Lecture 007

Trees 🌲🌴🌳

Edward Rubin
11 February 2021

Admin

Admin

Material

Last time: Classification

Today! Decision trees for regression and classification.

Admin

Upcoming

Readings

- *Today* *ISL* Ch. 8.1
- *Next* *ISL* Ch. 8.2

Problem sets

- *Penalized regression:* Due last week.
- *Classification:* Coming soon!
- Let Stephen know if you resubmit

Project See outline! (Think about prediction topics!)

Decision trees

Fundamentals

Decision trees

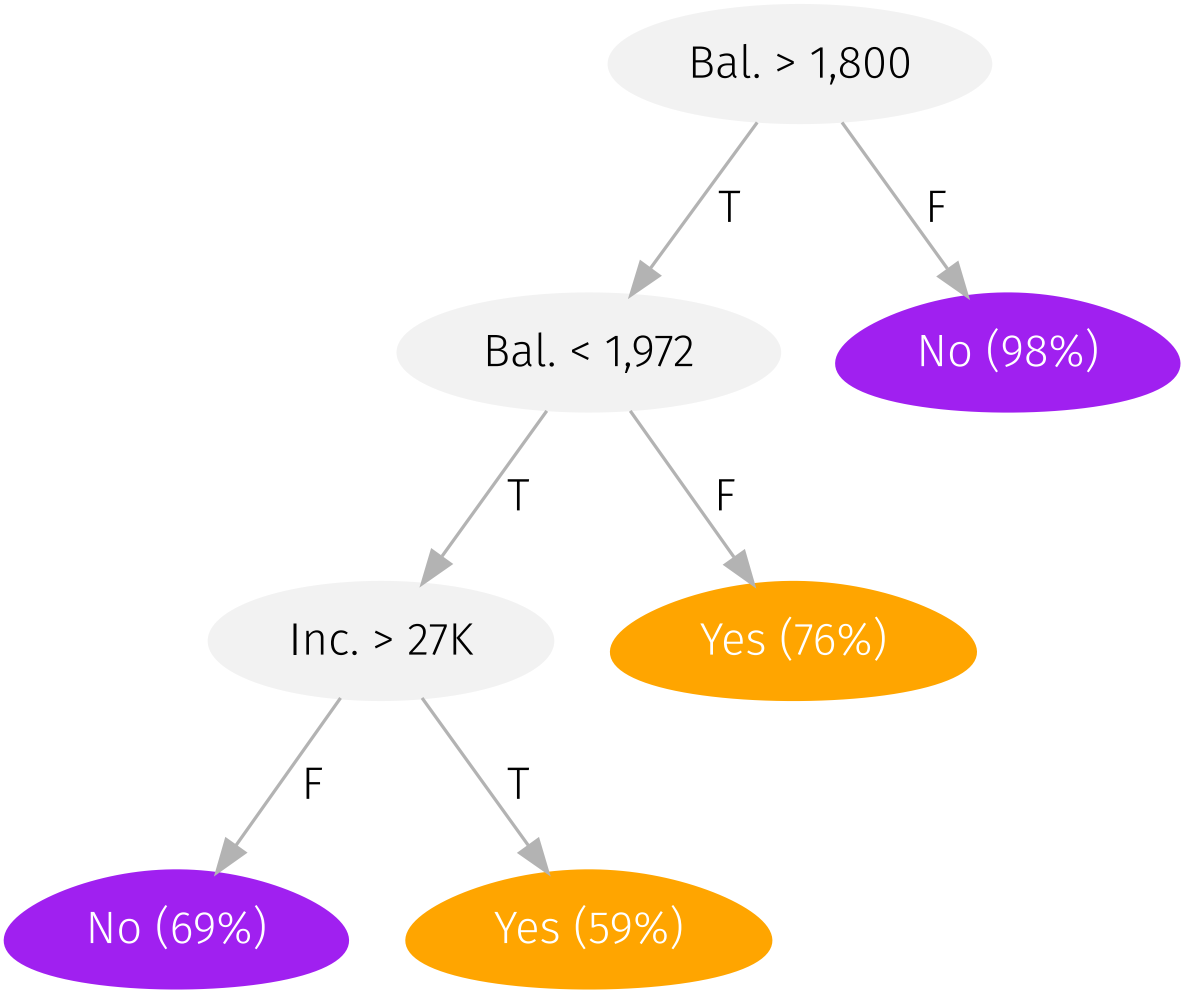
- split the *predictor space* (our $\mathbf{X}$) into regions
- then predict the most-common value within a region

Tree-based methods

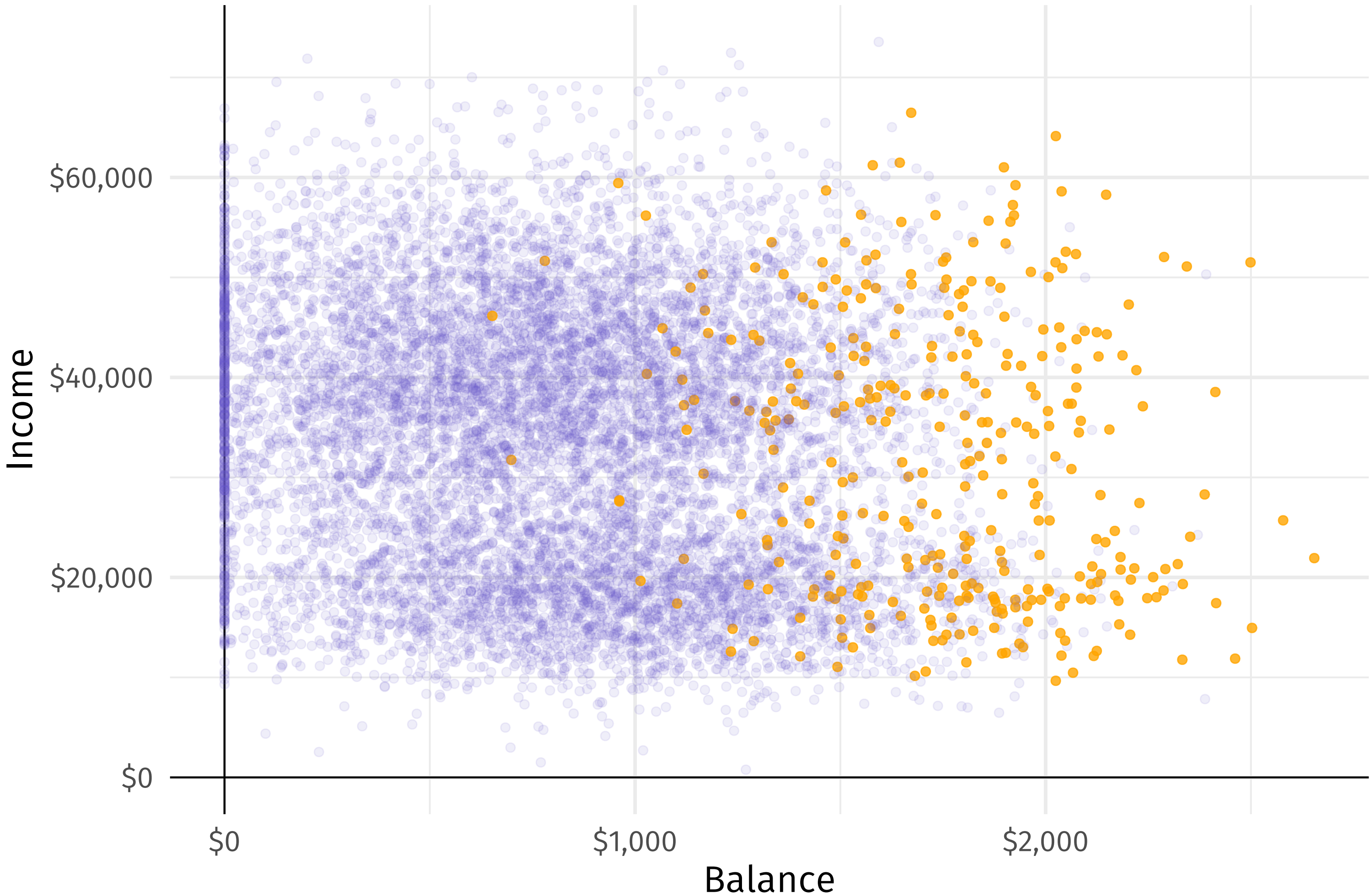
1. work for **both classification and regression**
2. are inherently **nonlinear**
3. are relatively **simple** and **interpretable**
4. often **underperform** relative to competing methods
5. easily extend to **very competitive ensemble methods** (*many* trees)🌲

🌲 Though the ensembles will be much less interpretable.

