

# Lecture 004

## Regression strikes back

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Admin

# Admin

## Today

### **In-class**

- A roadmap (where are we going?)
- Linear regression and model selection

# Admin

## Upcoming

### Readings

- *Today*
  - ISL Ch. 3 and 6.1
- *Next*
  - ISL Ch. 6 and 4

### Problem sets

- *Next one*: Soon! Possibly the next few days?

# Roadmap

## Where are we?

We've essentially covered the central topics in statistical learning<sup>†</sup>

- Prediction and inference
- Supervised vs. unsupervised methods
- Regression and classification problems
- The dangers of overfitting
- The bias-variance tradeoff
- Model assessment
- Holdouts, validation sets, and cross validation<sup>††</sup>
- Model training and tuning
- Simulation

<sup>†</sup> Plus a few of the "basic" methods: OLS regression and KNN.

<sup>††</sup> And the bootstrap!

# Roadmap

## Where are we going?

Next, we will cover many common machine-learning algorithms, *e.g.*,

- Decision trees and random forests
- SVM
- Neural nets
- Clustering
- Ensemble techniques

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- SVM
- Neural nets
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- Ensemble techniques

But first, we return to good old **linear regression**—in a new light...

- Linear regression
- Variable/model selection and LASSO/Ridge regression
- *Plus:* Logistic regression and discriminant analysis

# Roadmap

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### Motivation 2

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*E.g.*, did (cross) validation help you beat your old model?

### Motivation 3

many fancy statistical learning approaches can be seen as  
**generalizations or extensions of linear regression.**

*Source: ISL, p. 59; emphasis added*

# Linear regression

# Linear regression

## Regression regression

*Recall* Linear regression "fits" coefficients  $\beta_0, \dots, \beta_p$  for a model

$$y_i = \beta_0 + \beta_1 x_{1,i} + \beta_2 x_{2,i} + \dots + \beta_p x_{p,i} + \varepsilon_i$$

and is often applied in two distinct settings with fairly distinct goals:

1. **Causal inference** estimates and interprets **the coefficients**.
2. **Prediction** focuses on accurately estimating **outcomes**.

Regardless of the goal, the way we "fit" (estimate) the model is the same.

# Linear regression

## Fitting the regression line

As is the case with many statistical learning methods, regression focuses on minimizing some measure of loss/error.

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As is the case with many statistical learning methods, regression focuses on minimizing some measure of loss/error.

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Linear regression uses the  $L_2$  loss function—also called *residual sum of squares* (RSS) or *sum of squared errors* (SSE)

$$\text{RSS} = e_1^2 + e_2^2 + \cdots + e_n^2 = \sum_{i=1}^n e_i^2$$

Specifically: OLS chooses the  $\hat{\beta}_j$  that **minimize RSS**.

# Linear regression

## Performance

There's a large variety of ways to assess the fit<sup>†</sup> of linear-regression models.

### Residual standard error (RSE)

$$\text{RSE} = \sqrt{\frac{1}{n - p - 1} \text{RSS}} = \sqrt{\frac{1}{n - p - 1} \sum_{i=1}^n (y_i - \hat{y}_i)^2}$$

### R-squared ( $R^2$ )

$$R^2 = \frac{\text{TSS} - \text{RSS}}{\text{TSS}} = 1 - \frac{\text{RSS}}{\text{TSS}} \quad \text{where} \quad \text{TSS} = \sum_{i=1}^n (y_i - \bar{y})^2$$

<sup>†</sup> or predictive performance

# Linear regression

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**Add a new variable:** RSS ↓ and TSS is unchanged. Thus,  $R^2$  increases.

