Lecture 008

Ensembles 🌲🌲🌲🎄🌲

Edward Rubin

Admin

Today

Topic Ensembles (applied to decision trees)

Upcoming

Readings

- *Today* *ISL* Ch. 8.2
- *Next* *ISL* Ch. 9

Project Get the data together!

Decision trees

Review

Decision trees

Fundamentals

Decision trees

- split the *predictor space* (our $\mathbf{X}$) into regions
- then predict the most-common value within a region

Regression trees

- **Predict:** Region's mean
- **Split:** Minimize RSS
- **Prune:** Penalized RSS

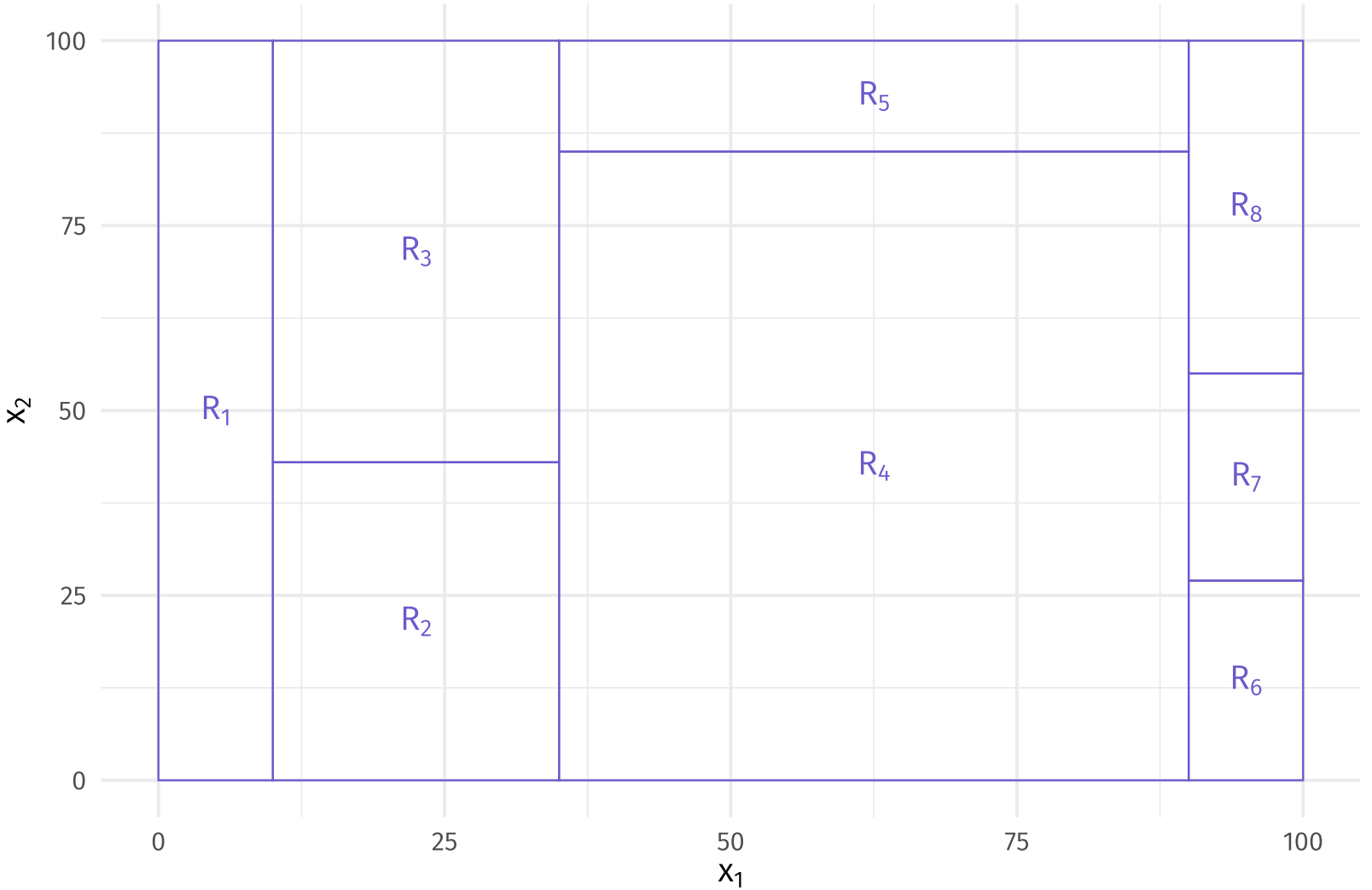
Classification trees

- **Predict:** Region's mode
- **Split:** Min. Gini or entropy.super
- **Prune:** Penalized error rate🌴

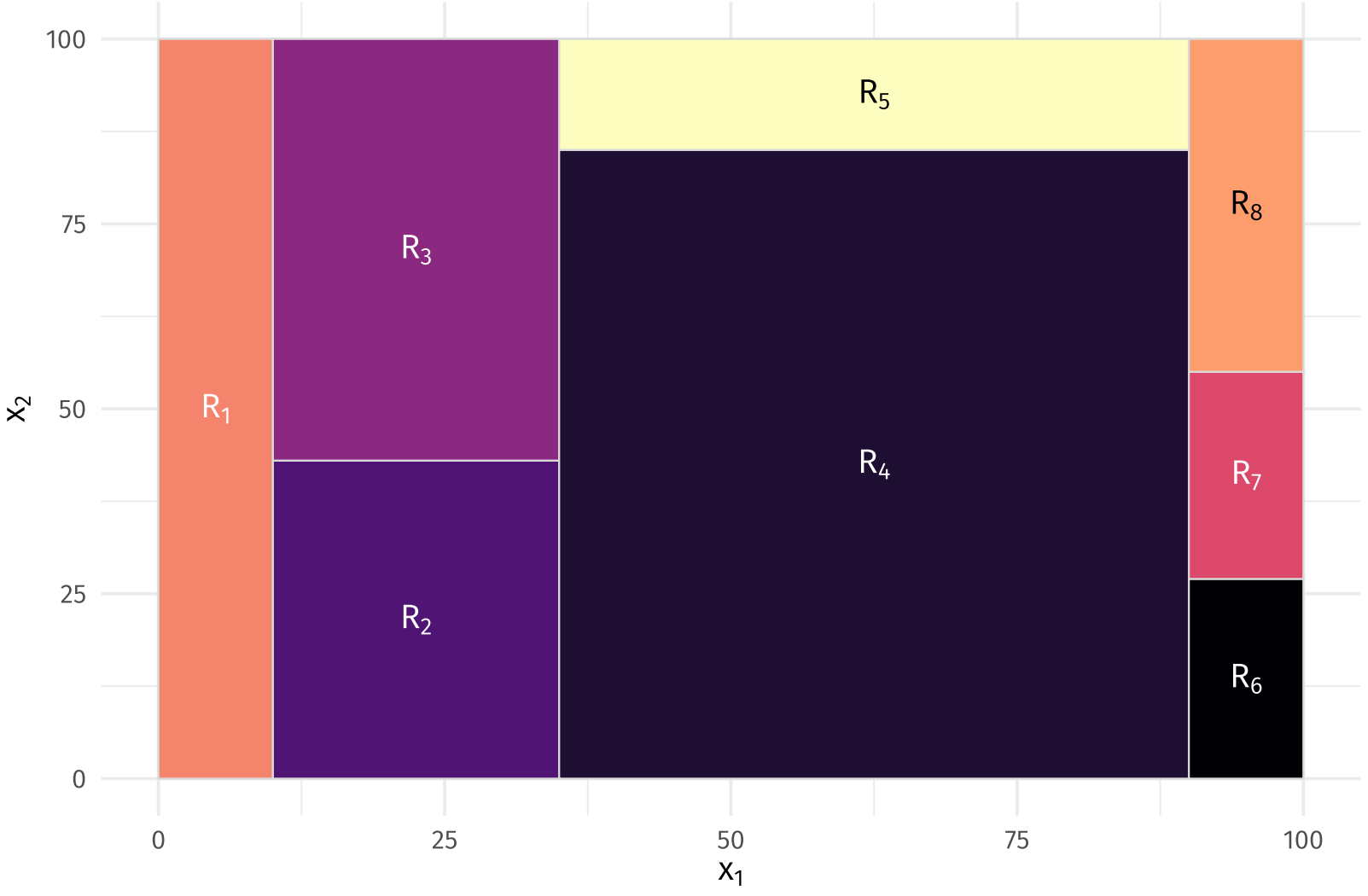
An additional nuance for classification trees: we typically care about the **proportions of classes in the leaves**—not just the final prediction.

