

Lecture 007

Trees 🌲🌴🌳

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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 and classification:* Very soon!

Project

- Group and topic **due today!**
- Start getting your data together!

Decision trees

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Fundamentals

Decision trees

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

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Decision trees

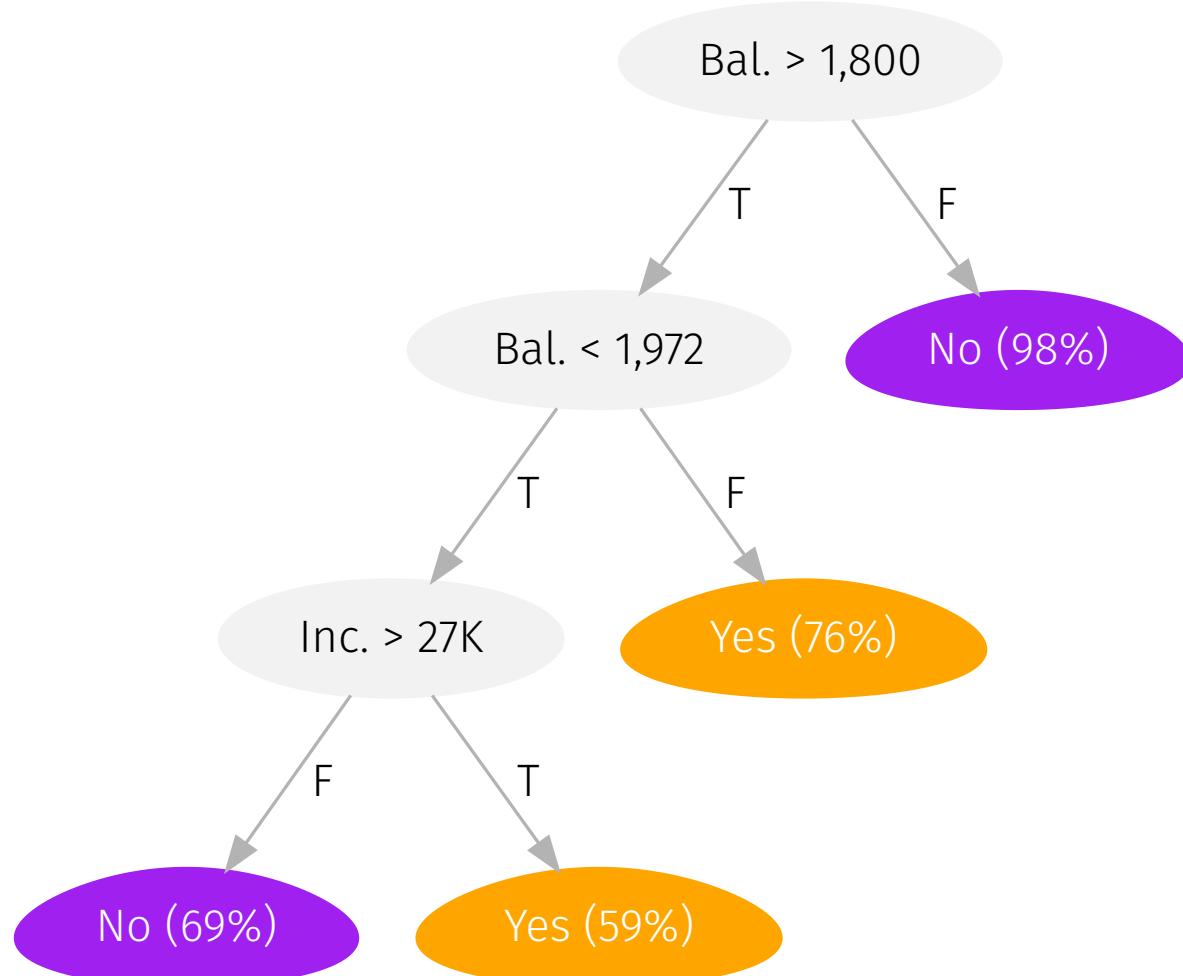
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Decision trees

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) 

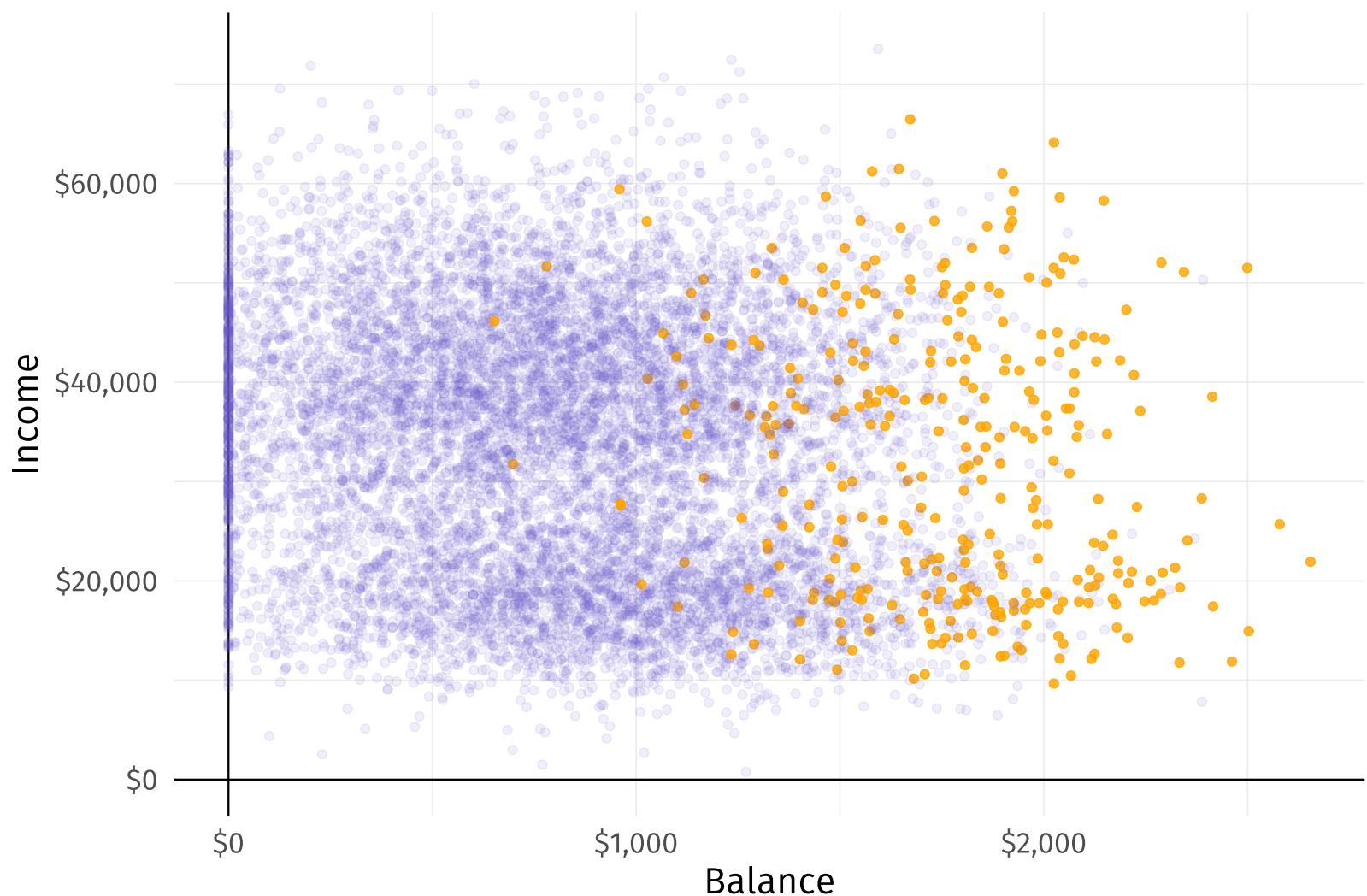
 Though the ensembles will be much less interpretable.

