(Some of) Machine Learning

EC 607, Set 13

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Spring 2021

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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What's different?

Machine-learning methods *typically* focus on **prediction**. What's different?

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

$$\mathbf{Y}_i = \mathbf{X}_i\beta + \boldsymbol{u}_i$$

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 $\hat{\beta}$.

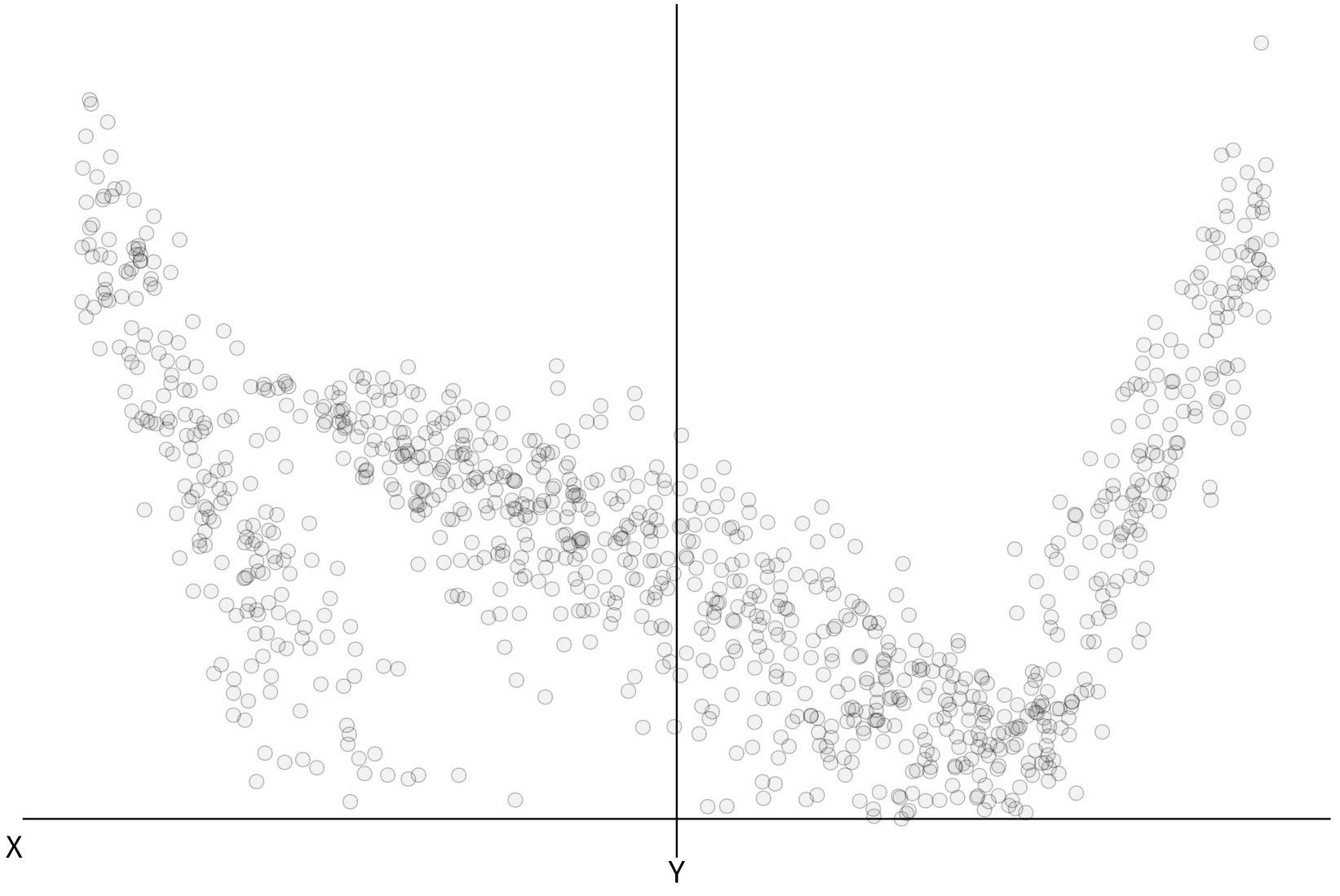
Q Can't we just use the same methods (*i.e.*, OLS)?

A It depends. How well does your **linear**-regression model approximate the underlying data? (And how do you plan to select your model?)

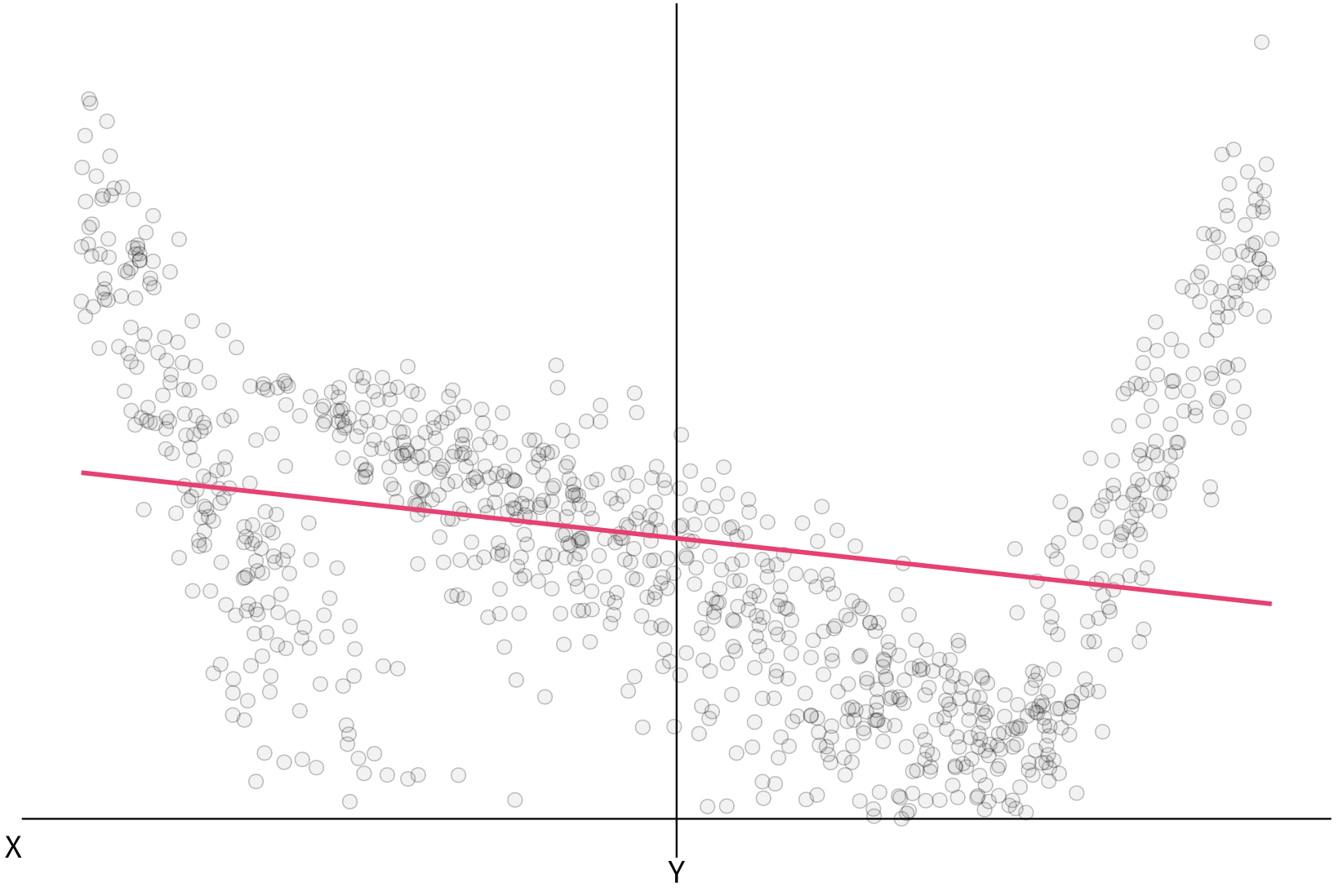
Recall Least-squares regression is a great **linear** estimator and predictor.

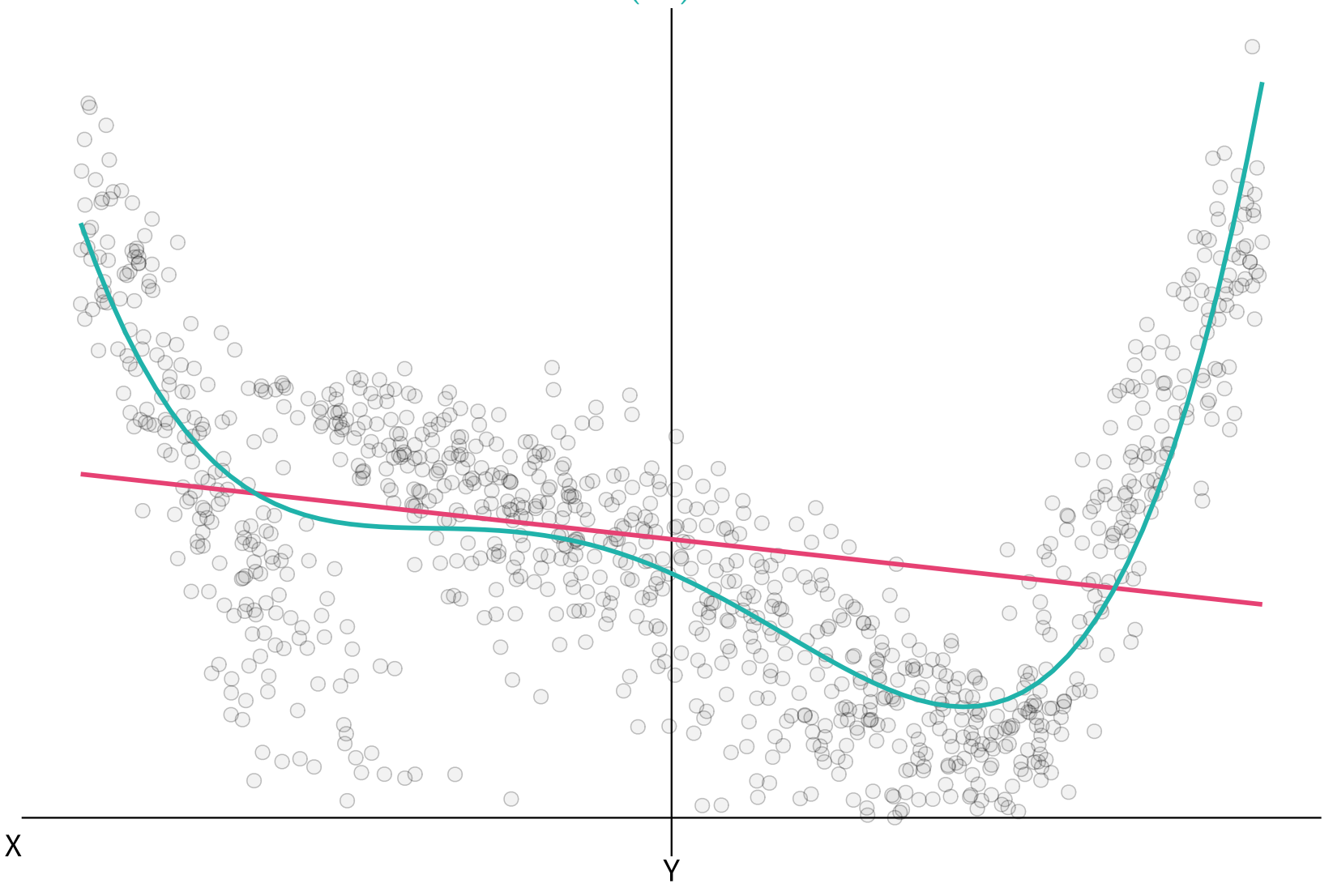
Data data be tricky[†]—as can understanding many relationships.

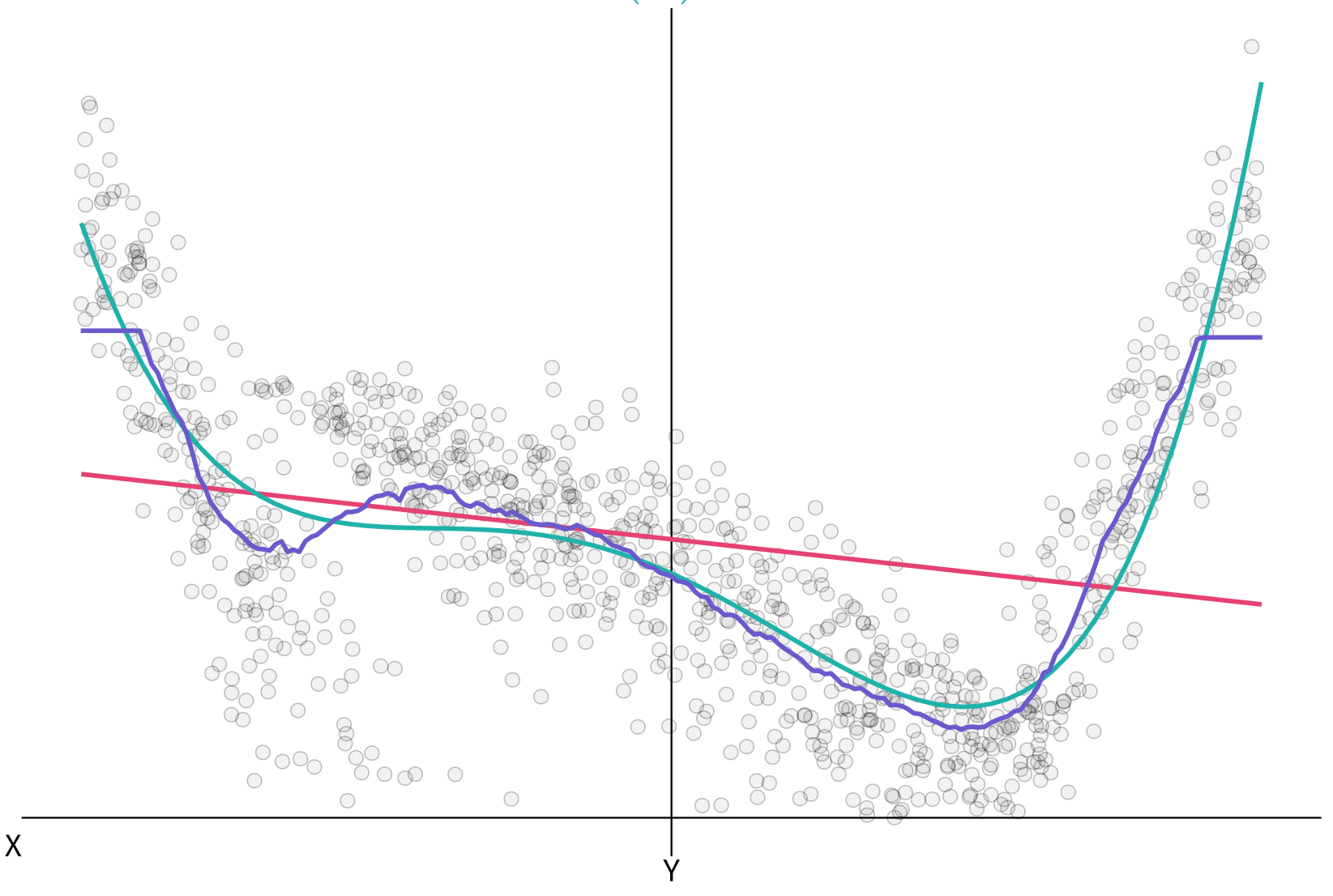
† "Tricky" might mean nonlinear... or many other things...

