The Role of Hyperparameters in Machine Learning Models and How to Tune Them (PSRM, 2023)

Christian Arnold, Luka Biedebach, Andreas Küpfer, and Marcel Neunhoeffer 2023-07-05

```
#install.packages("pacman")
pacman::p_load(here)
setwd(here::here())
# Figure 1
# Do you want to save the plot to disk at the end?
save_plot <- TRUE</pre>
plot_path <- "results/bivariate_example.png"</pre>
# Set seed for replicability (seed is date of our last run)
set.seed(12102021)
# Generate the true data
x <- rnorm(1000)
y \leftarrow 1 + x + 0.8 * x ^2 + 0.3 * x ^3 + rnorm(1000, 0, 2)
df <- data.frame(y, x)</pre>
# Set the number of folds for cross validation
n folds <- 10
# Generate fold ids
fold <- sample(rep(1:n_folds, nrow(df) %/% n_folds))</pre>
# Set up search grid. Here with only lambda to tune it is just a vector
search_grid <- 1:10
# Initialize object to collect results
res <- list()
# Loop over search_grid and calculate cross validation error
for (lambda in search_grid) {
  # Initialize object for results of one hyperparameter setting
  tmp <- NULL
```

```
# Start cross validation loop
  for (cv in 1:n_folds) {
    # Subset data to training folds and test fold
    train <- df[fold != cv, ]</pre>
    test <- df[fold == cv,]
    # Train model with current hyperparameter setting
    reg <- lm(y ~ poly(x, lambda, raw = T), data = train)</pre>
    # Make prediction with trained model on test set
    pred <- predict(reg, newdata = test)</pre>
    # Calculate error and store results
    tmp <- c(tmp, mean((test$y - pred) ^ 2))</pre>
  }
  # Store results of run in res object
  res[[paste0(lambda)]] <- tmp</pre>
}
# Get best hyperparameter setting. Here minimal cross validation error.
# Calculate average cross validation error for each value of lambda
avg_cv_error <- sapply(res, mean)</pre>
# Get the value of lambda with the minimal average cross validation error
best_lambda <- as.numeric(names(avg_cv_error)[avg_cv_error == min(avg_cv_error)])
# Plot results of linear regression (lambda = 1) and best model
plot(df$x, df$y, bty = "n", las = 1, ylab = "Y", xlab = "X", col = viridis::viridis(4, 0.4)[1], pch = 1
reg \leftarrow lm(y~poly(x, 1, raw = T), data = df)
q \leftarrow seq(-4, 4, 0.01)
lines(q, predict(reg, data.frame(x = q)), col = viridis::viridis(4, 0.7)[2], lwd = 3)
# Retrain model with best lambda on entire training data
reg <- lm(y~poly(x, best_lambda, raw = T), data = df)</pre>
lines(q, predict(reg, data.frame(x = q)), col = viridis::viridis(4, 0.7)[3], lwd = 3)
```

```
25 -
     20 -
     15 ·
     10 ·
       5
      0
     -5
                                                                 2
            -4
                              -2
                                                0
                                                                                   4
                                                Χ
if(save_plot){
  dev.copy(png, filename = plot_path, width = 695, height = 450)
  dev.off()
}
## pdf
##
     2
# Table 1
dat.temp <- read.csv("data/annotations_march22_2023.csv", sep = ',', header = TRUE)</pre>
dat <- subset(dat.temp,</pre>
 subset = dat.temp$Does.the.paper.use.machine.learning.in.the.sense.of.our.definition. == TRUE)
# Recoding some data
dat$journal <- car::recode(dat$journal, "</pre>
            'American Political Science Review' = 'APSR';
            'Political Analysis' = 'PA';
            'Political Science Research and Methods' = 'PSRM'
            ")
# Table for Main Paper
table(dat$model.replicability, dat$tuning.replicability)
##
##
           FALSE TRUE
##
     FALSE
              34
                    2
```

TRUE

##

15

13

```
round(prop.table(table(dat$model.replicability, dat$tuning.replicability)), 4)*100
```