

Lecture 007

Trees 🌲🌴🌳

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Material

Last time: Classification

Today! Decision trees for regression and classification.

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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

Decision trees

Fundamentals

Decision trees

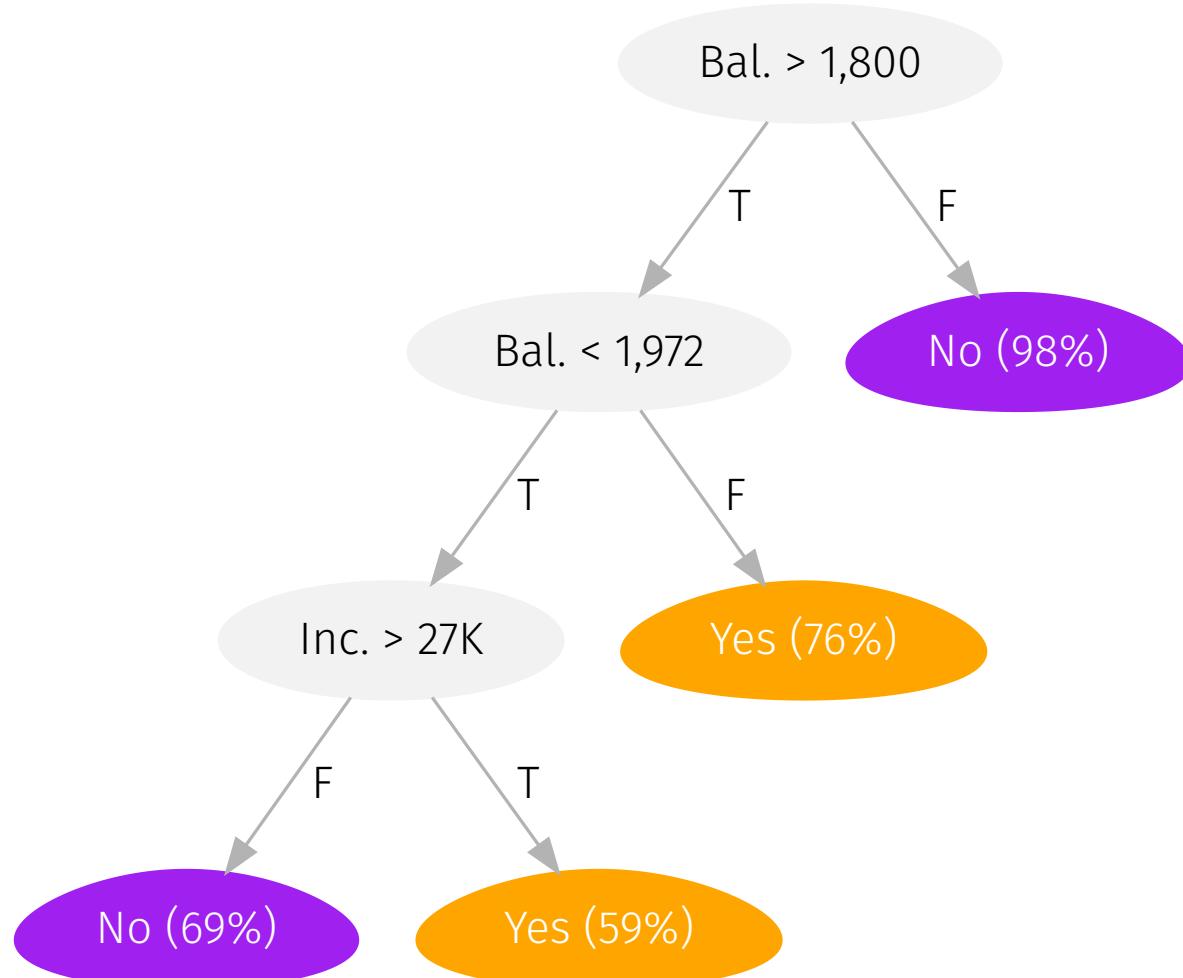
- split the *predictor space* (our \mathbf{X}) into regions
- then predict the most-common value within a region

Decision trees

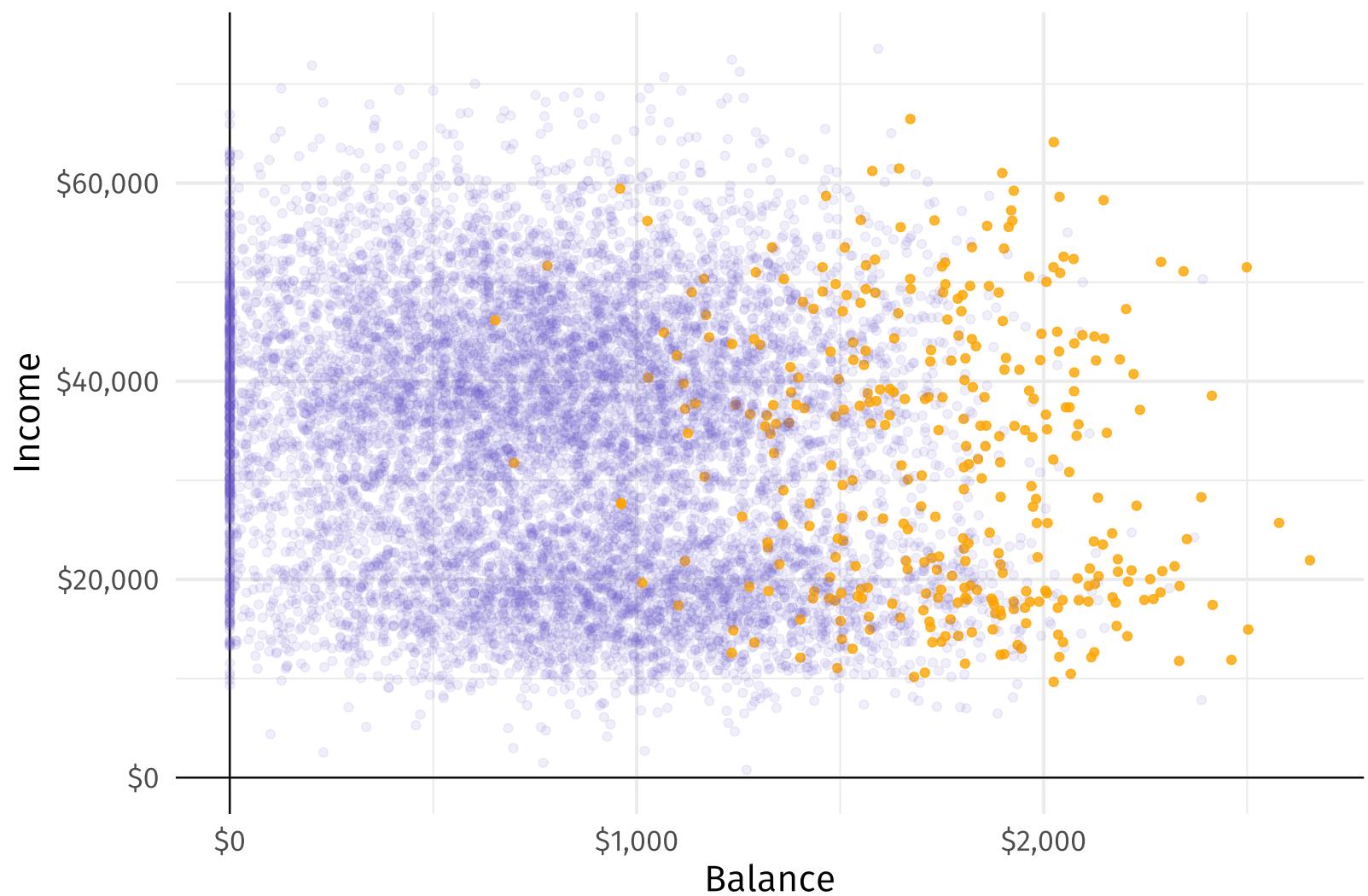
1. work for **both classification and regression**
2. are inherently **nonlinear**
3. are relatively **simple** and **interpretable**
4. often **underperform** relative to competing methods
5. easily extend to **very competitive ensemble methods** (*many trees*) 

 Though the ensembles will be much less interpretable.