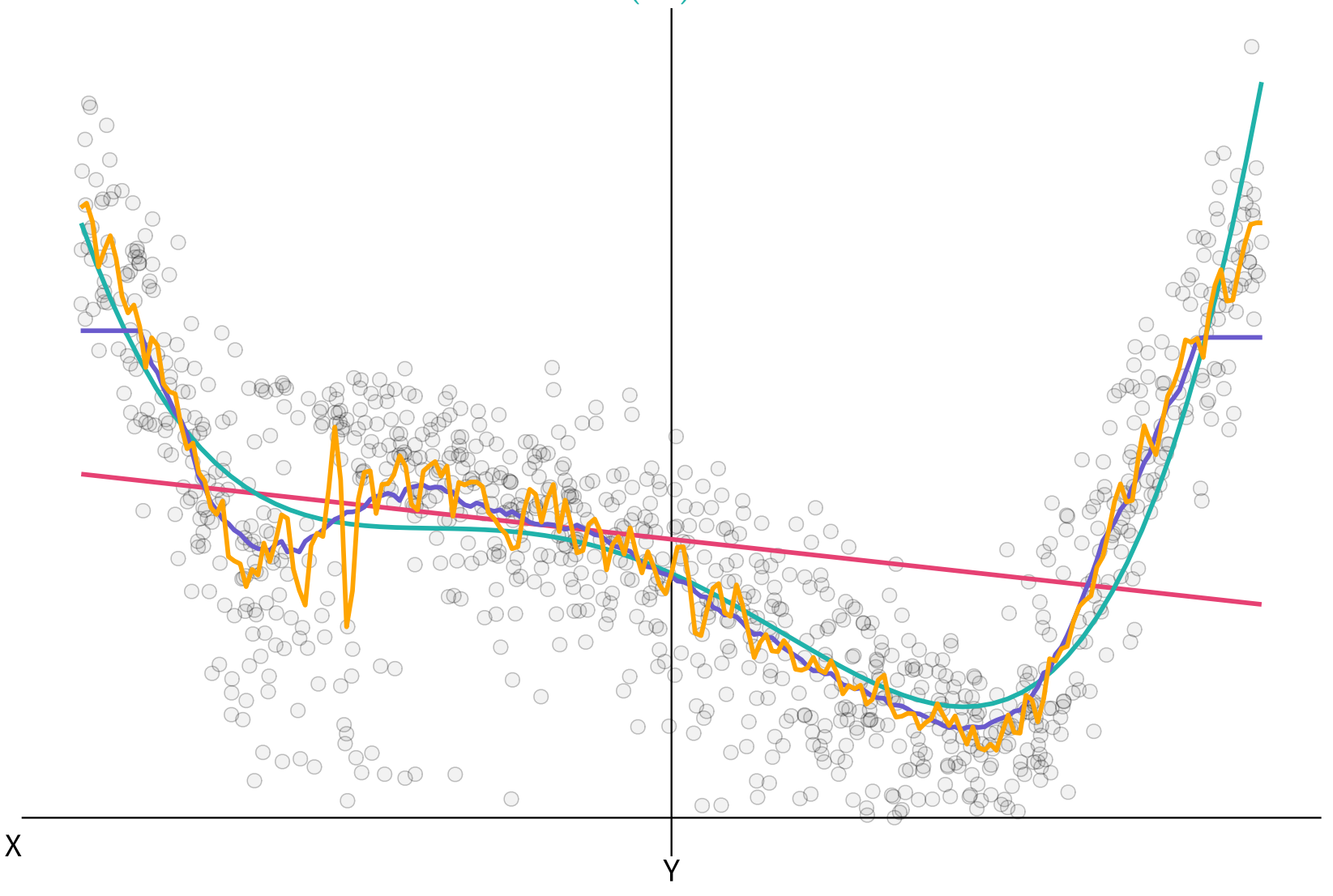

X
Y

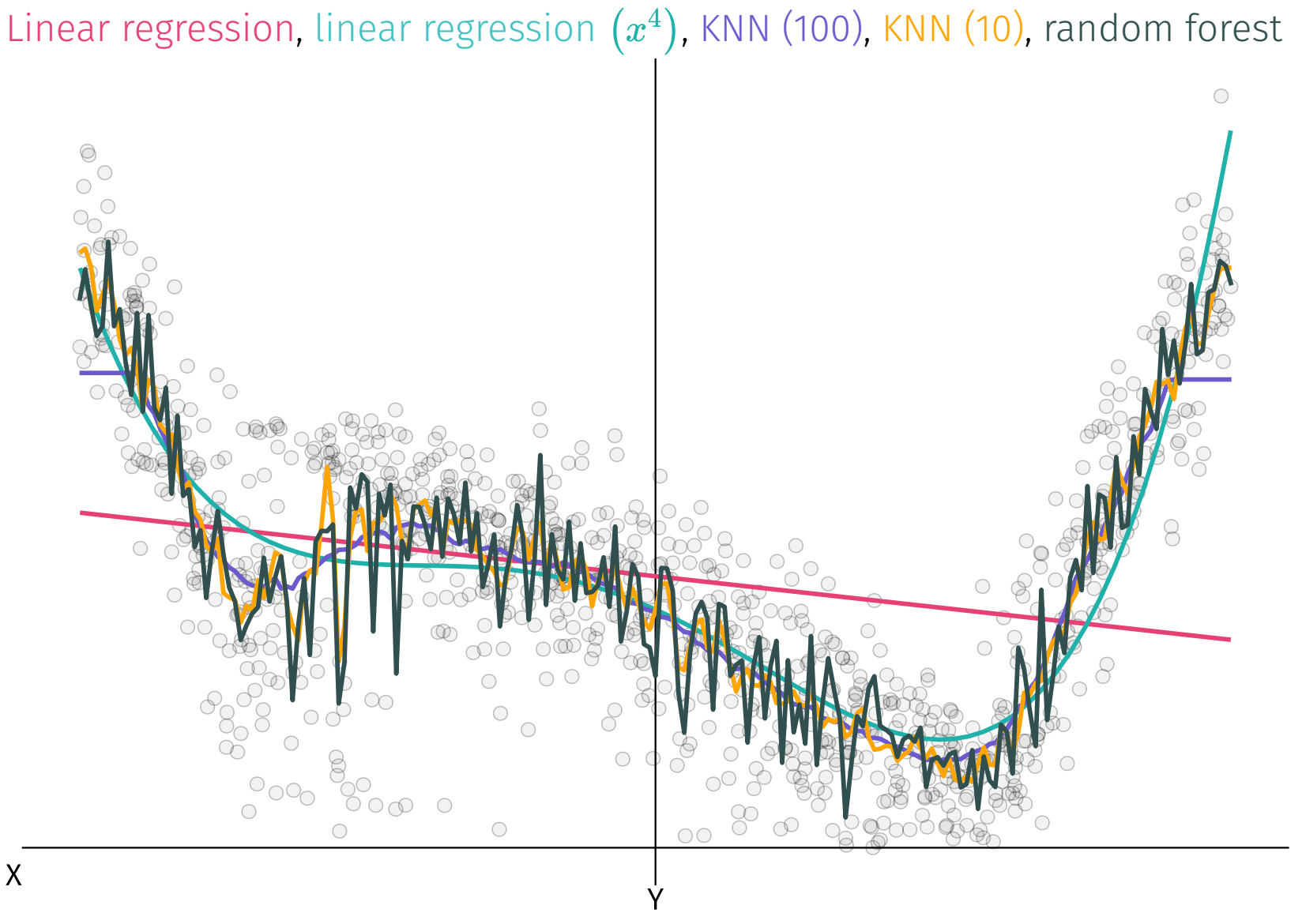
Linear regression




Linear regression, linear regression $\left(x^4\right)$
X
Y


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


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


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

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**

As your economic training should have predicted, in each setting, we need to **balance the additional benefits and costs** of adjusting these tradeoffs.

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

What's the goal?

There are many reasons to step outside the world of linear regression...

Multi-class classification problems

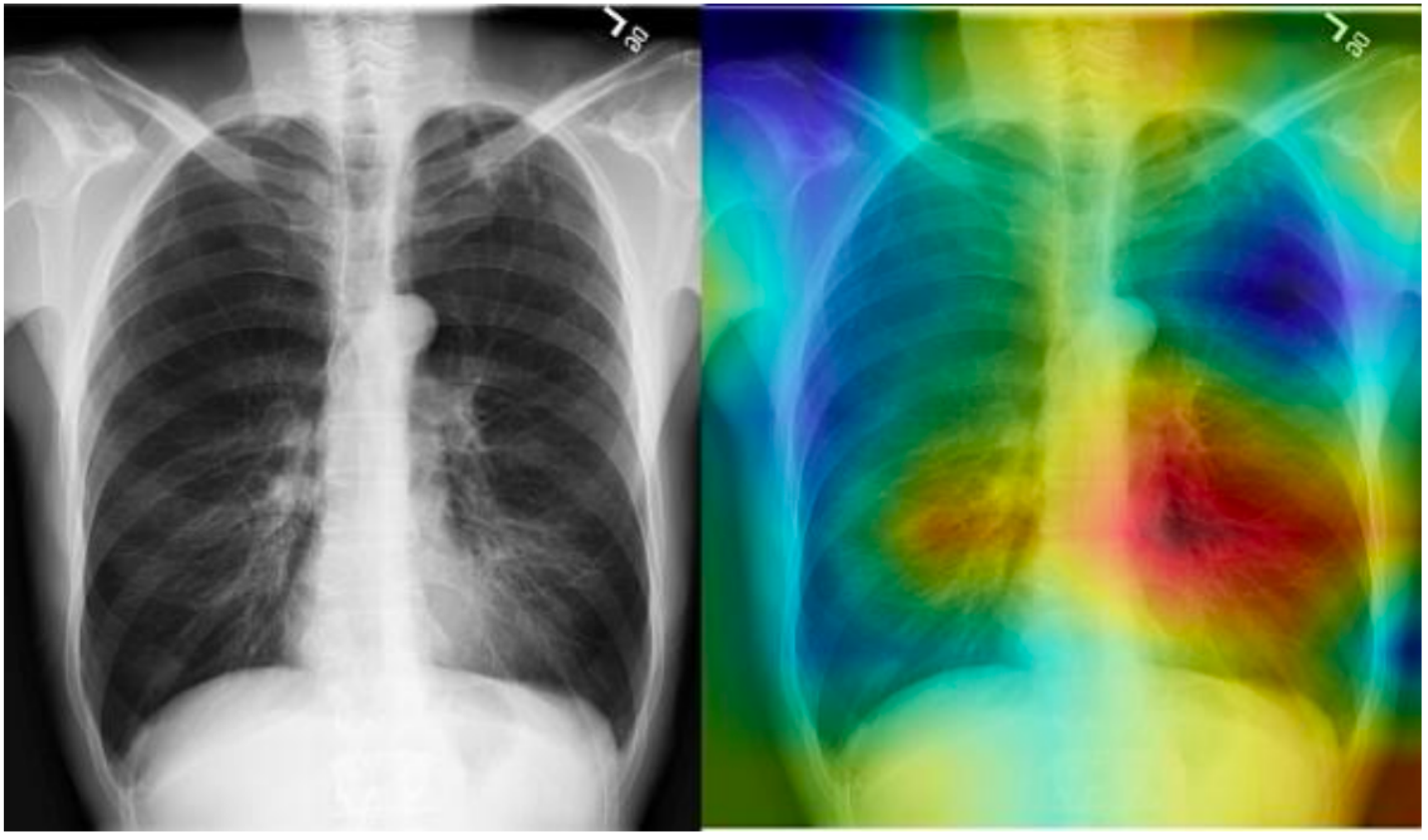
- Rather than {0,1}, we need to classify y_i into 1 of K classes
- *E.g.*, ER patients: {heart attack, drug overdose, stroke, nothing}

Text analysis and **image recognition**

- Comb though sentences (pixels) to glean insights from relationships
- *E.g.*, detect sentiments in tweets or roof-top solar in satellite imagery

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

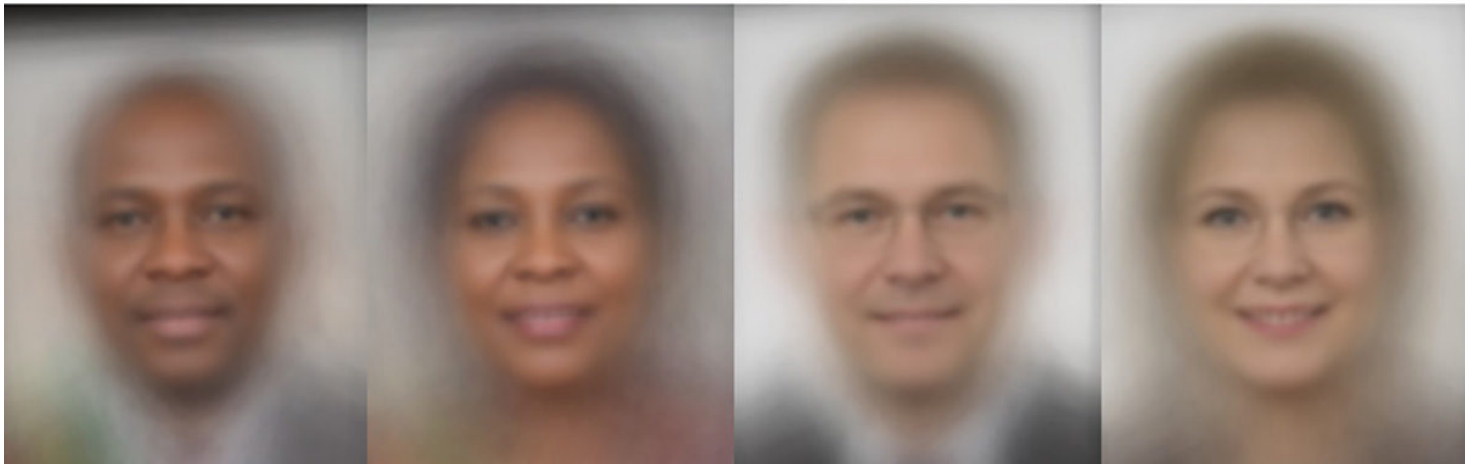
A REPORTER AT LARGE OCTOBER 14, 2019 ISSUE

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

What is it good for?

A lot of things. We tend to break statistical-learning into two(-ish) classes:

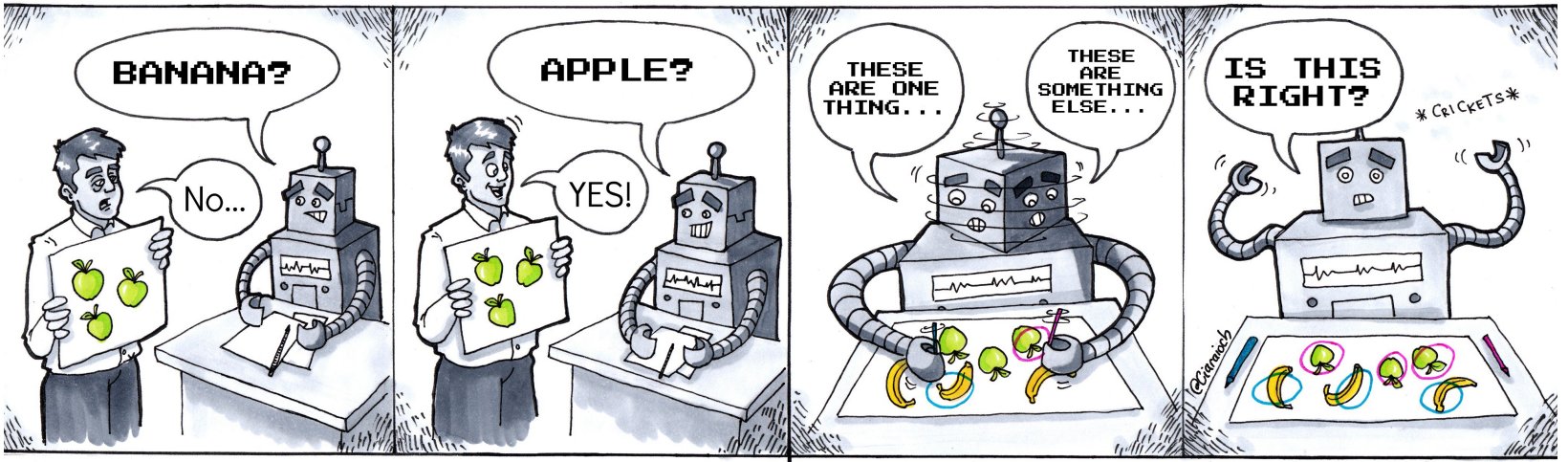
1. **Supervised learning** builds ("learns") a statistical model for predicting an **output** ($\mathbf{y}$) given a set of **inputs** ($\mathbf{x}_1, \ldots, \mathbf{x}_p$), *i.e.*, we want to build a model/function f

$$\mathbf{y} = f(\mathbf{x}_1, \ldots, \mathbf{x}_p)$$

   that accurately describes $\mathbf{y}$ given some values of $\mathbf{x}_1, \ldots, x_p$.

2. **Unsupervised learning** learns relationships and structure using only **inputs** ($x_1, \ldots, x_p$) without any *supervising* output—letting the data "speak for itself."

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

Output

We tend to further break **supervised learning** into two groups, based upon the **output** (the outcome we want to predict):

1. **Classification tasks** for which the values of $\mathbf{y}$ are discrete categories
   E.g., race, sex, loan default, hazard, disease, flight status

2. **Regression tasks** in which $\mathbf{y}$ takes on continuous, numeric values.
   E.g., price, arrival time, number of emails, temperature

$Note_1$ The use of *regression* differs from our use of *linear regression*.

$Note_2$ 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?

Statistical learning

The goal

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

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

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

Learning from $\hat{f}$

There are two main reasons we want to learn about f

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

   What we've done all quarter.

2. **Prediction problems** Predict $\mathbf{y}$ using our estimated f, *i.e.*,

$$\hat{\mathbf{y}} = \hat{f}(\mathbf{X})$$

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

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

† You shouldn't actually treat your prediction methods as total black boxes.

Prediction errors

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

The accuracy of $\hat{\mathbf{y}}$ depends upon **two errors**:

1. **Reducible error** The error due to $\hat{f}$ imperfectly estimating f.
   Reducible in the sense that we could improve $\hat{f}$.

2. **Irreducible error** The error component that is outside of the model f.
   Irreducible because we defined an error term ε unexplained by f.

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

Prediction errors

Why we're stuck with *irreducible* error

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

In less math:

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

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.

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}\left[y_i - \hat{f}\left(x_i\right)\right]^2$$

Recall: $y_i - \hat{f}\left(x_i\right) = y_i - \hat{y}_i$ is our prediction error.

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).

† *Most common* does not mean best—it just means lots of people use it.

Model accuracy

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**?

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 $\hat{f}$.

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

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

Model accuracy

Regression and loss

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

$$\text{error}_i = y_i - \hat{y}_i \qquad \text{loss}_i = |y_i - \hat{y}_i| = |\text{error}_i|$$

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

$$\text{L1 loss} = \sum_i |y_i - \hat{y}_i| \qquad \text{MAE} = \frac{1}{n} \sum_i |y_i - \hat{y}_i|$$

$$\text{L2 loss} = \sum_i (y_i - \hat{y}_i)^2 \qquad \text{MSE} = \frac{1}{n} \sum_i (y_i - \hat{y}_i)^2$$

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 $\mathbf{Pr}\big(y_0 = j \big| \mathbf{X} = \mathbf{x}_0\big)$ 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 $\mathbf{Pr}\big(y_0 = j \big| \mathbf{X} = \mathbf{x}_0\big)$.

Flexibility

The bias-variance tradeoff

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

Bias The error that comes from inaccurately estimating 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

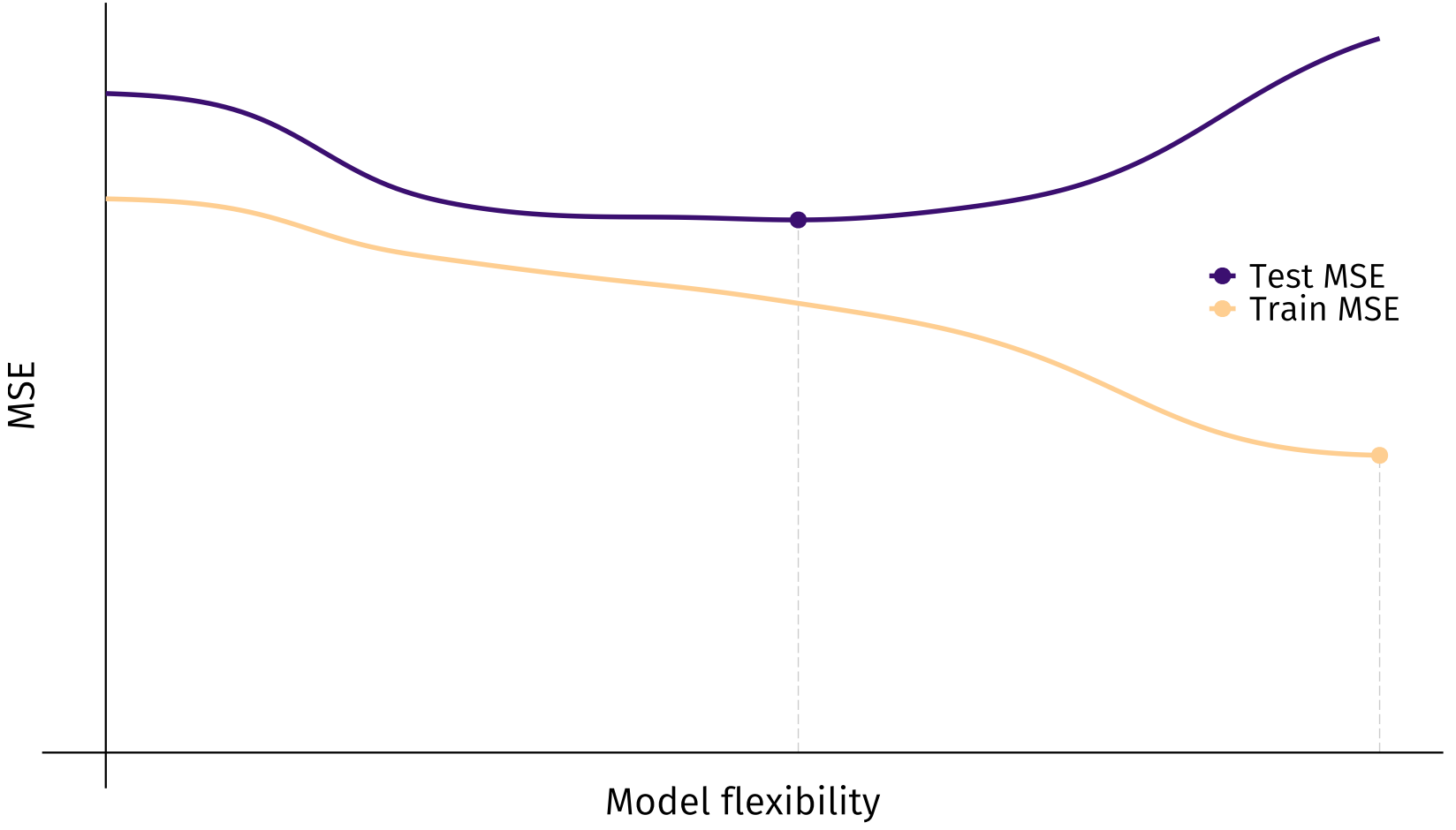
The expected value[†] of the **test MSE** can be written

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

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?