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

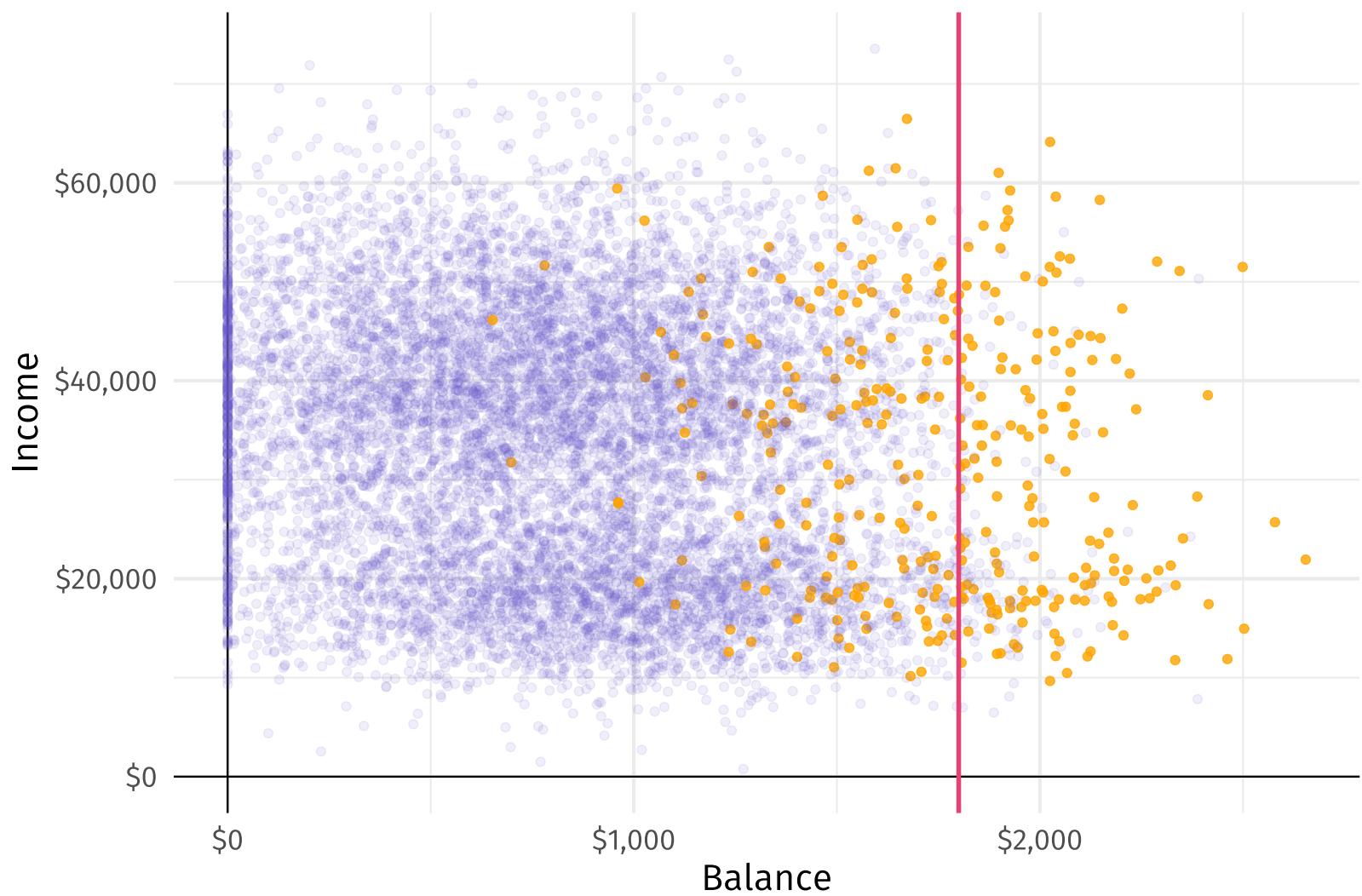


Let's see how the tree works

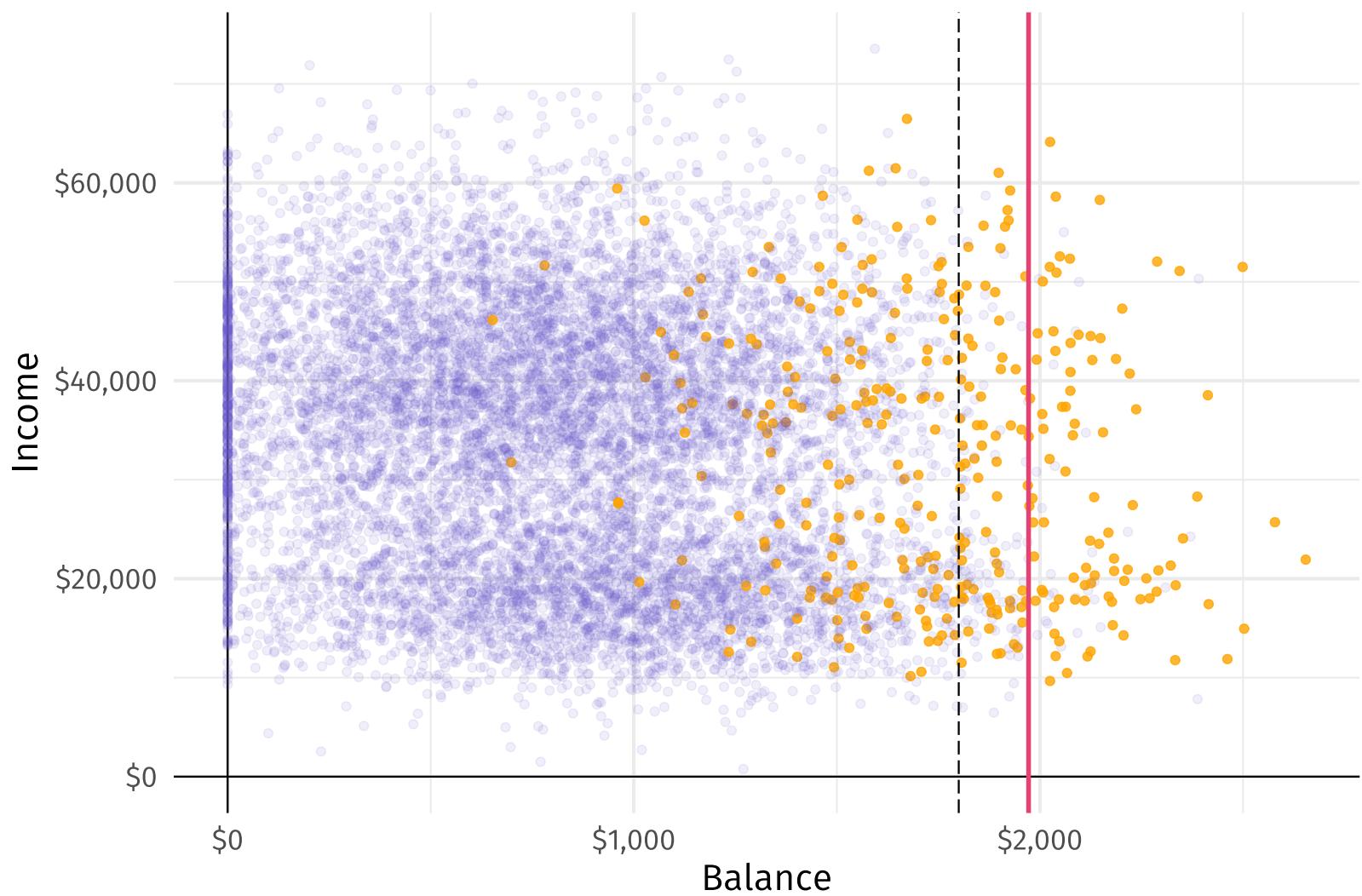
Let's see how the tree works—starting with our data (default: Yes vs. No).



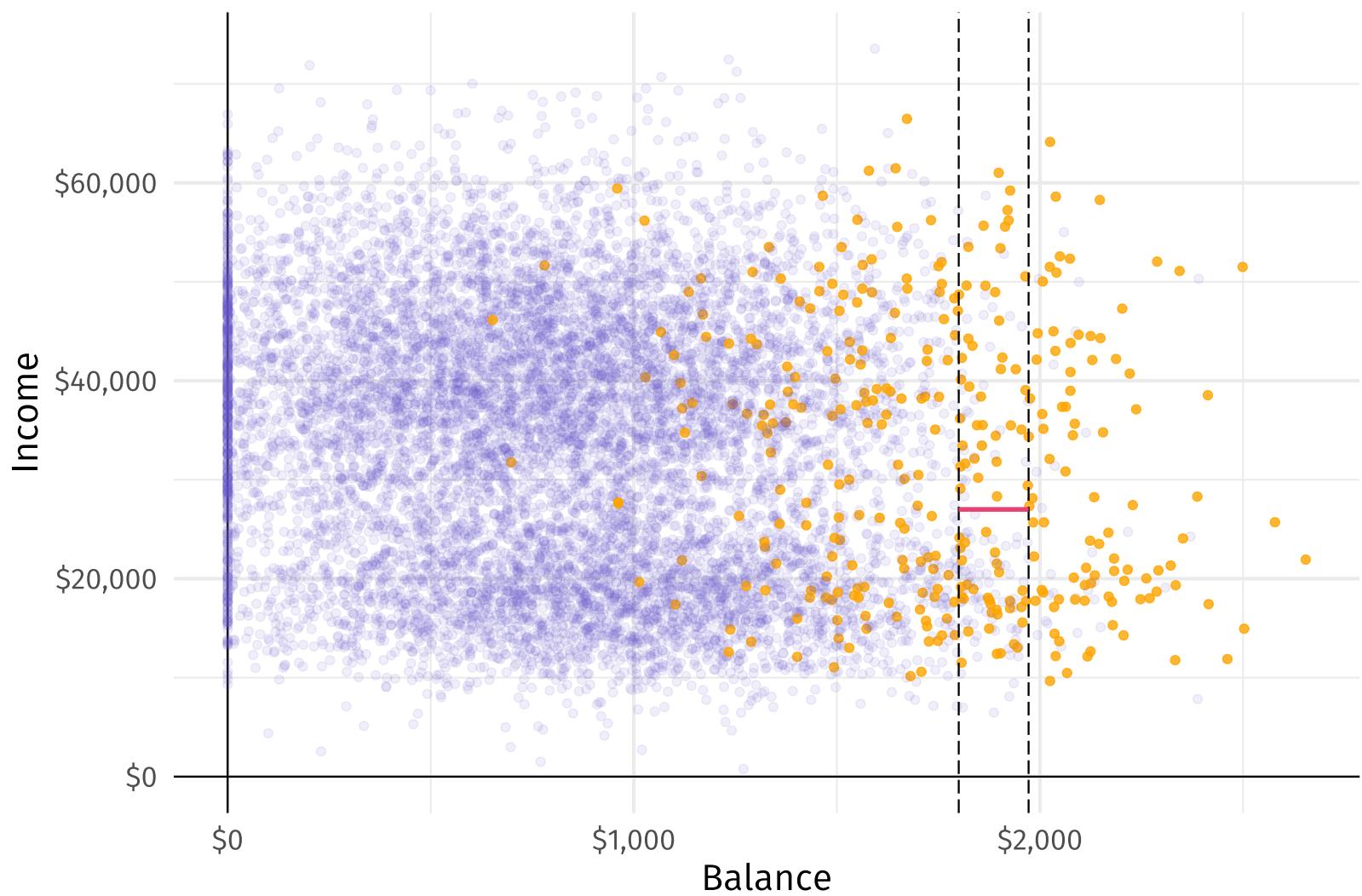
The **first partition** splits balance at \$1,800.