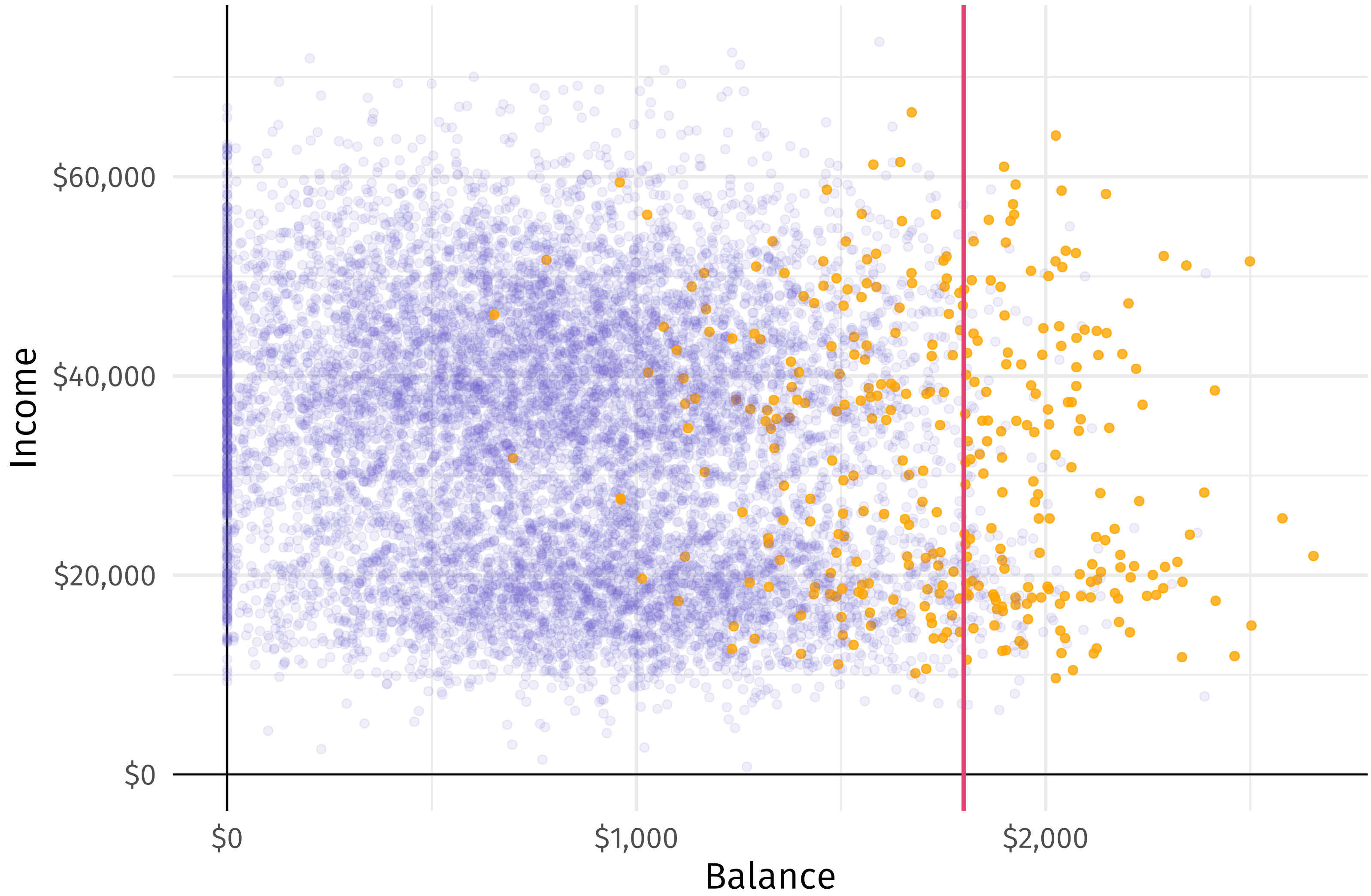
Example: **A simple decision tree** classifying credit-card default



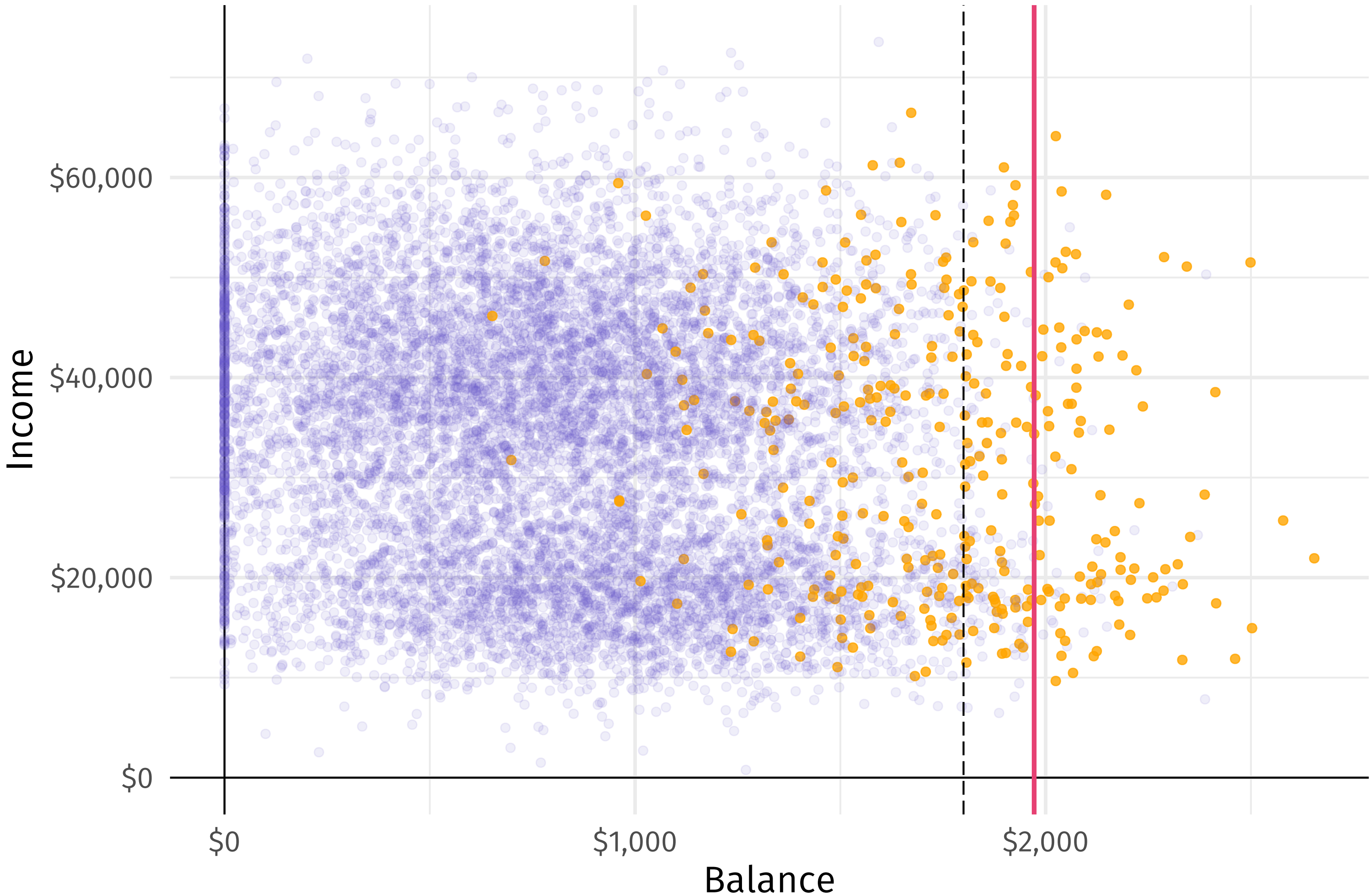
Let's see how the tree works—starting with our data (default: Yes *vs.* No).



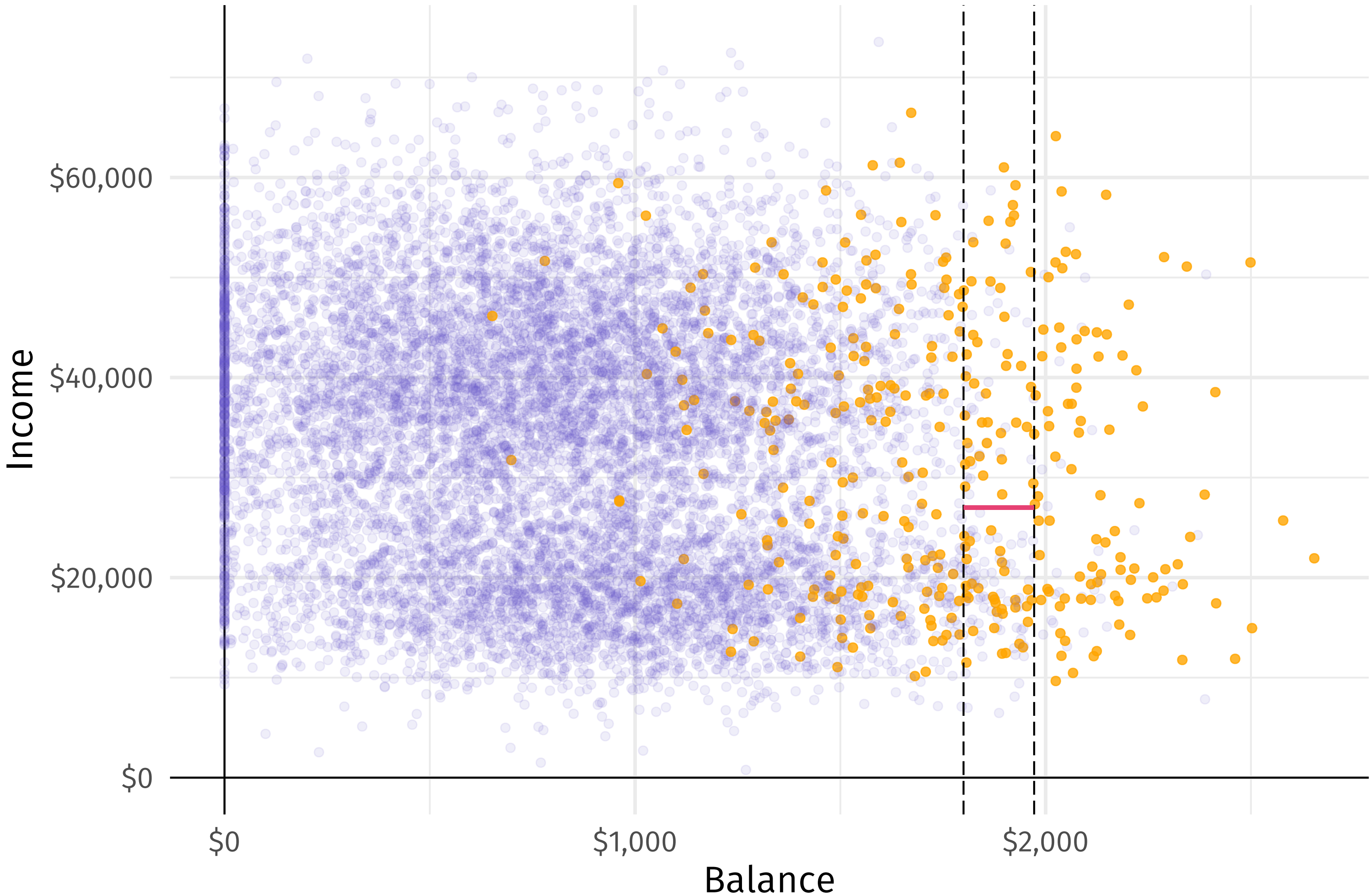
The **first partition** splits balance at $1,800.