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).

$\mathbf{Q}_1$ What if we don't have a test set?
$\mathbf{Q}_2$ What if we need to select and train a model?
$\mathbf{Q}_3$ How can we avoid overfitting our training[†] data during model selection?

$\mathbf{A}_{1,2,3}$ **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**
- The model only "sees" the non-validation subset of the **training data**.

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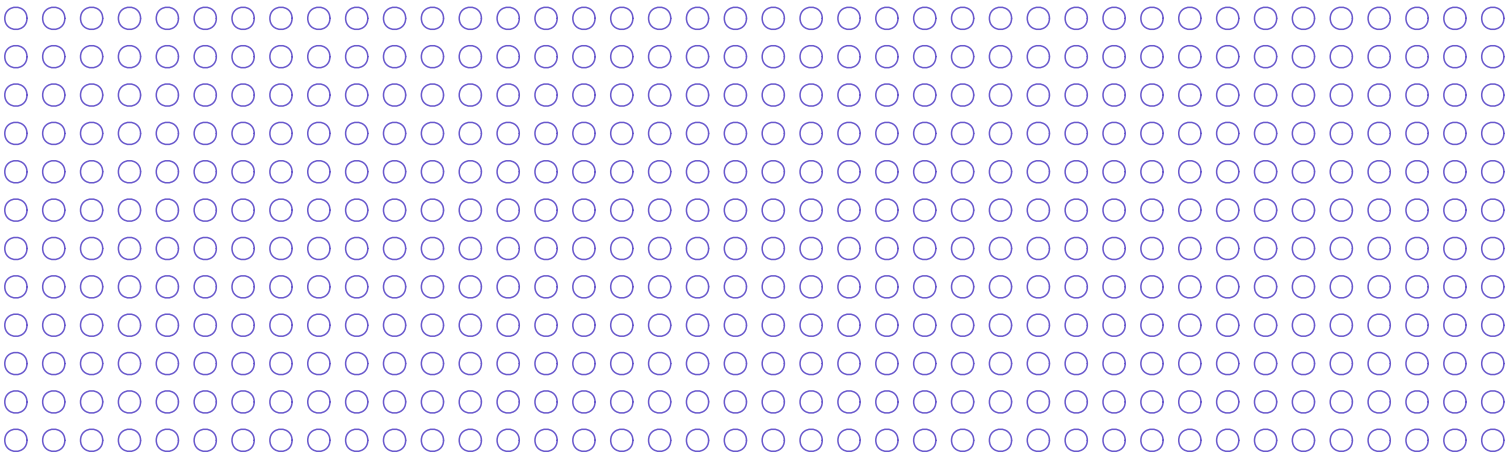

Initial training set

Hold-out methods

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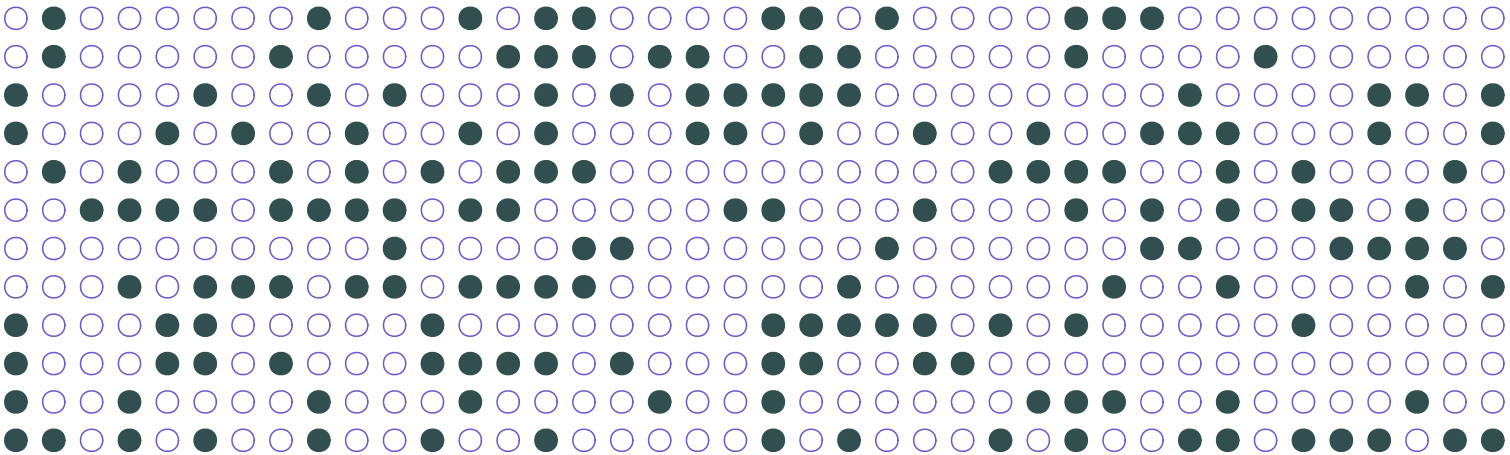

Validation (sub)set **Training set:** Model training

Hold-out methods

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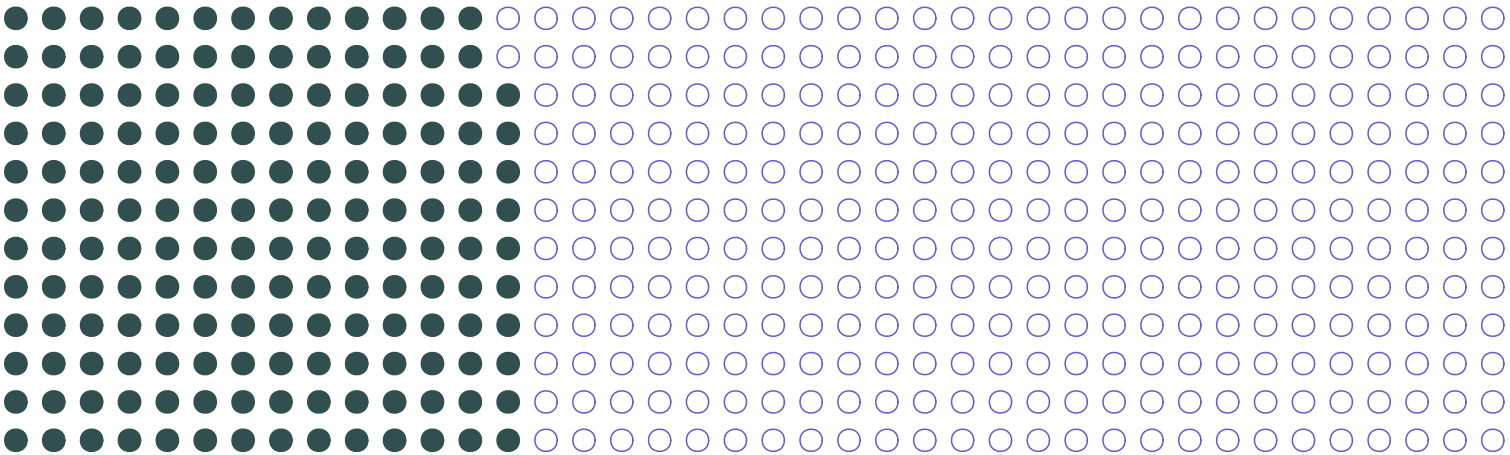


Validation (sub)set **Training set:** Model training

Hold-out methods

Option 1: The *validation set* approach

Example We could use the validation-set approach to help select the degree of a polynomial for a linear-regression model.

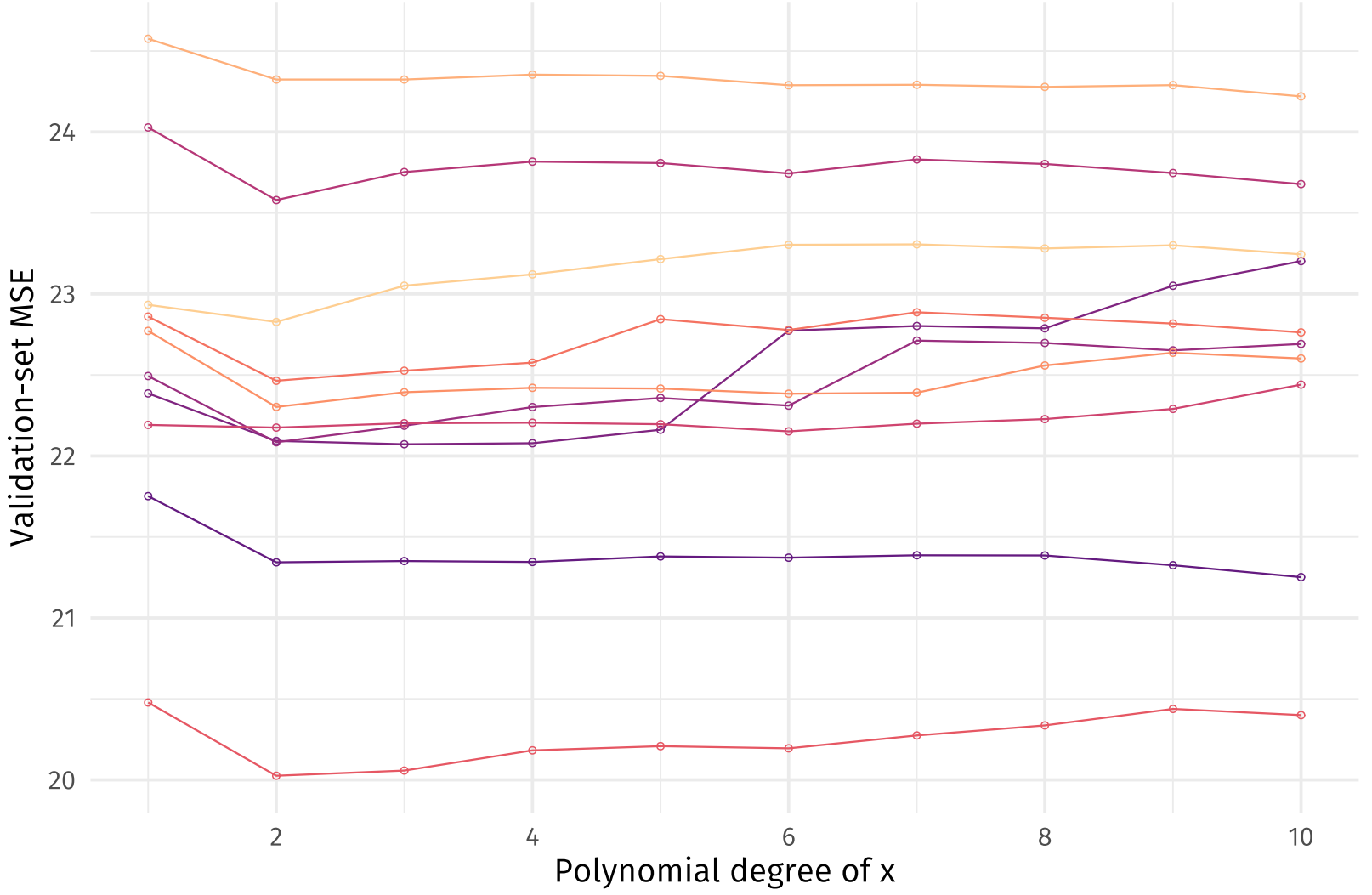
The goal of the validation set is to ***estimate* out-of-sample (test) error.**

Q So what?

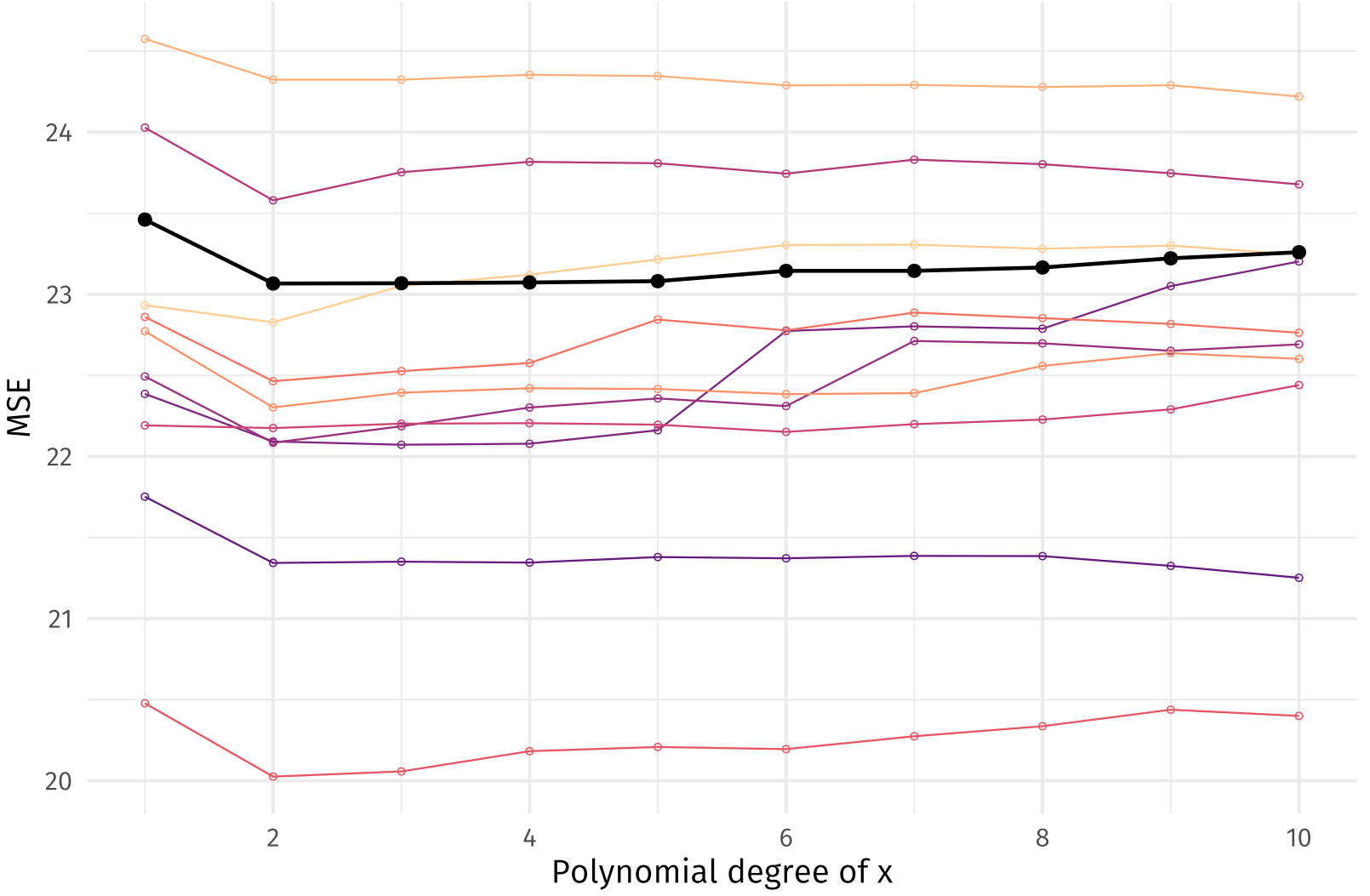
- Estimates come with **uncertainty**—varying from sample to sample.
- Variability (standard errors) is larger with **smaller samples**.

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 (≥) 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.

(2) $\Longrightarrow$ 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.

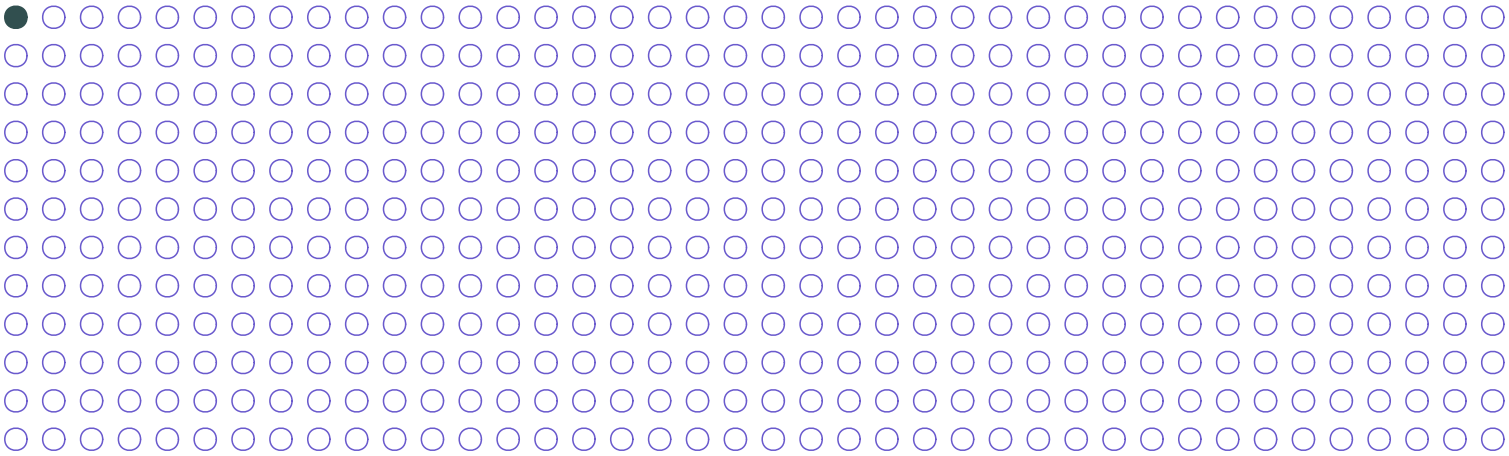
Leave-one-out cross validation (LOOCV) is perhaps the cross-validation method most similar to the validation-set approach.

- 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

Option 2: Leave-one-out cross validation

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.

