

(Some of) Machine Learning

EC 421, Set 12

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Prologue

Schedule

Last time

Resampling methods

Today

A one-lecture introduction to machine-learning methods

Upcoming

The end is near—as are the last problem set and the final.

Prediction: What's the goal?

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Up to this point, we've focused on causal **identification/inference** of β , *i.e.*,

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meaning we want an unbiased (consistent) and precise estimate $\hat{\beta}$.

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meaning we want an unbiased (consistent) and precise estimate $\hat{\beta}$.

With **prediction**, we shift our focus to accurately estimating outcomes.

In other words, how can we best construct $\hat{\mathbf{Y}}_i$?

Prediction: What's the goal?

... so?

So we want "nice"-performing estimates \hat{y} instead of $\hat{\beta}$.

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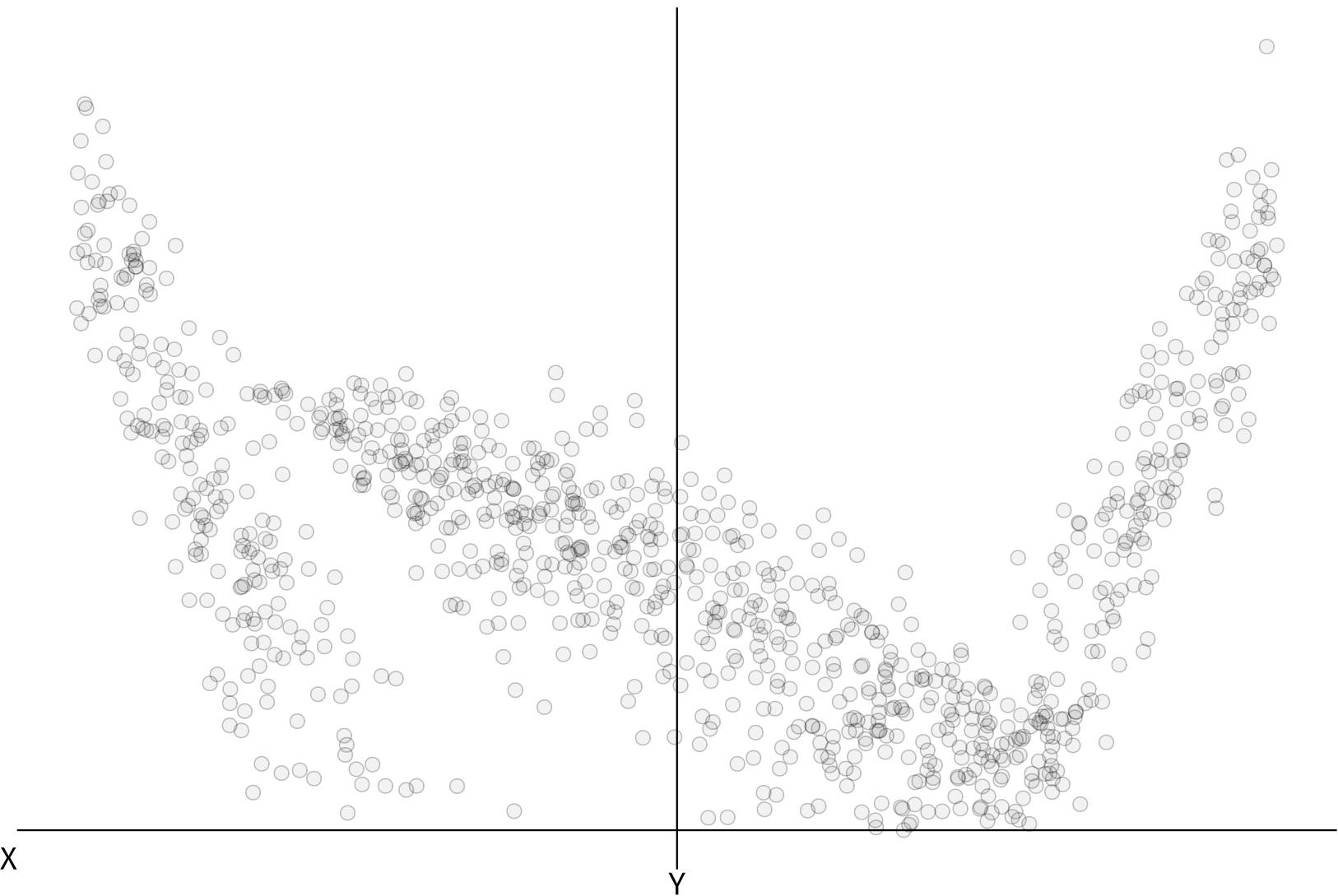
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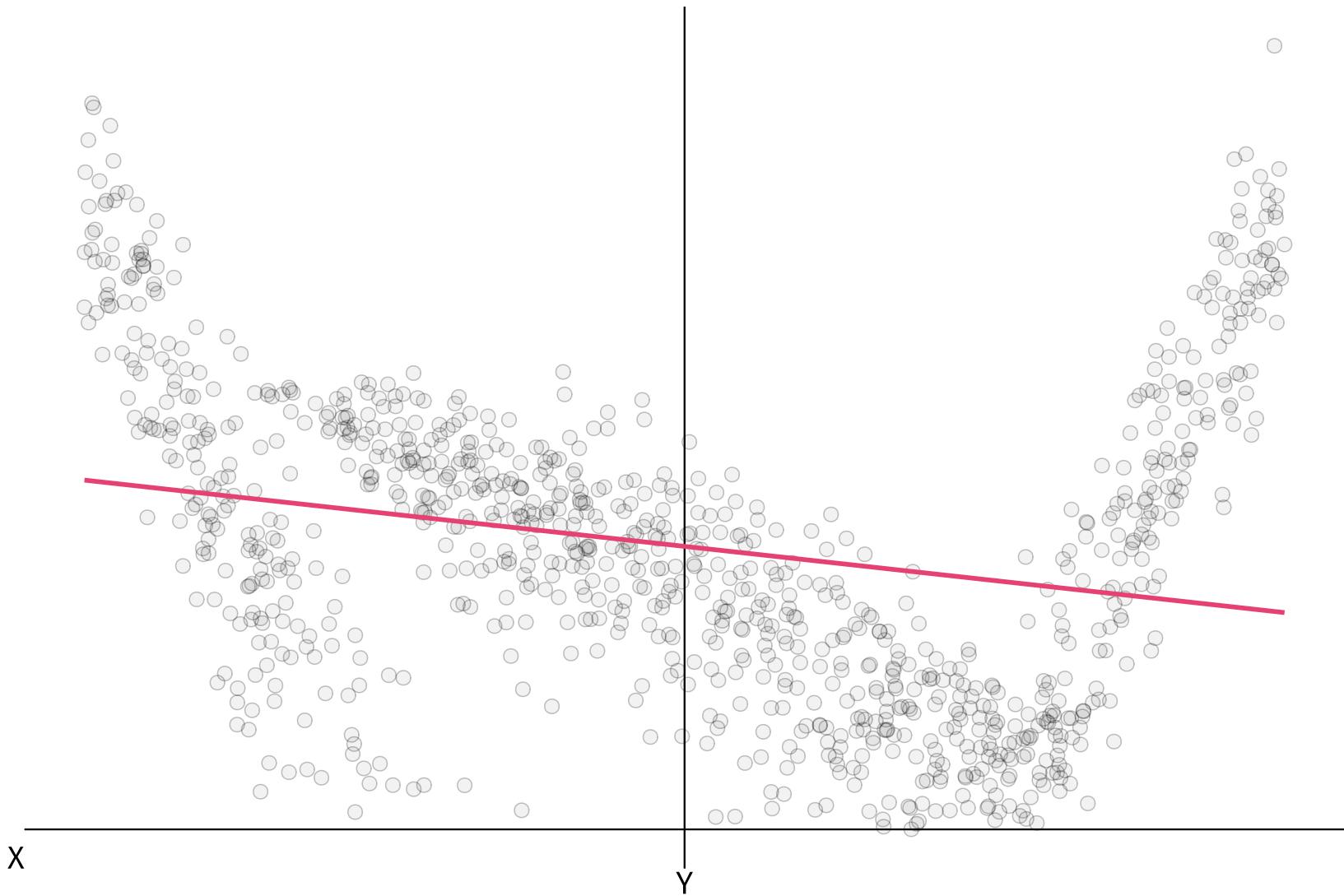
Recall Least-squares regression is a great **linear** estimator and predictor.

Data data be tricky[†]—as can understanding many relationships.

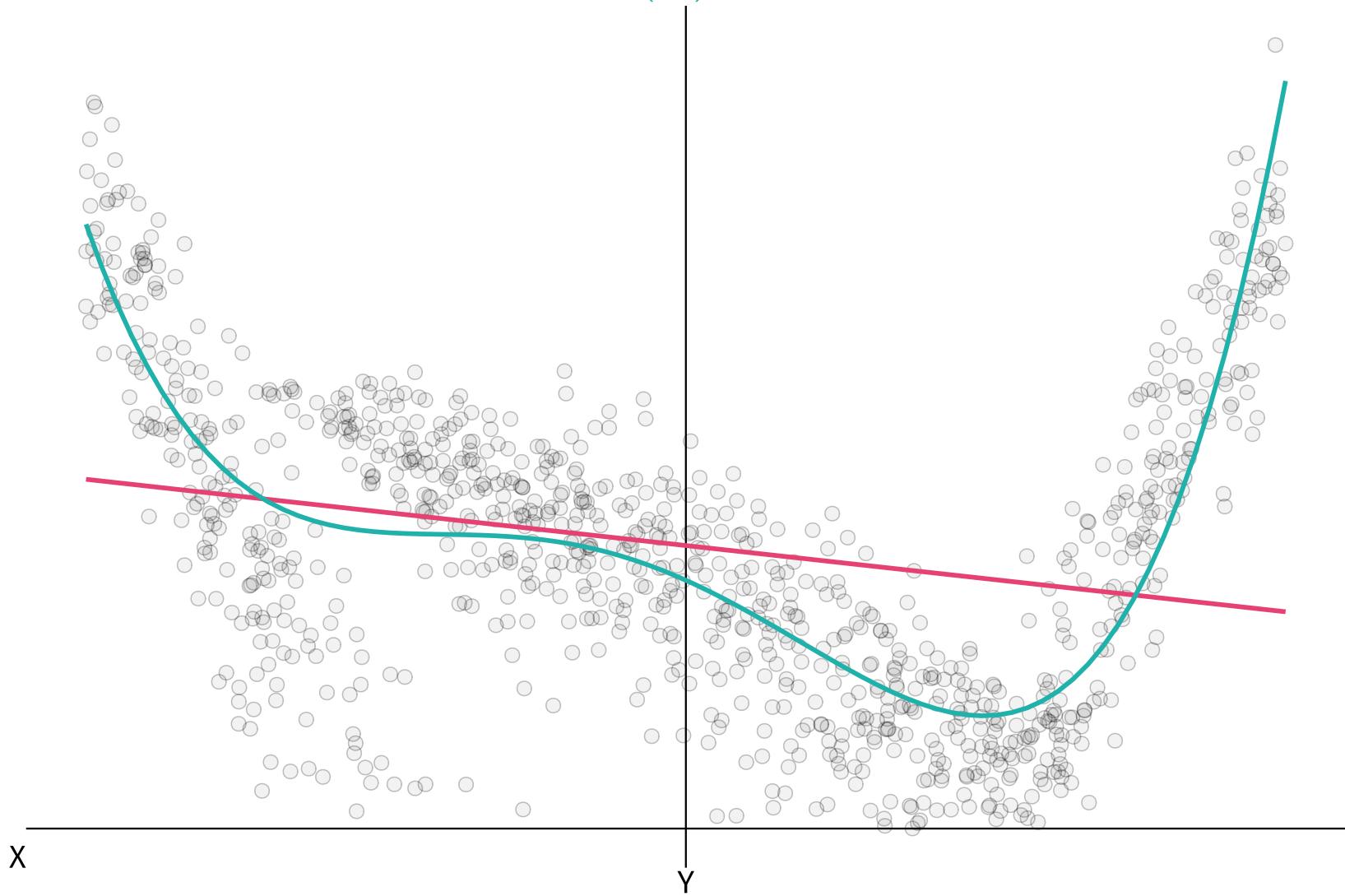
[†] "Tricky" might mean nonlinear... or many other things...



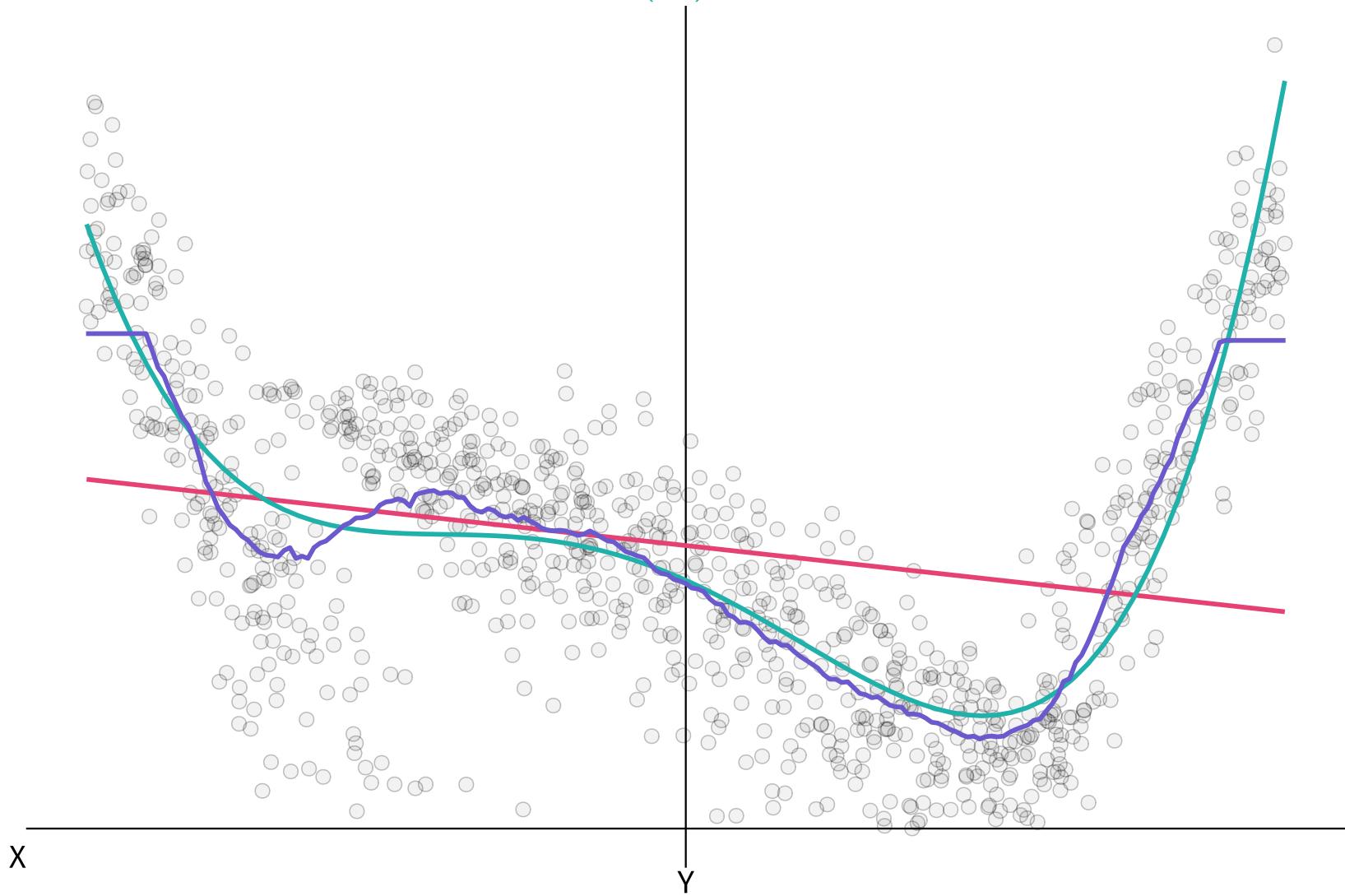
Linear regression



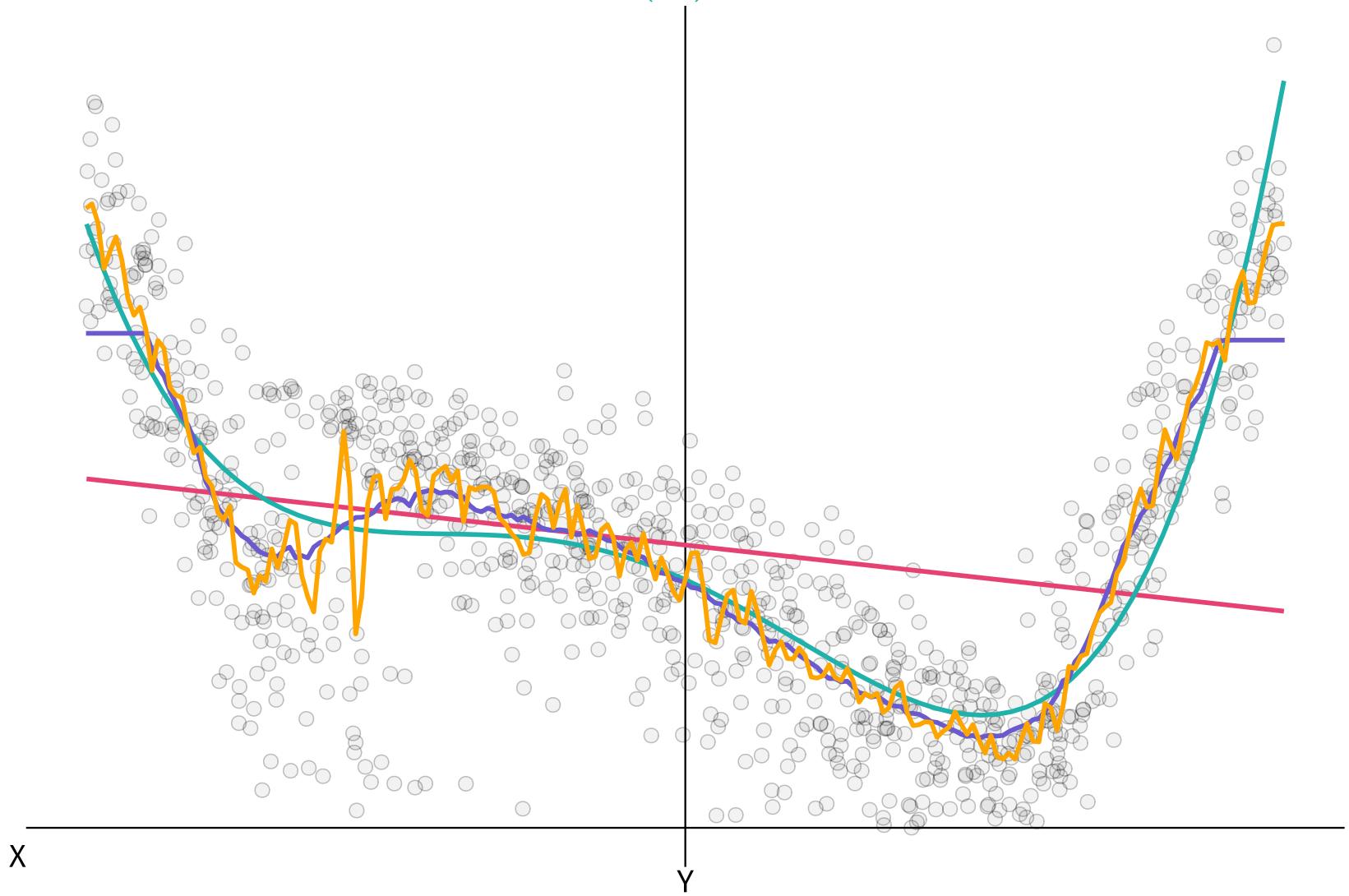
Linear regression, linear regression (x^4)



