Course Summary

Fundamental Techniques in Data Science

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Outline

Exam Information

Dates

- Exam: Wednesday 22 January
- Resit: Wednesday 12 February

Structure

- Approximately 25 questions
- Mixture of multiple-choice and short-answer questions
- Closed-book
- Remindo, computer-based exam

R TOPICS

R Fundamentals

Objects and assignment

```
1:3
```

```
[1] 1 2 3
```

```
x <- 1:3
x
```

```
[1] 1 2 3
```

```
x + 4
```

```
[1] 5 6 7
```

Data types

- Vectors, Matrices
- Lists, Data frames
- Factors

R Fundamentals

User-defined functions

```
helloWorld <- function() cat("Hello World!")
helloWorld()

Hello World!

add <- function(x, y) x + y
add(2, 3)

[1] 5

add(add(1, 2), 3)

[1] 6
```

Tidyverse Fundamentals

Working with pipes

```
library(magrittr)

iris %$% table(Species)

Species
    setosa versicolor  virginica
        50         50         50

add(1, 2) %>% add(3)

[1] 6
```

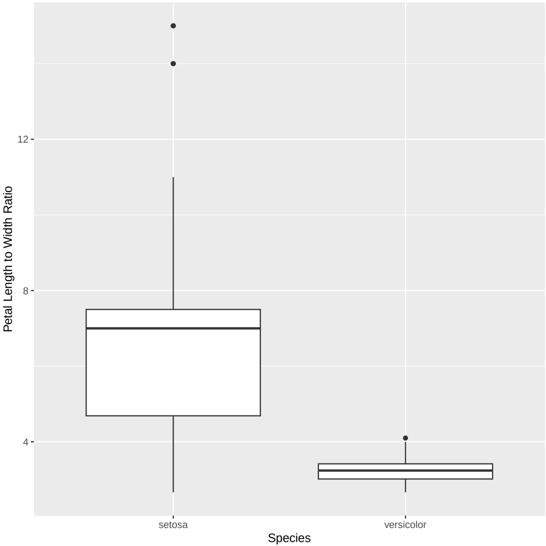
Tidyverse Fundamentals

Working with **dplyr** and **ggplot**

```
library(dplyr)
library(ggplot2)

iris %>%
    filter(Species != "virginica") %>%
    mutate(petal_ratio = Petal.Length / Petal.Width) %>%
    ggplot(aes(Species, petal_ratio)) +
    geom_boxplot() +
    ylab("Petal Length to Width Ratio")
```

Tidyverse Fundamentals



Manipulating Model Objects

```
fit1 <- lm(Petal.Length ~ Sepal.Length + Species, data = iris)
fit2 <- lm(Petal.Length ~ Sepal.Length*Species, data = iris)

coef(fit1)

      (Intercept)      Sepal.Length Speciesversicolor  Speciesvirginica
       -1.7023422         0.6321099         2.2101378         3.0900021

summary(fit2)$fstatistic

   value    numdf    dendf
1333.265    5.000  144.000
```

Manipulating Model Objects

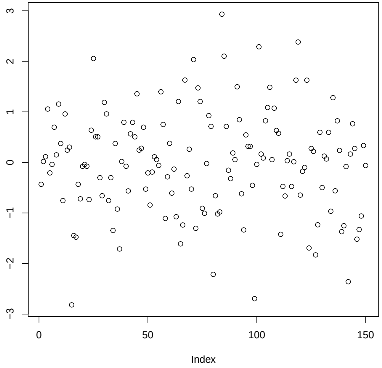
```
anova(fit2, fit1)

Analysis of Variance Table

Model 1: Petal.Length ~ Sepal.Length * Species
Model 2: Petal.Length ~ Sepal.Length + Species
  Res.Df     RSS Df Sum of Sq      F    Pr(>F)
1    144  9.8179
2    146 11.6571 -2   -1.8393 13.489 4.272e-06 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Manipulating Model Objects

