

Bagging

Data Sets

Attrition

```
attrition <- attrition %>% mutate_if(is.ordered, factor, order = F)
attrition.h2o <- as.h2o(attrition)

churn <- initial_split(attrition, prop = .7, strata = "Attrition")
churn.train <- training(churn)
churn.test <- testing(churn)
```

Ames, Iowa housing data.

```
set.seed(123)

ames <- AmesHousing::make_ames()
ames.h2o <- as.h2o(ames)

ames.split <- initial_split(ames, prop = .7, strata = "Sale_Price")

ames.train <- training(ames.split)
ames.test <- testing(ames.split)
```

Bagging Overview

Bagging (Bootstrap AGGREGatING) is a procedure that uses bootstrapping techniques to create an ensemble of predictions to improve the accuracy of regression and classification methods.

How Bagging Works

Bagging is a fairly straightforward algorithm that makes b bootstrap copies of the original training data, to which the (regression or classification) algorithm is applied (referred to as the “Base Learner”), and then the predictions are averaged together from the individual base learners.

For each record, X , we want to predict:

\hat{f}_{bag} is the bagged prediction, and $\hat{f}_1(X), \hat{f}_2(X), \dots, \hat{f}_b(X)$ are the predictions from the individual base learners.

So that,

$$\hat{f}(bag) = \hat{f}_1(X) + \hat{f}_2(X) + \dots + \hat{f}_b(X)$$

Bagging effectively reduces the variance of an individual base learning through the aggregation process. So, this process works especially well for high variance base learners (Decision Trees, KNN (small k)).

This is an example of the “Wisdom of the Crowd” approach to learners.

