Lecture 11: Machine Learning

Tree-Based Machine Learning Methods

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*Parts of these slides are adapted from **"Prediction and Machine-Learning in Econometrics"** by Ed Rubin, used under **CC BY-NC-SA 4.0**.

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Part 3: Tree-Based Methods

Prologue

Packages we'll use today:

```
pacman::p_load(grf, fixest, janitor, magrittr, parsnip, ranger, rpart, rpa
```

As well, let's use two datasets:

- The ISL default data again
- Heart disease data

```
default_df ← ISLR::Default

heart_df ← read_csv("data/Heart.csv") %>%
  dplyr::select(-1) %>%
  rename(HeartDisease = AHD) %>%
  clean_names()
```

Prologue

Throughout our econometric training, we've become experts in predicting an outcome by writing down a model with a **specific functional form** for the relationship between $\mathbf{y}$ and $\mathbf{X}$.

Decision Trees (or classification and regression trees, CART) are a supervised learning method that offers an alternative, **data-driven** way of generating predictions by partitioning the covariate space into groups and using the grouping to generate predictions.

After working through decision trees, we'll shift our focus to **forest methods** that combine many, many trees to overcome drawbacks of individual trees and yield predictions of alternate objects - including heterogeneous treatment effects.

 Decision Trees 

Decision Trees: Punchline

Goal

- Split the *predictor space* (our $\mathbf{X}$) into regions (partitions)
- Predict the most-common value within a region

Attributes of Decision Trees

1. Work for **both classification and regression**
2. Are inherently **nonlinear**
3. Are relatively **simple** and **interpretable**
4. Often **underperform** relative to competing methods
5. easily extend to **very competitive ensemble methods** (forests with *many* trees)🌲

🌲 Though the ensembles will be much less interpretable.

Growing Decision Trees

1. Divide the predictor space into J regions (using predictors $\mathbf{x}_1, \ldots, \mathbf{x}_p$)

- **Regression Trees:** Choose the regions to **minimize RSS** across all J regions

$$\sum_{j=1}^{J} \left(y_i - \hat{y}_{R_j} \right)^2$$

Growing Decision Trees: Steps

1. Divide the predictor space into J regions (using predictors $\mathbf{x}_1, \ldots, \mathbf{x}_p$)

- **Classification Trees:** Choose the regions to **minimize Gini index** or **Entropy**

$$G = \sum_{k=1}^{K} \hat{p}_{mk} (1 - \hat{p}_{mk}) \qquad Entropy = -\sum_{k=1}^{K} \hat{p}_{mk} \log(\hat{p}_{mk})$$

- Keep splitting until a specified threshold is reached (e.g. at most 5 observations per region)

Classification Tree

Q: Why are we using the Gini index or entropy (*vs.* error rate)?

A: The error rate isn't sufficiently sensitive to grow good trees.
The Gini index and entropy tell us about the **composition** of the leaf.

Consider two different leaves in a three-level classification.

Leaf 1

- A: 51, B: 49, C: 00
- **Error rate:** 49%
- **Gini index:** 0.4998
- **Entropy:** 0.6929

Leaf 2

- A: 51, B: 25, C: 24
- **Error rate:** 49%
- **Gini index:** 0.6198
- **Entropy:** 1.0325

The **Gini index** and **entropy** tell us about the distribution.

Growing Decision Trees: Steps

2. Make predictions using the regions' mean outcome.

For region R_j predict $\hat{y}_{R_j}$ where

$$\hat{y}_{R_j} = \frac{1}{n_j} \sum_{i \in R_j} y$$

Growing Decision Trees

Let's visualize this by growing a classification tree for predicting credit card defaults based on income and card balances.

Growing Decision Trees

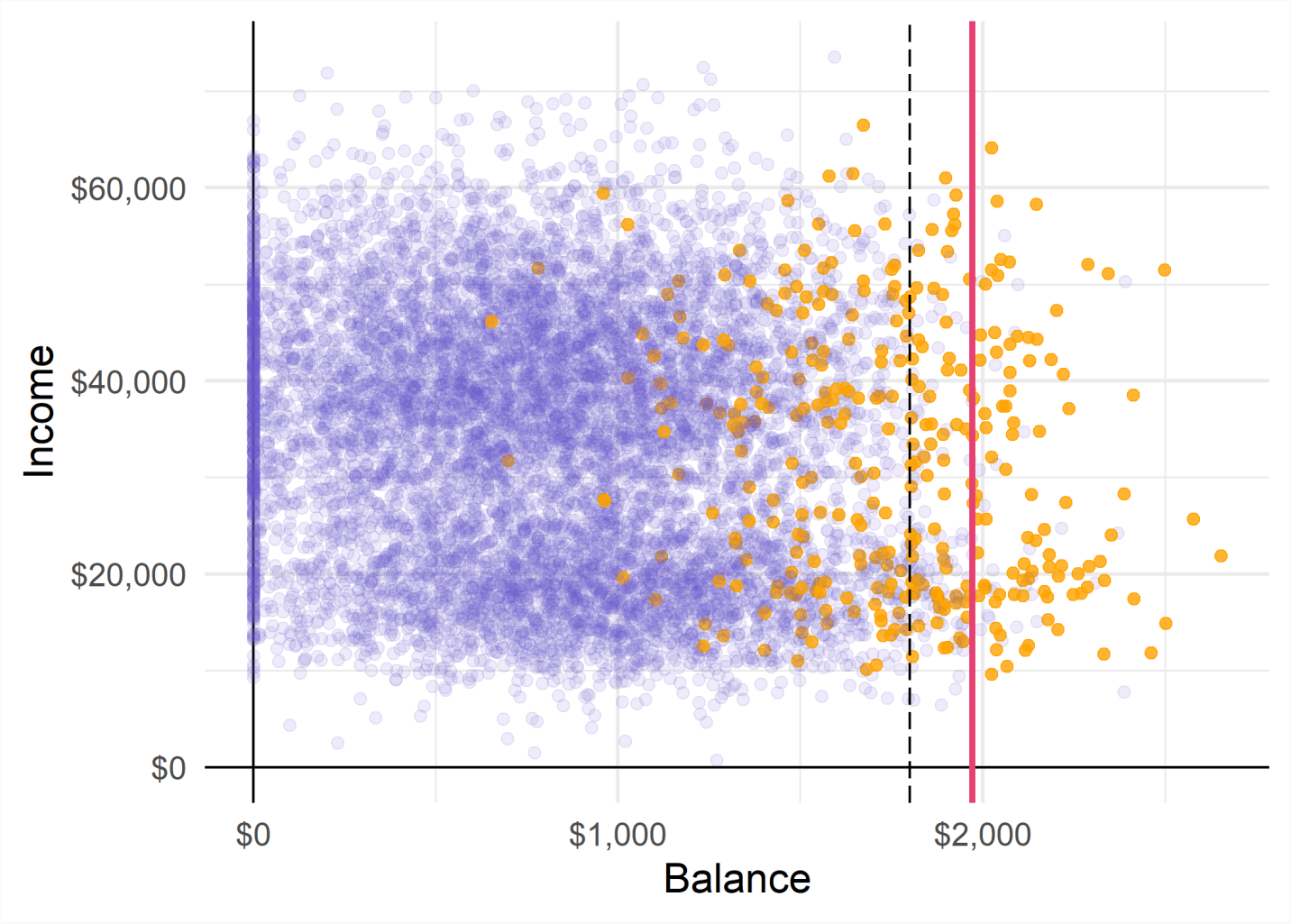
Consider our two-dimensional covariate space:

Growing Decision Trees

The **first partition** splits balance at $1,800.

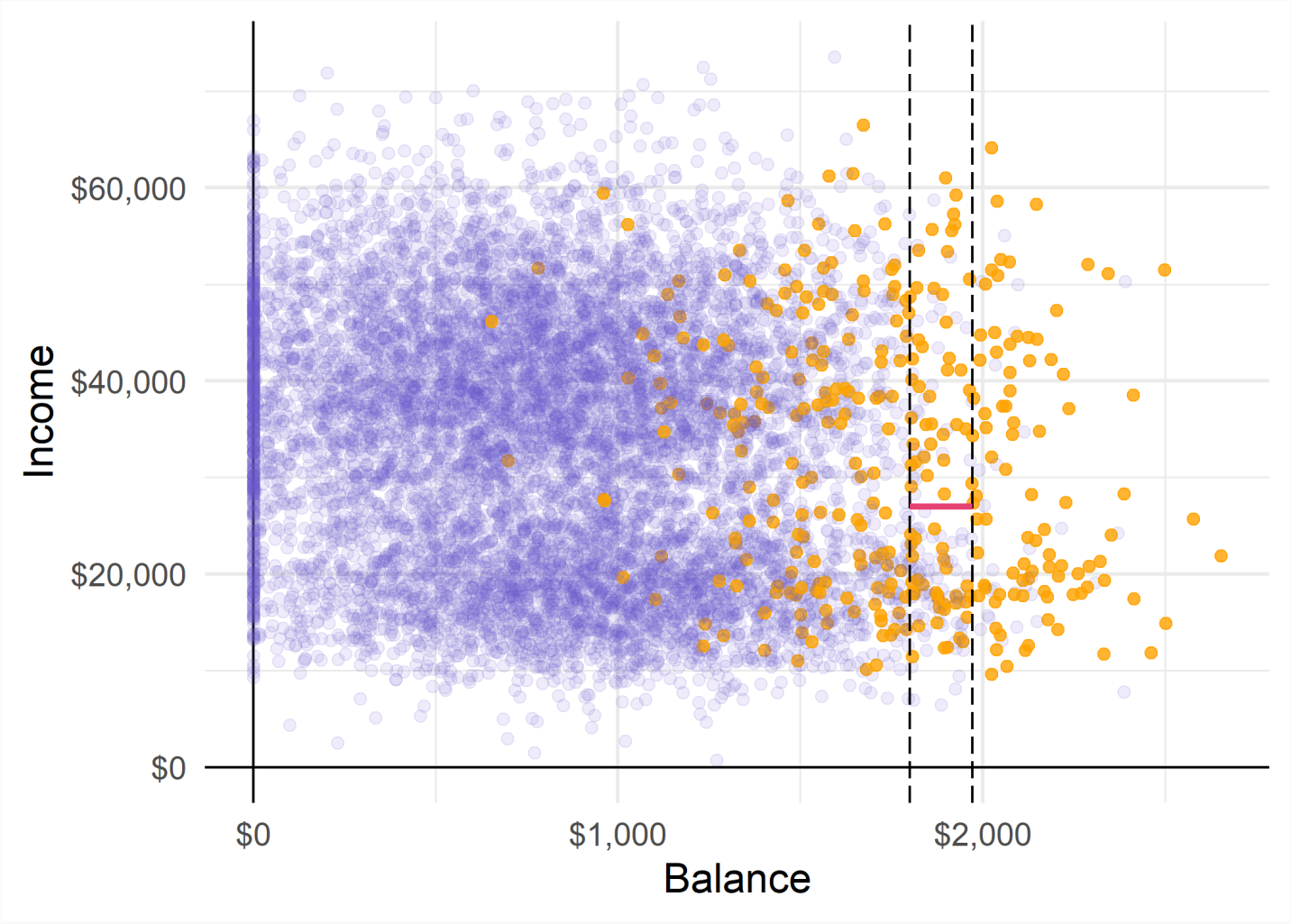
Growing Decision Trees

The **second partition** splits balance at \$1,972, (*conditional on bal. > \$1,800*).



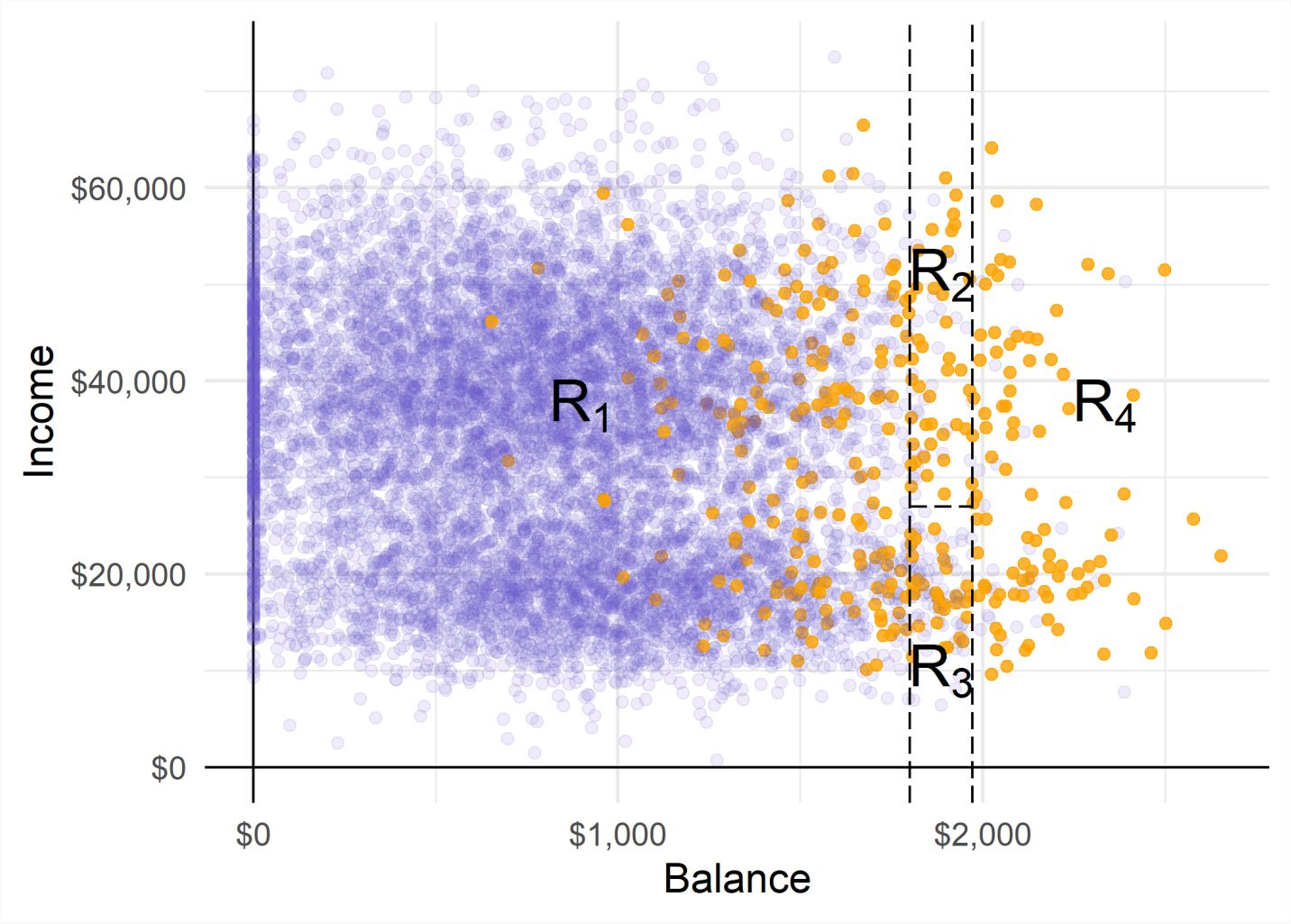
Growing Decision Trees

The **third partition** splits income at $27K for bal. between $1,800 and $1,972.