🌴 ... or Gini index or entropy

Example Each split in our tree creates **regions**.



Example Each region has its own **predicted value**.



Decision trees

Strengths and weaknesses

As with any method, decision trees have tradeoffs.

Strengths

+ Easily explained/interpretted
+ Include several graphical options
+ Mirror human decision making?
+ Handle num. or cat. on LHS/RHS🌳

Weaknesses

- Outperformed by other methods
- Struggle with linearity
- Can be very "non-robust"

Non-robust: Small data changes can cause huge changes in our tree.

Next: Create ensembles of trees🌲 to strengthen these weaknesses.🌴

🌳 Without needing to create lots of dummy variables!

🌲 Forests! 🌴 Which will also weaken some of the strengths.

Ensemble methods

Ensemble methods

Intro

Rather than focusing on training a **single**, highly accurate model, ensemble methods combine **many** low-accuracy models into a *meta-model*.

Today: Three common methods for **combining individual trees**

1. Bagging
2. Random forests
3. Boosting

Why? While individual trees may be highly variable and inaccurate, a combination of trees is often quite stable and accurate.🌲

🌲 We will lose interpretability.

Ensemble methods

Bagging

Bagging creates additional samples via **bootstrapping**.

Q How does bootstrapping help?

A *Recall:* Individual decision trees suffer from variability (*non-robust*).

This *non-robustness* means trees can change *a lot* based upon which observations are included/excluded.

We're essentially using many "draws" instead of a single one.🌴

🌴 Recall that an estimator's variance typically decreases as the sample size increases.

Ensemble methods

Bagging

Bootstrap aggregation (bagging) reduces this type of variability.

1. Create B bootstrapped samples
2. Train an estimator (tree) $\hat{f}^b(x)$ on each of the B samples
3. Aggregate across your B bootstrapped models:

$$\hat{f}_{\text{bag}}(x) = \frac{1}{B}\sum_{b=1}^{B}\hat{f}^b(x)$$

This aggregated model $\hat{f}_{\text{bag}}(x)$ is your final model.

Bagging trees

When we apply bagging to decision trees,

- we typically **grow the trees deep and do not prune**
- for **regression**, we **average** across the B trees' regions
- for **classification**, we have more options—but often take **plurality**

Individual (unpruned) trees will be very **flexible** and **noisy**,
but their **aggregate** will be quite **stable**.

The number of trees B is generally not critical with bagging.
$B = 100$ often works fine.

Out-of-bag error estimation

Bagging also offers a convenient method for evaluating performance.

For any bootstrapped sample, we omit ~n/3 observations.

Out-of-bag (OOB) error estimation estimates the test error rate using observations **randomly omitted** from each bootstrapped sample.

For each observation i:

1. Find all samples S_i in which i was omitted from training.
2. Aggregate the $|S_i|$ predictions $\hat{f}^b(x_i)$, *e.g.*, using their mean or mode
3. Calculate the error, *e.g.*, $y_i - \hat{f}_{i,\text{OOB},i}(x_i)$

Out-of-bag error estimation

When B is big enough, the OOB error rate will be very close to LOOCV.

Q Why use OOB error rate?

A When B and n are large, cross validation—with any number of folds—can become pretty computationally intensive.

Quick aside: Here is a tool to search `parsnip` models:

> https://www.tidymodels.org/find/parsnip/

Bagging in R

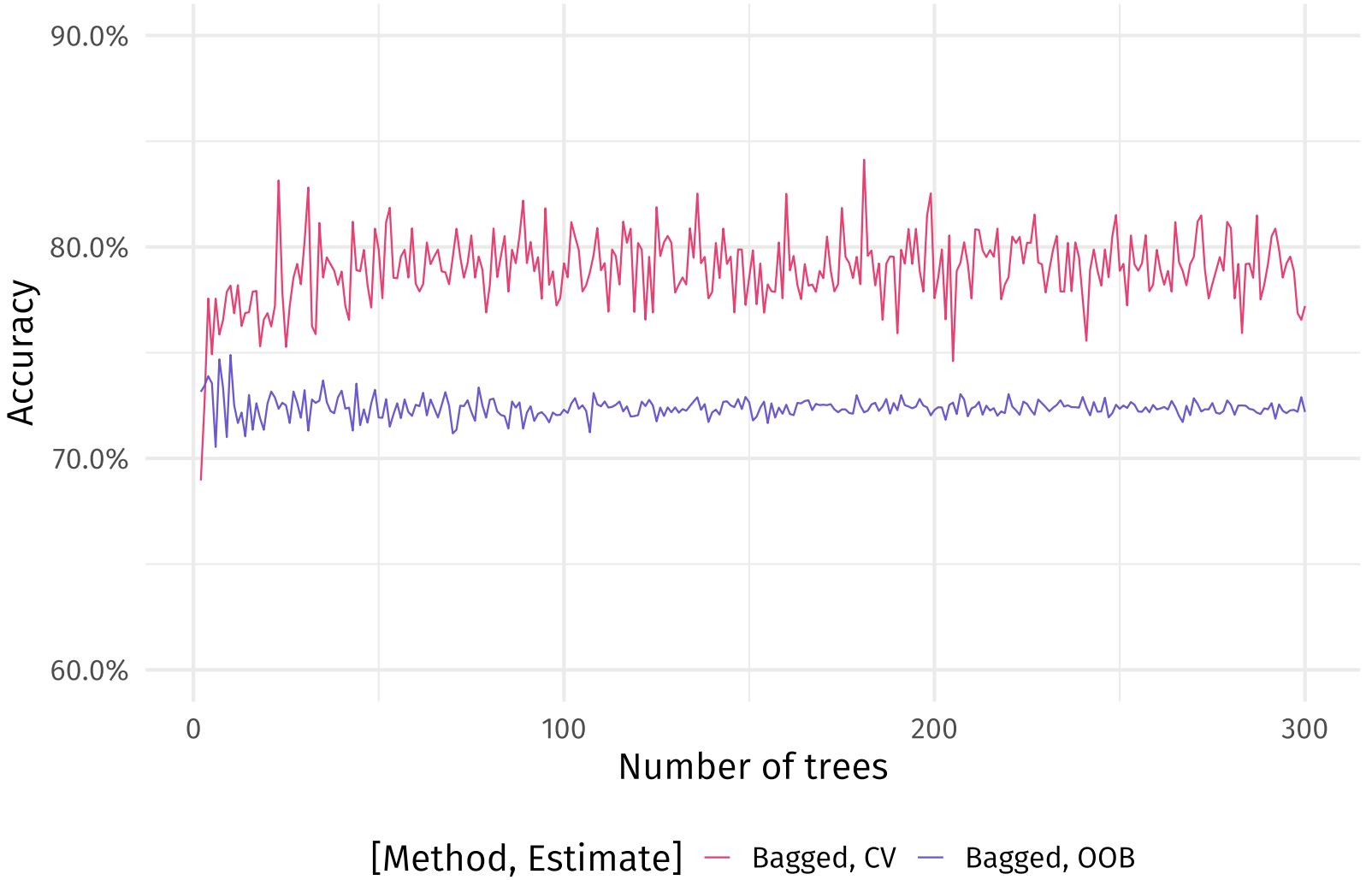
We can use `tidymodels` plus the `baguette` package to bag trees.