```
fit1 %>% rstudent() %>% plot()
```



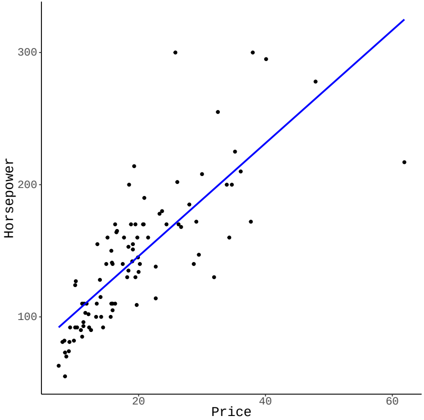
Linear Regression

Simple Linear Regression

In linear regression, we want to find the best fit line:

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

- For any X_n, the corresponding $\hat{Y}_n$ represents the model-implied, conditional mean of Y.



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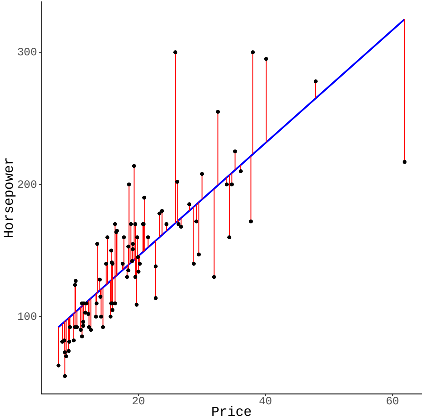
After accounting for the estimation error, we get the full regression equation:

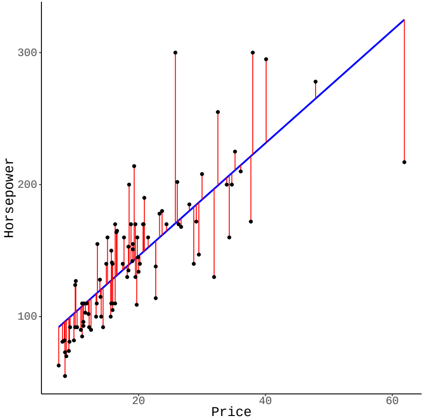
$$Y = \hat{\beta}_0 + \hat{\beta}_1 X + \hat{\varepsilon}$$



Residuals as the Basis of Estimation

We use the residuals, $\hat{\varepsilon}_n$, to estimate the model.

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



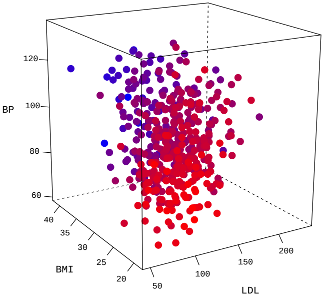
Assumptions

1. The model is linear in the parameters.
    - *Otherwise:* We are not working with linear regression.
2. The predictor matrix is *full rank*.
    - *Otherwise:* The model is not estimable.
3. The predictors are strictly exogenous.
    - *Otherwise:* The estimated regression coefficients will be biased.
4. The errors have constant, finite variance.
    - *Otherwise:* Standard errors will be biased.
5. The errors are uncorrelated.
    - *Otherwise:* Standard errors will be biased.
6. The errors are normally distributed.
    - *Otherwise:* Small-sample inferences and some estimates are not justified.

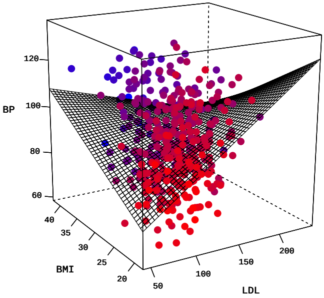
MODERATION

Moderated Regression

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



$\longrightarrow$



Interpretation

Given the following equation:

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

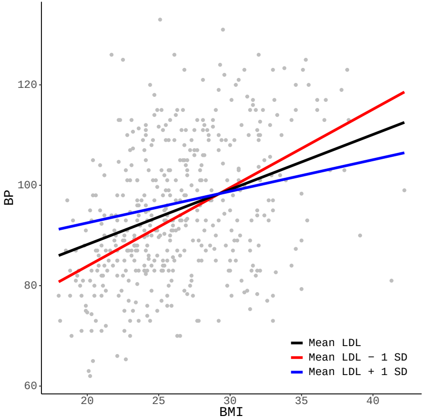
- $\hat{\beta}_3$ quantifies the effect of Z on the focal effect (the $X \rightarrow Y$ effect).
  - For a unit change in Z, $\hat{\beta}_3$ is the expected change in the effect of X on Y.
- $\hat{\beta}_1$ and $\hat{\beta}_2$ are *conditional effects*.
  - Interpreted where the other predictor is zero.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

Continuous Moderators

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

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



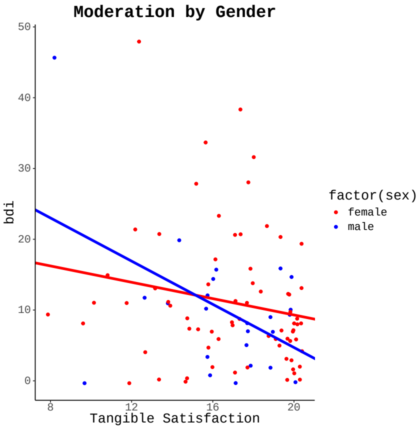
Categorical Moderators

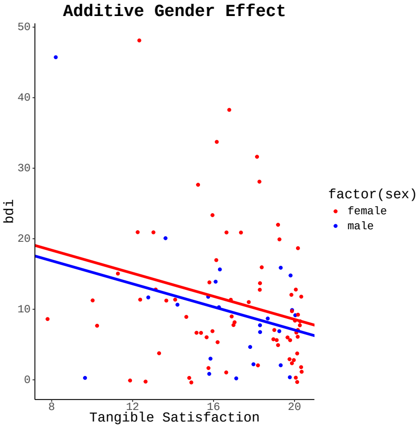
```
## Load data:
socSup <- readRDS("../data/social_support.rds")

## Estimate the moderated regression model:
out4 <- lm(bdi ~ tanSat * sex, data = socSup)
partSummary(out4, -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

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

$$\hat{Y}_{BDI} = 24.91 - 0.82X_{tsat} - 1.50Z_{male}$$





PREDICTION

Prediction Example

Let's fit the following model using the *diabetes* data:

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

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

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

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

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 Example

Two flavors of interval to quantify prediction uncertainty:

1. Confidence intervals
2. Prediction intervals

In our example, 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.