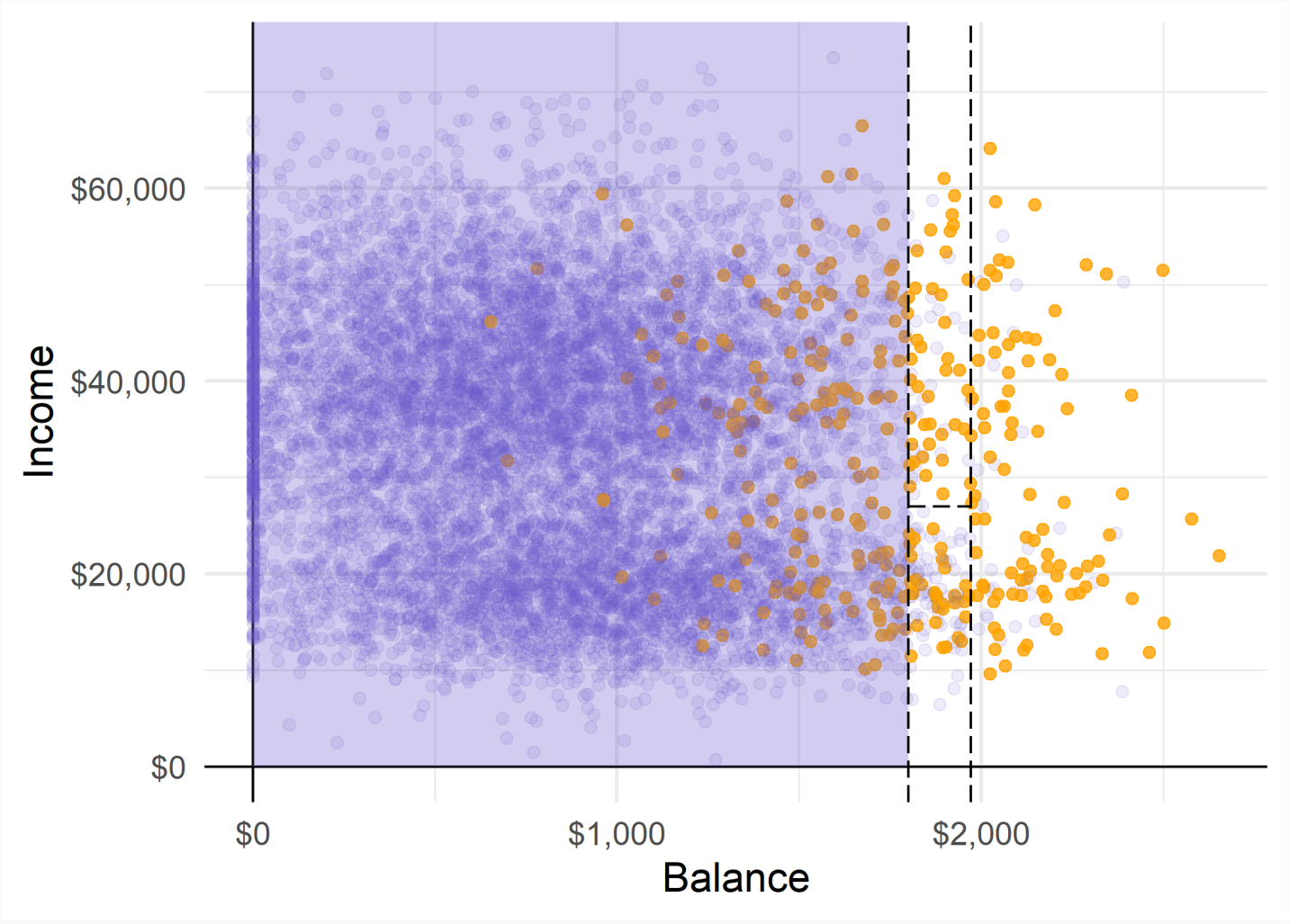
Growing Decision Trees

These three partitions give us four **regions**...



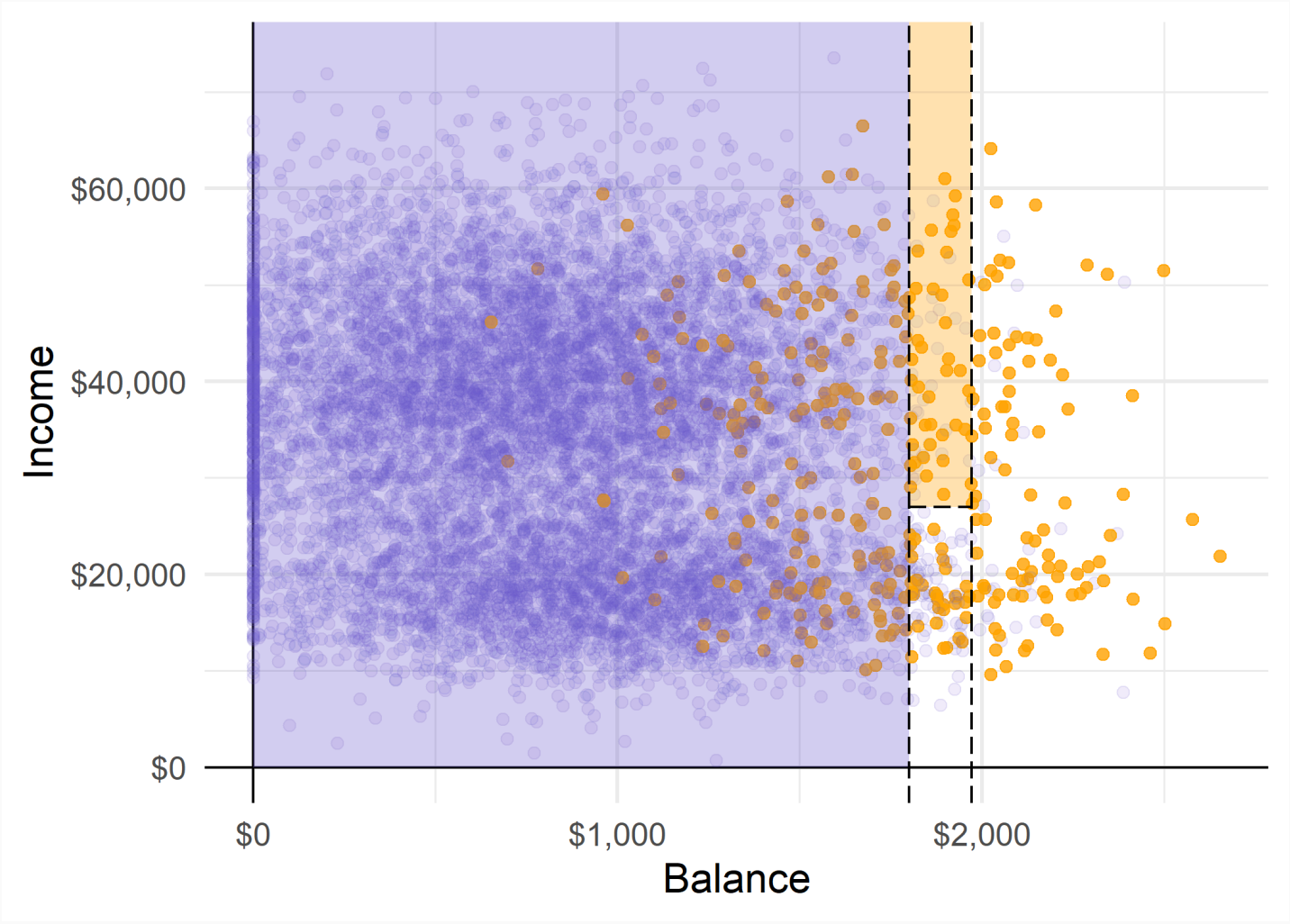
Growing Decision Trees

Predictions cover each region (e.g. using the region's **most common class**).



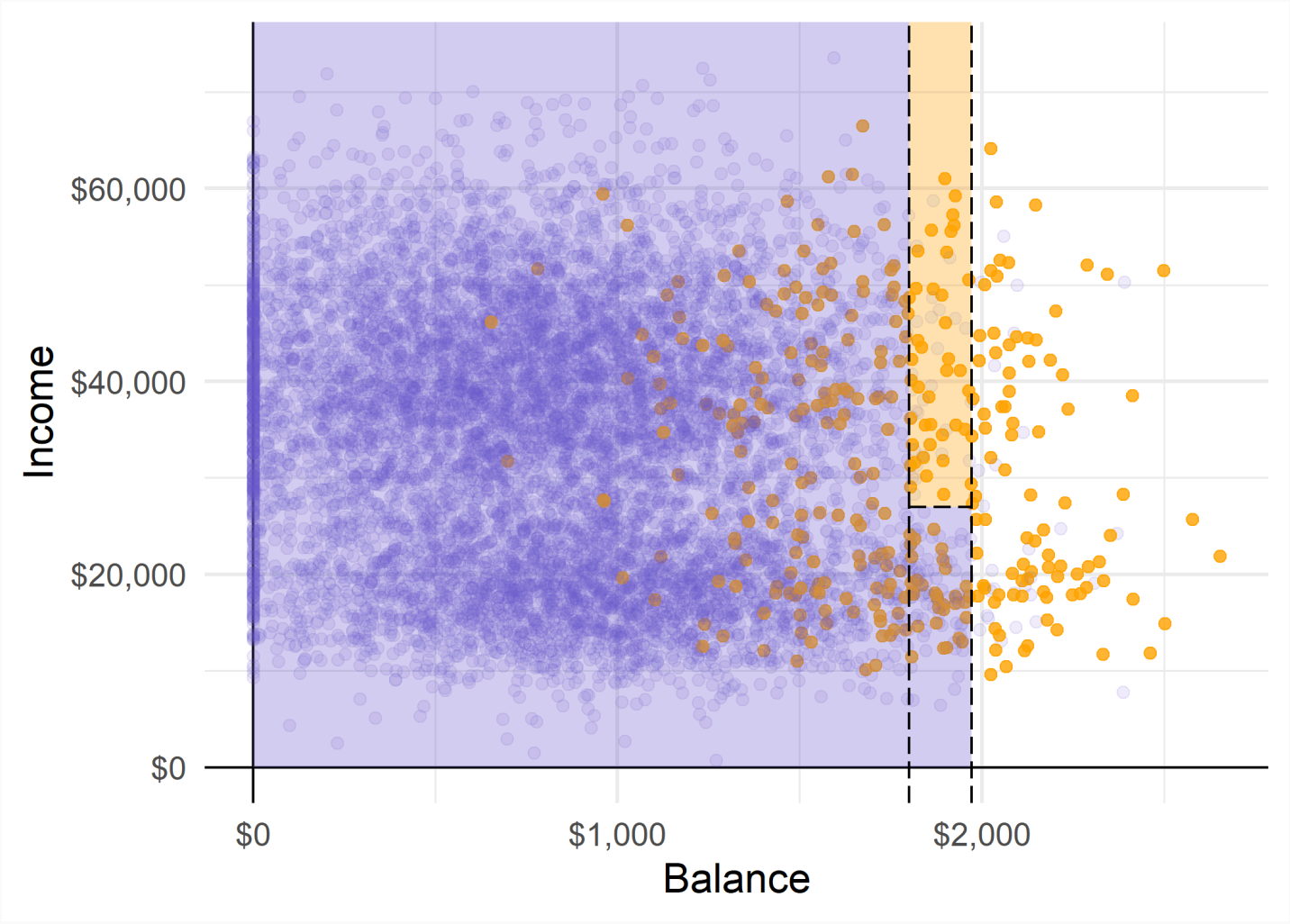
Growing Decision Trees

Predictions cover each region (e.g. using the region's **most common class**).



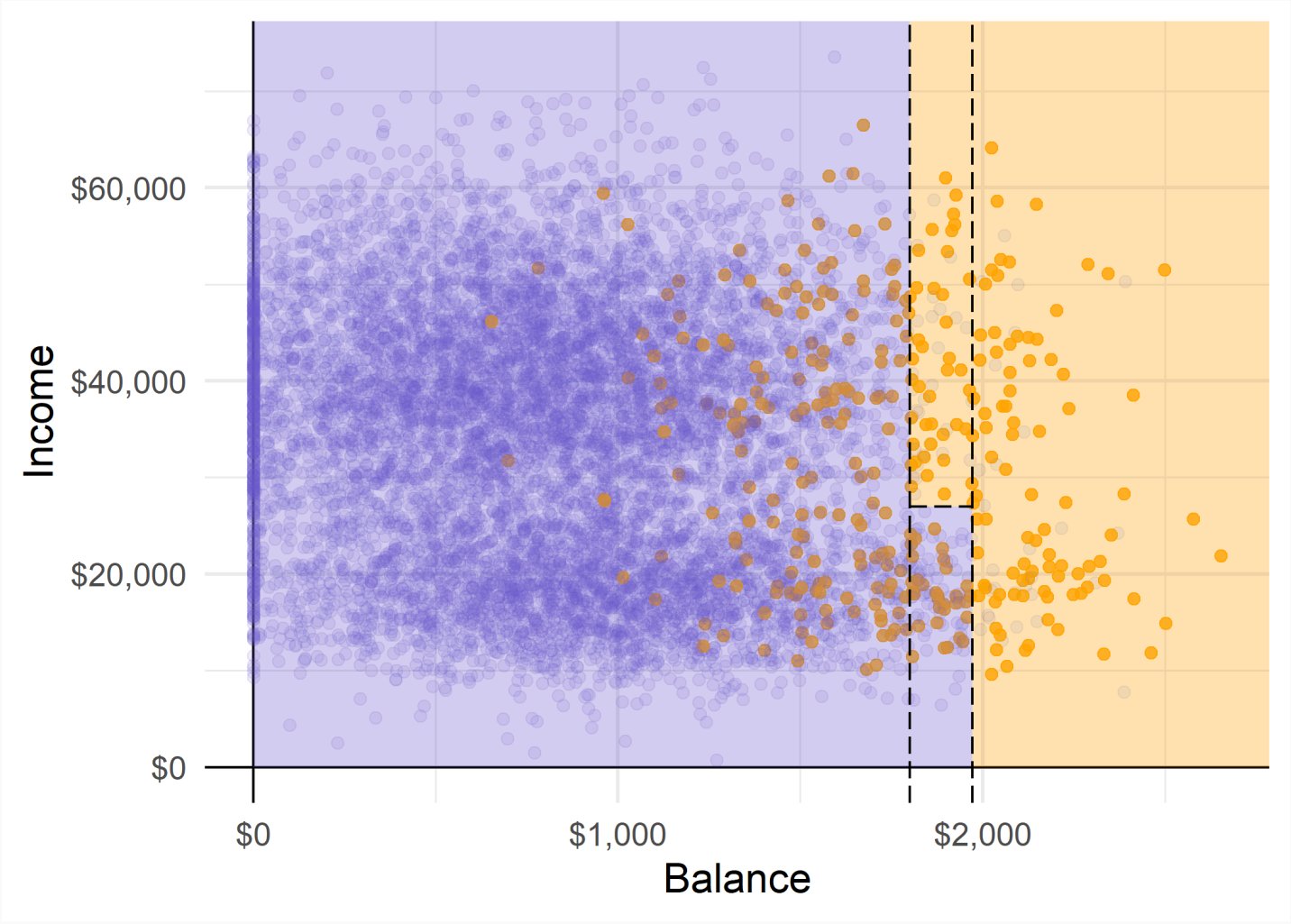
Growing Decision Trees

Predictions cover each region (e.g. using the region's **most common class**).



Growing Decision Trees

Predictions cover each region (e.g. using the region's **most common class**).