**RSE** *slightly* penalizes additional variables:

$$\text{RSE} = \sqrt{\frac{1}{n - p - 1} \text{RSS}}$$

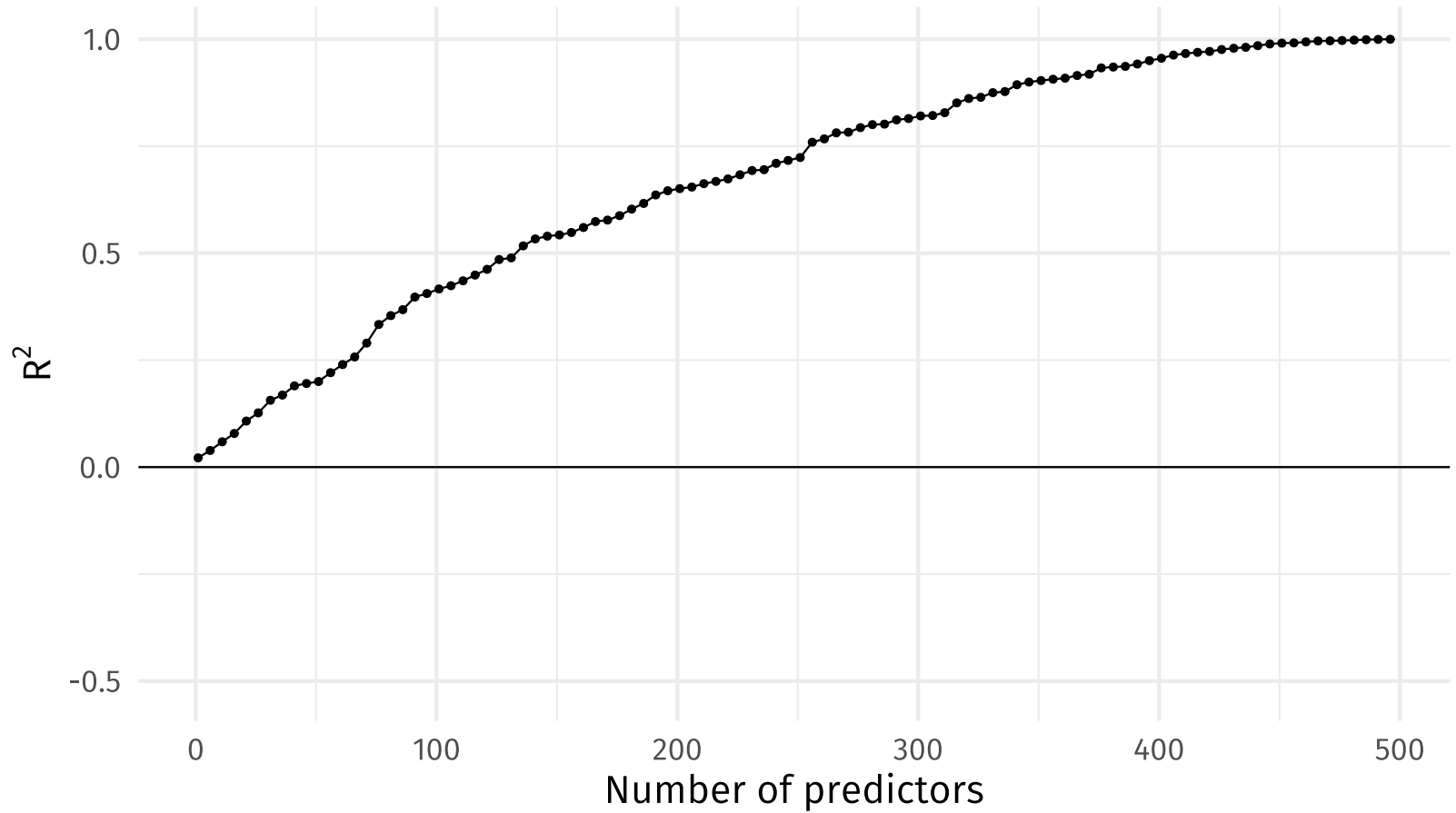
**Add a new variable:** RSS ↓ but  $p$  increases. Thus, RSE's change is uncertain.

## Example

Let's see how  **$R^2$**  and **RSE** perform with 500 very weak predictors.

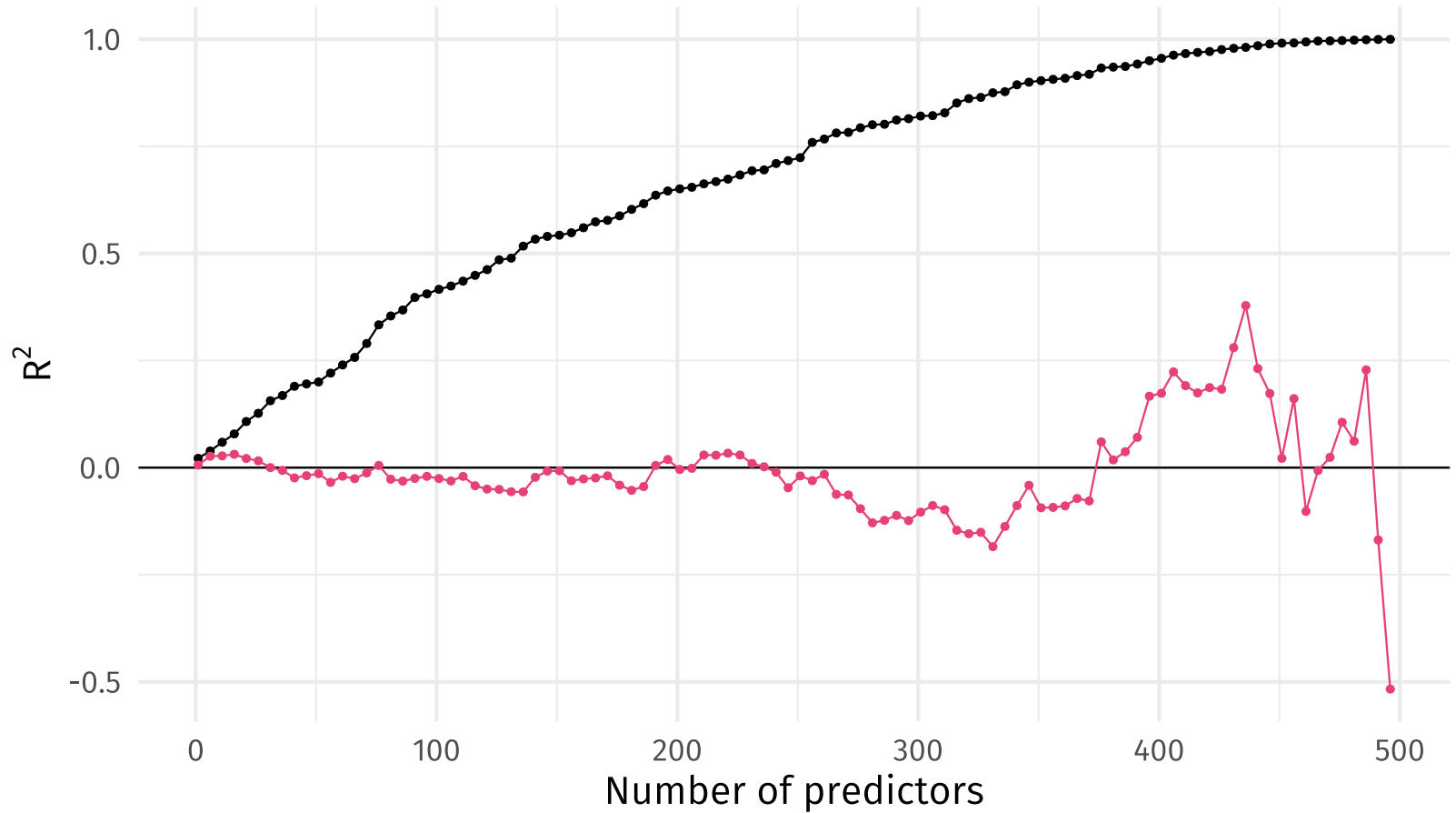
To address overfitting, we can compare **in-** vs. **out-of-sample** performance.