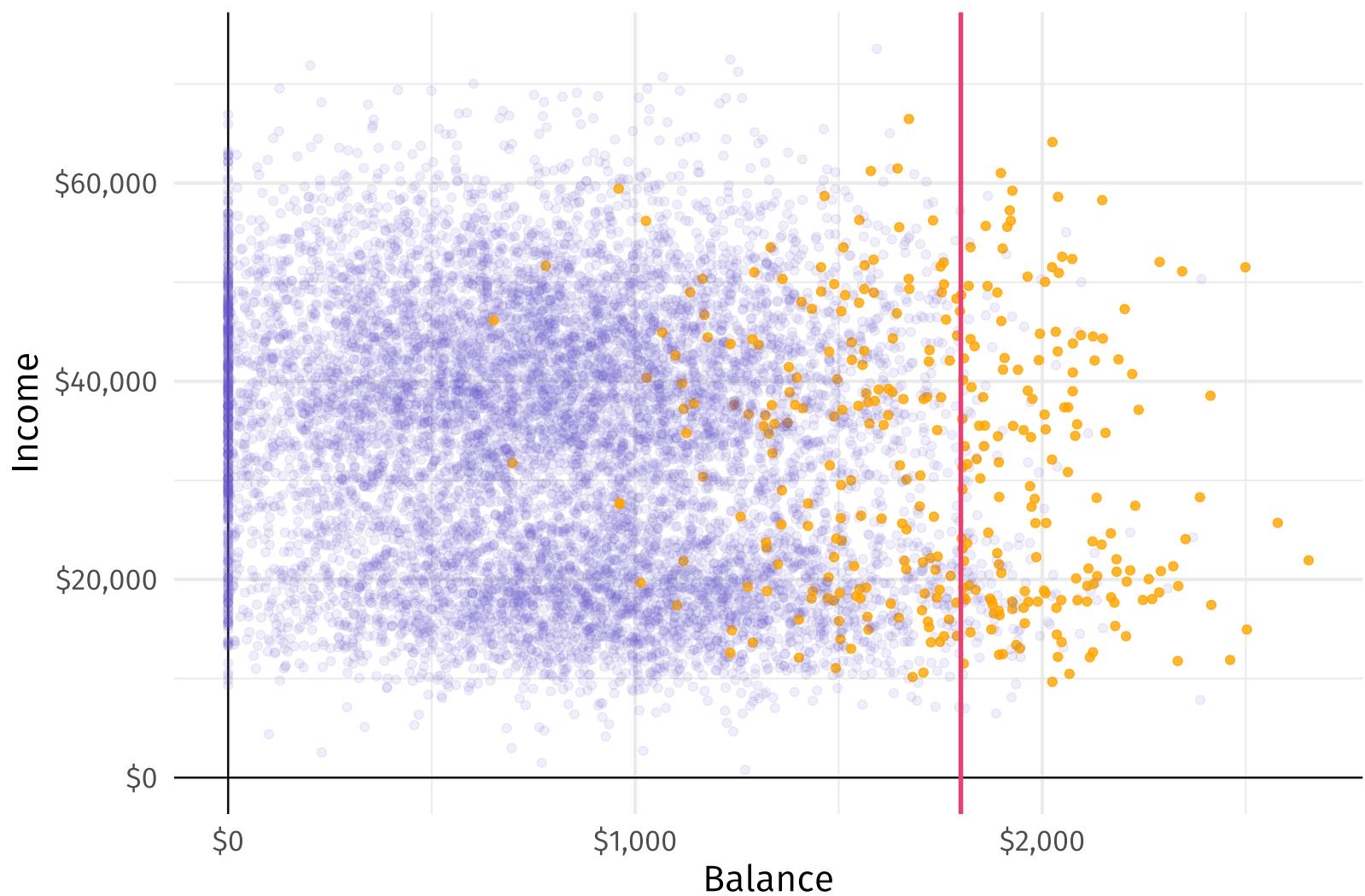
Example: **A simple decision tree** classifying credit-card default



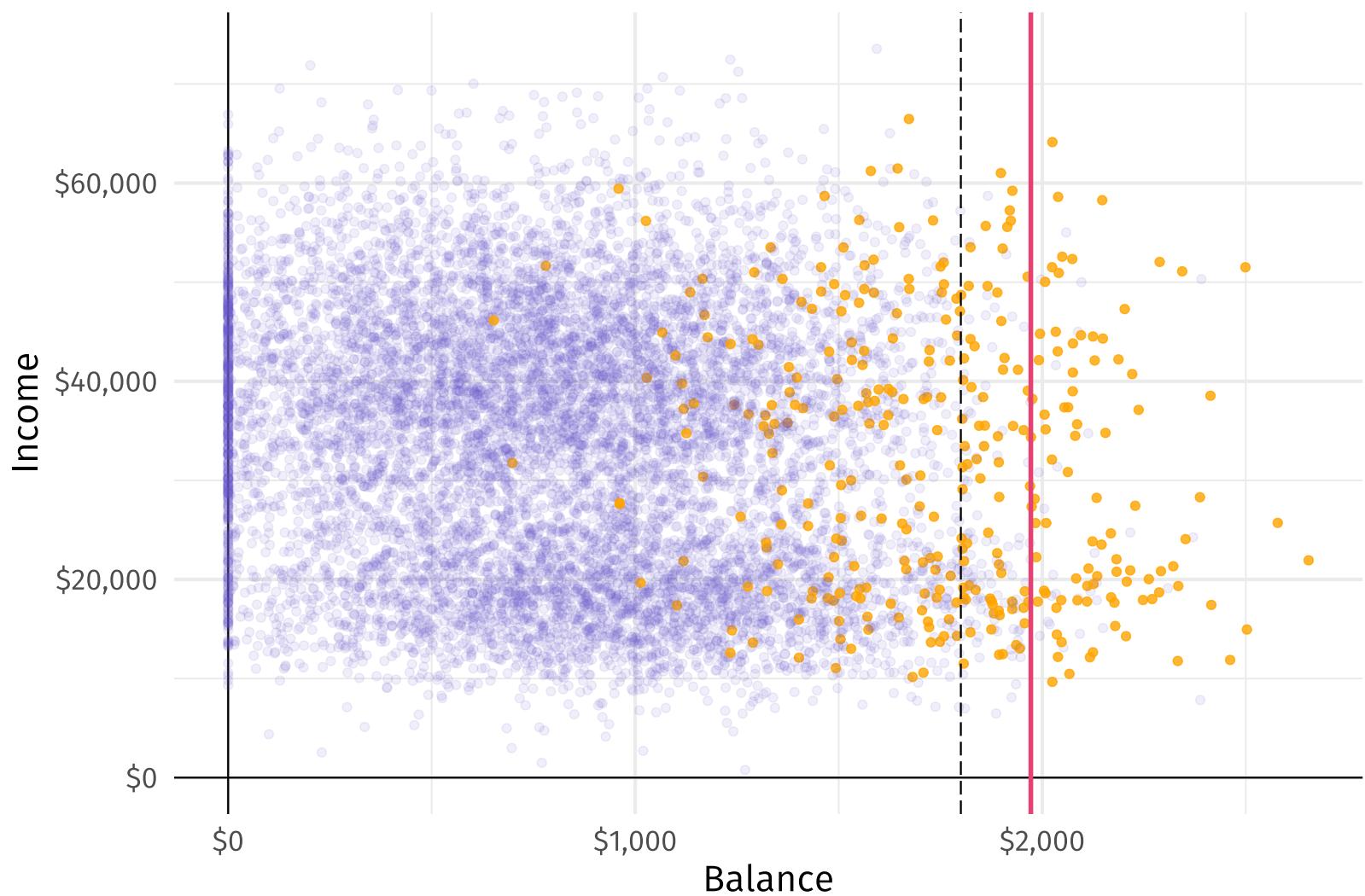
Let's see how the tree works—starting with our data (default: Yes vs. No).