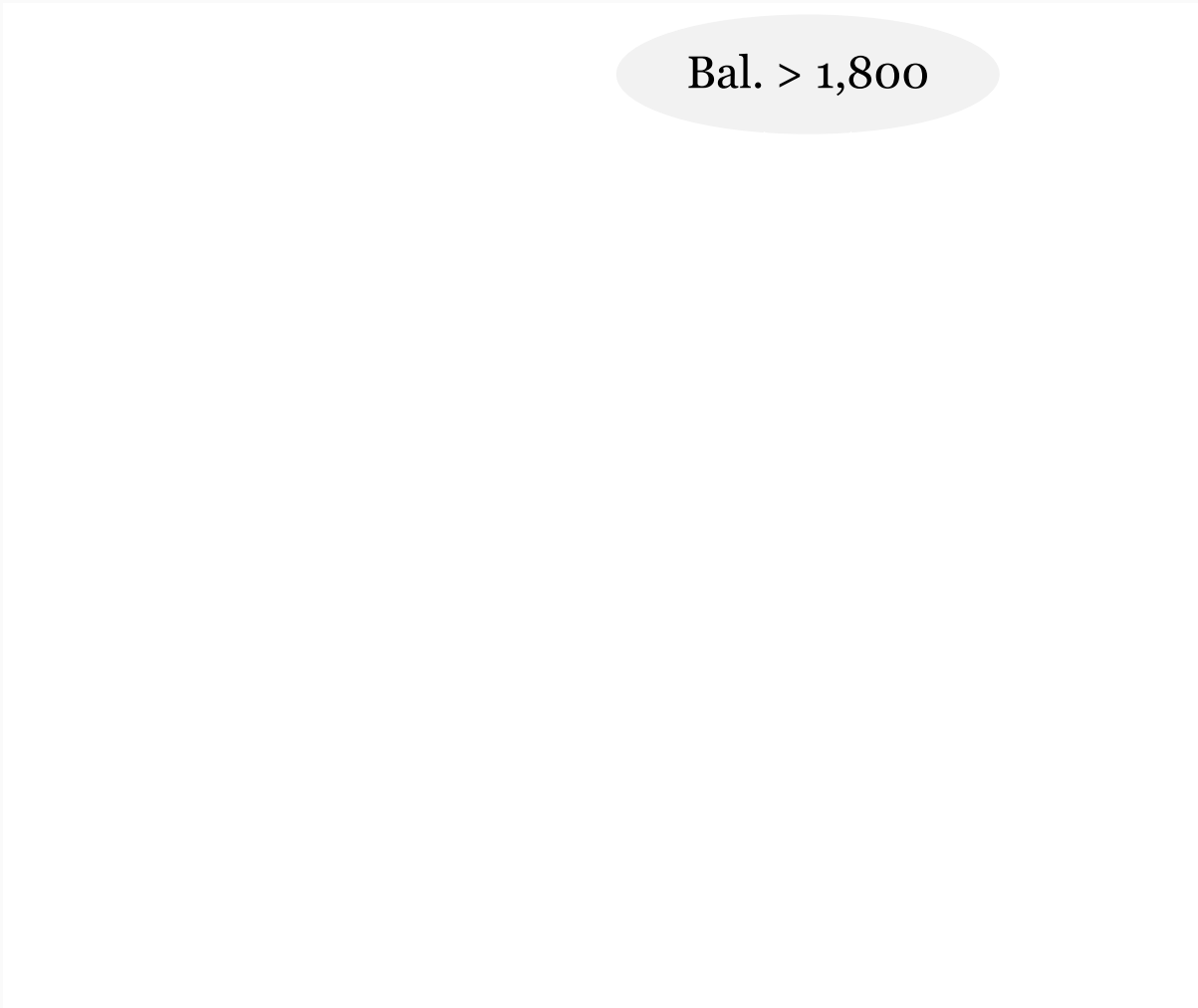
Visualizing the Decision Tree

Q: Why do we call it a tree?

A: Because we can easily represent this partitioning process in the form of a **decision tree!**

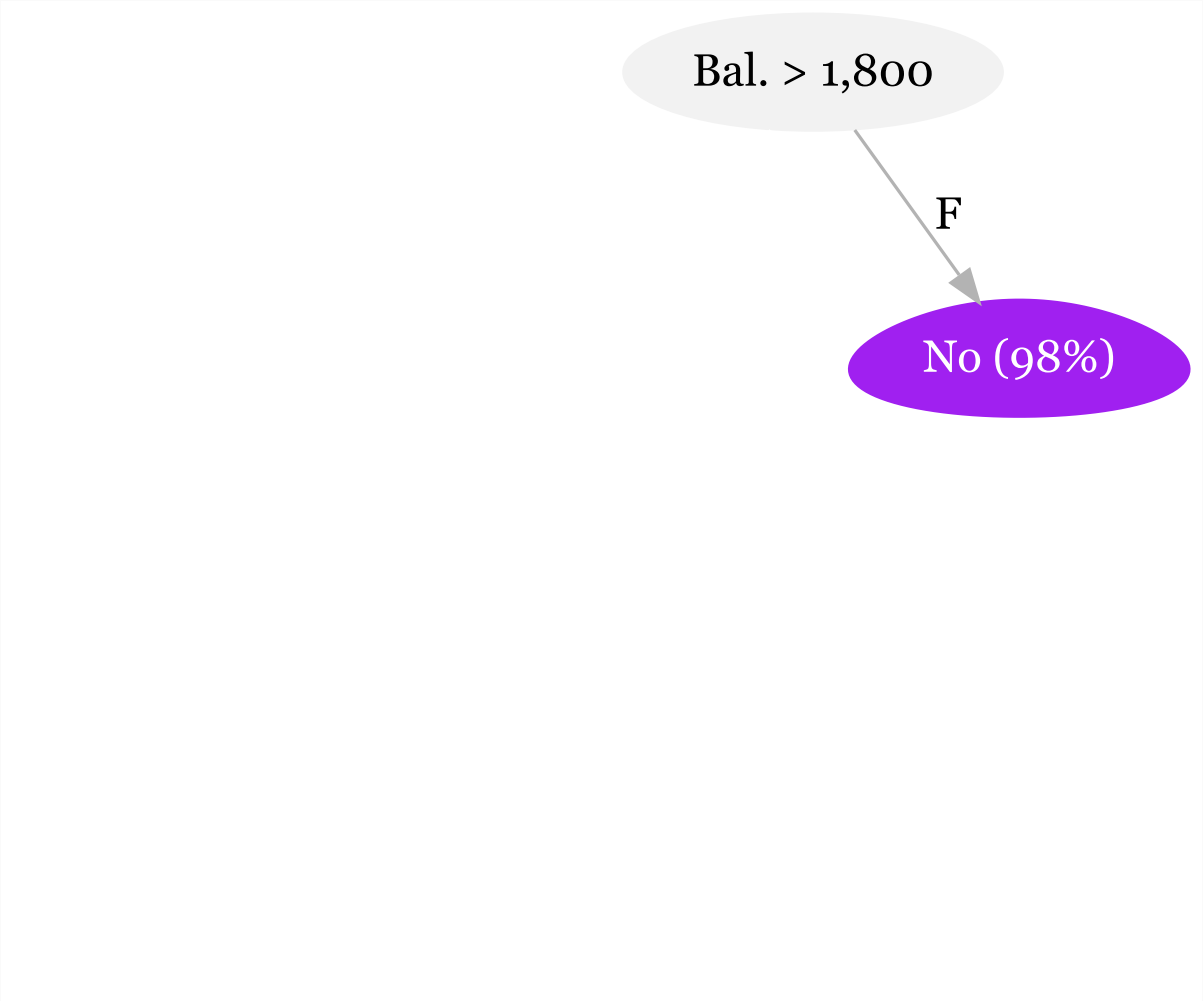
Visualizing the Decision Tree

Our first split occurs at a Balance of $1800:



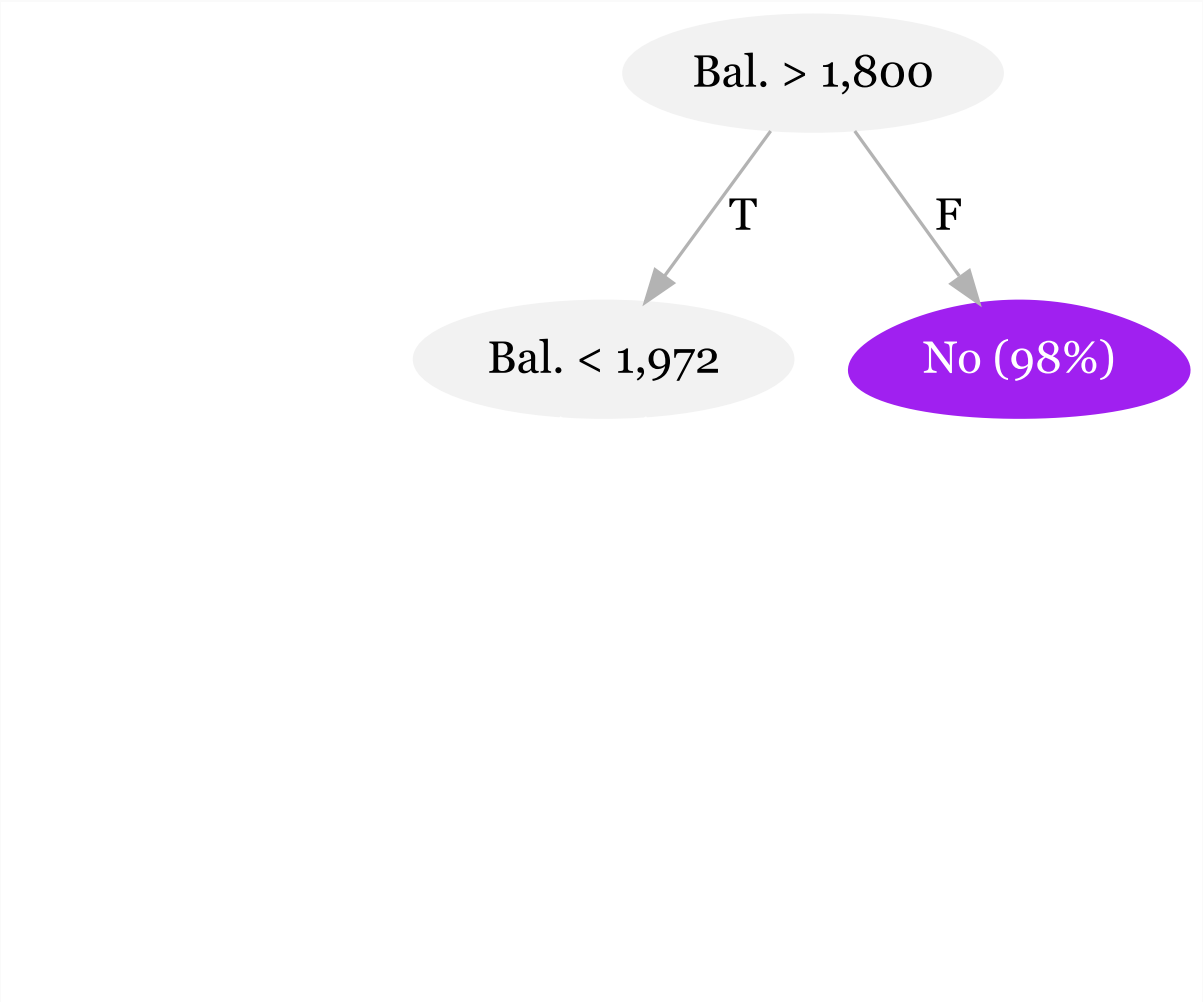
Visualizing the Decision Tree

If Balance > 1800 Is False, we get our first region:



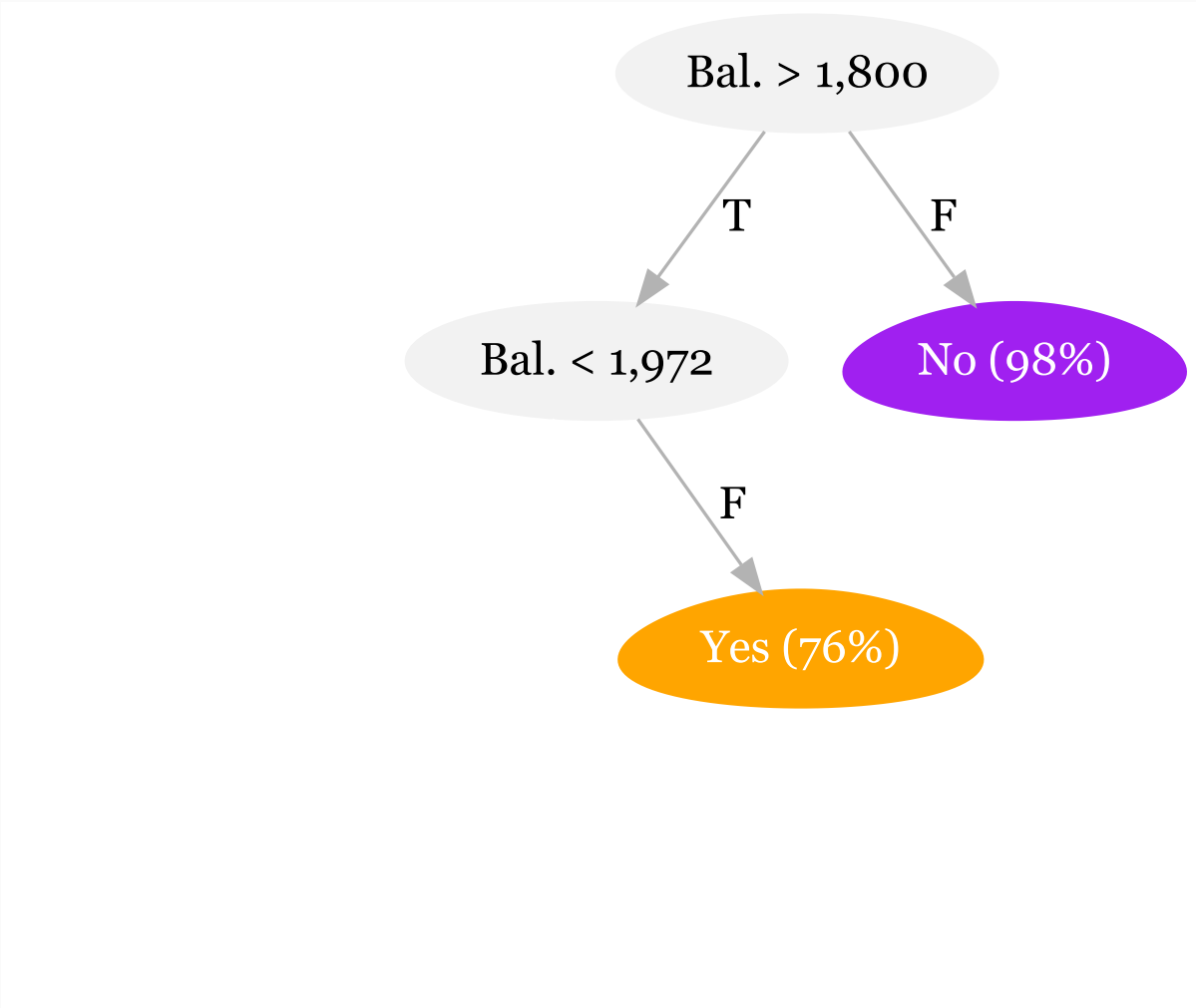
Visualizing the Decision Tree

If Balance < 1800 Is True, we next split on Balance < 1,972



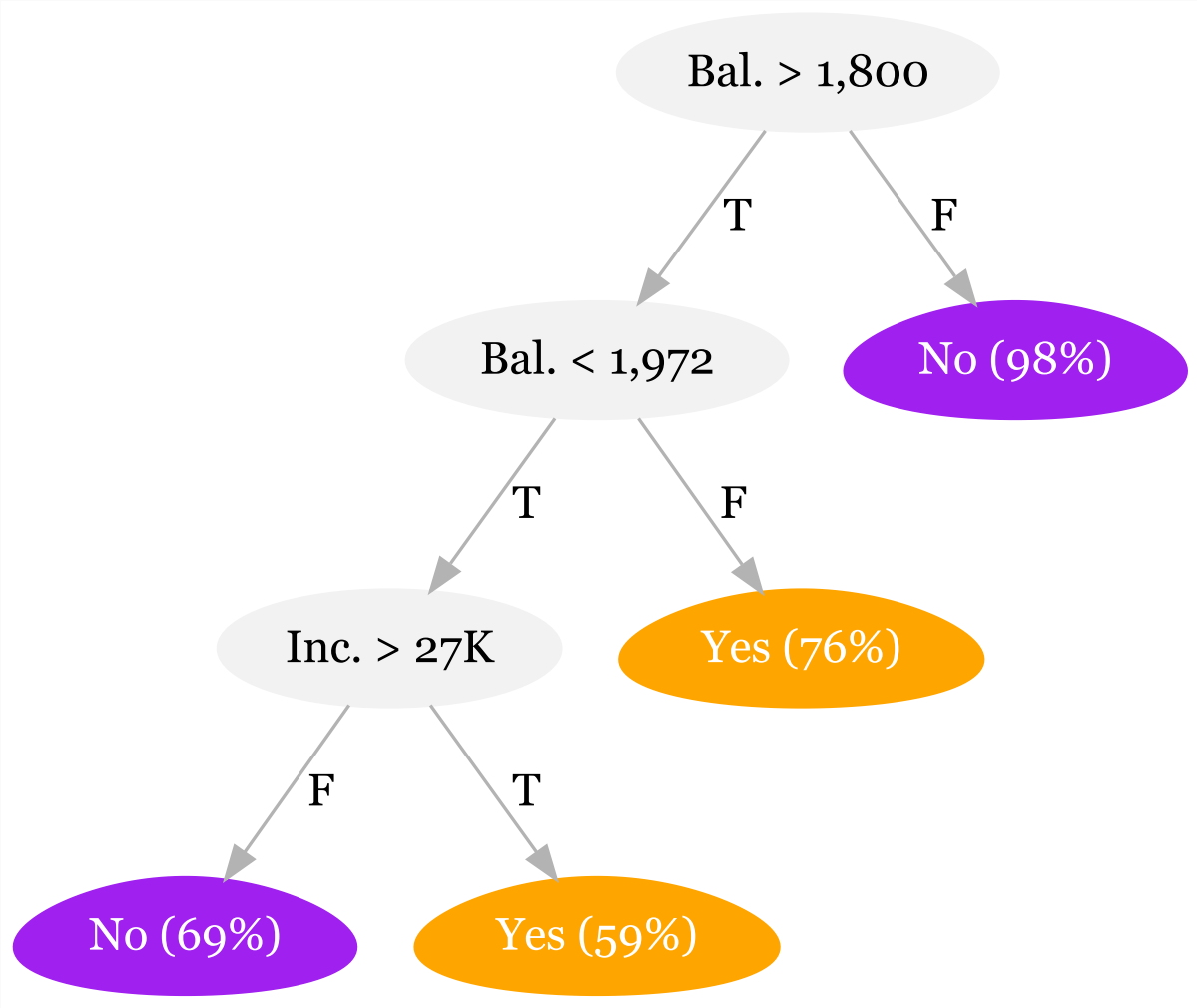
Visualizing the Decision Tree

If False, we get our second terminal node (76% default)



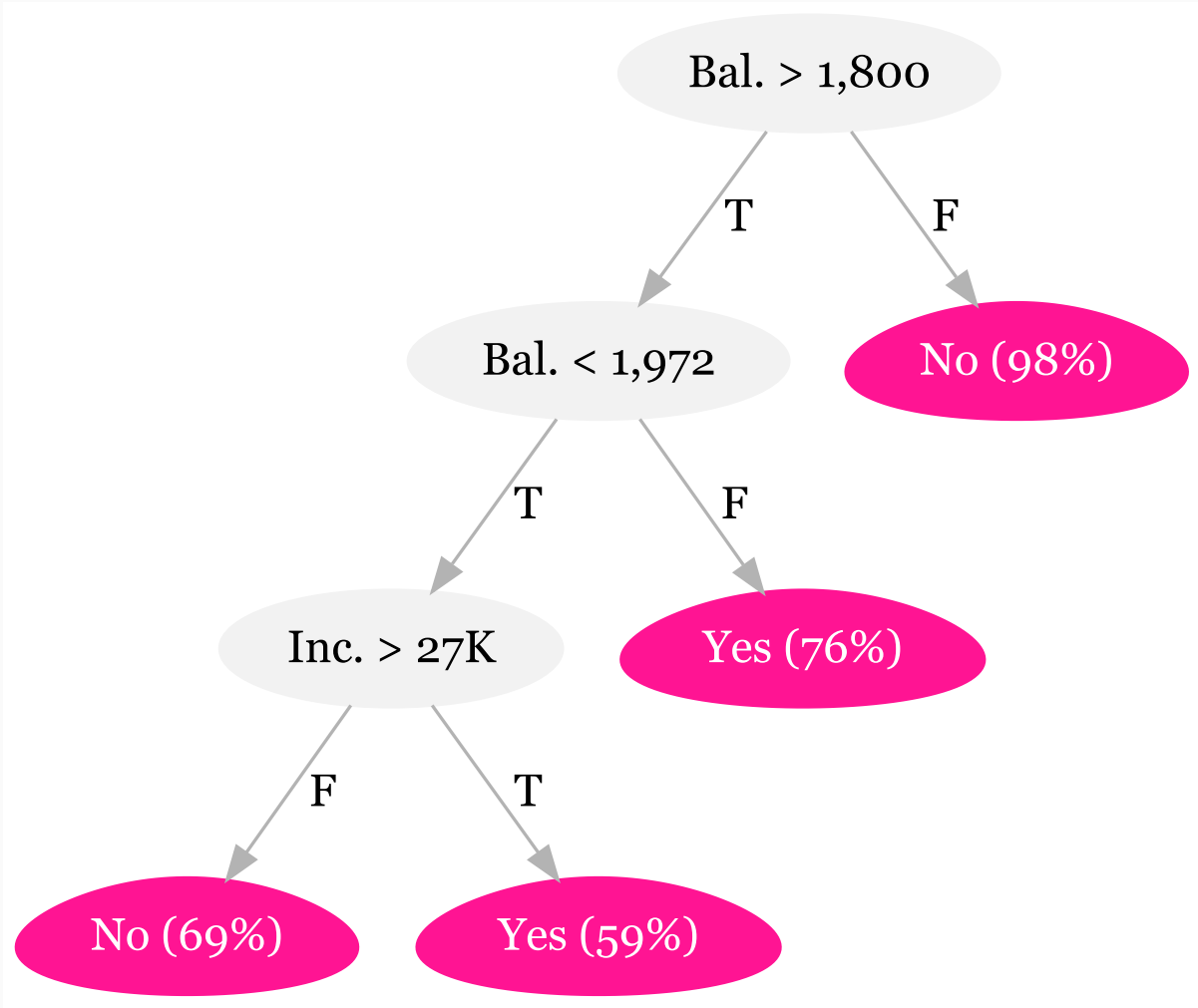
Visualizing the Decision Tree

If True, we get our final split at Income > 27,000



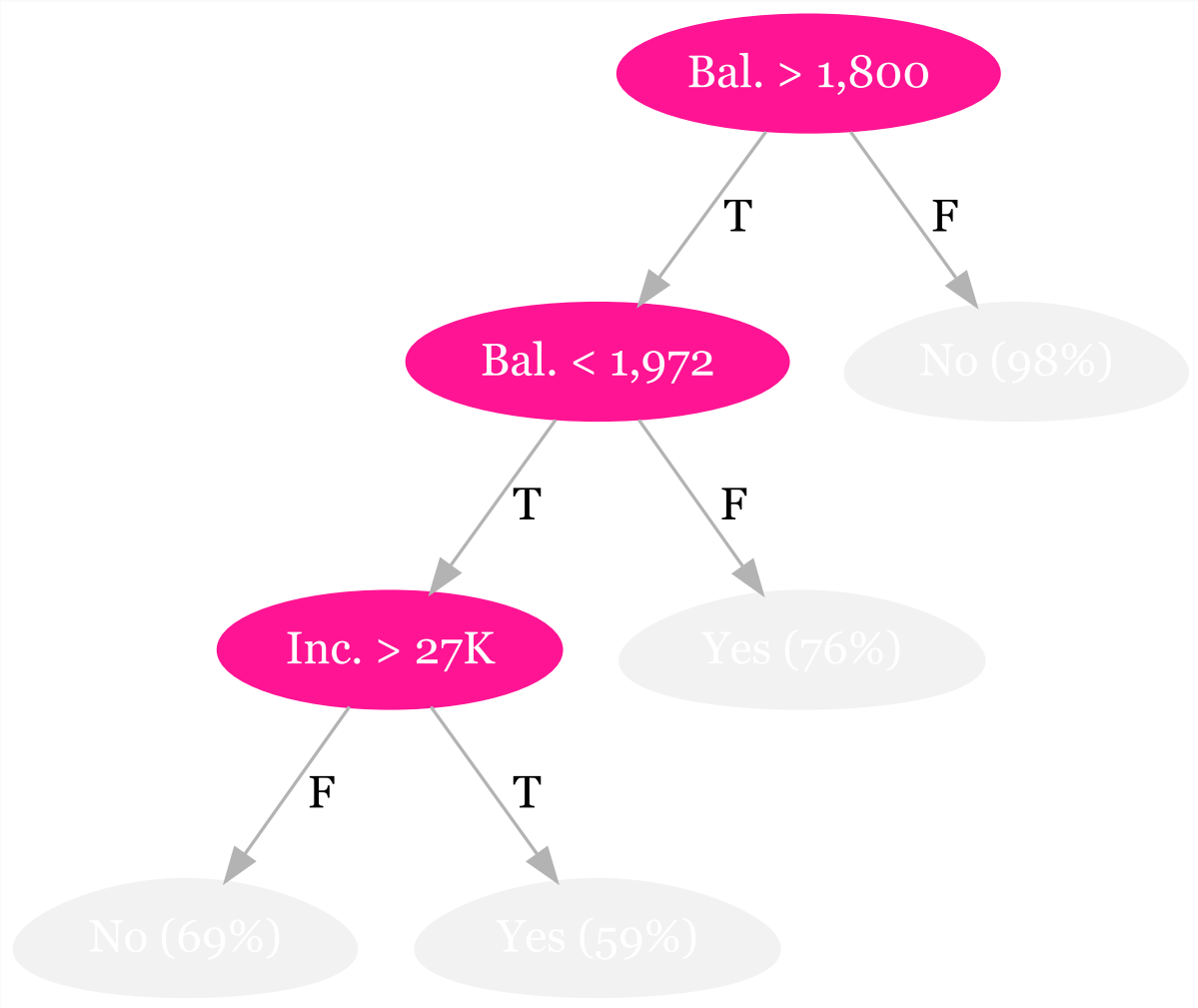
Decision Tree Anatomy

The **regions** correspond to the tree's **terminal nodes** (or **leaves**)



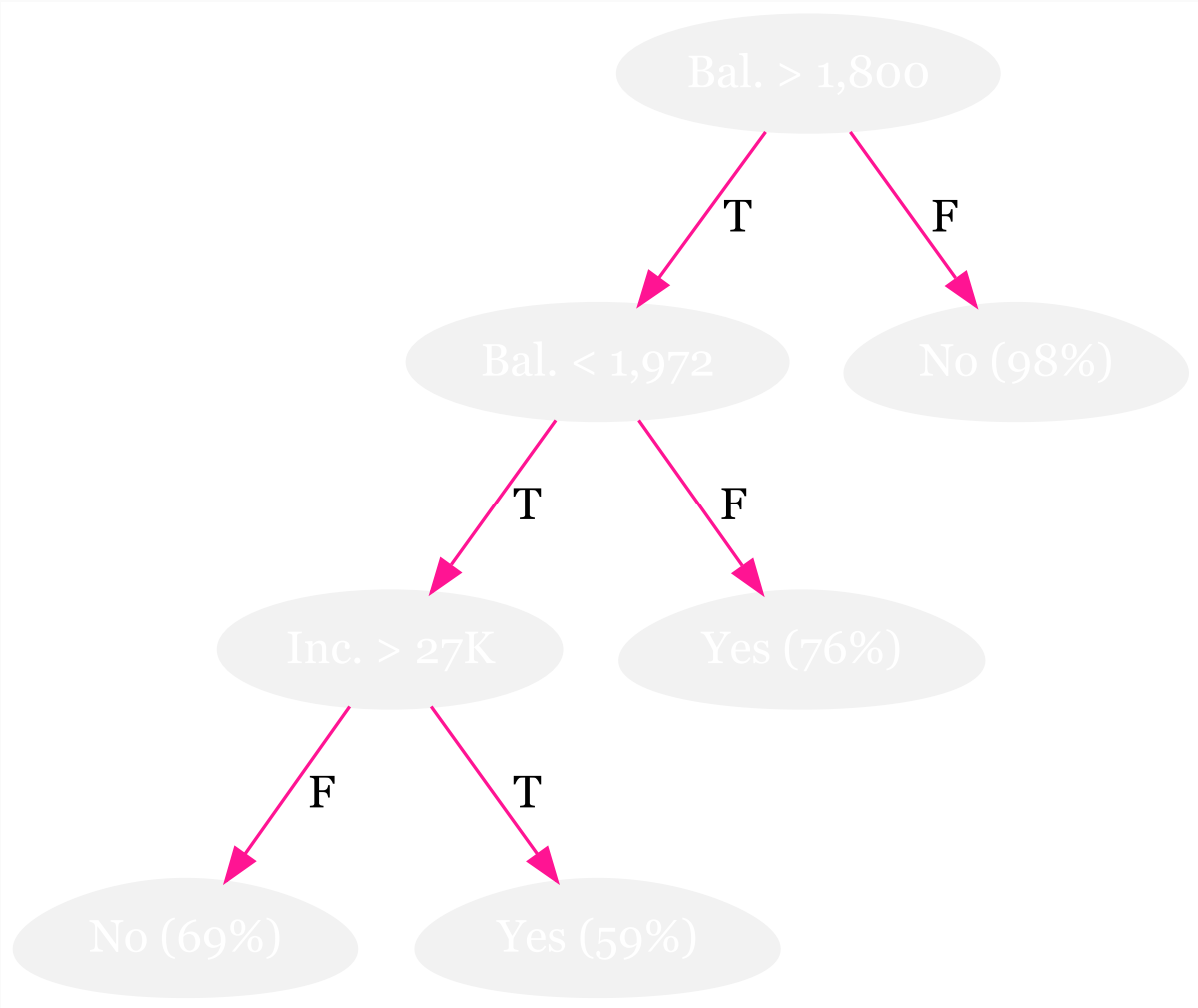
Decision Tree Anatomy

The graph's **separating lines** correspond to the tree's **internal nodes**



Decision Tree Anatomy

The segments connecting the nodes are the tree's **branches**



Growing The Tree

Problem: Examining every possible partition (every cutoff s of every predictor $\mathbf{x}_j$) is **computationally infeasible.**

Solution: a top-down, *greedy* algorithm named **recursive binary splitting**

- **Recursive:** starts with the "best" split, then find the next "best" split, etc.
- **Binary:** each split creates only two branches: "yes" and "no"
- **Greedy:** each step makes the "best" split without consideration for the overall process

Splitting Example

Consider the dataset

i	y	x1	x2
1	0	1	4
2	8	3	2
3	6	5	6

With just three observations, each variable only has two actual splits.