Example of “Bagging”:

```
# Simulate some nonlinear monotonic data
set.seed(123) # for reproducibility

x <- seq(from = 0, to = 2 * pi, length = 500)
y <- sin(x) + rnorm(length(x), sd = 0.3)
df <- data.frame(x, y) %>%
  filter(x < 4.5)

# bootstrapped polynomial model fit
bootstrap_n <- 100
bootstrap_results <- NULL
for(i in seq_len(bootstrap_n)) {
  # reproducible sampled data frames
  set.seed(i)
  index <- sample(seq_len(nrow(df)), nrow(df), replace = TRUE)
  df_sim <- df[index, ]

  # fit model and add predictions to results data frame
  fit <- lm(y ~ I(x^3), data = df_sim)
  df_sim$predictions <- predict(fit, df_sim)
  df_sim$model <- paste0("model", i)
  df_sim$ob <- index
  bootstrap_results <- rbind(bootstrap_results, df_sim)
}

p1 <- ggplot(bootstrap_results, aes(x, predictions)) +
  geom_point(data = df, aes(x, y), alpha = .25) +
  geom_line(aes(group = model), show.legend = FALSE, size = .5, alpha = .2) +
  stat_summary(fun.y = "mean", colour = "red", size = 1, geom = "line") +
  scale_y_continuous("Response", limits = c(-2, 2), expand = c(0, 0)) +
  scale_x_continuous(limits = c(0, 5), expand = c(0, 0)) +
  ggtitle("A) Polynomial regression")

# bootstrapped MARS model fit
bootstrap_n <- 100
bootstrap_results <- NULL
for(i in seq_len(bootstrap_n)) {
  # reproducible sampled data frames
  set.seed(i)
  index <- sample(seq_len(nrow(df)), nrow(df), replace = TRUE)
  df_sim <- df[index, ]
```

```

# fit model and add predictions to results data frame
fit <- earth::earth(y ~ x, data = df_sim)
df_sim$predictions <- predict(fit, df_sim)
df_sim$model <- paste0("model", i)
df_sim$ob <- index
bootstrap_results <- rbind(bootstrap_results, df_sim)
}

p2 <- ggplot(bootstrap_results, aes(x, predictions)) +
  geom_point(data = df, aes(x, y), alpha = .25) +
  geom_line(aes(group = model), show.legend = FALSE, size = .5, alpha = .2) +
  stat_summary(fun.y = "mean", colour = "red", size = 1, geom = "line") +
  scale_y_continuous(NULL, limits = c(-2, 2), expand = c(0, 0)) +
  scale_x_continuous(limits = c(0, 5), expand = c(0, 0)) +
  ggtitle("B) MARS")

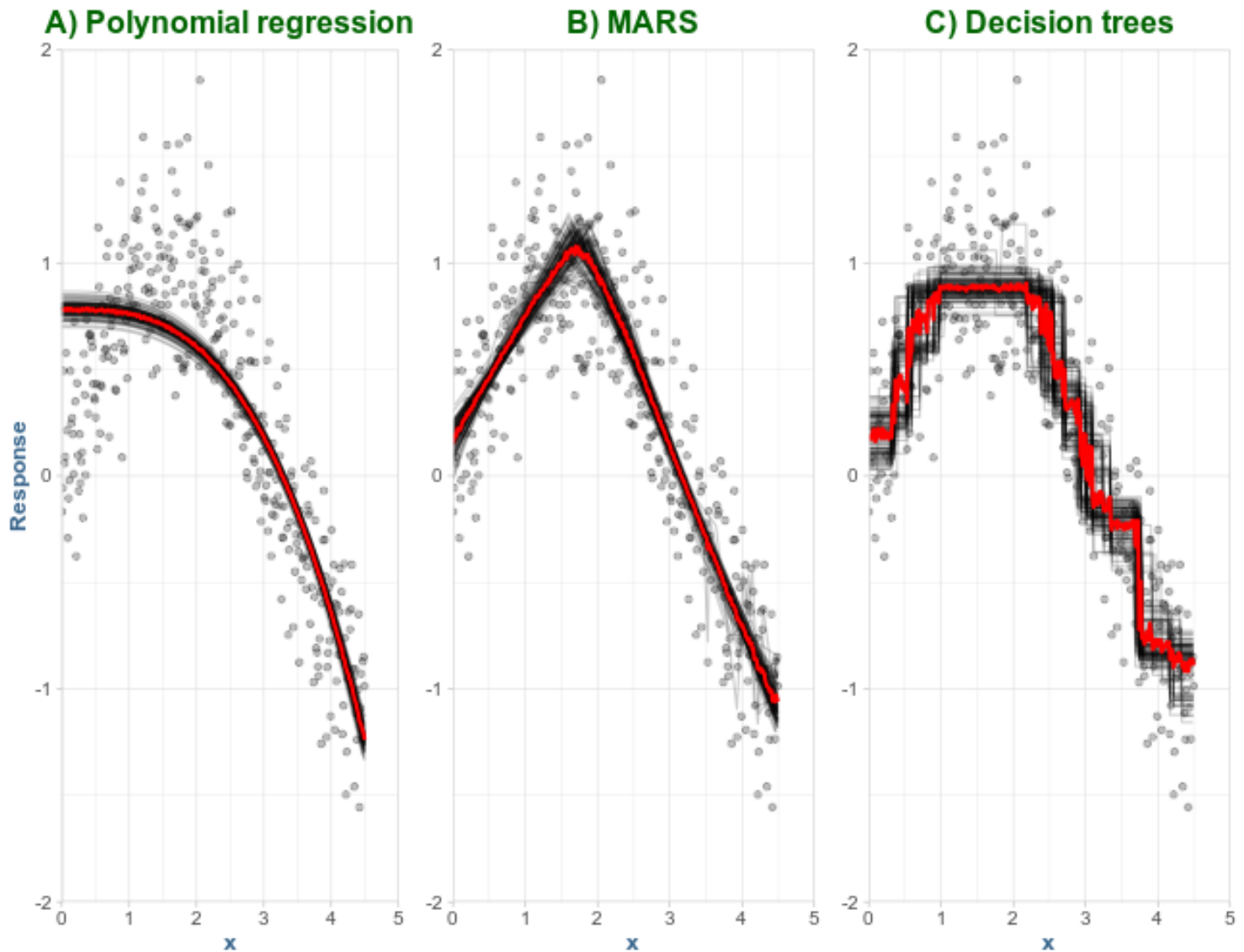
# bootstrapped decision trees fit
bootstrap_n <- 100
bootstrap_results <- NULL
for(i in seq_len(bootstrap_n)) {
  # reproducible sampled data frames
  set.seed(i)
  index <- sample(seq_len(nrow(df)), nrow(df), replace = TRUE)
  df_sim <- df[index, ]

  # fit model and add predictions to results data frame
  fit <- rpart::rpart(y ~ x, data = df_sim)
  df_sim$predictions <- predict(fit, df_sim)
  df_sim$model <- paste0("model", i)
  df_sim$ob <- index
  bootstrap_results <- rbind(bootstrap_results, df_sim)
}

p3 <- ggplot(bootstrap_results, aes(x, predictions)) +
  geom_point(data = df, aes(x, y), alpha = .25) +
  geom_line(aes(group = model), show.legend = FALSE, size = .5, alpha = .2) +
  stat_summary(fun.y = "mean", colour = "red", size = 1, geom = "line") +
  scale_y_continuous(NULL, limits = c(-2, 2), expand = c(0, 0)) +
  scale_x_continuous(limits = c(0, 5), expand = c(0, 0)) +
  ggtitle("C) Decision trees")

gridExtra::grid.arrange(p1, p2, p3, nrow = 1)