Hold-out methods

Option 2: Leave-one-out cross validation

Each observation takes a turn as the **validation set**,
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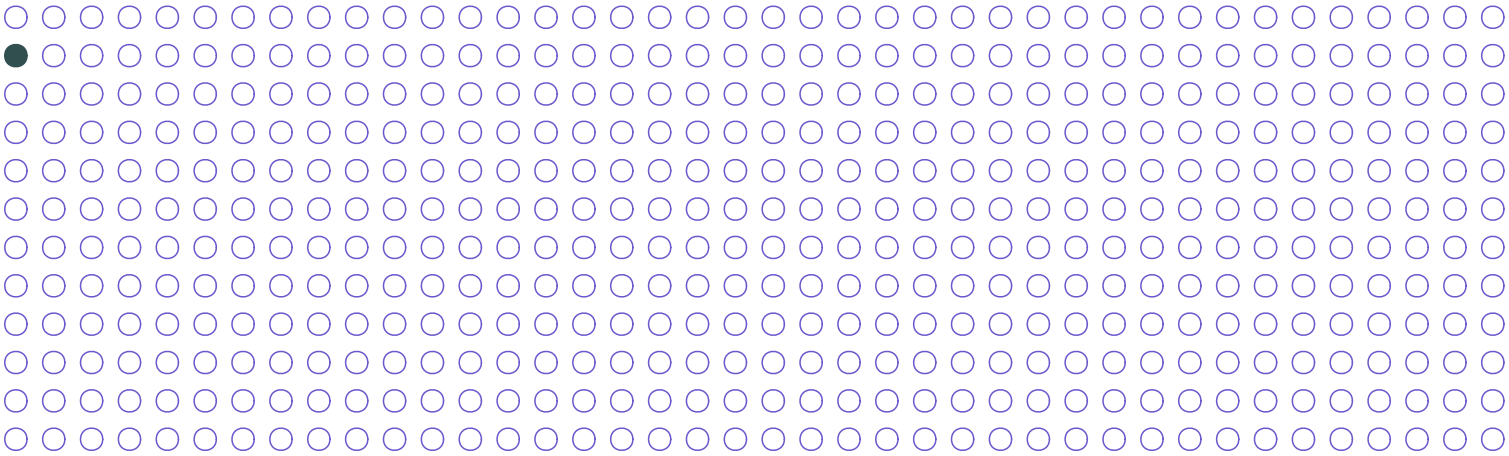
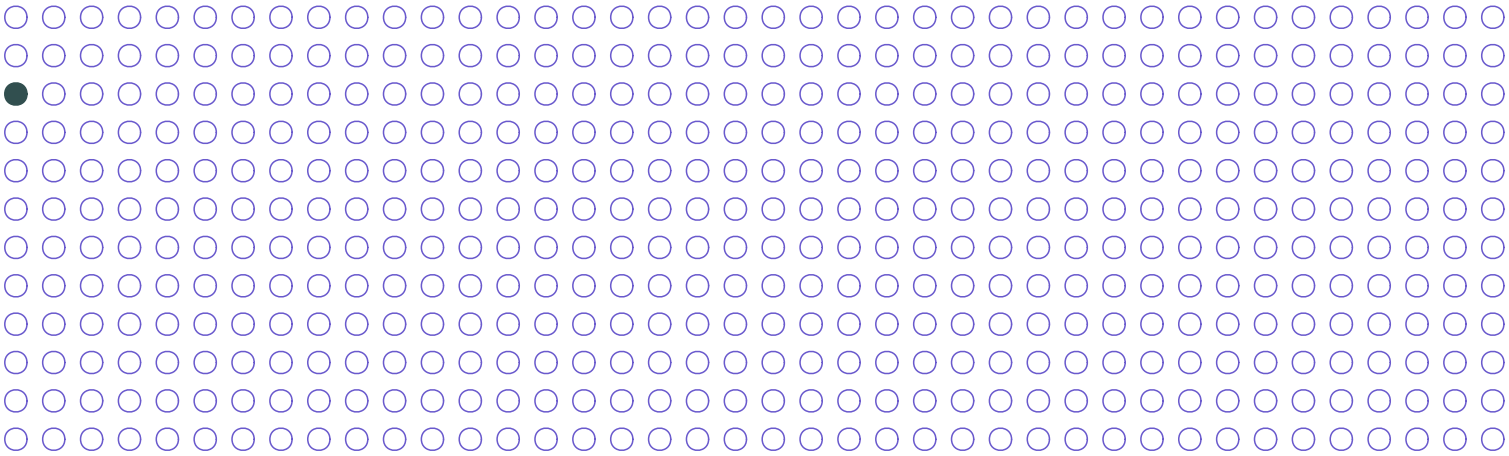


Observation 2's turn for validation produces MSE_2.

Hold-out methods

Option 2: Leave-one-out cross validation

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



Observation 3's turn for validation produces MSE_3.

Hold-out methods

Option 2: Leave-one-out cross validation

Each observation takes a turn as the **validation set**,
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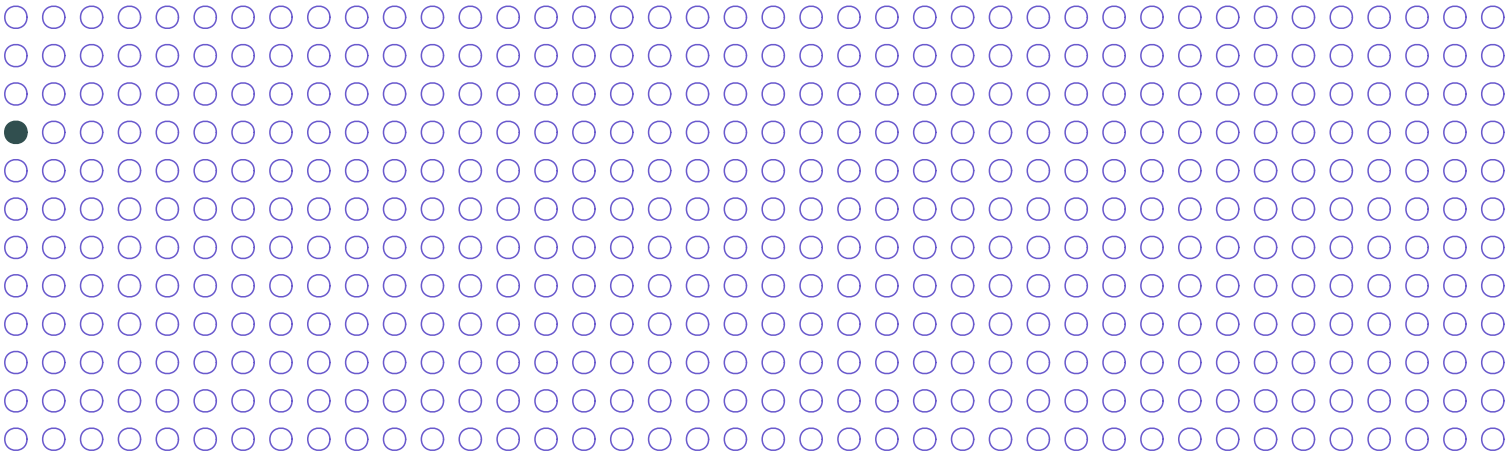
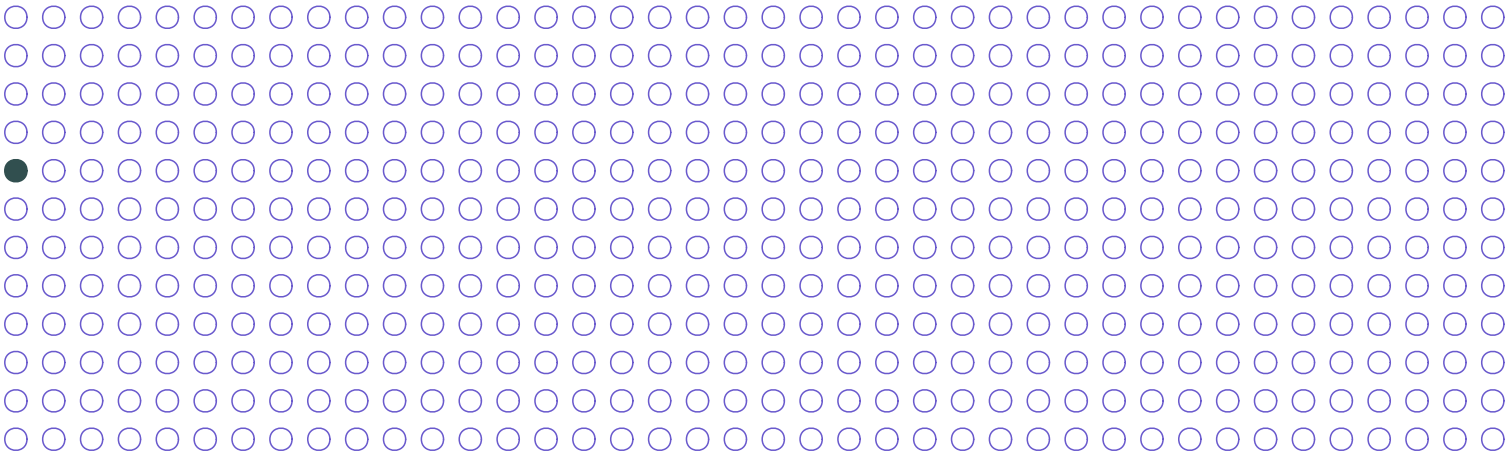


Observation 4's turn for validation produces MSE_4.

Hold-out methods

Option 2: Leave-one-out cross validation

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

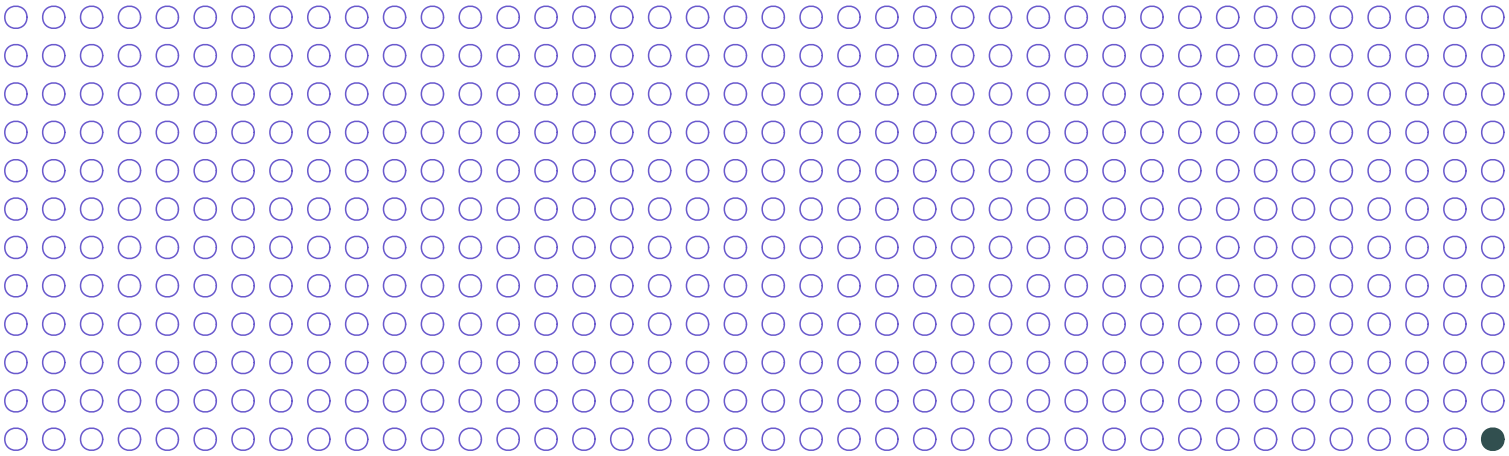


Observation 5's turn for validation produces MSE_5.

Hold-out methods

Option 2: Leave-one-out cross validation

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



Observation n's turn for validation produces MSE_n.

Hold-out methods

Option 2: Leave-one-out cross validation

Because **LOOCV uses n-1 observations** to train the model,[†] MSE_i (validation MSE from observation i) is approximately unbiased for test MSE.

Problem MSE_i is a terribly noisy estimator for test MSE (albeit ≈unbiased).

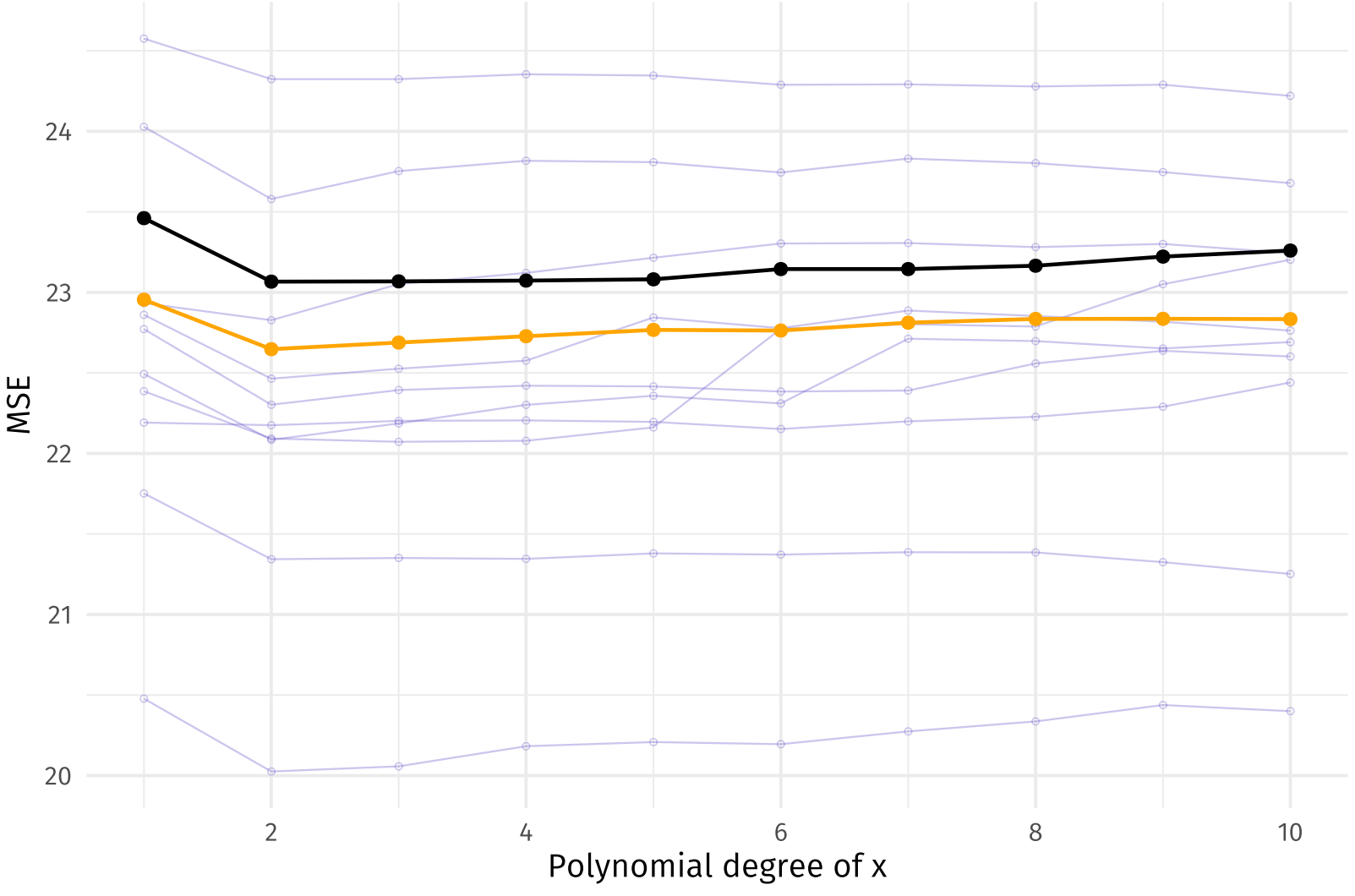
Solution Take the mean!

$$\text{CV}_{(n)} = \frac{1}{n}\sum_{i=1}^{n}\text{MSE}_i$$

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 ≈ 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).
2. **Iterate** over the k folds, treating each as a validation set once (training the model on the other $k-1$ folds).
3. **Average** the folds' MSEs to estimate test MSE.

Benefits?

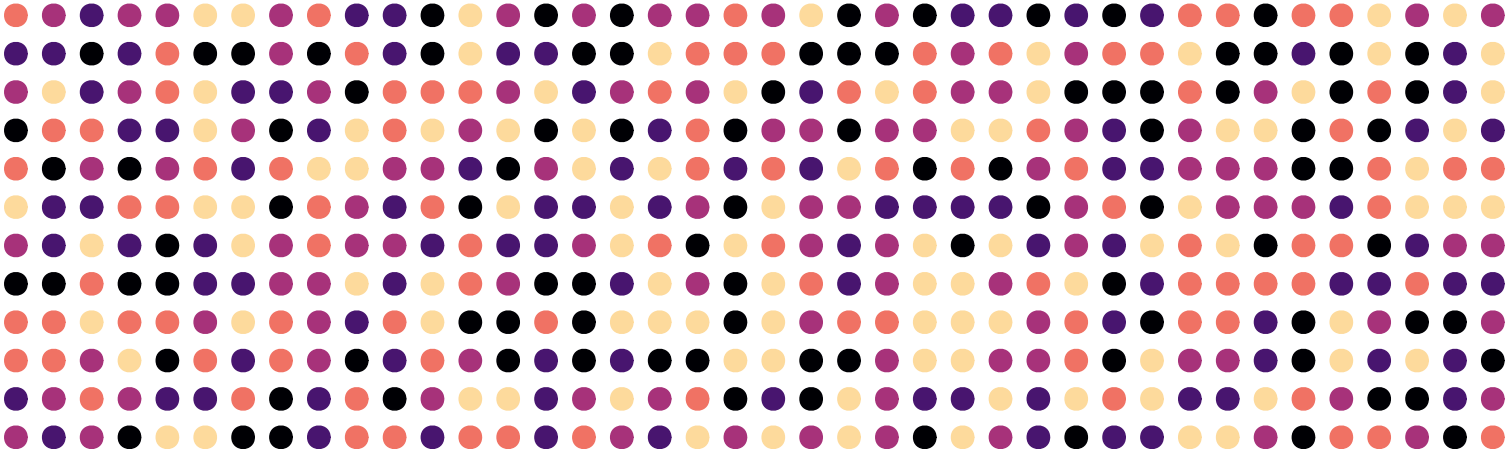
1. **Less computationally demanding** (fit model $k = 5$ or 10 times; not n).
2. **Greater accuracy** (in general) due to bias-variance tradeoff!
   - Somewhat higher bias, relative to LOOCV: $n-1$ *vs.* $(k-1)/k$.
   - Lower variance due to high-degree of correlation in LOOCV MSE_i.🤯

Hold-out methods

Option 3: k-fold cross validation

With k-fold cross validation, we estimate test MSE as

$$\text{CV}_{(k)} = \frac{1}{k} \sum_{i=1}^{k} \text{MSE}_i$$



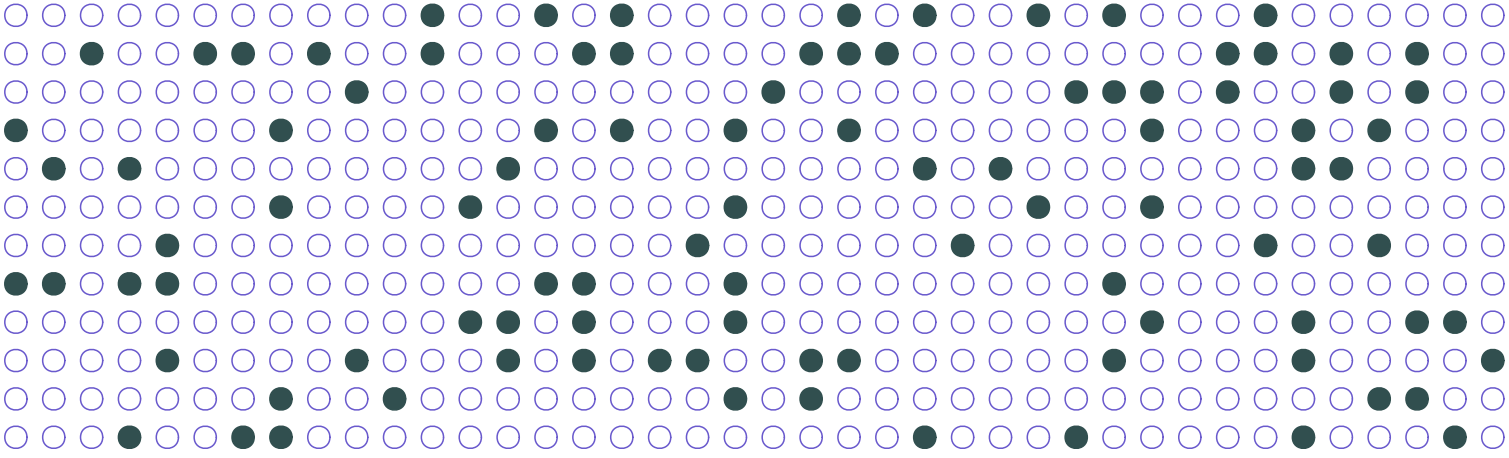
Our $k = 5$ folds.

