Evauluation Metrics

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2025-07-31

Evaluation metrics

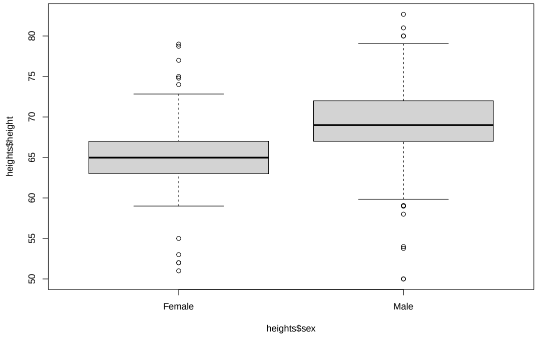
Before we start describing approaches to optimize the way we build algorithms, we first need to define what we mean when we say one approach is better than another. We use the caret package and the height data in dslabs.

```r
library(tidyverse)
library(caret)
library(dslabs)
data(heights)
```

Evaluation metrics

To summarize the data, consider the following boxplot:

```
boxplot(heights$height~heights$sex)
```



Evaluation metrics

We will start with a simple example: suppose we want to predict sex using height. We start by defining the outcome and predictors.

```
y <- heights$sex
x <- heights$height
```

Evaluation metrics

In this case, we have only one predictor, height, and `y` is clearly a categorical outcome since observed values are either `Male` or `Female`.

We know that we will not be able to predict Y very accurately based on X because male and female average heights are not that different relative to within group variability. But can we do better than guessing? To answer this question, we need a quantitative definition of better.

Training and test sets

A machine learning algorithm is evaluated on how it performs in the real world with completely new datasets. Te typically split the data into two parts and act as if we don't know the outcome for one of these. We refer to the group for which we know the outcome, and use to develop the algorithm, as the **training** set. We refer to the group for which we pretend we don't know the outcome as the **test** set.

Training and test sets

The caret package includes the function createDataPartition for randomly splitting the data into training and test sets:

```r
set.seed(2007)
test_index <- createDataPartition(y, times = 1,
                                  p = 0.5, list = FALSE)
```

The argument times defines how many random samples of indexes to return, p is thr proportion of the data is represented by the index, and list decides if we want the indexes returned as a list or not.

Training and test sets

We can define the training and test sets like this:

```
test_set <- heights[test_index, ]
train_set <- heights[-test_index, ]
```

We develop an algorithm using **only** the training set. Once we are done developing the algorithm, we will **freeze** it and evaluate it using the test set. The simplest way to evaluate the algorithm is to use the **overall accuracy**.

Overall accuracy

To demonstrate the use of overall accuracy, let’s start by developing the simplest possible machine algorithm: guessing the outcome.

```r
y_hat <- sample(c("Male", "Female"),
                length(test_index), replace = TRUE)
```

We are completely ignoring the predictor and simply guessing the sex.

Overall accuracy

R functions developed for machine learning usually require that categorical outcomes be coded as factors. So convert `y_hat` to factors:

```r
y_hat <- sample(c("Male", "Female"),
                length(test_index), replace = TRUE) %>%
  factor(levels = levels(test_set$sex))
```

Overall accuracy

The *overall accuracy* is simply the proportion predicted correctly:

```r
mean(y_hat == test_set$sex)
```

```
## [1] 0.5104762
```

Not surprisingly, our accuracy is about 50%. We are guessing!

Overall accuracy

Can we do better? Exploratory data analysis suggests we can because, on average, males are slightly taller than females:

```r
heights %>% group_by(sex) %>%
  summarize(mean(height), sd(height))
```

```
## # A tibble: 2 x 3
##   sex    `mean(height)` `sd(height)`
##   <fct>           <dbl>        <dbl>
## 1 Female           64.9         3.76
## 2 Male             69.3         3.61
```

Overall accuracy

Let's try another simple approach: predict `Male` if height is within two standard deviations from the average male:

```r
y_hat <- ifelse(x > 62, "Male", "Female") %>%
  factor(levels = levels(test_set$sex))
```

The accuracy goes up from 0.50 to about 0.80:

```r
mean(y == y_hat)
```

```
## [1] 0.7933333
```

Overall accuracy

But can we do even better? In the example above, we used a cutoff of 62, but we can examine the accuracy obtained for other cutoffs and then pick the value that provides the best results.

