Introduction to Linear Modeling

Fundamental Techniques in Data Science with R

Kyle M. Lang

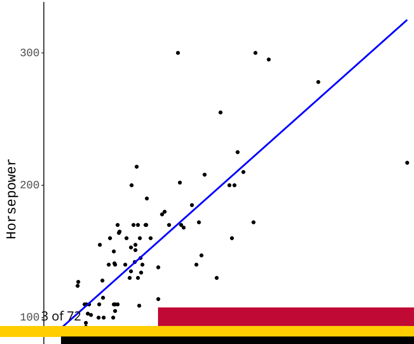
Department of Methodology & Statistics
Utrecht University

Outline

Visualizations of Simple Linear Regression

```
data(Cars93)
out1 <- lm(Horsepower
  Price, data = Cars93)
Cars93yHat< −fitted(out1)Cars93yMean
<- mean(Cars93Horsepower)
p <- ggplot(data = Cars93, aes(x =
Price, y = Horsepower)) +
coordcartesian()+themeclassic()+theme(text=e
```

$< -p$



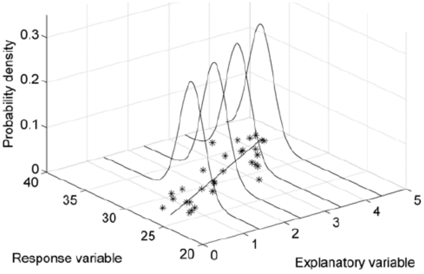


Image retrieved from:
`http://www.seaturtle.org/mtn/archives/mtn122/mtn122p1.shtml`

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 $X = 0$.

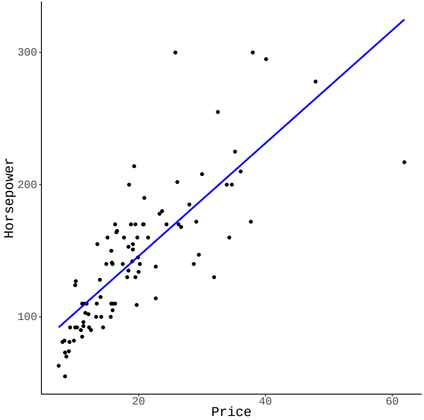
$\hat{\beta}_1$ is the *slope*.

- 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.



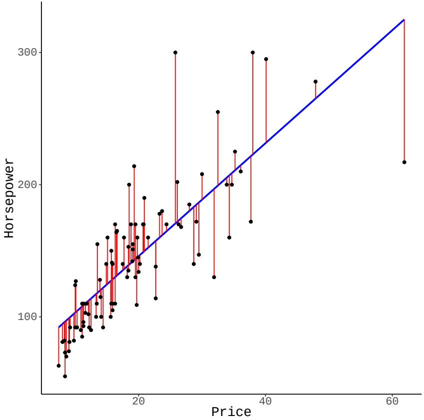
Thinking about Error

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

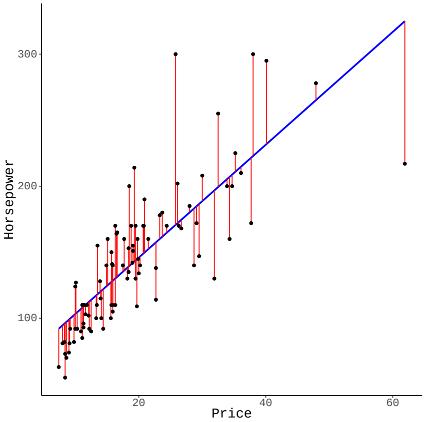
Residuals as the Basis of Estimation

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

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

Each $\hat{\varepsilon}_n$ 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:

```
#data(Cars93)
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: $\hat{\beta}_1 = 4.27$.

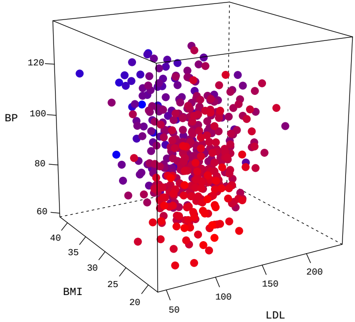
- For every additional $1000 in price, a car is expected to gain 4.27 horsepower.

Multiple Linear Regression

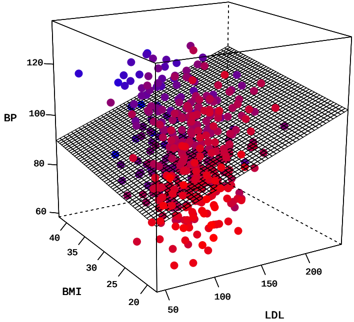
Graphical Representations

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

```r
## 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?