You can think about cutoffs as the ways we divide observations into two groups.

Splitting Example

One possible split: x_1 at 2, which yields (1) $x_1 < 2$ *vs.* (2) $x_1 \geq 2$

i	y	x1	x2
1	0	1	4
2	8	3	2
3	6	5	6

Splitting Example

One possible split: x_1 at 2, which yields (1) $x_1 < 2$ *vs.* (2) $x_1 \geq 2$

i	pred	y	x1	x2
1	**0**	0	1	4
2	**7**	8	3	2
3	**7**	6	5	6

This split yields an RSS of $0^2 + 1^2 + (-1)^2 = 2$.

Note$_1$ Splitting x_1 at 2 yields the same results as 1.5, 2.5—anything in (1, 3).

Splitting Example

An alternative split: x_1 at 4, which yields (1) $x_1 < 4$ *vs.* (2) $x_1 \geq 4$

i	pred	y	x1	x2
1	**4**	0	1	4
2	**4**	8	3	2
3	**6**	6	5	6

This split yields an RSS of $(-4)^2 + 4^2 + 0^2 = 32$.

Previous: Splitting x_1 at 4 yielded RSS = 2. *(Much better)*

Splitting Example

Another split: x_2 at 3, which yields (1) $x_1 < 3$ *vs.* (2) $x_1 \geq 3$

i	pred	y	x1	x2
1	**3**	0	1	4
2	**8**	8	3	2
3	**3**	6	5	6

This split yields an RSS of $(-3)^2 + 0^2 + 3^2 = 18$.

Splitting Example

Final split: x_2 at 5, which yields (1) $x_1 < 5$ *vs.* (2) $x_1 \geq 5$

i	pred	y	x1	x2
1	**4**	0	1	4
2	**4**	8	3	2
3	**6**	6	5	6

This split yields an RSS of $(-4)^2 + 4^2 + 0^2 = 32$.

Splitting Example

Across our four possible splits (two variables each with two splits)

- x_1 with a cutoff of 2: RSS = 2
- x_1 with a cutoff of 4: RSS = 32
- x_2 with a cutoff of 3: RSS = 18
- x_2 with a cutoff of 5: RSS = 32

our split of x_1 at 2 generates the lowest RSS.

Splitting

Note: Categorical predictors work in exactly the same way.
We want to try all possible combinations of the categories.

Ex: For a four-level categorical predictor (levels: A, B, C, D)

- Split 1: A|B|C *vs.* D
- Split 2: A|B|D *vs.* C
- Split 3: A|C|D *vs.* B
- Split 4: B|C|D *vs.* A
- Split 5: A|B *vs.* C|D
- Split 6: A|C *vs.* B|D
- Split 7: A|D *vs.* B|C

we would need to try 7 possible splits.

Splitting

Once we make our a split, we then continue splitting, conditional on the regions from our previous splits.

So if our first split creates R_1 and R_2, then our next split searches the predictor space only in R_1 or R_2.

The tree continue to grow until it hits some specified threshold, *e.g.*, at most 5 observations in each leaf.

We are no longer searching the full space—it is conditional on the previous splits.

Too many Splits?

One can have **too many splits.**

Q: Why?

A: "More splits" means

1. more flexibility (think about the bias-variance tradeoff/overfitting)
2. less interpretability (one of the selling points for trees)

Q: So what can we do?

A: Prune your trees!

Pruning

The idea: Some regions may increase **variance** more than they reduce **bias**.

- By removing these regions, we gain in test MSE.

Candidates for trimming: Regions that do not reduce RSS very much.

Updated strategy: Grow big trees T_0 and then trim T_0 to an optimal subtree.

Updated problem: Considering all possible subtrees can get expensive.

Pruning

Updated solution: add a penalty for complexity with **cost-complexity pruning**

- Pay a penalty to become more complex with a greater number of regions $|T|$

For regression trees[1]:

$$\sum_{m=1}^{|T|} \sum_{i:x \in R_m} \left(y_i - \hat{y}_{R_m}\right)^2 + \alpha |T|$$

For any value of $\alpha (\geq 0)$, we get a subtree $T \subset T_0$.

We choose α via cross validation.

1 For classification trees we instead penalize the error rate

Decision Trees in R

To train decision trees in R, we'll use **tidymodels** (and several others) for modeling and machine learning using **tidyverse** principles[2]

Let's first set the seed and define our cross-validation with `vfold_cv` from **rsample**

- `v` the number of folds (here we'll use 5)

```
# Define our CV split
set.seed(12345)
default_cv ← default_df %>% vfold_cv(v = 5)
```

2. **tidymodels** allow you to do a *ton* of stuff that we're just scratching the surface of.

Decision Trees in R

Next, let's use the `decision_tree()` function from **parsnip** to set up the parameters of the tree:

- `mode`: `"regression"` or `"classification"`
- `cost_complexity`: the cost (penalty) paid for complexity
- `tree_depth`: *max.* tree depth (max. number of splits in a "branch")
- `min_n`: *min.* # of observations for a node to split
- Use the **rpart** "engine" to grow the tree

```
# Define the decision tree
default_tree ← decision_tree(
  mode = "classification", #
  cost_complexity = tune(),
  tree_depth = tune(),
  min_n = 10 # Arbitrarily choosing '10'
) %>% set_engine("rpart")
```

Decision Trees in R

Next, use `recipe()` to build a recipe describing the formula/data

```
# Define recipe
default_recipe ← recipe(default ~ ., data = default_df)
```

And define the workflow, first adding the model then the recipe

```
# Define the workflow
default_flow ← workflow() %>%
  add_model(default_tree) %>% add_recipe(default_recipe)
```

Decision Trees in R

Lastly, execute the workflow through cross-validation!

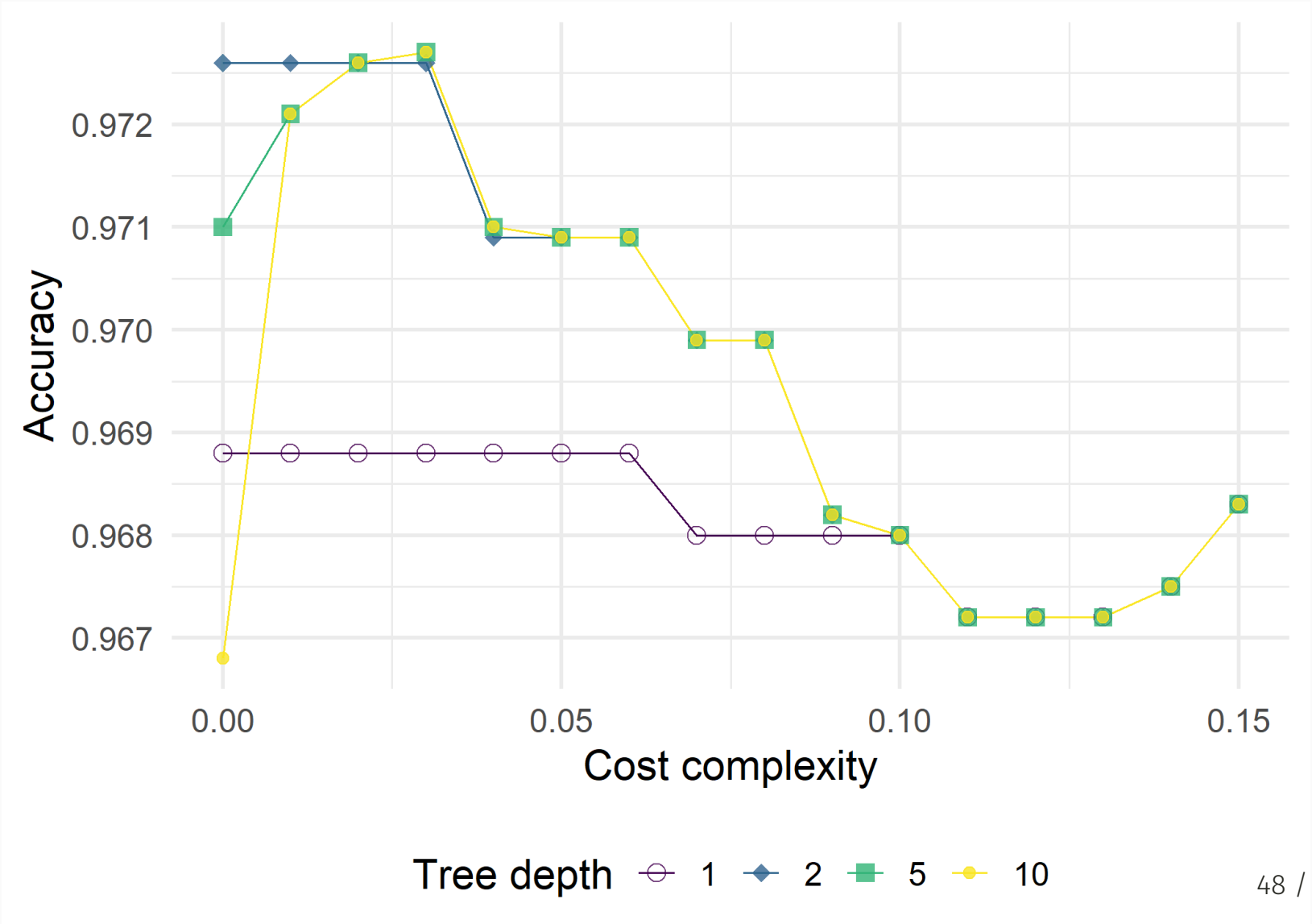
```
# Tune!
default_cv_fit ← default_flow %>% tune_grid(
  default_cv,
  grid = expand_grid(
    cost_complexity = seq(0, 0.15, by = 0.01),
    tree_depth = c(1, 2, 5, 10),
  ),
  metrics = metric_set(accuracy)
)
```

Decision Trees in R

Plotting

```
ggplot(
  data = default_cv_fit %>% collect_metrics() %>% filter(.metric == "accu
  aes(
    x = cost_complexity,
    y = mean,
    color = tree_depth %>% factor(levels = c(1,2,5,10), ordered = T),
    shape = tree_depth %>% factor(levels = c(1,2,5,10), ordered = T)
  )
) +
geom_line(linewidth = 0.4) +
geom_point(size = 3, alpha = 0.8) +
scale_y_continuous("Accuracy") +
scale_x_continuous("Cost complexity") +
scale_color_viridis_d("Tree depth") +
scale_shape_manual("Tree depth", values = c(1, 18, 15, 20)) +
theme_minimal(base_size = 16) +
theme(legend.position = "bottom")
```

Decision Trees in R



Decision Trees in R

To plot the CV-chosen tree...

1. **Fit** the chosen/best model with `finalize_workflow()` and `select_best()`

```
best_flow ←
  default_flow %>%
  finalize_workflow(select_best(default_cv_fit, metric = "accuracy")) %>%
  fit(data = default_df)
```

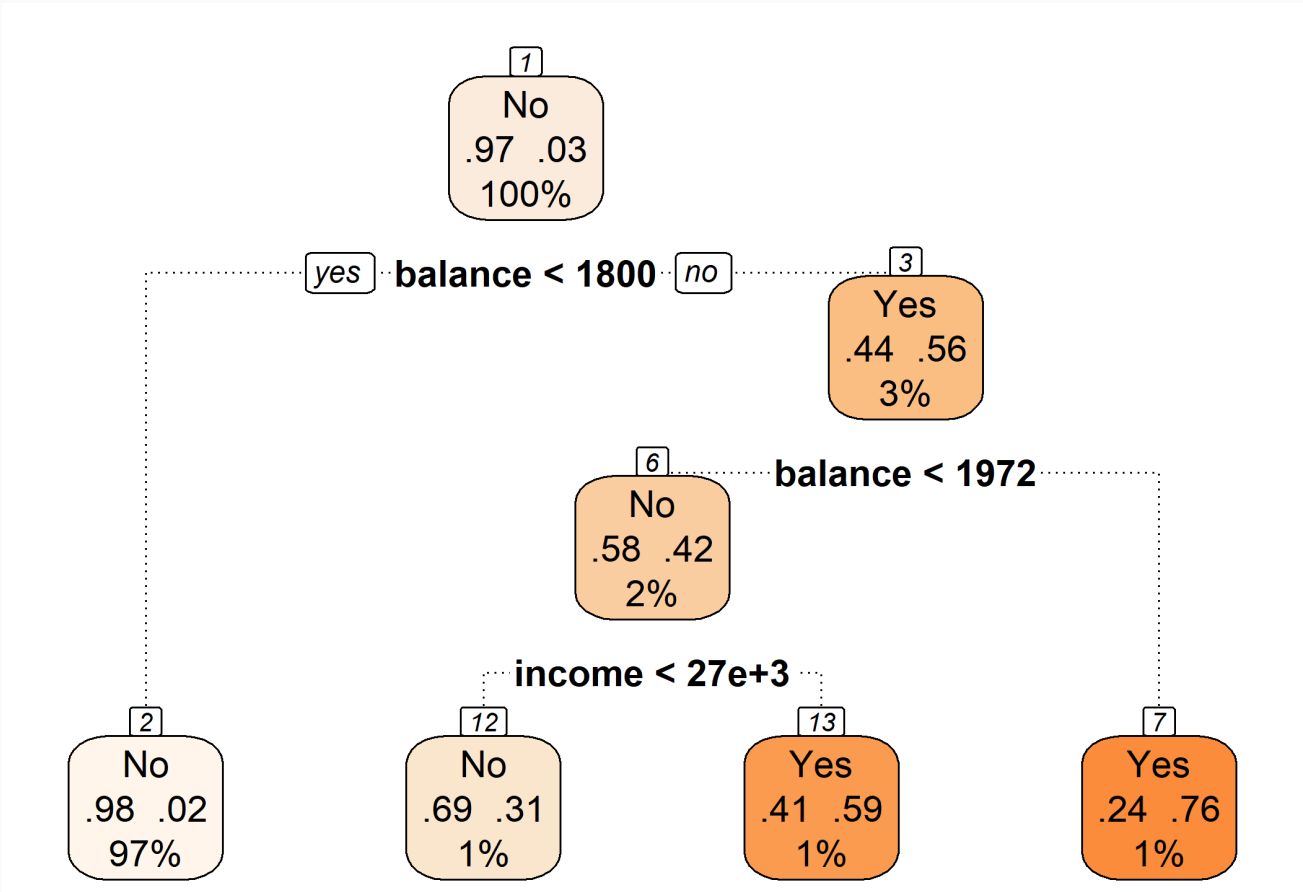
2. **Extract** the fitted model with `extract_fit_parsnip()`

```
best_tree ← best_flow %>% extract_fit_parsnip()
```

Decision Trees in R

3. **Plot** the tree with `rpart.plot()` from **rpart.plot**.

```
best_tree$fit %>% rpart.plot()
```