**In-sample  $R^2$**  mechanically increases as we add predictors.



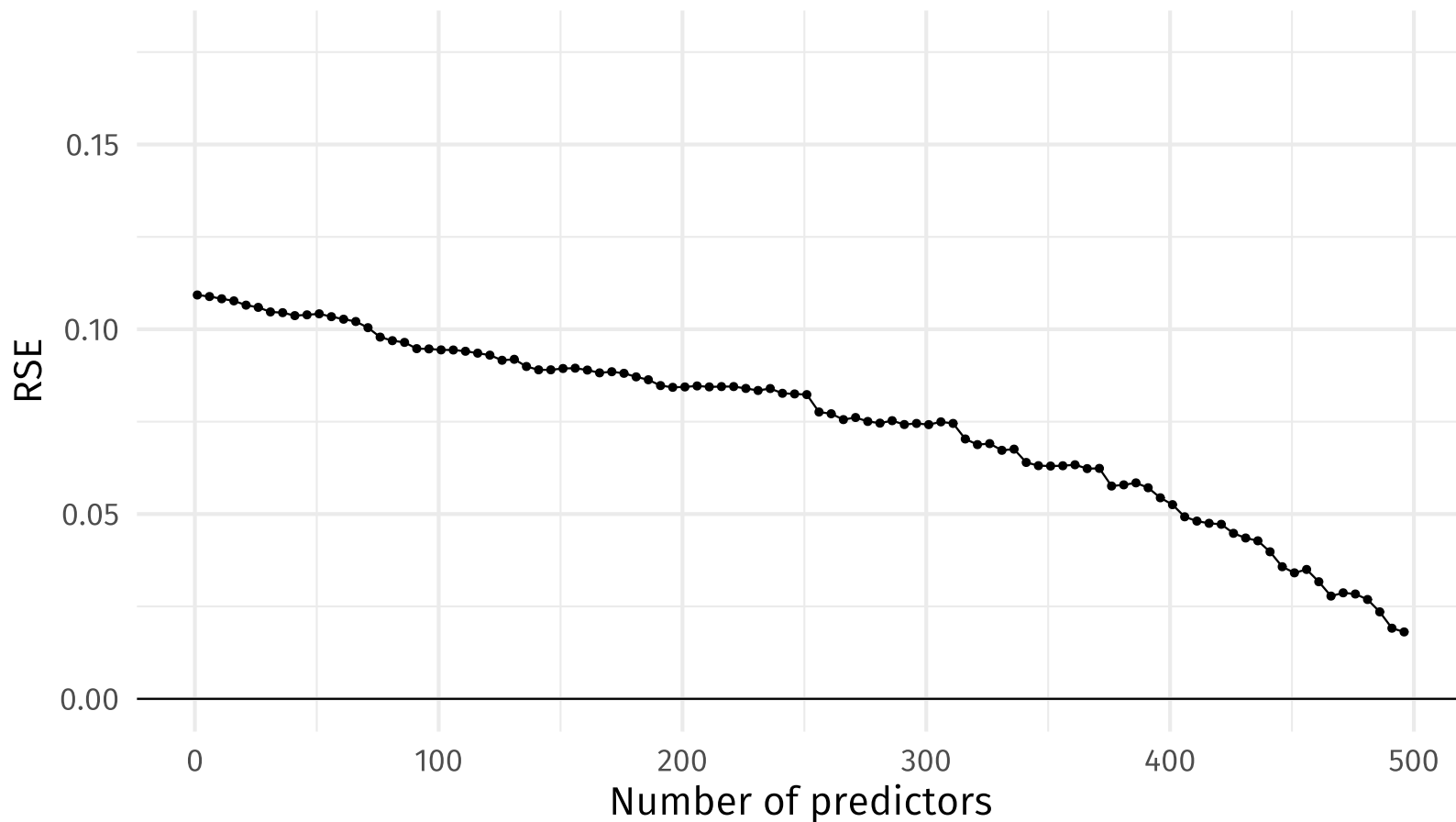
**In-sample  $R^2$**  mechanically increases as we add predictors.