```



Optimal performance is typically found using 50-500 trees.

Interestingly, bagging decision trees does not tend to overfit, however, using a CV approach with bagging does begin to become computationally burdensome.

The out-of-bag (OOB) is an internal estimate of the predictive performance. Think of this as a “free” CV statistic.

Implementation

Here we will use a bag of unpruned (we don't prune the individual trees because the bagging process will reduce the variance, and therefore have the largest impact) decision trees on the ames data set.

```
set.seed(123)
```

```
# train bagged model
```

```
ames.bag1 <- bagging(  
  formula = Sale_Price ~ .,  
  data = ames.train,  
  nbagg = 100,  
  coob = T,  
  control = rpart.control(minsplit = 2, cp = 0)  
)  
  
ames.bag1
```

Bagging regression trees with 100 bootstrap replications

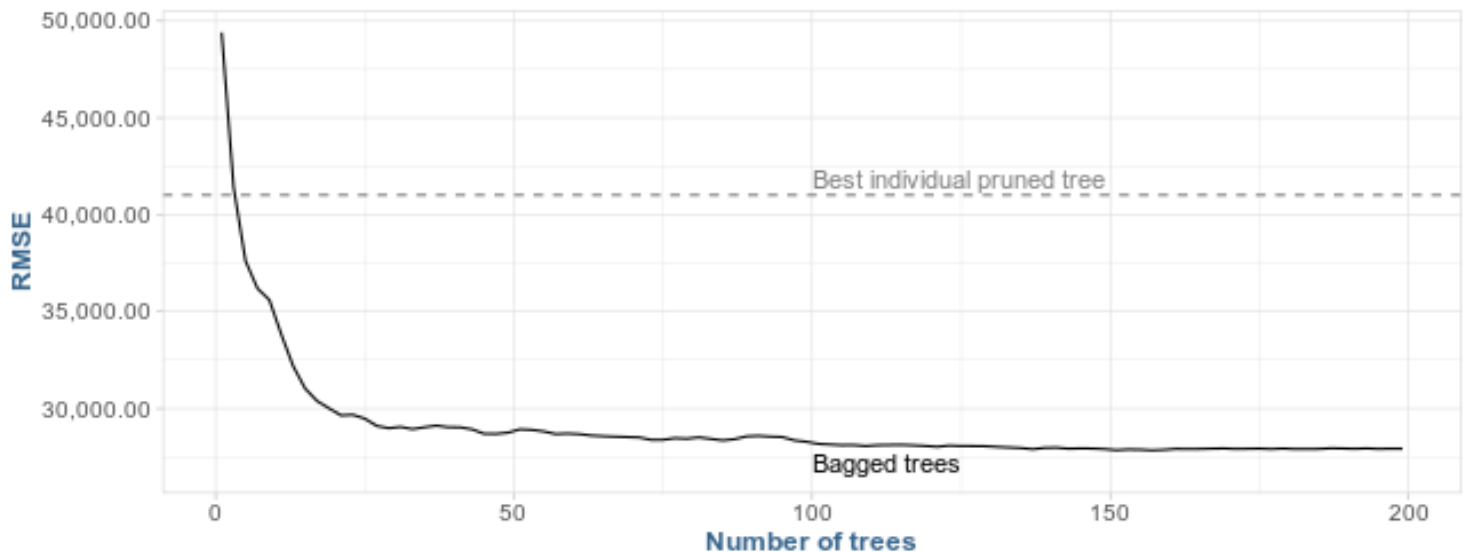
```
Call: bagging.data.frame(formula = Sale_Price ~ ., data = ames.train,  
  nbagg = 100, coob = T, control = rpart.control(minsplit = 2,  
    cp = 0))
```