Function: `bag_tree()`

- "Specifies" model for `parsnip`.
- `mode`: class., reg., or unknown
- `cost_complexity`: the penalty for model complexity (`Cp`)
- `tree_depth`: max. tree depth
- `min_n`: min. # obs. to split
- `class_cost`: magnify *cost*
- `rpart` is the defaul engine
- `times`: the number of trees

```
# Train a bagged tree model
bag_tree(
  mode = "classification",
  cost_complexity = 0,
  tree_depth = NULL,
  min_n = 2,
  class_cost = NULL
) %>% set_engine(
  engine = "rpart",
  times = 100
)
```

Bagging and the number of trees



Unfortunately, this combination of `rpart` / `baguette` / `parsnip` / `yardstick` doesn't (currently) offer OOB-based metrics. 😞

We *can* "trick" random forests (`ranger`) into doing OOB for bagged trees.

But first, we need to learn about random forests...

... and before *that*, let's briefly talk about variable importance.

Ensemble methods

Variable importance

While ensemble methods tend to **improve predictive performance**, they also tend **reduce interpretability**.

We can illustrate **variables' importance** by considering their splits' reductions in the model's performance metric (RSS, Gini, entropy, *etc.*).🌳

Note By default, many variable-importance functions will scale importance.

🌳 This idea isn't exclusive to bagging/ensembles; it also works for a single tree.

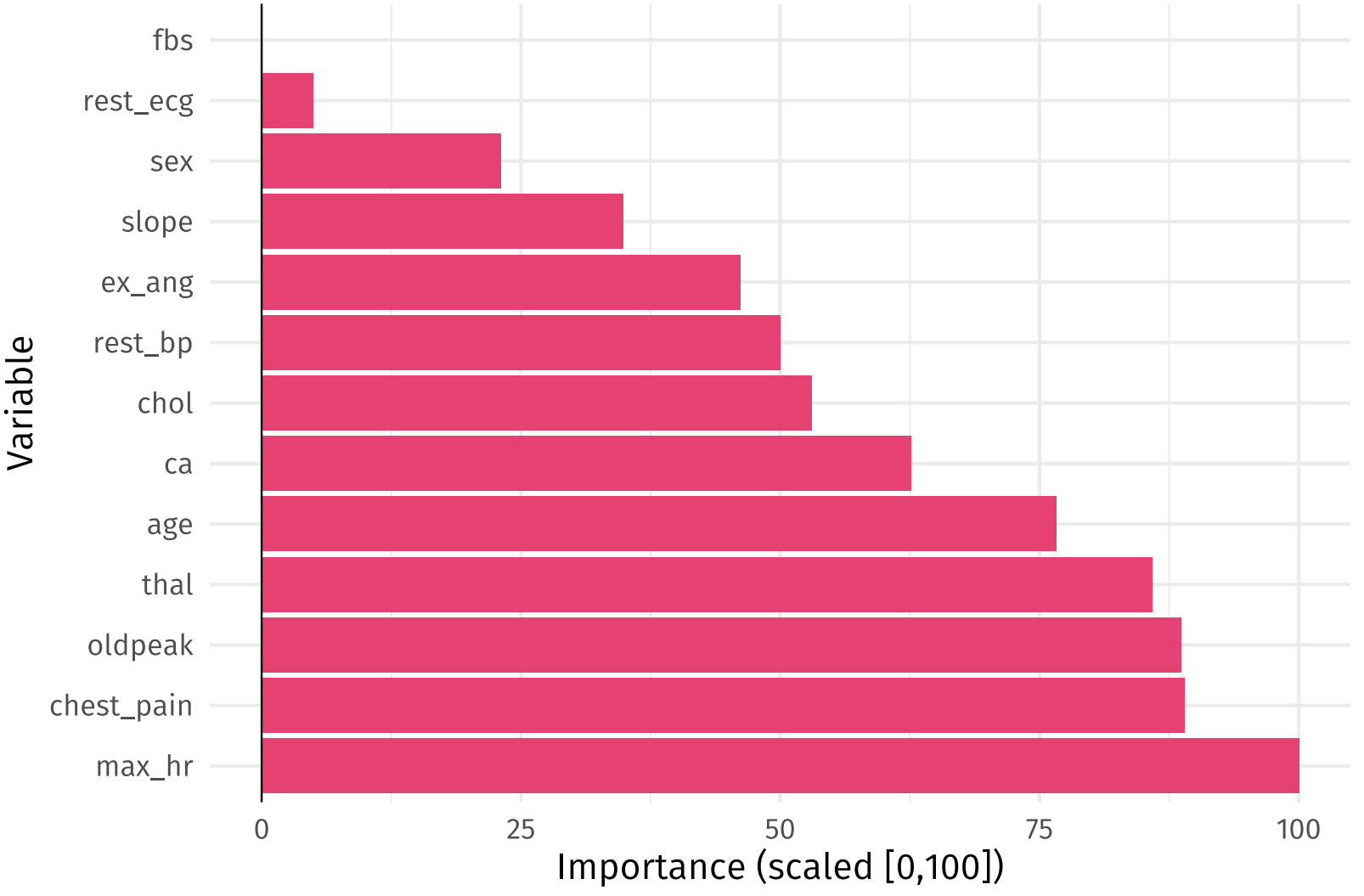
In the case of `"rpart"` bagged trees...

```
# Recipe to clean data (impute NAs)
heart_recipe = recipe(heart_disease ~ ., data = heart_df) %>%
  step_medianimpute(all_predictors() & all_numeric()) %>%
  step_modeimpute(all_predictors() & all_nominal())
# Define the bagged tree model
heart_bag = bag_tree(
  mode = "classification",
  cost_complexity = 0,
  tree_depth = NULL,
  min_n = 2,
  class_cost = NULL
) %>% set_engine(
  engine = "rpart",
  times = 100
)
# Define workflow
heart_bag_wf = workflow() %>%
  add_model(heart_bag) %>%
  add_recipe(heart_recipe)
# Fit/assess with CV
heart_bag_fit = heart_bag_wf %>% fit(heart_df)
```

