Eltecon Data Science Course by Emarsys

Introduction to Prediction

Tamás Koncz

November 4, 2020

Homeworks from last week

- Im Seongwon - Kim Yeonggyeong
- Szőnyi Máté - Tran, Dung
- Sármány Áron - Schmall Róbert

Goal of the lesson

- Understand what *prediction* is, and how it differs from *causal inference*
- Try basic `R` commands for fitting & evaluating simple regression and classification models

Section 1

What is prediction?

What is prediction?

You have an assumed relationship:

$$Y \approx f(X) + \epsilon$$

where:

- Y is your target variable
- X are your predictors
- $f()$: is the relationship between X and Y
- ϵ: is the irreducible error

Prediction is:

- estimating $f()$ based on the available observations (X) ...
- **... to minimize the error** $E(Y - \hat{Y})$

Error metric: RMSE

- Root Mean Square Error (RMSE)
- It is the standard deviation of the residuals i.e. prediction errors
- RMSE penalizes the model for large errors

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

Bike rental - the dataset

- Source: Kaggle
- Goal: Predict the total count of bikes rented during each hour

count	season_1	season_2	workingday	holiday	hour	weather_1	weather_2	temp	atemp	humidity	windspeed
16	TRUE	FALSE	0	0	0	TRUE	FALSE	9.84	14.395	81	0.0000
40	TRUE	FALSE	0	0	1	TRUE	FALSE	9.02	13.635	80	0.0000
32	TRUE	FALSE	0	0	2	TRUE	FALSE	9.02	13.635	80	0.0000
13	TRUE	FALSE	0	0	3	TRUE	FALSE	9.84	14.395	75	0.0000
1	TRUE	FALSE	0	0	4	TRUE	FALSE	9.84	14.395	75	0.0000
1	TRUE	FALSE	0	0	5	FALSE	TRUE	9.84	12.880	75	6.0032

Bike rental - variables

field	description
season	1 = spring, 2 = summer, 3 = fall, 4 = winter
holiday	whether the day is considered a holiday
workingday	whether the day is neither a weekend nor holiday
weather	1 ~ Clear, 2 ~ Cloudy, 3 ~ Light Rain, 4 ~ Heavy Rain
temp	temperature in Celsius
atemp	feels like temperature in Celsius
humidity	relative humidity
windspeed	wind speed
count	number of total rentals

Benchmark “model”

```
calculateRMSE <- function(actual, predictions) {
  sqrt(mean((actual - predictions) ^ 2))
}
```

```
predictions_benchmark_model <- rep(
  bike_sharing_train[, mean(count)], bike_sharing_train[, .N]
)

bike_sharing_benchmark_model_rmse <- calculateRMSE(
  actual = bike_sharing_train$count,
  predictions = predictions_benchmark_model
)

bike_sharing_benchmark_model_rmse
```

```
## [1] 170.2384
```

Section 2

Regression

Linear regression

When to use it:

- We want to estimate a numerical target (e.g. price)
- Assuming an approximate linear relationship between X and Y

Simple linear regression formula:

$$\hat{Y} = \beta_0 + \beta_1 X$$

The OLS estimate for β will conveniently minimize RMSE for us for given X!

(So what is Machine Learning?)

"A computer program is said to ***learn from experience*** *E with respect to some class of tasks T and performance measure P,* ***if its performance*** *at tasks in T, as measured by P,* ***improves with experience*** *E."* (Tom Mitchell)

Bike rental - minimal model

```r
bike_sharing_min_model <- glm(
  formula = count ~ atemp,
  family = gaussian,
  data = bike_sharing_train
)
```

Bike rental - minimal model

```r
summary(bike_sharing_min_model)
```

```
##
## Call:
## glm(formula = count ~ atemp, family = gaussian, data = bike_sharing_train)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -282.73  -103.86   -27.63    72.96   709.89
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) -19.5412     4.6755   -4.18 2.95e-05 ***
## atemp         8.3048     0.1841   45.10  < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for gaussian family taken to be 23649.64)
##
##     Null deviance: 261264747  on 9014  degrees of freedom
## Residual deviance: 213154213  on 9013  degrees of freedom
## AIC: 116378
##
## Number of Fisher Scoring iterations: 2
```