**Out-of-sample  $R^2$**  does not.

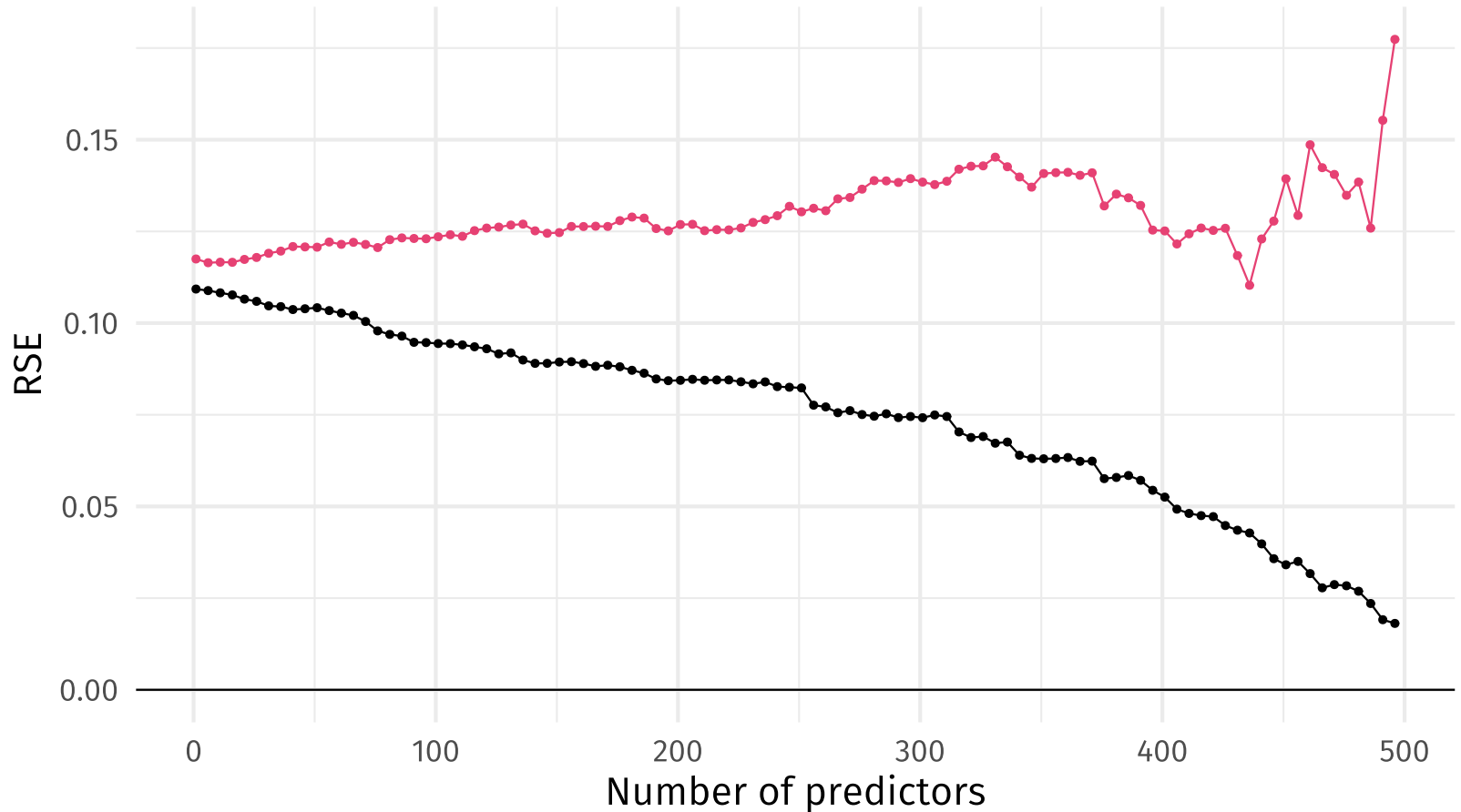


What about RSE? Does its penalty *help*?

Despite its penalty for adding variables, **in-sample RSE** still can overfit,



Despite its penalty for adding variables, **in-sample RSE** still can overfit, as evidenced by **out-of-sample RSE**.





# Linear regression

## Penalization

RSE is not the only way to penalization the addition of variables.<sup>†</sup>

**Adjusted  $R^2$**  is another *classic* solution.

$$\text{Adjusted } R^2 = 1 - \frac{\text{RSS}/(n - p - 1)}{\text{TSS}/(n - 1)}$$

Adj.  $R^2$  attempts to "fix"  $R^2$  by **adding a penalty for the number of variables**.

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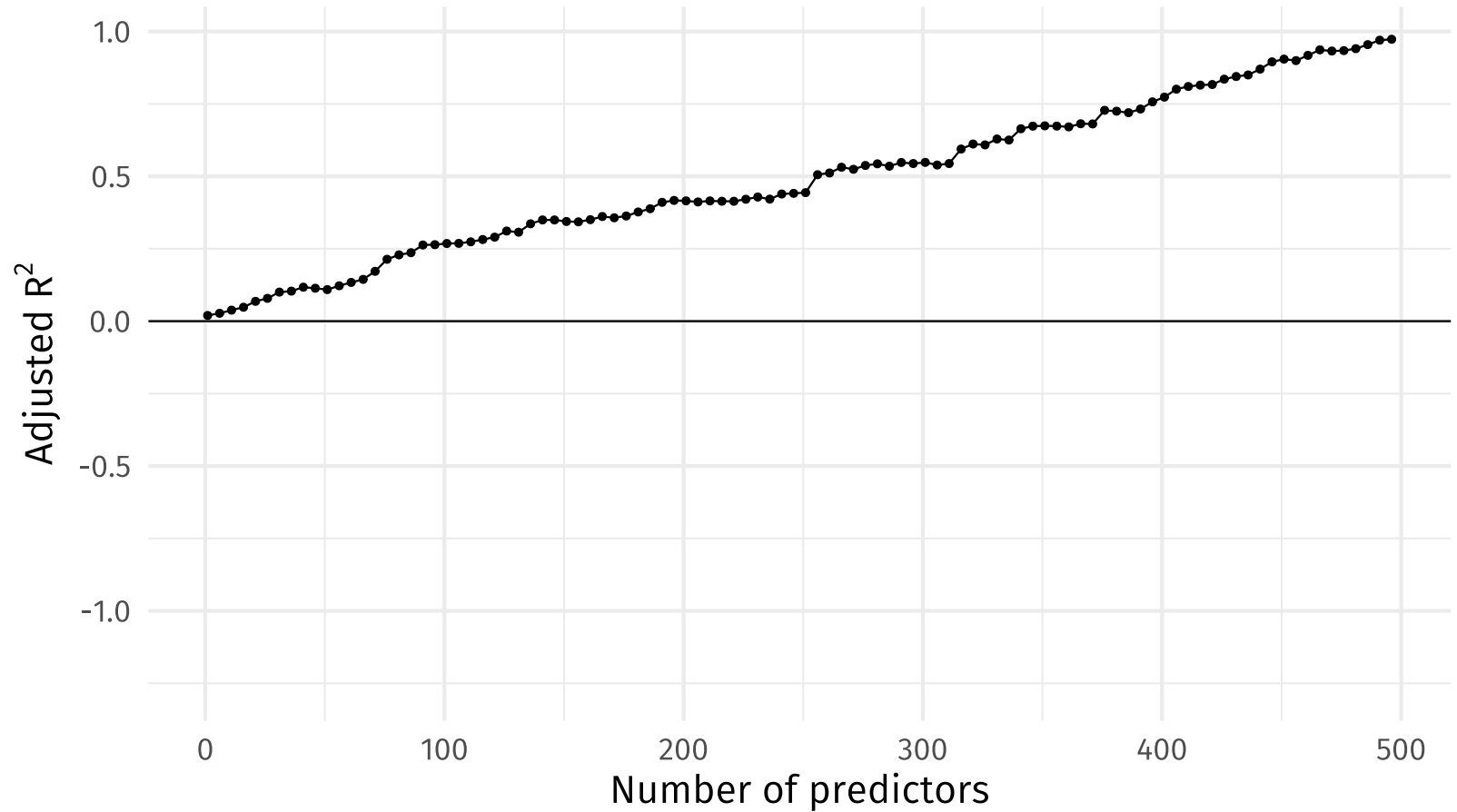
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Adj.  $R^2$  attempts to "fix"  $R^2$  by **adding a penalty for the number of variables**.