Example

```
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
```

Example

```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?*

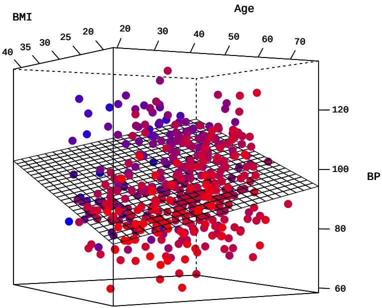
- We're partialing age out of the effect of BMI on blood pressure.

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.



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

```
Error in data.frame(y =
Cars93$Horsepower, r =
resid(out1)):  arguments imply
differing number of rows:  93,
442
Error in ggplot(data = dat3,
aes(x = y)):  object 'dat3'
not found
Error in eval(expr, envir,
enclos):  object 'p10' not
found
```

$\longrightarrow$

```
Error in ggplot(data = dat3,
aes(x = r)):  object 'dat3'
not found
Error in eval(expr, envir,
enclos):  object 'p11' not
found
```

Model Fit

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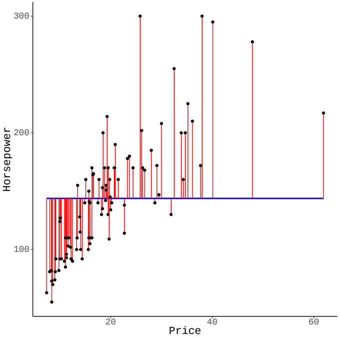
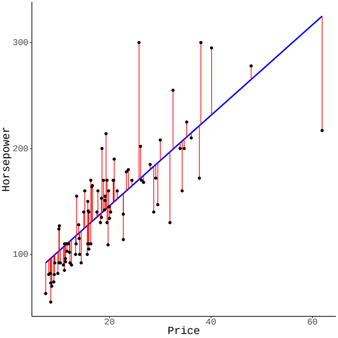


$\longrightarrow$



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

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

For our example problem, we get:

$$R^2 = 1 - \frac{74873}{252363} \approx 0.7$$

Indicating that car price explains 70% 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.

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

For our example problem, we get:

$$
MSE = \frac{74873}{93} \approx 805.09
$$

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:

$$RMSE = \sqrt{\frac{74873}{93}} \approx 28.37$$

- When using price as the only predictor of horsepower, we expect prediction errors with magnitudes of 28.37 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:

$$\begin{aligned} AIC &= 2(3) - 2(-1761.4) \\ &= 3528.79 \end{aligned}$$

$$\begin{aligned} BIC &= 3\ln(93) - 2(-1761.4) \\ &= 3541.07 \end{aligned}$$

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

```
AIC(out1)
```

```
[1] 3528.792
```

```
BIC(out1)
```

```
[1] 3541.066
```

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

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

How to Model Categorical Predictors

```
mDat <- readRDS("../data/major_data.rds")
mDat[seq(25, 150, 25), ]

    sat majF majN
25  1.9  law    1
50  1.4  law    1
75  4.3 econ    2
100 4.1 econ    2
125 5.7   ds    3
150 5.1   ds    3

out1 <- lm(sat ~ majN, data = mDat)
```

How to Model Categorical Predictors

```
partSummary(out1, -1)

Residuals:
   Min     1Q Median     3Q    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.

Example

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

out3 <- lm(price ~ front + rear, data = cDat)
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
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.

Example

Include two sets of dummy codes:

```
out4 <- lm(price ~ mtOpt + front + rear, data = cDat)
partSummary(out4, -c(1, 2))

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  21.7187     2.9222   7.432 6.25e-11
mtOpt        -5.8410     1.8223  -3.205  0.00187
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
```

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.

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.

```
out2 <- lm(price ~ mtOpt, data = cDat)
partSummary(out2, -c(1, 2))

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)   23.841      1.623  14.691   <2e-16
mtOpt         -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
mtOpt        -5.8410     1.8223  -3.205  0.00187
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
```

Significance Testing

```
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)
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
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
```

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:

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

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:

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

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

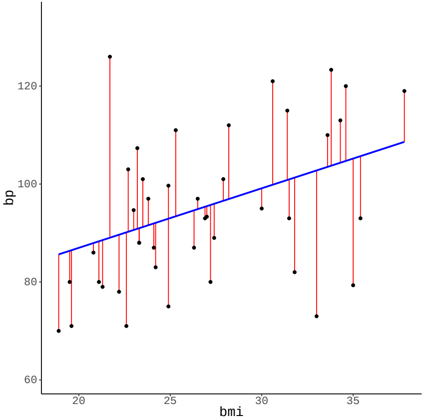
- The CI for $\hat{Y}_m$ gives a likely range (in the sense of coverage probability and “confidence”) for the *m*th value of the true conditional mean.
  - CIs only account for uncertainty in the estimated regression coefficients, $\{\hat{\beta}_0, \hat{\beta}_p\}$.

- 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, ε.

Confidence vs. Prediction Intervals

Let's visualize the predictions from a simple model:

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

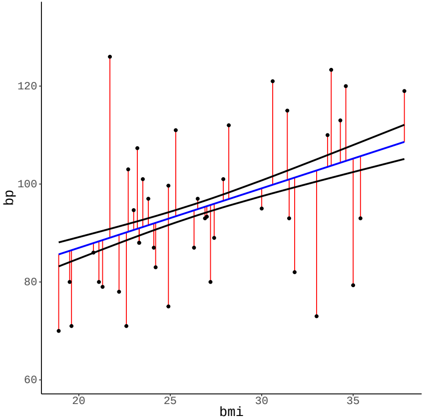


Confidence vs. Prediction Intervals

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, $\beta_0 + \beta_1 X_{BMI}$.