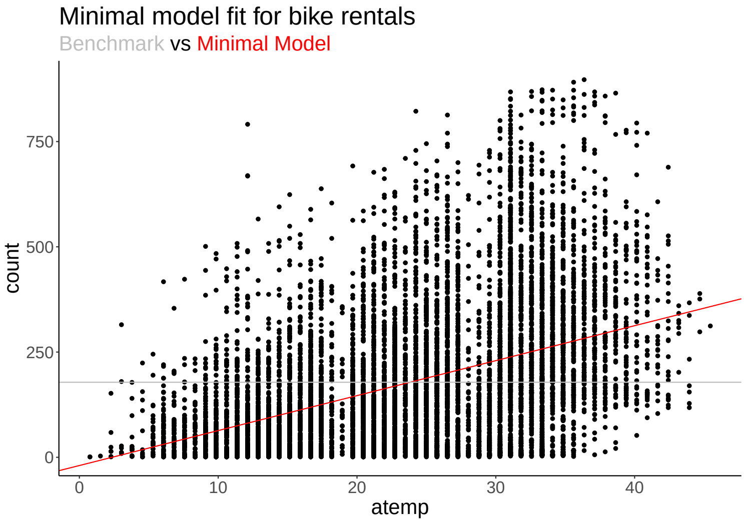
Bike rental - minimal model - coefficients

```
str(bike_sharing_min_model$coefficients)
```

```
##  Named num [1:2] -19.5 8.3
##  - attr(*, "names")= chr [1:2] "(Intercept)" "atemp"
```

```
intercept <- bike_sharing_min_model$coefficients[1]
slope <- bike_sharing_min_model$coefficients[2]
```

Bike rental - minimal model - predictive fit



Bike rental - minimal model - prediction error

```
predictions_min_model <- predict.glm(
  bike_sharing_min_model, newdata = bike_sharing_train
)

predictions_min_model[1:5]
```

```
##         1         2         3         4         5
## 100.00620  93.69456  93.69456 100.00620 100.00620
```

```
bike_sharing_train[1:5, count]
```

```
## [1] 16 40 32 13  1
```

Bike rental - minimal model - prediction error

```
calculateRMSE <- function(actual, predictions) {
  sqrt(mean((actual - predictions) ^ 2))
}
```

```
bike_sharing_min_model_rmse <- calculateRMSE(
  actual = bike_sharing_train[, count],
  predictions = predictions_min_model
)

bike_sharing_min_model_rmse
```

```
## [1] 153.7673
```

Bike rental - improving predictions

```r
bike_sharing_2nd_model <- glm(
  formula = count ~ atemp + humidity,
  data = bike_sharing_train
)

predictions_2nd_model <- predict.glm(
  bike_sharing_2nd_model, newdata = bike_sharing_train
)

calculateRMSE(
  actual = bike_sharing_train[, count],
  predictions = predictions_2nd_model
)
```

```
## [1] 144.5333
```

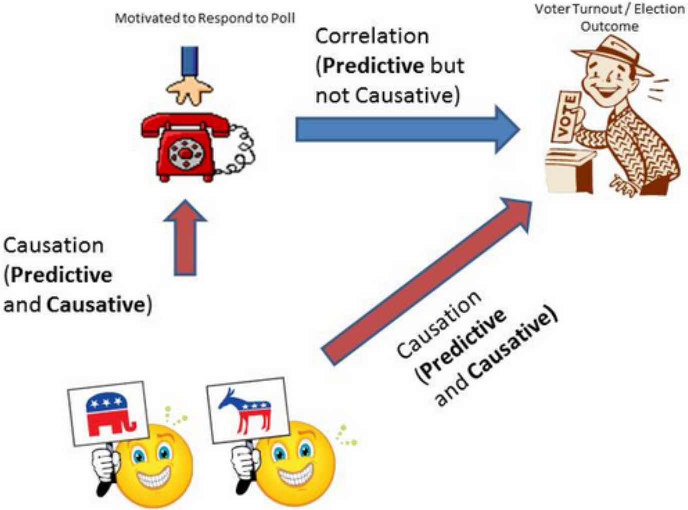
Practice time

- Task: improve the model to be as accurate as possible!
- Share your regression formula + achieved RMSE in Socrative!
- You have 20 minutes - feel free to take a break if needed.