Hold-out methods

Option 3: k-fold cross validation

With k-fold cross validation, we estimate test MSE as

$$\text{CV}_{(k)} = \frac{1}{k} \sum_{i=1}^{k} \text{MSE}_i$$

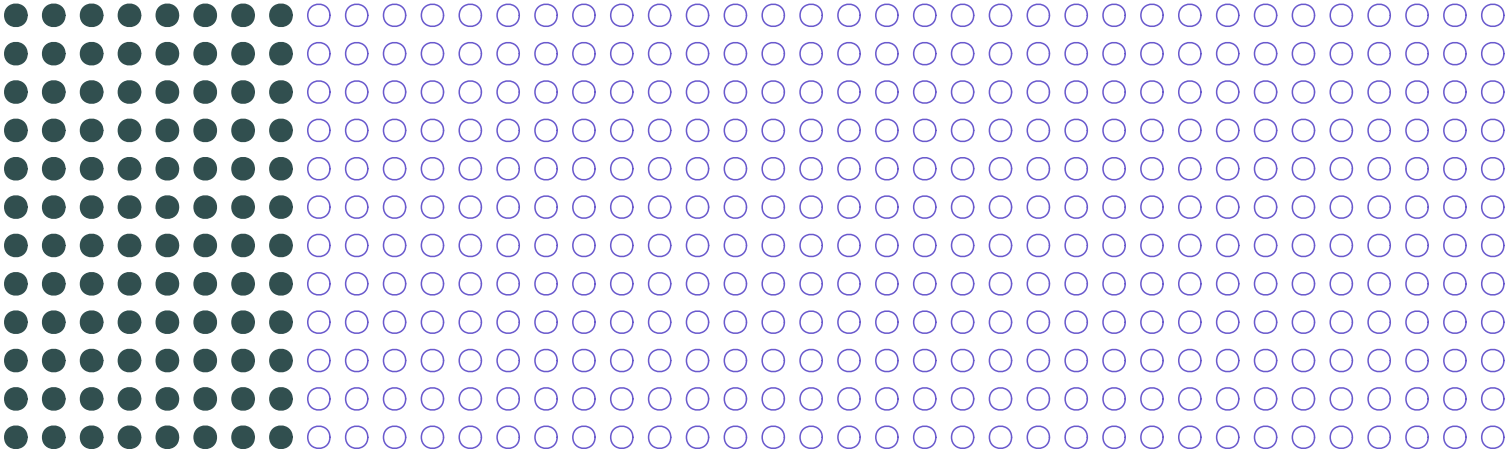


Each fold takes a turn at **validation**. The other $k - 1$ folds **train**.

Option 3: k-fold cross validation

With k-fold cross validation, we estimate test MSE as

$$\text{CV}_{(k)} = \frac{1}{k} \sum_{i=1}^{k} \text{MSE}_i$$

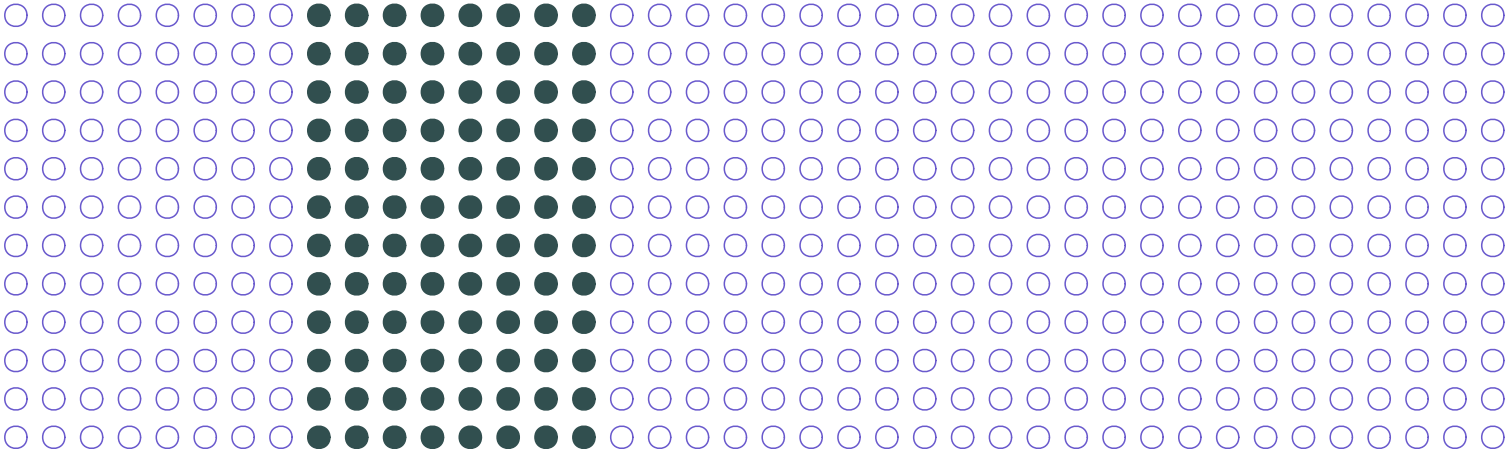


For $k = 5$, fold number 1 as the **validation set** produces $\text{MSE}_{k=1}$.

Option 3: k-fold cross validation

With k-fold cross validation, we estimate test MSE as

$$\text{CV}_{(k)} = \frac{1}{k} \sum_{i=1}^{k} \text{MSE}_i$$



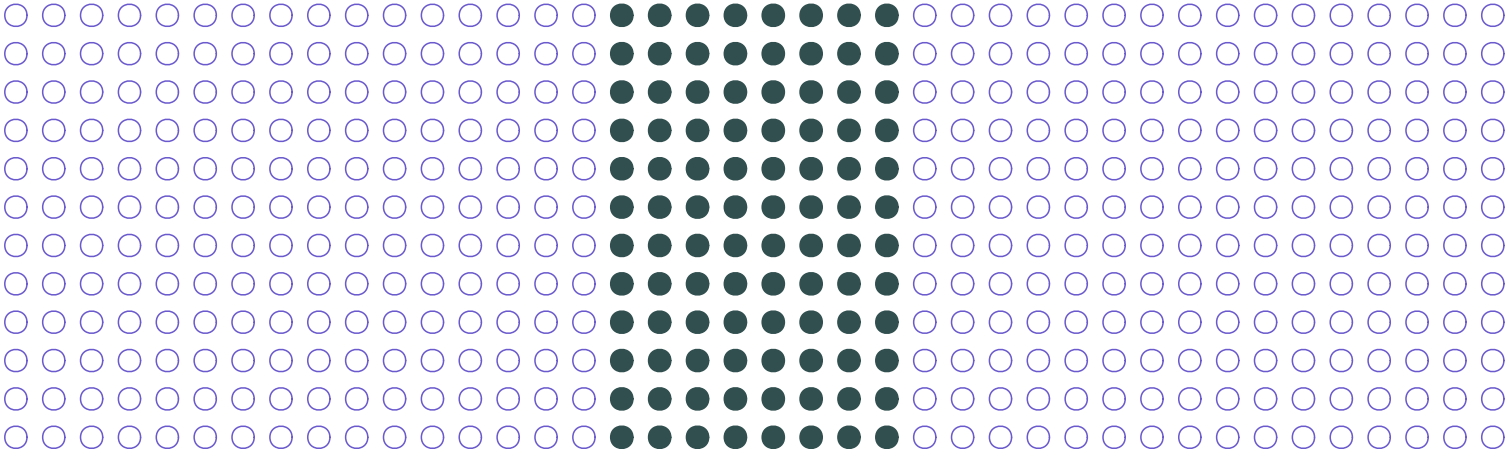
For $k = 5$, fold number 2 as the **validation set** produces $\text{MSE}_{\text{k=2}}$.

Hold-out methods

Option 3: k-fold cross validation

With k-fold cross validation, we estimate test MSE as

$$\text{CV}_{(k)} = \frac{1}{k} \sum_{i=1}^{k} \text{MSE}_i$$



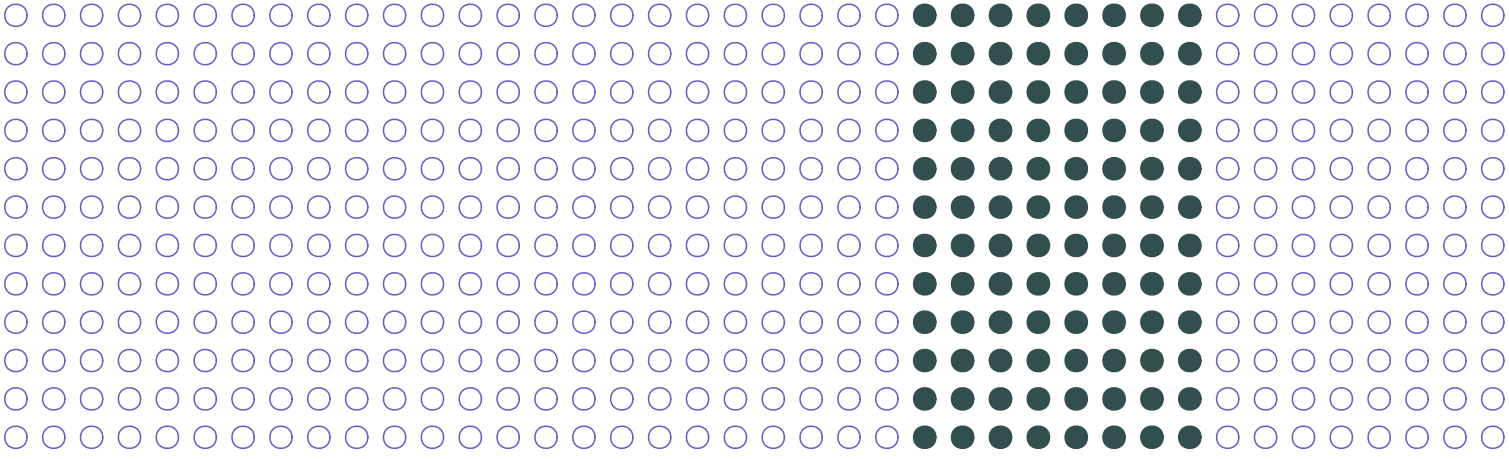
For $k = 5$, fold number 3 as the **validation set** produces $\text{MSE}_{\text{k=3}}$.

Hold-out methods

Option 3: k-fold cross validation

With k-fold cross validation, we estimate test MSE as

$$\text{CV}_{(k)} = \frac{1}{k} \sum_{i=1}^{k} \text{MSE}_i$$

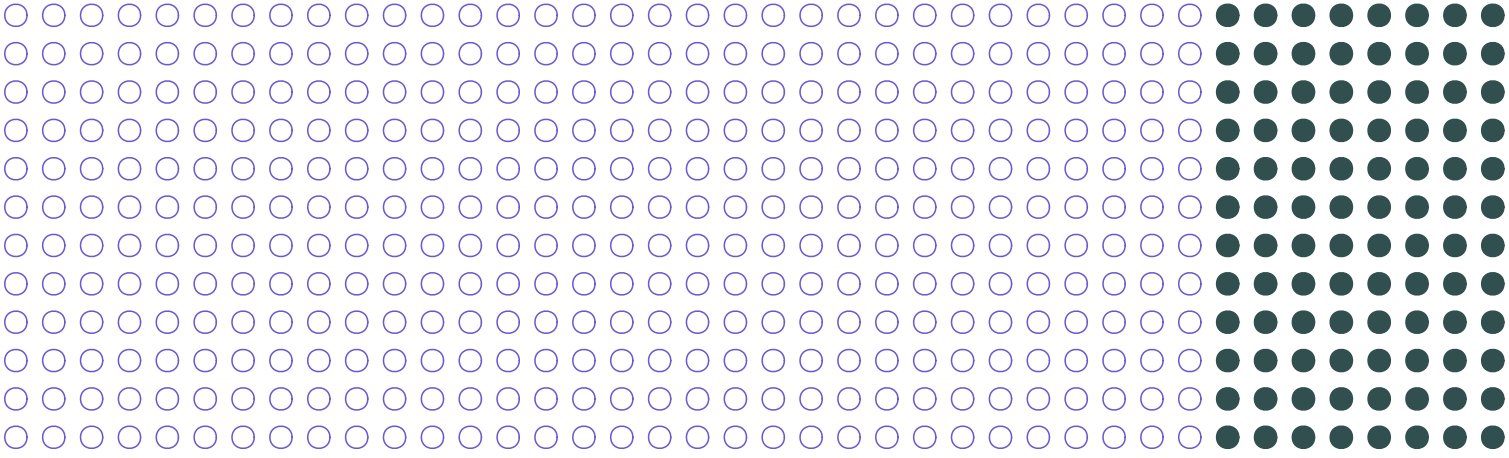


For $k = 5$, fold number 4 as the **validation set** produces $\text{MSE}_{\text{k=4}}$.

Option 3: k-fold cross validation

With k-fold cross validation, we estimate test MSE as

$$\text{CV}_{(k)} = \frac{1}{k} \sum_{i=1}^{k} \text{MSE}_i$$



For $k = 5$, fold number 5 as the **validation set** produces $\text{MSE}_{\text{k=5}}$.

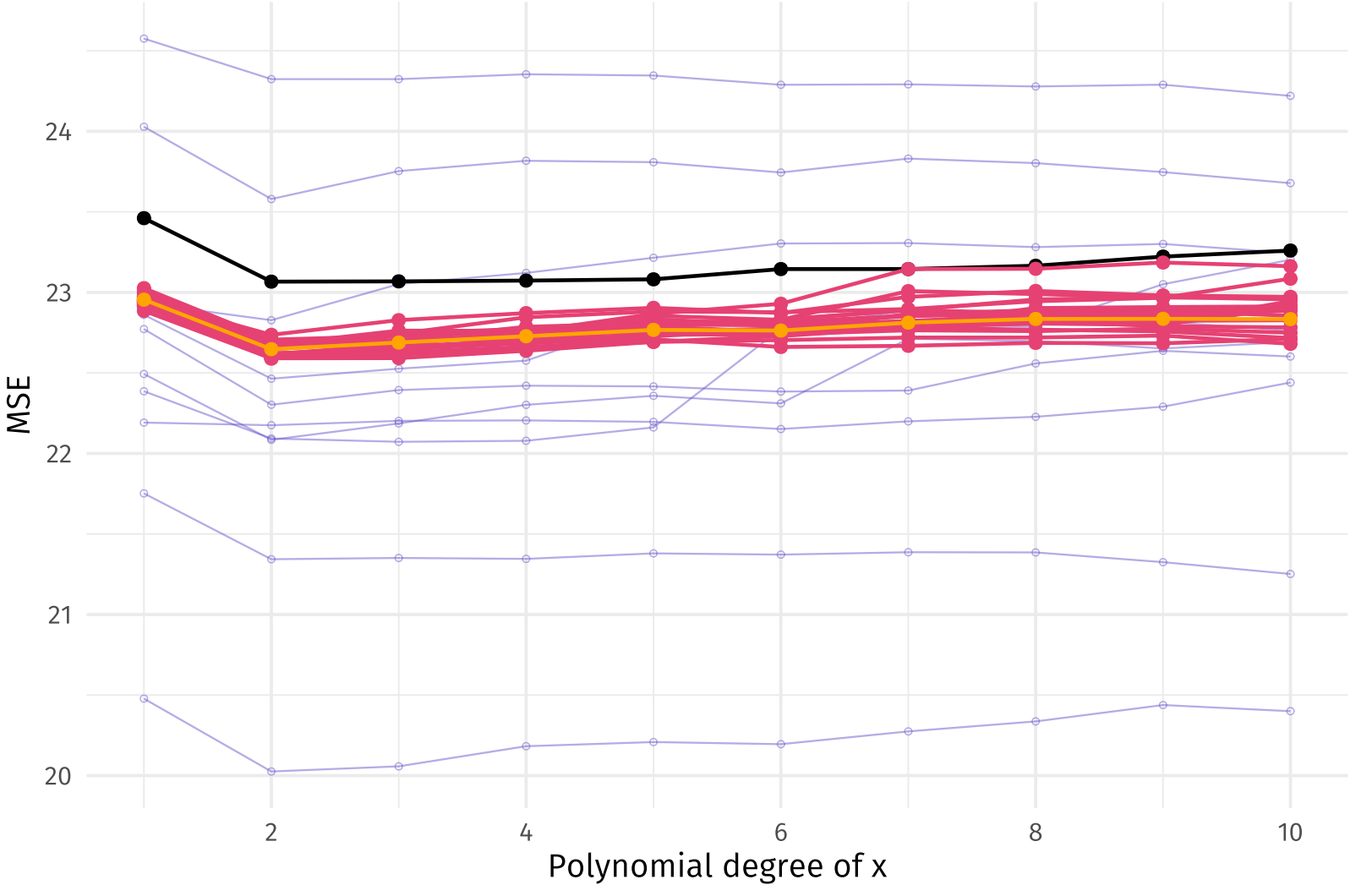
Hold-out methods

Option 3: k-fold cross validation

With k-fold cross validation, we estimate test MSE as

$$\text{CV}_{(k)} = \frac{1}{k} \sum_{i=1}^{k} \text{MSE}_i$$

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

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

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

Alternative approach: **Shrinkage methods**

- fit a model that contains all p predictors
- simultaneously: shrink[†] coefficients toward zero

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 twoard zero help or predictions?