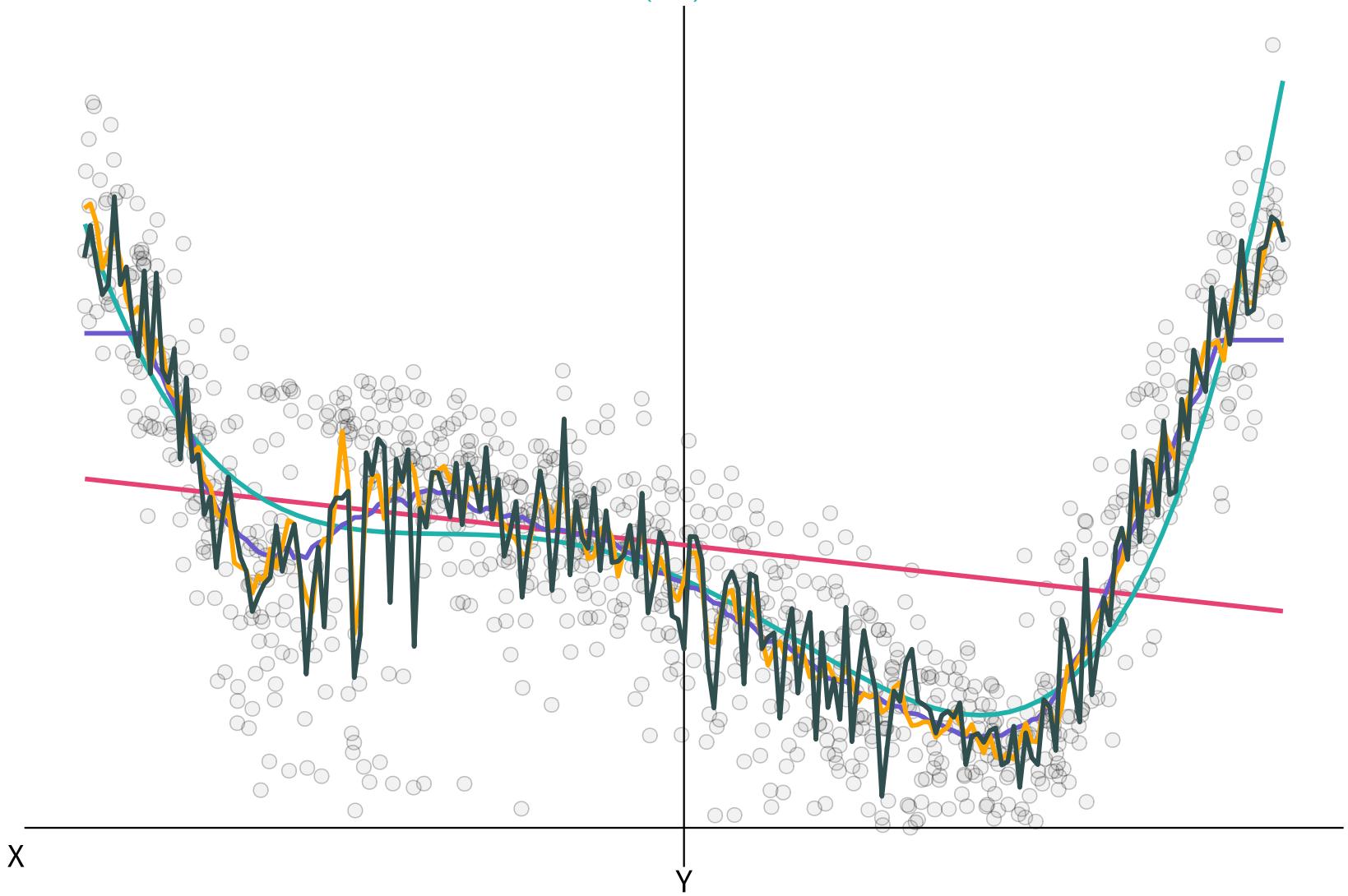
Linear regression, linear regression (x^4), KNN (100)



Linear regression, linear regression (x^4), KNN (100), KNN (10)



Linear regression, linear regression (x^4), KNN (100), KNN (10), random forest



Note That example only had one predictor...

What's the goal?

Tradeoffs

In prediction, we constantly face many tradeoffs, *e.g.*,

- **flexibility** and **parametric structure** (and interpretability)
- performance in **training** and **test** samples
- **variance** and **bias**

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Many machine-learning (ML) techniques/algorithms are crafted to optimize with these tradeoffs, but the practitioner (you) still needs to be careful.

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Multi-class classification problems

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Text analysis and **image recognition**

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Unsupervised learning

- You don't know groupings, but you think there are relevant groups
- *E.g.*, classify spatial data into groups



Stanford University (Stanford, CA) researchers have developed a deep-learning algorithm that can evaluate chest X-ray images for signs of disease at a level exceeding practicing radiologists.



Parking Lot Vehicle Detection Using Deep Learning

THE
NEW YORKER

A REPORTER AT LARGE OCTOBER 14, 2019 ISSUE

The Next Word |

Where will predictive text take us?

Text by John Seabrook



Gender Classifier	Darker Male	Darker Female	Lighter Male	Lighter Female	Largest Gap
Microsoft	94.0%	79.2%	100%	98.3%	20.8%
FACE++	99.3%	65.5%	99.2%	94.0%	33.8%
IBM	88.0%	65.3%	99.7%	92.9%	34.4%



Flexibility is huge, but we still want to avoid overfitting.

Statistical learning

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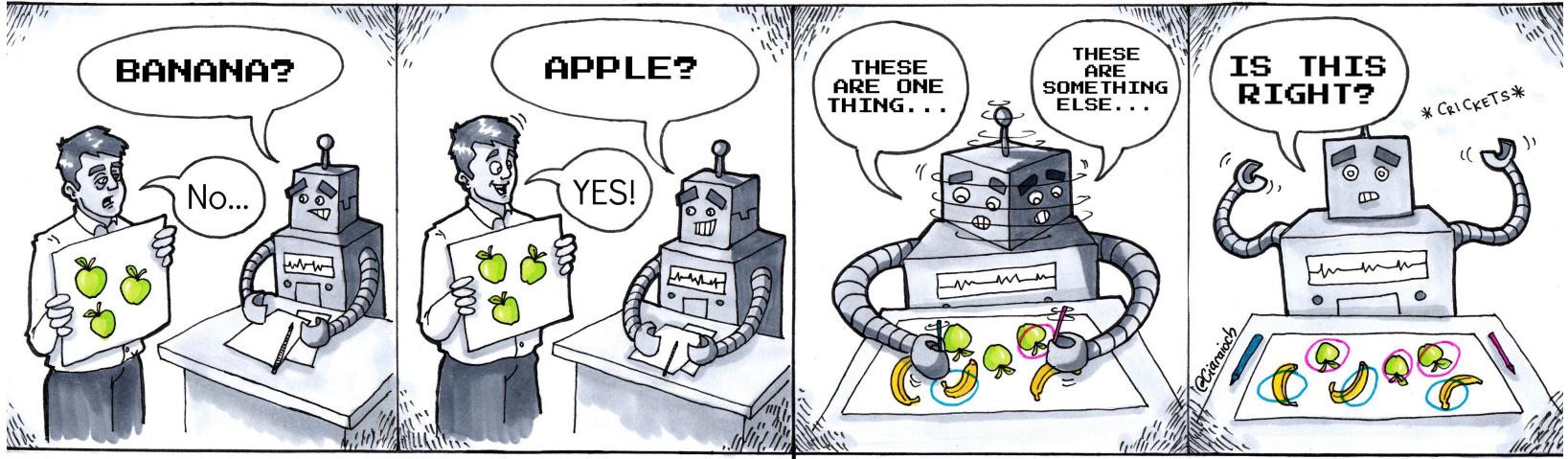
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Semi-supervised learning falls somewhere between these supervised and unsupervised learning—generally applied to supervised tasks when labeled **outputs** are incomplete.



Supervised Learning

Unsupervised Learning

Source

Statistical learning

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Note₂ Don't get tricked: Not all numbers represent continuous, numerical values—e.g., zip codes, industry codes, social security numbers.[†]

[†] **Q** Where would you put responses to 5-item Likert scales?

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As defined before, we want to *learn* a model to understand our data.

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1. Take our (numeric) **output \mathbf{y}** .
2. Imagine there is a **function f** that takes **inputs $\mathbf{X} = \mathbf{x}_1, \dots, \mathbf{x}_p$** and maps them, plus a random, mean-zero **error term ε** , to the **output**.

$$\mathbf{y} = f(\mathbf{X}) + \varepsilon$$

Statistical learning

Learning from \hat{f}

There are two main reasons we want to learn about \hat{f}

1. **Causal inference settings** How do changes in \mathbf{X} affect \mathbf{y} ?

What we've done all quarter.

Statistical learning

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our *black-box setting* where we care less about f than \hat{y} .[†]

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Similarly, in causal-inference settings, we don't particularly care about \hat{y} .

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As tends to be the case in life, you will make errors in predicting $\hat{\mathbf{y}}$.

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Irreducible because we defined an error term ε unexplained by f .

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Note As its name implies, you can't get rid of *irreducible* error—but we can try to get rid of *reducible* errors.

Statistical learning

Prediction errors

Why we're stuck with *irreducible* error

$$\begin{aligned} E[\{\mathbf{y} - \hat{\mathbf{y}}\}^2] &= E\left[\left\{\mathbf{f}(\mathbf{X}) + \varepsilon + \hat{\mathbf{f}}(\mathbf{X})\right\}^2\right] \\ &= \underbrace{\left[\mathbf{f}(\mathbf{X}) - \hat{\mathbf{f}}(\mathbf{X})\right]^2}_{\text{Reducible}} + \underbrace{\text{Var}(\varepsilon)}_{\text{Irreducible}} \end{aligned}$$

In less math:

- If ε exists, then \mathbf{X} cannot perfectly explain \mathbf{y} .
- So even if $\hat{\mathbf{f}} = \mathbf{f}$, we still have irreducible error.

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Thus, to form our **best predictors**, we will **minimize reducible error**.

Model accuracy

MSE

Mean squared error (MSE) is the most common[†] way to measure model performance in a regression setting.

$$\text{MSE} = \frac{1}{n} \sum_{i=1}^n \left[\mathbf{y}_i - \hat{\mathbf{f}}(\mathbf{x}_i) \right]^2$$

Recall: $\mathbf{y}_i - \hat{\mathbf{f}}(\mathbf{x}_i) = \mathbf{y}_i - \hat{\mathbf{y}}_i$ is our prediction error.

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Two notes about MSE

1. MSE will be (relatively) very small when **prediction error** is nearly zero.
2. MSE **penalizes** big errors more than little errors (the squared part).

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Training or testing?

Low MSE (accurate performance) on the data that trained the model isn't actually impressive—maybe the model is just overfitting our data.[†]

What we want: How well does the model perform **on data it has never seen?**

[†] Recall the kNN performance for k=1.

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This introduces an important distinction:

1. **Training data:** The observations (y_i, x_i) used to **train** our model \hat{f} .
2. **Testing data:** The observations (y_0, x_0) that our model has yet to see—and which we can use to evaluate the performance of \hat{f} .

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Real goal: Low test-sample MSE (not the training MSE from before).

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Model accuracy

Regression and loss

For **regression settings**, the loss is our **prediction**'s distance from **truth**, i.e.,

$$\text{error}_i = \mathbf{y}_i - \hat{\mathbf{y}}_i \quad \text{loss}_i = |\mathbf{y}_i - \hat{\mathbf{y}}_i| = |\text{error}_i|$$

Depending upon our ultimate goal, we choose **loss/objective functions**.

$$\text{L1 loss} = \sum_i |\mathbf{y}_i - \hat{\mathbf{y}}_i|$$

$$\text{MAE} = \frac{1}{n} \sum_i |\mathbf{y}_i - \hat{\mathbf{y}}_i|$$

$$\text{L2 loss} = \sum_i (\mathbf{y}_i - \hat{\mathbf{y}}_i)^2$$

$$\text{MSE} = \frac{1}{n} \sum_i (\mathbf{y}_i - \hat{\mathbf{y}}_i)^2$$

Whatever we're using, we care about **test performance** (e.g., test MSE), rather than training performance.

Model accuracy

Classification

For **classification problems**, we often use the **test error rate**.

$$\frac{1}{n} \sum_{i=1}^n \mathbb{I}(y_i \neq \hat{y}_i)$$

The **Bayes classifier**

1. predicts class j when $\Pr(y_0 = j | \mathbf{X} = \mathbf{x}_0)$ exceeds all other classes.
2. produces the **Bayes decision boundary**—the decision boundary with the lowest test error rate.
3. is unknown: we must predict $\Pr(y_0 = j | \mathbf{X} = \mathbf{x}_0)$.

Flexibility

The bias-variance tradeoff

Finding the optimal level of flexibility highlights the **bias-variance tradeoff**.

Bias The error that comes from inaccurately estimating \hat{f} .

- More flexible models are better equipped to recover complex relationships (f), reducing bias. (Real life is seldom linear.)
- Simpler (less flexible) models typically increase bias.

Variance The amount \hat{f} would change with a different **training sample**

- If new **training sets** drastically change \hat{f} , then we have a lot of uncertainty about f (and, in general, $\hat{f} \not\approx f$).
- More flexible models generally add variance to f .

Flexibility

The bias-variance tradeoff

The expected value[†] of the **test MSE** can be written

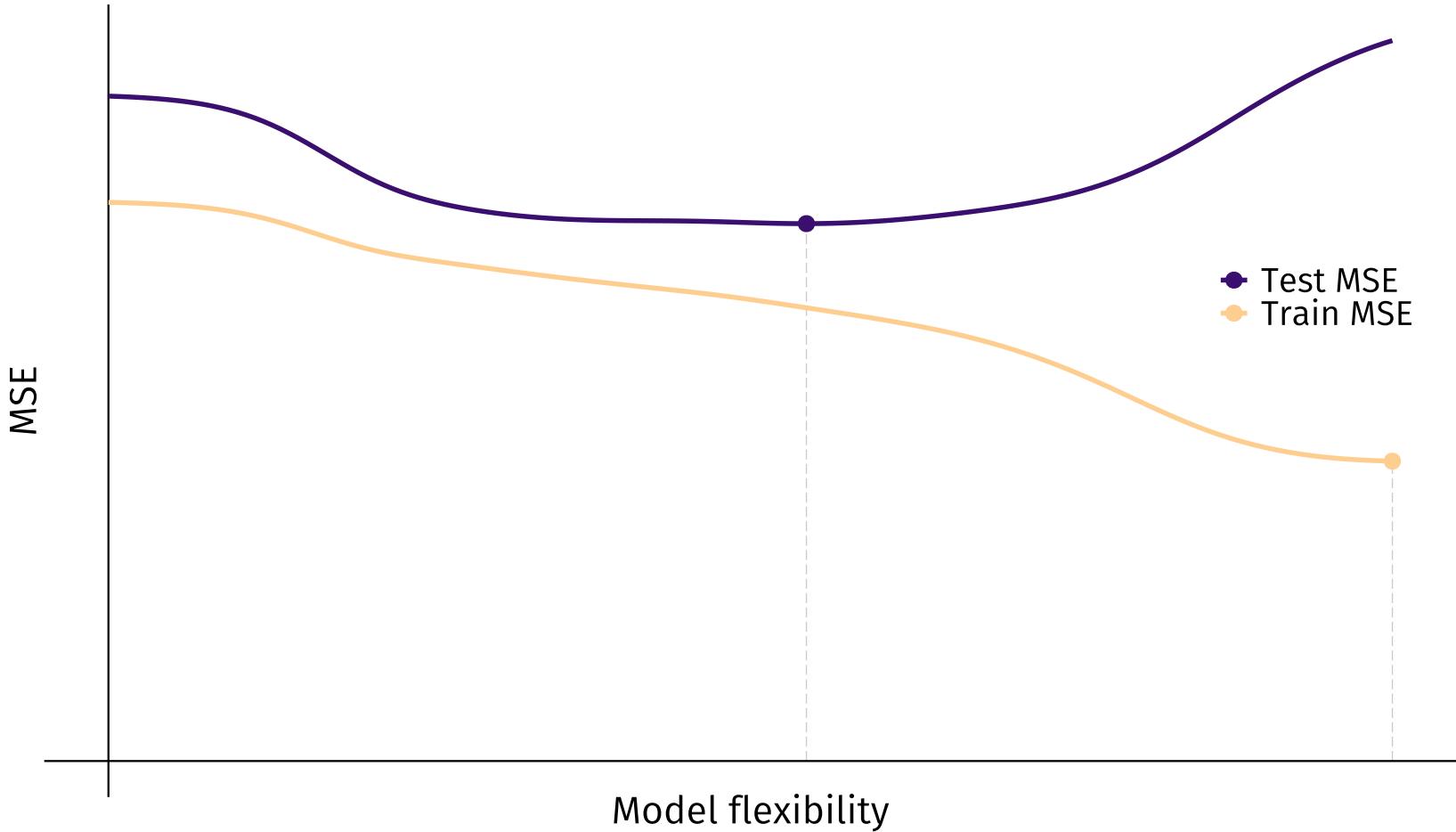
$$E\left[\left(\mathbf{y}_0 - \hat{\mathbf{f}}(\mathbf{X}_0)\right)^2\right] = \underbrace{\text{Var}\left(\hat{\mathbf{f}}(\mathbf{X}_0)\right)}_{\text{Variance}} + \underbrace{\left[\text{Bias}\left(\hat{\mathbf{f}}(\mathbf{X}_0)\right)\right]^2}_{\text{Bias}} + \underbrace{\text{Var}(\varepsilon)}_{\text{Irr. error}}$$

The tradeoff in terms of model flexibility

- Increasing flexibility *from total inflexibility* generally **reduces bias more** than it increases variance (reducing test MSE).
- At some point, the marginal benefits of flexibility **equal** marginal costs.
- Past this point (optimal flexibility), we **increase variance more** than we reduce bias (increasing test MSE).

U-shaped test MSE with respect to model flexibility (KNN here).

Increases in variance eventually overcome reductions in (squared) bias.



Resampling refresher

Resampling methods help understand uncertainty in statistical modeling.

The process behind the magic of resampling methods:

1. **Repeatedly draw samples** from the **training data**.
2. **Fit your model**(s) on each random sample.
3. **Compare** model performance (or estimates) **across samples**.
4. Infer the **variability/uncertainty in your model** from (3).

Sounds familiar, right?

Resampling

Hold out

Recall: We want to find the model that **minimizes out-of-sample test error.**

If we have a large test dataset, we can use it (once).