... the fitted object automatically includes variable importance.

```
#> Bagged CART (classification with 100 members)
#>
#> Variable importance scores include:
#>
#> # A tibble: 13 × 4
#>    term       value std.error  used
#>    <chr>      <dbl>     <dbl> <int>
#>  1 max_hr     41.1      0.839   100
#>  2 chest_pain 36.9      1.18    100
#>  3 oldpeak    36.8      0.806   100
#>  4 thal       35.7      1.35    100
#>  5 age        32.2      0.702   100
#>  6 ca         26.8      1.18    100
#>  7 chol       23.2      0.685   100
#>  8 rest_bp    22.1      0.589   100
#>  9 ex_ang     20.6      0.818    99
#> 10 slope      16.3      0.772   100
#> 11 sex        11.8      0.678   100
#> 12 rest_ecg    4.92     0.311    95
#> 13 fbs         3.02     0.210    93
```

Variable importance from our bagged tree model.



Bagging

Bagging has one additional shortcoming...

If one variable dominates other variables, the **trees will be very correlated**.

If the trees are very correlated, then bagging loses its advantage.

Solution We should make the trees less correlated.

Random forests

Random forests improve upon bagged trees by *decorrelating* the trees.

In order to decorrelate its trees, a **random forest** only considers a random subset of m ($\approx \sqrt{p}$) predictors when making each split (for each tree).

Restricting the variables our tree sees at a given split

- nudges trees away from always using the same variables,
- increasing the variation across trees in our forest,
- which potentially reduces the variance of our estimates.

If our predictors are very correlated, we may want to shrink m.

Random forests

Random forests thus introduce **two dimensions of random variation**

1. the **bootstrapped sample**
2. the m **randomly selected predictors** (for the split)

Everything else about random forests works just as it did with bagging.🎄

🎄 And just as it did with plain, old decision trees.

Ensemble methods

Random forests in R

You have several options for training random forests with `tidymodels`.🎄
E.g., `ranger`, `randomForest`, `spark`.

`rand_forest()` accesses each of these packages via their *engines*.

- The default engine is `"ranger"` (`ranger` package).
- The argument `mtry` gives m, the # of predictors at each split.

You've already seen the other hyperparameters for `ranger`:

- `trees` the number of trees in your (random) forest
- `min_n` min. # of observations

🎄 And even more if you look outside of `tidymodels`.

Ensemble methods

Training a random forest in R using `tidymodels`...

... and `ranger`

- Goal: Classification
- Three variables per split
- 100 trees in the forest
- At least 2 obs. to split
- Choose the `ranger` engine
- Set a splitting rule

```
# Define the random forest
heart_rf = rand_forest(
  mode = "classification",
  mtry = 3,
  trees = 100,
  min_n = 2
) %>% set_engine(
  engine = "ranger",
  splitrule = "gini"
)
```

Step 1: Define our parameter grid

```
# Define the parameter grid
rf_grid = expand_grid(
  mtry = 1:13,
  min_n = 1:15
)
```

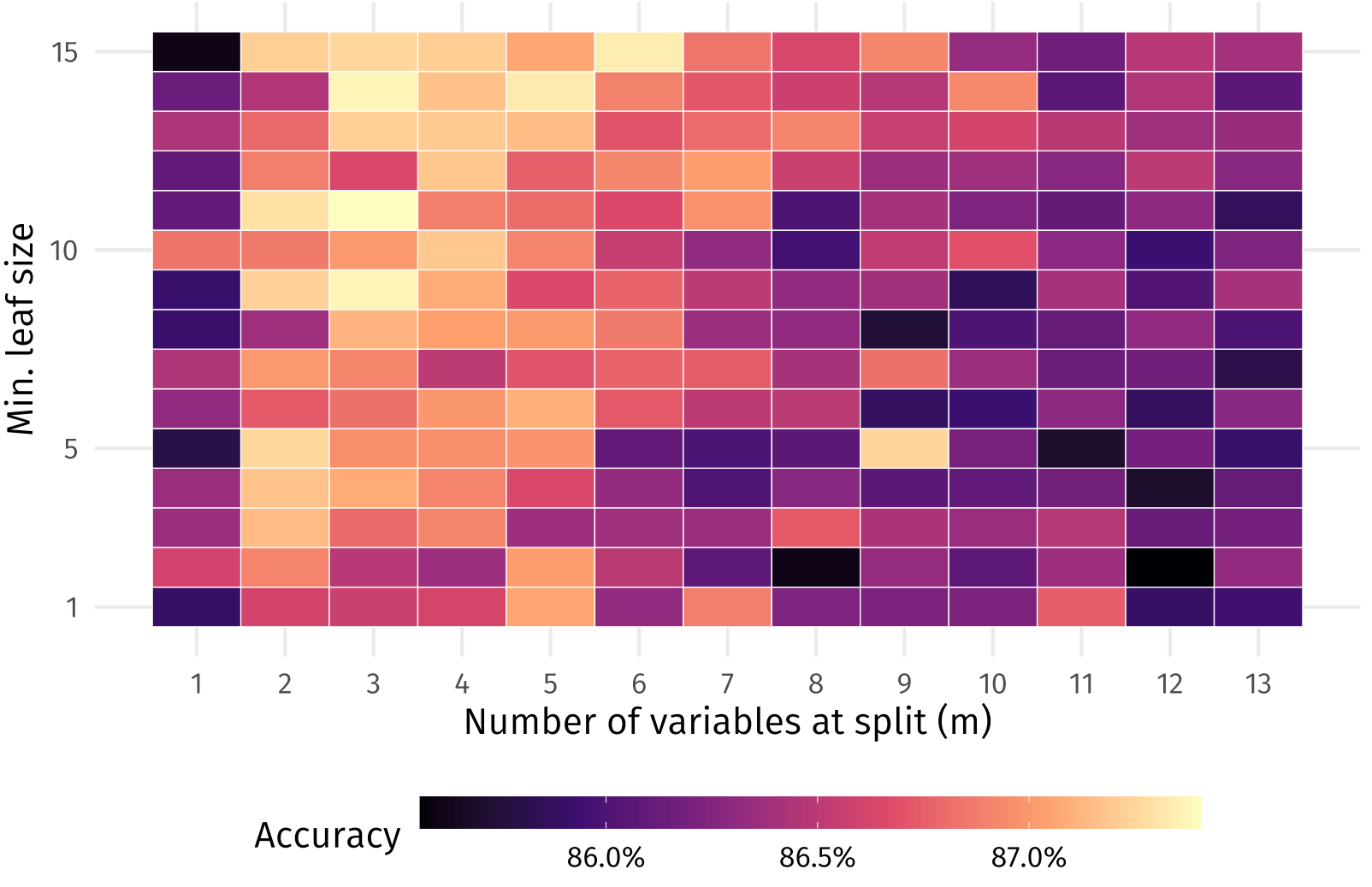
Step 2: Write a function that fits a RF using **given hyperparameters**.

```
# Function: One set of hyperparam
rf_i = function(i) {
  # Define the random forest
  heart_rf_i = rand_forest(
    mode = "classification",
    mtry = rf_grid$mtry[i],
    trees = 100,
    min_n = rf_grid$min_n[i]
  ) %>% set_engine(engine = "ranger", splitrule = "gini")
  # Define workflow
  heart_rf_wf_i =
    workflow() %>% add_model(heart_rf_i) %>% add_recipe(heart_recipe)
  # Fit
  heart_rf_fit_i = heart_rf_wf_i %>% fit(heart_df)
  # Return DF w/ OOB error and the hyperparameters
  tibble(
    mtry = rf_grid$mtry[i],
    min_n = rf_grid$min_n[i],
    # Note: OOB error is buried
    error_oob = heart_rf_fit_i$fit$fit$fit$prediction.error
  )
}
```

