# Validating Models

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DATA 2010—Tools and Techniques in Data Science

# Lecture Objectives

- Understand the difference between training and test data.
- Describe the workflow of model evaluation.
- Compute the different metrics used in model evaluation.

# Motivation

- After building a model, you should probably ask yourself **is it any good**?
    - Or **could you improve it**?
    - Or given two models, **which one is the best**?
- In this lecture, we will discuss strategies for validating and evaluating a model.
- These ideas will be important for the rest of the semester, when we actually start building models!

# Basic setup i

- Models typically have parameters that need to be estimated.
    - E.g. regression coefficients in linear regression; decision rules in classification trees.
- With data-driven models, we learn (or estimate) these parameters using data.
    - This dataset is called the **training dataset**.
- Some models are very expressive and do a great job of describing the training data.
- But what we want is to apply the model to *new data*.
- Therefore, when we evaluate models, we want to do it on a separate dataset.

# Basic setup ii

    - This separate dataset is called the **test dataset**.
- The workflow is as follows:
    - Train model on *training data*.
    - Validate/evaluate on *test data*.
    - When changing the model, go back to the *training data*.
- **Note**: there is always a risk of being overconfident in our model if we look at the test data.
    - You could implicitly or explicitly start optimizing for the test data...
- Best practice: build several models using the training data, then evaluate all at the same time.

# Classification vs Regression

- We will discuss several ways to evaluate models.
- These metrics usually depend on the task at hand.
- **Classification**: The model outputs a class label (e.g. cats, dogs, birds, etc.)
- **Regression**: The model outputs a numerical value (e.g. predicted value of stock, probability of rain, etc.)

# Evaluating Classifiers

- Correct vs Incorrect classification for binary classifiers:

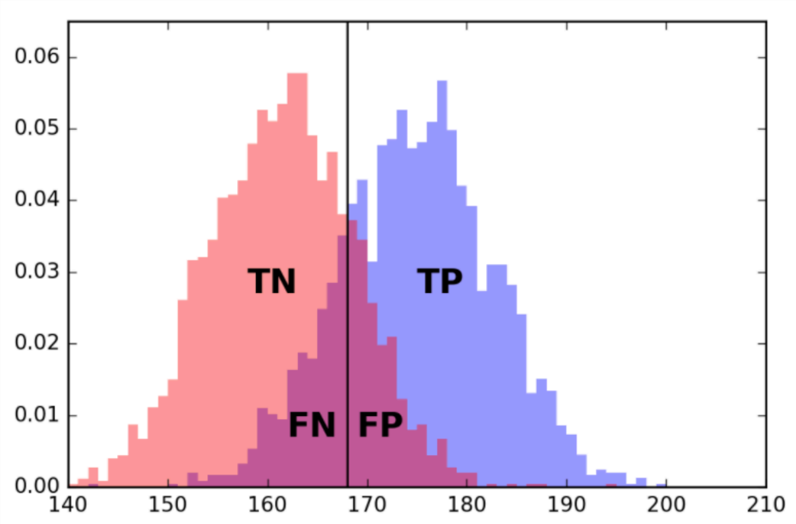
| | | Predicted Class | |
|---|---|---|---|
| | | Yes | No |
| Actual Class | Yes | TP | FN |
| | No | FP | TN |

- This is sometimes called a **confusion matrix**.

# Threshold classifiers i

- Some classifiers are built by taking a *score* and using a threshold:
  - If the score is greater than threshold, then classify as positive.
  - If the score is lower than threshold, then classify as negative.
- To choose a threshold, we would want to maximize the number of TPs and TNs, while minimizing the number of FPs and FNs.
  - On the test data!

# Threshold classifiers ii



# Accuracy

- **Accuracy** is the ratio of correct predictions over total predictions:

$$\text{Accuracy} = \frac{TP + TN}{TP + FP + FN + TN}.$$

- In balanced datasets (i.e. same number of observations in each class), randomly guessing will have an accuracy of 50%.
- In highly unbalanced datasets (e.g. 95% of observations are from a single class), then always guessing the majority class will lead to high accuracy...

# Precision

- Also called **Positive Predictive Value**: proportion of correct calls among the positive calls.

$$\text{Precision} = \frac{TP}{TP + FP}.$$

- In medicine: probability of having the disease, given that the test was positive.

# Exercise

Assume we have 100 observations: 90 are negative and 10 are positive. What would be the accuracy and the precision of:

- Someone making random guesses (with equal probability for each class)?
- Someone always guessing positive?