Q₁ What if we don't have a test set?

Q₂ What if we need to select and train a model?

Q₃ How can we avoid overfitting our training[†] data during model selection?

[†] Also relevant for *testing* data.

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A_{1,2,3} **Hold-out methods** (e.g., cross validation) use training data to estimate test performance—**holding out** a mini "test" sample of the training data that we use to estimate the test error.

[†] Also relevant for *testing* data.

Hold-out methods

Option 1: The *validation set* approach

To estimate the **test error**, we can *hold out* a subset of our **training data** and then **validate** (evaluate) our model on this held out **validation set**.

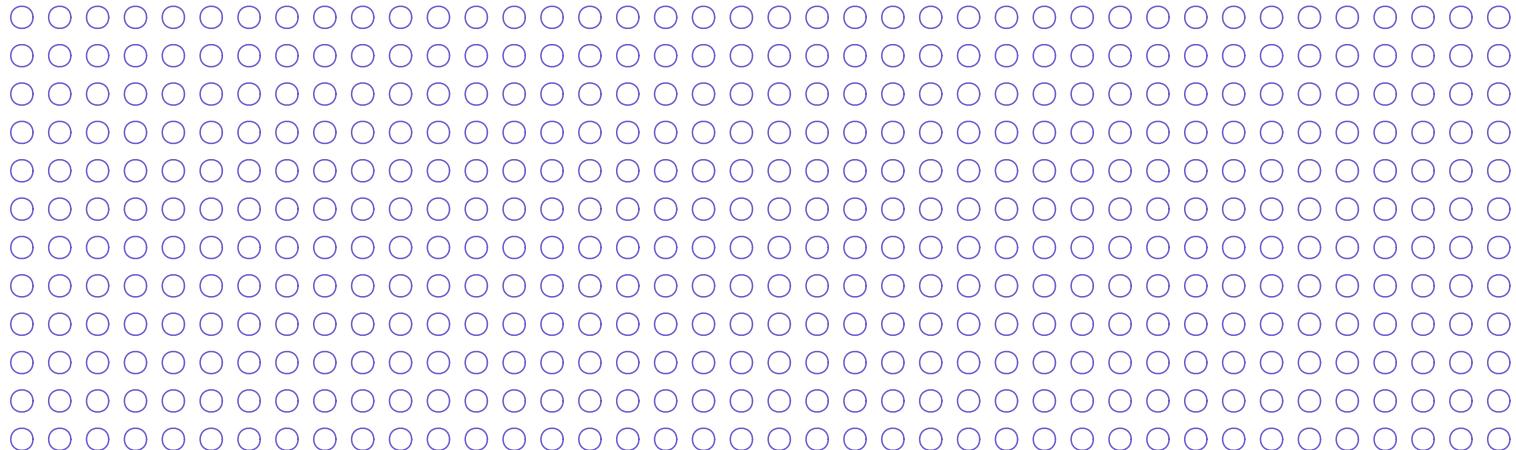
- The **validation error rate** estimates the **test error rate**
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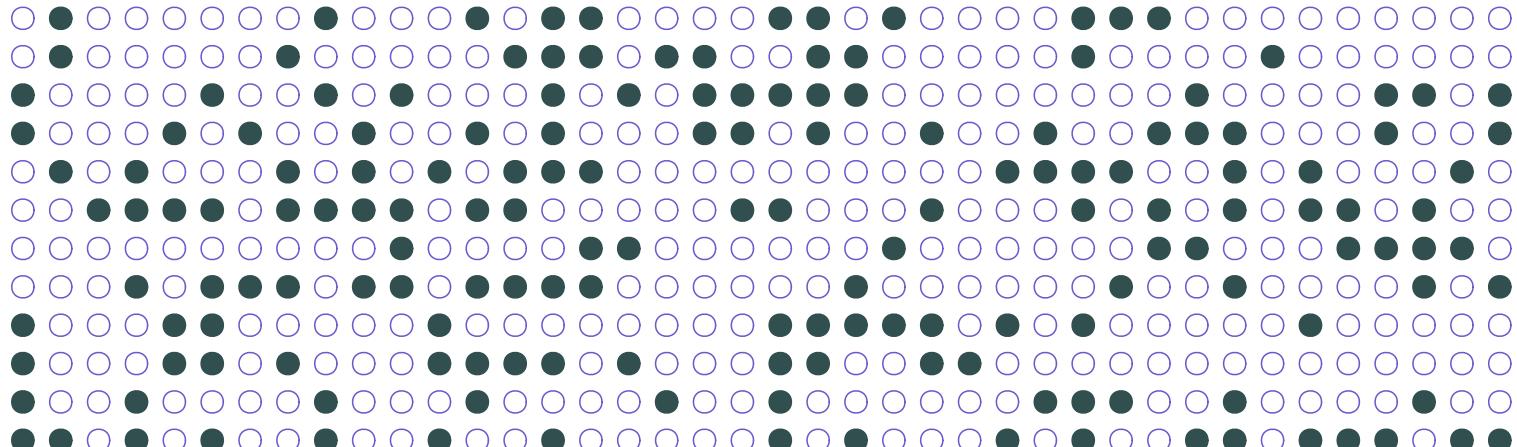
Initial training set

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Validation (sub)set

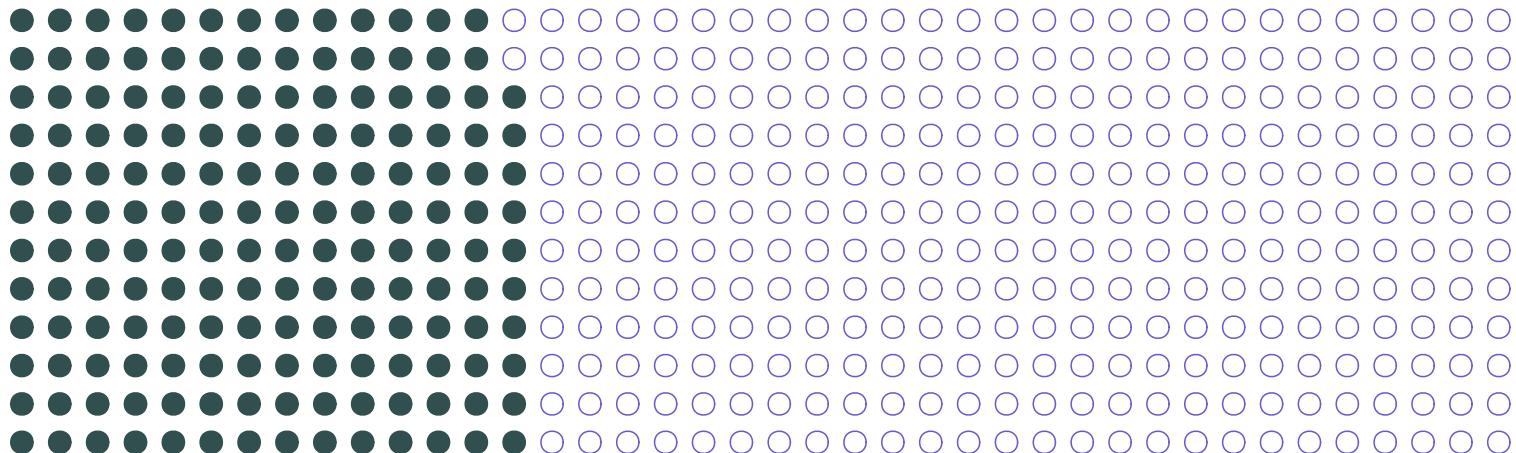
Training set: Model training

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The goal of the validation set is to **estimate out-of-sample (test) error.**

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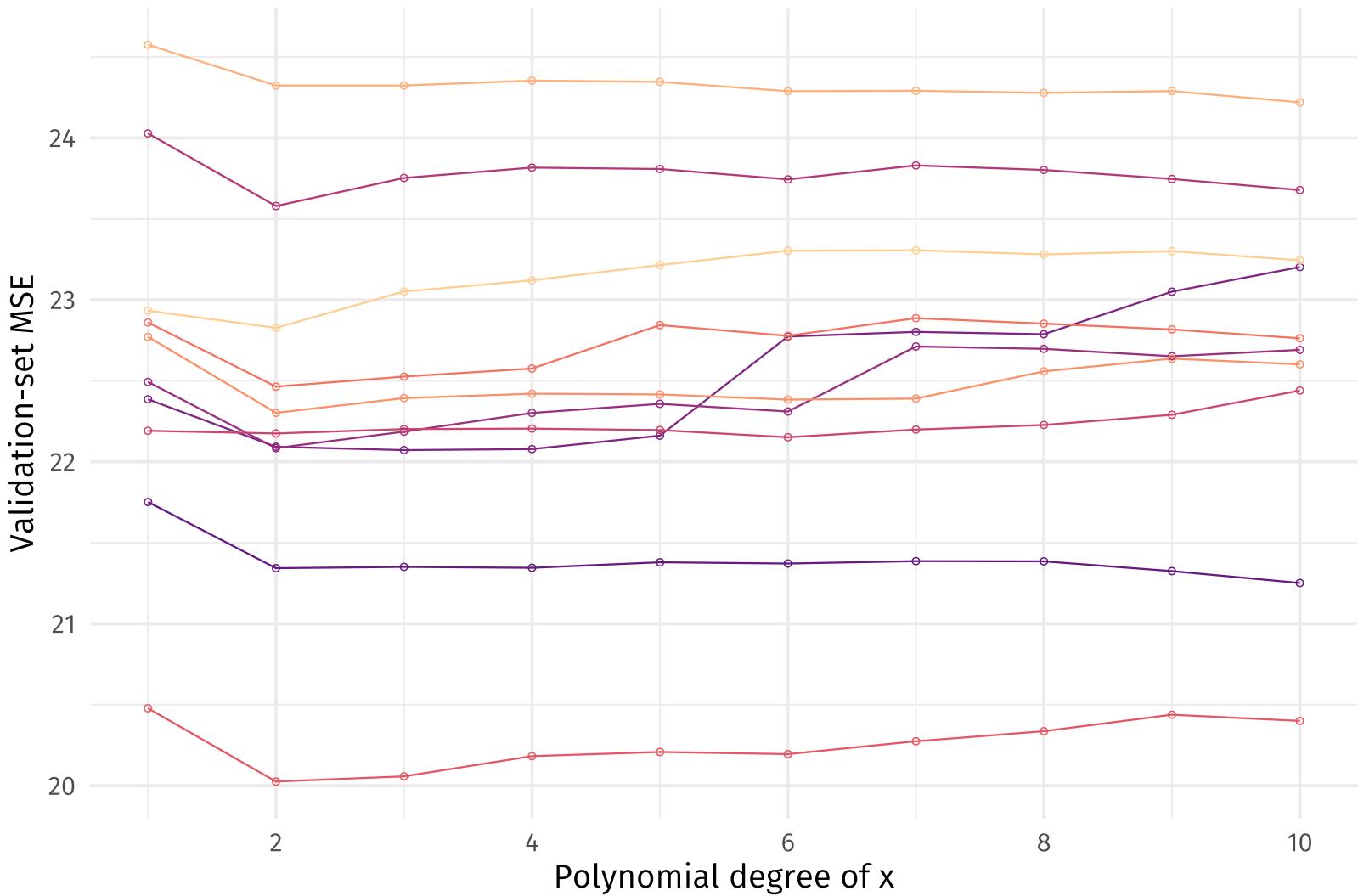
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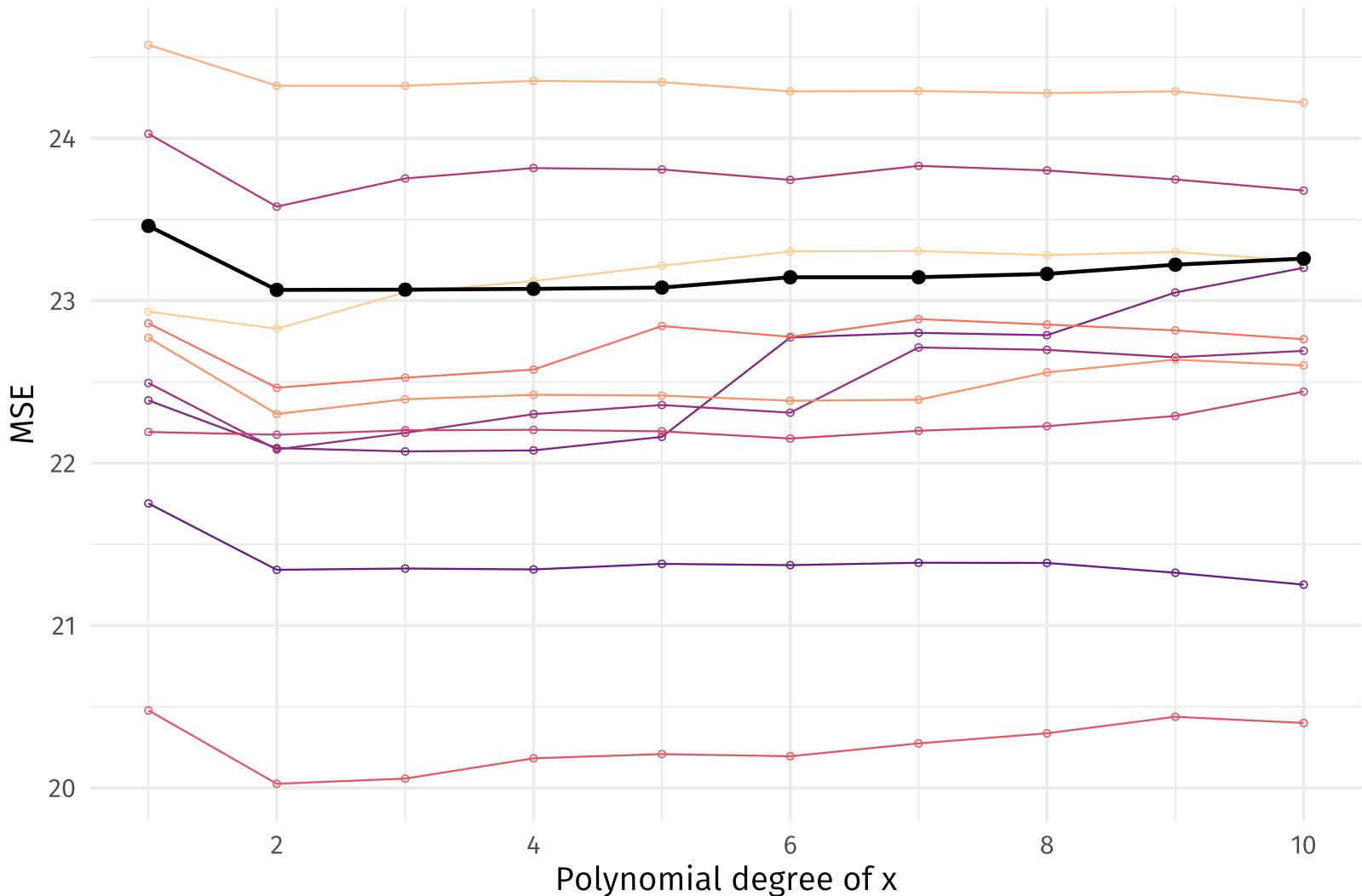
- Estimates come with **uncertainty**—varying from sample to sample.
- Variability (standard errors) is larger with **smaller samples**.

Problem This estimated error is often based upon a fairly small sample (<30% of our training data). So its variance can be large.

Validation MSE for 10 different validation samples



True test MSE compared to validation-set estimates



Hold-out methods

Option 1: The *validation set* approach

Put differently: The validation-set approach has (\geq) two major drawbacks:

1. **High variability** Which observations are included in the validation set can greatly affect the validation MSE.
2. **Inefficiency in training our model** We're essentially throwing away the validation data when training the model—"wasting" observations.

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(2) \Rightarrow validation MSE may overestimate test MSE.

Even if the validation-set approach provides an unbiased estimator for test error, it is likely a pretty noisy estimator.

Hold-out methods

Option 2: Leave-one-out cross validation

Cross validation solves the validation-set method's main problems.

- Use more (= all) of the data for training (lower variability; less bias).
- Still maintains separation between training and validation subsets.

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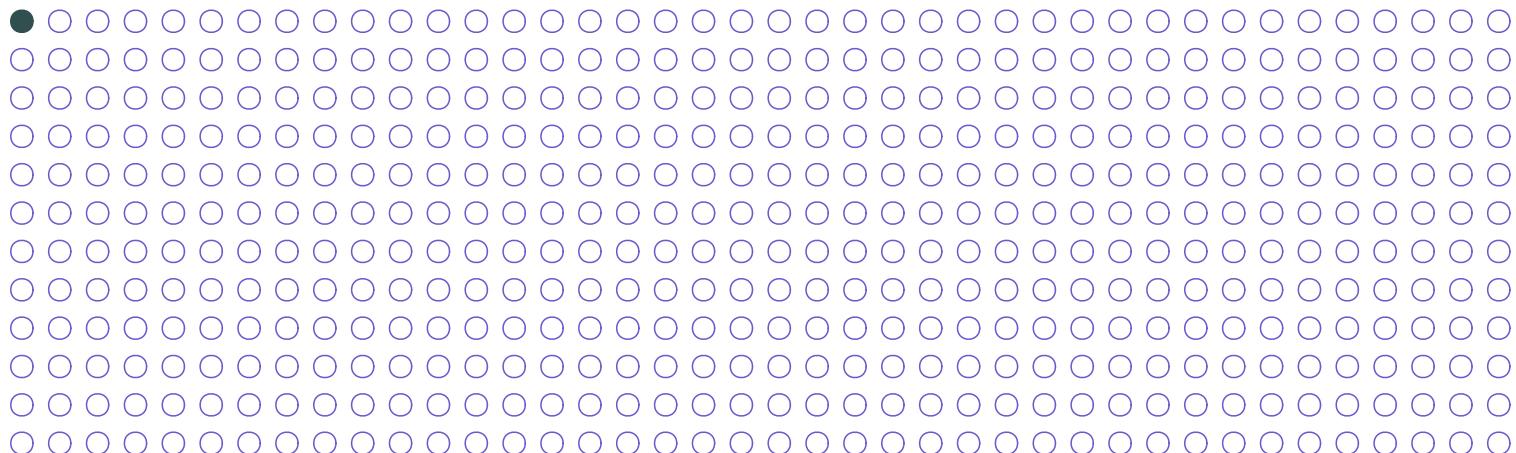
Leave-one-out cross validation (LOOCV) is perhaps the cross-validation method most similar to the validation-set approach.

- Your validation set is exactly one observation.
- *New* You repeat the validation exercise for every observation.
- *New* Estimate MSE as the mean across all observations.

Hold-out methods

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Each observation takes a turn as the **validation set**,
while the other $n-1$ observations get to **train the model**.