- RSS always decreases when a new variable is added.
- $\text{RSS}/(n - p - 1)$  may increase or decrease with a new variable.

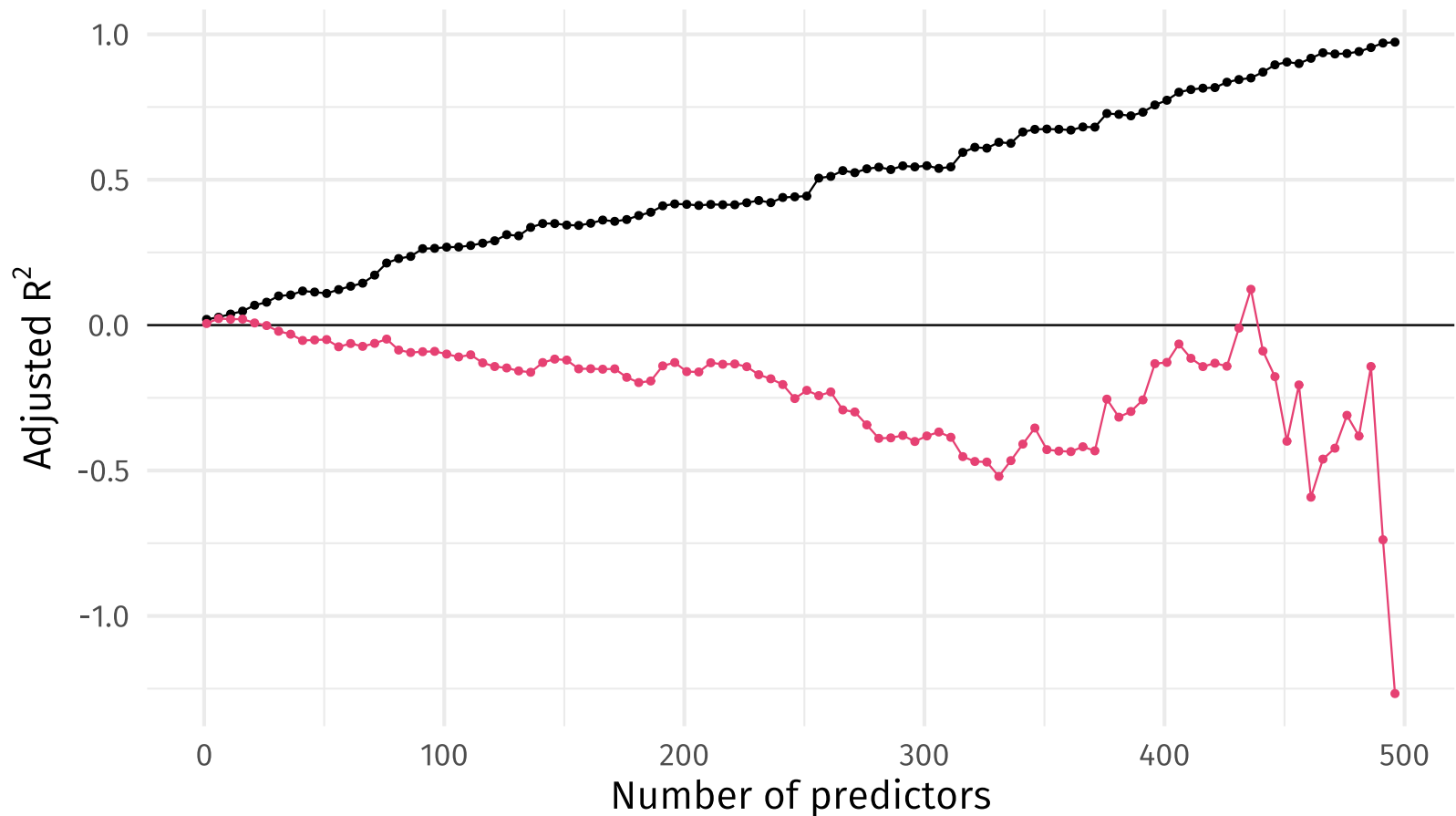
<sup>†</sup> We'll talk about other penalization methods (LASSO and Ridge) shortly.