# Solution i

Let's start with random guesses:

- out of the 90 negative observations, we would expect 45 would be TNs and 45 would be FPs.
- out of the 10 positive observations, we would expect 5 would be TPs and 5 would be FNs.

$$\begin{aligned}
\text{Accuracy} &= \frac{TP+TN}{TP+FP+FN+TN} &= \frac{50}{100} = 50\%, \\
\text{Precision} &= \frac{TP}{TP+FP} &= \frac{5}{50} = 10\%.
\end{aligned}$$

# Solution ii

Now let's consider all positive guesses:

- out of the 90 negative observations, we would expect 0 would be TNs and 90 would be FPs.
- out of the 10 positive observations, we would expect 10 would be TPs and 0 would be FNs.

$$
\begin{aligned}
\text{Accuracy} &= \frac{TP + TN}{TP + FP + FN + TN} &&= \frac{10}{100} = 10\%, \\
\text{Precision} &= \frac{TP}{TP + FP} &&= \frac{10}{100} = 10\%.
\end{aligned}
$$

# Solution iii

What would happen to precision if someone always guesses negative?

# Recall

- Also called **Sensitivity** and **hit rate**: proportion of correct calls among the positive observations.

$$\mathrm{Recall} = \frac{TP}{TP + FN}.$$

- Don't confuse this with precision, even if they look similar. Think of conditional probabilities.
- Someone always guessing positive will have perfect recall...

# F-score

- The **F-score** is a way to balance precision and recall.

$$\text{F-score} = 2\frac{\text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}}.$$

- The F-score is actually the *harmonic mean* of precision and recall.
    - And the harmonic mean is always less than or equal to the (usual) arithmetic mean.

# Exercise

Given the same setting as the previous exercise, compute the recall and F-score for the two classifiers.

# General comments

- Accuracy is generally misleading with unbalanced test data.
- High precision is difficult to achieve with unbalanced test data.
    - Even minimal error can lead to a large number of FPs.
- The F-score is a good way to balance all these things.
- **Recommendation**: Compute and report all metrics.

# Evaluating Regression Models

- In regression problems, for each observation in the test data, we will have
    - A predicted value, coming from the model.
    - An actual/observed value, coming from the test data.
- In evaluating a regression model, we want to assess how *close* the predicted values are to the observed values.
    - Think distance metrics.

# Numerical Errors i

- We will use $f_i$ for the $i$-th predicted (or forecasted) value, and $o_i$ for the corresponding observed value.
- Mean Squared Error: Average of squared differences:

$$\mathrm{MSE} = \frac{1}{n} \sum_{i=1}^{n} \left(f_i - o_i\right)^2 .$$

- The RMSE is the square root of the MSE.
  - And it is on the same scale as the observations, so easier to interpret.

# Numerical Errors ii

- **Mean Absolute Error**: Average of absolute differences:

$$\mathrm{MAE} = \frac{1}{n}\sum_{i=1}^{n}\left|f_i - o_i\right|.$$

- **Mean Absolute Percentage Error**: Average of absolute *relative* differences:

$$\mathrm{MAPE} = \frac{1}{n}\sum_{i=1}^{n}\left|\frac{f_i - o_i}{o_i}\right|.$$

# Numerical Errors iii

- MAPE is typically reported on the percentage scale.
    - Easier to interpret over multiple scale/problems, but can run into problems with small observed values.

# Example i

- We will use the famous prostate cancer dataset.

```
url <- paste0("https://web.stanford.edu/~hastie/",
              "ElemStatLearn/datasets/prostate.data")
data <- read.table(url)

names(data)
```

```
## [1] "lcavol" "lweight" "age" "lbph" "svi"
"lcp" "gleason"
## [8] "pgg45" "lpsa" "train"
```

# Example ii

```r
# Separate train and test
library(tidyverse)
count(data, train)
```

```
##   train  n
## 1 FALSE 30
## 2  TRUE 67
```

```r
data_train <- filter(data, train)
data_test <- filter(data, train)
```

# Example iii

- We will build a simple regression model for predicting the log-PSA value (`lpsa`):
    - We always predict the sample mean from the training data.
- We will look at better models in the next lectures.

```
prediction <- data_train |>
  pull(lpsa) |>
  mean(na.rm = TRUE)

prediction
```

```
## [1] 2.452345
```

# Example iv

```
# Now compute metrics----
actual_vals <- pull(data_test, lpsa)
# MSE
mse <- mean((actual_vals - prediction)^2)
rmse <- sqrt(mse)

c(mse, rmse)
```

```
## [1] 1.437036 1.198765
```

# Example v

```r
# MAE
mae <- mean(abs(actual_vals - prediction))
mae
```

```
## [1] 0.9610855
```

```r
# MAPE
ratios <- (actual_vals - prediction)/actual_vals
mape <- 100*mean(abs(ratios))
mape
```

```
## [1] 124.9439
```

# Example vi

```
# All together
c(mse, rmse, mae, mape)
```

```
## [1] 1.4370365 1.1987646 0.9610855 124.9438741
```

- MAPE is the only one we can interpret without more context—and it's large!