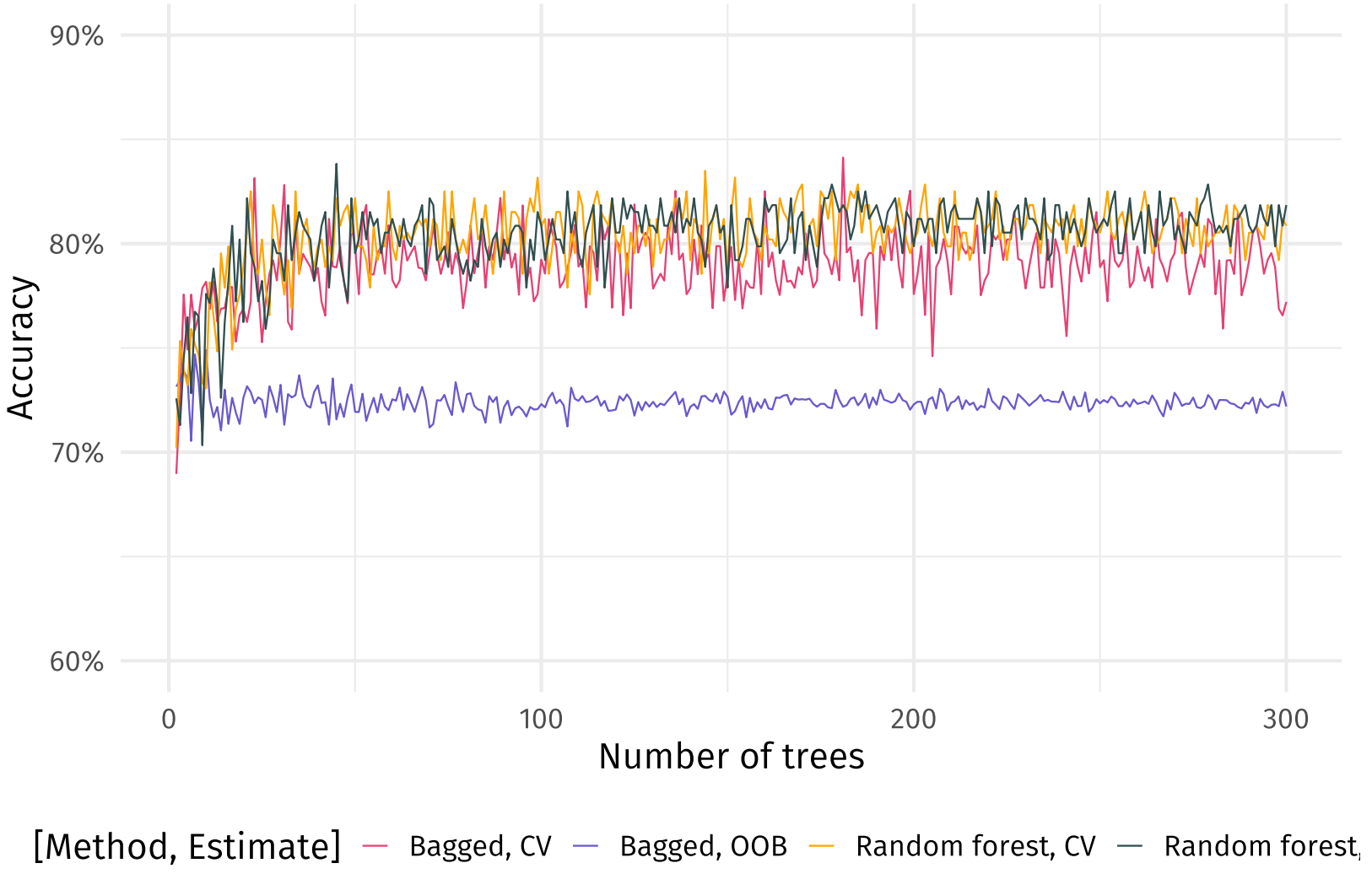
Step 3: Fit all of the forests (in `parallel`)!

```
# Fit the RFs on the grid
rf_tuning = mclapply(
  X = 1:nrow(rf_grid),
  FUN = rf_i,
  mc.cores = 12
) %>% rbindlist()
```

Accuracy (OOB) across the grid of our parameters.



Tree ensembles and the number of trees



Ensemble methods

Boosting

So far, the elements of our ensembles have been acting independently: any single tree knows nothing about the rest of the forest.

Boosting allows trees to pass on information to eachother.

Specifically, **boosting** trains its trees🌲 *sequentially*—each new tree trains on the residuals (mistakes) from its predecessors.

- We add each new tree to our model $\hat{f}$ (and update our residuals).
- Trees are typically small—slowly improving $\hat{f}$ *where it struggles*.

🌲 As with bagging, boosting can be applied to many methods (in addition to trees).

Boosting

Boosting has three **tuning parameters**.

1. The **number of trees** B can be important to prevent overfitting.
2. The **shrinkage parameter** λ, which controls boosting's *learning rate* (often 0.01 or 0.001).
3. The **number of splits** d in each tree (trees' complexity).
   - Individual trees are typically short—often $d = 1$ ("stumps").
   - *Remember* Trees learn from predecessors' mistakes, so no single tree needs to offer a perfect model.

Ensemble methods

How to boost

Step 1: Set $\hat{f}(x) = 0$, which yields residuals $r_i = y_i$ for all i.

Step 2: For $b = 1, 2 \ldots, B$ do:

A. Fit a tree $\hat{f}^b$ with d splits.

B. Update the model $\hat{f}$ with "shrunken version" of new treee $\hat{f}^b$

$$\hat{f}(x) \leftarrow \hat{f}(x) + \lambda \hat{f}^b(x)$$

C. Update the residuals: $r_i \leftarrow r_i - \lambda \hat{f}^b(x)$.

Step 3: Output the boosted model: $\hat{f}(x) = \sum_b \lambda \hat{f}^b(x)$.