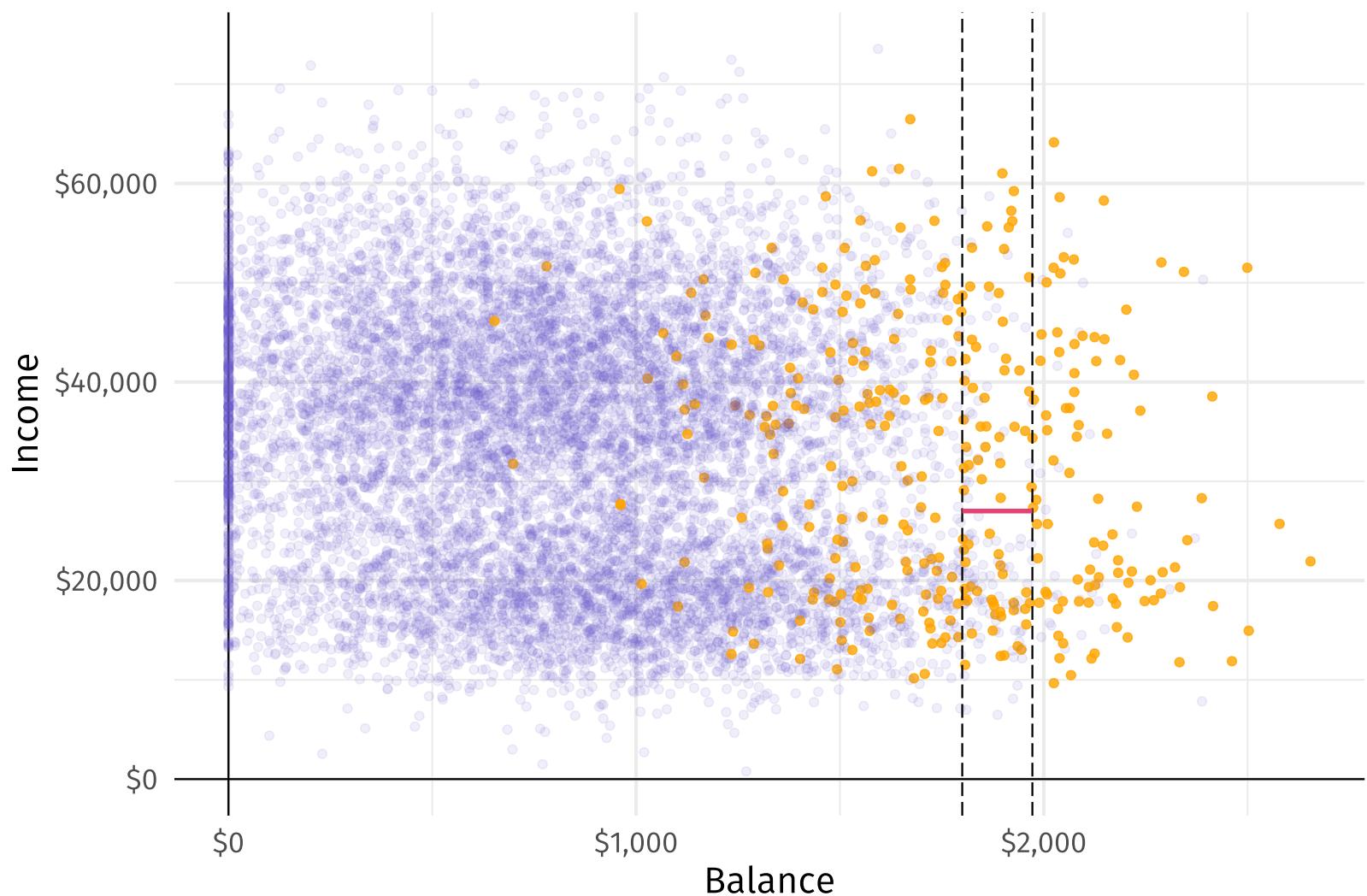
The **first partition** splits balance at \$1,800.



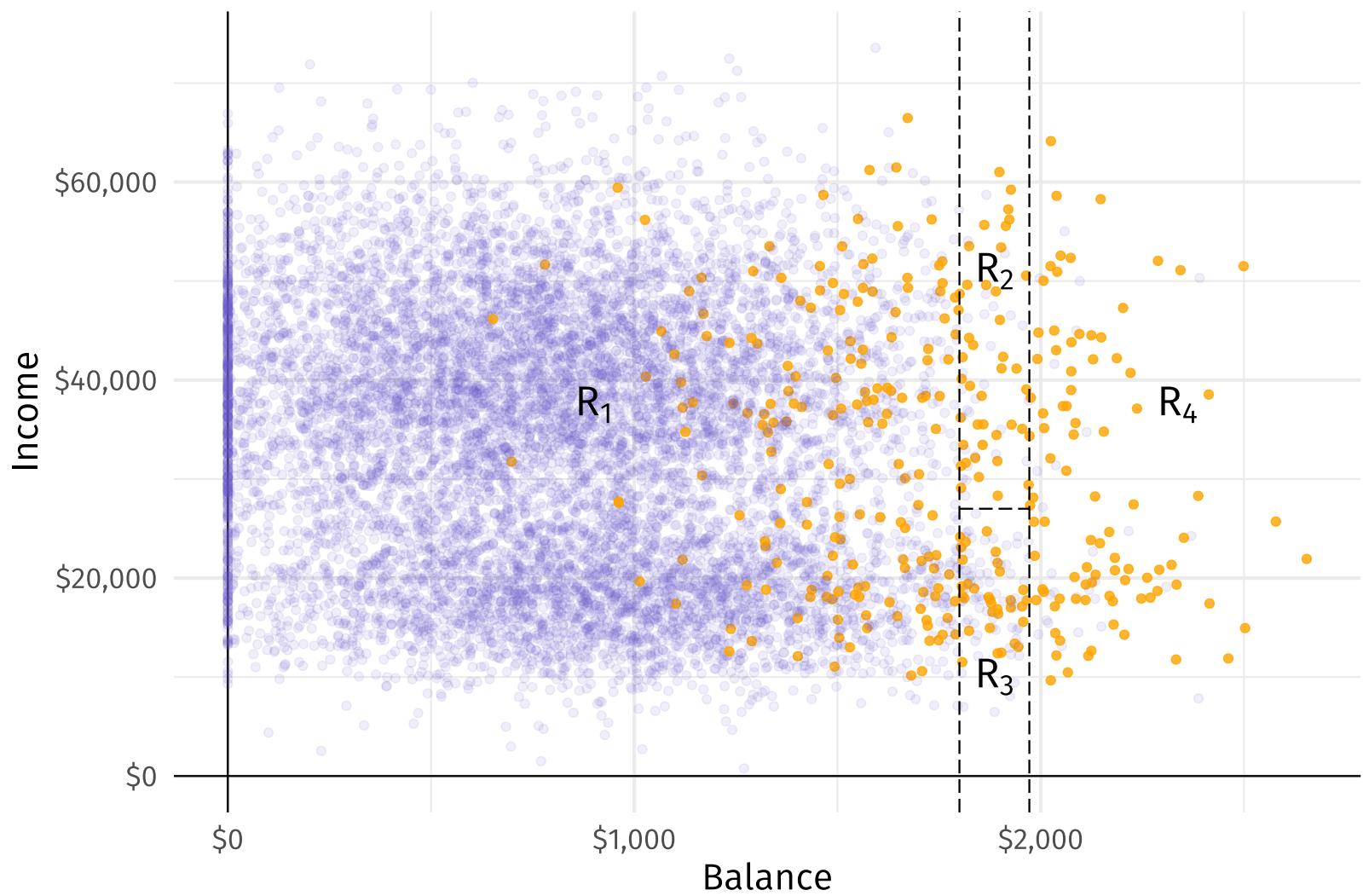
The **second partition** splits balance at \$1,972, (conditional on bal. > \$1,800).