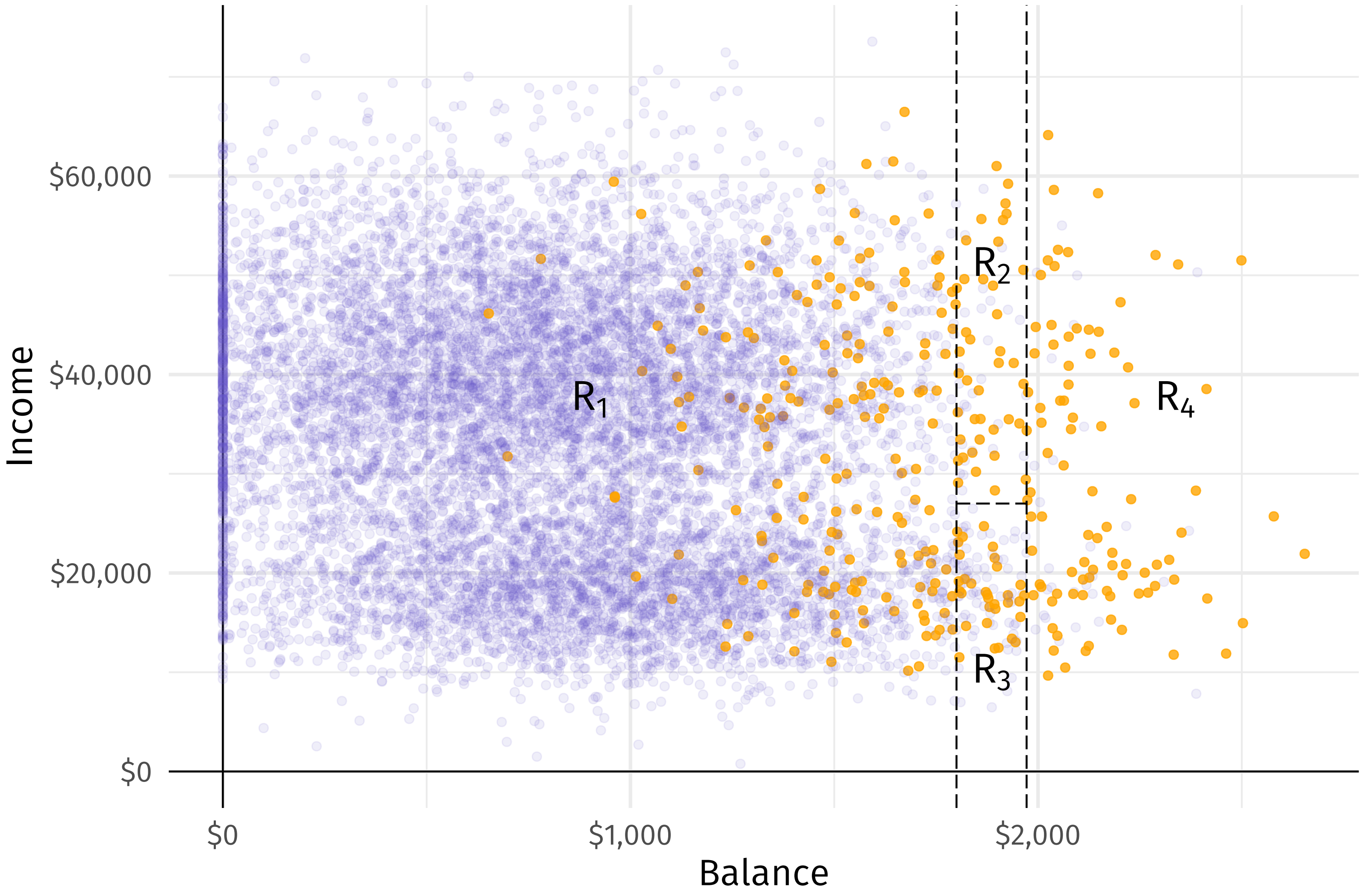
The **second partition** splits balance at $1,972, (*conditional on bal. > $1,800*).



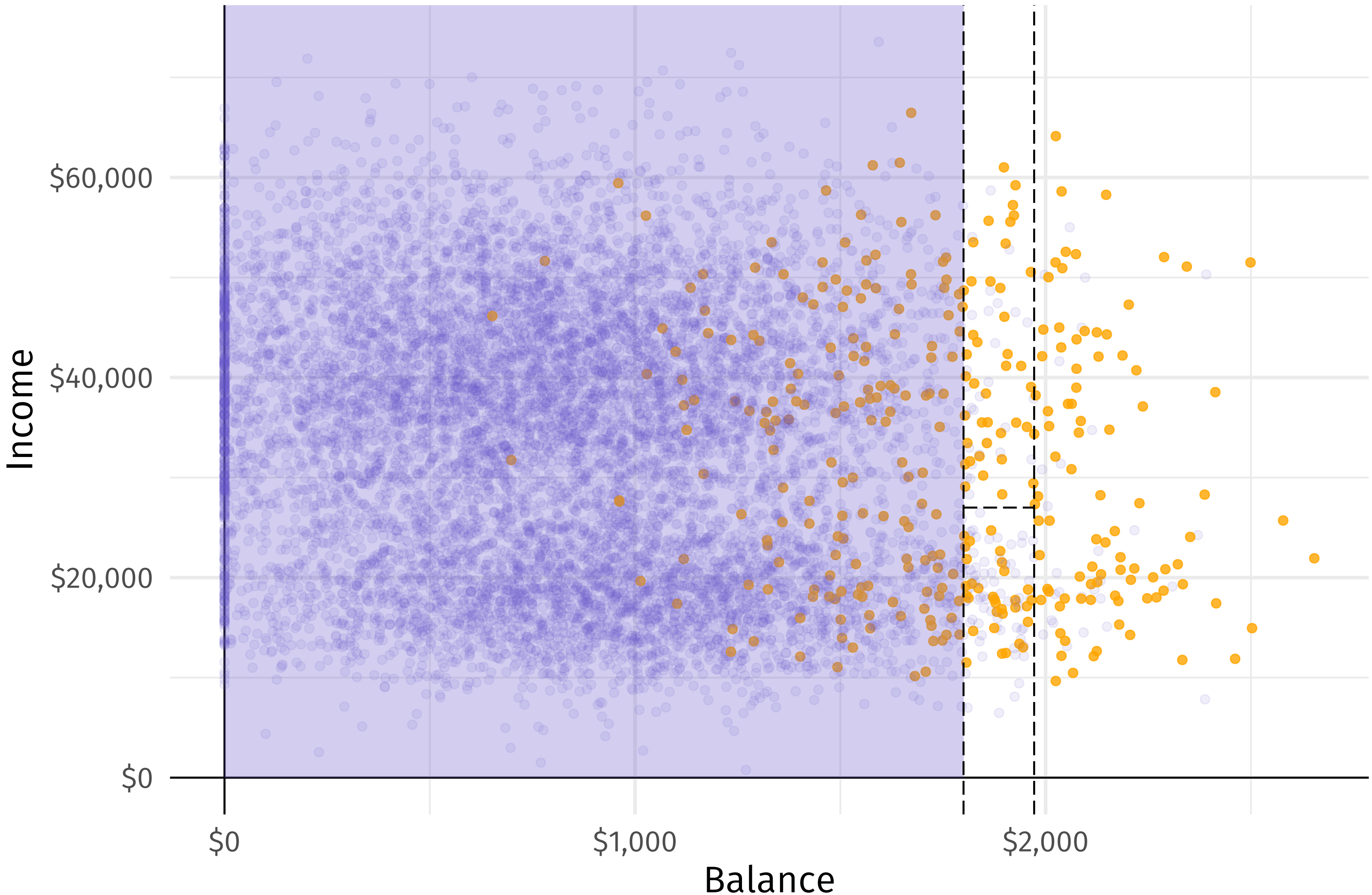
The **third partition** splits income at $27K **for** bal. between $1,800 and $1,972.



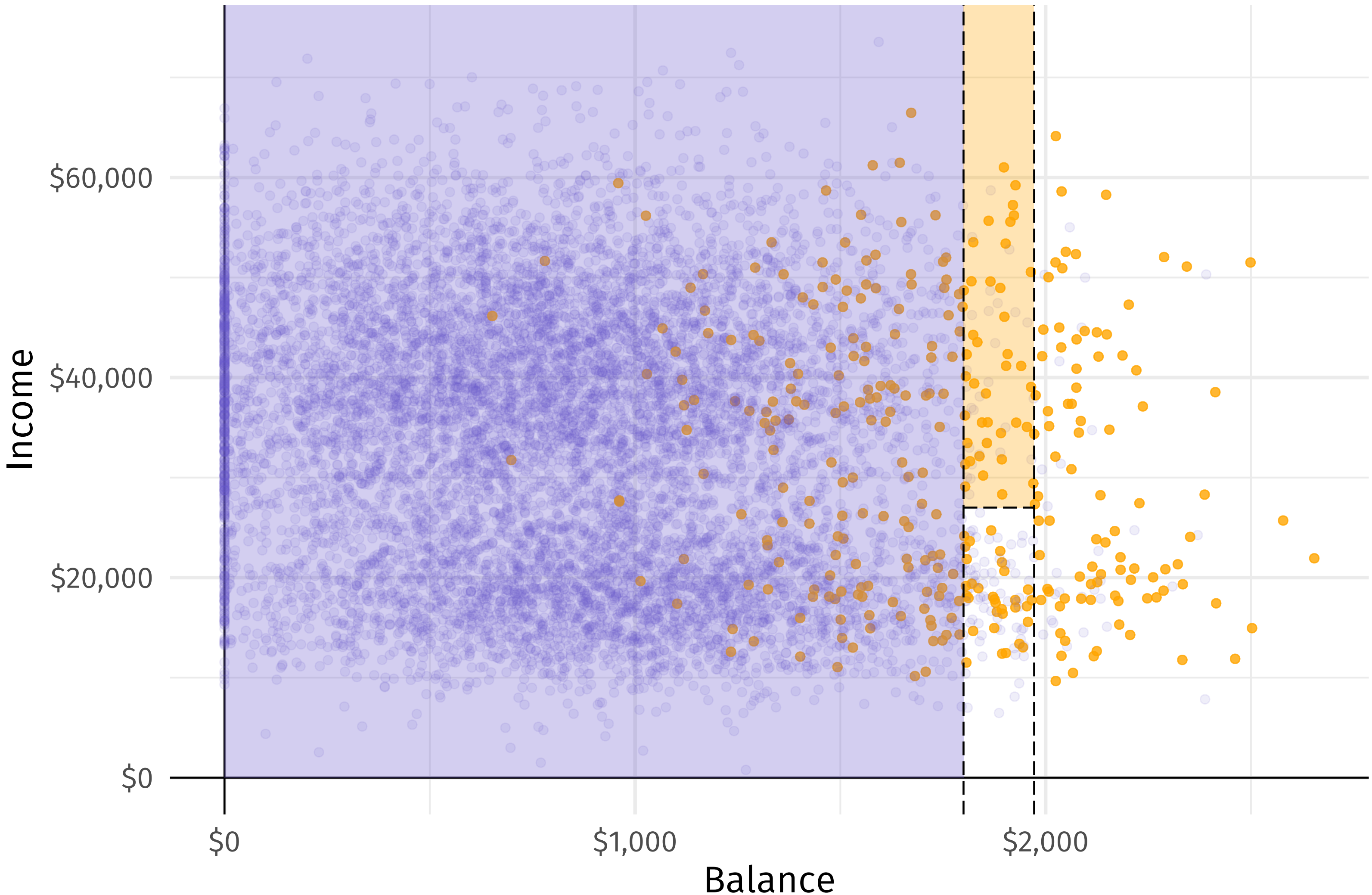
These three partitions give us four **regions**...