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Illustrated by **out-of-sample adjusted  $R^2$** .



# Model selection

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$R^2$ , adjusted  $R^2$ , and RSE each offer some flavor of model fit, but they appear **limited in their abilities to prevent overfitting**.

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We want a method to optimally select a (linear) model—balancing variance and bias and avoiding overfit.

We'll discuss two (related) methods today:

1. **Subset selection** chooses a (sub)set of our  $p$  potential predictors
2. **Shrinkage** fits a model using all  $p$  variables but "shrinks" its coefficients



# Model selection

## Subset selection

In **subset selection**, we

1. whittle down the  $p$  potential predictors (using some magic/algorithm)
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How do we do the *whittling* (selection)?

# Model selection

## Subset selection

In **subset selection**, we

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2. estimate the chosen linear model using OLS

How do we do the *whittling* (selection)? We've got **options**.

- **Best subset selection** fits a model for every possible subset.
- **Forward stepwise selection** starts with only an intercept and tries to build up to the best model (using some fit criterion).
- **Backward stepwise selection** starts with all  $p$  variables and tries to drop variables until it hits the best model (using some fit criterion).
- **Hybrid approaches** are what their name implies (*i.e.*, hybrids).

# Model selection

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*E.g.,*

- 10 predictors → 1,024 models to fit
- 25 predictors → >33.5 million models to fit
- 100 predictors → ~1.5 trillion models to fit

# Model selection

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*E.g.,*

- 10 predictors  $\rightarrow$  1,024 models to fit
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Even with plentiful, cheap computational power, we can run into barriers.



# Model selection

## Best subset selection

Computational constraints aside, we can implement **best subset selection** as

1. Define  $\mathcal{M}_0$  as the model with no predictors.
2. For  $k$  in 1 to  $p$ :
  - Fit every possible model with  $k$  predictors.
  - Define  $\mathcal{M}_k$  as the "best" model with  $k$  predictors.
3. Select the "best" model from  $\mathcal{M}_0, \dots, \mathcal{M}_p$ .

As we've seen, RSS declines (and  $R^2$  increases) with  $p$ , so we should use a cross-validated measure of model performance in step 3.<sup>†</sup>

<sup>†</sup> Back to our distinction between test vs. training performance.

# Model selection

## Example dataset: Credit

We're going to use the Credit dataset from *ISL*'s R package ISLR.

# Model selection

## Example dataset: Credit

We're going to use the `Credit` dataset from *ISL*'s R package `ISLR`.

ID	Income	Limit	Rating	Cards	Age	Education	Gender	Student	Married	Ethnicity	Balance
1	14.9	3606	283	2	34	11	Male	No	Yes	Caucasian	333
2	106.0	6645	483	3	82	15	Female	Yes	Yes	Asian	903
3	104.6	7075	514	4	71	11	Male	No	No	Asian	580
4	148.9	9504	681	3	36	11	Female	No	No	Asian	964
5	55.9	4897	357	2	68	16	Male	No	Yes	Caucasian	331
6	80.2	8047	569	4	77	10	Male	No	No	Caucasian	1151
7	21.0	3388	259	2	37	12	Female	No	No	African American	203

The `credit` dataset has 400 observations on 12 variables.