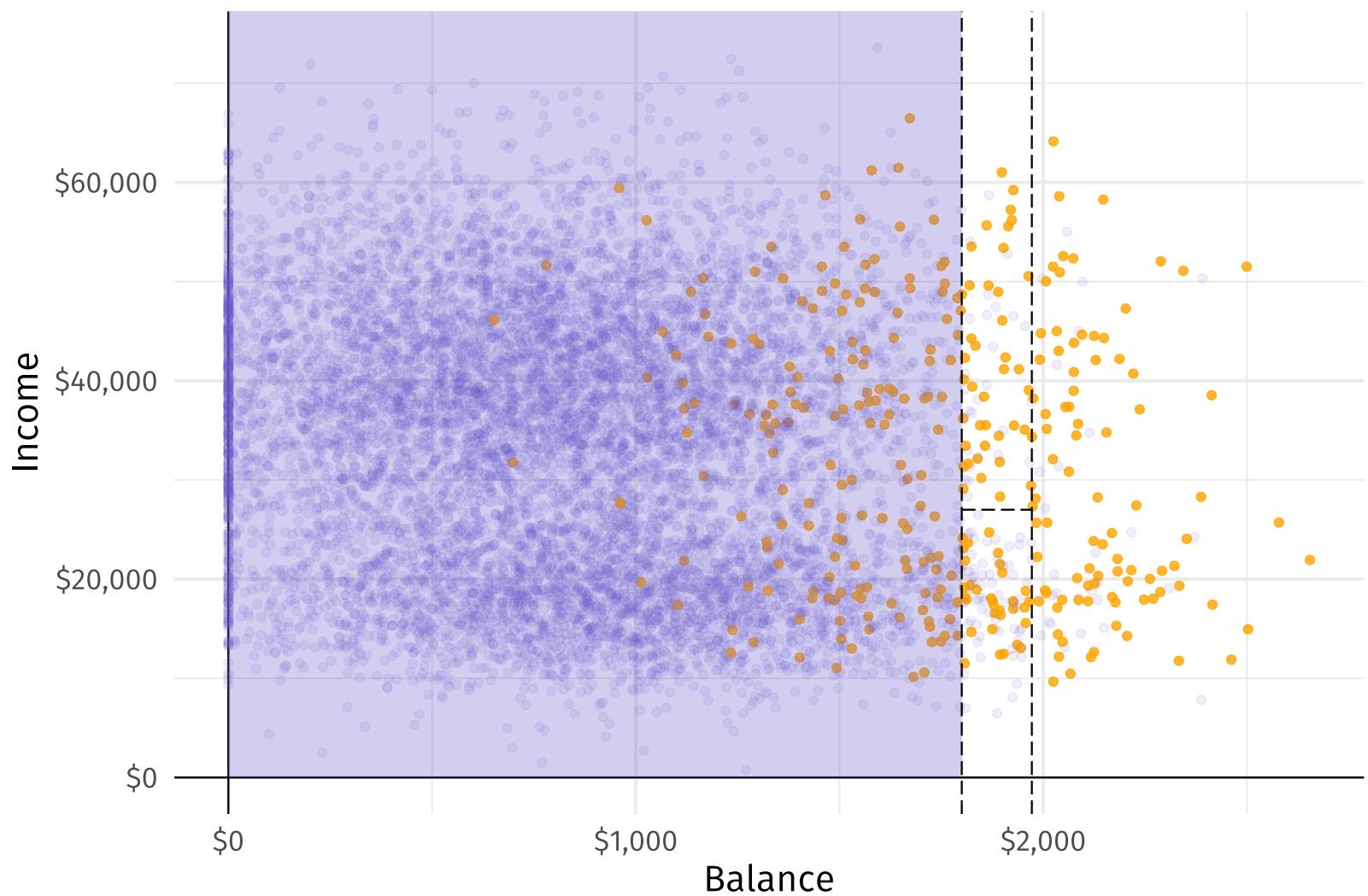
The **third partition** splits income at \$27K **for** bal. between \$1,800 and \$1,972.



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).



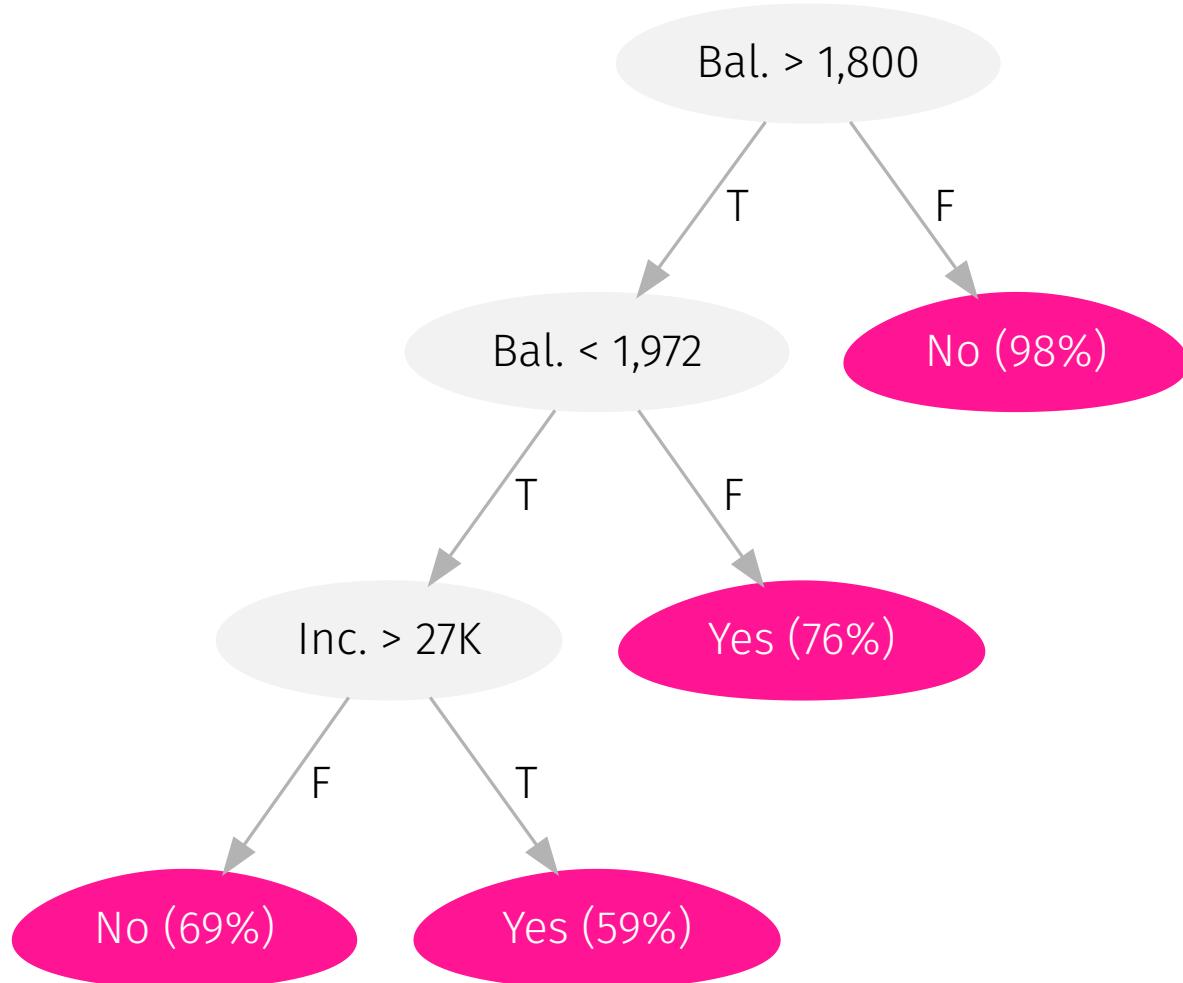
Predictions cover each region (e.g., using the region's most common class).