But remember, **it is important that we optimize the cutoff using only the training set**: the test set is only for evaluation.

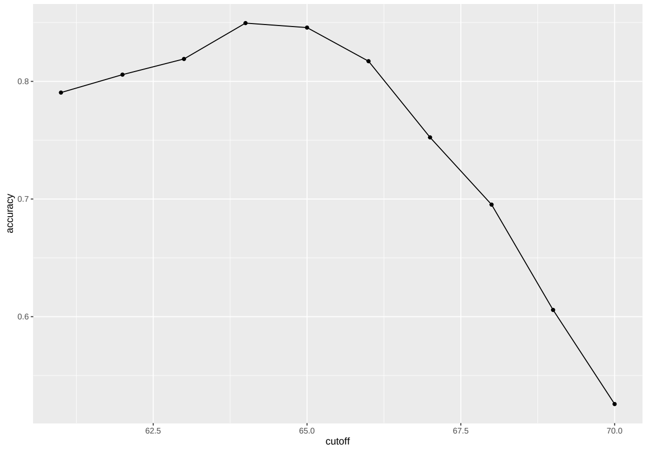
Overall accuracy

We can examine the accuracy of 10 different cutoffs and pick the one yielding the best result:

```r
cutoff <- seq(61, 70)
accuracy <- map_dbl(cutoff, function(x){
  y_hat <- ifelse(train_set$height > x, "Male", "Female") %>%
    factor(levels = levels(test_set$sex))
  mean(y_hat == train_set$sex)
})
```

We can make a plot showing the accuracy obtained on the training set for males and females:

Overall accuracy



Overall accuracy

We see that the maximum value is:

```
max(accuracy)
```

```
## [1] 0.8495238
```

The cutoff resulting in this accuracy is:

```
best_cutoff <- cutoff[which.max(accuracy)]
best_cutoff
```

```
## [1] 64
```

Overall accuracy

We can now test this cutoff on our test set to make sure our accuracy is not overly optimistic:

```r
y_hat <- ifelse(test_set$height >
  best_cutoff,"Male","Female") %>%
  factor(levels = levels(test_set$sex))
y_hat <- factor(y_hat)
mean(y_hat == test_set$sex)
```

```
## [1] 0.8038095
```

The confusion matrix

Generally speaking, overall accuracy can be a deceptive measure. We construct the *confusion matrix*. We can do this in R using the function `table`:

```r
table(predicted = y_hat, actual = test_set$sex)
```

```
##            actual
## predicted Female Male
##    Female     48   32
##    Male       71  374
```

The confusion matrix

If we study this table closely, it reveals a problem. If we compute the accuracy separately for each sex, we get:

```
test_set %>%
  mutate(y_hat = y_hat) %>%
  group_by(sex) %>%
  summarize(accuracy = mean(y_hat == sex))
```

```
## # A tibble: 2 x 2
##   sex    accuracy
##   <fct>     <dbl>
## 1 Female    0.403
## 2 Male      0.921
```

The confusion matrix

There is an imbalance in the accuracy for males and females: too many females are predicted to be male. This is because the **prevalence** of males in this dataset is high:

```r
prev <- mean(y == "Male")
prev
```

```
## [1] 0.7733333
```

The confusion matrix

So when computing overall accuracy, the high percentage of mistakes made for females is outweighed by the gains in correct calls for men. **This can actually be a big problem in machine learning.**

Sensitivity and specificity

We name the four entries of the **confusion matrix**:

	Actually Positive	Actually Negative
Predicted positive	True positives (TP)	False positives (FP)
Predicted negative	False negatives (FN)	True negatives (TN)

Sensitivity and specificity

Sensitivity is typically quantified by $TP/(TP + FN)$, the proportion of actual positives (the first column $= TP + FN$) that are called positives (TP). This quantity is referred to as the **true positive rate** (TPR) or **recall**.