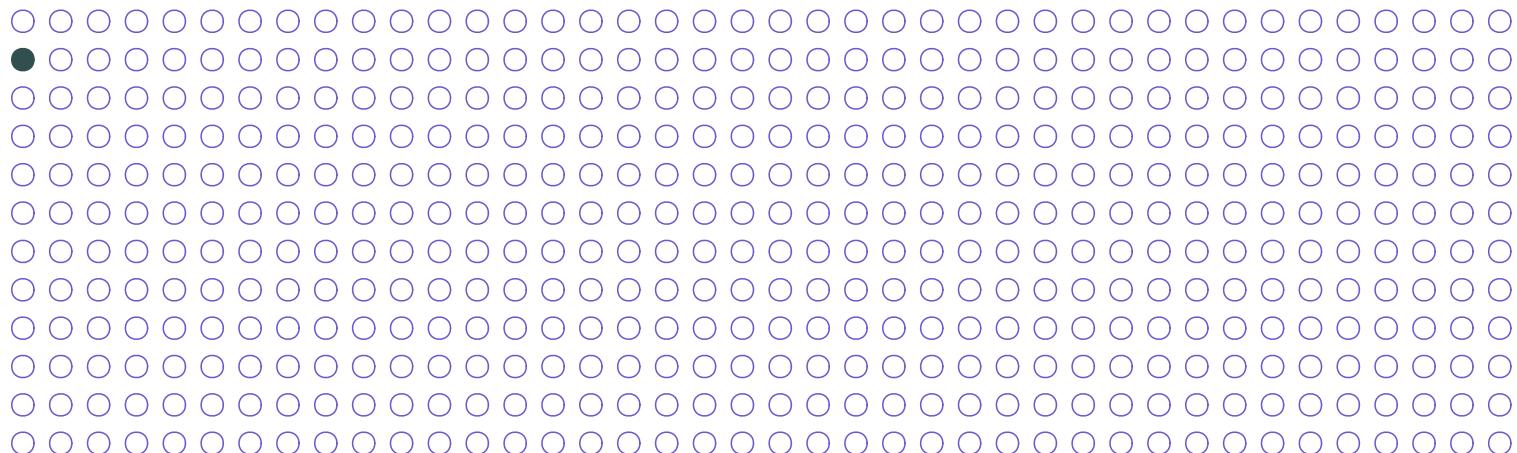


Observation 1's turn for validation produces MSE_1 .

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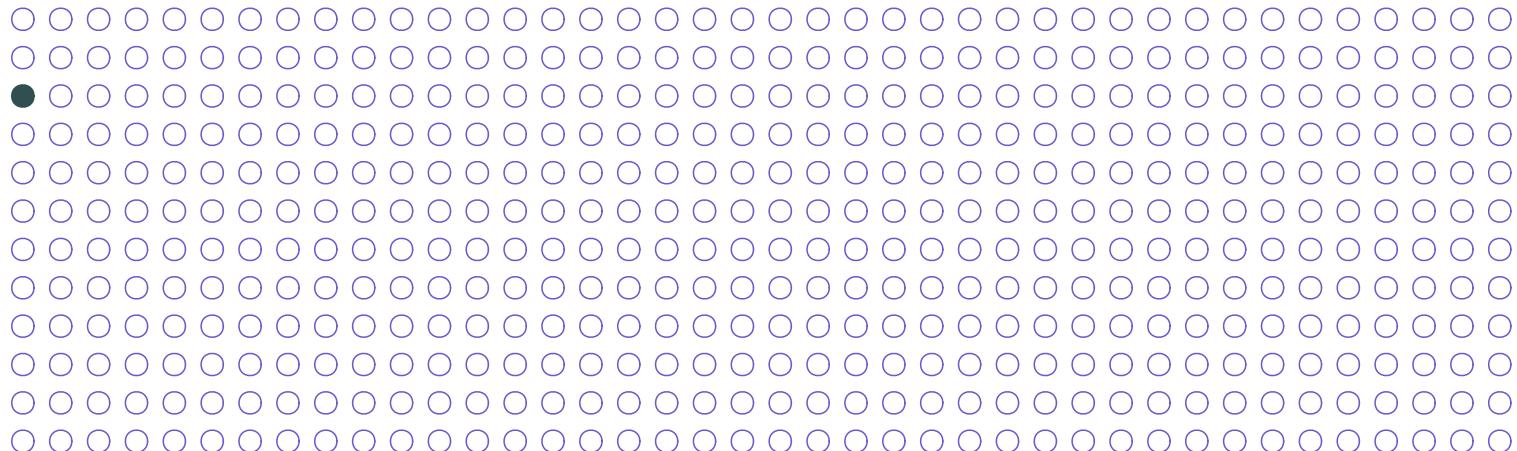


Observation 2's turn for validation produces MSE_2 .

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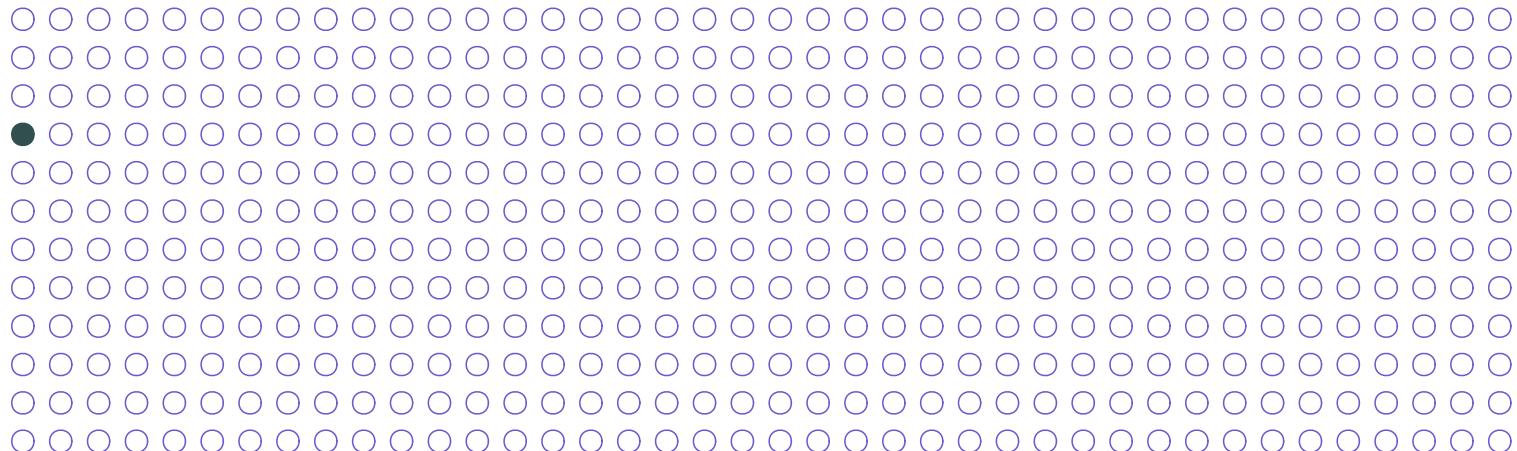


Observation 3's turn for validation produces MSE_3 .

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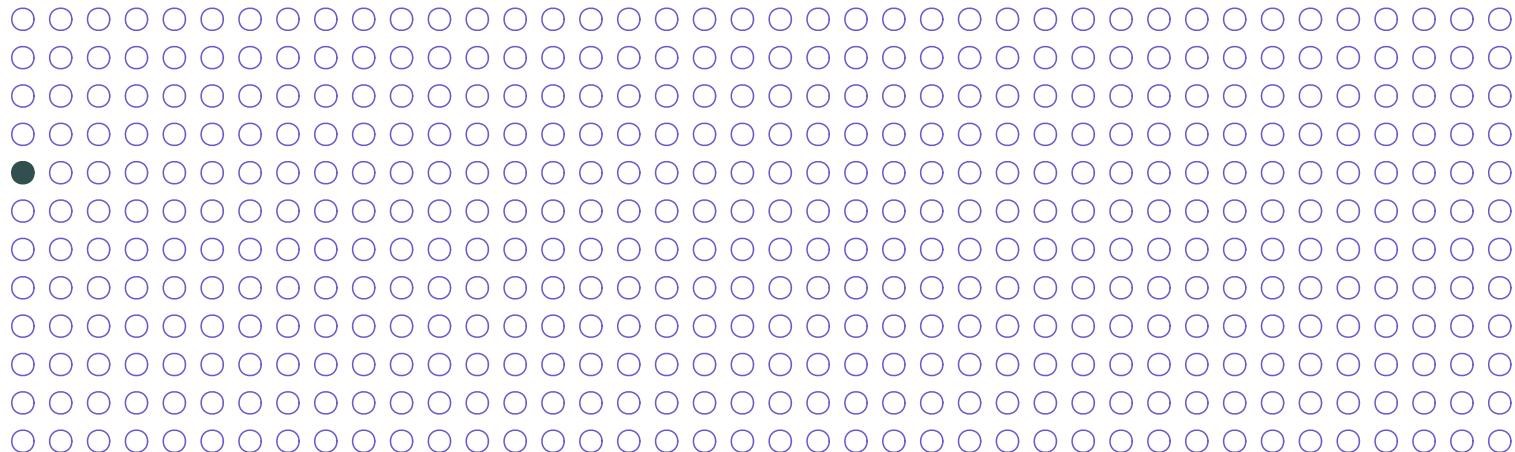


Observation 4's turn for validation produces MSE_4 .

Hold-out methods

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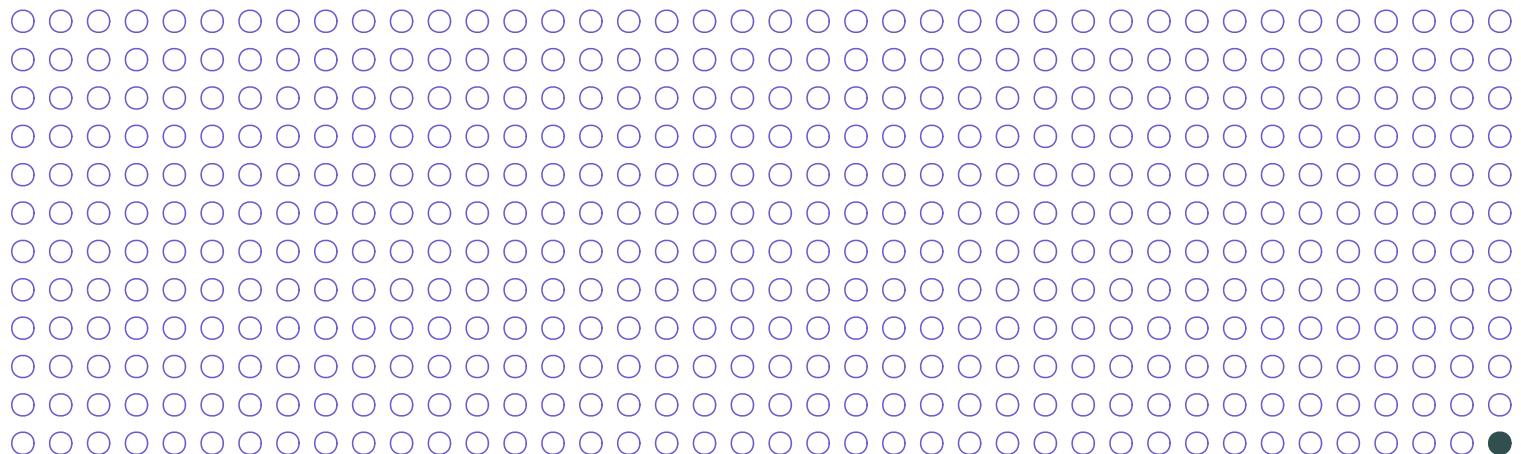


Observation 5's turn for validation produces MSE_5 .

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Observation n's turn for validation produces MSE_n .

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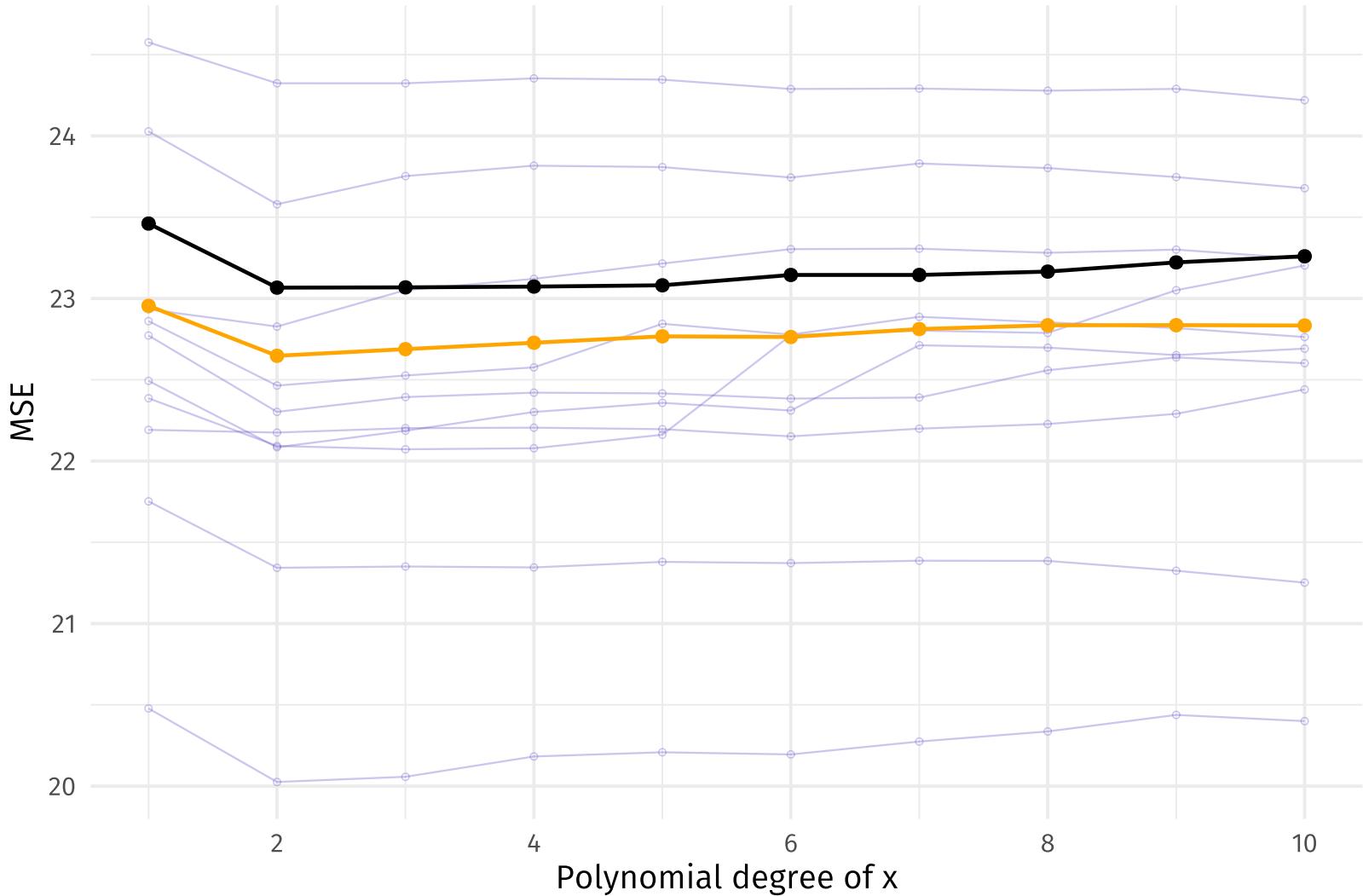
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1. LOOCV **reduces bias** by using n-1 (almost all) observations for training.
2. LOOCV **resolves variance**: it makes all possible comparison
(no dependence upon which validation-test split you make).

[†] And because often $n-1 \approx n$.

True test MSE and LOOCV MSE compared to validation-set estimates



Hold-out methods

Option 3: k-fold cross validation

Leave-one-out cross validation is a special case of a broader strategy:
k-fold cross validation.

1. **Divide** the training data into k equally sized groups (folds).
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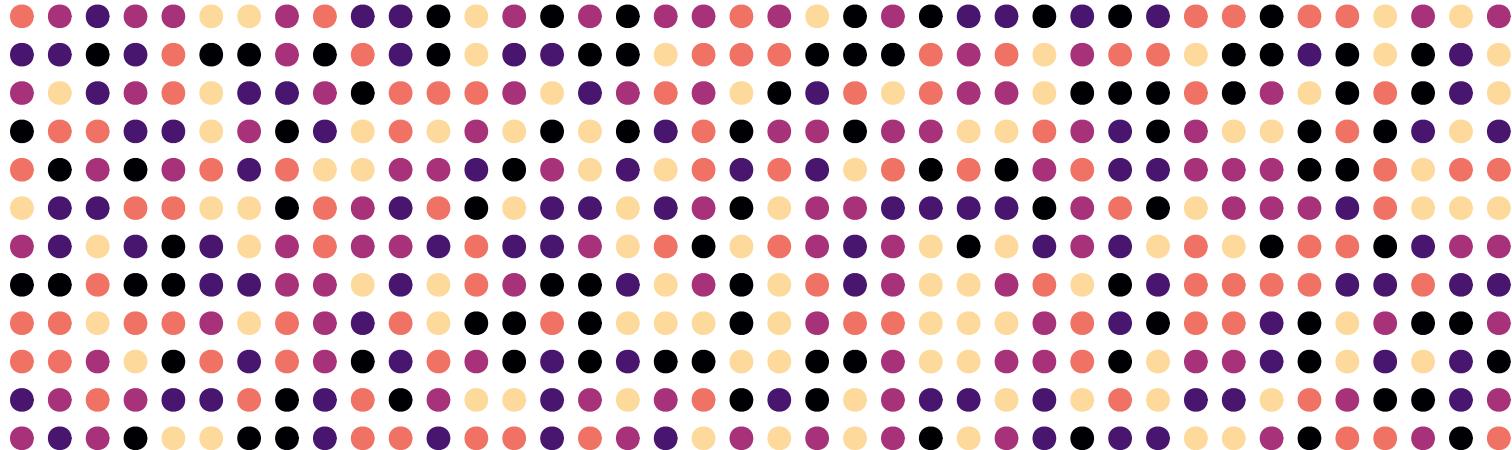
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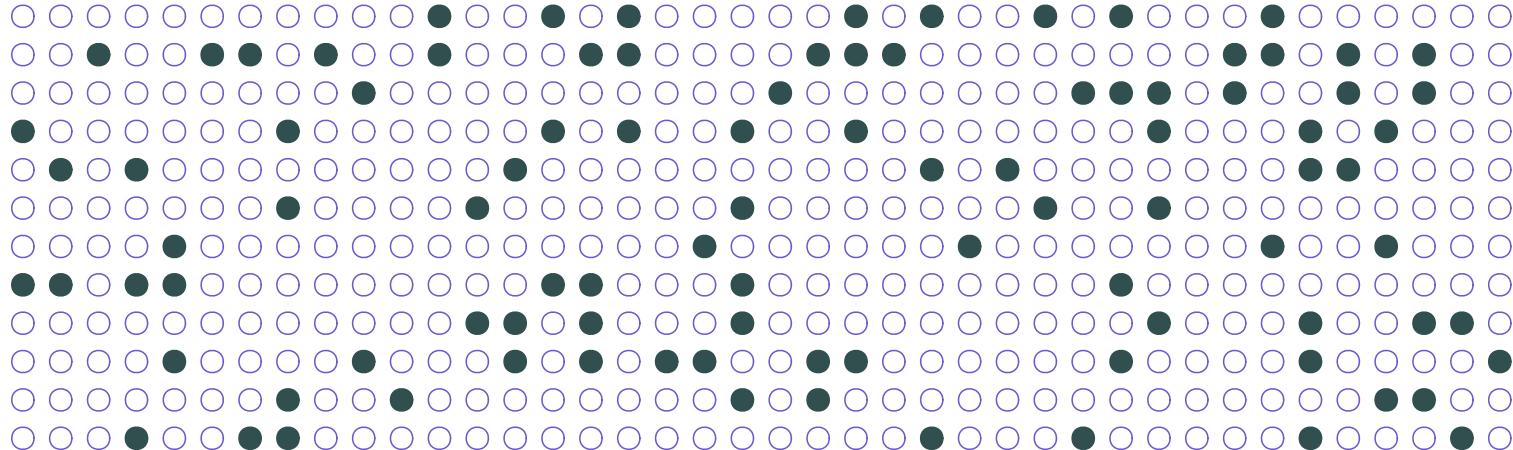
Our $k = 5$ folds.

