

# **ETC3250/5250: Introduction to Machine Learning**

## **Review of regression**

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CALENDAR  
Week 2a



# Multiple Regression



$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \cdots + \beta_p X_{ip} + \varepsilon_i, \quad i = 1, \dots, n$$

- Each  $X_j$  is called a **predictor**, or independent variable or input variable.
- The coefficients  $\beta_1, \dots, \beta_p$  measure the **effect** of each predictor after taking account of the effect of all other predictors in the model.
- Predictors may be **transforms** of other predictors. e.g.,  $x_2 = x_1^2$ . Then the model form would be nonlinear. Categorical predictors need to be converted into dummy variables (see a few slides along).
- Once we **estimate** the model, we will have estimated coefficients  $\hat{\beta}_1, \dots, \hat{\beta}_p$ , predicted values,  $\hat{Y}$ , and residuals,  $e_i, i = 1, \dots, n$ .

# Multiple Regression

The model describes a **line, plane or hyperplane** in the predictor space.



(Chapter3/3.1.pdf)

The model describes a **line, plane or hyperplane** in the predictor space.



(Chapter3/3.5.pdf)

# Categorical Variables

Qualitative variables need to be converted to numeric, by making a set of dummy variables.

$$x_i = \begin{cases} 1 & \text{if } i^{\text{th}} \text{ obs is a koala} \\ 0 & \text{otherwise} \end{cases}$$

which would result in the model

$$\hat{y}_i = \begin{cases} \beta_0 + \beta_1 & \text{if } i^{\text{th}} \text{ obs is a koala} \\ \beta_0 & \text{otherwise} \end{cases}$$

# Categorical Variables

More than two categories

$$x_{i1} = \begin{cases} 1 & \text{if } i^{\text{th}} \text{ obs is a koala} \\ 0 & \text{otherwise} \end{cases}$$

$$x_{i2} = \begin{cases} 1 & \text{if } i^{\text{th}} \text{ obs is a bilby} \\ 0 & \text{otherwise} \end{cases}$$

which would result in the model using **dummy variables**.

$$\hat{y}_i = \begin{cases} \beta_0 + \beta_1 & \text{if } i^{\text{th}} \text{ obs is a koala} \\ \beta_0 + \beta_2 & \text{if } i^{\text{th}} \text{ obs is a bilby} \\ \beta_0 & \text{otherwise} \end{cases}$$

# Interactions are induced by categorical predictors



When you have a categorical variable, it can be convenient to allow **BOTH** slope and intercept to **vary** across category levels. This is called an **interaction**.



(Chapter3/3.7.pdf)

# Inference

- Is at least one of the predictors useful in predicting the response?
- Do all the predictors help to explain  $Y$ , or is only a subset of the predictors useful?
- How well does the model fit the data?
- Given a set of predictor values, what response value should we predict and how accurate is our prediction?

## Model fitting

Least squares is a common way to fit the model, where  $\hat{\beta}_j$  are chosen to minimise

$$RSS = \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

The smaller the sum of differences, the better the model fits the data.

## Goodness-of-fit

$R^2$  is the proportion of variation explained by the model, and measures the goodness of the fit, close to 1 the model explains most of the variability in  $Y$ , close to 0 it explains very little.

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

where  $TSS = \sum_{i=1}^n (y_i - \bar{y})^2$ . RSS is residual sum of squares, and TSS is total sum of squares.

## Model Diagnostics

Residual Standard Error (RSE) is an estimate of the standard deviation of  $\varepsilon$ . This is meaningful with the assumption that  $\varepsilon \sim N(0, \sigma^2)$ .

$$RSE = \sqrt{\frac{1}{n-p-1} RSS}$$

This is another way to examine the variation around the model. Unlike  $R^2$  it is not on a standard scale.

# Maximum Likelihood Estimation and Least Squares

If the errors are iid and normally distributed, then

$$Y \sim N(X\beta, \sigma^2 I)$$

So the likelihood is

$$L = \frac{1}{\sigma^n (2\pi)^{n/2}} \exp\left(-\frac{1}{2\sigma^2} \sum_{i=1}^n (Y_i - \hat{Y}_i)^2\right)$$

which is maximized when  $\sum_{i=1}^n (Y_i - \hat{Y}_i)^2$  is minimized.



MLE  $\equiv$  OLS.

# Significance tests

An  $F$ -test can be computed to assess if **any** predictor explains response, by testing this hypothesis

$$H_0 : \beta_1 = \beta_2 = \dots = \beta_p = 0 \text{ vs } H_a : \text{at least one is not 0}$$

where the test statistic is  $F = \frac{(TSS - RSS)/p}{RSS/(n-p-1)}$ .

## Individual variables

The strength of relationship between the response and an individual variable can be tested using a  $t$ -test for the hypothesis:

$$H_0 : \beta_j = 0 \text{ vs } H_a : \beta_j \neq 0$$

where the test statistic is  $t = \frac{\hat{\beta}_j}{SE(\hat{\beta}_j)}$

## Interpreting the effect of any predictor

We interpret  $\beta_j$  as the average effect on  $Y$  of a one unit increase in  $X_j$ , holding all other predictors fixed.