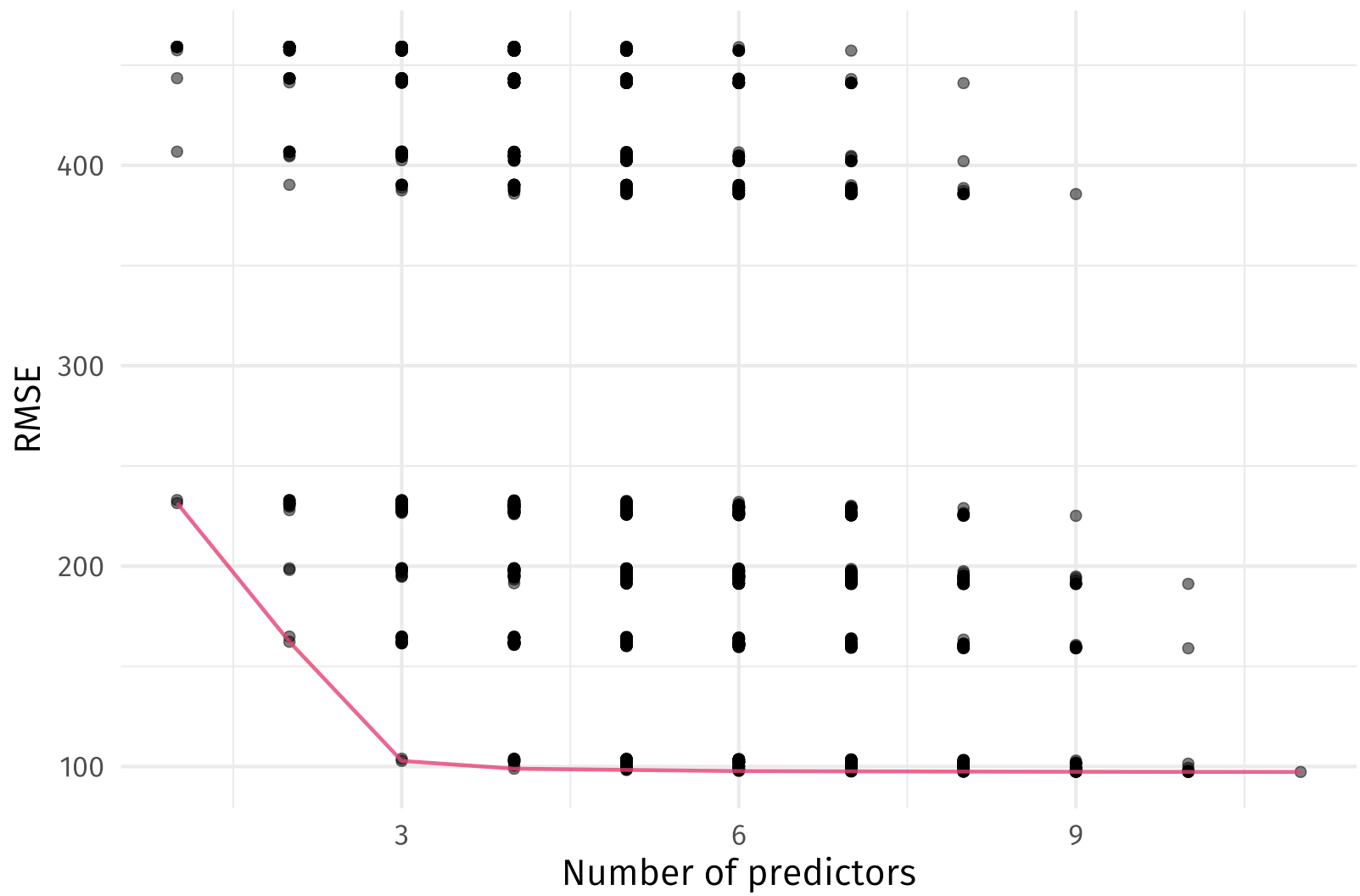
# Model selection

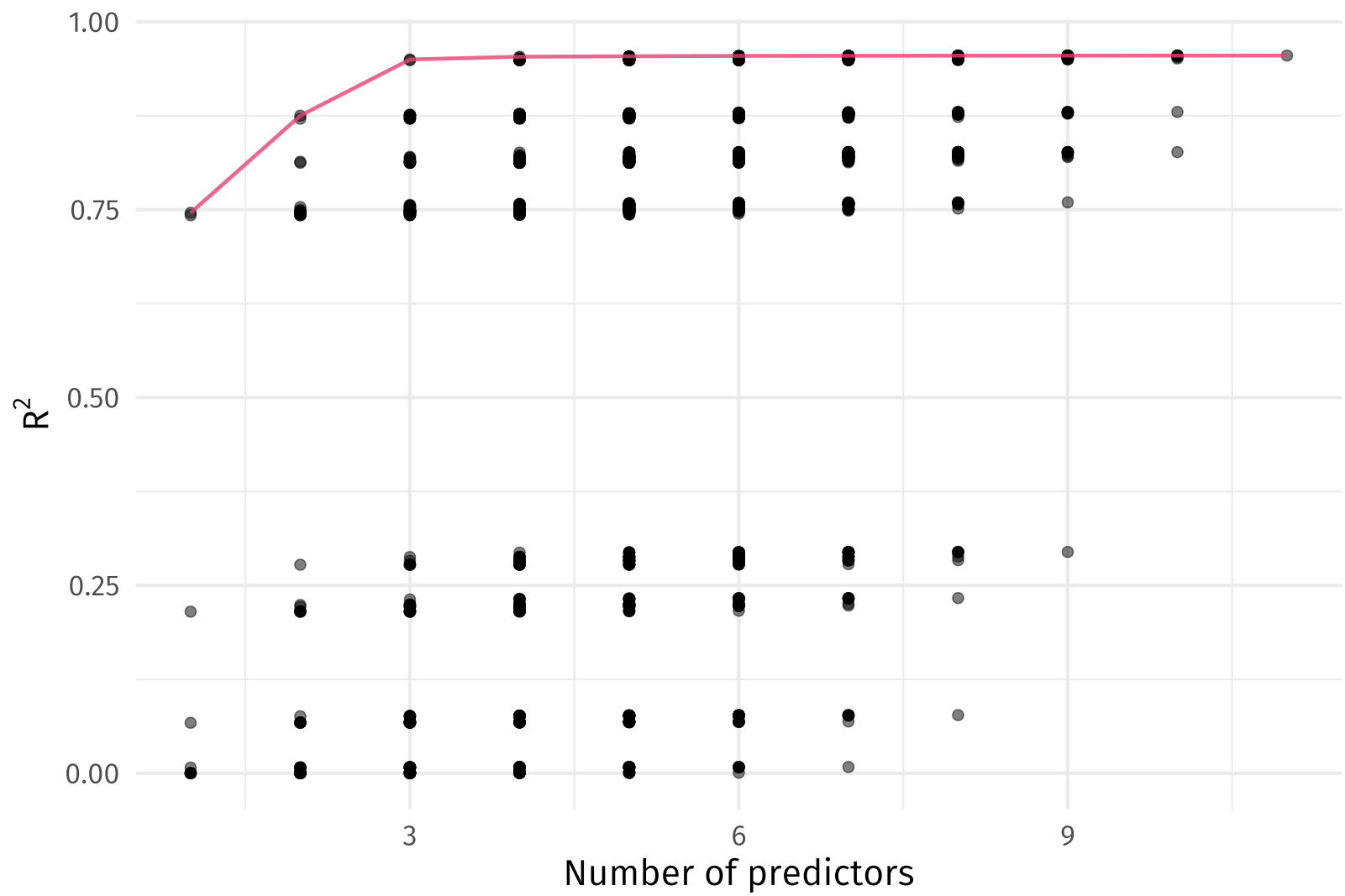
## Example dataset: Credit

We need to pre-process the dataset before we can select a model...

income	limit	rating	cards	age	education	i_female	i_student	i_married	i_asian	i_african_american	balance
14.9	3606	283	2	34	11	0	0	1	0	0	333
106.0	6645	483	3	82	15	1	1	1	1	0	903
104.6	7075	514	4	71	11	0	0	0	1	0	580
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80.2	8047	569	4	77	10	0	0	0	0	0	1151
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Now the dataset on has 400 observations on 12 variables (2,048 subsets).