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

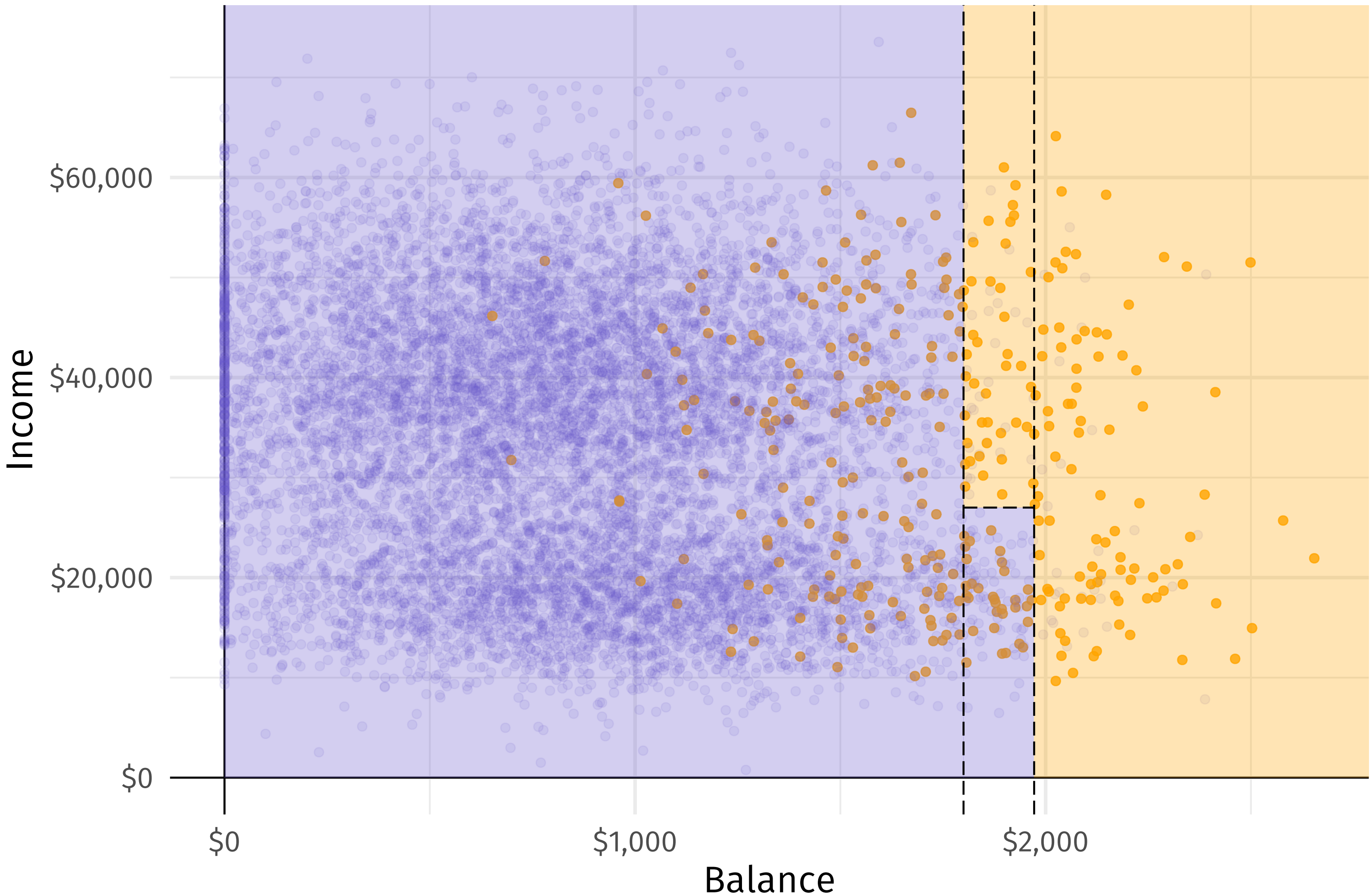


Predictions cover each region (*e.g.*, using the region's most common class).

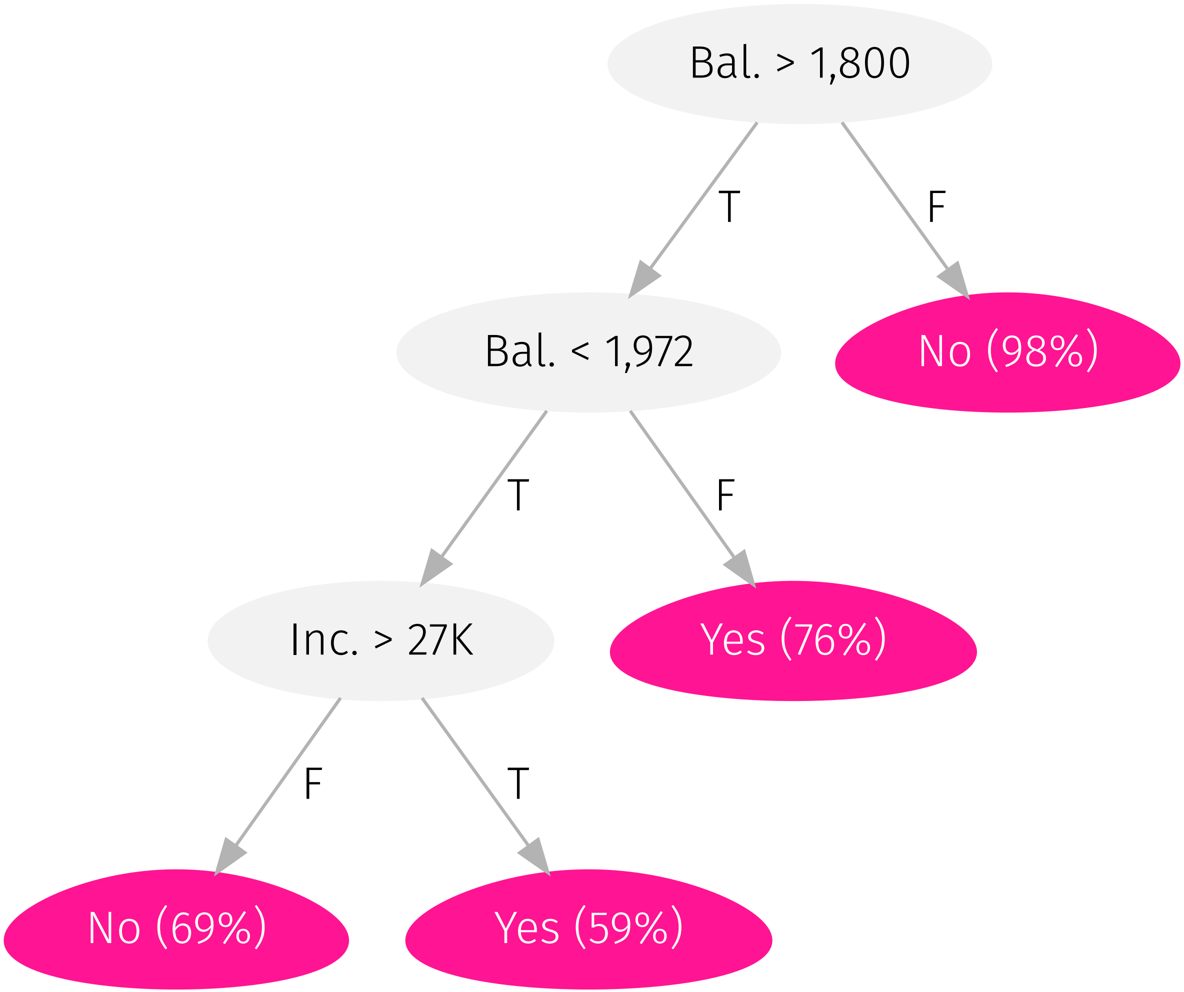


Predictions cover each region (*e.g.*, using the region's most common class).