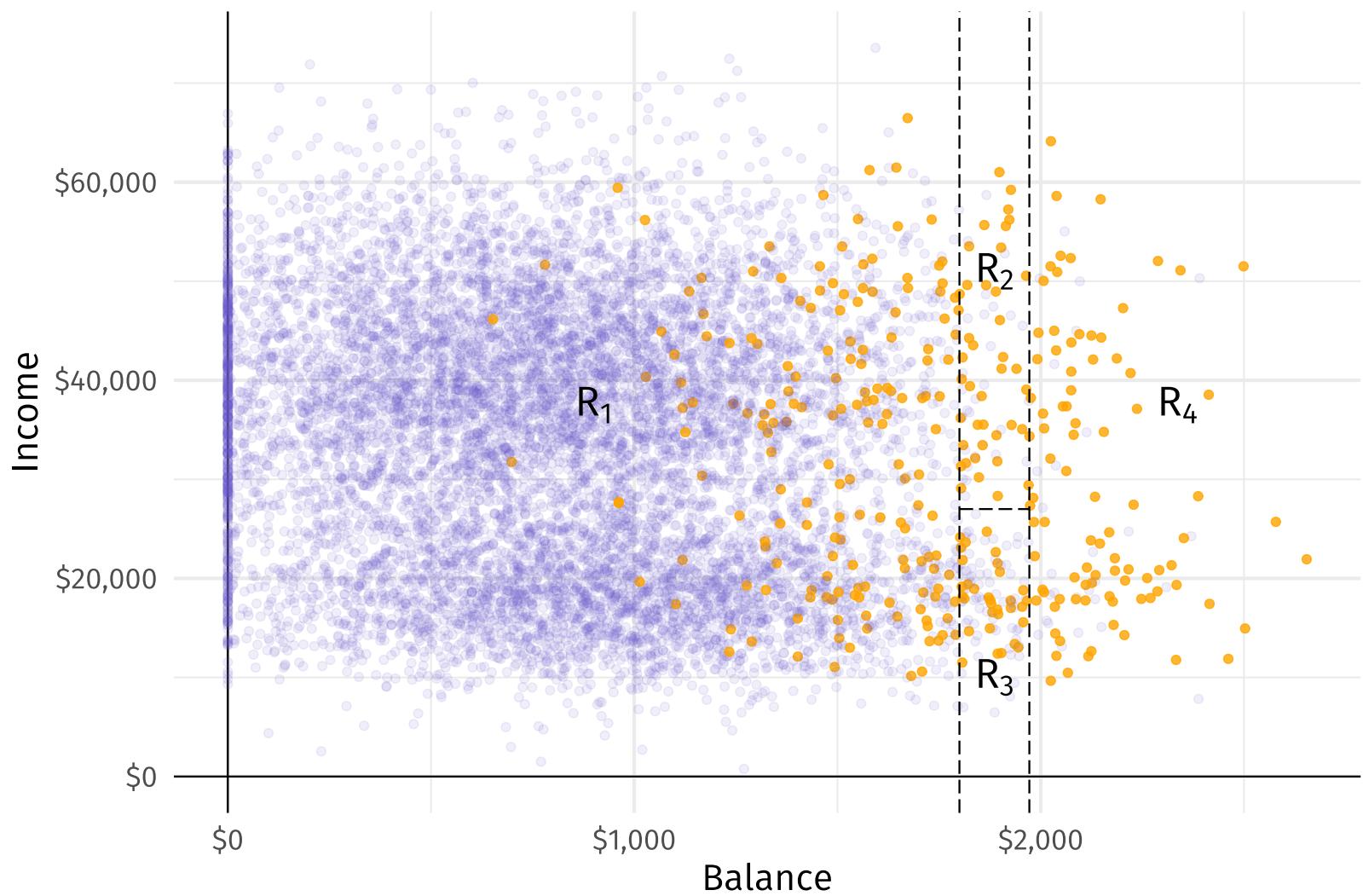
The **second partition** splits balance at \$1,972, (conditional on bal. > \$1,800).



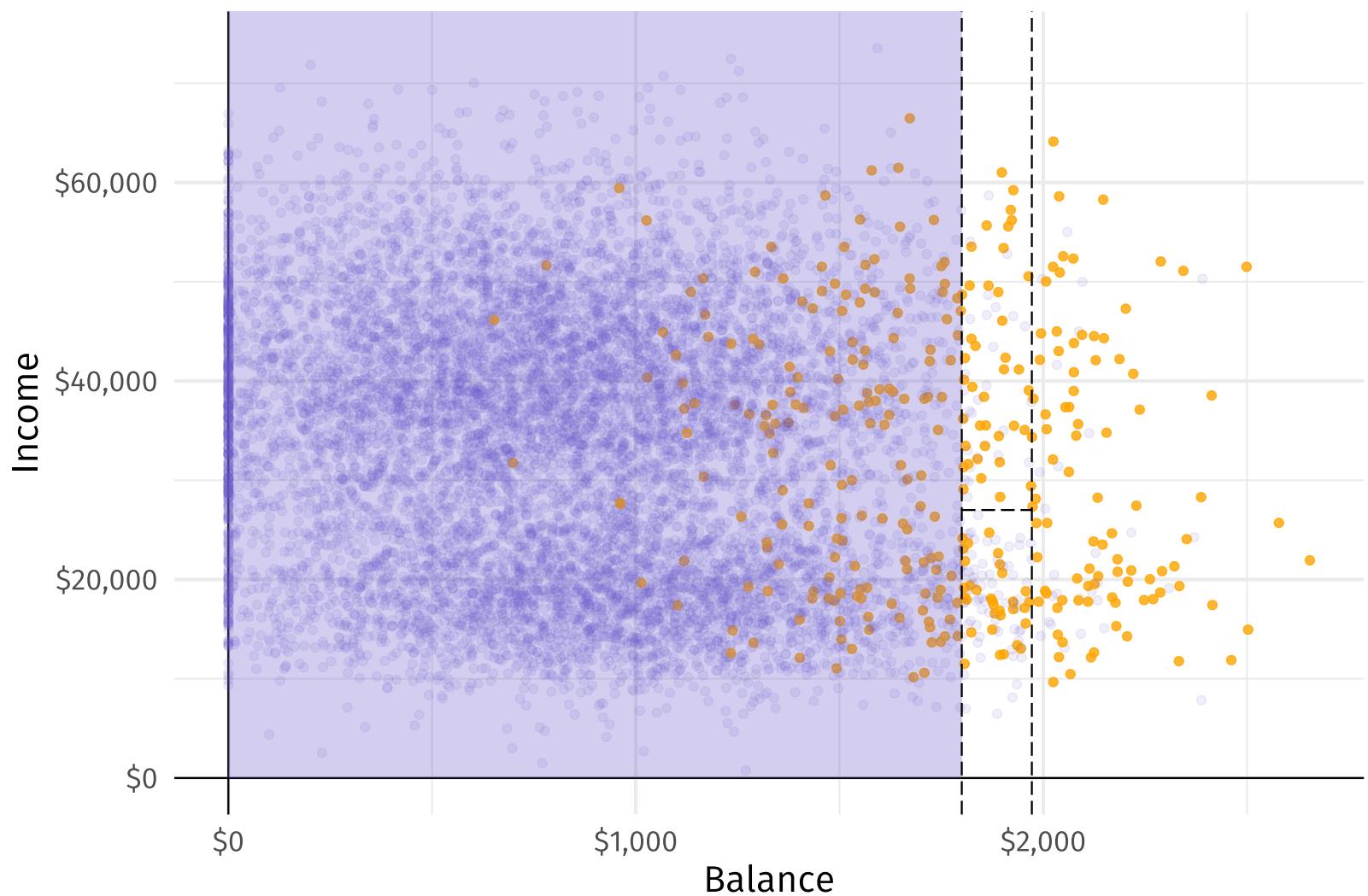
The **third partition** splits income at \$27K **for** bal. between \$1,800 and \$1,972.



