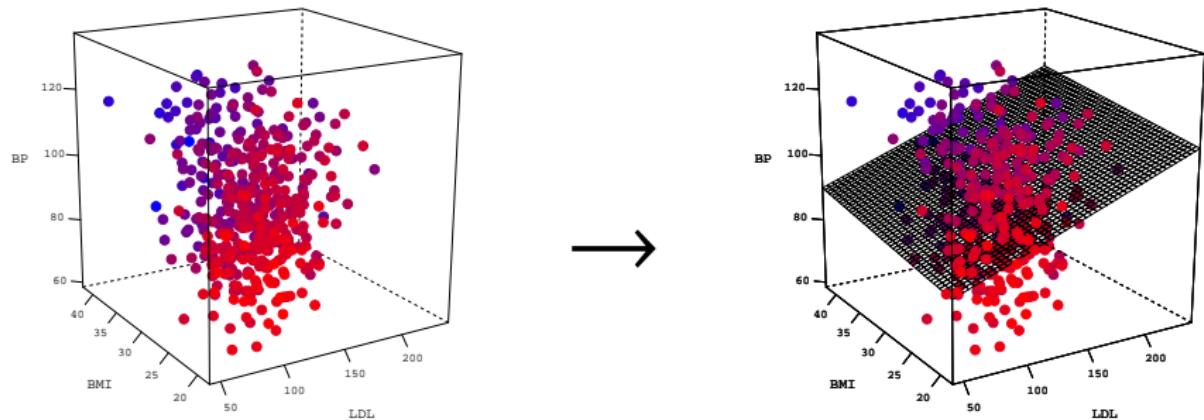
When X and Z are independent predictors, the following are true:

- X and Z *can* be correlated.
- 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.
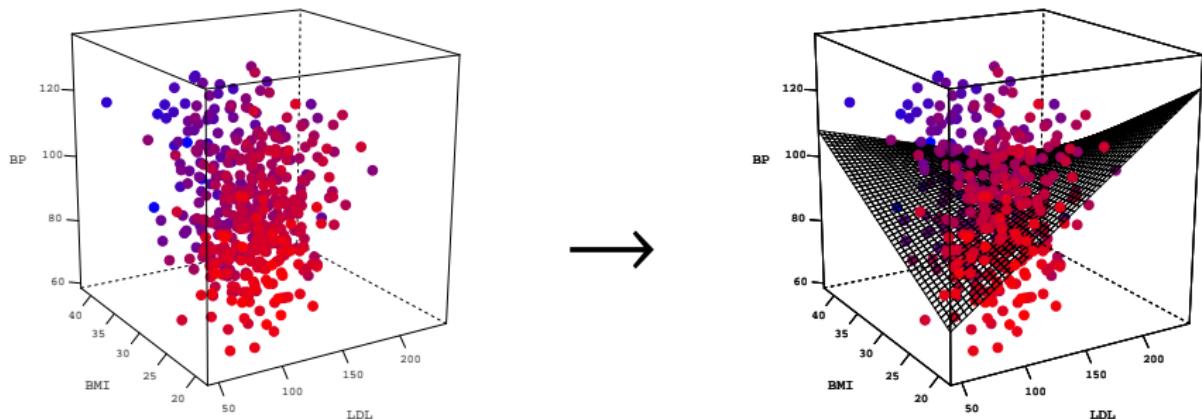
Additive Regression

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

$\longrightarrow$

Moderated Regression

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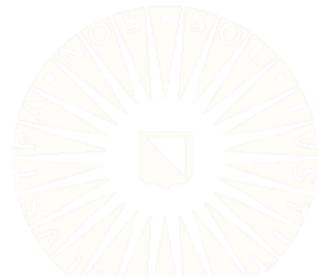
Equations

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:

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

Equations
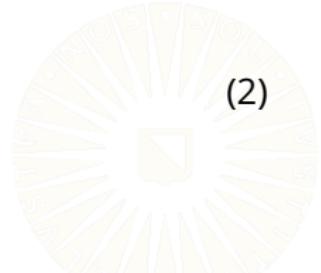
The following derivation is adapted from Hayes (2017).