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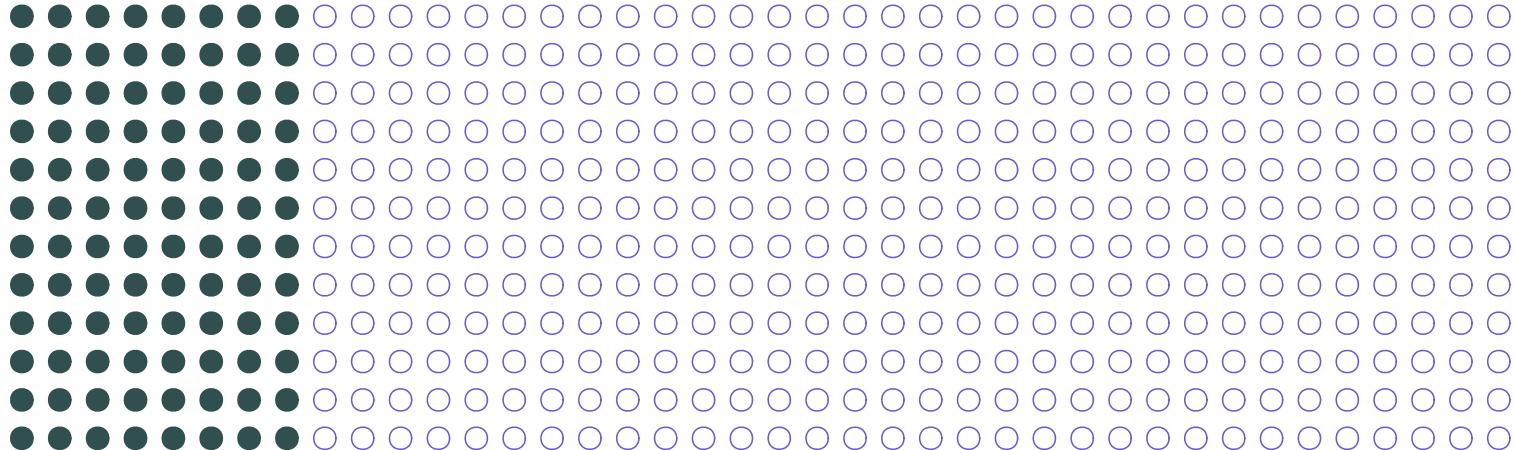
Each fold takes a turn at **validation**. The other $k - 1$ folds **train**.

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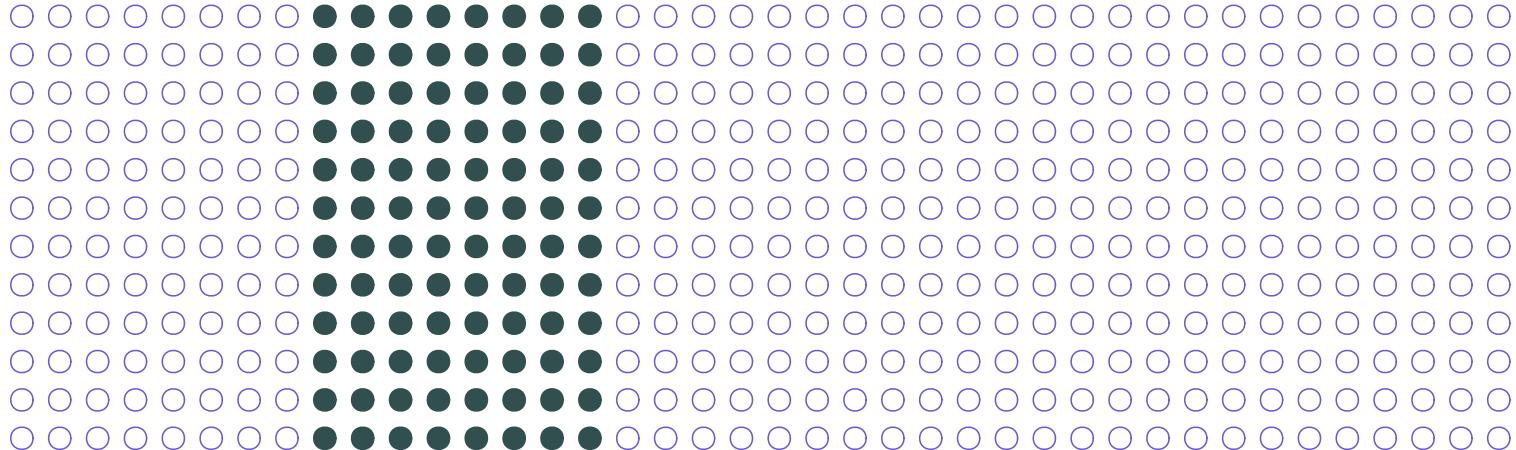
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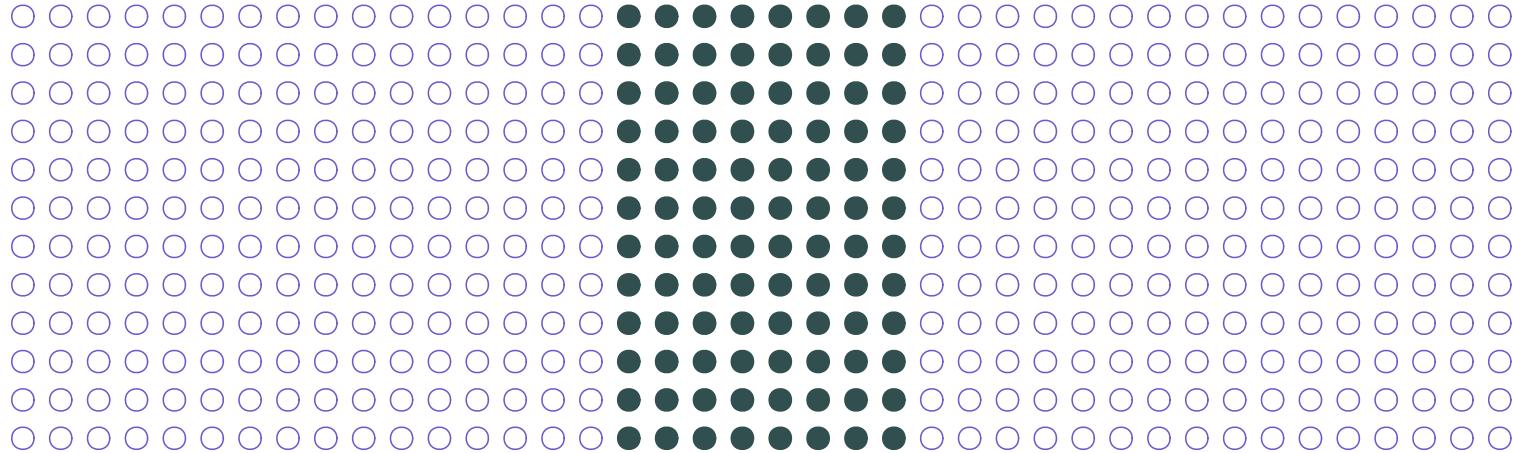
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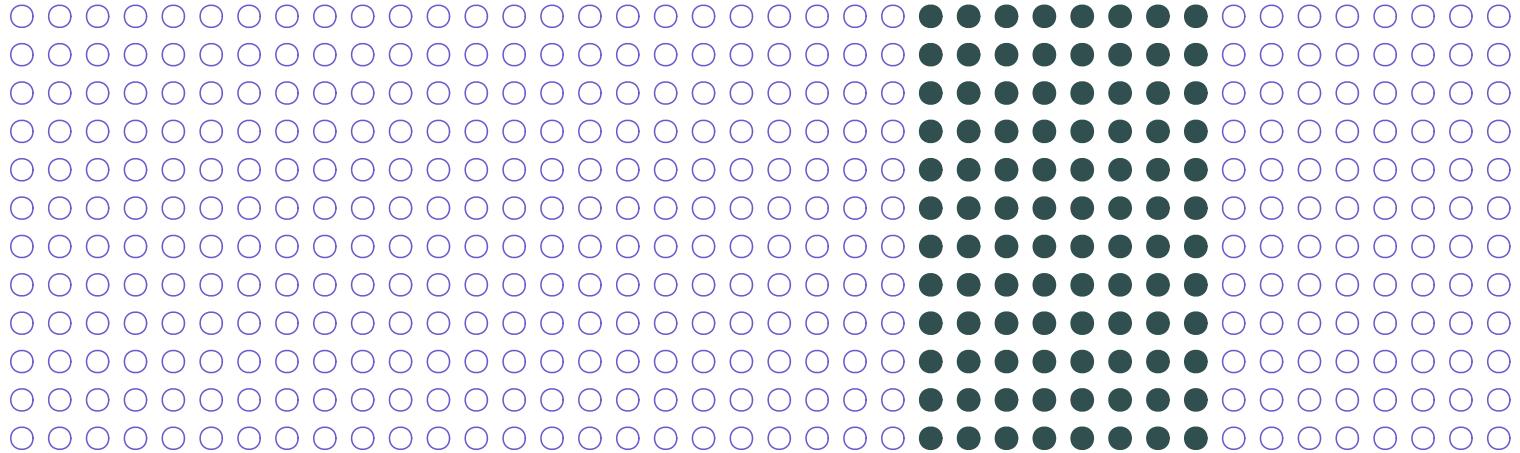
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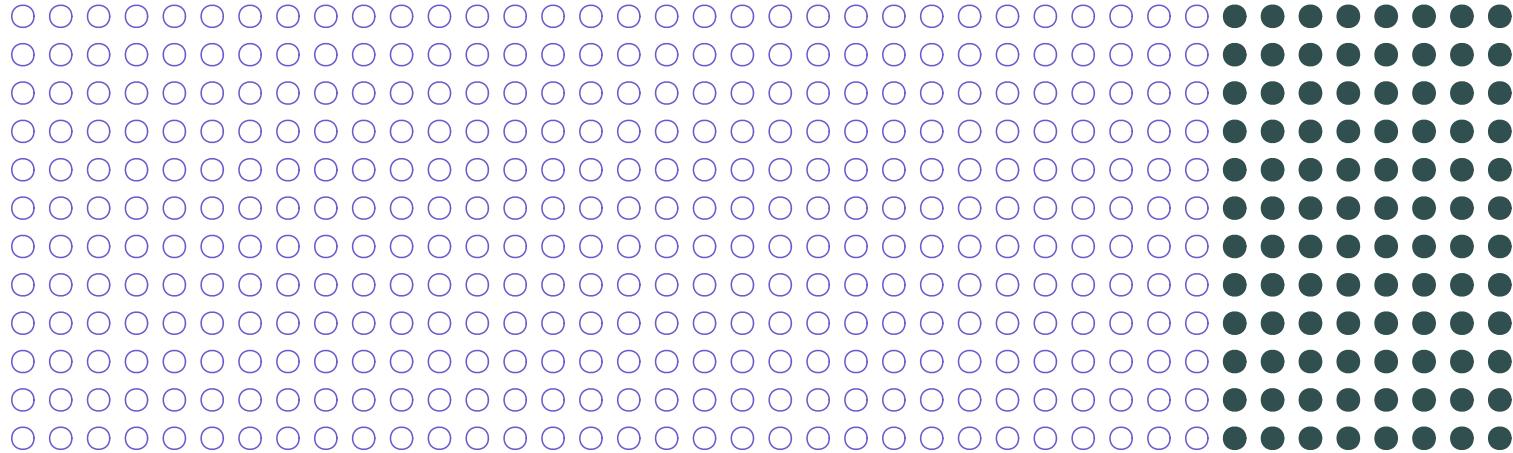
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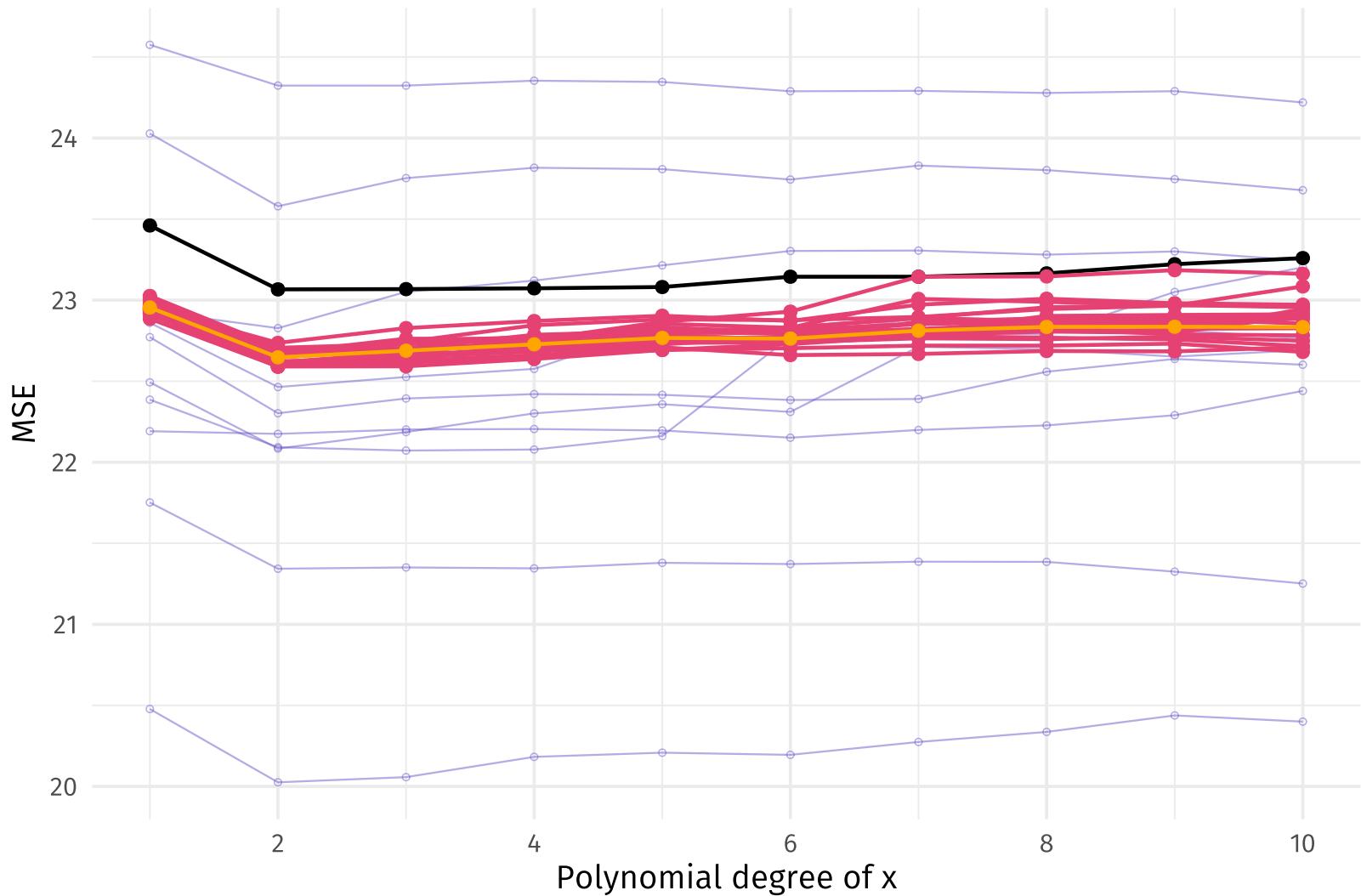
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Test MSE vs. estimates: LOOCV, 5-fold CV (20x), and validation set (10x)



Note: Each of these methods extends to classification settings, e.g., LOOCV

$$\text{CV}_{(n)} = \frac{1}{n} \sum_{i=1}^n \mathbb{I}(\textcolor{orange}{y_i} \neq \hat{y}_i)$$

Hold-out methods

Caveat

So far, we've treated each observation as separate/independent from each other observation.

The methods that we've defined so far actually need this independence.

Hold-out methods

Goals and alternatives

You can use CV for either of two important **modeling tasks**:

- **Model selection** Choosing and tuning a model
- **Model assessment** Evaluating a model's accuracy

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- fit a model that contains *all p* predictors
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Idea: Penalize the model for coefficients as they move away from zero.

[†] Synonyms for *shrink*: constrain or regularize

Shrinkage

Why?

Q How could shrinking coefficients toward zero help or predictions?

Shrinkage

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- Shrinking our coefficients toward zero **reduces the model's variance**.[†]
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- The **optimal penalty** will balance reduced variance with increased bias.

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Now you understand shrinkage methods.

- **Ridge regression**
- **Lasso**
- **Elasticnet**

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Ridge regression

Ridge regression

Back to least squares (again)

Remember OLS? Least-squares regression finds $\hat{\beta}_j$'s by minimizing RSS

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Ridge's approach to the bias-variance tradeoff: **Balance**

- reducing **RSS**, i.e., $\sum_i (\mathbf{y}_i - \hat{\mathbf{y}}_i)^2$
- reducing **coefficients' magnitudes** (ignoring the intercept)

λ determines how much ridge "cares about" these two quantities.[†]

[†] With $\lambda = 0$, least-squares regression only "cares about" RSS.

Ridge regression

λ and penalization

Choosing a *good* value for λ is key.

- If λ is too small, then our model is essentially back to OLS.
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A Cross validate!

(You saw that coming, right?)

Ridge regression

Penalization and standardization

Important Predictors' **units** can drastically **affect ridge regression results**.

Why?

Ridge regression

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If x_1 is *meters* and $\beta_1 = 3$, then when x_1 is *km*, $\beta_1 = 3,000$.

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Solution Standardize your variables, *i.e.*, $x_{\text{stnd}} = (x - \text{mean}(x))/\text{sd}(x)$.

Lasso

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Intro

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Lasso

$$\min_{\hat{\beta}^L} \sum_{i=1}^n (\textcolor{orange}{y_i} - \hat{y}_i)^2 + \lambda \sum_{j=1}^p |\beta_j|$$

Everything else will be the same—except one aspect...