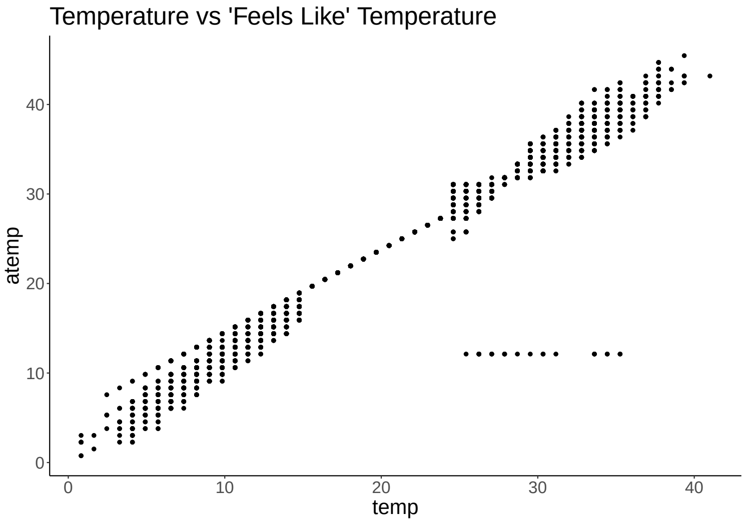
Practice time

DEMO - 1 SOLUTION

Don't worry about Confounding!



Don't worry about Confounding!



Why should you still care about model inputs?

- Model explainability is often desirable in business (and other applications)
- Example: Google Flu Trends
- Emarsys example: all models are retrained every 30 days

Section 3

Classification

Binary classification

- Binary: target can take on two values (0 or 1)
- Typical example is predicting if an event is happening or not
- Examples:
  - Patient has a medical condition or not
  - Loan will be repaid in full
  - User will make a purchase in the next 30 days (BPS - Buying Probability Score)

Question time

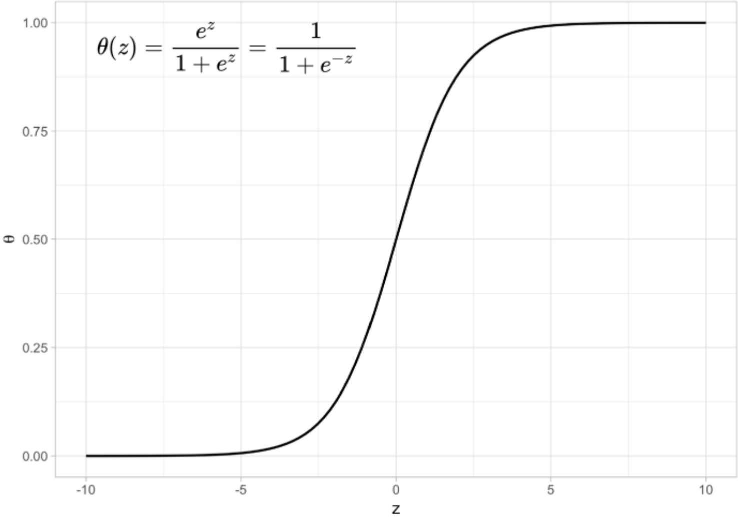
- **Why should we not use linear regression for binary classification**?
- Please record your answers in Socrative!
- You have 5 minutes

Logistic regression

- A linear model makes continuous predictions that are unbounded.
- In classification, we are interested in the probability of an outcome occurring
- So we want **predictions that are bounded between 0 and 1.**

$$Pr(Y_i = 1|X_i) = \frac{exp(\beta_0 + \beta_1 X_i)}{1 + exp(\beta_0 + \beta_1 X_i)}$$

The sigmoid function



The Titanic dataset

```
install.packages("titanic")
library(titanic)
head(titanic_train)
```

PassengerId	Survived	Pclass	Name	Sex	Age	SibSp	Parch	Ticket	Fare	Cabin	Embarked
1	0	3	Braund, Mr. Owen Harris	male	22	1	0	A/5 21171	7.2500		S
2	1	1	Cumings, Mrs. John Bradley (Florence Briggs Thayer)	female	38	1	0	PC 17599	71.2833	C85	C
3	1	3	Heikkinen, Miss. Laina	female	26	0	0	STON/O2. 3101282	7.9250		S
4	1	1	Futrelle, Mrs. Jacques Heath (Lily May Peel)	female	35	1	0	113803	53.1000	C123	S
5	0	3	Allen, Mr. William Henry	male	35	0	0	373450	8.0500		S
6	0	3	Moran, Mr. James	male	NA	0	0	330877	8.4583		Q

Example - binary model

```
model <- glm(
    Survived ~ Fare,
    data = titanic_train,
    family = binomial(link = "logit")
)
```