Boosted residuals: The expansion

Recall: Boosting trains

- successive models $\hat{f}_i(y, x)$
- on previous models' residuals, r_{i-1} (shrunk by λ)

$$
\begin{aligned}
r_0 &= y \\
r_1 &= r_0 - \lambda \hat{f}_1(r_0, x) \\
&= y - \lambda \hat{f}_1(y, x) \\
r_2 &= r_1 - \lambda \hat{f}_2(r_1, x) \\
&= y - \lambda \hat{f}_1(y, x) - \lambda \hat{f}_2(y - \lambda \hat{f}_1(y, x), x) \\
&\dots
\end{aligned}
$$

Boosting in R

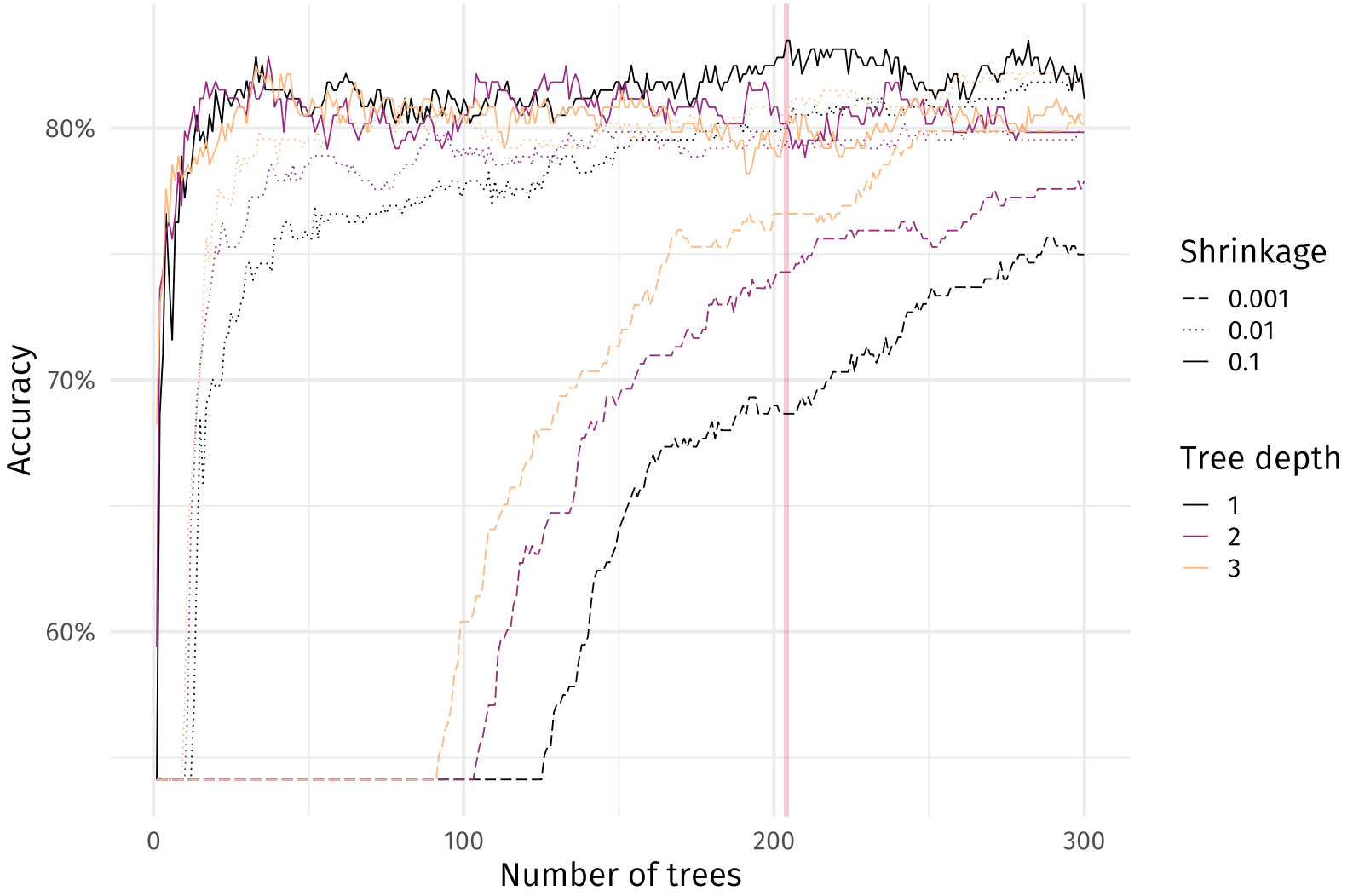
We will use `parsnips`'s `boost_tree()` to train boosted trees.🌴

`boost_tree()` takes several parameters you've seen—plus one more:

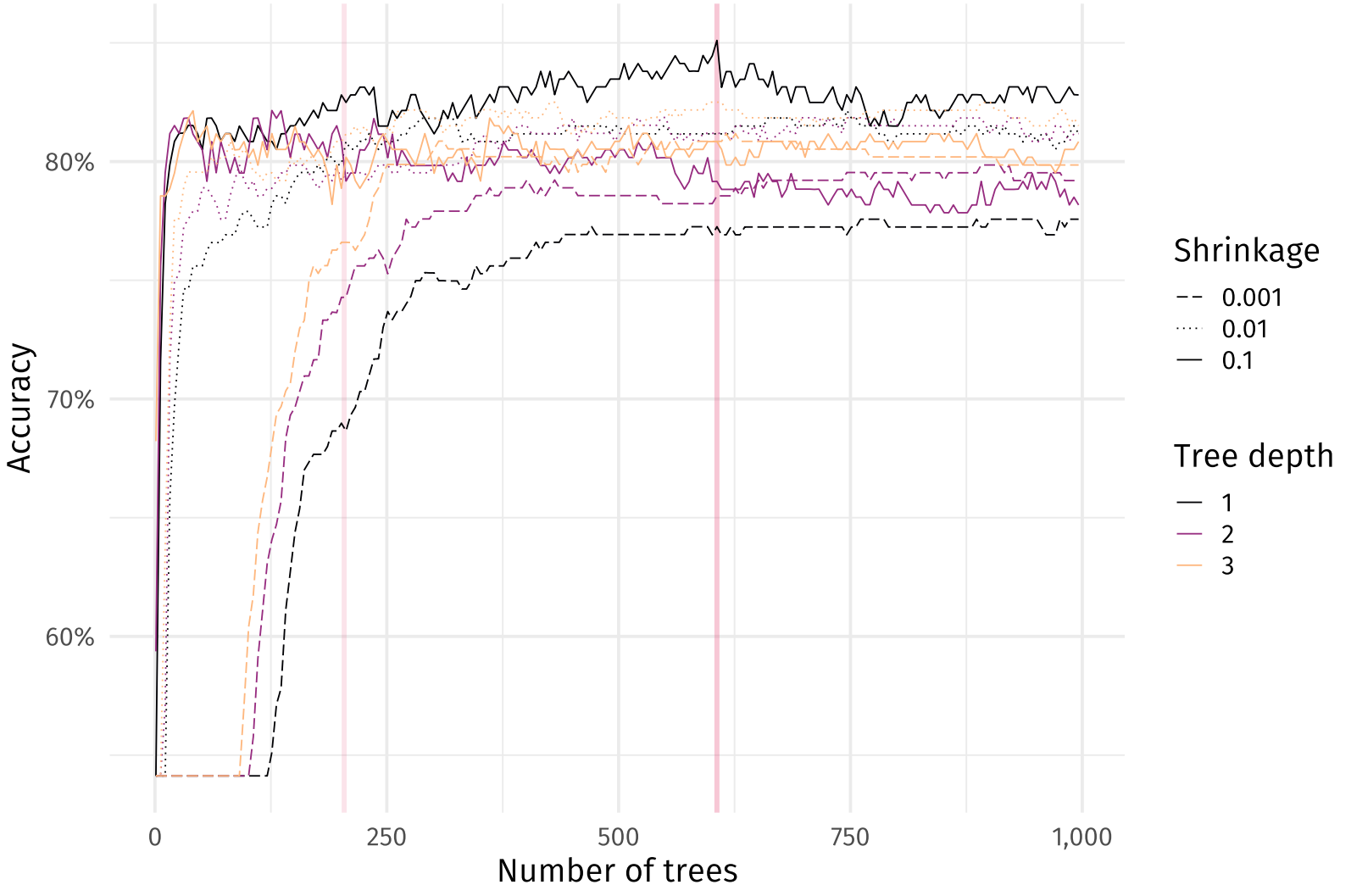
1. `mtry` number of predictors to try at each split
2. `trees`, the number of trees (B)
3. `min_n`, minimum observations to split
4. `tree_depth`, max. tree depth (max. splits from top)
5. `learn_rate`, the learning rate (λ)