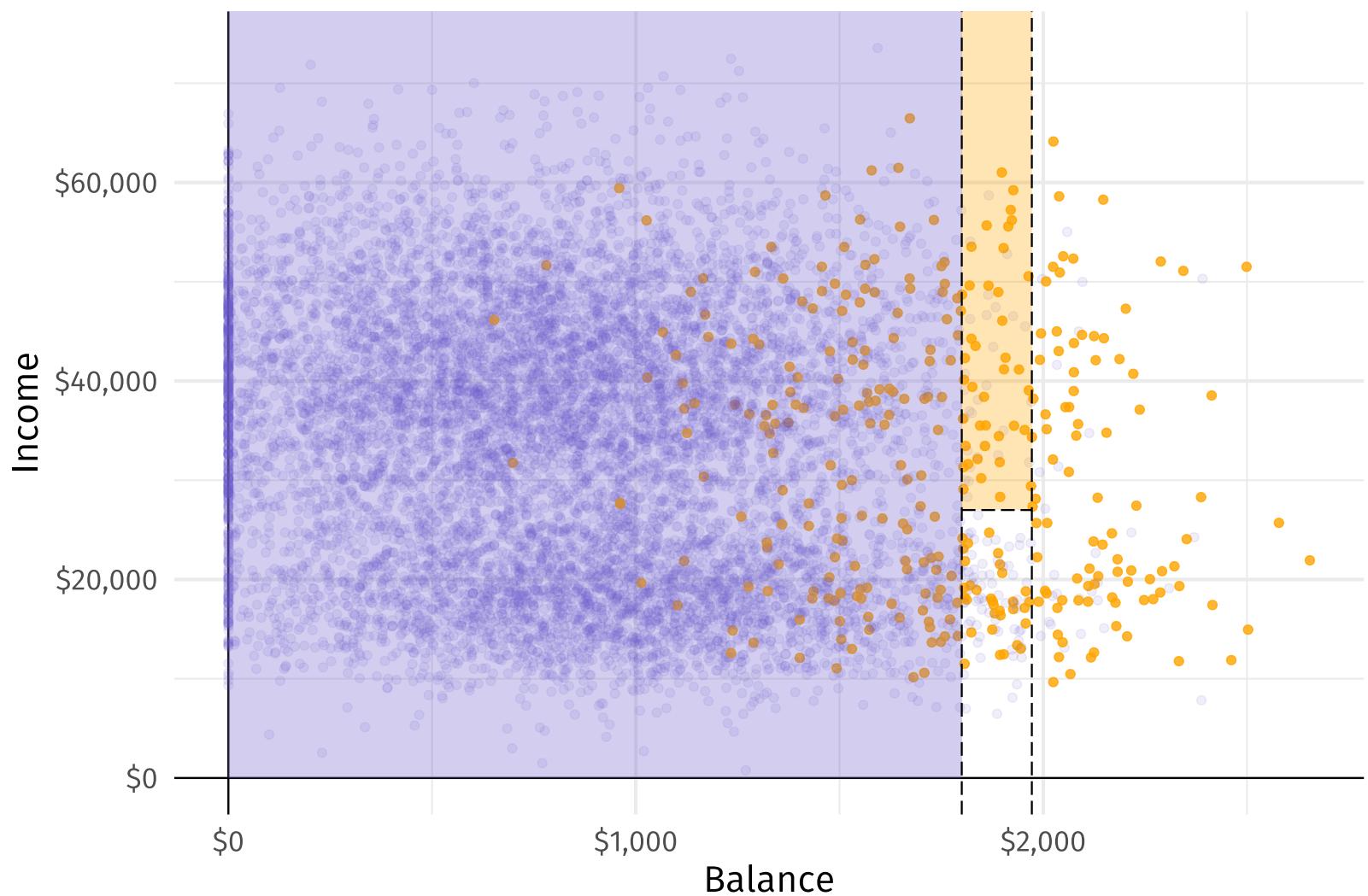
These three partitions give us four **regions**...