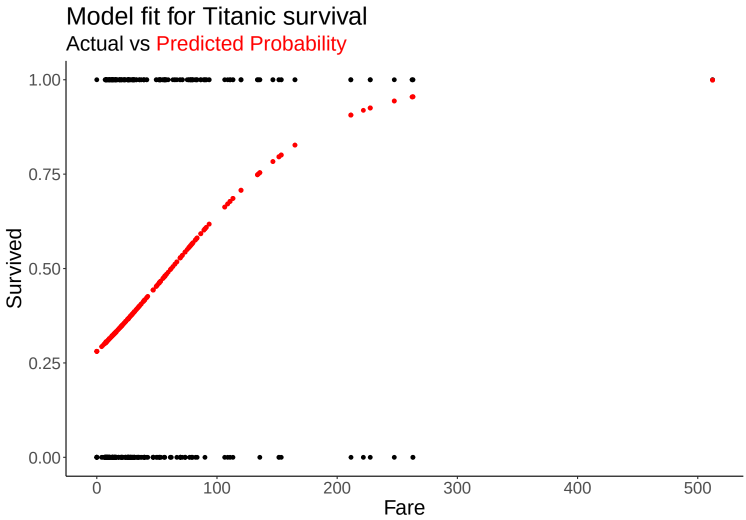
Making predictions

```
predicted_prob <- predict.glm(
  model,
  newdata = titanic_train,
  type = "response"
)

predicted_prob[1:5]
```

```
##         1         2         3         4         5
## 0.3034014 0.5354287 0.3055738 0.4664564 0.3059770
```

Predictive fit



Converting probabilities to predictions

```
titanic_train[1:5, "Survived"]
```

```
## [1] 0 1 1 1 0
```

Using `cutoff = 0.5`:

```
predicted_class <- ifelse(predicted_prob > 0.5, 1, 0)
predicted_class[1:5]
```

```
## 1 2 3 4 5
## 0 1 0 0 0
```

Evaluating binary models - Accuracy

```r
calculateAccuracy <- function(actual, predicted) {
    N <- length(actual)
    accuracy <- sum(actual == predicted) / N

    return(accuracy)
}
```

```r
calculateAccuracy(titanic_train$Survived, predicted_class)
```

```
## [1] 0.6655443
```

Evaluating binary models - Confusion Matrix

```
table(
  titanic_train$Survived,
  predicted_class,
  dnn = c("actual", "predicted")
)
```

```
##        predicted
## actual    0   1
##      0 511  38
##      1 260  82
```

Practice time

- Task: improve the model to be as accurate as possible!
- Share your regression formula + achieved Accuracy & Confusion Matrix in Socrative!
- You have 20 minutes - feel free to take a break if needed.

Practice time

DEMO - 1 SOLUTION

Section 4

Generalization performance

Why do we care?

- It's easy to predict something we already know...
- Actually, it would be silly to build predictive models to predict what we already know!
- What we are after is **out-of-sample** performance

Example on the Bike Sharing dataset

```r
simple_model <- glm(
  count ~ hour + temp + workingday,
  data = bike_sharing_train
)
```

Accuracy on our training data

```
simple_model_predictions <- predict.glm(
  simple_model,
  newdata = bike_sharing_train
)

calculateRMSE(bike_sharing_train$count, simple_model_predictions)
```

```
## [1] 141.4175
```

Accuracy out-of-sample

```
bike_sharing_test <- fread("bike_sharing_test.csv")

simple_model_predictions <- predict.glm(
  simple_model,
  newdata = bike_sharing_test
)

calculateRMSE(bike_sharing_test$count, simple_model_predictions)
```

```
## [1] 208.0325
```

Section 5

Homework

Homework - Final project

- **Have a high level outline of how you plan to answer your research question**
- Should be around half a page
- Can be in bullet point format: our goal is to make sure you have a question and some idea how to answer it
- Please send it email to us - no need to present next week

Homework - prediction

- If you haven't finished the binary classification practice, do so.
  - Create at least two models to predict Titanic Survival
  - Show your Logit formulas, and the achieved Accuracy & Confusion Matrix!
  - Reason why you would use one model or another if you had to perform an out-of-sample prediction
  - (No right or wrong answers!)
- Presenters:
  - Alexandrov Dániel - Földesi Attila
  - Nguyen Thai Duong - Szentistványi János
  - Kovács Ádám - Nguyen Nam Son