Lasso

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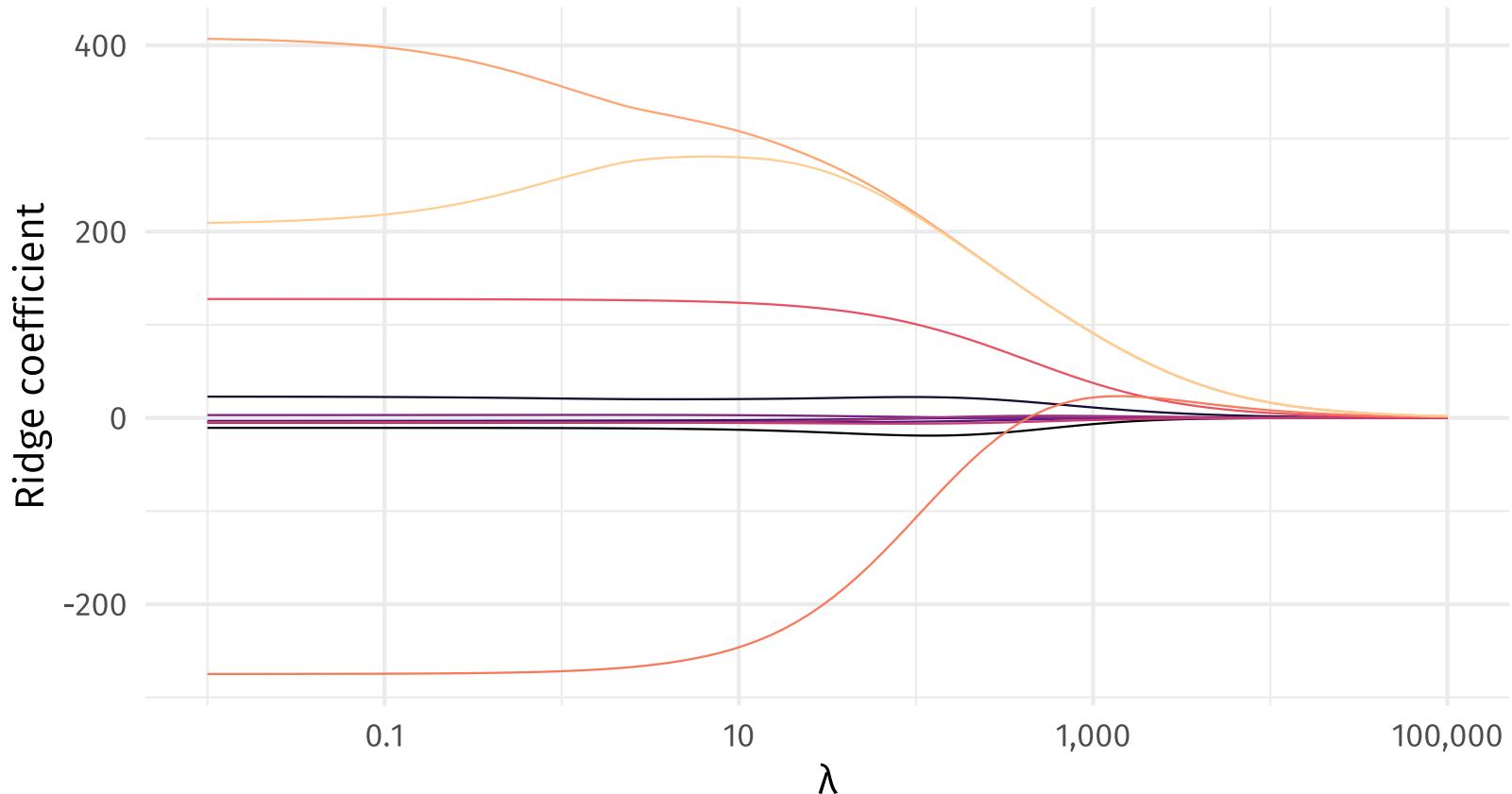
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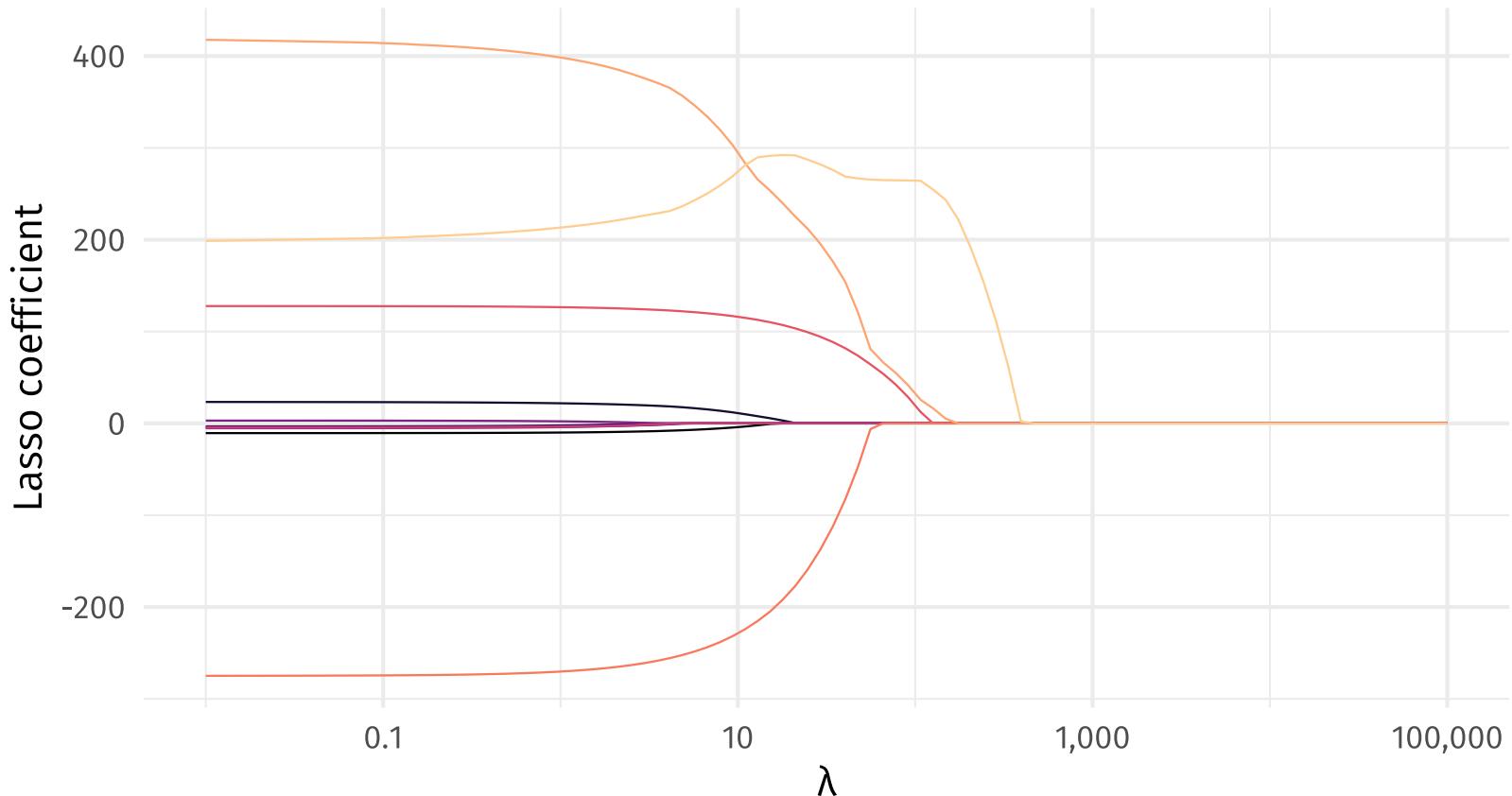
We will still need to carefully select λ .

Ridge regression coefficients for λ between 0.01 and 100,000



Predictor	— age	— i_african_american	— i_married	— limit
	— cards	— i_asian_american	— i_student	— rating
	— education	— i_female	— income	

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i_student	—	—	—	—
income	—	—	—	—
rating	—	—	—	—

Machine learning

Summary

Now you understand the basic tenants of machine learning:

- How **prediction** differs from causal inference
- **Bias-variance tradeoff** (the benefits and costs of flexibility)
- **Cross validation:** Performance and tuning
- In- vs. out-of-sample **performance**

But there's a lot more...

Trees (🌲🌴🌳)

Trees ()

Fundamentals

Decision trees

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

Trees ()

Fundamentals

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Decision trees

1. work for **both classification and regression**

Trees ()

Fundamentals

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- then predict the most-common value within a region

Decision trees

1. work for **both classification and regression**
2. are inherently **nonlinear**

Trees (🌲🌴🌳)

Fundamentals

Decision trees

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Trees ()

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Trees (

Fundamentals

Decision trees

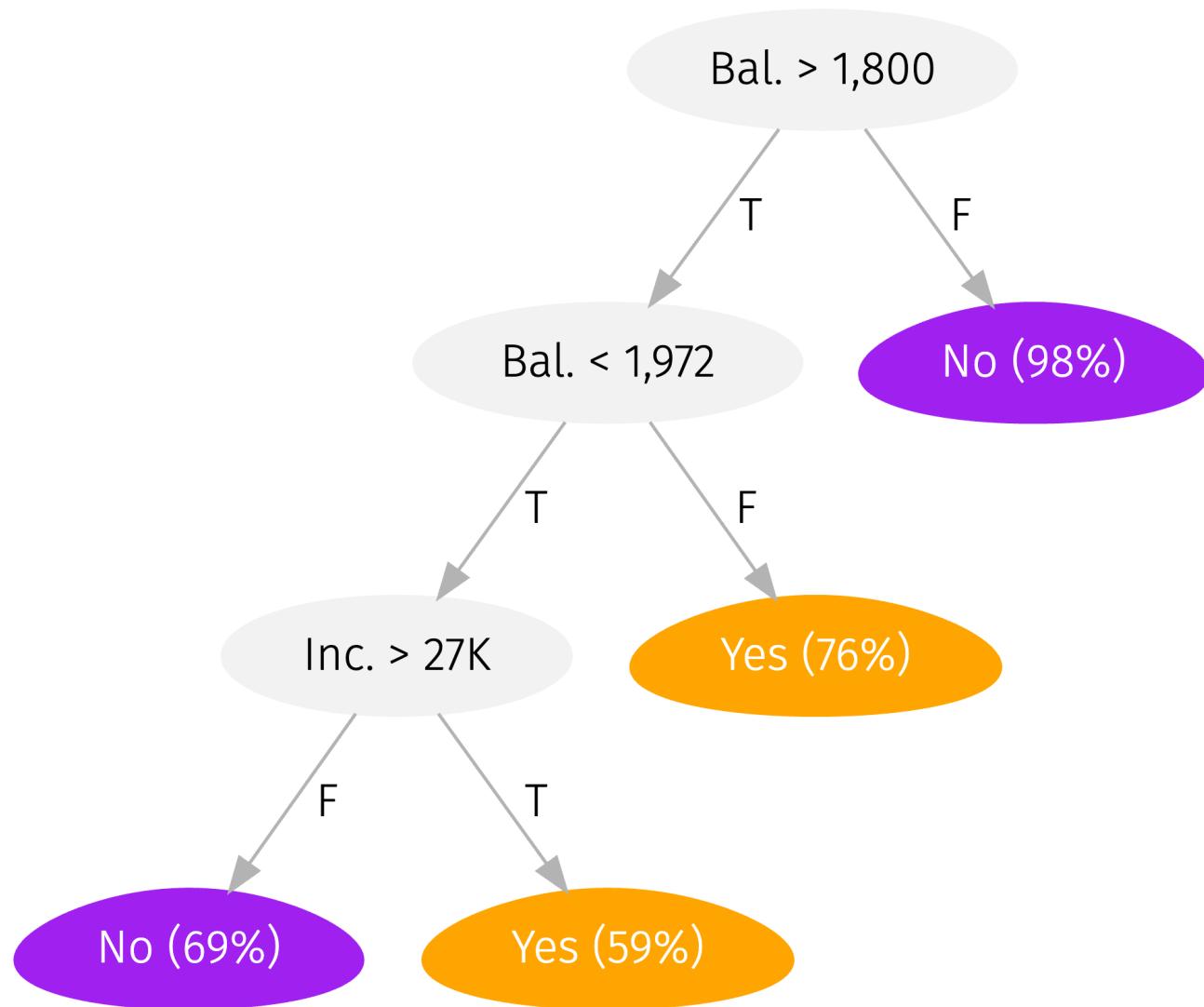
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Decision trees

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) 

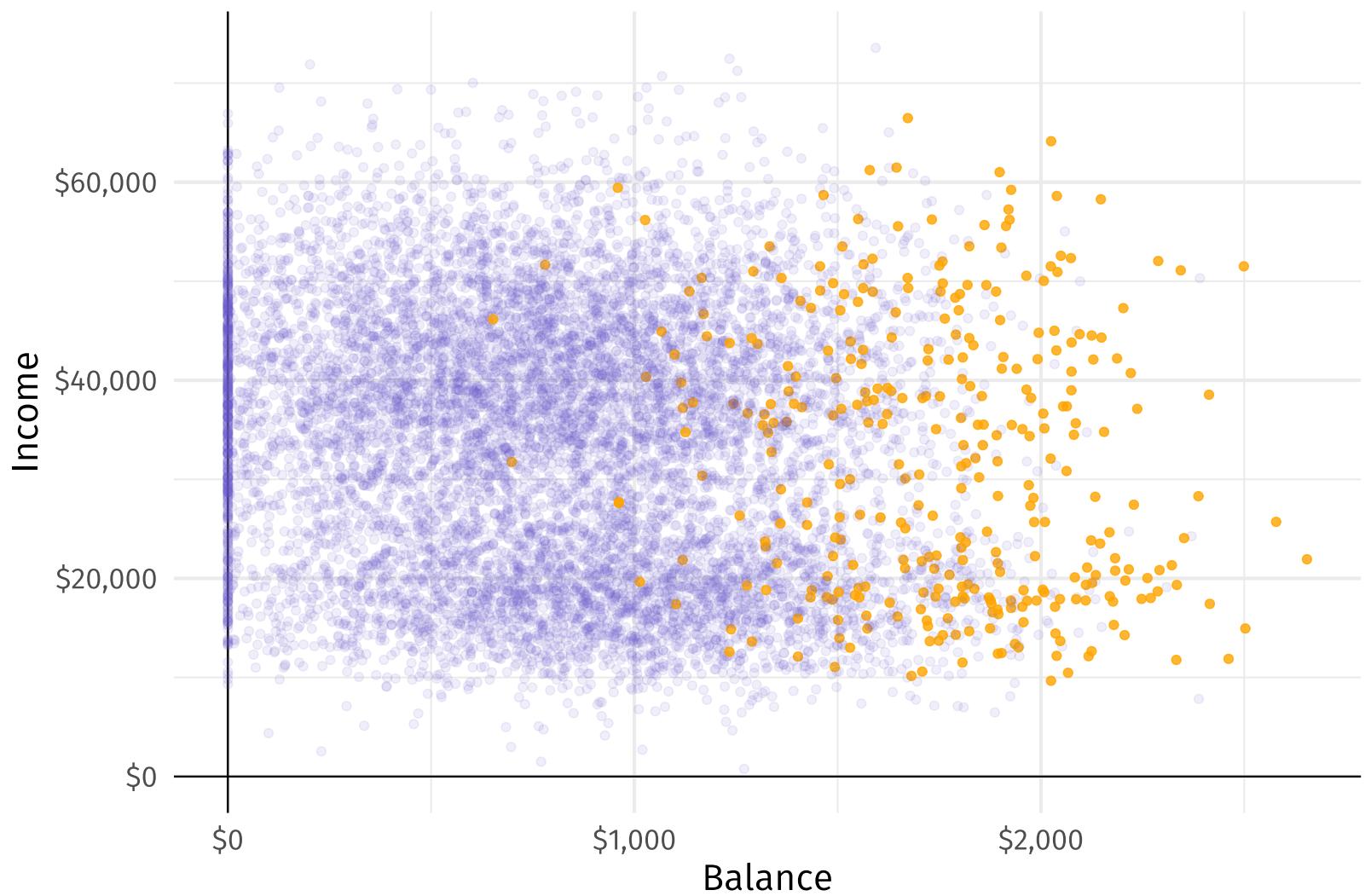
 Though the ensembles will be much less interpretable.