- 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:

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

- If we assume that Z linearly (and deterministically) affects the relationship between X and Y, then we can take:
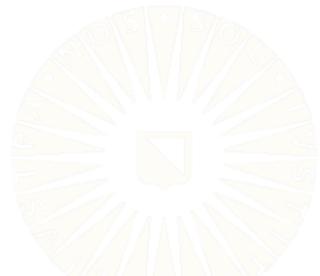
$$f(Z) = \beta_1 + \beta_3 Z \tag{2}$$

Equations

- Substituting Equation 2 into Equation 1 leads to:
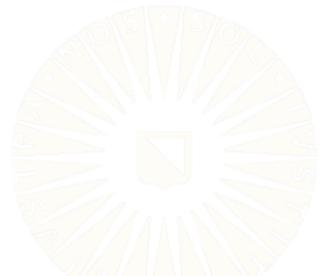
$$Y = \beta_0 + (\beta_1 + \beta_3 Z)X + \beta_2 Z + \varepsilon$$

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:

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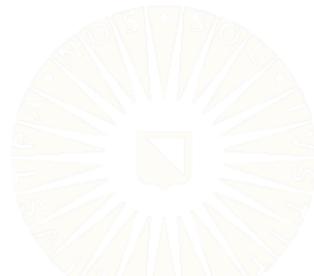
Testing Moderation

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.
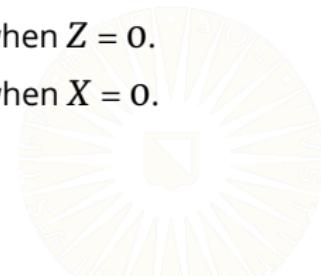
Interpretation

Given the following equation:

$$Y = \hat{\beta}_0 + \hat{\beta}_1 X + \hat{\beta}_2 Z + \hat{\beta}_3 XZ + \hat{\varepsilon}$$
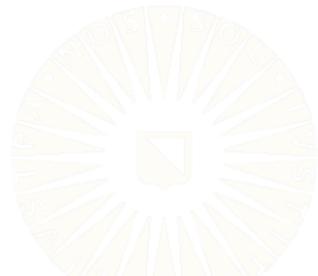
- $\hat{\beta}_3$ quantifies the effect of Z on the focal effect (the $X \rightarrow Y$ effect).
  - For a unit change in Z, $\hat{\beta}_3$ is the expected change in the effect of X on Y.

- $\hat{\beta}_1$ 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
```
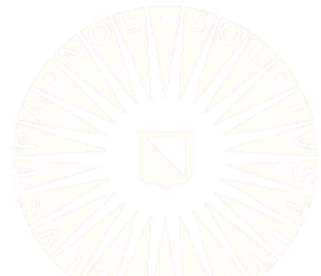
Interpretation

INTERACTION

LDL cholesterol level significantly influences the effect of BMI on average blood pressure ($\beta = -0.02$, $t[438] = -3.26$, $p = 0.001$).

- For each additional point of LDL cholesterol, the effect of BMI on BP decreases by 0.02 units.

Interpretation

CONDITIONAL EFFECTS

There is significant conditional effect of BMI on average blood pressure, when LDL = 0 ($\beta = 2.87$, $t[438] = 5.3$, $p < 0.001$).

- For patients with zero LDL cholesterol, each additional point of BMI produces a change of 2.87 units in expected average blood pressure.

There is significant conditional effect of LDL cholesterol level on average blood pressure, when BMI = 0 ($\beta = 0.45$, $t[438] = 3.53$, $p < 0.001$).

- For patients with BMI = 0, each additional point of LDL cholesterol increases their expected average blood pressure by 0.45 units.

Interpretation
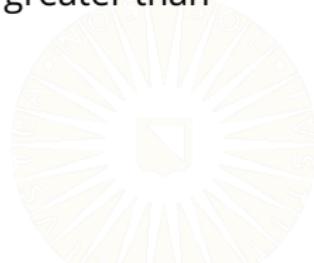
INTERCEPT

The expected average blood pressure for a patient with BMI = 0 and zero LDL cholesterol is 14.48.

MODEL FIT

BMI, LDL cholesterol level, and the interaction therebetween explain approximately 18.3% of the variability in average blood pressure.
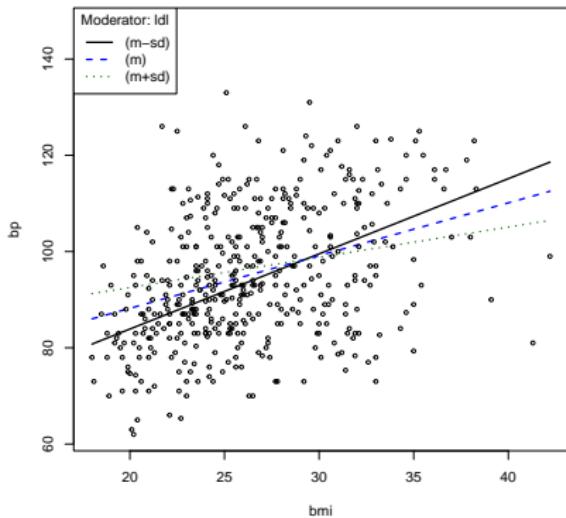
- This proportion of explained variability is significantly greater than zero ($F[3, 438] = 32.78$, $p < 0.001$).

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
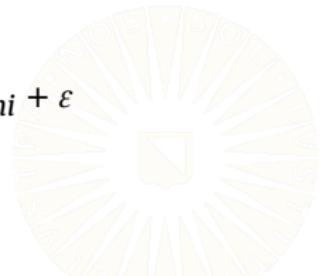
Categorical moderators encode *group-specific* effects.

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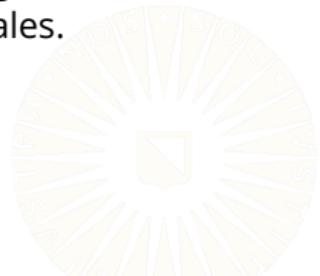
```
## Load data:
socSup <- readRDS(here::here("data", "social_support.rds"))