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



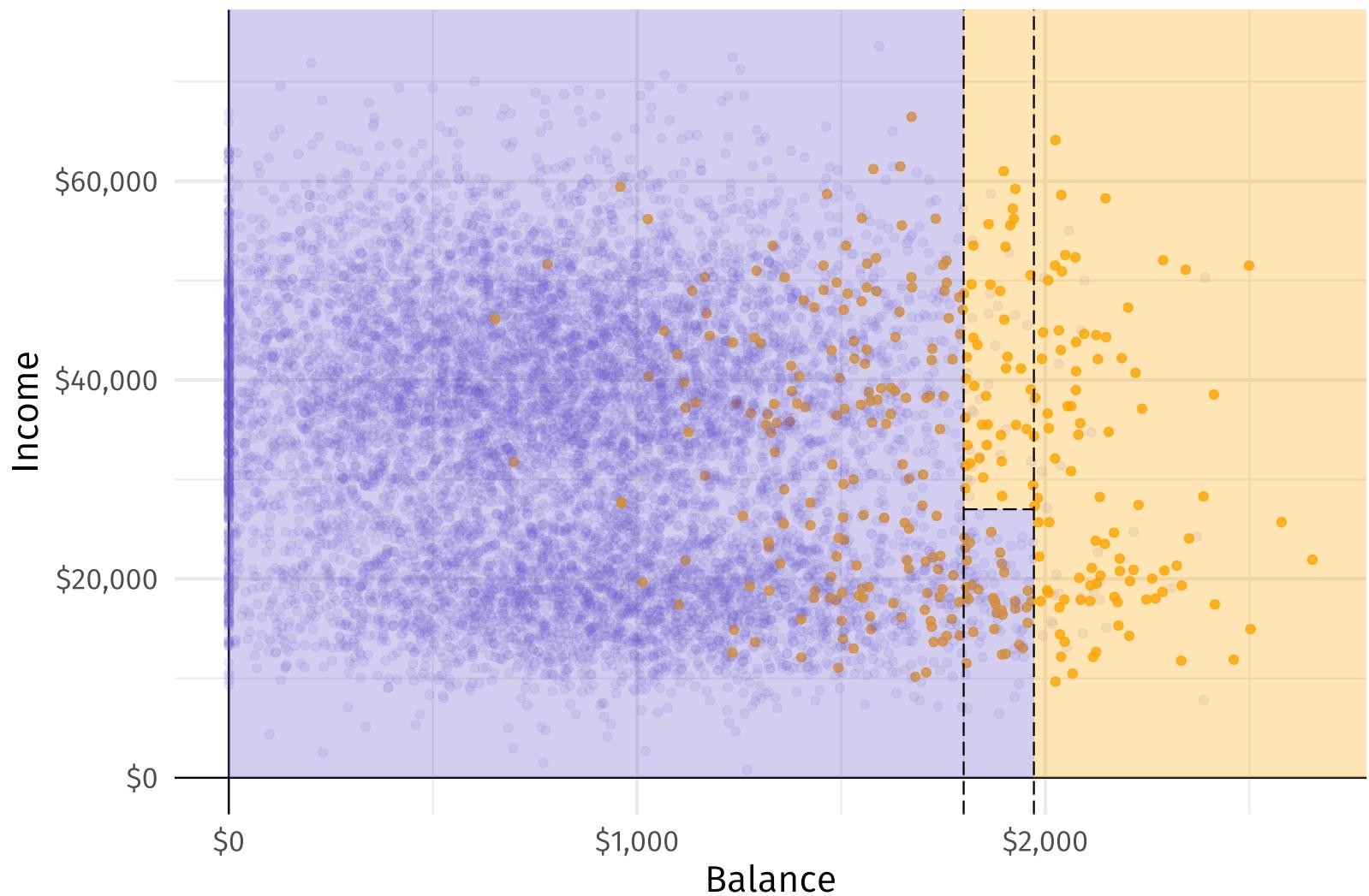
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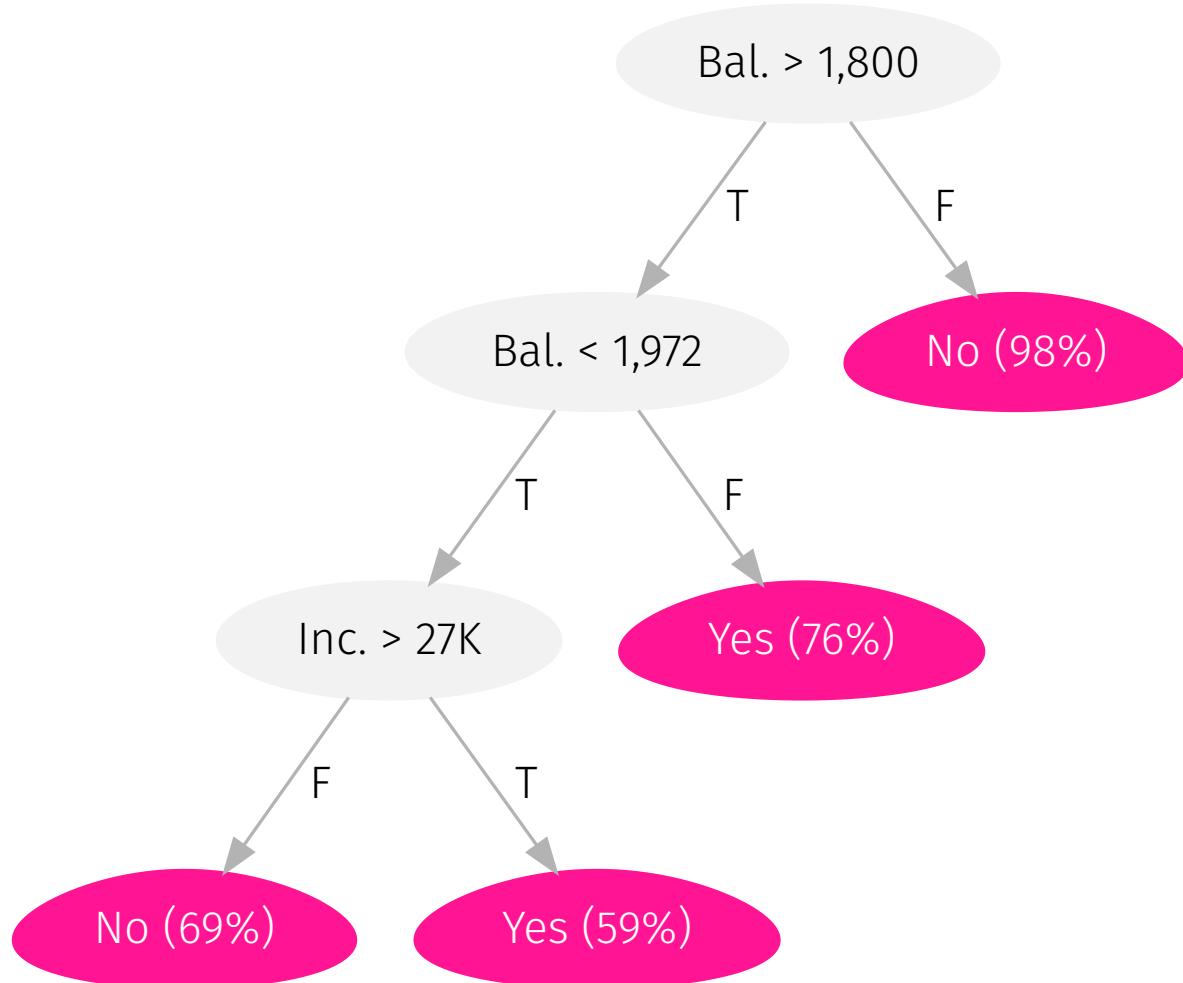
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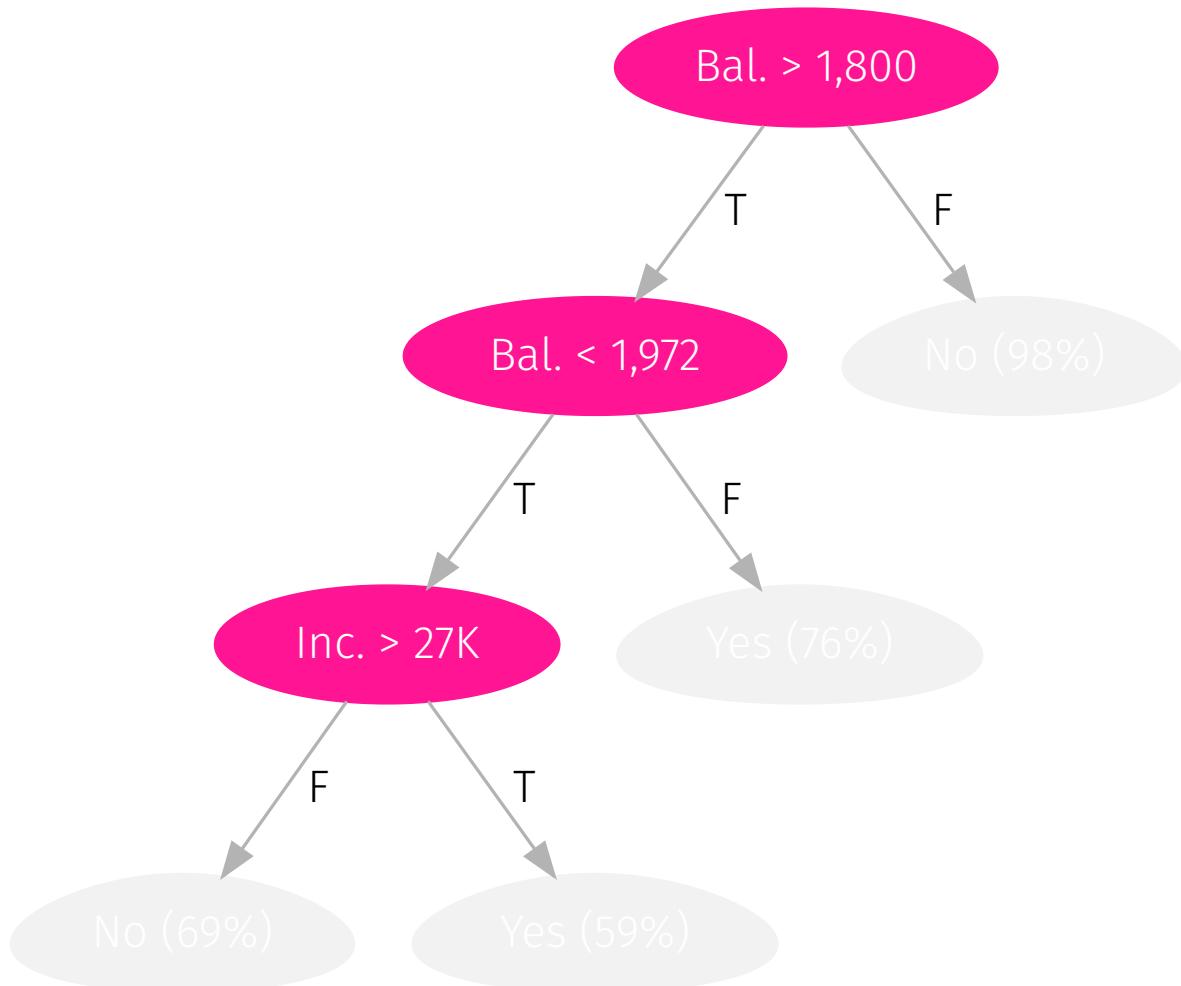
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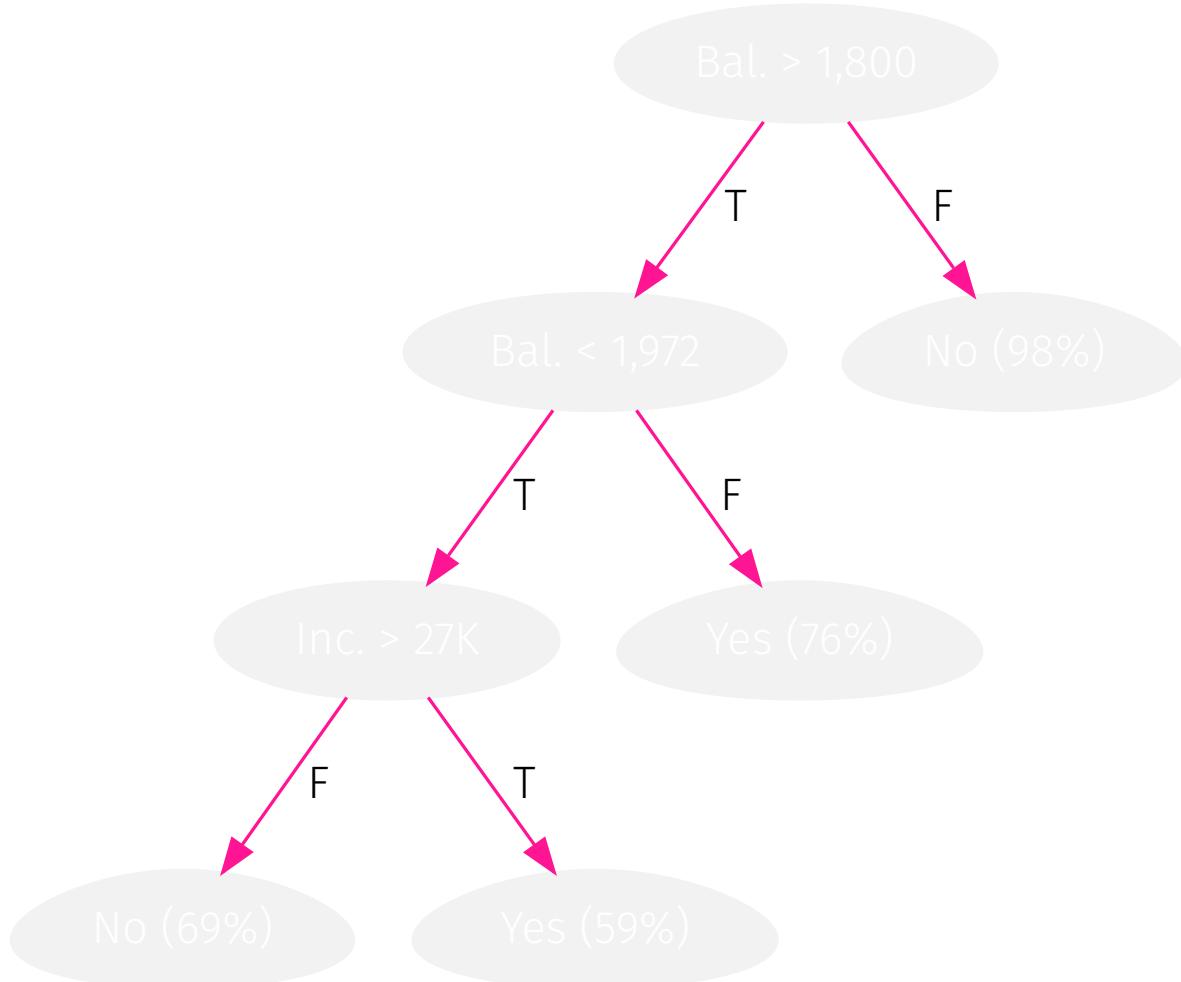
The **regions** correspond to the tree's **terminal nodes** (or **leaves**).



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?

 grow

Decision trees

Growing trees

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

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

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

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.,

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

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Problem: Examining every possible partition is computationally infeasible.

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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) $\mathbf{x}_j \geq s$

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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

Decision trees

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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) $x_1 \geq 2$

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Decision trees

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i	pred.	y	x_1	x_2
1	0	0	1	4
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This split yields an RSS of $0^2 + 1^2 + (-1)^2 = 2$.

Decision trees

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

Decision trees

Example: Splitting

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

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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 . 

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

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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?

Decision trees

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A "More splits" means

1. more flexibility (think about the bias-variance tradeoff/overfitting)
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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.

Decision trees

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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 $T \subset T_0$.

Decision trees

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We choose α via cross validation.

Decision trees

Classification trees

Classification with trees is very similar to regression.

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Regression trees

- **Predict:** Region's mean
- **Split:** Minimize RSS
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Decision trees

Classification trees

Classification with trees is very similar to regression.

Regression trees

- **Predict:** Region's mean
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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 .

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.