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

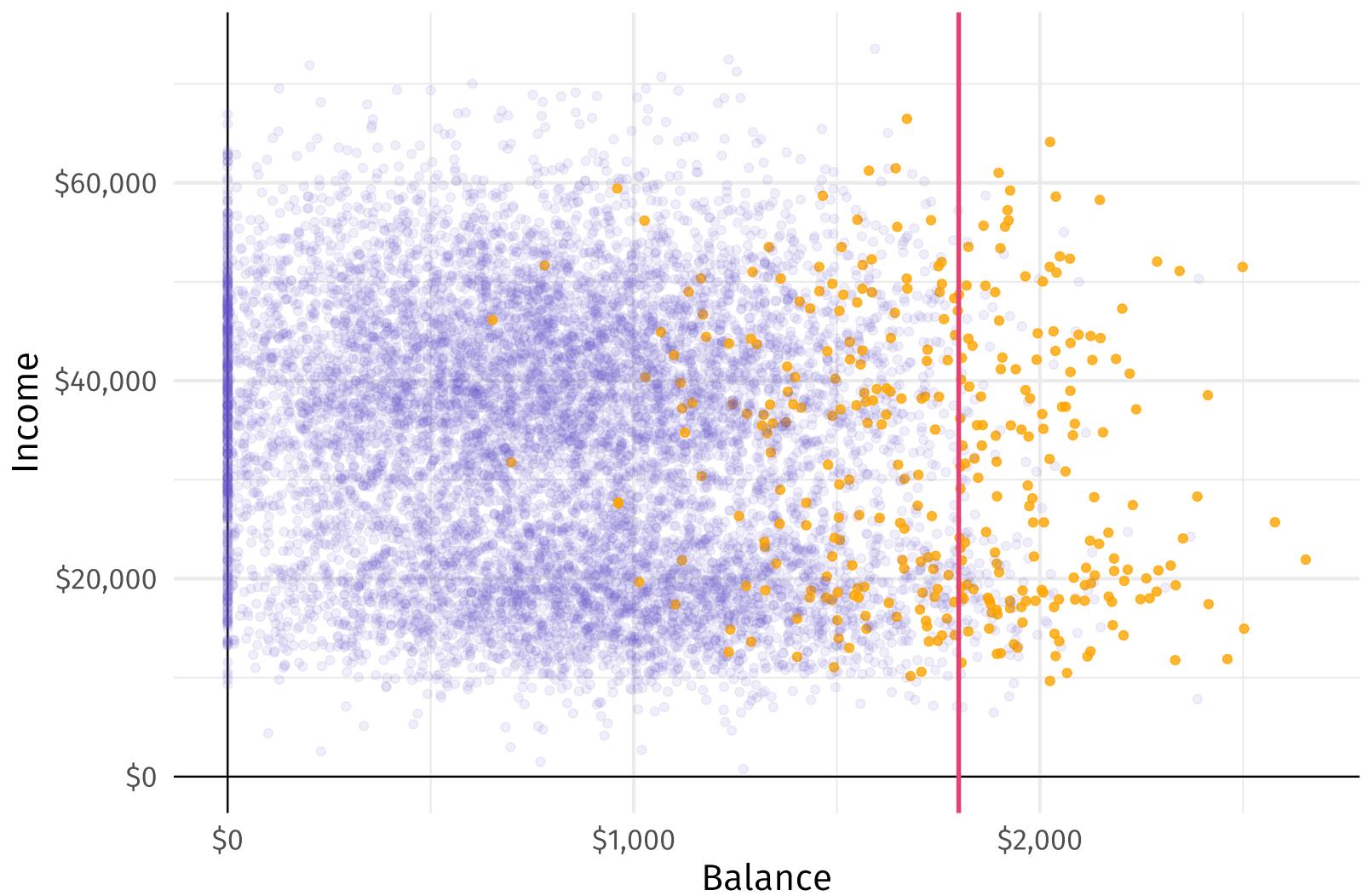


Let's see how the tree works

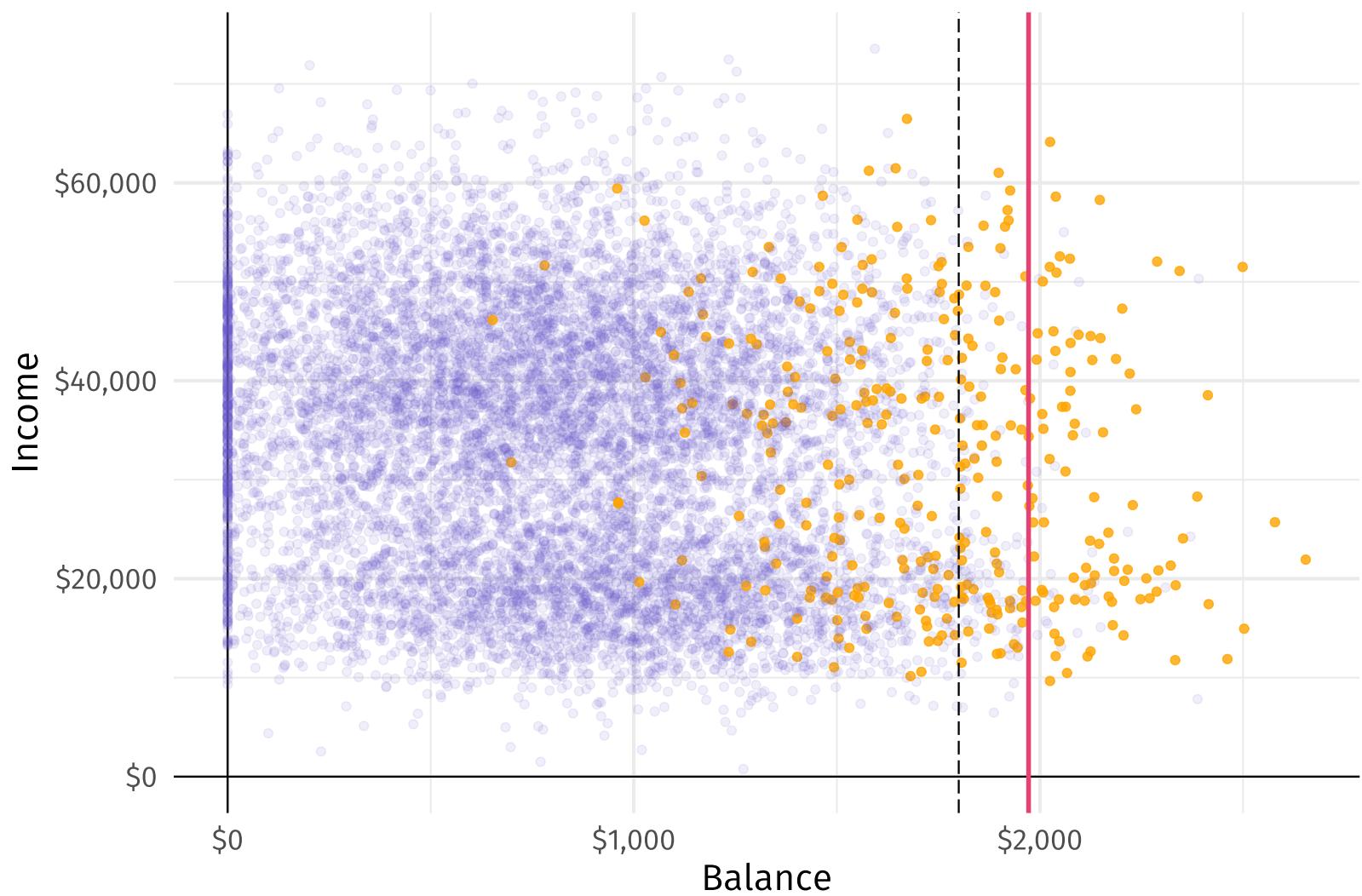
Let's see how the tree works—starting with credit data (default: Yes vs. No).



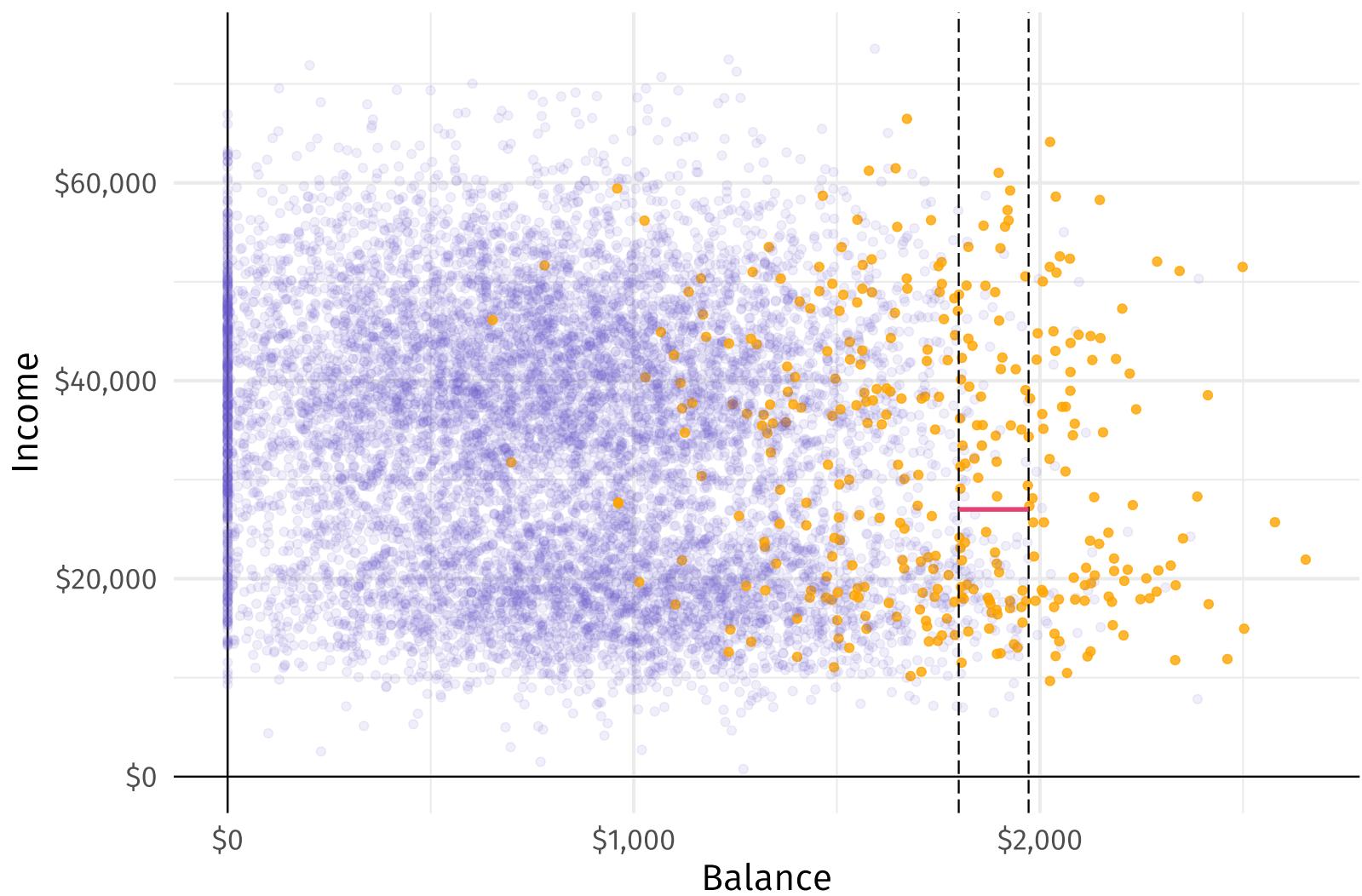
The **first partition** splits balance at \$1,800.



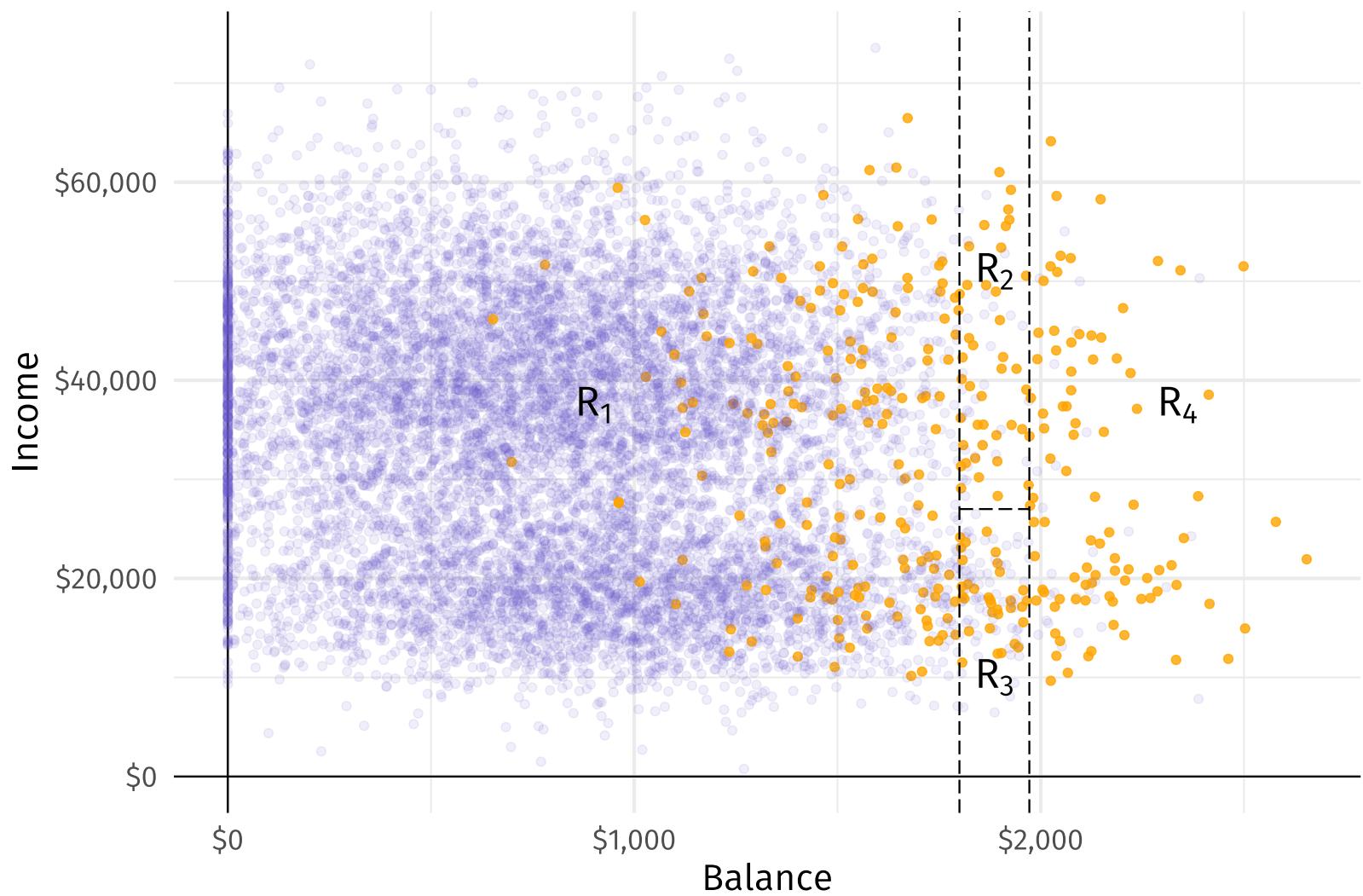
The **second partition** splits balance at \$1,972, (conditional on bal. > \$1,800).



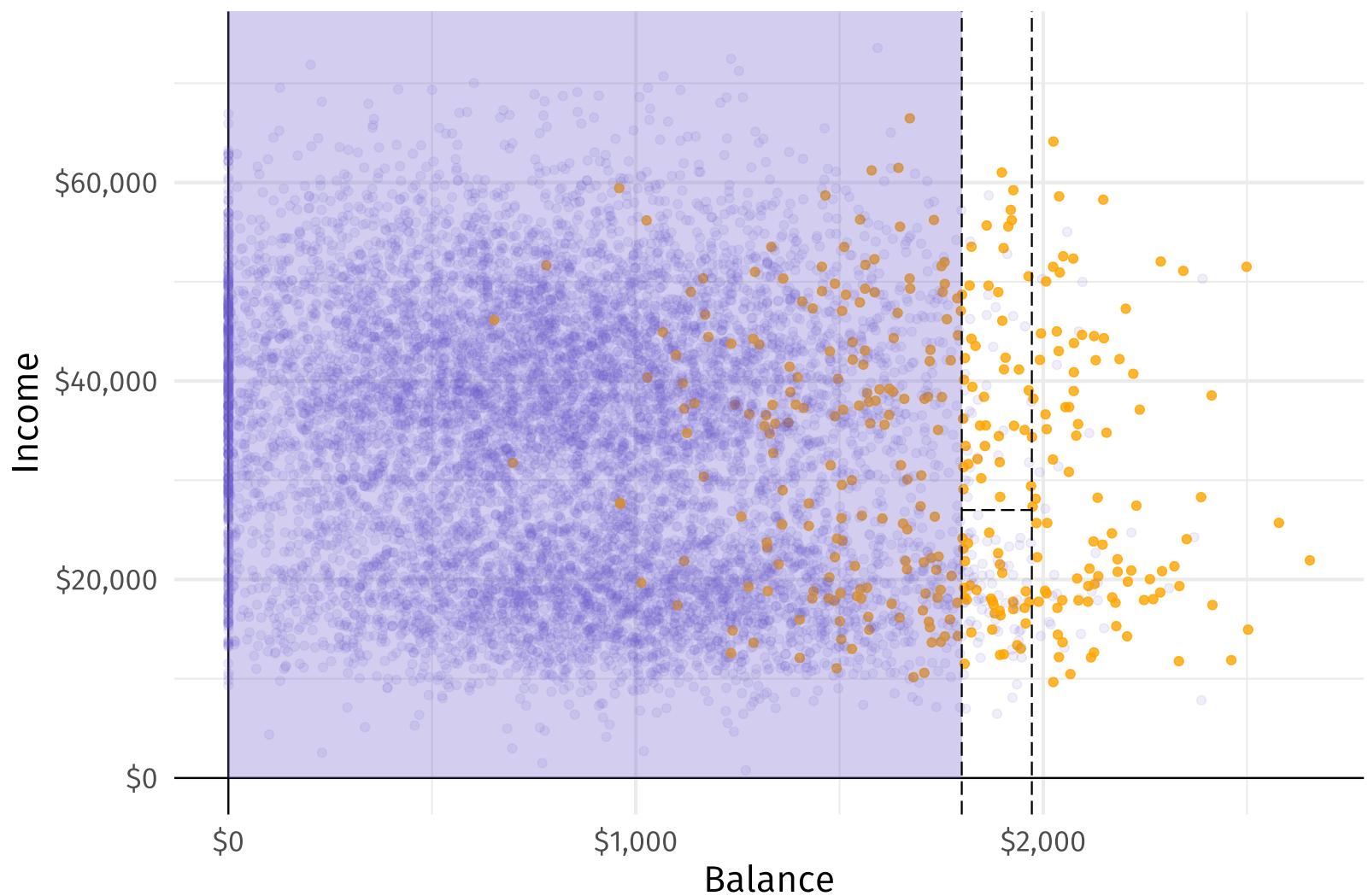
The **third partition** splits income at \$27K **for** bal. between \$1,800 and \$1,972.



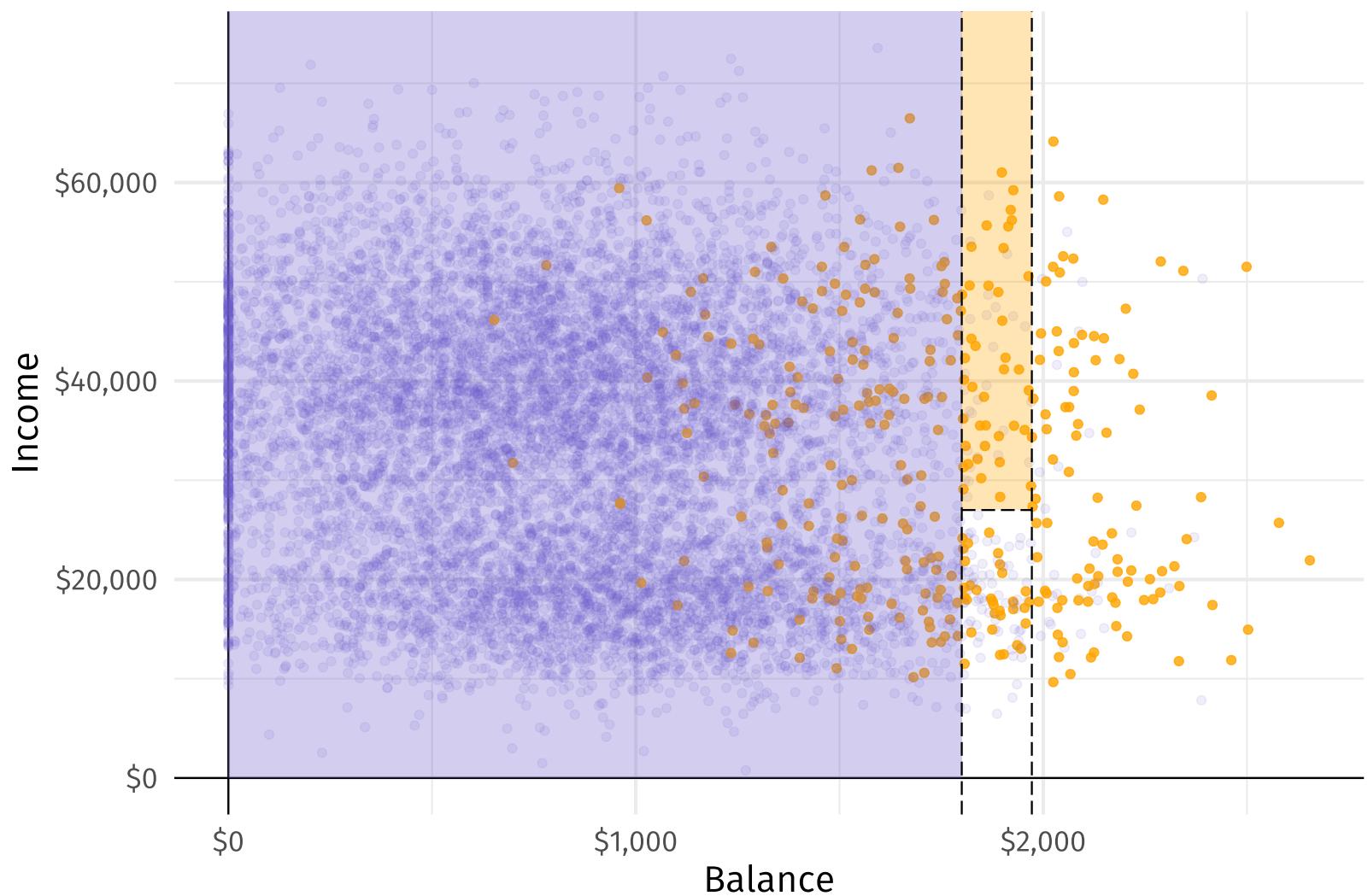
These three partitions give us four **regions**...