A Remember we're generally facing a tradeoff between bias and variance.

- Shrinking our coefficients toward zero **reduces the model's variance**.†
- **Penalizing** our model for **larger coefficients** shrinks them toward zero.
- The **optimal penalty** will balance reduced variance with increased bias.

Now you understand shrinkage methods.

- Ridge regression
- Lasso
- Elasticnet

† Imagine the extreme case: a model whose coefficients are all zeros has no variance.

Ridge regression

Ridge regression

Back to least squares (again)

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

$$\min_{\hat{\beta}} \text{RSS} = \min_{\hat{\beta}} \sum_{i=1}^{n} e_i^2 = \min_{\hat{\beta}} \sum_{i=1}^{n} \left(y_i - \underbrace{\left[\hat{\beta}_0 + \hat{\beta}_1 x_{i,1} + \cdots + \hat{\beta}_p x_{i,p} \right]}_{=\hat{y}_i} \right)^2$$

Ridge regression makes a small change

- adds a shrinkage penalty = the sum of squared coefficents $\left(\lambda \sum_j \beta_j^2 \right)$
- minimizes the (weighted) sum of RSS and the shrinkage penalty

$$\min_{\hat{\beta}^R} \sum_{i=1}^{n} \left(y_i - \hat{y}_i \right)^2 + \lambda \sum_{j=1}^{p} \beta_j^2$$

Ridge regression

Ridge regression

$$\min_{\hat{\beta}^R} \sum_{i=1}^{n} \left(y_i - \hat{y}_i \right)^2 + \lambda \sum_{j=1}^{p} \beta_j^2$$

Least squares

$$\min_{\hat{\beta}} \sum_{i=1}^{n} \left(y_i - \hat{y}_i \right)^2$$

λ (≥ 0) is a tuning parameter for the harshness of the penalty.

$\lambda = 0$ implies no penalty: we are back to least squares.

Each value of λ produces a new set of coefficents.

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

- reducing **RSS**, *i.e.*, $\sum_i \left(y_i - \hat{y}_i \right)^2$
- 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.
- If λ is too large, then we shrink all of our coefficients too close to zero.

Q So what do we do?

A Cross validate!

(You saw that coming, right?)

Ridge regression

Penalization and standardization

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

Why? Because $\mathbf{x}_j$'s units affect β_j, and ridge is very sensitive to β_j.

Example Let x_1 denote distance.

Least-squares regression
If x_1 is *meters* and $\beta_1 = 3$, then when x_1 is *km*, $\beta_1 = 3,000$.
The scale/units of predictors do not affect least squares' estimates.

Ridge regression pays a much larger penalty for $\beta_1 = 3,000$ than $\beta_1 = 3$.
You will not get the same (scaled) estimates when you change units.

Solution Standardize your variables, *i.e.*, `x_stnd = (x - mean(x))/sd(x)`.

Lasso

Lasso

Intro

Lasso simply replaces ridge's *squared* coefficients with absolute values.

Ridge regression

$$\min_{\hat{\beta}^R} \sum_{i=1}^{n} \left(y_i - \hat{y}_i\right)^2 + \lambda \sum_{j=1}^{p} \beta_j^2$$

Lasso

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

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

Lasso

Shrinkage

Unlike ridge, lasso's penalty does not increase with the size of β_j.

You always pay λ to increase $|\beta_j|$ by one unit.

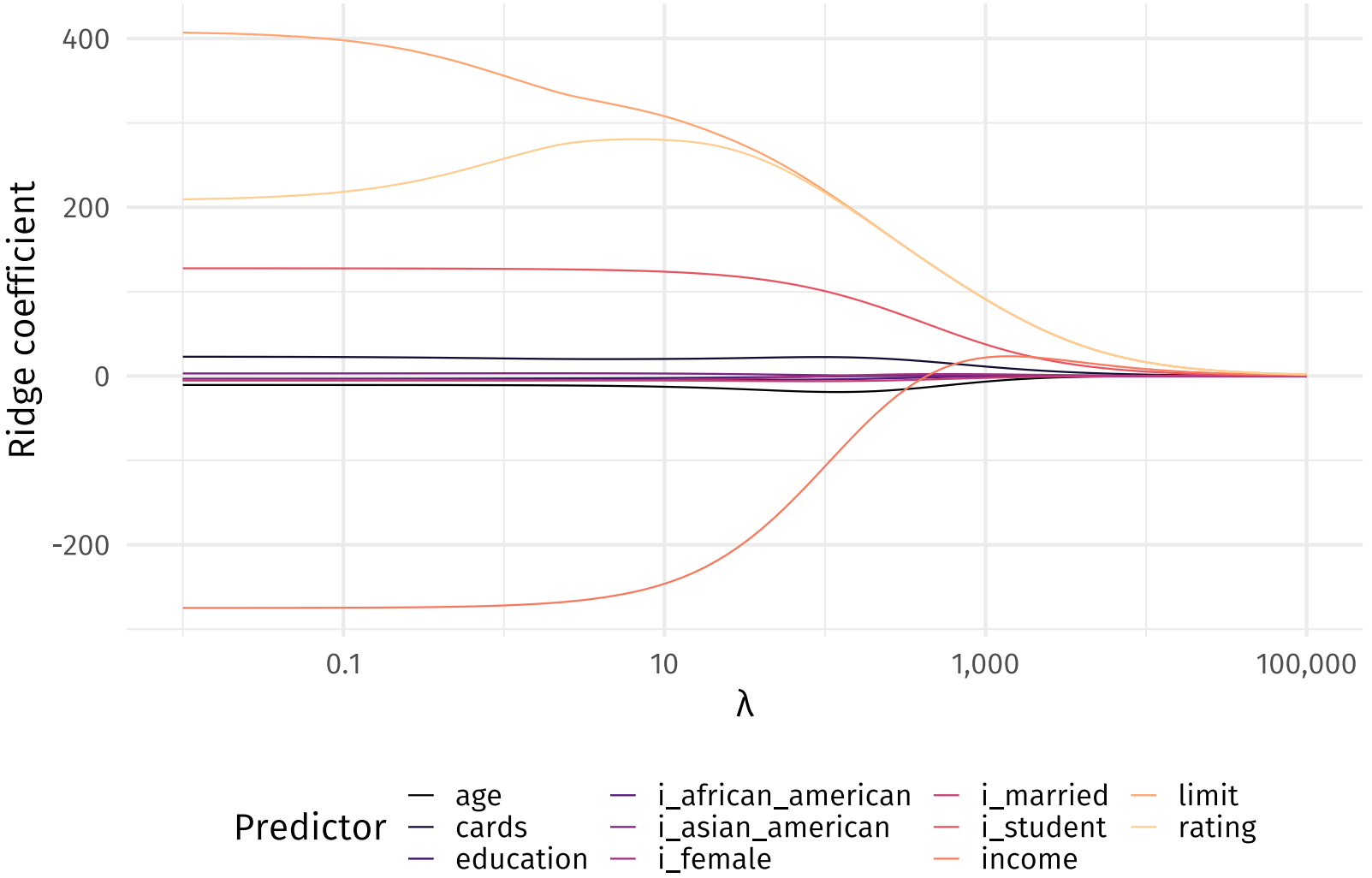
The only way to avoid lasso's penalty is to **set coefficents to zero**.

This feature has two **benefits**

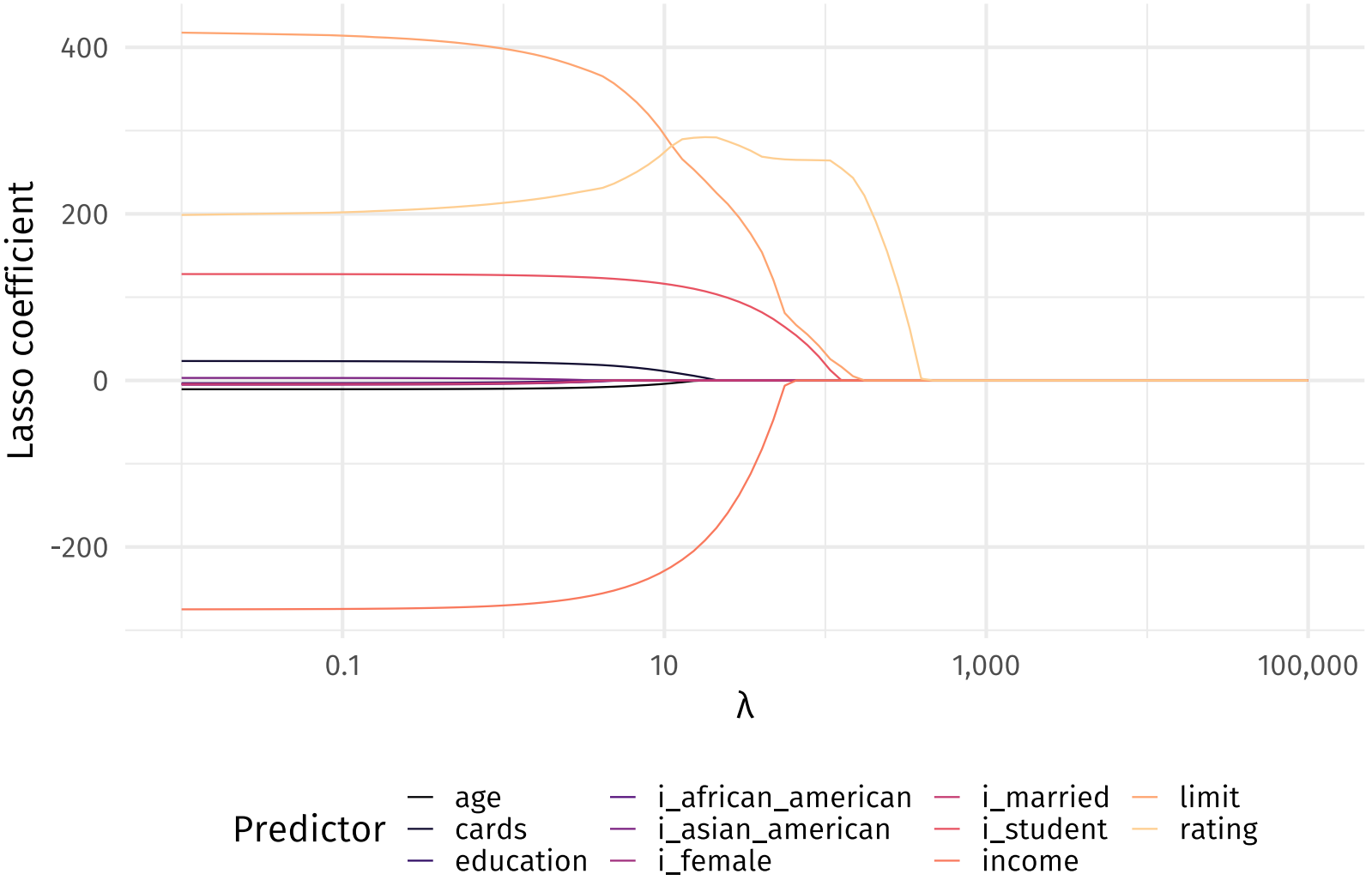
1. Some coefficients will be **set to zero**—we get "sparse" models.
2. Lasso can be used for subset/feature **selection**.

We will still need to carefully select λ.

Ridge regression coefficents for λ between 0.01 and 100,000



Lasso coefficents for λ between 0.01 and 100,000



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 (🌲🌴🌳)

Fundamentals

Decision trees

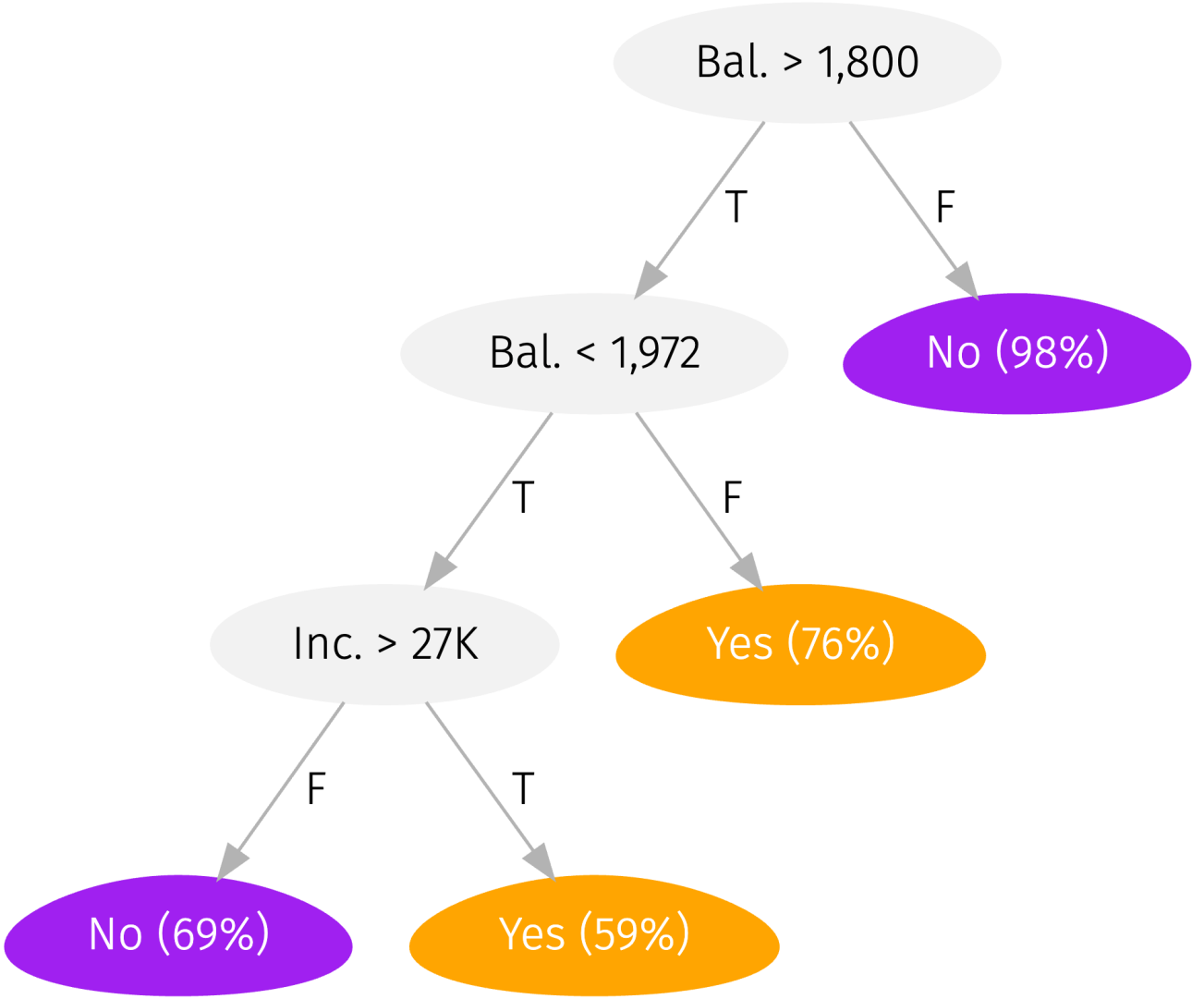
- split the *predictor space* (our $\mathbf{X}$) into regions
- then predict the most-common value within a region

Decision trees

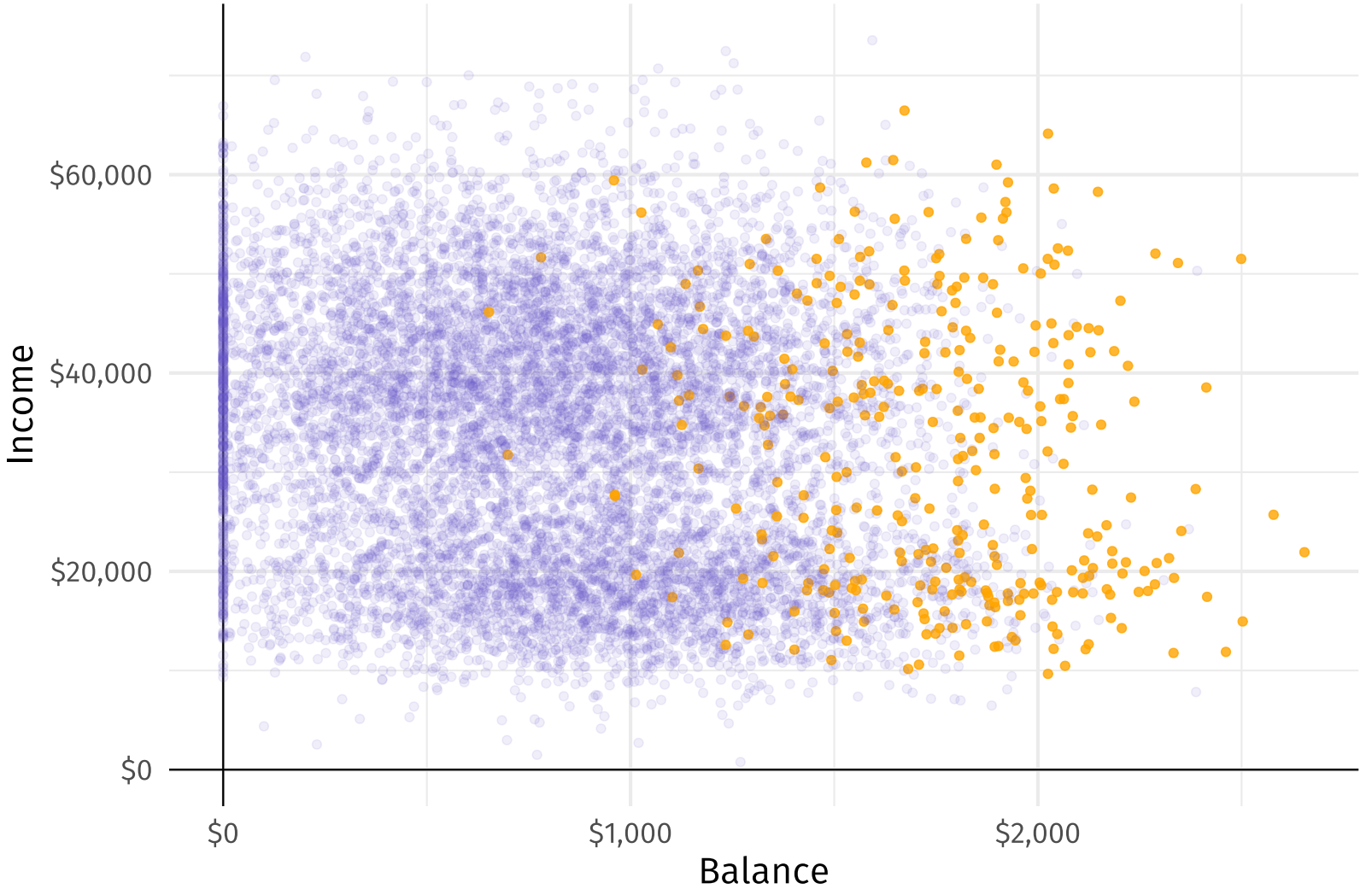
1. work for **both classification and regression**
2. are inherently **nonlinear**
3. are relatively **simple** and **interpretable**
4. often **underperform** relative to competing methods
5. easily extend to **very competitive ensemble methods** (*many* trees)🌲

🌲 Though the ensembles will be much less interpretable.