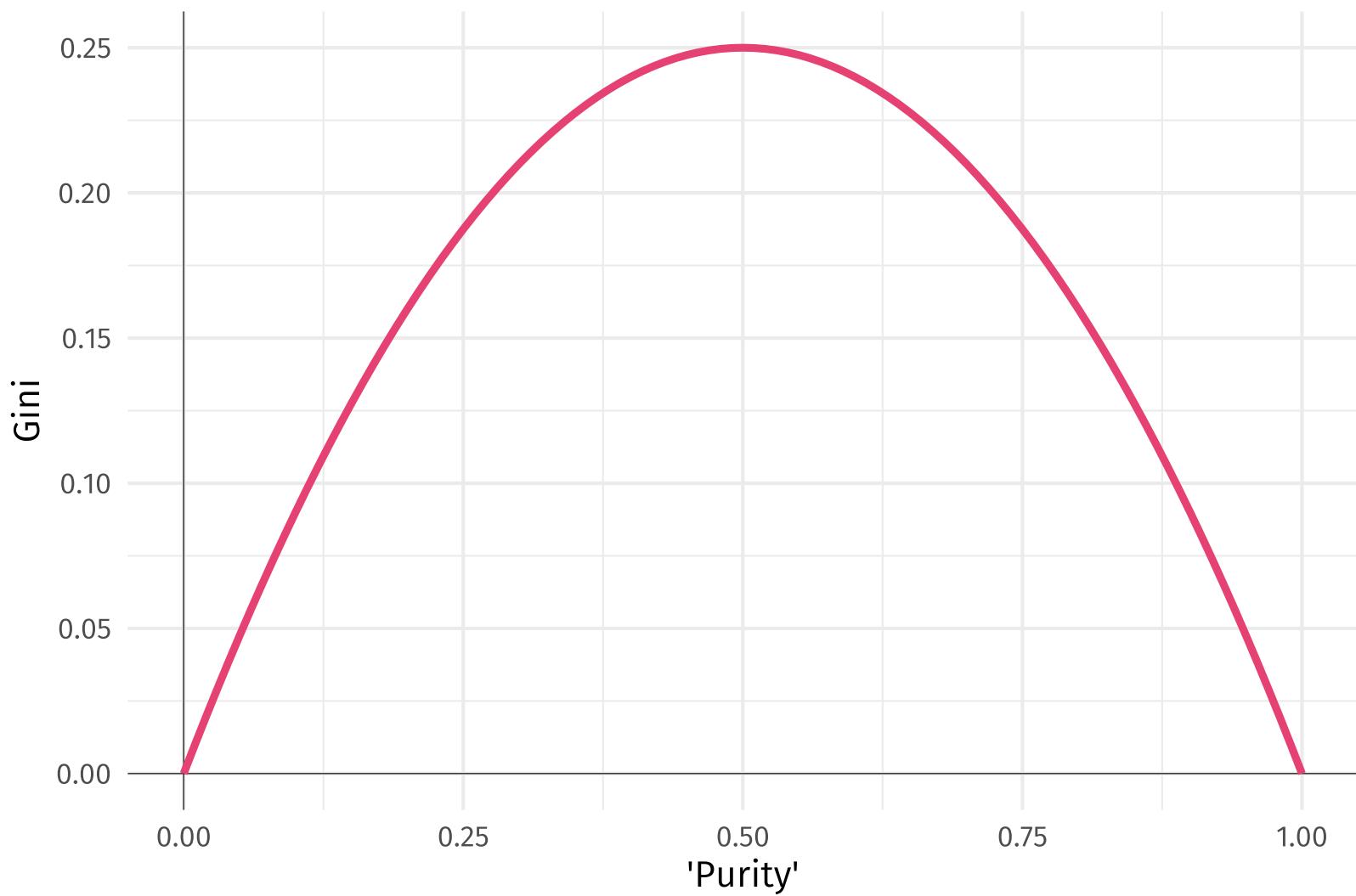
Reducing the Gini index yields to more homogeneous regions

.
∴ We want to minimize the Gini index.



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

Gini as a function of 'purity'



Decision trees

Entropy

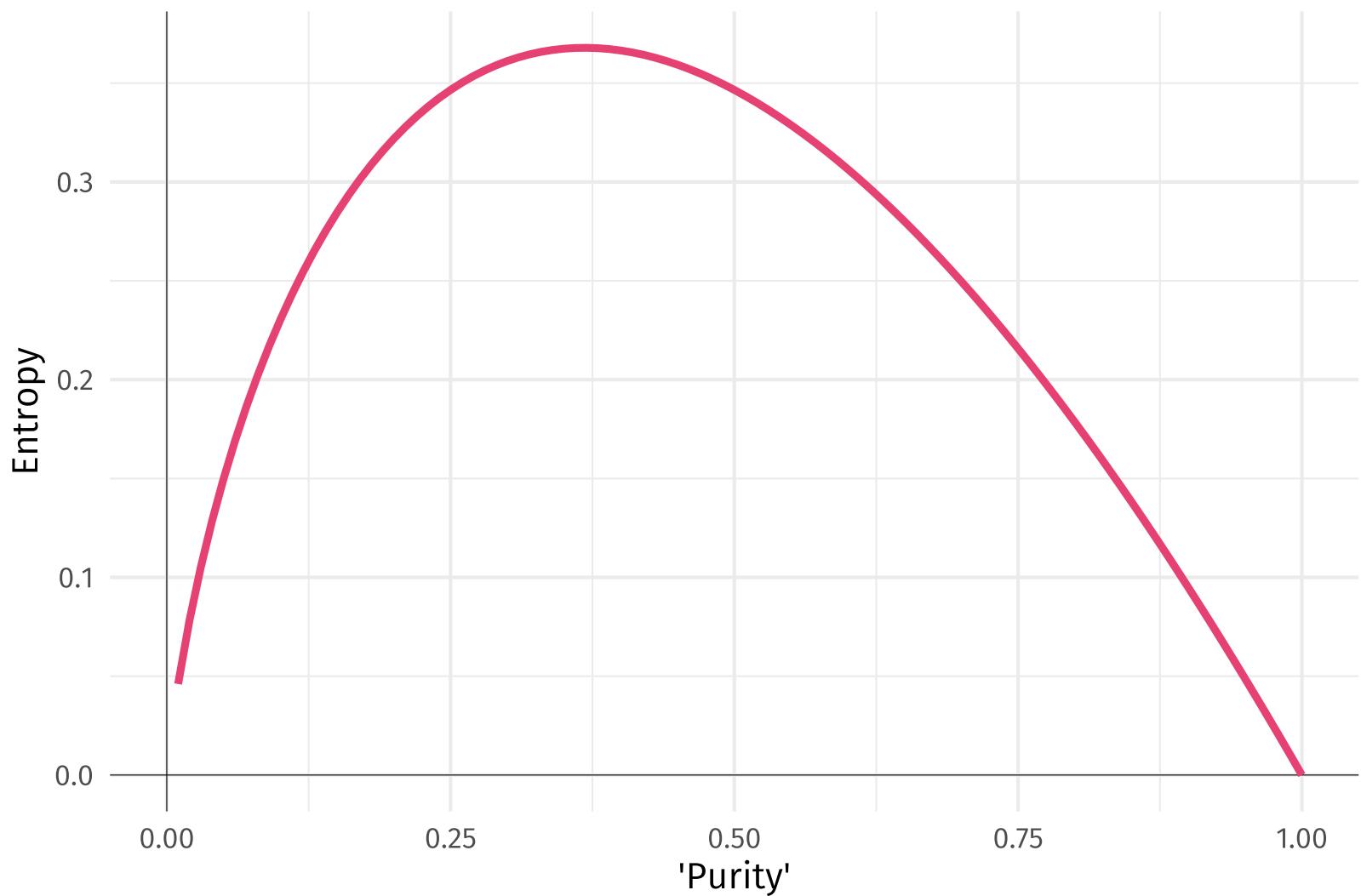
Let \hat{p}_{mk} denote the proportion of observations in class k and region m .

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.

Entropy as a function of 'purity'



Decision trees

Rational

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

Decision trees

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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.

Decision trees

Rational

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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.