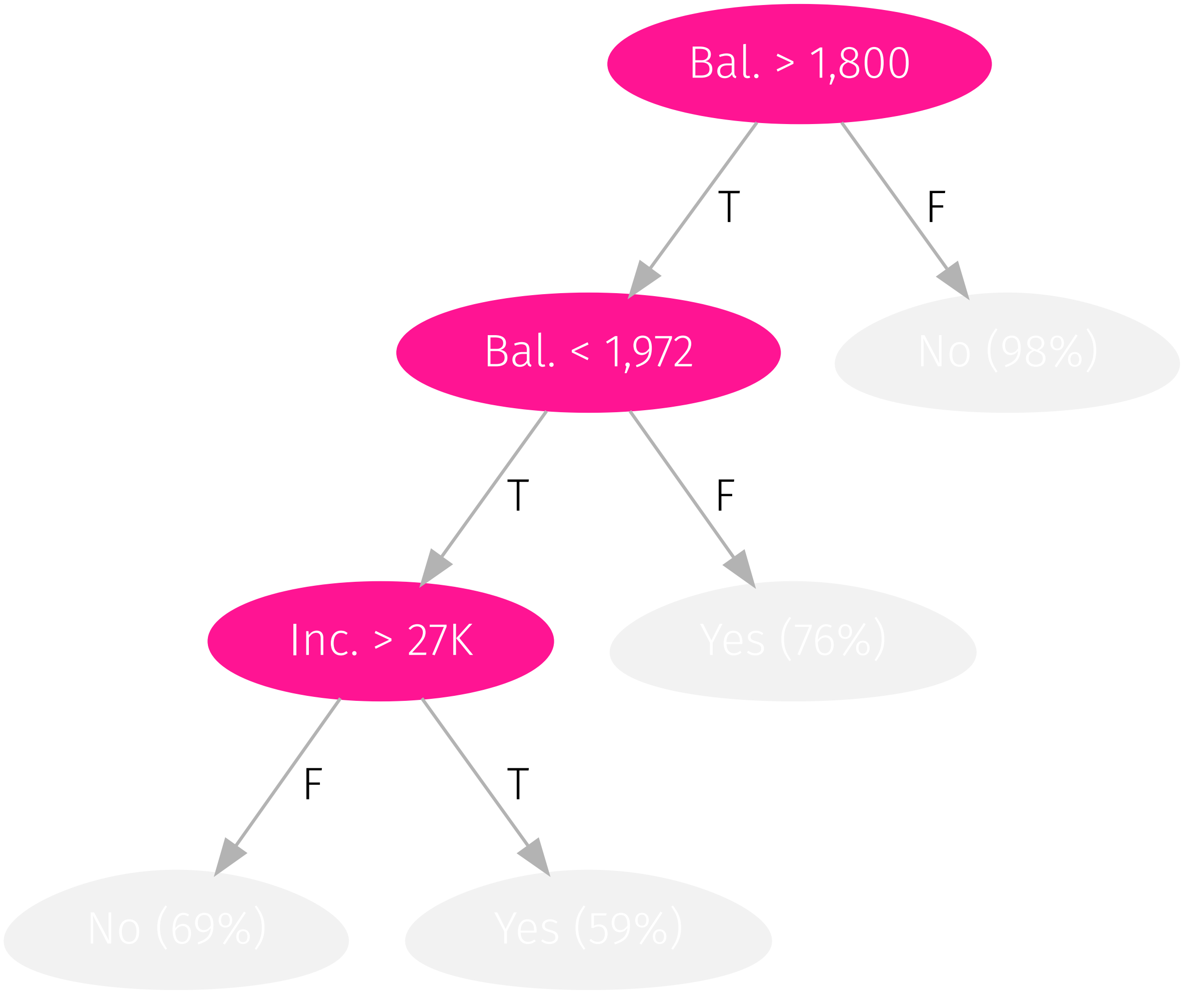
Predictions cover each region (*e.g.*, using the region's most common class).



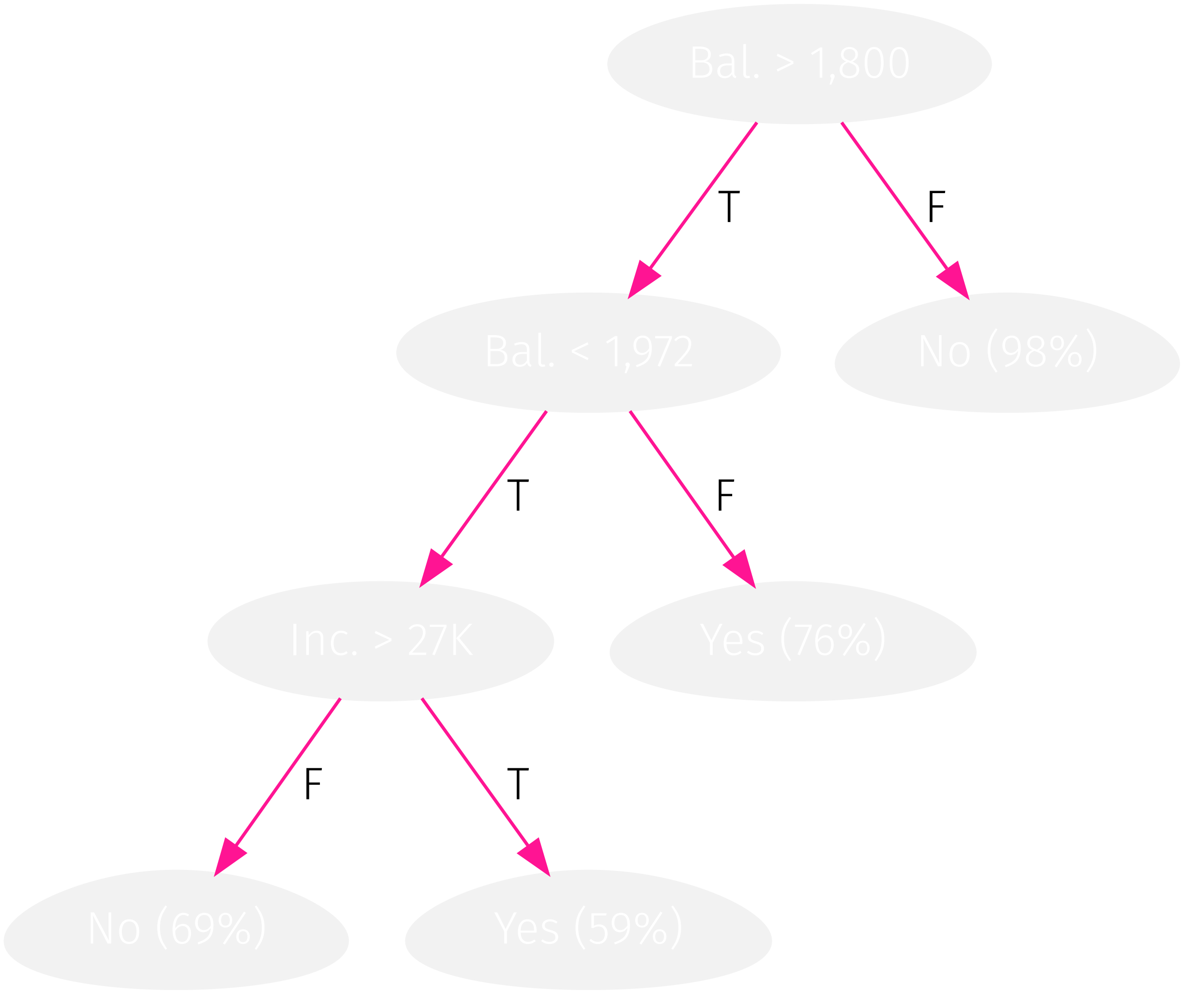
The **regions** correspond to the tree's **terminal nodes** (or **leaves**).



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



The segments connecting the nodes within the tree are its **branches**.



You now know the anatomy of a decision tree.

But where do trees come from—how do we train🌲 a tree?

Growing trees

We will start with regression trees, *i.e.*, trees used in regression settings.

As we saw, the task of **growing a tree** involves two main steps:

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

2. **Make predictions** using the regions' mean outcome.
   For region R_j predict $\hat{y}_{R_j}$ where

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

Decision trees

Growing trees

We **choose the regions to minimize RSS** *across all* J [regions], *i.e.*,

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

Problem: Examining every possible parition is computationally infeasible.

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

- recursive start with the "best" split, then find the next "best" split, ...
- binary each split creates two branches—"yes" and "no"
- greedy each step makes *best* split—no consideration of overall process

Growing trees: Choosing a split

Recall Regression trees choose the split that minimizes RSS.

To find this split, we need

1. a predictor, $\mathbf{x}_j$
2. a **cutoff** s that splits $\mathbf{x}_j$ into two parts: (1) $\mathbf{x}_j < s$ and (2) $\mathbf{x}_j \geq s$

Searching across each of our predictors j and all of their cutoffs s, we choose the combination that **minimizes RSS**.

Example: Splitting

Example Consider the dataset

i	**y**	$\mathbf{x_1}$	$\mathbf{x_2}$
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.

Decision trees

Example: Splitting

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

i	**y**	$\mathbf{x_1}$	$\mathbf{x_2}$
1	0	1	4
2	8	3	2
3	6	5	6

Decision trees

Example: Splitting

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

i	pred.	y	x_1	x_2
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).

Note$_2$ Trees often grow until they hit some number of observations in a leaf.

Example: Splitting

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

i	pred.	y	x_1	x_2
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)*

Example: Splitting

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

i	pred.	y	x_1	x_2
1	**3**	0	1	4
2	**8**	8	3	2
3	**3**	6	5	6

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

Example: Splitting

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

i	pred.	y	x_1	x_2
1	**4**	0	1	4
2	**4**	8	3	2
3	**6**	6	5	6

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

Example: Splitting

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.

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 predicator (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.

More splits

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!

Decision trees

Pruning

Pruning allows us to trim our trees back to their "best selves."

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

Cost-complexity pruning🌲 offers a solution.

Just as we did with lasso, **cost-complexity pruning** forces the tree to pay a price (penalty) to become more complex

Complexity here is defined as the number of regions $|T|$.

🌲 Also called: *weakest-link pruning.*

Pruning

Specifically, cost-complexity pruning adds a penalty of $\alpha|T|$ to the RSS, *i.e.*,

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

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

$\alpha = 0$ generates T_0, but as α increases, we begin to cut back the tree.

We choose α via cross validation.

Classification trees

Classification with trees is very similar to regression.

Regression trees

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

Classification trees

- **Predict:** Region's mode
- **Split:** Min. Gini or entropy🌲
- **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.

🌲 Defined on the next slide. 🌴 ... or Gini index or entropy

Decision trees

The Gini index

Let $\hat{p}_{mk}$ denote the proportion of observations in class k and region m.

The **Gini index** tells us about a region's "purity"🌲

$$G = \sum_{k=1}^{K} \hat{p}_{mk} \left(1 - \hat{p}_{mk}\right)$$

if a region is very homogeneous, then the Gini index will be small.