🌴 This method uses the `xgboost` package.

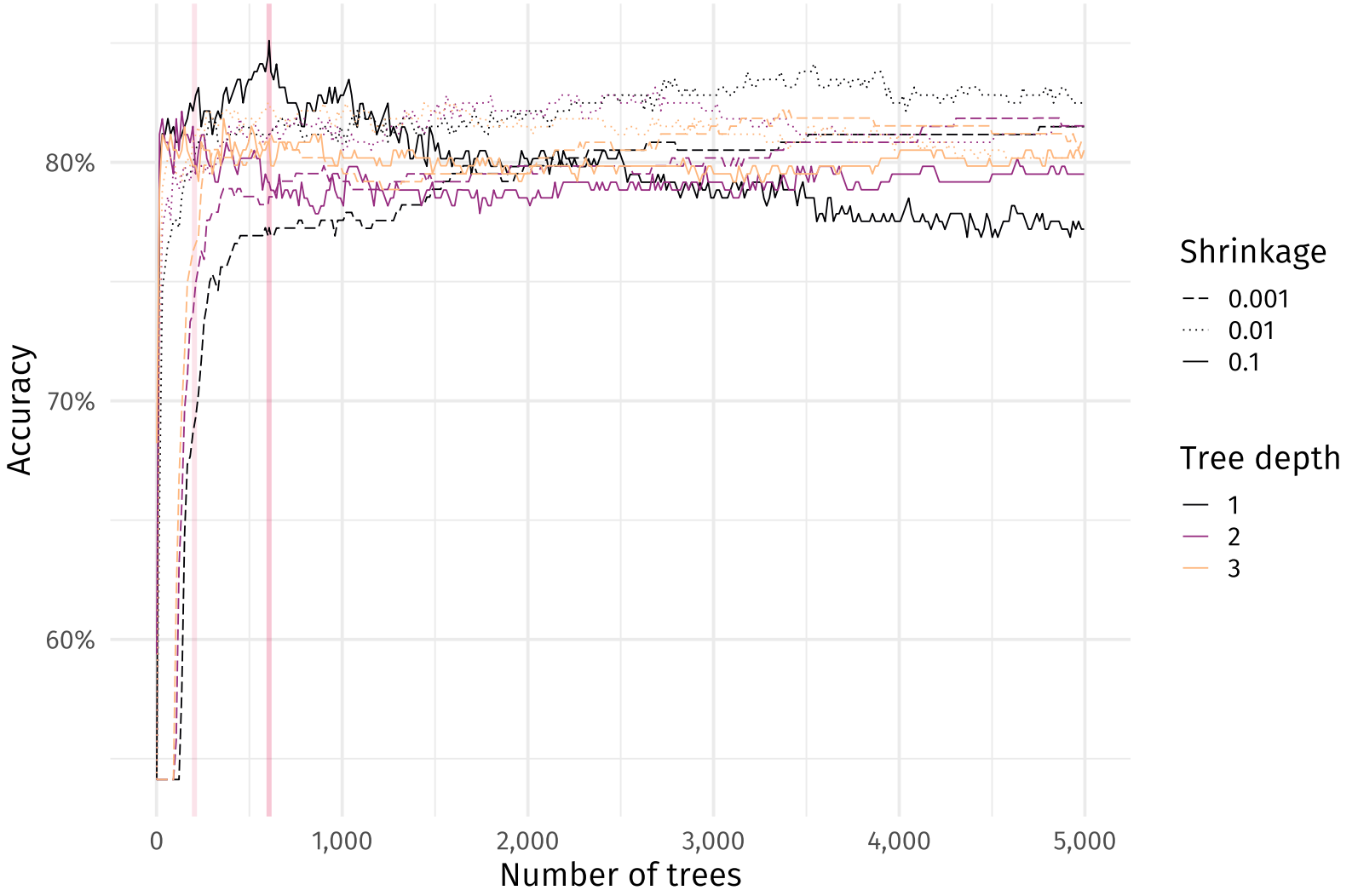
Comparing boosting parameters—notice the rates of learning