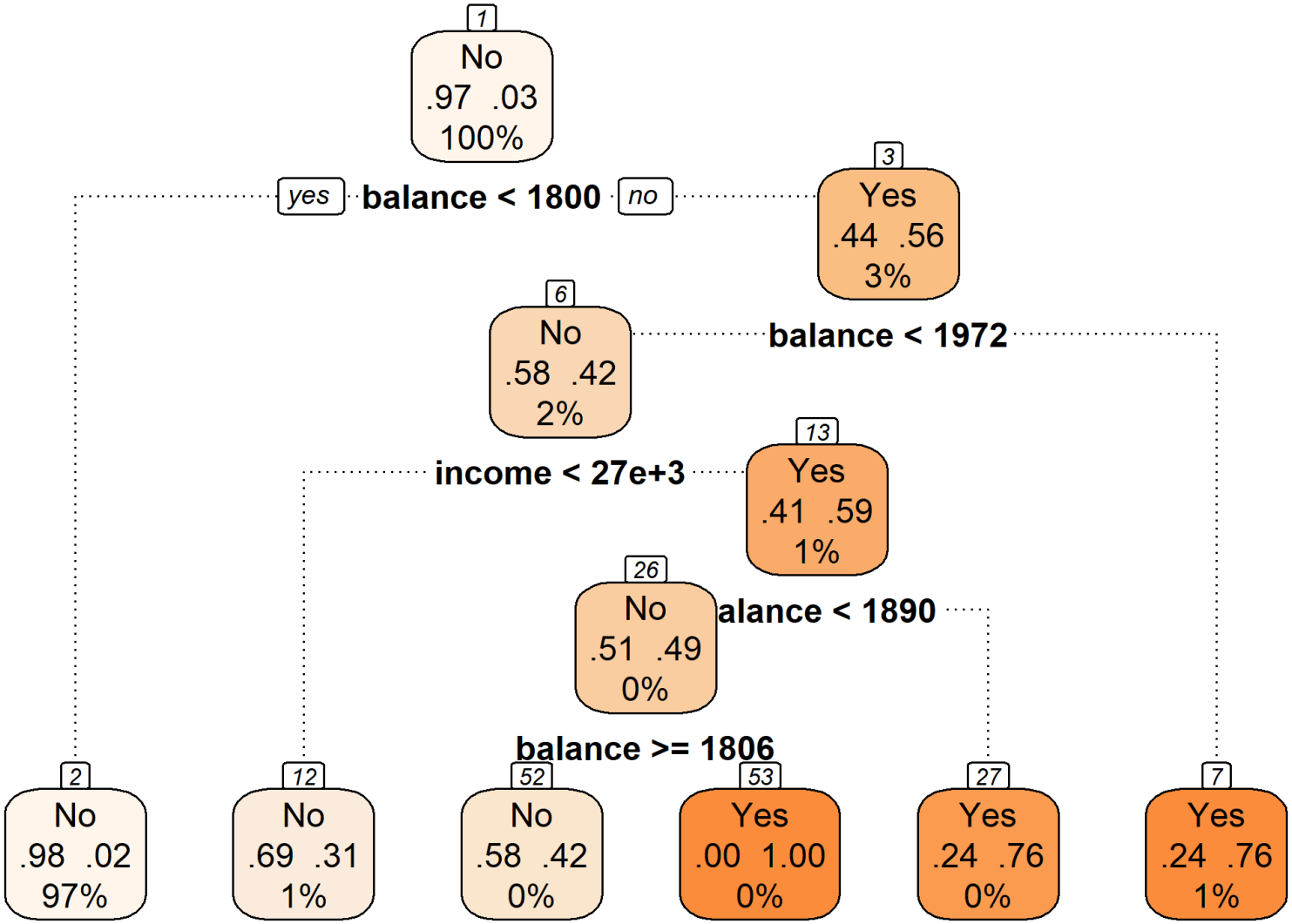
Decision Trees in R

The previous tree has cost complexity of 0.03 (and a max. depth of 5).

We can compare this "best" tree to a less pruned/penalized tree

- `cost_complexity = 0.005`
- `tree_depth = 5`

Decision Trees in R



Decision Trees vs. Linear Models

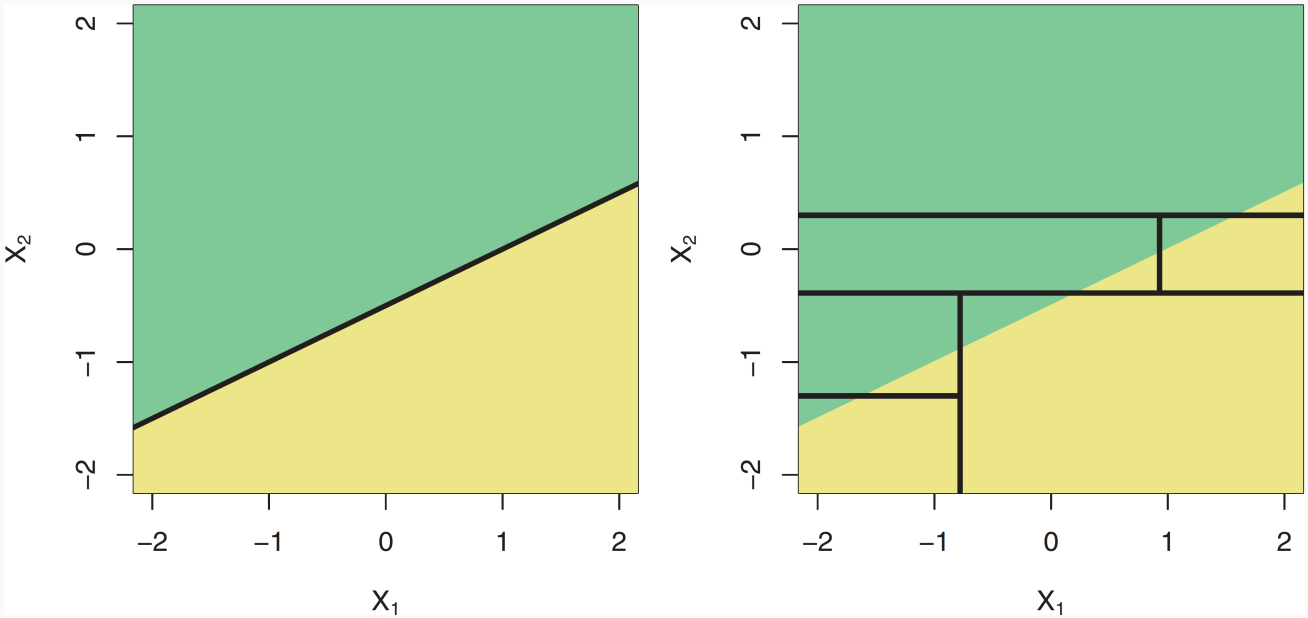
Q How do trees compare to linear models?

A It depends how linear the true boundary is.

Linear Boundary

Linear models recreate the line

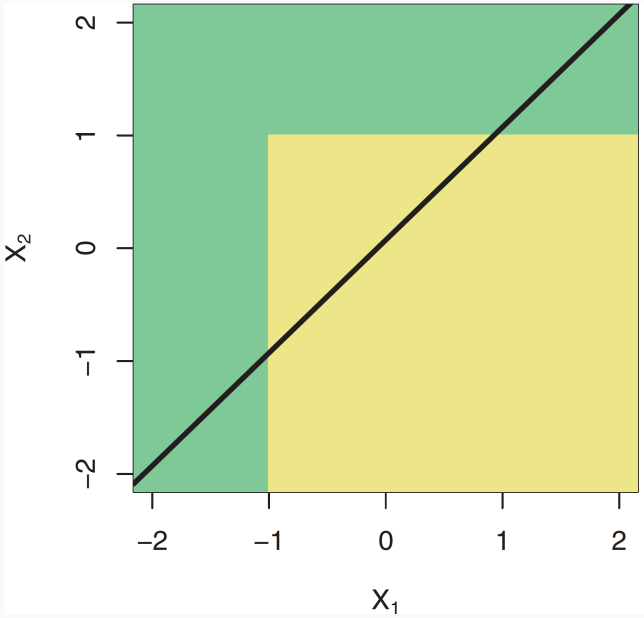
trees struggle at replicating linearity



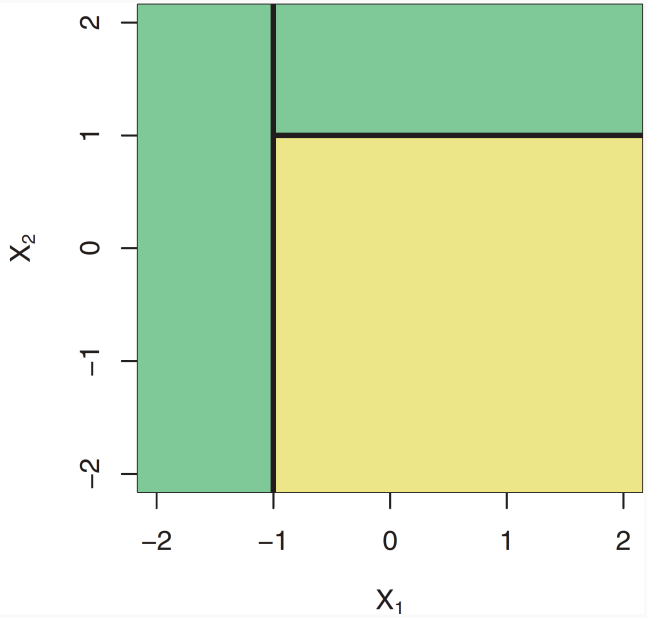
Source: ISL, p. 315

Nonlinear Bounday

Linear models struggle with nonlinear boundaries



trees easily replicate these relationships



Source: ISL, p. 315

Strengths and weaknesses

As with any method, decision trees have **tradeoffs**.

Strengths	Weaknesses
+ Easily explained/interpretted	- Outperformed by other methods
+ Include several graphical options	- Struggle with linearity
+ Mirror human decision making?	- Can be very "non-robust" - small data changes can cause huge changes in our tree
+ Handle num. or cat. on LHS/RHS	

Next: Create ensembles of trees to strengthen these weaknesses. with...

Forests! Which will also weaken some of the strengths.


Random Forests

Random Forests

The gist: combine many individual trees into a single **forest** via **bootstrap aggregation (bagging)**

Bagging:

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

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**.

Out-of-Bag Error

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

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.

Random Forests

Random forests overcome a major shortcoming of bagging: **very correlated trees**

- Since trees consider all predictors at every split of every tree, the trees will often be highly related.

Solution: decorrelate the trees!

- Only consider a **random subset** of m $(\approx \sqrt{p})$ predictors when making each split (for each tree)
- This nudges trees away from always using the same variables, increasing variation across trees, and potentially reducing 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 decision trees.

Random Forests in R

Let's see how to train a random forest using **tidymodels**.

Let's try and predict heart disease occurrence as a function of

- `age` Patient age
- `sex` Gender (`sex=1` for male)
- `chest_pain` Type of chest pain
- `rest_bp` Resting blood pressure
- `chol` Serum cholesterol level
- `fbs` Fasting blood sugar above 120mg/dl
- `restecg` Resting ECG results
  - 0 normal, 1 have ST-T wave abnormality, 2 probable/definite left ventricular hypertrophy
- `max_hr` Max heart rate
- `ex_ang` Exercised induced angina (pain from reduced blood flow)
  - 1 yes
- `oldpeak` ST depression induced by exercise relative to rest (observed in ECG)
- `slope` Slope of the peak exercise ST segment (observed in ECG)
  - 0 upsloping, 1 flat, 2 downsloping
- `ca` Number of major vessels colored by fluoroscopy (`ca`)
- `thal` Thalium stress test result
  - 0 normal, 1 fixed defect, 2 reversible defect, 3 not described

Random Forests in R

Let's first define our recipe and do some preprocessing.

- **Recipe:** predict heart disease (Yes/No) as a function of everything else
- **Cleaning:** imput missing values (median for numeric, mode for categorical)

```
# Impute missing values
heart_recipe ← recipe(heart_disease ~ ., data = heart_df) %>%
  step_impute_median(all_predictors() & all_numeric()) %>%
  step_impute_mode(all_predictors() & all_nominal())
```

Now we can use `prep()` and `juice()` to replace our data frame with the cleaned version:

```
heart_df_clean ← heart_recipe %>% prep() %>% juice()
```

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`.

Random Forests in R

Training a random forest in R using **tidymodels** and **ranger**:

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

Random Forests in R

Training a random forest in R using **tidymodels** and **ranger**:

- Goal: Classification

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

Random Forests in R

Training a random forest in R using **tidymodels** and **ranger**:

- Goal: Classification
- Try 3 variables per split

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

Random Forests in R

Training a random forest in R using **tidymodels** and **ranger**:

- Goal: Classification
- Try 3 variables per split
- 100 trees in the forest

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

Random Forests in R

Training a random forest in R using **tidymodels** and **ranger**:

- Goal: Classification
- Try 3 variables per split
- 100 trees in the forest
- At least 2 obs. to split

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

Random Forests in R

Training a random forest in R using **tidymodels** and **ranger**:

- Goal: Classification
- Try 3 variables per split
- 100 trees in the forest
- At least 2 obs. to split
- Choose the `ranger` engine

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

)
```

Random Forests in R

Training a random forest in R using **tidymodels** and **ranger**:

- Goal: Classification
- Try 3 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",
  importance = "impurity"
)
```

Random Forests in R

Training a random forest in R using **tidymodels** and **ranger**:

- Goal: Classification
- Try 3 variables per split
- 100 trees in the forest
- At least 2 obs. to split
- Choose the `ranger` engine
- Set a **splitting rule**
- Set the method for calculating variable importance

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

Random Forests in R

We can then build our workflow and fit the random forest:

Interpreting Random Forests

While ensemble methods like random forests tend to **improve predictive performance**, they also tend to **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.

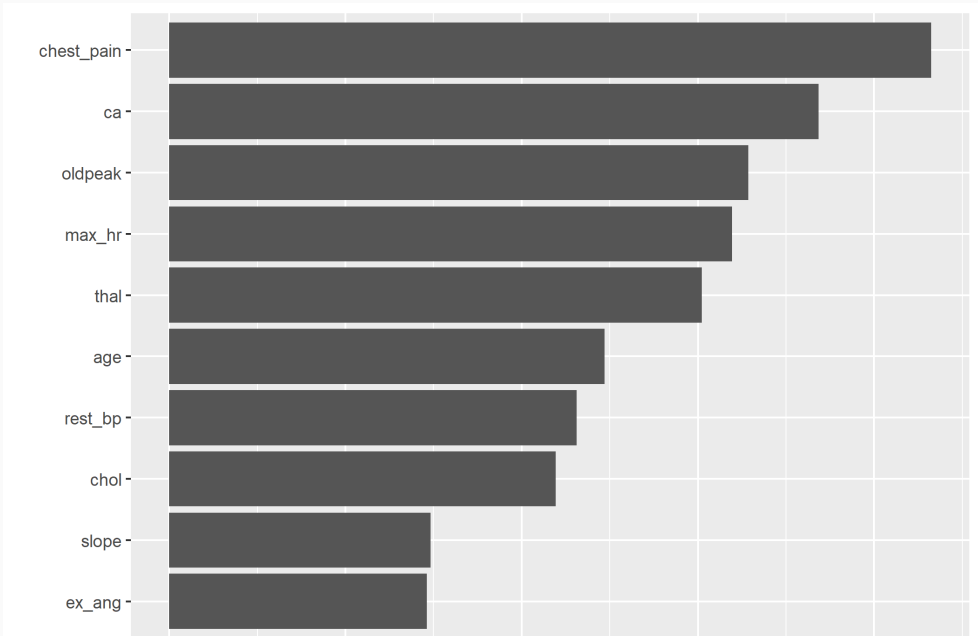
This idea isn't exclusive to forests; it also works for a single tree.