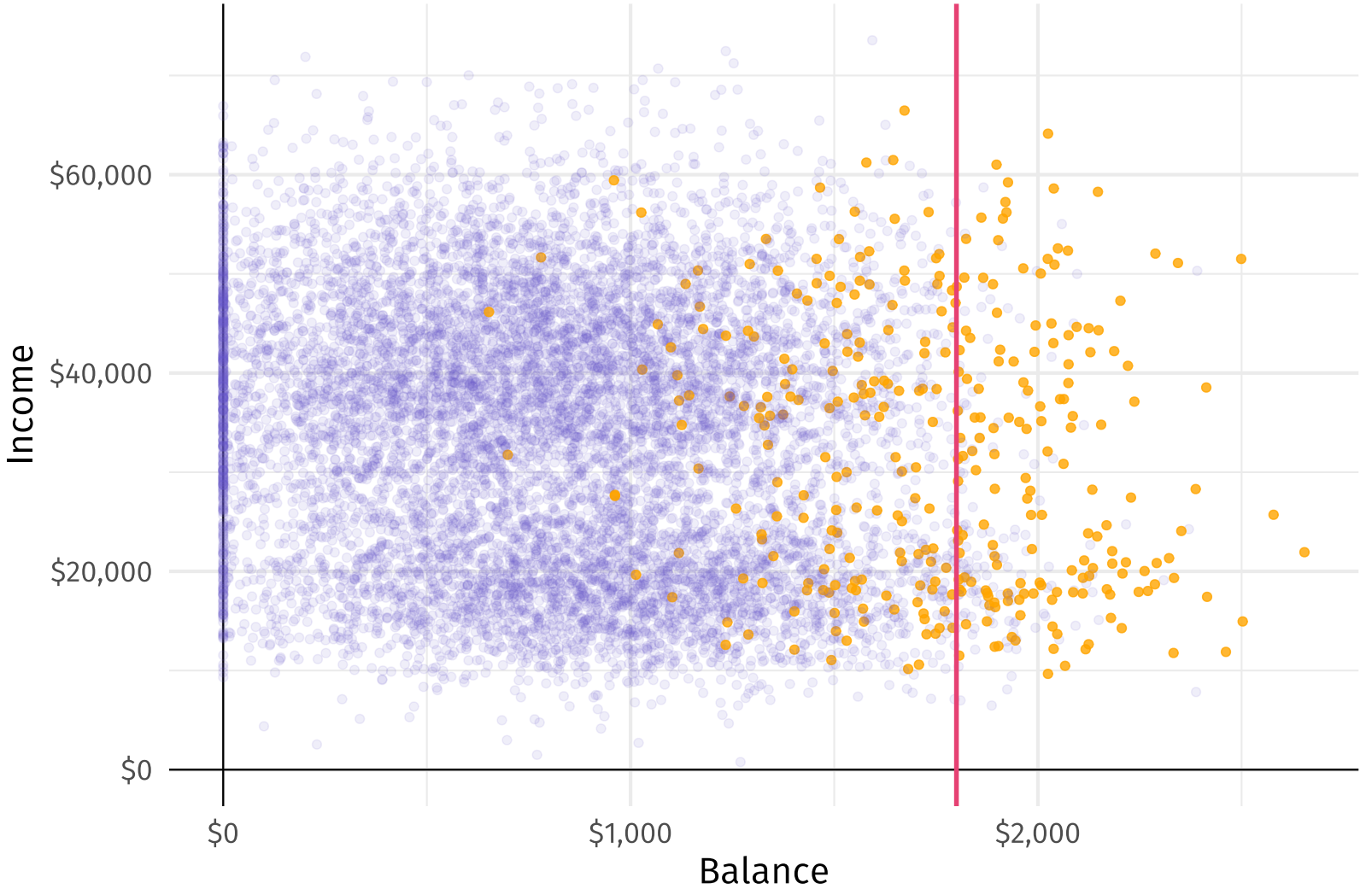
Example: **A simple decision tree** classifying credit-card default



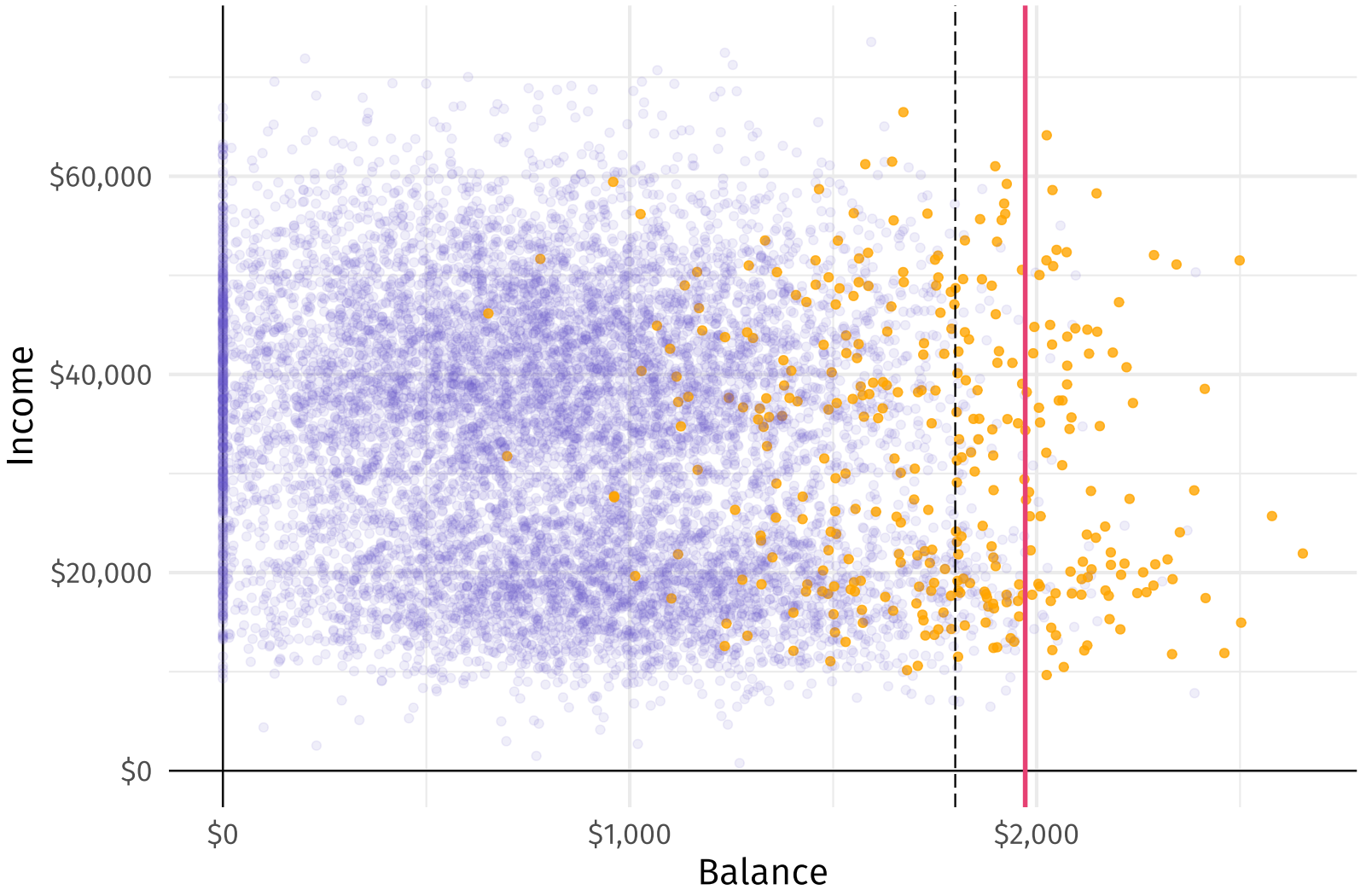
Let's see how the tree works—starting with credit data (default: Yes *vs.* No).



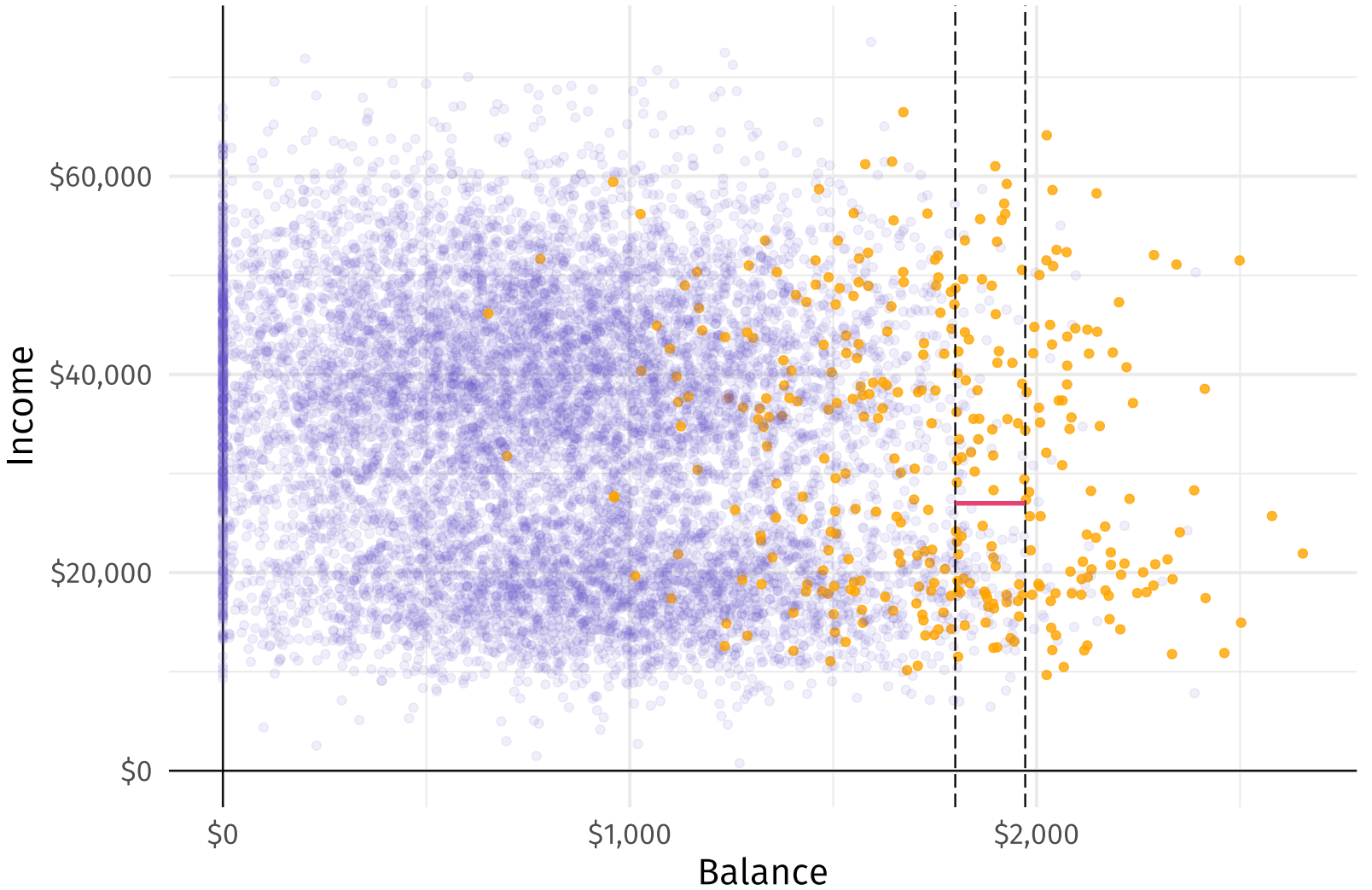
The **first partition** splits balance at $1,800.



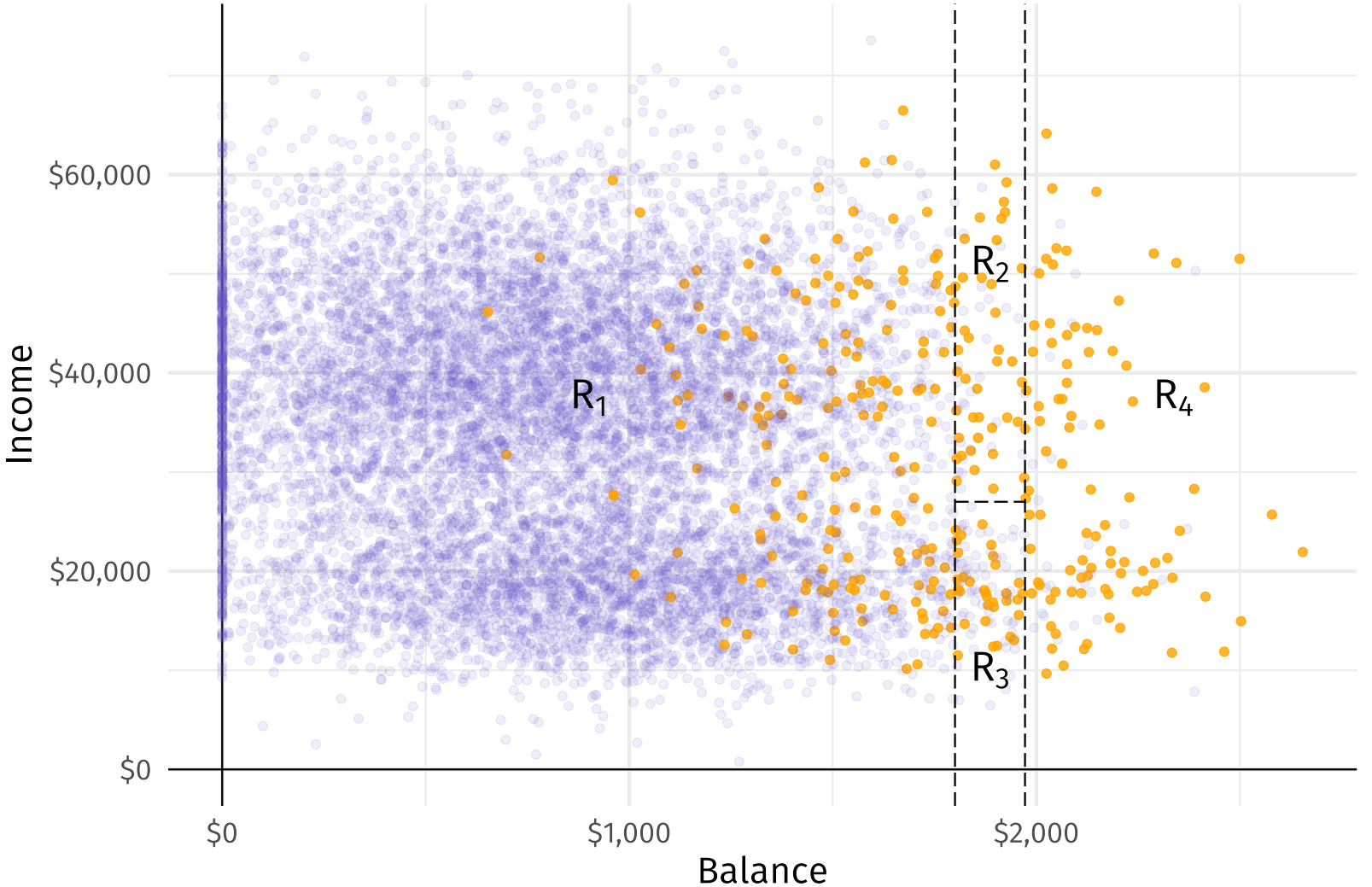
The **second partition** splits balance at $1,972, (*conditional on bal. > $1,800*).



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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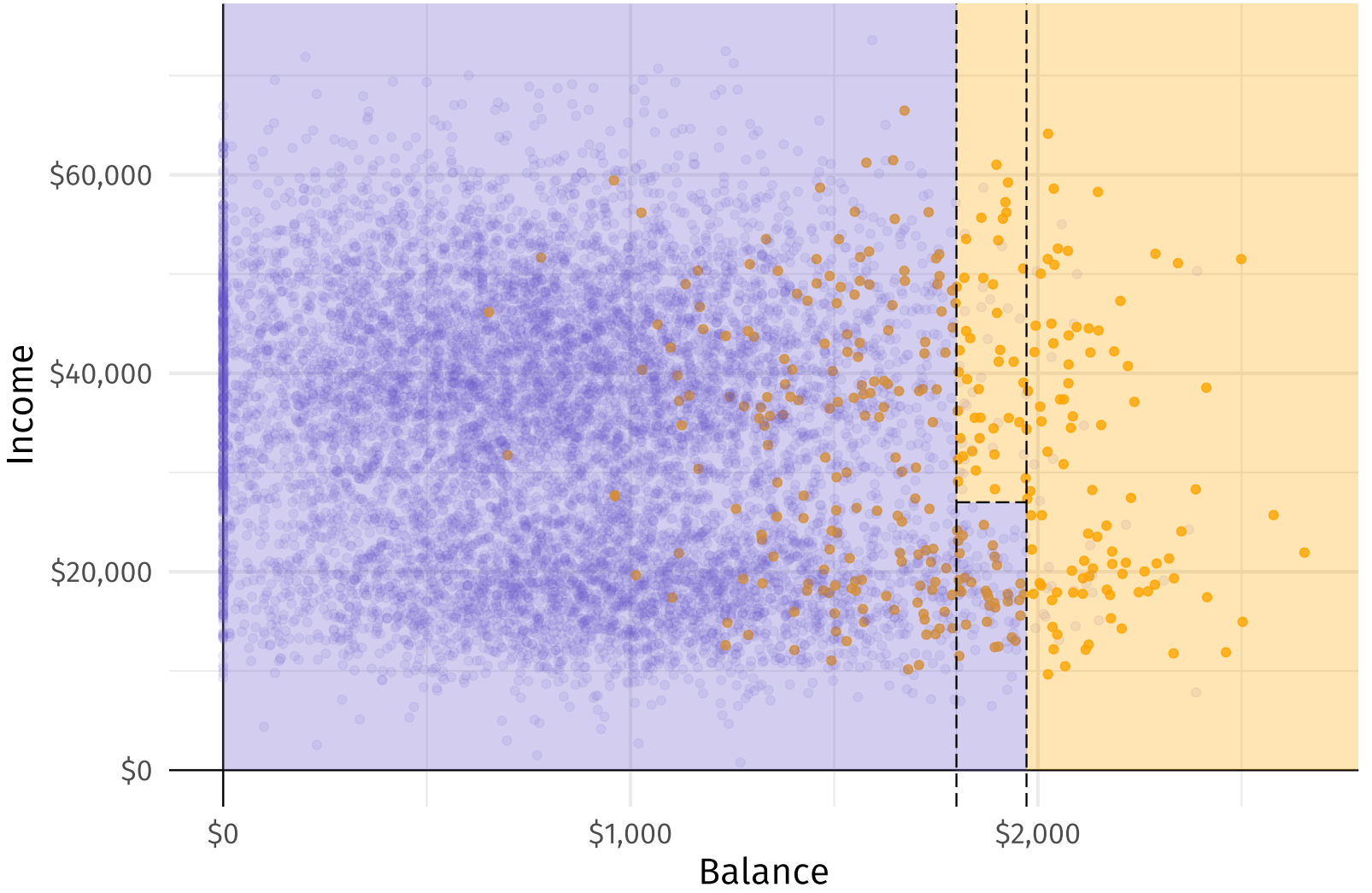


Q Where do trees come from?