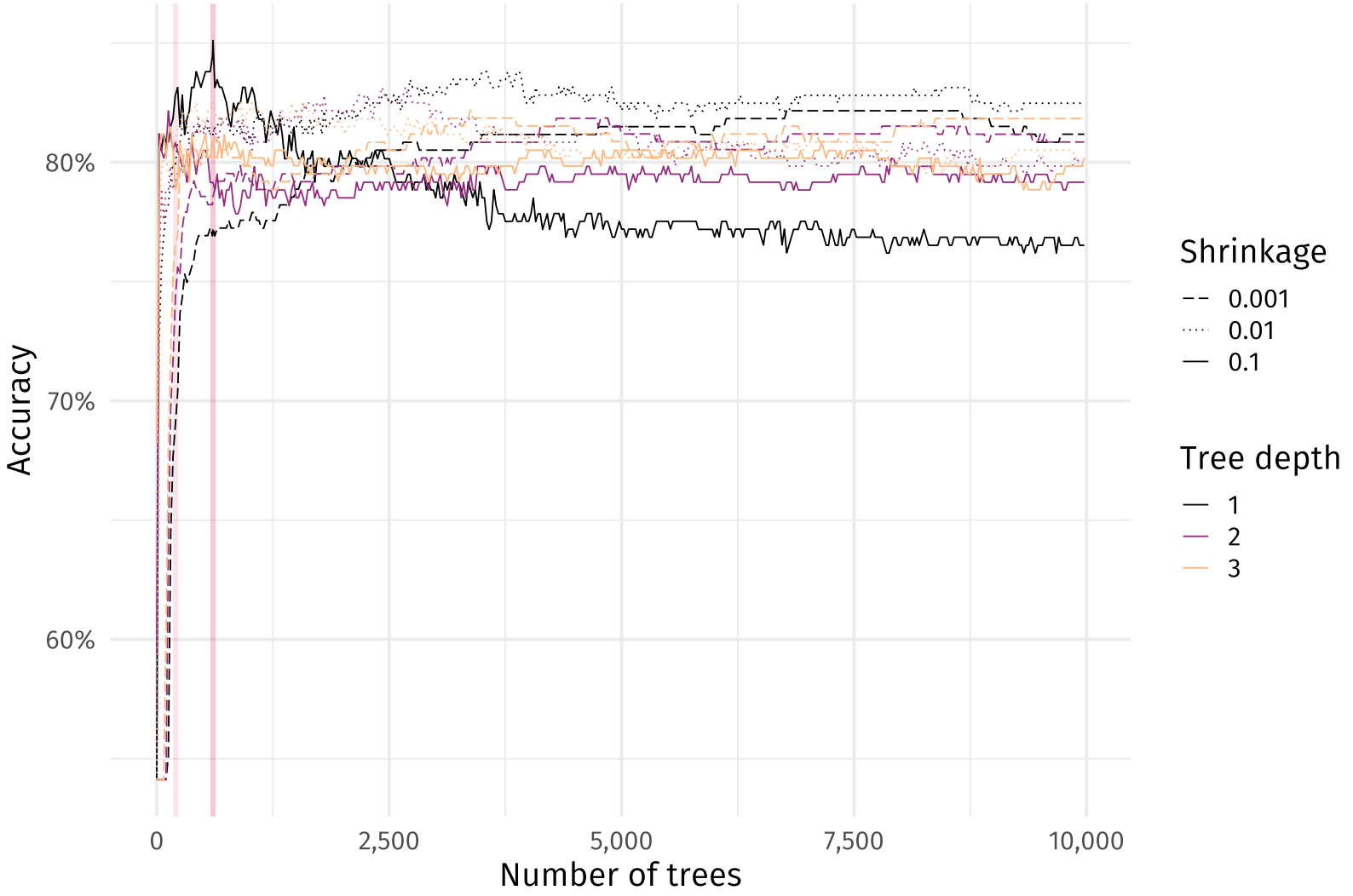
Comparing boosting parameters—more trees!



Comparing boosting parameters—even more trees!



Comparing boosting parameters—and even more trees!



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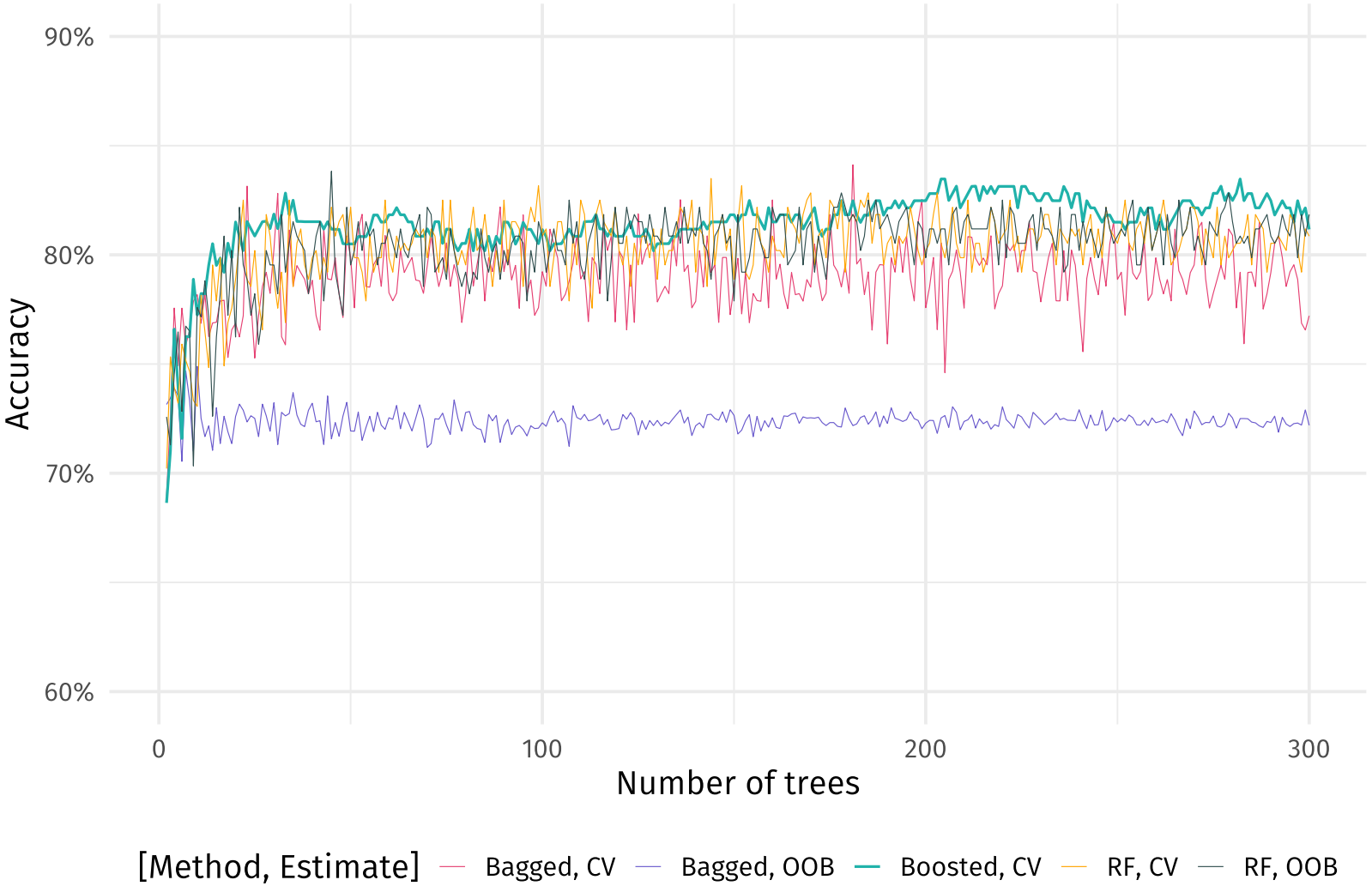

Of course, there are a lot of other tree-based learning options:

- CatBoost (R)
- LightGBM (R)
- TabNet (R)

Sources

These notes draw upon

- An Introduction to Statistical Learning (*ISL*)
  James, Witten, Hastie, and Tibshirani

Table of contents