Out-of-bag estimate of root mean squared error: 27767.13

Error curve for bagging 1-200 deep, unpruned decision trees:

```
n.tree <- seq(1, 200, by = 2)  
  
rmse <- vector(mode = "numeric", length = length(n.tree))  
  
for(i in seq_along(n.tree))  
{  
  set.seed(123)  
  
  # perform bagged model  
  model <- ranger::ranger(  
    formula = Sale_Price ~ .,  
    data = ames.train,  
    num.trees = n.tree[i],  
    mtry = ncol(ames.train) - 1,  
    min.node.size = 1  
  )  
  
  rmse[i] <- sqrt(model$prediction.error)  
}  
  
bagging.errors <- data.table(n.tree, rmse)  
  
ggplot(bagging.errors, aes(n.tree, rmse)) +  
  geom_line() +
```

```
geom_hline(yintercept = 41019, lty = "dashed", color = "grey50") +
annotate("text", x = 100, y = 41385, label = "Best individual pruned tree", vjust = 0, hjust = 0) +
annotate("text", x = 100, y = 26750, label = "Bagged trees", vjust = 0, hjust = 0) +
scale_y_continuous(labels = comma) +
ylab("RMSE") +
xlab("Number of trees")
```



```
ames.bag2 <- train(
  Sale_Price ~ .,
  data = ames.train,
  method = "treebag",
  trControl = trainControl(method = "cv", number = 10),
  nbagg = 200,
  control = rpart.control(minsplit = 2, cp = 0)
)

ames.bag2
```

Bagged CART

2053 samples
80 predictor

No pre-processing

Resampling: Cross-Validated (10 fold)

Summary of sample sizes: 1847, 1849, 1847, 1847, 1848, 1847, ...

Resampling results:

RMSE	Rsquared	MAE
------	----------	-----

27460.99 0.8862784 16755.65

Since each tree is trained on independent samples of the data, we can easily parallelize this process.

```
cl <- makeCluster(8)

registerDoParallel(cl)

# fit trees in parallel and compute predictions on the test set

predictions <- foreach(
  icount(160),
  .packages = "rpart",
  .combine = cbind
) %dopar% {
  # bootstrap copy of training data
  index <- sample(nrow(ames.train), replace = T)
  ames.train.boot <- ames.train[index, ]

  # fit tree to bootstrap copy
  bagged.tree <- rpart(
    Sale_Price ~ .,
    control = rpart.control(minsplit = 2, cp = 0),
    data = ames.train.boot
  )

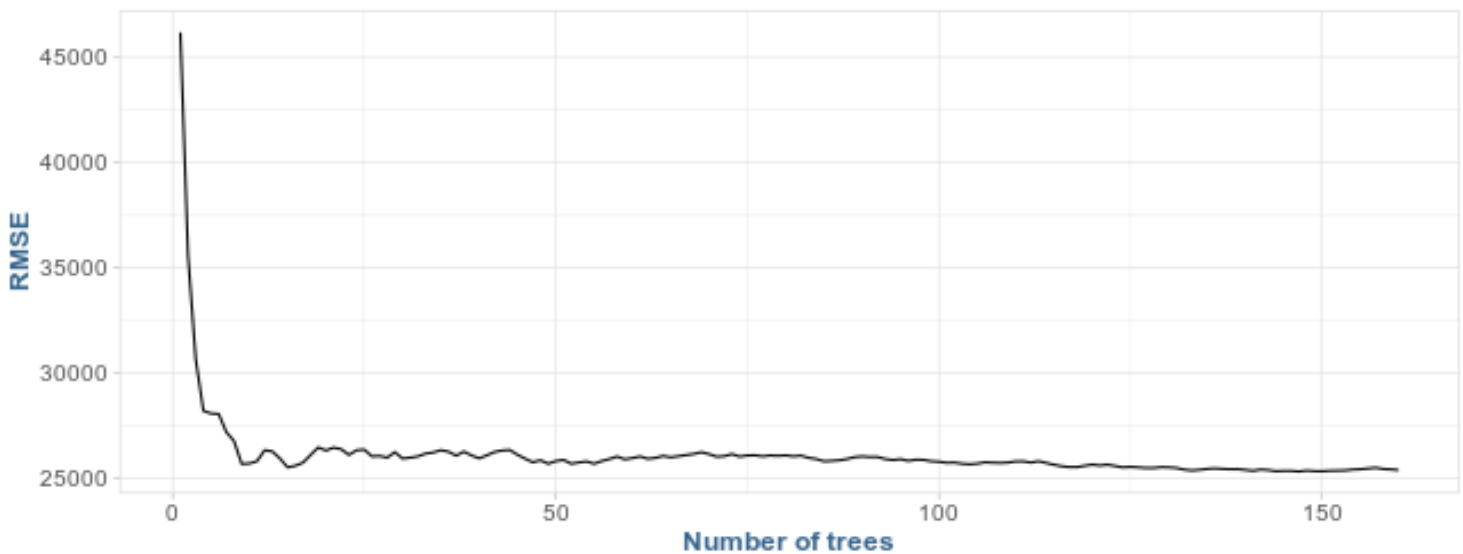
  predict(bagged.tree, newdata = ames.test)
}

predictions[1:5, 1:7]
```

	result.1	result.2	result.3	result.4	result.5	result.6	result.7
1	375000	206900	165000	243000	206900	226500	167000
2	173000	183000	196500	235000	185000	193000	173000
3	189000	213750	201000	187500	180000	183600	130000
4	174000	162500	173000	165500	156820	167900	173000
5	278000	226500	301000	187500	239500	251000	130000

```
predictions %>%
  as.data.frame() %>%
  mutate(
    observation = 1:n(),
    actual = ames.test$Sale_Price) %>%
  tidyr::gather(tree, predicted, -c(observation, actual)) %>%
  group_by(observation) %>%
  mutate(tree = stringr::str_extract(tree, '\\d+') %>% as.numeric()) %>%
```

```
ungroup() %>%  
arrange(observation, tree) %>%  
group_by(observation) %>%  
mutate(avg_prediction = cummean(predicted)) %>%  
group_by(tree) %>%  
summarize(RMSE = RMSE(avg_prediction, actual)) %>%  
ggplot(aes(tree, RMSE)) +  
geom_line() +  
xlab('Number of trees')
```



```
stopCluster(cl)
```

Feature Interpretation

Unfortunately, due to the many trees involved feature interpretation becomes tricky. Typically, the bagging process will use many features, at lower levels of importance.

```
vip::vip(ames.bag2, num_features = 40, bar = FALSE)
```

Warning in vip.default(ames.bag2, num_features = 40, bar = FALSE): The `bar` argument has been deprecated in favor of the new `geom` argument. It will be removed in version 0.3.0.



```
# clean up
rm(list = ls())
```