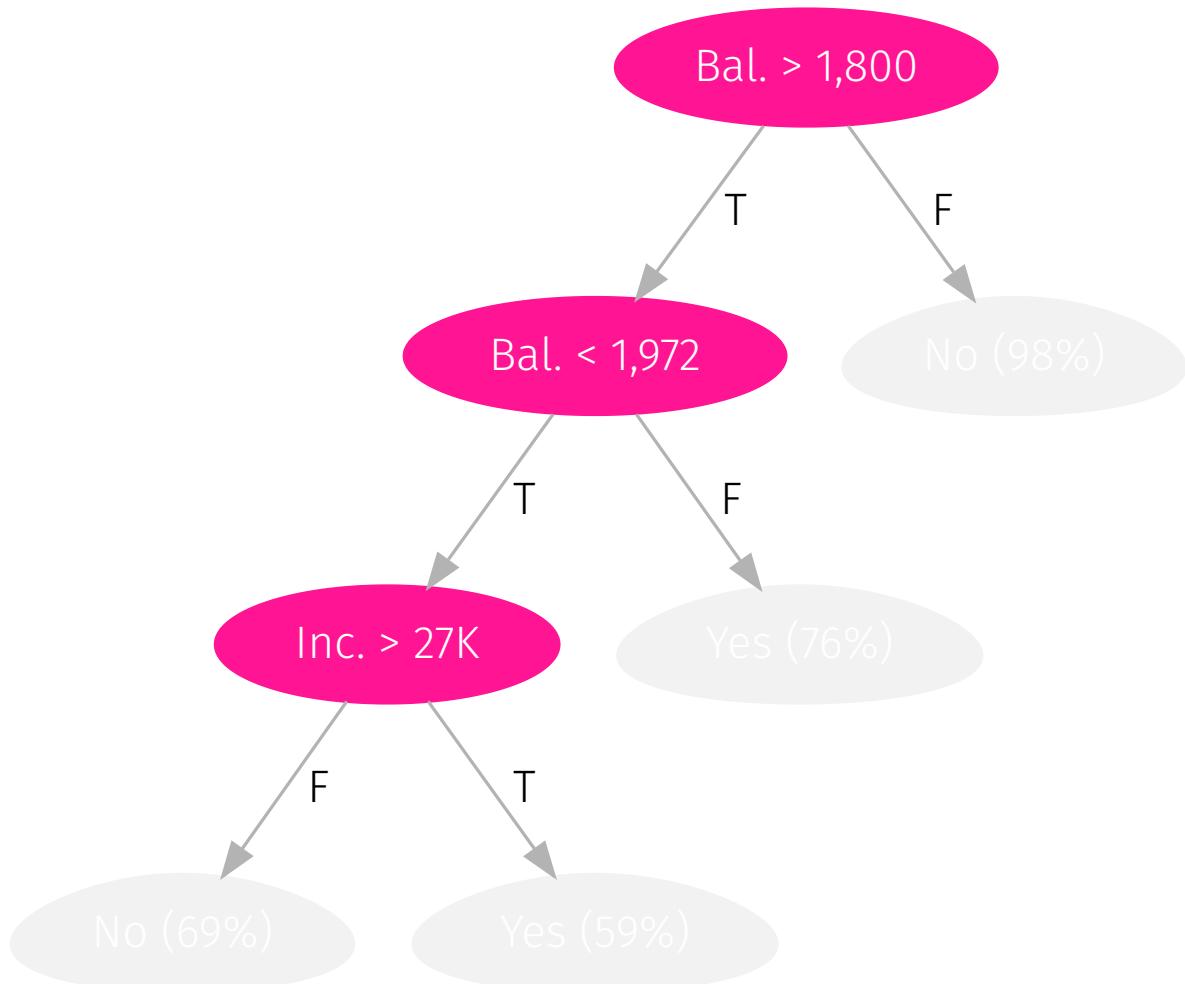
Predictions cover each region (e.g., using the region's most common class).



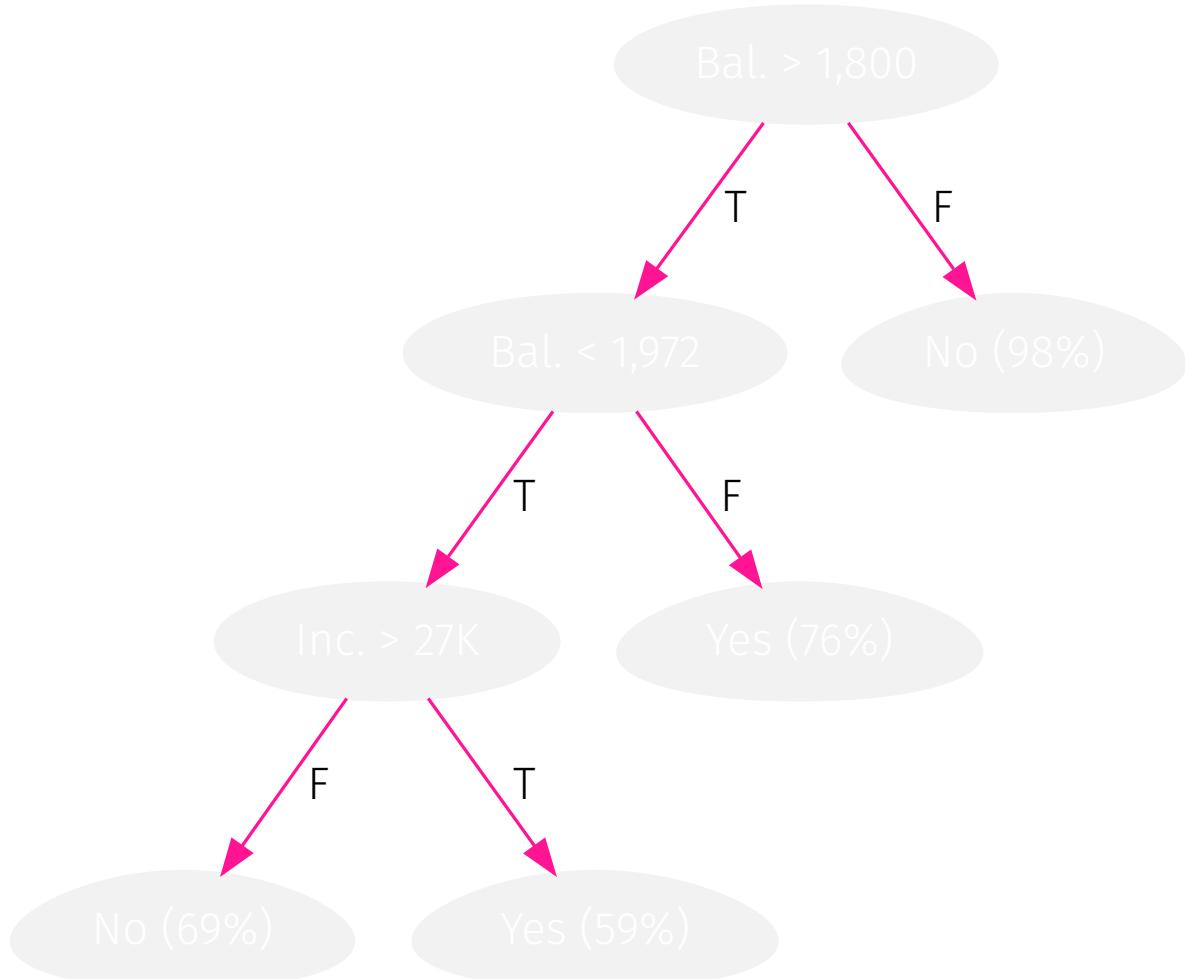
The **regions** correspond to the tree's **terminal nodes** (or **leaves**).