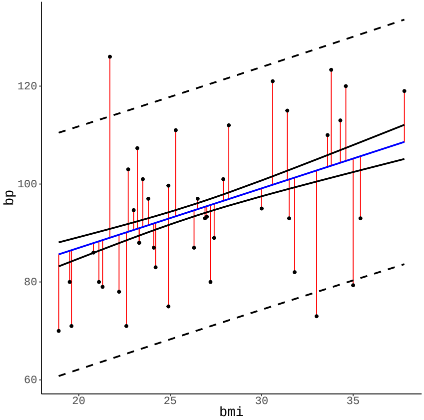


Confidence vs. Prediction Intervals

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:

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

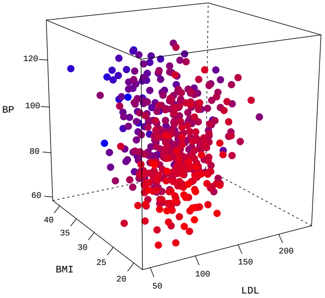
This additive equation assumes that X and Z are independent predictors of Y.

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

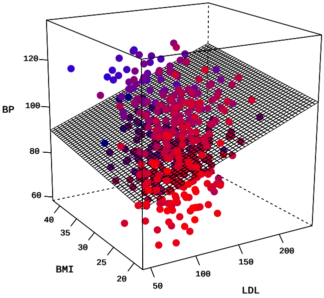
- X and Z *can* be correlated.
- β_1 and β_2 are *partial* regression coefficients.
- The effect of X on Y is the same at **all levels** of Z, and the effect of Z on Y is the same at **all levels** of X.

Additive Regression

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

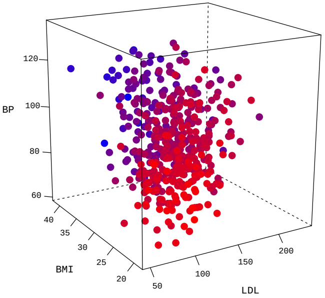


$\longrightarrow$

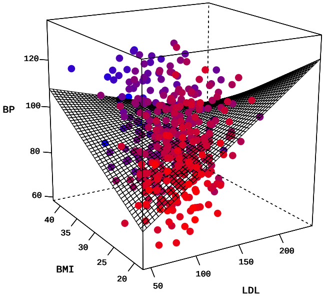


Moderated Regression

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



$\longrightarrow$



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.

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

- 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

```
## Focal Effect:
out0 <- lm(bp ~ bmi, data = dDat)
partSummary(out0, -c(1, 2))

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  61.9973     3.6659   16.91   <2e-16
bmi           1.2379     0.1371    9.03   <2e-16

Residual standard error: 12.72 on 440 degrees of freedom
Multiple R-squared:  0.1563,Adjusted R-squared:  0.1544
F-statistic: 81.54 on 1 and 440 DF,  p-value: < 2.2e-16
```

Example

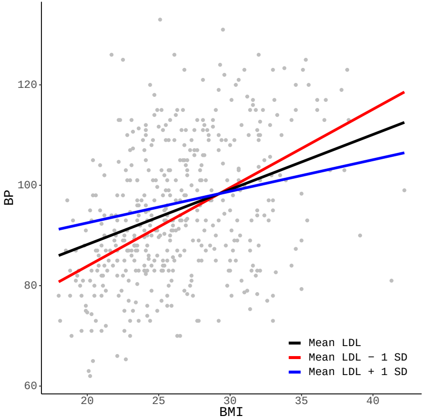
```
## Additive Model:
out1 <- lm(bp ~ bmi + ldl, data = dDat)
partSummary(out1, -c(1, 2))

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 59.26577    3.91281  15.147  < 2e-16
bmi          1.16567    0.14156   8.235 2.08e-15
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
```

Example

```
## Moderated Model:
out2 <- lm(bp ~ bmi * ldl, data = dDat)
partSummary(out2, -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.



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:

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

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

Example

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

Error in paste0(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
```

Example

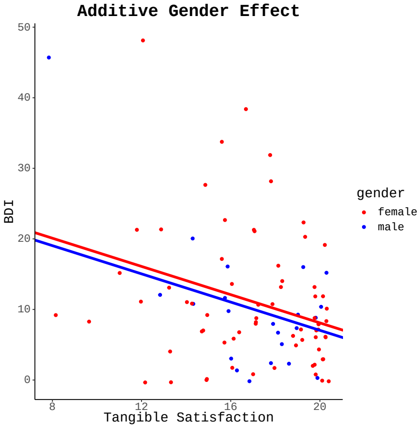
```
## Estimate the interaction:
out4 <- lm(bdi ~ tanSat * sex, data = socSup)

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
mtOpt        -5.8410     1.8223  -3.205  0.00187
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

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

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

```
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
```



References

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