Homogenous regions are easier to predict.
Reducing the Gini index yields to more homogeneous regions
$\therefore$ We want to minimize the Gini index.

🌲 This vocabulary is Voldemort's contribution to the machine-learning literature.

Decision trees

Entropy

Let $\hat{p}_{mk}$ denote the proportion of observations in class k and region m.

Entropy also measures the "purity" of a node/leaf

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

Entropy is also minimized when $\hat{p}_{mk}$ values are close to 0 and 1.

Decision trees

Rational

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.

Ex. 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.

Classification trees

When **growing** classification trees, we want to use the Gini index or entropy.

However, when **pruning**, the error rate is typically fine—especially if accuracy will be the final criterion.

Decision trees

In R

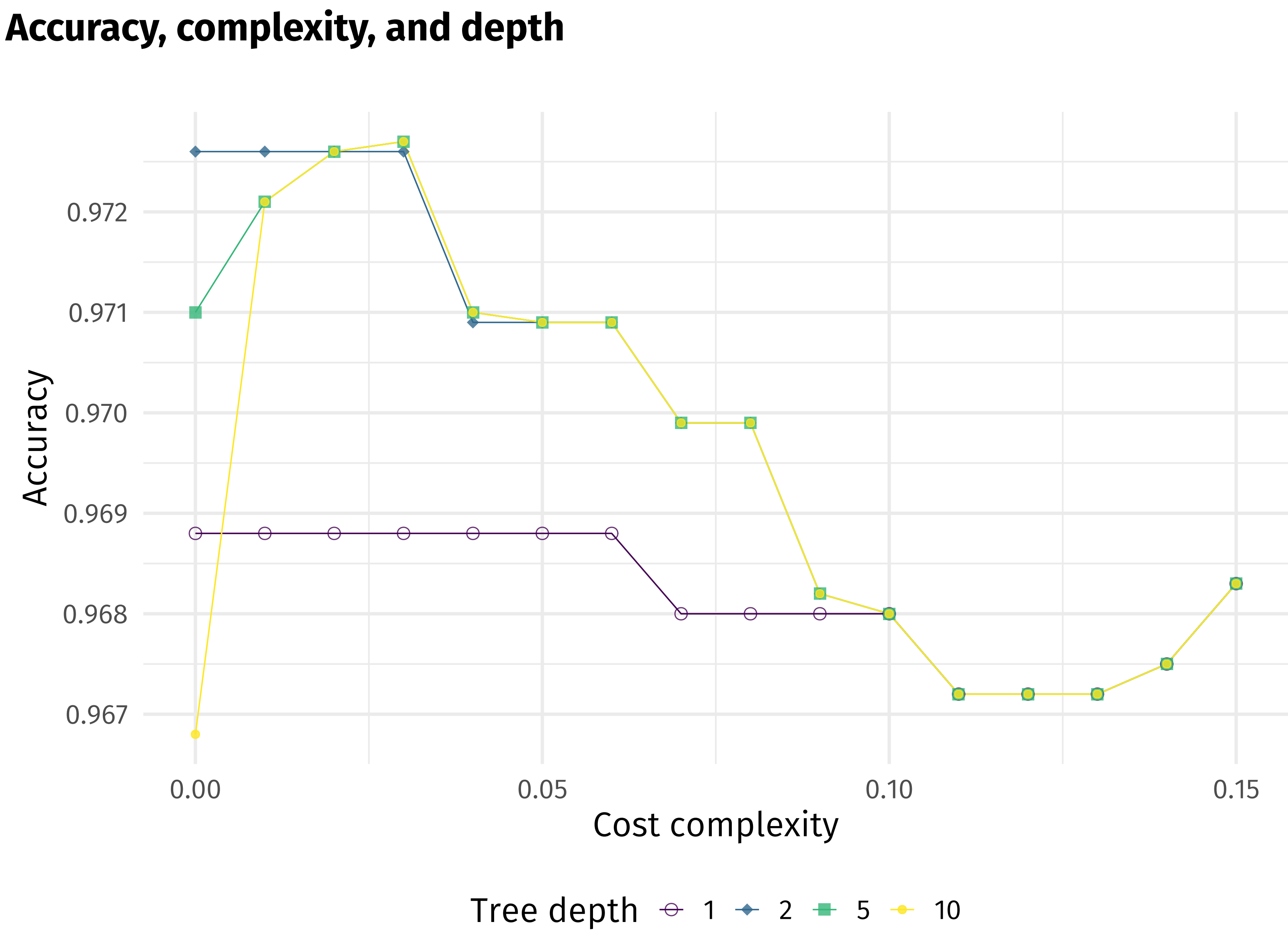
To train decision trees in R, we can use `parsnip`, which draws upon `rpart`.

In `parsnip`, we use the aptly named `decision_tree()` function.

The `decision_tree()` model (with `rpart` engine) wants four inputs:

- `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

```r
# Define our CV split
set.seed(12345)
default_cv = default_df %>% vfold_cv(v = 5)
# 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")
# Define recipe
default_recipe = recipe(default ~ ., data = default_df)
# Define the workflow
default_flow = workflow() %>%
  add_model(default_tree) %>% add_recipe(default_recipe)
# 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, roc_auc)
)
```


Accuracy, complexity, and depth
Accuracy
0.972
0.971
0.970
0.969
0.968
0.967
0.00
0.05
0.10
0.15
Cost complexity
Tree depth
1
2
5
10

To plot the CV-chosen tree...

1. **Fit** the chosen/best model.

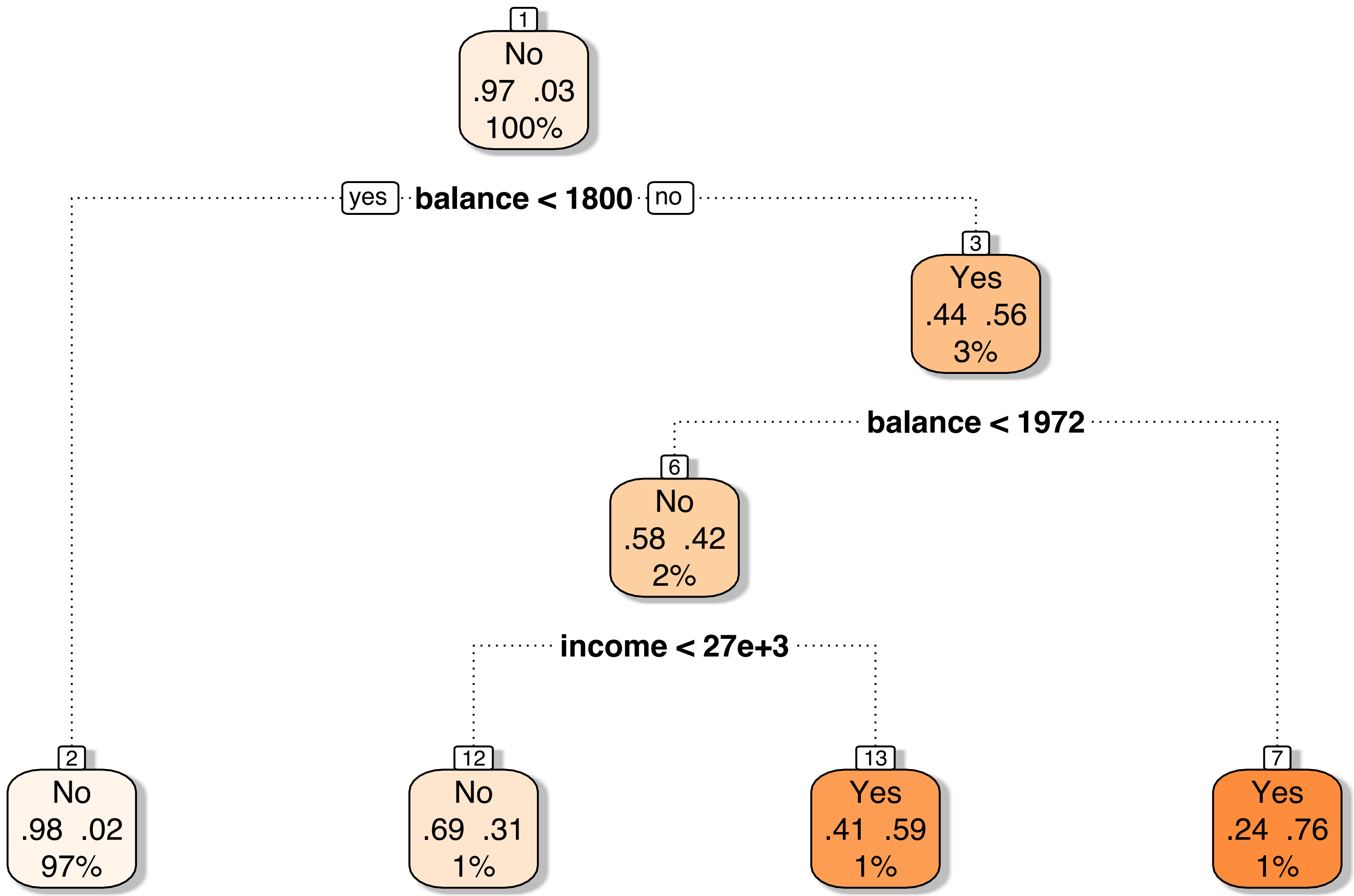
```
best_flow =
  default_flow %>%
  finalize_workflow(select_best(default_cv_fit, metric = "accuracy")) %>%
  fit(data = default_df)
```

2. **Extract** the fitted model, *e.g.*, with `pull_workflow_fit()`.

```
best_tree = best_flow %>% pull_workflow_fit()
```