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



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Q Where do trees come from?

A Seeds! 

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Q How do we train (grow) trees?

Decision trees

Growing trees

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

Decision trees

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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.,

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

Decision trees

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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
2	7	8	3	2
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This split yields an RSS of $0^2 + 1^2 + (-1)^2 = 2$.

Decision trees

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

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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) $x_1 \geq 4$

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 . 

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

Decision trees

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A "More splits" means

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

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Decision trees

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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.

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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 $T \subset T_0$.

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We choose α via cross validation.

Decision trees

Classification trees

Classification with trees is very similar to regression.

Decision trees

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Regression trees

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

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.

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)?

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.

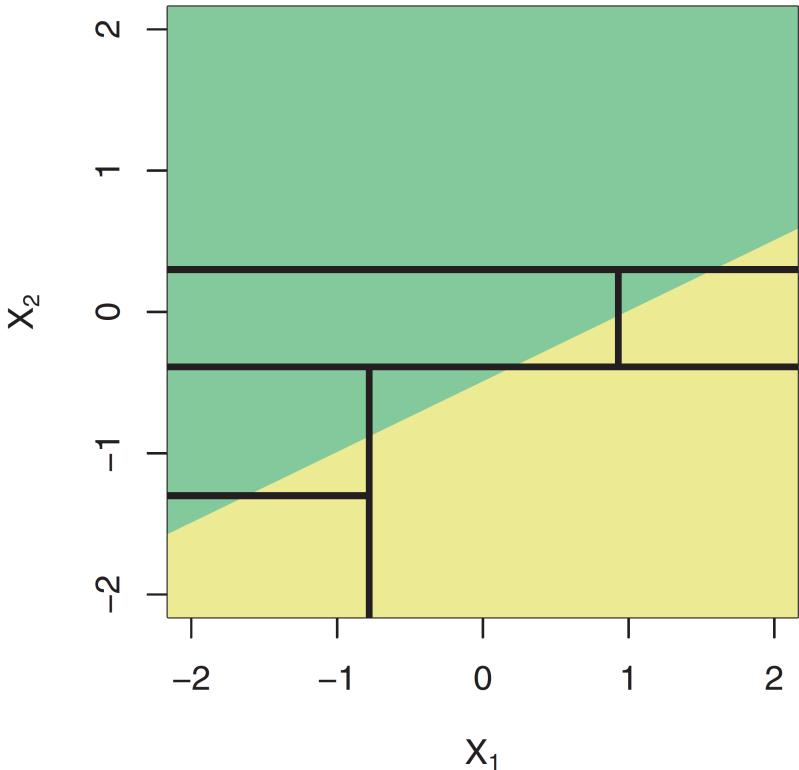
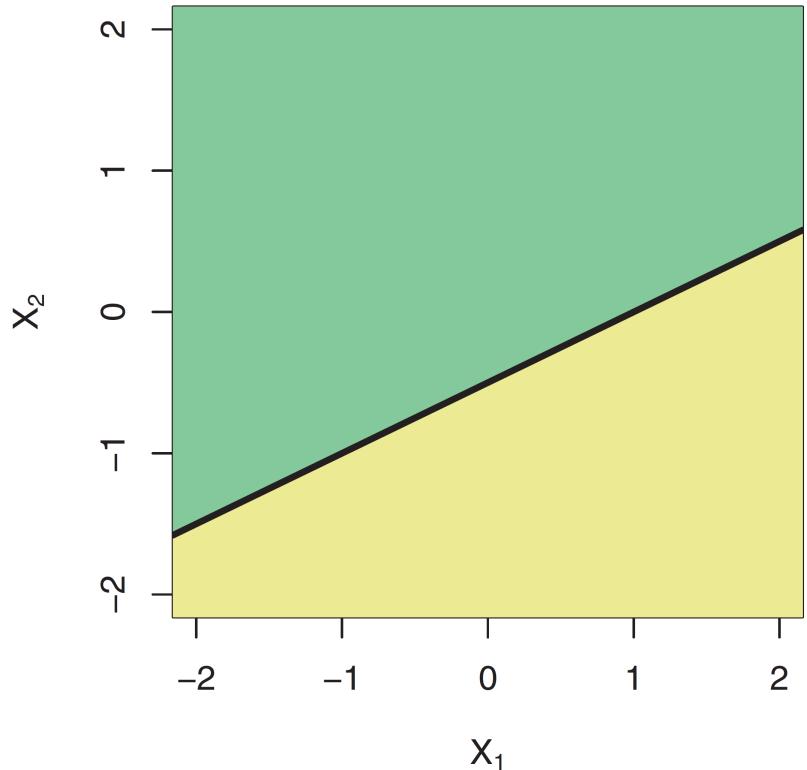
However, when **pruning**, the error rate is typically fine—especially if accuracy will be the final criterion.

Q How do trees compare to linear models?

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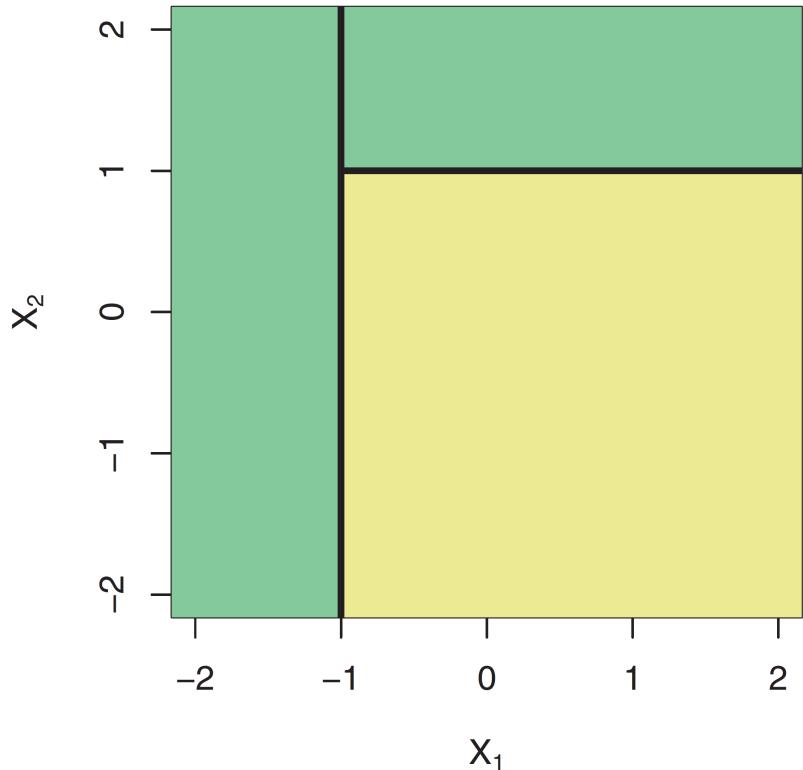
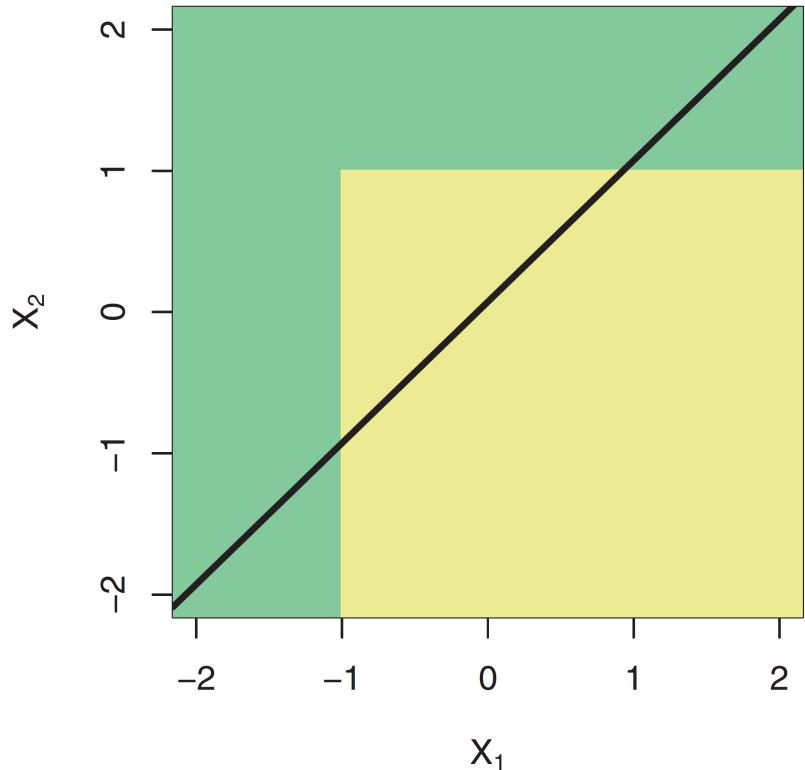
A It depends how linear the true boundary is.

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

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

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

Next: Create ensembles of trees  to strengthen these weaknesses. 

-  Without needing to create lots of dummy variables!
-  Forests!  Which will also weaken some of the strengths.

Ensemble methods

Ensemble methods

Intro

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

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

1. **Bagging**
2. **Random forests**
3. **Boosting**

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

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

 We will lose interpretability.

Ensemble methods

Bagging

Bagging creates additional samples via bootstrapping.

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Q How does bootstrapping help?

Ensemble methods

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

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Q How does bootstrapping help?

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

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

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

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

Ensemble methods

Bagging

Bootstrap aggregation (bagging) reduces this type of variability.

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

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

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

Ensemble methods

Bagging trees

When we apply bagging to decision trees,

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

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

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Bagging trees

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

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

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

Ensemble methods

Out-of-bag error estimation

Bagging also offers a convenient method for evaluating performance.

Ensemble methods

Out-of-bag error estimation

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For any bootstrapped sample, we omit $\sim n/3$ observations.

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

Ensemble methods

Out-of-bag error estimation

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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 $\hat{f}^b(\mathbf{x}_i)$, e.g., using their mean or mode
3. Calculate the error, e.g., $y_i - \hat{f}_{i,\text{OOB},i}(x_i)$

Ensemble methods

Out-of-bag error estimation

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

Ensemble methods

Out-of-bag error estimation

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

Q Why use OOB error rate?

Ensemble methods

Out-of-bag error estimation

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

Q Why use OOB error rate?

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

Ensemble methods

Bagging

Bagging has one additional shortcoming...

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

Ensemble methods

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

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Bagging has one additional shortcoming...

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

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

Solution We should make the trees less correlated.

Ensemble methods

Random forests

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

Ensemble methods

Random forests

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

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

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

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

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

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

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

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

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

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

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

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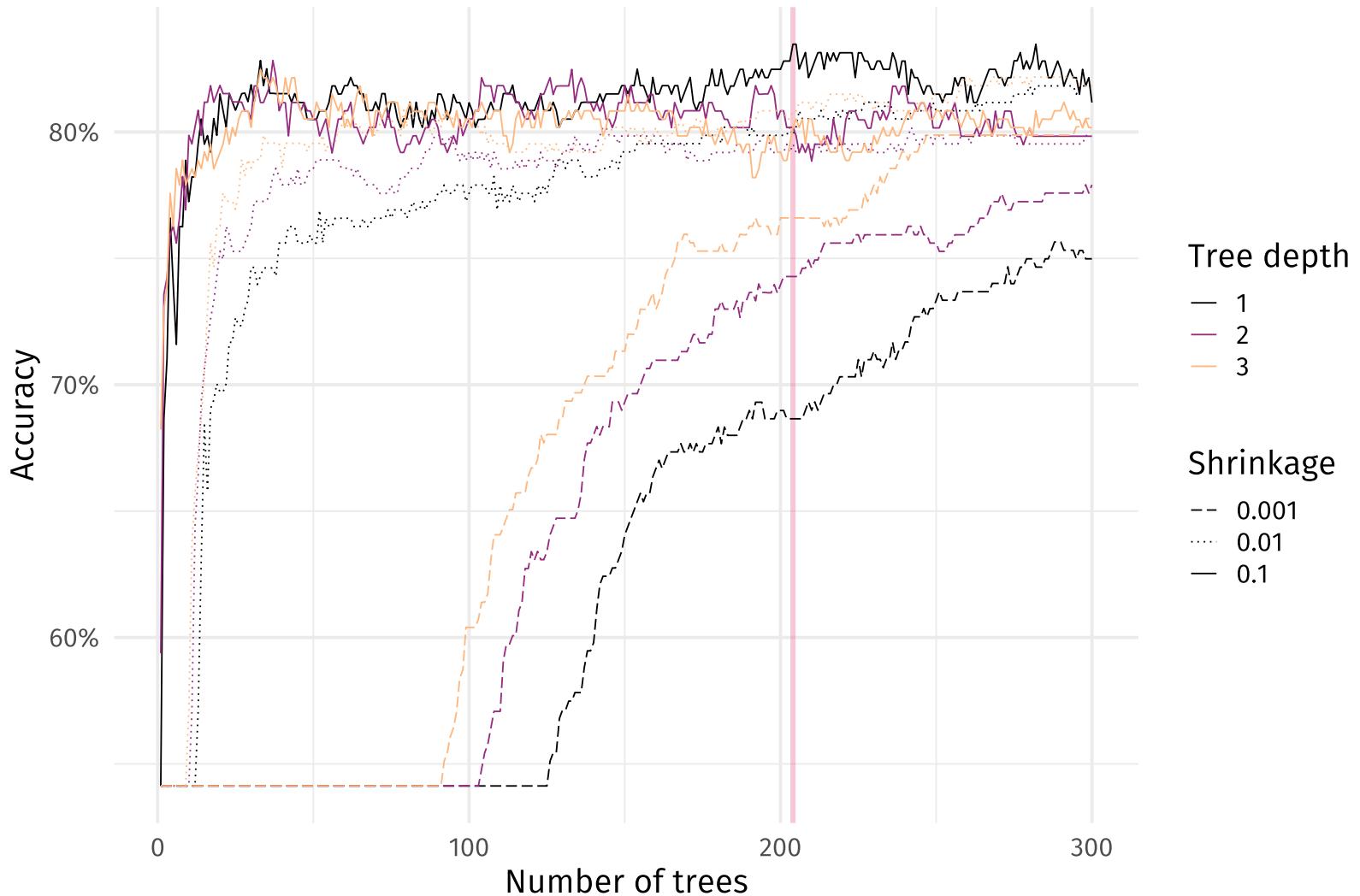
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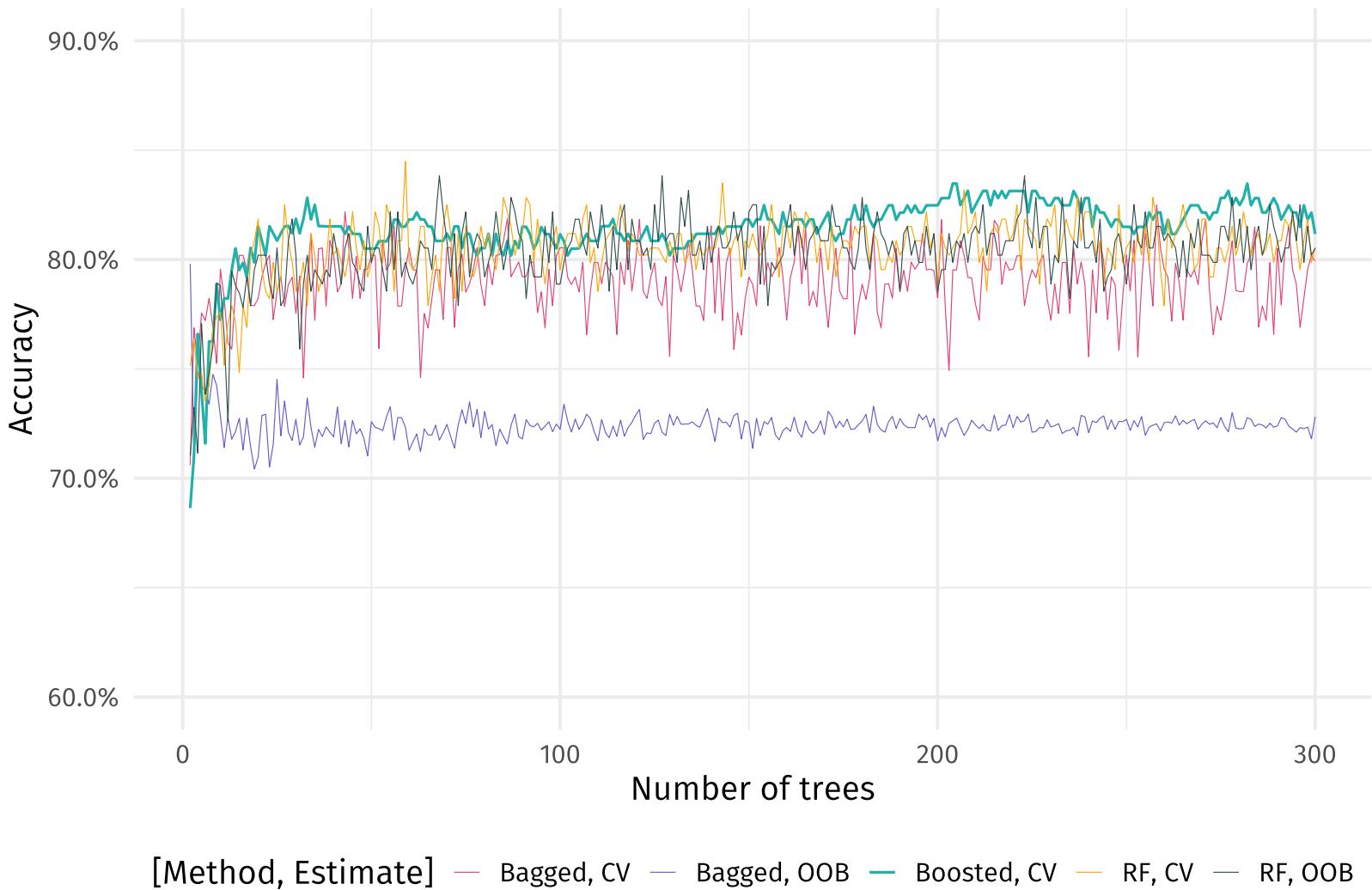
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Step 3: Output the boosted model: $\hat{f}(x) = \sum_b \lambda \hat{f}^b(x)$.

Comparing boosting parameters—notice the rates of learning



Tree ensembles and the number of trees



Sources

Sources (articles) of images

- Deep learning and radiology
- Parking lot detection
- *New Yorker* writing
- Gender Shades

Tree-classification boundary examples come from [ISL](#).

I pulled the comic from [Twitter](#).