Sensitivity and specificity

Specificity is defined as $TN/(TN+FP)$ or the proportion of negatives (the second column $= FP + TN$) that are called negatives (TN). This quantity is also called the true negative rate (TNR).

Sensitivity and specificity

There is another way of quantifying accuracy which is $TP/(TP + FP)$ or the proportion of outcomes called positives (the first row or $TP + FP$) that are actually positives (TP). This quantity is referred to as **positive predictive value (PPV)** and also as **precision**. Note that, unlike TPR and TNR, precision depends on prevalence since higher prevalence implies you can get higher precision even when guessing.

Sensitivity and specificity

The multiple names can be confusing, so we include a table to help us remember the terms. The table includes a column that shows the definition if we think of the proportions as probabilities.

Measure of	Name 1	Name 2	Definition	Probability representation
sensitivity	TPR	Recall	$\frac{\text{TP}}{\text{TP+FN}}$	$\Pr(\hat{Y} = 1 \mid Y = 1)$
specificity	TNR	1-FPR	$\frac{\text{TN}}{\text{TN+FP}}$	$\Pr(\hat{Y} = 0 \mid Y = 0)$
Precision	PPV		$\frac{\text{TP}}{\text{TP+FP}}$	$\Pr(Y = 1 \mid \hat{Y} = 1)$

Here TPR is True Positive Rate, FPR is False Positive Rate, and PPV is Positive Predictive Value.

Sensitivity and specificity

he caret function confusionMatrix computes all these metrics for us once we define what category “positive” is. The function expects factors as input, and the first level is considered the positive outcome or $Y = 1$. In our example, Female is the first level because it comes before Male alphabetically. If you type this into R you will see several metrics including accuracy, sensitivity, specificity, and PPV.

```r
cm <- confusionMatrix(data = y_hat,
                      reference = test_set$sex)
```

Sensitivity and specificity

You can access these directly, for example, like this:

```
cm$overall["Accuracy"]
```

```
##  Accuracy
## 0.8038095
```

```
cm$byClass[c("Sensitivity","Specificity", "Prevalence")]
```

```
## Sensitivity Specificity  Prevalence
##   0.4033613   0.9211823   0.2266667
```

Sensitivity and specificity

We can see that the high overall accuracy is possible despite relatively low sensitivity. As we hinted at above, the reason this happens is because of the low prevalence (0.23): the proportion of females is low. Because prevalence is low, failing to predict actual females as females (low sensitivity) does not lower the accuracy as much as failing to predict actual males as males (low specificity).

Session Info

```r
sessionInfo()
```

```
## R version 4.5.1 (2025-06-13)
## Platform: aarch64-apple-darwin20
## Running under: macOS Sequoia 15.5
##
## Matrix products: default
## BLAS:   /Library/Frameworks/R.framework/Versions/4.5-arm64/Resources/lib/libRblas.0.dylib
## LAPACK: /Library/Frameworks/R.framework/Versions/4.5-arm64/Resources/lib/libRlapack.dylib;  LAPACK version 3.12.1
##
## locale:
## [1] en_US.UTF-8/en_US.UTF-8/en_US.UTF-8/C/en_US.UTF-8/en_US.UTF-8
##
## time zone: America/New_York
## tzcode source: internal
##
## attached base packages:
## [1] stats     graphics  grDevices utils     datasets  methods   base
##
## other attached packages:
##  [1] dslabs_0.8.0    caret_7.0-1     lattice_0.22-7  lubridate_1.9.4
##  [5] forcats_1.0.0   stringr_1.5.1   dplyr_1.1.4     purrr_1.1.0
##  [9] readr_2.1.5     tidyr_1.3.1     tibble_3.3.0    ggplot2_3.5.2
## [13] tidyverse_2.0.0
##
## loaded via a namespace (and not attached):
##  [1] tidyselect_1.2.1     viridisLite_0.4.2    timeDate_4041.110
```