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?

Decision trees

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 $\mathbf{x}_1, \dots, \mathbf{x}_p$)
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 partition 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

Decision trees

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**.

Decision trees

Example: Splitting

Example Consider the dataset

i	y	x ₁	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	x_1	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 $0^2 + 1^2 + (-1)^2 = 2$.

Note₁ Splitting x_1 at 2 yields the same results as 1.5, 2.5—anything in (1, 3).

Note₂ Trees often grow until they hit some number of observations in a leaf.

Decision trees

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*)

Decision trees

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 $(-3)^2 + 0^2 + 3^2 = 18$.

Decision trees

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 $(-4)^2 + 4^2 + 0^2 = 32$.

Decision trees

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 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.

Decision trees

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.

Decision trees

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.

Decision trees

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*.

Decision trees

Pruning

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

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

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.

Decision trees

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" 

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

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

.
∴ 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.

Decision trees

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`.

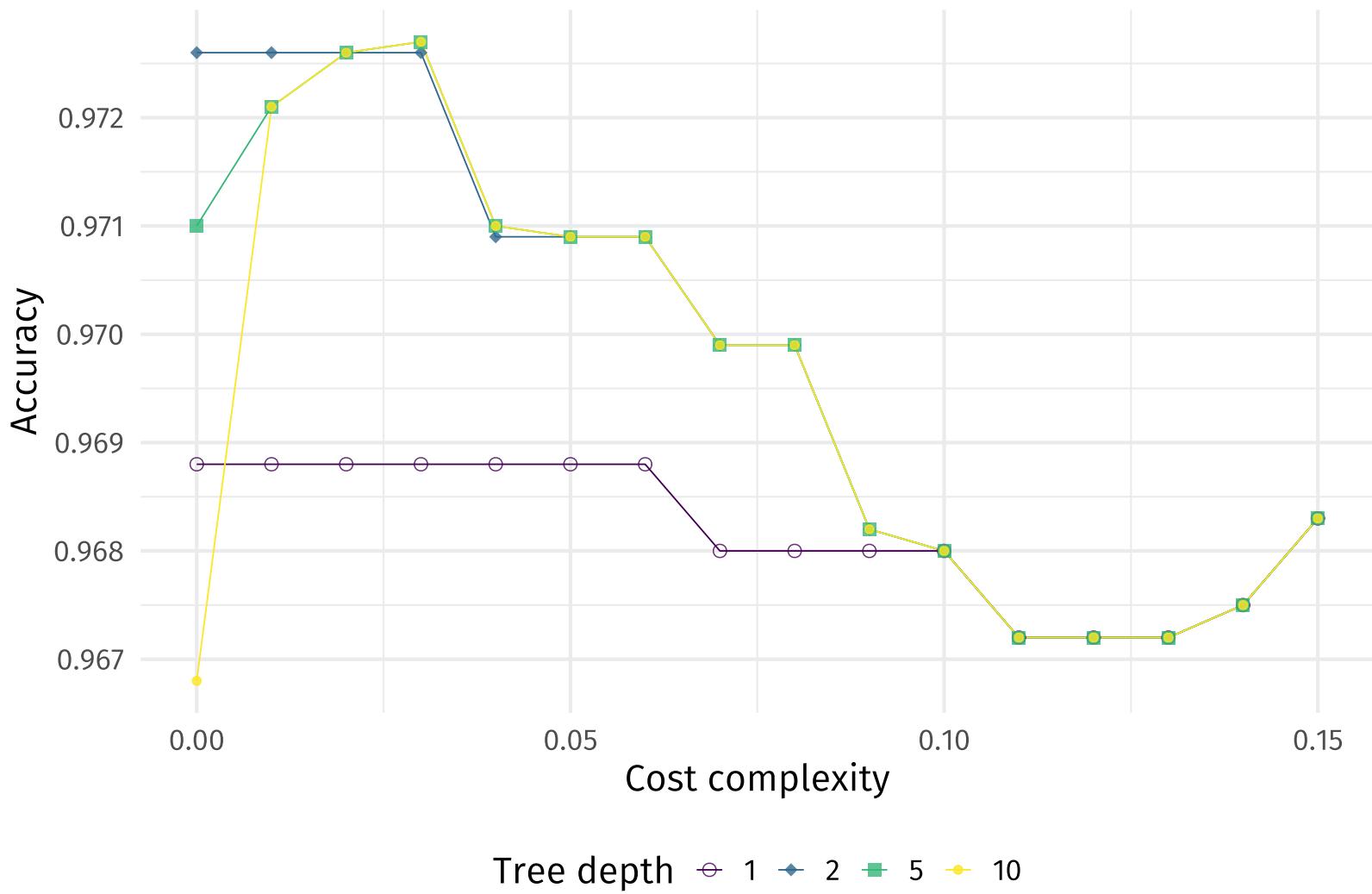
In `parsnip`, we use the aptly named `decision_tree()` function.