A Seeds!🌱🙄

Q How do we train (grow) 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 $\mathbf{x}_1, \ldots, \mathbf{x}_p$)
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 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

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	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.

Example: Splitting

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

i
1
2
3

y	x_1	x_2
0	1	4
8	3	2
6	5	6

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!

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[1] 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 $|T|$.

[1] 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

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
$\therefore$ We want to minimize the Gini index.

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

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.

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.

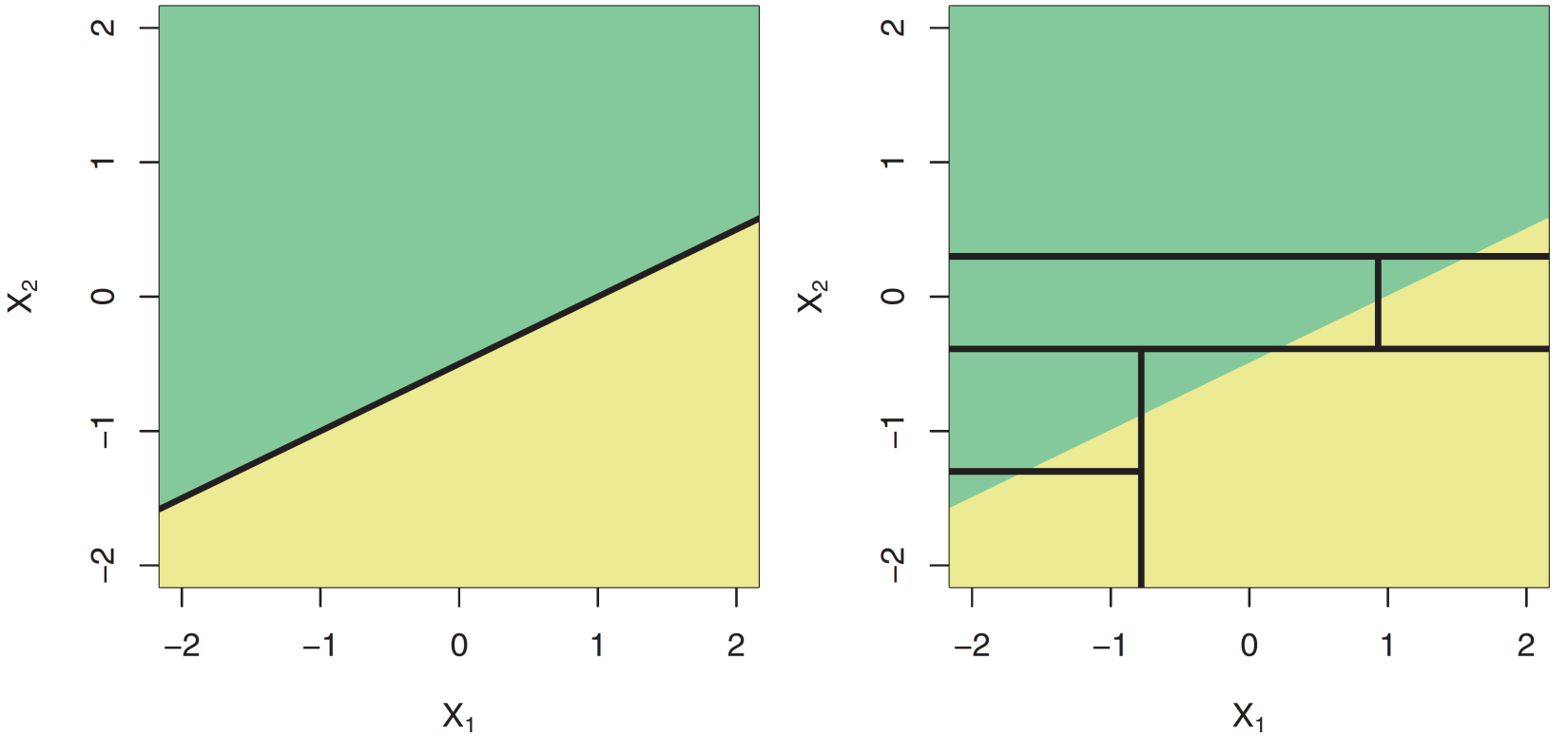
However, when **pruning**, the error rate is typically fine—especially if accuracy will be the final criterion.

Q How do trees compare to linear models?

Q How do trees compare to linear models?

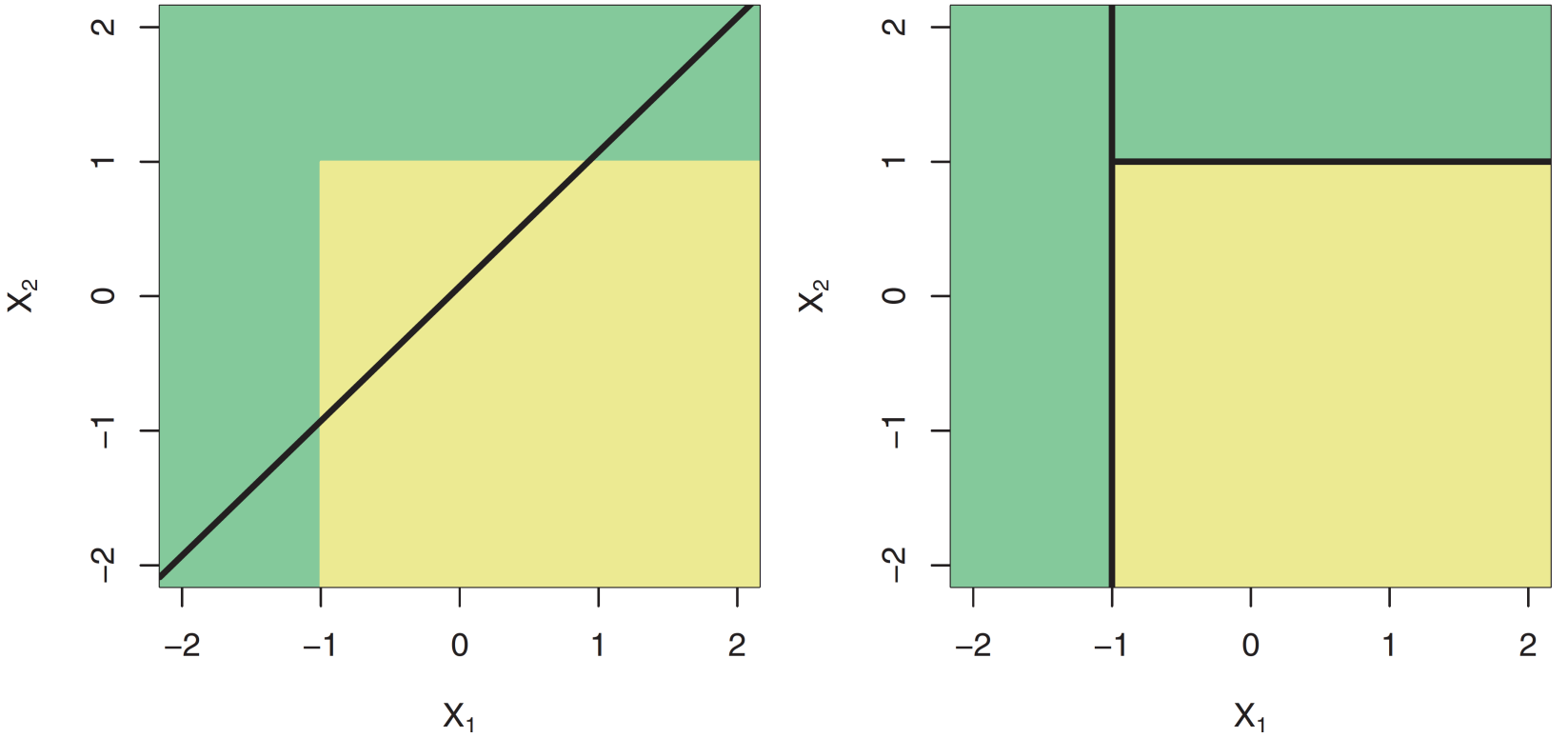
A It depends how linear the true boundary is.

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.

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*.

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

1. Bagging
2. Random forests
3. Boosting

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**.

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.

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.

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**

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.

Out-of-bag error estimation

Bagging also offers a convenient method for evaluating performance.

For any bootstrapped sample, we omit ~n/3 observations.

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

For each observation i:

1. Find all samples S_i in which i was omitted from training.
2. Aggregate the $|S_i|$ predictions $\hat{f}^b(x_i)$, *e.g.*, using their mean or mode
3. Calculate the error, *e.g.*, $y_i - \hat{f}_{i,\text{OOB},i}(x_i)$

Out-of-bag error 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.

Bagging

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.

Random forests

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

In order to decorrelate its trees, a **random forest** only considers a random subset of m $(\approx \sqrt{p})$ predictors when making each split (for each tree).

Restricting the variables our tree sees at a given split

- nudges trees away from always using the same variables,
- increasing the variation across trees in our forest,
- which potentially reduces the variance of our estimates.

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

Random forests

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

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

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

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

Boosting

So far, the elements of our ensembles have been acting independently: any single tree knows nothing about the rest of the forest.

Boosting allows trees to pass on information to eachother.

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).

Boosting

Boosting has three **tuning parameters**.

1. The **number of trees** B can be important to prevent overfitting.
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).
    - Individaul trees are typically short—often $d = 1$ ("stumps").
    - *Remember* Trees learn from predecessors' mistakes, so no single tree needs to offer a perfect model.

How to boost

Step 1: Set $\hat{f}(x) = 0$, which yields residuals $r_i = y_i$ for all i.

Step 2: For $b = 1, 2 \ldots, B$ do:

A. Fit a tree $\hat{f}^b$ with d splits.

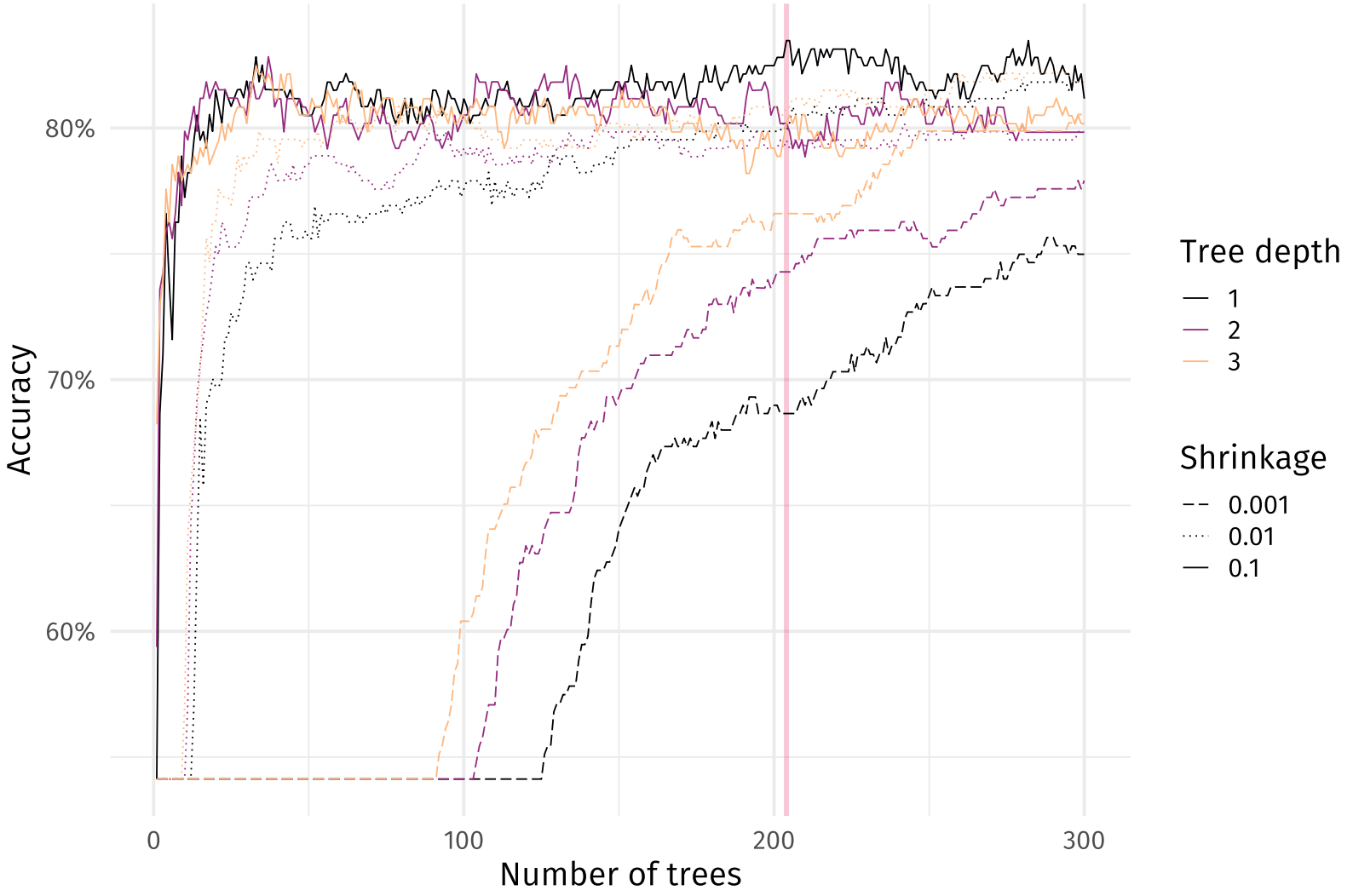
B. Update the model $\hat{f}$ with "shrunken version" of new treee $\hat{f}^b$

$$\hat{f}(x) \leftarrow \hat{f}(x) + \lambda \hat{f}^b(x)$$

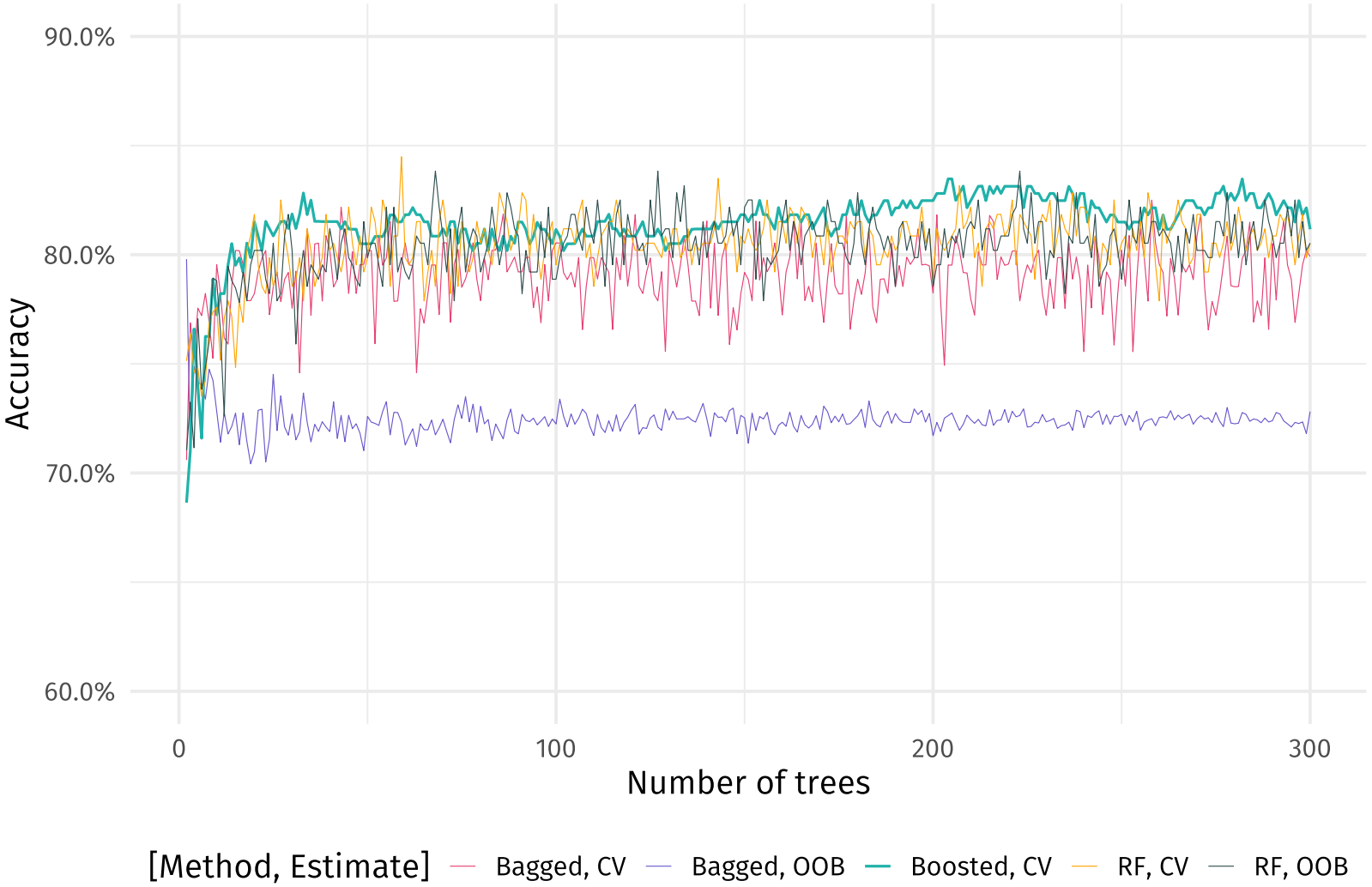
C. Update the residuals: $r_i \leftarrow r_i - \lambda \hat{f}^b(x)$.

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.