Variable Importance

Plotting the most important variables using `vip()` from **vip**:

```
# extract the fitted forest
extr ← heart_rf_fit %>%
  extract_fit_parsnip()

# plot variable importance
extr %>% vip::vip()
```



Variable Importance

Or extracting manually:

```
var_imp ← data.frame(variable = names(extr$fit$variable.importance),
                     importance = extr$fit$variable.importance %>% as.numeric() #
                     ) %>% arrange(desc(importance))
var_imp
```

variable	importance
chest_pain	21.6
ca	18.4
oldpeak	16.4
max_hr	16
thal	15.1
age	12.4

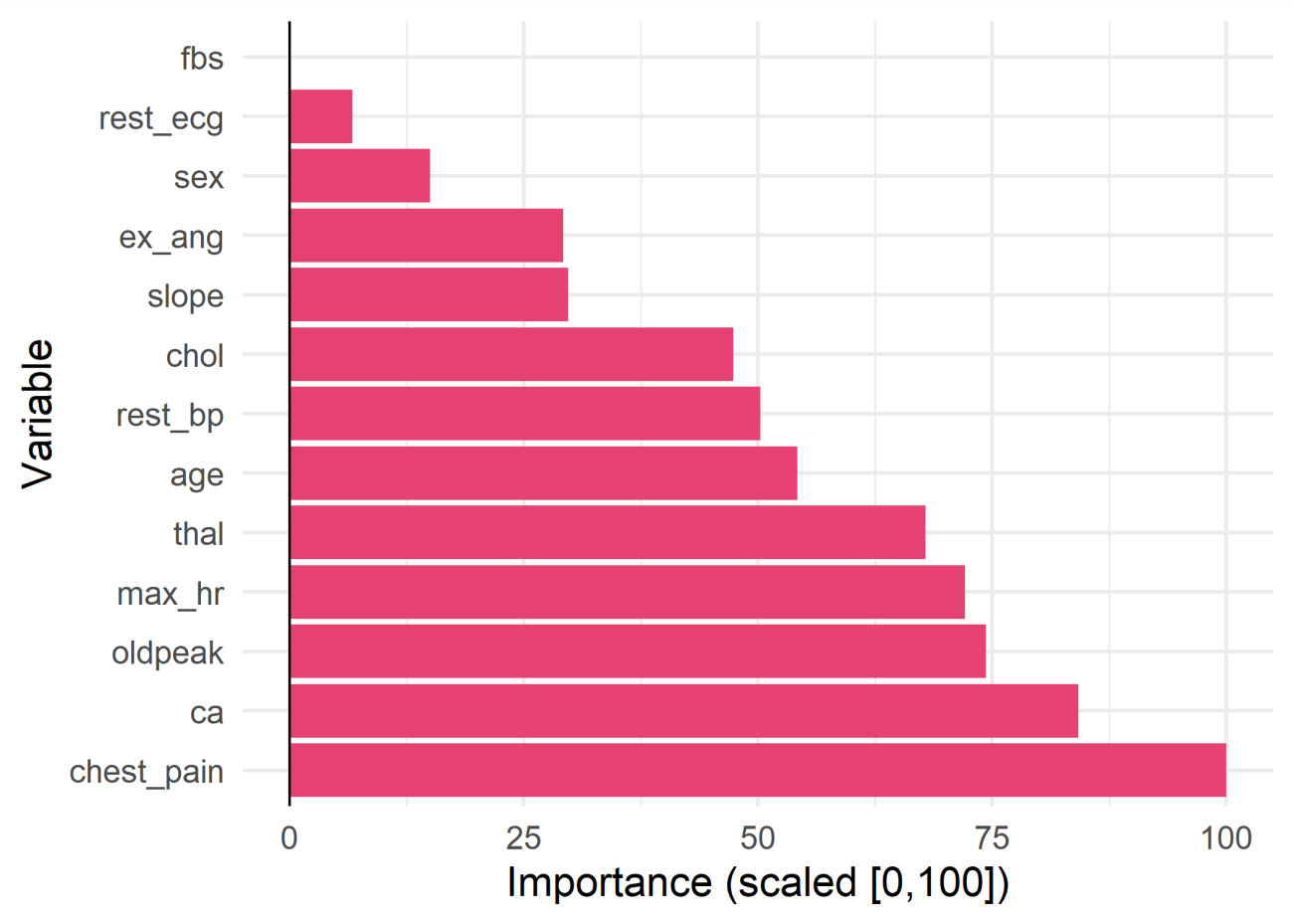
Variable Importance

Standardizing to 0-100 scale:

```
var_imp ← var_imp %>%
  # standardize importance
  mutate(imp_std = importance - min(importance),
         imp_std = 100 * imp_std/ max(imp_std))
```

Variable Importance

Plotting standardized importance:



Random Forest Error

Out-of-bag error is hidden pretty deep in the fitted model:

```
rf_error ← heart_rf_fit$fit$fit$fit$prediction.error
```

Which means we predicted 87% of heart disease cases correctly with our forest!

Random Forest Predictions

Extracting the predictions confirms another **interpretability challenge** of random forests/ensemble methods:

since we **average over all tree predictions**, our predicted classifications represent the **share of trees that assign the observation to class** s.[3]

3. The result of this averaging is more interpretable for regression forests

Random Forest Predictions

Extracting the predictions and viewing them:

```
rf_fit ← heart_rf_fit %>% extract_fit_parsnip()
rf_pred ← rf_fit$fit$predictions %>% as.data.frame()
head(rf_pred)
```

No	Yes
0.6	0.4
0.0303	0.97
0.025	0.975
0.526	0.474
1	0
0.935	0.0645

Random Forest Predictions

Like with the predicted probabilities with the Bayes classifier, we can assign each observation to the **most frequently predicted class**:

```
rf_pred ← rf_pred %>% mutate(heart_disease_hat = case_when(
  Yes > No ~ "Yes", # assign yes if more trees assign the obs to Yes
  TRUE ~ "No" # otherwise assign to No
))
```

Adding the predictions into the cleaned data frame:

```
heart_df_clean ← mutate(heart_df_clean,
                        heart_disease_hat = rf_pred$heart_disease_hat,
                        correct = ifelse(
                          heart_disease == heart_disease_hat, 1, 0))
```

Random Forest Predictions

Seeing how we did at predicting each class:

```
group_by(heart_df_clean, heart_disease) %>%
  summarise(Correct = mean(correct) %>% round(4),
            Count = n())
```

heart_disease	Correct	Count
No	0.86	164
Yes	0.748	139

So we did relatively better at predicting the more frequent "No Heart Disease" cases.[4.]

4. Note that the unconditional average would get us a different value than the model's error rate. That's because the error rate is calculated at the individual tree level while the above error is a summary/average across all the trees' predictions

Random Forest Cross-Validation

Just like with our single tree, we can **tune** our random forest parameters via **cross-validation**.

1. Partition the data into training/test samples

```
set.seed(12345)
split ← initial_split(data = heart_df_clean, prop = 0.5) # split 50/50

train_set ← training(split)
test_set ← testing(split)
```

Random Forest Cross-Validation

2. Setup the cross-validation with `vfold_cv()`

```
# 3-fold cross-validation
heart_cv ← vfold_cv(train_set, v = 3)
```

Random Forest Cross-Validation

3. Set up the random forest for cross-validating parameters

```
# Define the random forest
heart_rf_cv ← rand_forest(
  mode = "classification",
  mtry = tune(),
  trees = 100,
  min_n = tune()
) %>% set_engine(
  engine = "ranger",
  splitrule = "gini",
  importance = "impurity"
)
```

Random Forest Cross-Validation

4. Build a grid of possible hyperparameter values

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

Random Forest Cross-Validation

5. Set the workflow

```
rf_cv_wf ← workflow() %>%
  add_model(heart_rf_cv) %>% # new CV random forest setup
  add_recipe(heart_recipe) # same recipe as before
```

Random Forest Cross-Validation

6. Tune!

```
rf_tune ← rf_cv_wf %>%
  tune_grid(
    resamples = heart_cv, # the CV setup
    grid = rf_grid # the grid of hyperparameter values to try
  )
```

Random Forest Cross-Validation

Showing the 5 best-performing models:

```
show_best(x = rf_tune, metric = "accuracy", n = 5) %>%
   select(mtry:min_n, mean, std_err)
```

mtry	min_n	mean	std_err
2	1	0.847	0.0273
3	5	0.841	0.0352
4	1	0.841	0.0405
3	9	0.834	0.0183
3	6	0.834	0.0248

Random Forests

Random Forests offer a lot of improvement over single decision trees from a performance standpoint.

However, they can often be harder to interpret.

Perhaps more limiting to the types of questions we economists are interested in: it's not always a **conditional mean** that we're interested in.

What if we want to harness the benefits of **forest-based ensemble methods** for identifying **any conditional object of interest?**

Machine Learning for Causal Treatment Effect Estimation

Machine Learning for Causal Treatment

The goal of **Random Forests** is to estimate a **conditional mean**,

$$\mu(x_0) = E[Y \mid X = x_0]$$

But what if instead we wanted to estimate... **any** conditional function $\theta(x_0)$?

- Conditional linear regression coefficients
- Conditional causal treatment effects
- Conditional local average treatment effects using instruments
- Quantiles of the conditional distribution of $Y \mid X = x_0$
- Conditional class probabilities

Enter **Athey, Tibshirani, and Wager (2019)**.

Generalized Random Forests

Generalized Random Forests by **Athey, Tibshirani, and Wager (2019)** extends the ensemble methods of Random Forests to essentially any conditional function $\theta(x)$ that can be identified by local moment conditions.

They recast forests as an **adaptive locally weighted estimator**

1. Use the forest to calculate weighted set of neighbors for each observation (sound familiar?)
    - Employ problem-specific splitting rules to maximize the likelihood of capturing heterogeneity in $\theta(x)$
2. Use those neighbors to estimate $\theta(x)$ as the solution to a local moment equation

GRF Setup

More formally:

Suppose you have an IID sample with N observations.

You observe:

- O_i an observable quantity that encodes information relevant to estimating $\theta(\cdot)$
  - For nonparametric regression, this is just our our outcome $O_i = \{Y_i\}$
  - For treatment effect estimation, $O_i = \{Y_i, W_i\}$
  - Generally can contain more info
- Auxiliary covariates Xi

GRF

Goal: Estimate solutions to local estimating equations of the form

$$E[\psi_{\theta(x),\, \nu(x)}(O_i \mid X_i = x)] = 0$$

- $\theta(x)$ the parameter we care about (i.e. conditional mean, treatment effect, regression slope)
- $\nu(x)$ a (optional) nuisance parameter

If conditional mean without noise, then $\psi_{\mu(x)}(Y_i) = Y_i - \mu(x)$

GRF Forest-Based Local Estimation

One approach to estimating functions like $\theta(x)$:

- Find $\hat{\theta}(x), \hat{\nu}(x)$ that solve

$$\sum_{i=1}^{n} \alpha_i \psi_{\hat{\theta}(x),\hat{\nu}(x)}(O_i) = 0$$

- α_i: weights measuring relevance of the i^{th} observation for fitting $\theta(\cdot)$ at x
  - Traditionally obtained using a kernel function (and sometimes a bandwidth)
  - Traditionally sensitive to curse of dimensionality

GRF Forest-Based Local Estimation

GRF Approach: use forests to derive α_i.

1. Grow $b = 1, \ldots, B$ trees
2. Choose weights $\alpha_i(x)$ to capture how frequently the i^{th} training example falls into the same leaf as x.

Weights within a given tree, $\alpha_{bi}(x)$, are calculated as

$$\alpha_{bi}(x) = \frac{I[X_i \in L_b(x)]}{|L_b(x)|}$$

- $L_b(x)$ the set of observations falling within the same leaf as x

Overall weights for observation i are then the average across all trees:

$$\alpha_i(x) = \frac{1}{B} \sum_{b=1}^{B} \alpha_{bi}(x)$$

GRF Weights

For example, we can reframe random forests and our estimate of the conditional mean function as

$$\hat{\mu}(x) = \sum_{i=1}^{n} \frac{1}{B} \sum_{b=1}^{B} Y_i \frac{I[X_i \in L_b(x)]}{|L_b(x)|}$$

Or as the weighted sum of single tree predictions $\hat{\mu}_b(\cdot)$:

$$\hat{\mu}(x) = \frac{1}{B} \sum_{b=1}^{B} \hat{\mu}_b(x)$$

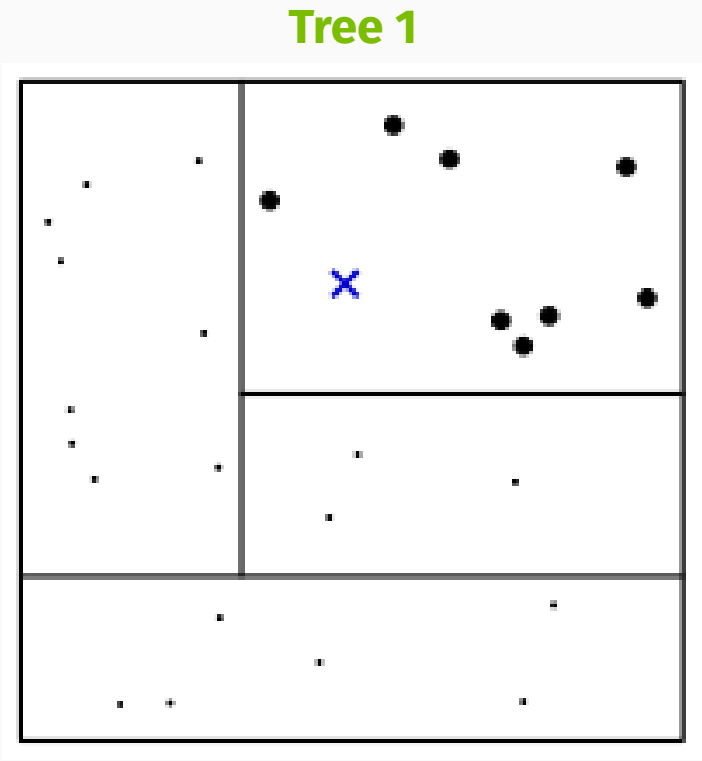
Or more simply, as

$$\hat{\mu}(x) = \sum_{i=1}^{n} Y_i \alpha_i(x)$$

GRF Weights Visually

Let's see how these weights are developed with a simple example: a forest with three trees and two covariates.