Decision trees

In R

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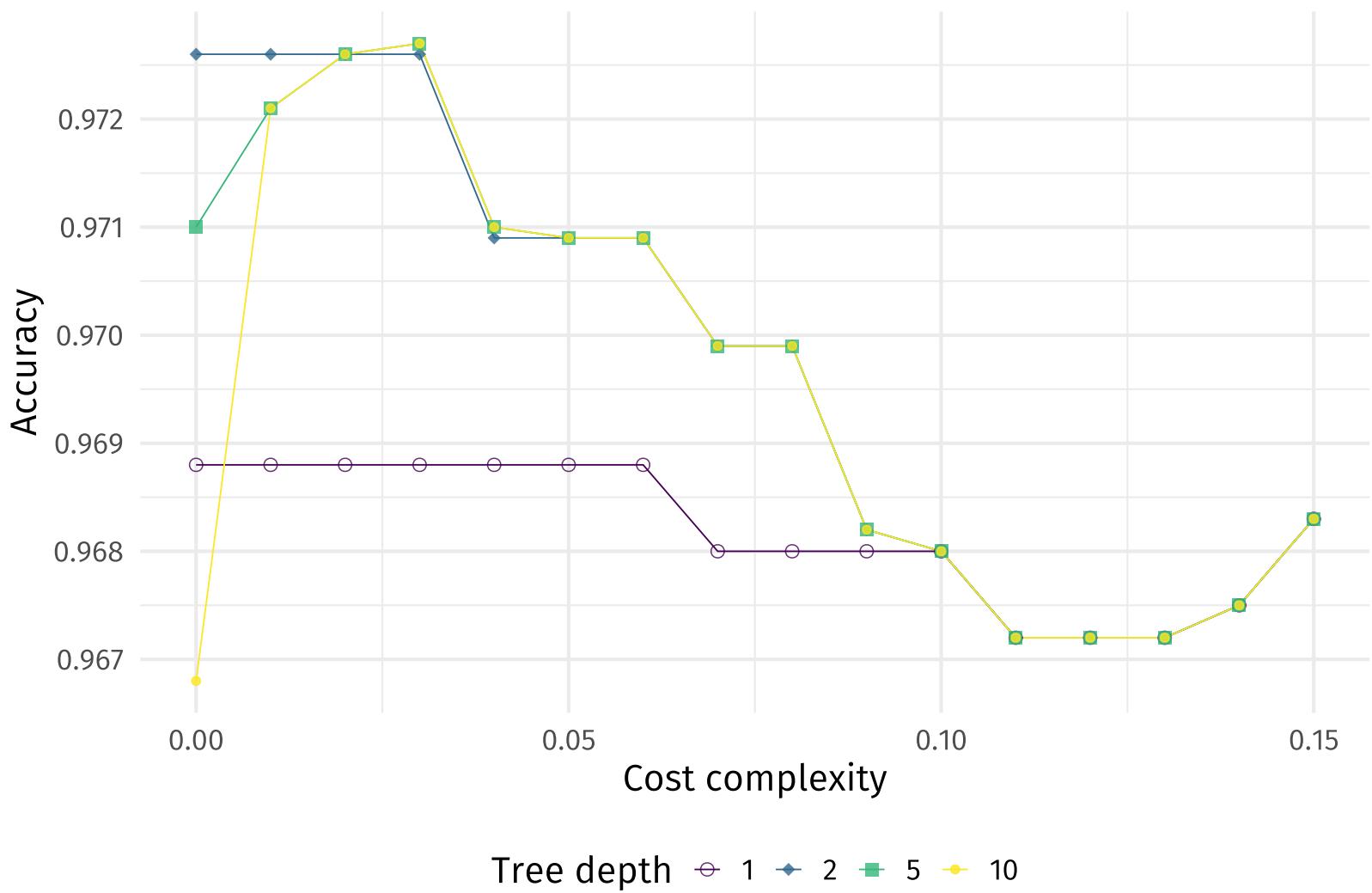
In `parsnip`, we use the aptly named `decision_tree()` function.