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

```
# 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



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%

6
No
.58 .42
2%

balance < 1972

income < 27e+3

2
No
.98 .02
97%

12
No
.69 .31
1%

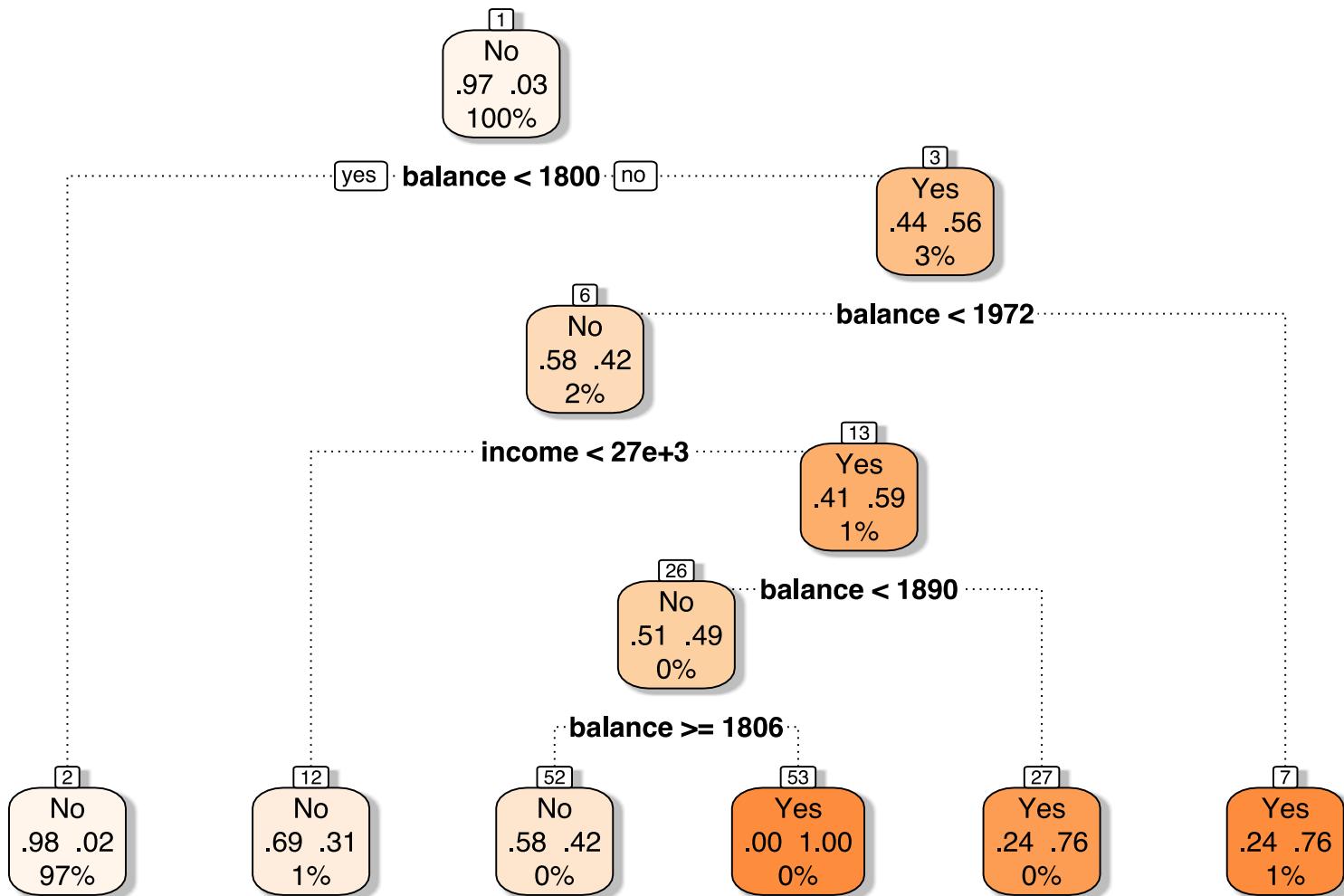
13
Yes
.41 .59
1%

7
Yes
.24 .76
1%

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

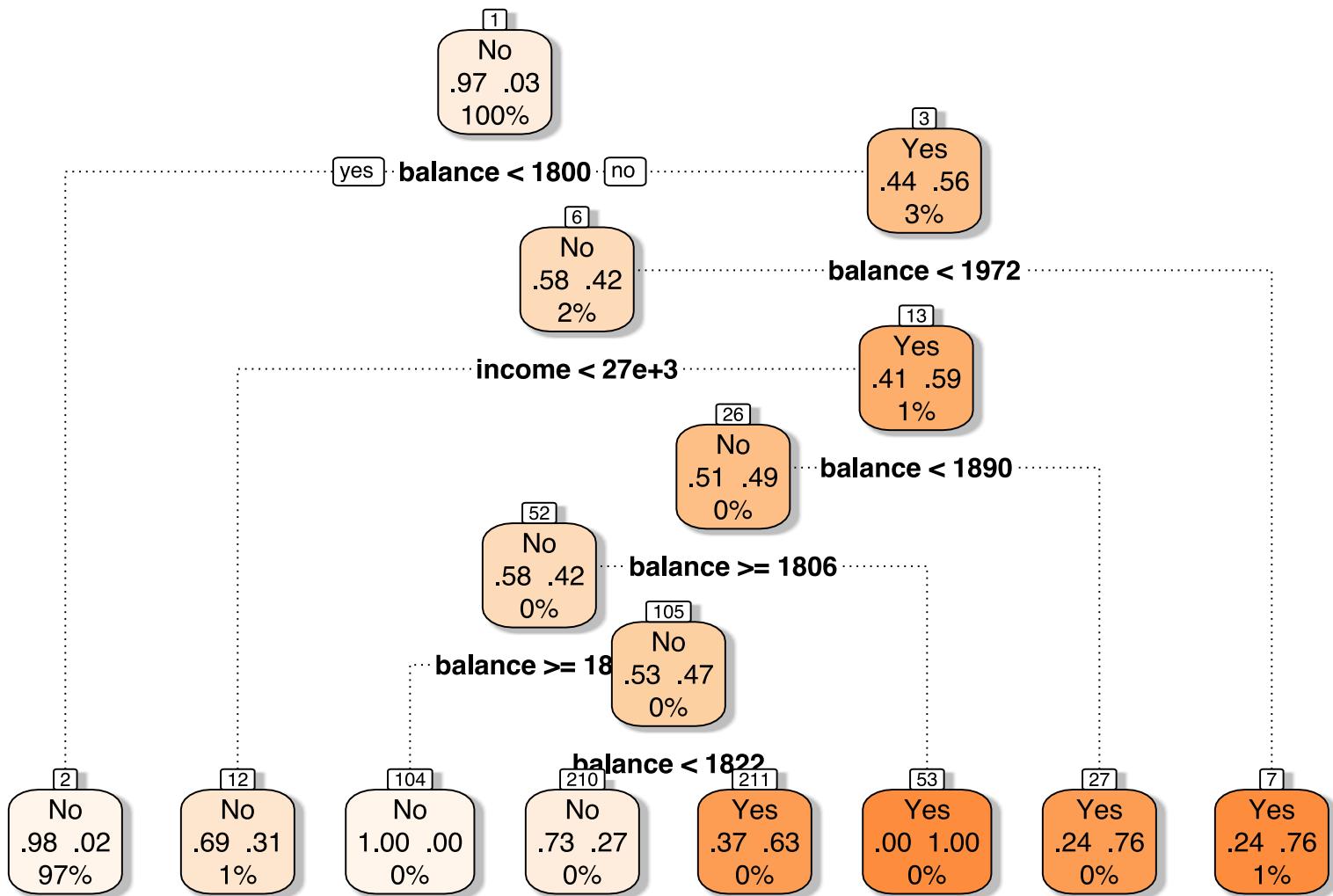
We can compare this "best" tree to a less pruned/penalized tree

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



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