- x the point of interest
  - lines our splits
  - darker dots the points within the same leaf



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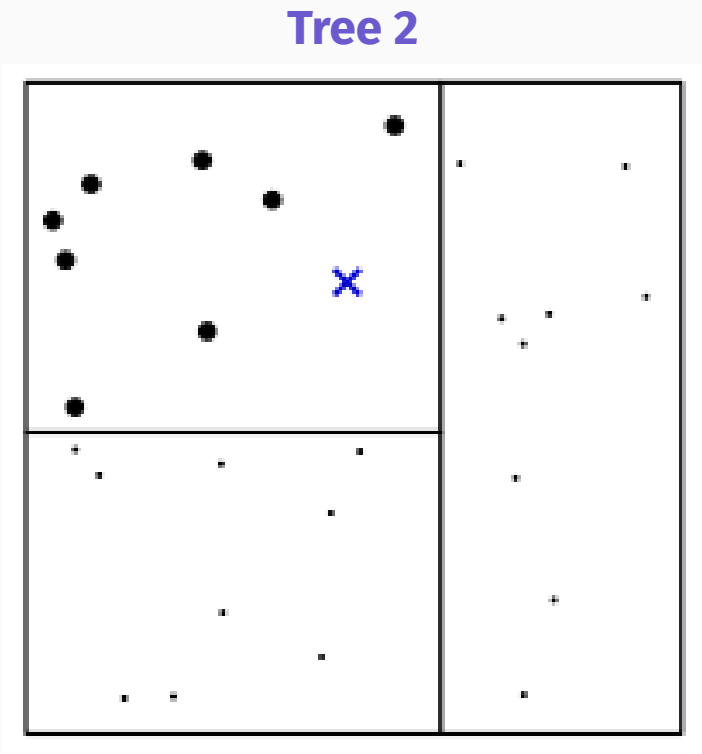

GRF Weights Visually

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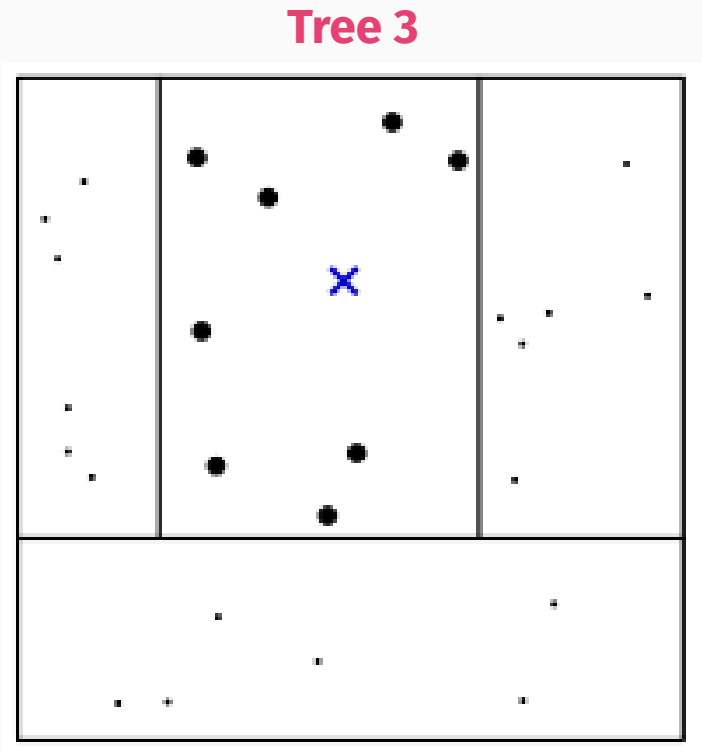
  - lines our splits
  - darker dots the points within the same leaf

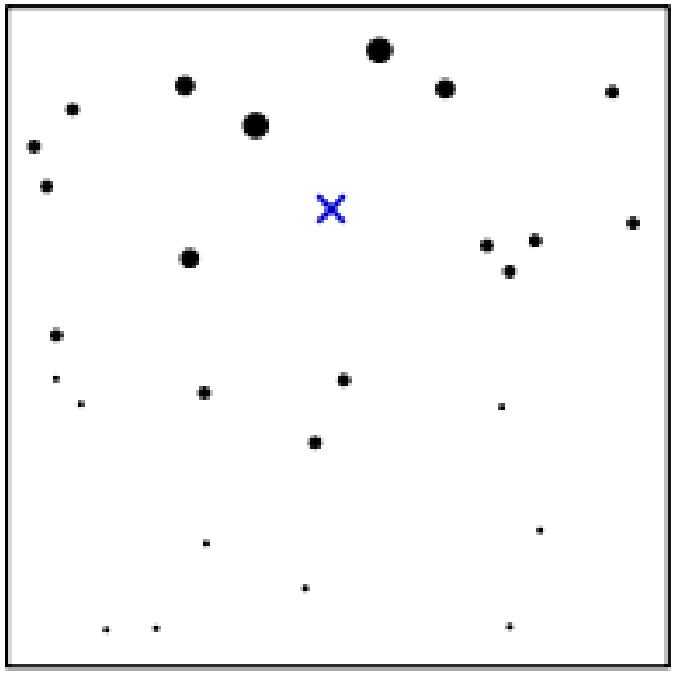


GRF Weights Visually

Let's see how these weights are developed with a simple example: a forest with three trees and two covariates.

Then we average across all the individual tree-based weights to obtain the overall $\alpha_i(x)$.

Forest Weights for x



Honesty

One additional benefit of using GRF: growing **honest** forests

Honesty aims to reduce bias in tree predictions by using **distinct subsamples** for 1. Building the tree, and 2. Making predictions

Classic Random Forest

- Draws a single subsample, use that subsample for both choosing a tree's splits and making predictions in that tree

Honest Forests

- Draw a training sample
- Use part of that sample to choose the tree's splits
- Use the rest of the training sample to make predictions
- Prune away any remaining empty leaves

GRF Functions

Conveniently for us, the **grf** package contains tons of features and **extensive documentation** to estimate a wide range of forests, including...

Causal Treatment Effects

Approach	Forest Function
Causal Treatment Effects	`causal_forest()`
Causal Treatment Effects with right-censored outcomes	`causal_survival_forest()`
Multi-arm/multi-outcome causal treatment effects	`multi_arm_causal_forest()`

GRF Functions

Conveniently for us, the **grf** package contains tons of features and **extensive documentation** to estimate a wide range of forests, including...

Moments of Conditional Distributions

Approach	Forest Function
Conditional Mean	`regression_forest()`
Multi-outcome conditional means	`multi_regression_forest()`
Right-censored Survival	`survival_forest()`
Conditional Quantiles	`quantile_forest()`
Conditional Class Probabilities	`probability_forest()`

GRF Functions

Conveniently for us, the **grf** package contains tons of features and **extensive documentation** to estimate a wide range of forests, including...

Regression Outcomes

Approach	Forest Function
Conditional Linear Model	`lm_forest()`
Local Average Treatment Effects (IV)	`instrumental_forest()`

Causal Forests

When $W_i \in \{0, 1\}$ and **unconfoundedness holds**, we can estimate heterogeneous causal treatment effects with **causal forests**.

1. Build Phase: greedily choose splits to maximize the **squared difference in subgroup treatment effects**

$$n_L n_R (\hat{\tau}_L - \hat{\tau}_R)^2$$

- $\hat{\tau}$'s chosen through a centered residual-on-residual regression (Robinson 1988)

Causal Forests

2. Estimate $\tau(x)$, where

$$\tau(x) := lm\left(Y_i - \hat{m}^{-1}(X_i) \sim W_i - \hat{e}^{-1}(X_i),\ \mathbf{weights} = \alpha_i(x)\right)$$

- $\left(Y_i - \hat{m}^{-1}(X_i),\ W_i - \hat{e}^{-1}(X_i)\right)$: orthogonalized outcome/treatment
  - Residual after "regressing out" the main effect of X_i on Y_i (W_i)
  - $\hat{m}^{-1}(X_i), \hat{e}^{-1}(X_i)$ obtained from separate regression forests

Causal Forests Example

Let's load in some data to see how we can run causal forests, using a sample from the **National Study of Learning Mindsets**.

ARTICLE

OPEN

https://doi.org/10.1038/s41586-019-1466-y

A national experiment reveals where a growth mindset improves achievement

David S. Yeager[1*], Paul Hanselman[2*], Gregory M. Walton[3], Jared S. Murray[1], Robert Crosnoe[1], Chandra Muller[1], Elizabeth Tipton[4], Barbara Schneider[5], Chris S. Hulleman[6], Cintia P. Hinojosa[7], David Paunesku[8], Carissa Romero[9], Kate Flint[10], Alice Roberts[10], Jill Trott[10], Ronaldo Iachan[10], Jenny Buontempo[1], Sophia Man Yang[1], Carlos M. Carvalho[1], P. Richard Hahn[11], Maithreyi Gopalan[12], Pratik Mhatre[1], Ronald Ferguson[13], Angela L. Duckworth[14] & Carol S. Dweck[3]

```
nslm ← read.csv("data/NSLM.csv") %>%
  mutate(schoolid = factor(schoolid))
```

Causal Forests Example

Taking a look at the data, we have the following variables:

- `schoolid` the ID of randomly selected US public high schools
- `Y`: continuous measure of achievement
- `Z`: treatment status
- `S3`: students' self-reported expectations for future success
- `C1`: student race (categorical)
- `C2`: student gender (categorical)
- `C3`: first-generation status (categorical)
- `XC`: school urbanicity (categorical)
- `X1`: school-level mean of students' fixed mindsets
- `X2`: school achievement level (test scores + college prep)
- `X3`: school racial minority composition (% black, latino, native american)
- `X4`: school poverty (% in familes below FPL)
- `X5`: school size

Causal Forests Example

We want to answer the following research questions:

1. Was a nudge-like mindset intervention designed to instill a "growth mindset" in students effective at improving achievement?

2. Do schools' prior achievement levels (`X2`) and pre-existing mindset norms (`X2`) effect the magnitude of this effect?

Let's find out!

Causal Forests Example

We *could* just run an (interacted) OLS regression...

```
reg1 ← feols(Y ~ Z + S3 + C1 + C2 + C3 + XC + X1 + X2 + X3 + X4 + X5, data  = nsl
reg2 ← feols(Y ~ Z + Z:X2 + Z:X3 + S3 + C1 + C2 + C3 + XC + X1 + X2 + X3 + X4 + X
etable(reg1, reg2, keep = c("Z", "X2", "X1"))
```

	reg1	reg2
Dependent Var.:	Y	Y
Z	0.2549*** (0.0115)	0.2539*** (0.0115)
X1	-0.0954*** (0.0073)	-0.0954*** (0.0073)
X2	-0.0163. (0.0087)	-0.0263** (0.0098)
Z x X2		0.0313* (0.0141)
Z x X3		0.0152 (0.0134)

Causal Forests Example

...which gives us an estimate of the mean treatment effect and mean mediating effect of `X1/X2`.

Instead, let's use `causal_forest()` to obtain heterogeneous treatment effects for each school.

Let's first build some data objects we'll use as arguments.

1. Convert `C1` and `XC` to dummies:

- `C1` has 15 levels, so rather than code each one by hand let's use `model.matrix`
  - Argument: formula

```
# expand C1 categorical variable into dummies (with intercept)
C1.exp = model.matrix(~ factor(nslm$C1) + 0)
```

Causal Forests Example

...which gives us an estimate of the mean treatment effect and mean mediating effect of `X1/X2`.

Instead, let's use `causal_forest()` to obtain heterogeneous treatment effects for each school.

Let's first build some data objects we'll use as arguments.

Repeat for `XC`:

```
XC.exp = model.matrix(~ factor(nslm$XC) + 0)
```

Causal Forests Example

Next, build the predictor matrix

```
# first select all covariates except for XC and C1
X ← select(nslm, -schoolid:-Y, -XC, - C1)

# Add in the dummies for XC and C1
Xmat ← cbind(X, XC.exp, C1.exp) %>%
  as.matrix()
```

And get the outcome and treatment vectors:

```
Y ← nslm$Y # our outcome
Z ← nslm$Z # our treatment indicator
```

Causal Forests Example

To perform the residual-on-residual regression step, our forest wants predictions for $\hat{Y}$ and $\hat{W}$. We can either

1. Omit them from the forest setup
    - The forest will estimate them for us in a separate regression forest
2. Run the initial regression forests manually and supply the predictions

Let's do the latter, but first an important consideration...

Causal Forests Example

As with random forests, by default GRF methods assume **independent observations**.

Here, we know that treatment assignment occurred at the **school level**, so students' treatment is dependent on which school that they're at.

The good news is, we can account for this **clustering** within our forest to draw our random units at the school level.

- `clusters` the clustering variable (here our `schoolid` factor)
- `equalize.cluster.weights = TRUE` ensures we draw the same fraction frmo each cluster

Causal Forests Example

Running the initial regression forests for our $\hat{Y}$ and $\hat{W}$ predictions:

```
Y_forest ← regression_forest(X = Xmat,
                             Y = Y,
                             clusters = nslm$schoolid,
                             equalize.cluster.weights = TRUE)
Y_hat ← predict(Y_forest)$predictions

W_forest ← regression_forest(X = Xmat,
                             Y = Z,
                             clusters = nslm$schoolid,
                             equalize.cluster.weights = TRUE)
W_hat ← predict(W_forest)$predictions
```

Causal Forests Example

Setting up the causal forest:

- `X`: the covariate matrix

```
# Define the random forest
cf ← causal_forest(X = Xmat,
                   Y = Y,
                   Y.hat = Y_hat,
                   W = Z,
                   W.hat = W_hat,
                   clusters = nslm$schoo
                   equalize.cluster.weig
                   num.trees = 200,
                   honesty = TRUE,
                   honesty.fraction = 0.
                   tune.parameters = "al
                   )
```

Causal Forests Example

Setting up the causal forest:

- `X`: the covariate matrix
- `Y`: the outcome vector (our measure of student achievement)
- `W`: the treatment vector

```
# Define the random forest
cf ← causal_forest(X = Xmat,
                   Y = Y,
                   W = Z,
                   Y.hat = Y_hat,
                   W.hat = W_hat,
                   clusters = nslm$schoo
                   equalize.cluster.weig
                   num.trees = 200,
                   honesty = TRUE,
                   honesty.fraction = 0.
                   tune.parameters = "al
                   )
```

Causal Forests Example

Setting up the causal forest:

- `X`: the covariate matrix
- `Y`: the outcome vector (our measure of student achievement)
- `W`: the treatment vector
- `Y.hat`: our prediction of Y as a function of X
- `W.hat`: our prediction of W as a function of X

```
# Define the random forest
cf ← causal_forest(X = Xmat,
                   Y = Y,
                   W = Z,
                   Y.hat = Y_hat,
                   W.hat = W_hat,
                   clusters = nslm$schoo
                   equalize.cluster.weig
                   num.trees = 200,
                   honesty = TRUE,
                   honesty.fraction = 0.
                   tune.parameters = "al
                   )
```

Causal Forests Example

Setting up the causal forest:

- `X`: the covariate matrix
- `Y`: the outcome vector (our measure of student achievement)
- `W`: the treatment vector
- `Y.hat`: our prediction of Y as a function of X
- `W.hat`: our prediction of W as a function of X
- `clusters`: the cluster identier vector
- `equalize.cluster.weights`: whether to draw equal sample sizes from each

```
# Define the random forest
cf ← causal_forest(X = Xmat,
                   Y = Y,
                   W = Z,
                   Y.hat = Y_hat,
                   W.hat = W_hat,
                   clusters = nslm$schoo
                   equalize.cluster.weig
                   num.trees = 200,
                   honesty = TRUE,
                   honesty.fraction = 0.
                   tune.parameters = "al
                   )
```

Causal Forests Example

Setting up the causal forest:

- `num.trees`: size of forest to grow (default is 2000)

```
# Define the random forest
cf ← causal_forest(X = Xmat,
                   Y = Y,
                   W = Z,
                   Y.hat = Y_hat,
                   W.hat = W_hat,
                   clusters = nslm$schoo
                   equalize.cluster.weig
                   num.trees = 200,
                   honesty = TRUE,
                   honesty.fraction = 0.
                   tune.parameters = "al
                   )
```

Causal Forests Example

Setting up the causal forest:

- `num.trees`: size of forest to grow (default is 2000)
- `honesty`: whether or not to grow honestly (default to TRUE)
- `honesty.fraction`: the subsample portion used for growing trees (defaults to 50%)

```
# Define the random forest
cf ← causal_forest(X = Xmat,
                   Y = Y,
                   W = Z,
                   Y.hat = Y_hat,
                   W.hat = W_hat,
                   clusters = nslm$schoo
                   equalize.cluster.weig
                   num.trees = 200,
                   honesty = TRUE,
                   honesty.fraction = 0.
                   tune.parameters = "al
                   )
```

Causal Forests Example

Setting up the causal forest:

- `num.trees`: size of forest to grow (default is 2000)
- `honesty`: whether or not to grow honestly (default to TRUE)
- `honesty.fraction`: the subsample portion used for growing trees (defaults to 50%)
- `tune.parameters`: which/whether to tune parameters
  - `none, all, sample.fraction`

```
# Define the random forest
cf ← causal_forest(X = Xmat,
                   Y = Y,
                   W = Z,
                   Y.hat = Y_hat,
                   W.hat = W_hat,
                   clusters = nslm$schoo
                   equalize.cluster.weig
                   num.trees = 200,
                   honesty = TRUE,
                   honesty.fraction = 0.
                   tune.parameters = "al
                   )
```

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Part 3: Tree-Based Methods