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

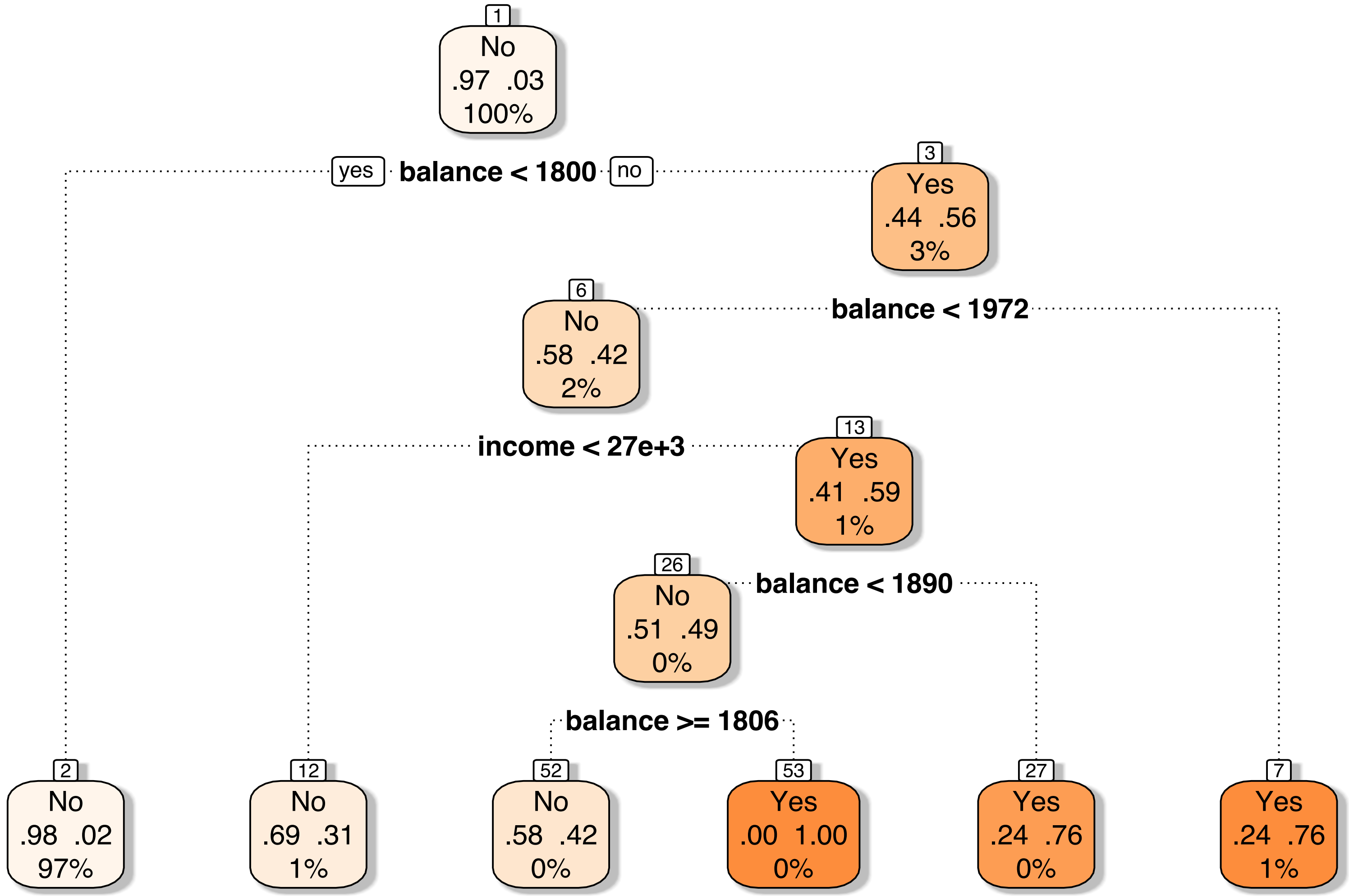
```
best_tree$fit %>% rpart.plot()
```


1
No
.97 .03
100%
yes
balance < 1800
no
3
Yes
.44 .56
3%
balance < 1972
6
No
.58 .42
2%
income < 27e+3
2
No
.98 .02
97%
12
No
.69 .31
1%
13
Yes
.41 .59
1%
7
Yes
.24 .76
1%

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

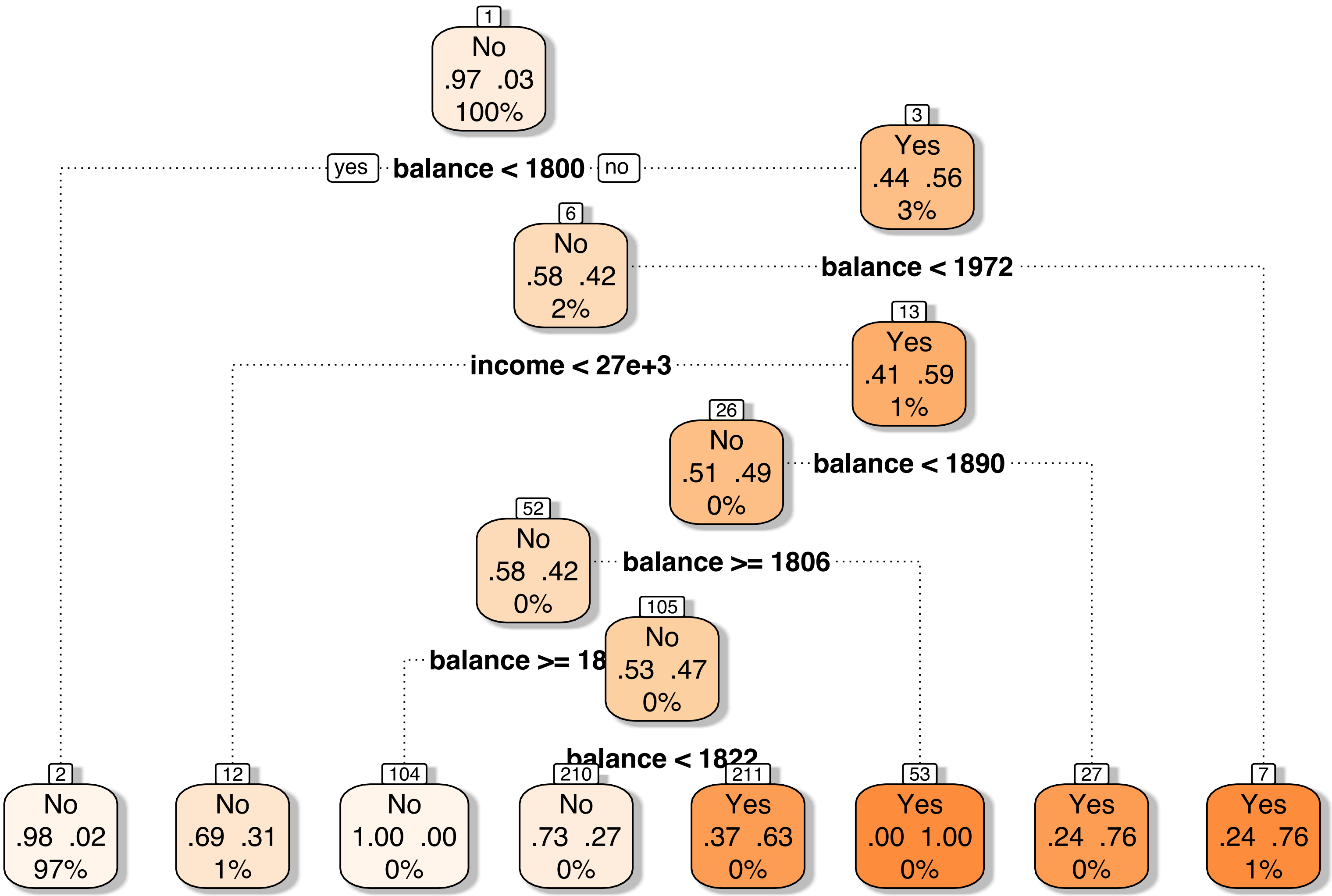
We can compare this "best" tree to a less pruned/penalized tree

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


1
No
.97 .03
100%
yes
balance < 1800
no
3
Yes
.44 .56
3%
6
No
.58 .42
2%
balance < 1972
income < 27e+3
13
Yes
.41 .59
1%
26
No
.51 .49
0%
balance < 1890
balance >= 1806
2
No
.98 .02
97%
12
No
.69 .31
1%
52
No
.58 .42
0%
53
Yes
.00 1.00
0%
27
Yes
.24 .76
0%
7
Yes
.24 .76
1%

What if we hold the cost complexity constant but increase the max. depth?

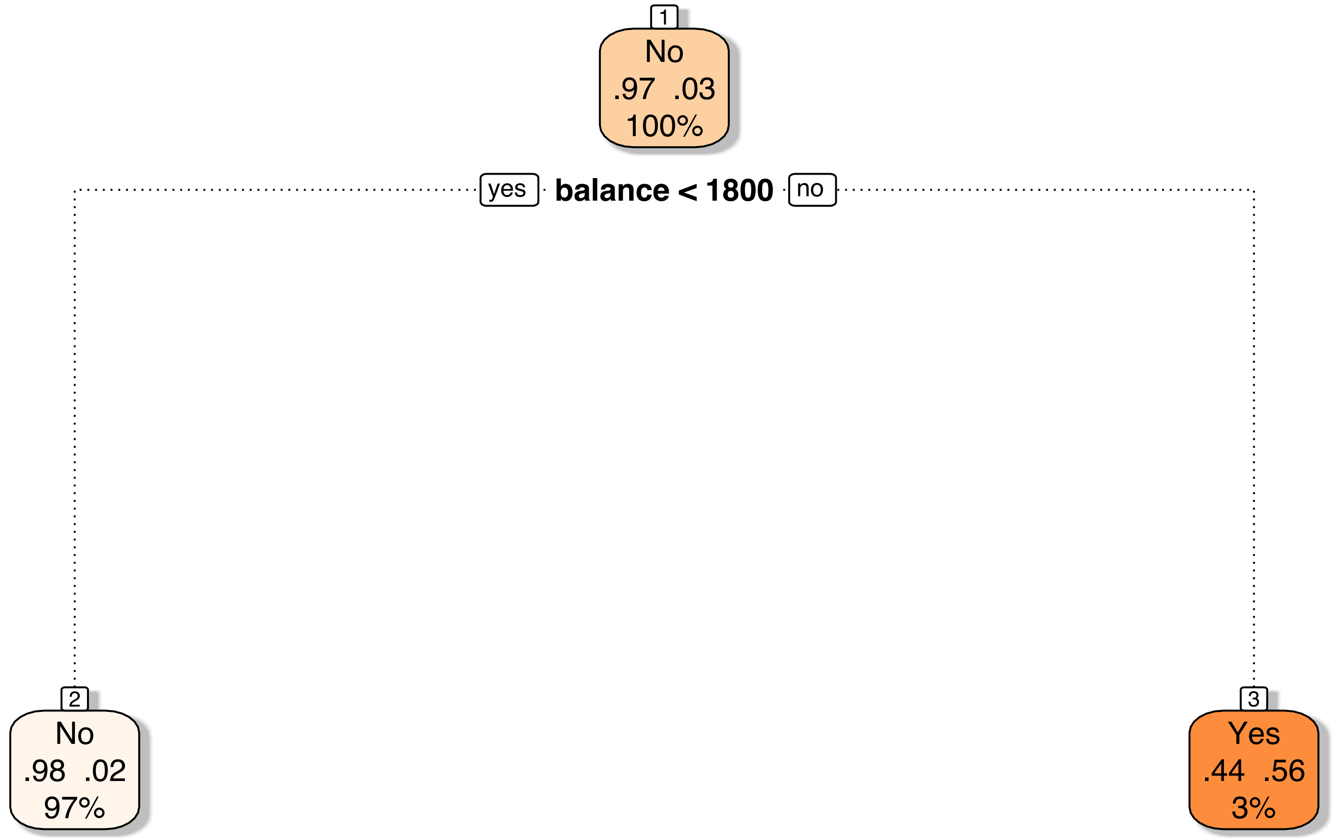
- `cost_complexity = 0.005`
- `tree_depth = 10` (moved up from `5`)