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



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%

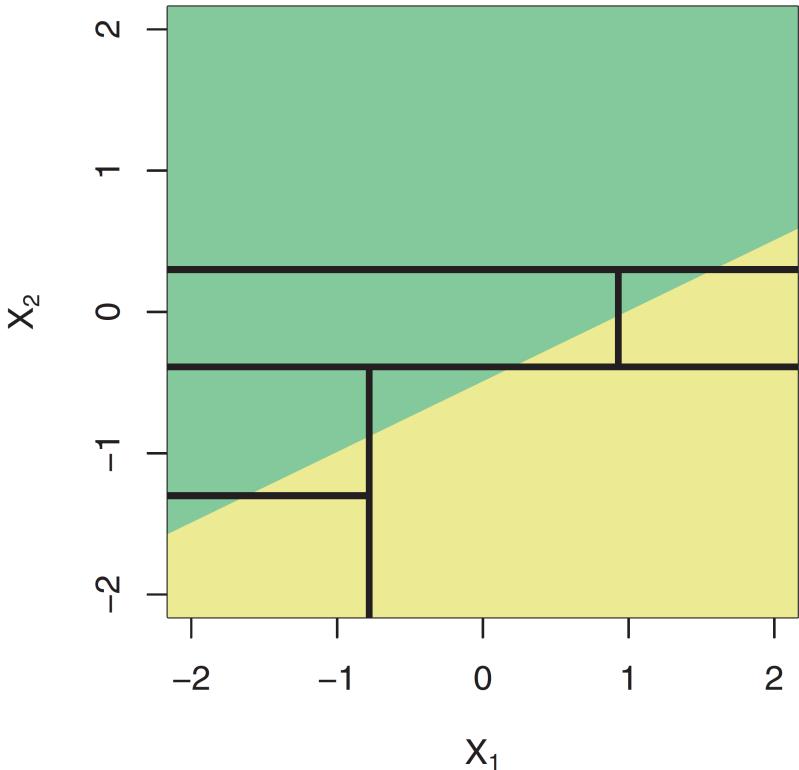
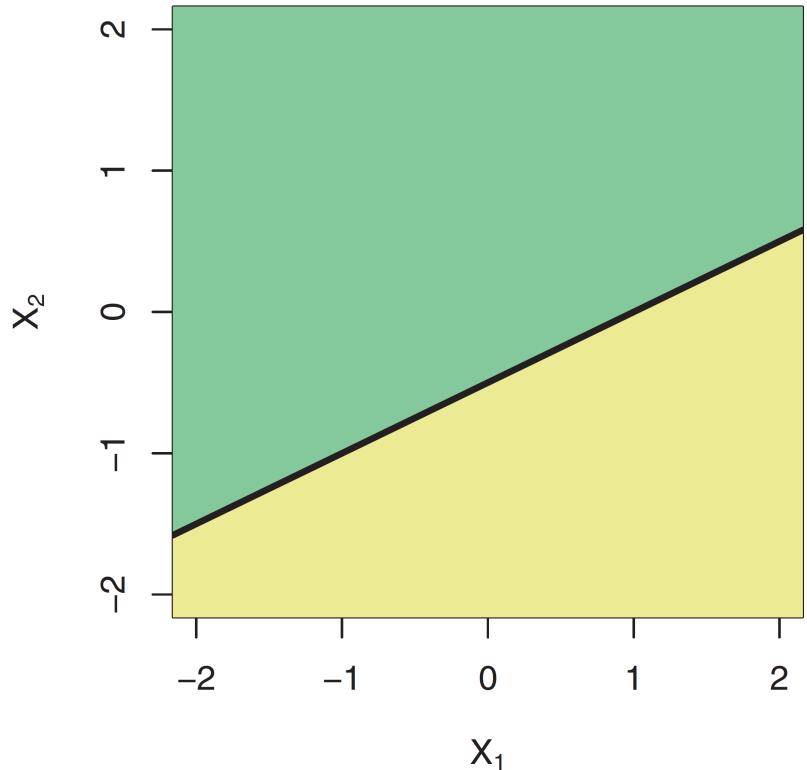
3
Yes
.44 .56
3%

Q How do trees compare to linear models?

Q How do trees compare to linear models?

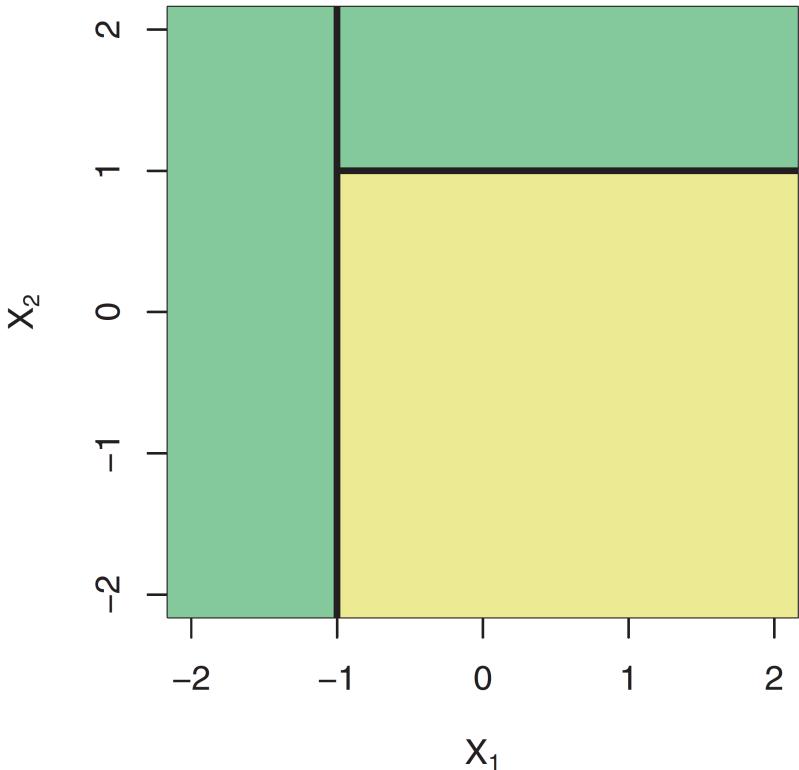
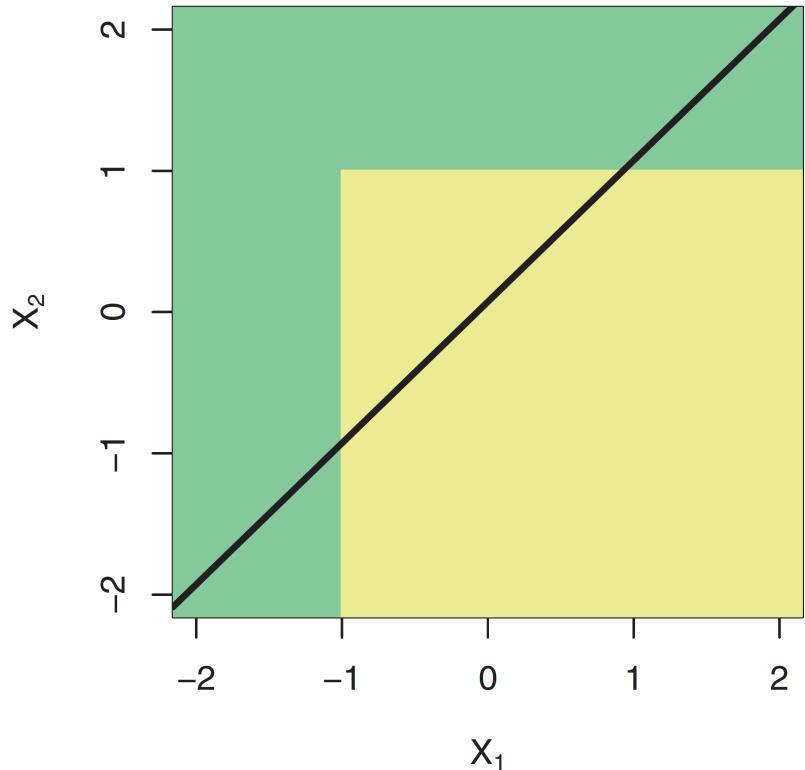
A It depends how linear the true boundary is.

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/interpreted
- + 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

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