This is association and **not causation**.

# Assessing model fit using residuals

- If a plot of the residuals vs any predictor in the model shows a pattern, then the relationship is nonlinear.
- If a plot of the residuals vs any predictor **not** in the model shows a pattern, then the predictor should be added to the model.
- If a plot of the residuals vs fitted values shows a pattern, then there is heteroscedasticity in the errors. (Try a transformation, but may not fix.)



(Chapter3/3.9.pdf)

# Comparing models

An  $F$ -test can be computed to assess if **any additional** predictors significantly help to explain response, by testing this hypothesis

$$H_0 : \beta_{p-q+1} = \beta_{p-q+2} = \dots = \beta_p = 0 \text{ vs } H_a : \text{at least one is not 0}$$

where the test statistic is  $F = \frac{(RSS_0 - RSS)/q}{RSS/(n-p-1)}$ .

(We are considering a model with just  $q$  variables as opposed to all  $p$ .)

# Common pitfalls

1. Non-linearity of the response-predictor relationships.
2. Correlation of error terms.
3. Non-constant variance of error terms.
4. Outliers.
5. High-leverage points.
6. Collinearity.

# Example - Wages

Wage and other data for a group of 3000 male workers in the Mid-Atlantic region. Goal: Predict wage based on worker characteristics.

```
## Rows: 3,000
## Columns: 11
## $ year      <int> 2006, 2004, 2003, 2003, 2005, 2008, 2009, 2008, 2006, 2004
## $ age       <int> 18, 24, 45, 43, 50, 54, 44, 30, 41, 52, 45, 34, 35, 39, 54
## $ maritl    <fct> 1. Never Married, 1. Never Married, 2. Married, 2. Married
## $ race      <fct> 1. White, 1. White, 1. White, 3. Asian, 1. White, 1. White
## $ education <fct> 1. < HS Grad, 4. College Grad, 3. Some College, 4. College
## $ region    <fct> 2. Middle Atlantic, 2. Middle Atlantic, 2. Middle Atlantic
## $ jobclass   <fct> 1. Industrial, 2. Information, 1. Industrial, 2. Information
## $ health     <fct> 1. <=Good, 2. >=Very Good, 1. <=Good, 2. >=Very Good, 1. <
## $ health_ins <fct> 2. No, 2. No, 1. Yes, 1. Yes, 1. Yes, 1. Yes, 1. Yes, 1. Y
## $ logwage    <dbl> 4.318063, 4.255273, 4.875061, 5.041393, 4.318063, 4.845098
## $ wage       <dbl> 75.04315, 70.47602, 130.98218, 154.68529, 75.04315, 127.11
```

# Take a look

What do the following pairwise comparisons of the variables `year`, `age` and, `education` against `wage` show us?



# Take a look

If we examine `logwage` instead of `wage` as response variable - what changes?



# Take a look



- Examine the predictors. *Ideally values are spread out without any associations.*
- There is no evidence of any association between the predictors here.
- One category of "education" has much fewer observations than the others - this is not ideal.

# Model for wage data

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \varepsilon$$

where  $Y$  = `logwage`,  $X_1$  = `year`,  $X_2$  = `age`, and  $X_3$  = `education`.

# Fitting the model in R

```
library(broom)
library(parsnip)
library(kableExtra)
lm_mod <-
  linear_reg() %>%
  set_engine("lm")

fit <- lm_mod %>%
  fit(logwage~year+age+education, data=Wage)
```

# Parameter estimates

```
tidy(fit) %>%  
  kable(digits = 3) %>%  
  kable_styling(bootstrap_options = "striped", full_width = FALSE)
```

term	estimate	std.error	statistic	p.value
(Intercept)	-17.450	5.469	-3.191	0.001
year	0.011	0.003	3.952	0.000
age	0.006	0.000	11.447	0.000
education2. HS Grad	0.120	0.021	5.762	0.000
education3. Some College	0.244	0.022	11.115	0.000
education4. College Grad	0.368	0.022	16.894	0.000
education5. Advanced Degree	0.541	0.024	22.909	0.000

# Model fit

```
glance(fit) %>%  
  kable(digits = 2) %>%  
  kable_styling(bootstrap_options = "striped", full_width = FALSE)
```

r.squared	adj.r.squared	sigma	statistic	p.value	df	logLik	AIC	BIC	deviance	df.residual	nobs
0.26	0.26	0.3	178.09		0	6	-663.9	1343.8	1391.85	273.44	2993 3000

# Polynomial regression

A simple non-linear model can be achieved by adding polynomial terms, like

$$\text{mpg} = \beta_0 + \beta_1 \text{horsepower} + \beta_2 \text{horsepower}^2 + \varepsilon$$



(Chapter3/3.8.pdf,3.9.pdf)



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