1
No
.97 .03
100%
yes
balance < 1800
no
3
Yes
.44 .56
3%
6
No
.58 .42
2%
balance < 1972
13
Yes
.41 .59
1%
income < 27e+3
26
No
.51 .49
0%
balance < 1890
52
No
.58 .42
0%
balance >= 1806
105
No
.53 .47
0%
balance >= 18
balance < 1822
2
No
.98 .02
97%
12
No
.69 .31
1%
104
No
1.00 .00
0%
210
No
.73 .27
0%
211
Yes
.37 .63
0%
53
Yes
.00 1.00
0%
27
Yes
.24 .76
0%
7
Yes
.24 .76
1%

What if we ratchet up complexity constant?

- `cost_complexity = 0.1` (increased from `0.005`)
- `tree_depth = 10`

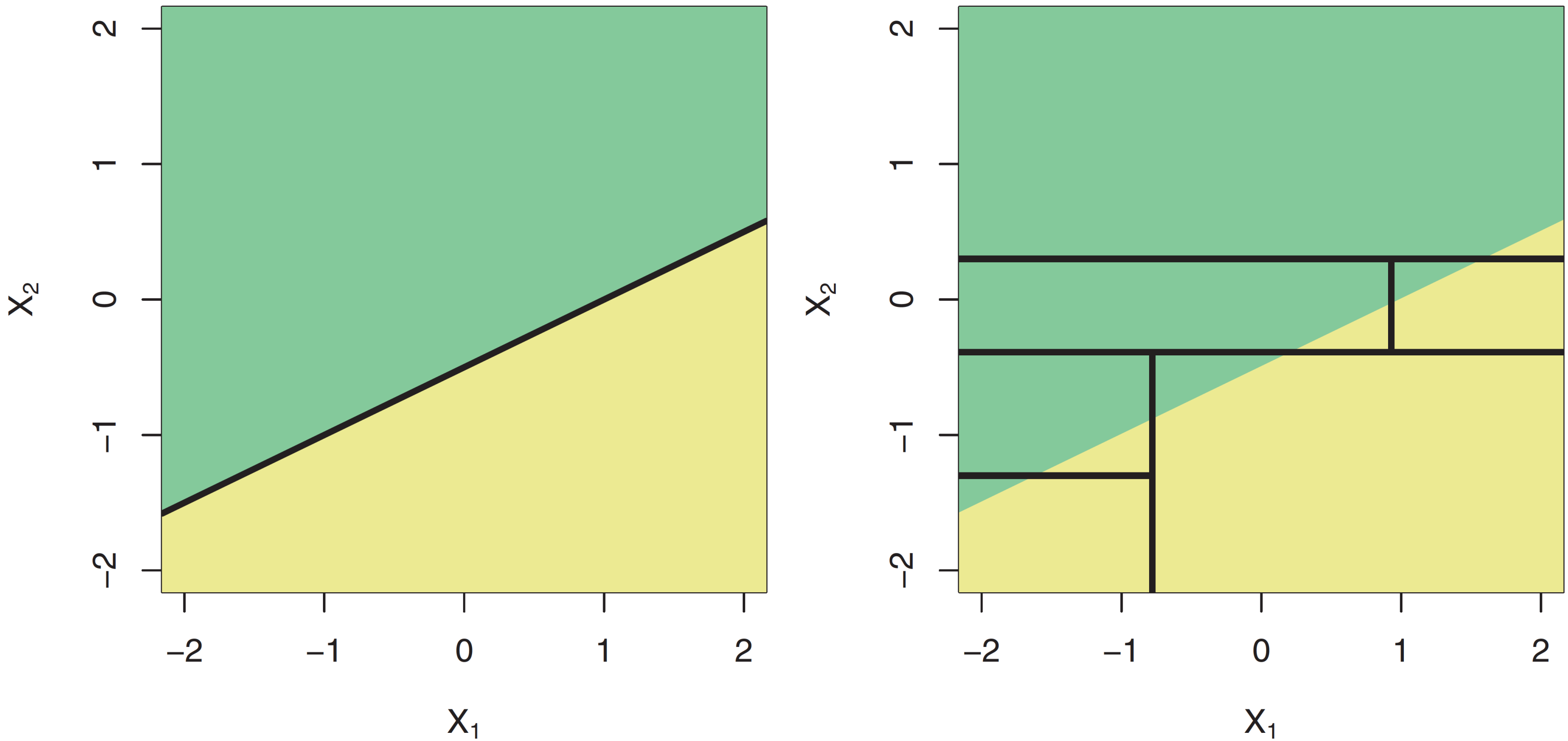

1
No
.97 .03
100%
yes
balance < 1800
no
2
No
.98 .02
97%
3
Yes
.44 .56
3%

Q How do trees compare to linear models?

Q How do trees compare to linear models?

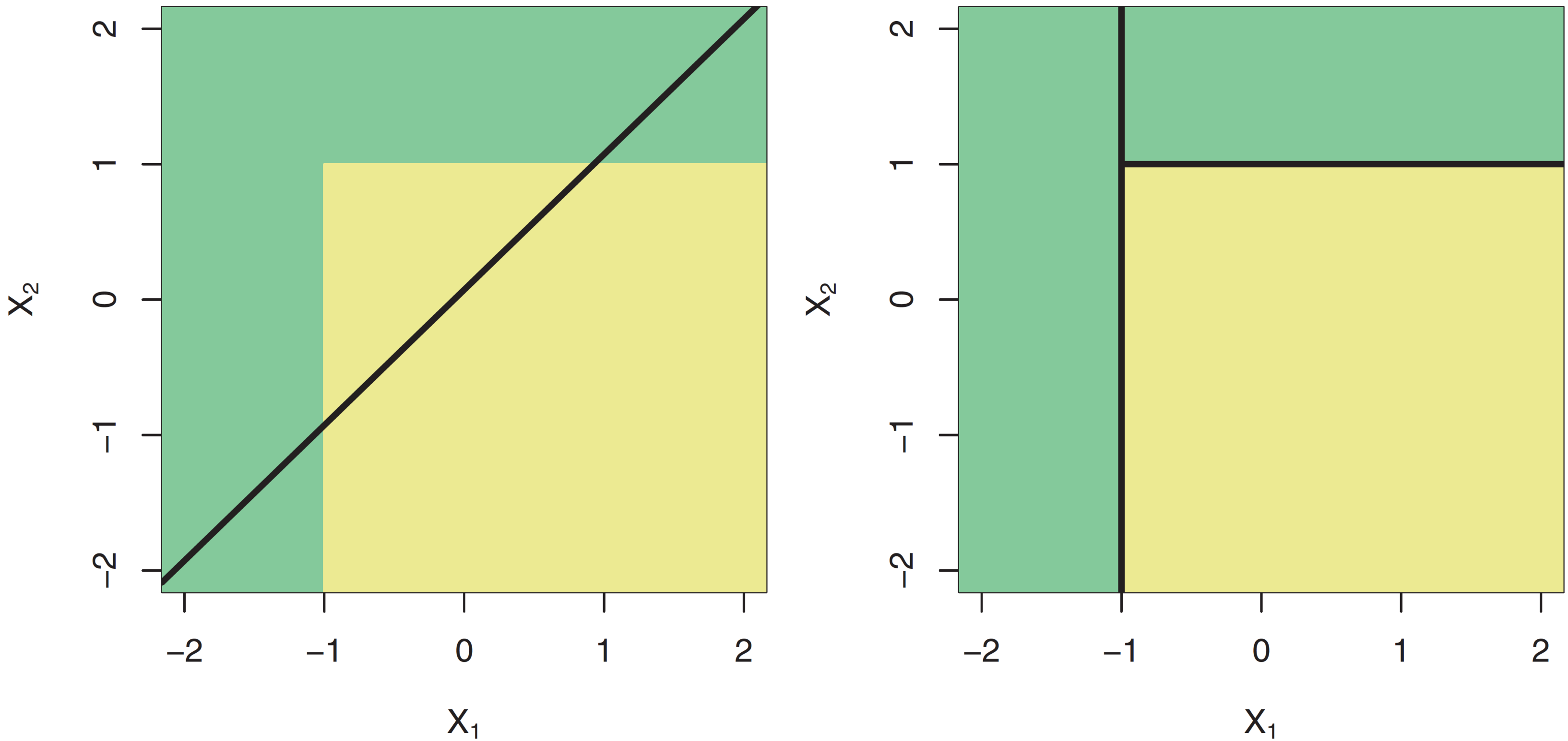
A It depends how linear the true boundary is.

Linear boundary: trees struggle to recreate a line.



Source: ISL, p. 315

Nonlinear boundary: trees easily replicate the nonlinear boundary.



Source: ISL, p. 315

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.

Sources

These notes draw upon

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

Table of contents