Model Fit

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

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

For the model we estimated in the above prediction example, we get:

$$R^2 = 1 - \frac{315383}{361704} \approx 0.13$$

Model Fit for Prediction

We use the *mean squared error* (MSE) to assess predictive performance.

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

For our example problem, we get:

$$
MSE = \frac{315383}{400} \approx 788.46
$$

Information Criteria

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

- Akaike's Information Criterion (AIC)

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

- Bayesian Information Criterion (BIC)

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

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

$$\begin{aligned} AIC &= 2(3) - 2(-1901.59) \\ &= 3813.18 \end{aligned}$$

$$\begin{aligned} BIC &= 3\ln(400) - 2(-1901.59) \\ &= 3833.14 \end{aligned}$$

LOGISTIC REGRESSION

Probabilities & Odds

Sex	Complete No	Yes
Female	95	147
Male	753	1540

$$P(C|M) = \frac{1540}{1540 + 753} = 0.672 \qquad O(C|M) = \frac{1540}{753} = 2.045 \approx \frac{0.672}{1 - 0.672}$$

$$P(C|F) = \frac{147}{147 + 95} = 0.607 \qquad O(C|F) = \frac{147}{95} = 1.547 \approx \frac{0.607}{1 - 0.607}$$

The Generalized Linear Model

Every GLM is built from three components:

1. The systematic component, η.
   - A linear function of the predictors, $\{X_p\}$.
   - Describes the association between $\mathbf{X}$ and Y.
2. The link function, $g(\mu_Y)$.
   - Transforms μ_Y so that it can take any value on the real line.
3. The random component, $P(Y|g^{-1}(\eta))$
   - The distribution of the observed Y.
   - Quantifies the error variance around η.

The Logistic Regression Model

The logistic regression model can be represented as:

$$Y \sim \text{Bin}(\pi, 1)$$

$$\text{logit}(\pi) = \beta_0 + \sum_{p=1}^{P} \beta_p X_p$$

The fitted model can be represented as:

$$\text{logit}(\hat{\pi}) = \hat{\beta}_0 + \sum_{p=1}^{P} \hat{\beta}_p X_p$$

To convert fitted values, $\hat{\eta} = \hat{\beta}_0 + \sum_{p=1}^{P} \hat{\beta}_p X_p$, from a logit scale to a probability scale, we apply the *logistic* function:

$$\text{logistic}(\hat{\eta}) = \frac{e^{\hat{\eta}}}{1 + e^{\hat{\eta}}}$$

Logistic Regression Example

```
## Coarsen the blood glucose variable:
diabetes %<>% mutate(highGlu = as.numeric(glu > 90))

## Estimate the model:
out1 <- glm(highGlu ~ age + bmi + bp, data = diabetes, family = binomial())
partSummary(out1, -c(1, 2))

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 610.42  on 441  degrees of freedom
Residual deviance: 538.18  on 438  degrees of freedom
AIC: 546.18

Number of Fisher Scoring iterations: 4
```

Assumptions

We can state the assumptions of logistic regression as follows:

1. The predictors are linearly related to $logit(\pi)$.
2. The predictor matrix is full-rank.
3. The outcome is iid binomial with mean $\pi_n = \text{logistic}\left(\eta_n\right)$.

Unlike linear regression, we don't need to assume

- Constant, finite error variance
- Normally distributed errors

For computational reasons, we also need the following:

- Large (enough) sample
- Relatively well-balance outcome
- No perfect prediction

Classification

Classification Example

Say we want to classify a new patient into either the “high glucose” group or the “not high glucose” group using the model fit above.

- Assume this patient has the following characteristics:
  - They are 57 years old
  - Their BMI is 28
  - Their average blood pressure is 92

First we plug their predictor data into the fitted model to get their model-implied η:

$$\begin{aligned}\hat{\eta} &= -6.479 + 0.035 \times 57 + 0.107 \times 28 + 0.023 \times 92 \\ &= 0.572\end{aligned}$$

Classification Example

Next we convert the predicted η value into a model-implied success probability by applying the logistic function:

$$\hat{\pi} = \text{logistic}(0.572) = \frac{e^{0.572}}{1 + e^{0.572}} = 0.639$$

Finally, to make the classification, assume a threshold of $\hat{\pi} = 0.5$ as the decision boundary.

- Because $0.639 > 0.5$ we would classify this patient into the “high glucose” group.

Confusion Matrix

	Predicted	
True	Low	High
Low	123	82
High	62	175

Confusion Matrix of Blood Glucose Level

$$Sensitivity = \frac{175}{175 + 62} = 0.738$$

$$Specificity = \frac{123}{123 + 82} = 0.6$$

$$Accuracy = \frac{175 + 123}{175 + 123 + 62 + 82} = 0.674$$

ROC Curve