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)
```

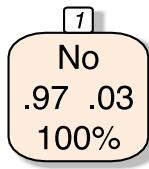
2. **Extract** the fitted model, e.g., with `extract_fit_parsnip`.

Old/deprecated way: `pull_workflow_fit()`

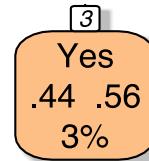
```
best_tree = best_flow %>% extract_fit_parsnip()
```

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

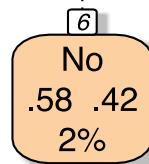
```
best_tree$fit %>% rpart.plot()
```



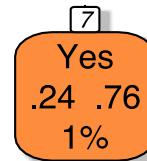
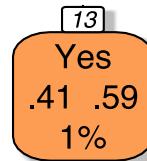
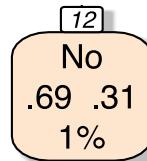
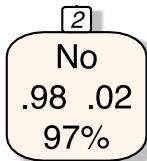
yes · **balance < 1800** · no



balance < 1972



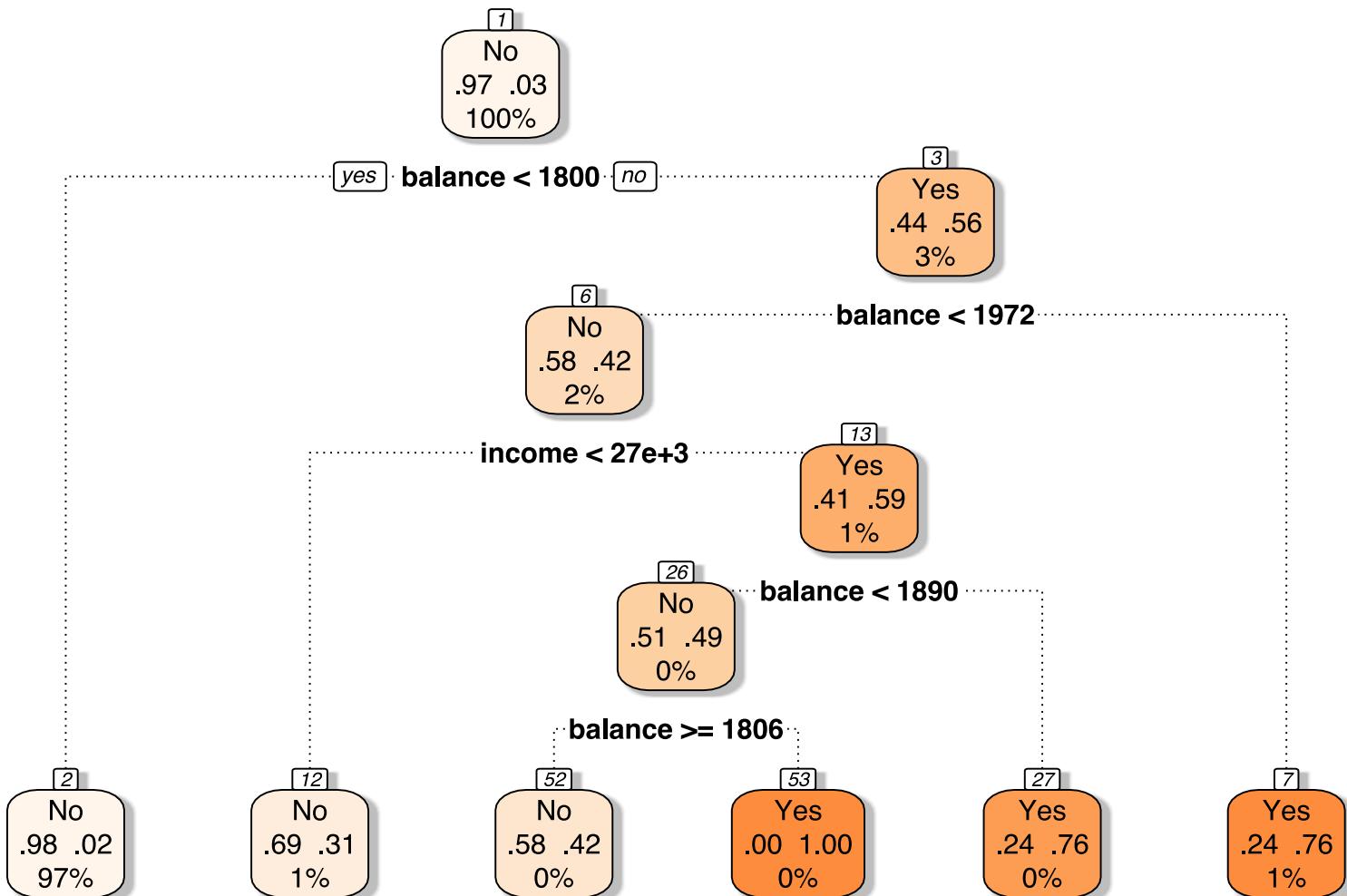
income < 27e+3



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

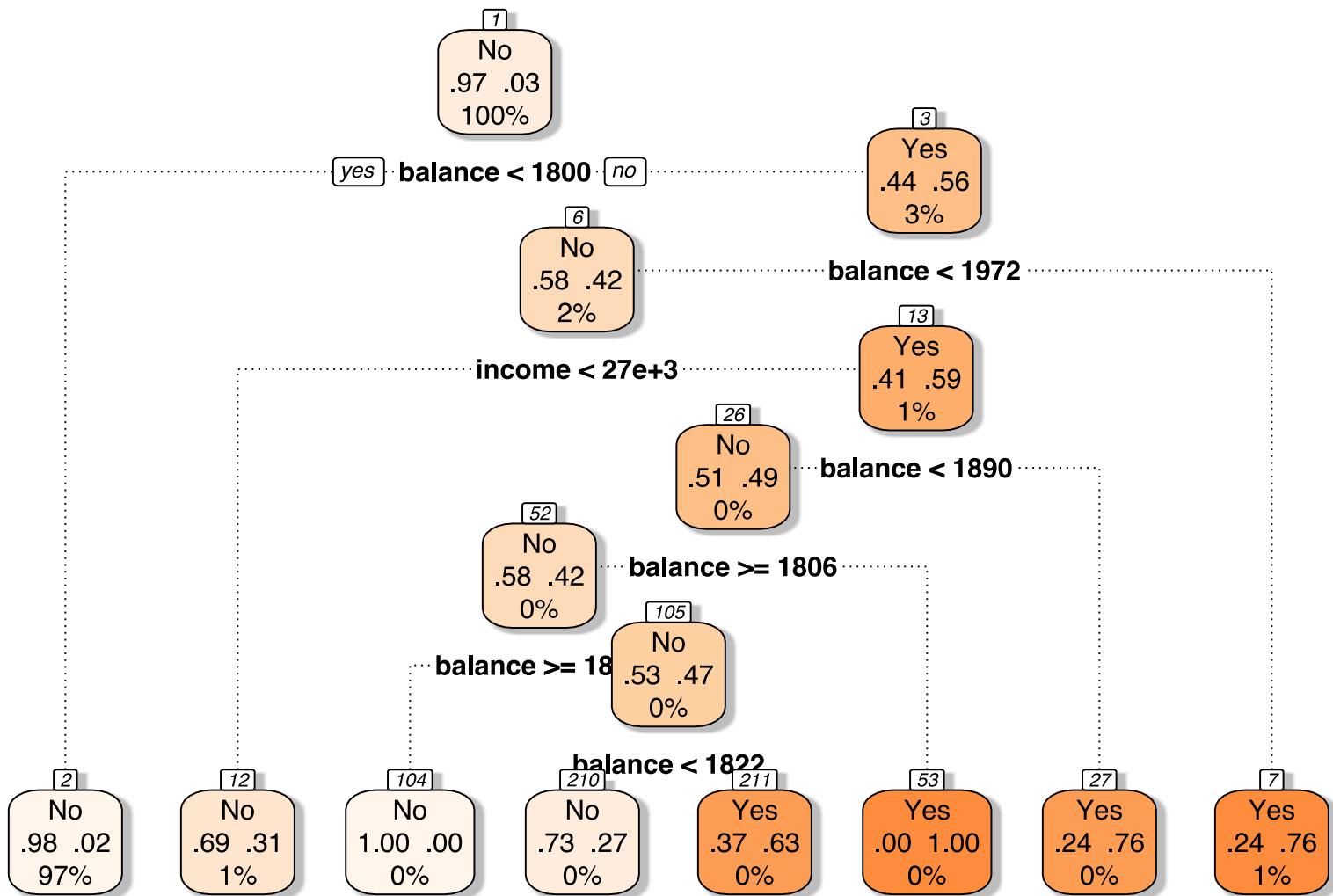
We can compare this "best" tree to a less pruned/penalized tree

- `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%

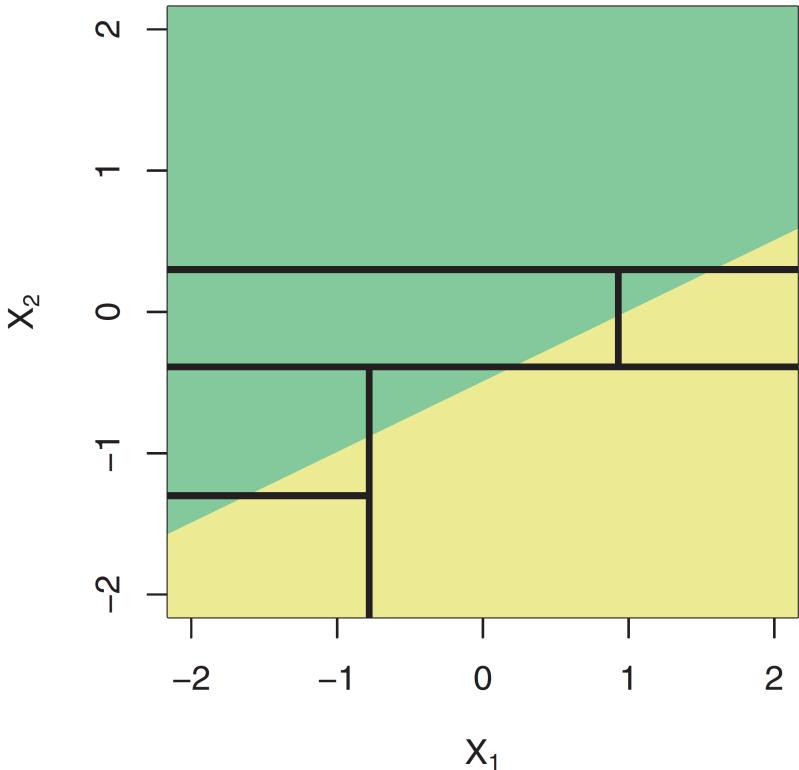
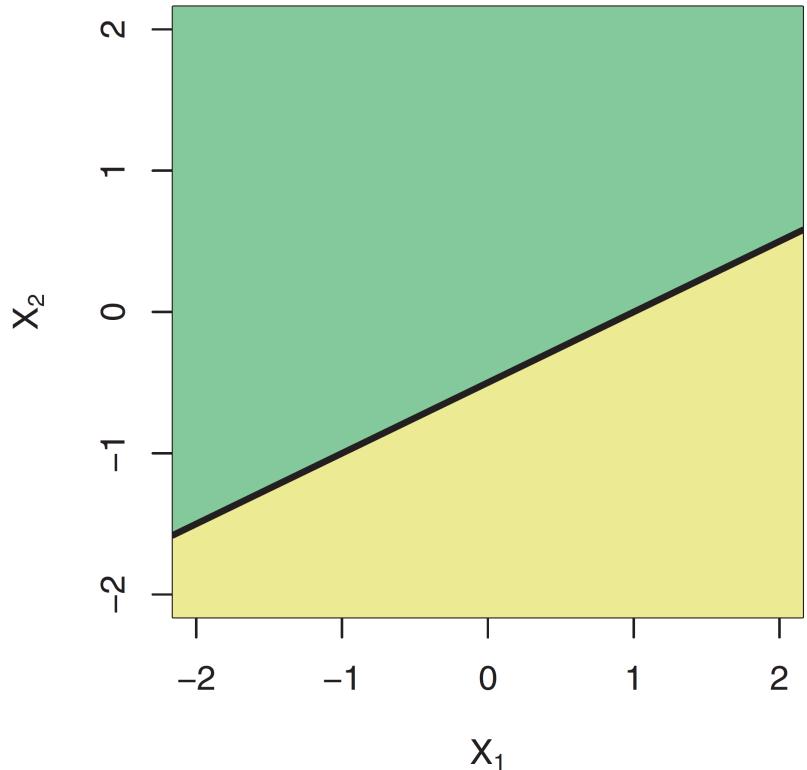
3
Yes
.44 .56
3%

Q How do trees compare to linear models?

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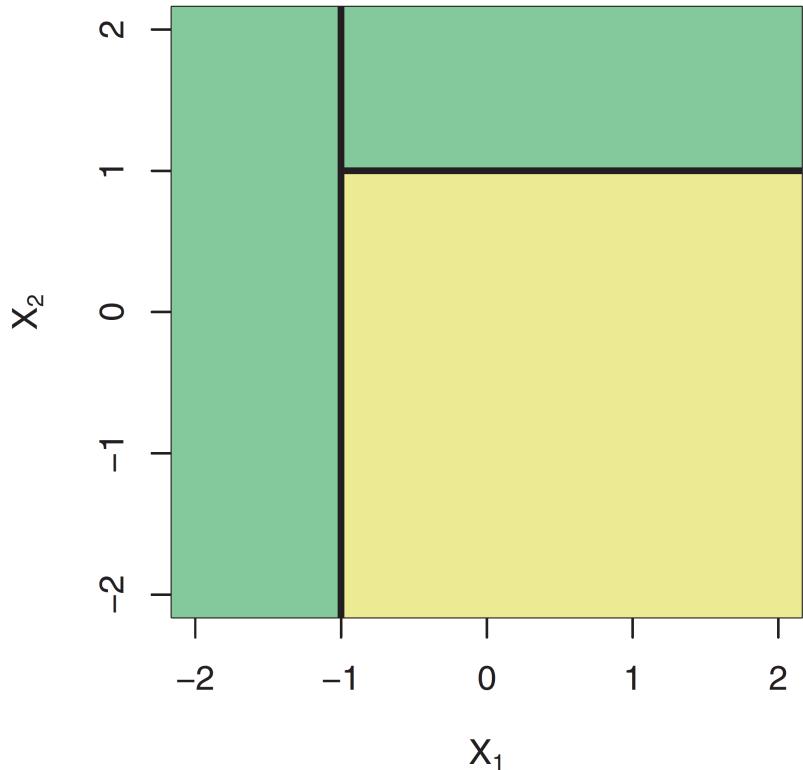
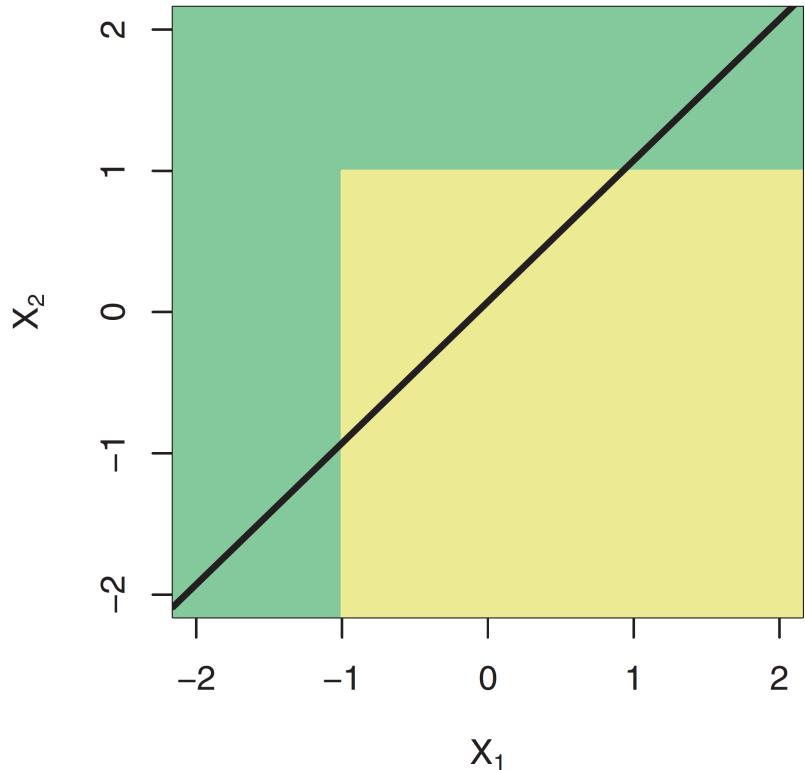
A It depends how linear the true boundary is.

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 

-  Without needing to create lots of dummy variables!

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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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