## 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
```

Interpretation

INTERACTION

Sex does not significantly influence the effect of tangible satisfaction ratings on depression levels ($\beta = -0.95$, $t[91] = -1.32$, $p = 0.19$).

- In other words, there is not significant a difference between males and females in the way that tangible satisfaction ratings affect depression levels.

- In this sample, the effect of tangible satisfaction ratings on depression is 0.95 units lower for males than for females.

Interpretation
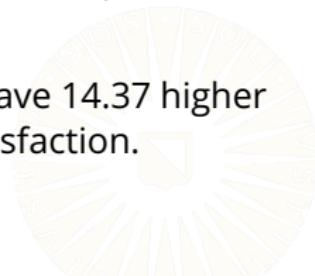
CONDITIONAL EFFECTS

There is not a significant effect of tangible satisfaction ratings on depression levels for females ($\beta = -0.58$, $t[91] = -1.6$, $p = 0.114$).

- For females in this sample, each additional point of rated tangible satisfaction produces a change of -0.58 units in expected depression level.

There is not a significant conditional effect of sex on depression levels, when tangible satisfaction rating is zero ($\beta = 14.37$, $t[91] = 1.18$, $p = 0.242$).

- In this sample, males with zero tangible satisfaction have 14.37 higher depression levels than females with zero tangible satisfaction.

Interpretation

INTERCEPT

The expected depression level for females with a zero tangible satisfaction rating is 20.85.

MODEL FIT
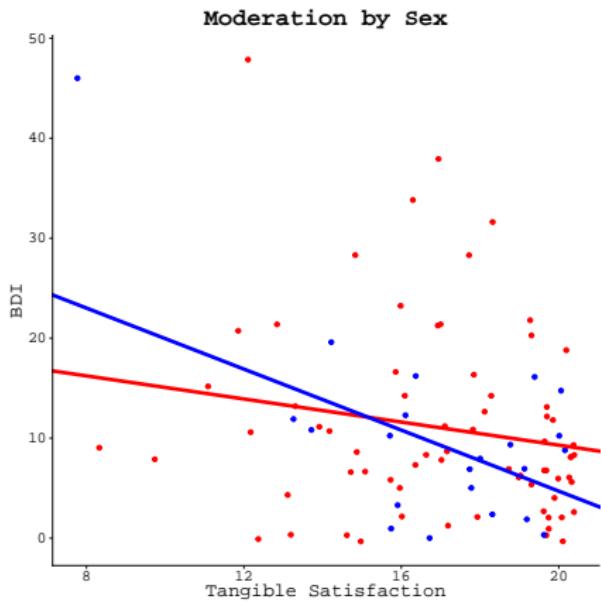
Sex, tangible satisfaction rating, and their interaction explain approximately 9% of the variability in depression levels.

- This proportion of explained variability is significantly greater than zero ($F[3, 91] = 2.98$, $p = 0.035$).
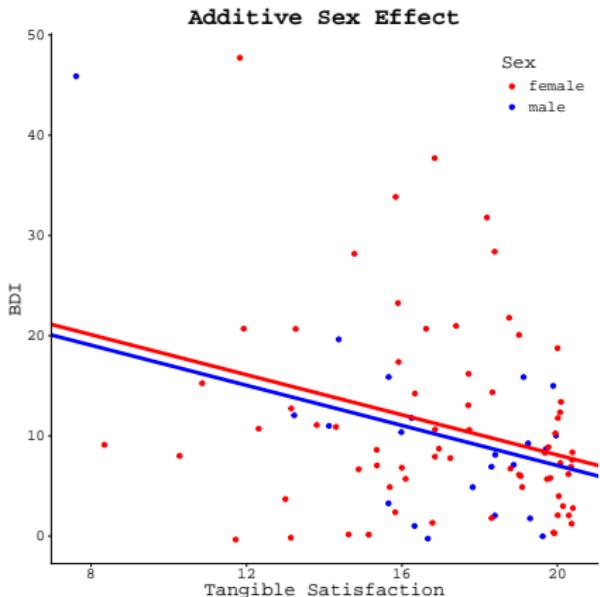
Visualizing Categorical Moderation

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

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

References

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