# Model selection

## Best subset selection

From here, you would

1. Estimate cross-validated error for each  $\mathcal{M}_k$ .
2. Choose the  $\mathcal{M}_k$  that minimizes the CV error.
3. Train the chosen model on the full dataset.

# Model selection

## Best subset selection

### Warnings

- Computationally intensive
- Selected models may not be "right" (squared terms with linear terms)
- You need to protect against overfitting when choosing across  $\mathcal{M}_k$
- Also should worry about overfitting when  $p$  is "big"
- Dependent upon the variables (transformations) you provide

### Benefits

- Comprehensive search across provided variables
- Resulting model—when estimated with OLS—has OLS properties
- Can be applied to other (non-OLS) estimators



# Model selection

## Stepwise selection

**Stepwise selection** provides a less computational intensive alternative to best subset selection.

The basic idea behind **stepwise selection**

1. Start with an arbitrary model.
2. Try to find a "better" model by adding/removing variables.
3. Repeat.
4. Stop when you have the best model. (Or choose the best model.)

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The two most-common varieties of stepwise selection:

- **Forward** starts with only intercept ( $\mathcal{M}_0$ ) and adds variables
- **Backward** starts with all variables ( $\mathcal{M}_p$ ) and removes variables

# Model selection

## Forward stepwise selection

The process...

1. Start with a model with only an intercept (no predictors),  $\mathcal{M}_0$ .
2. For  $k = 0, \dots, p$ :
  - Estimate a model for each of the remaining  $p - k$  predictors, separately adding the predictors to model  $\mathcal{M}_k$ .
  - Define  $\mathcal{M}_{k+1}$  as the "best" model of the  $p - k$  models.
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What do we mean by "best"?

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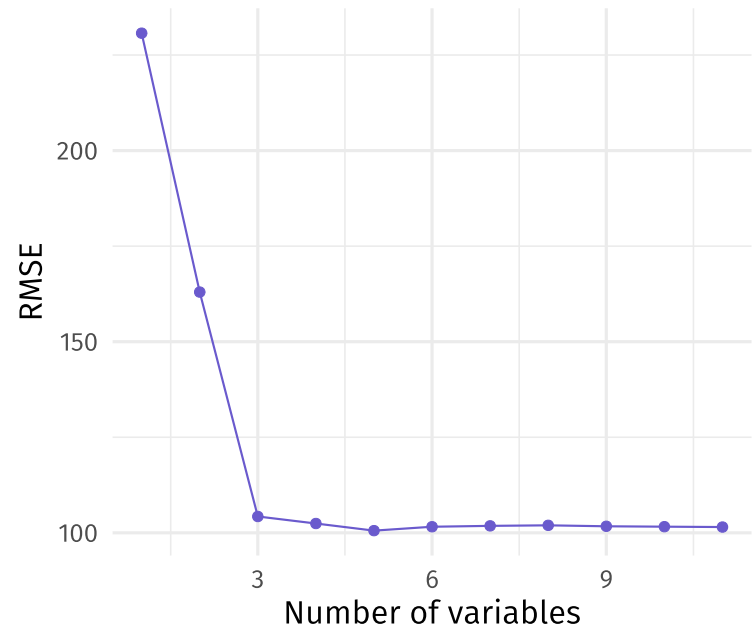
## Forward stepwise selection with caret in R

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train_forward = train(  
  y = credit_dt[["balance"]],  
  x = credit_dt %>% dplyr::select(-balance),  
  trControl = trainControl(method = "cv", number = 5),  
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N vars ⬆	RMSE ⬆	R2 ⬆	MAE ⬆
1	230.72	0.750	175.1
2	162.98	0.878	122.1
3	104.27	0.950	84.5
4	102.44	0.952	82.5
5	100.57	0.954	80.3
6	101.59	0.953	81.7
7	101.82	0.953	81.7
8	101.96	0.953	81.7
9	101.71	0.953	81.5
10	101.61	0.953	81.5



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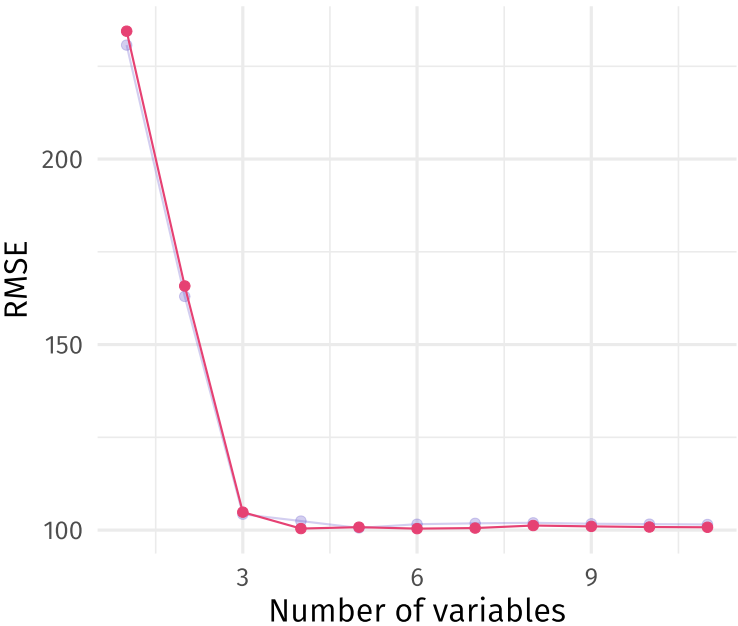
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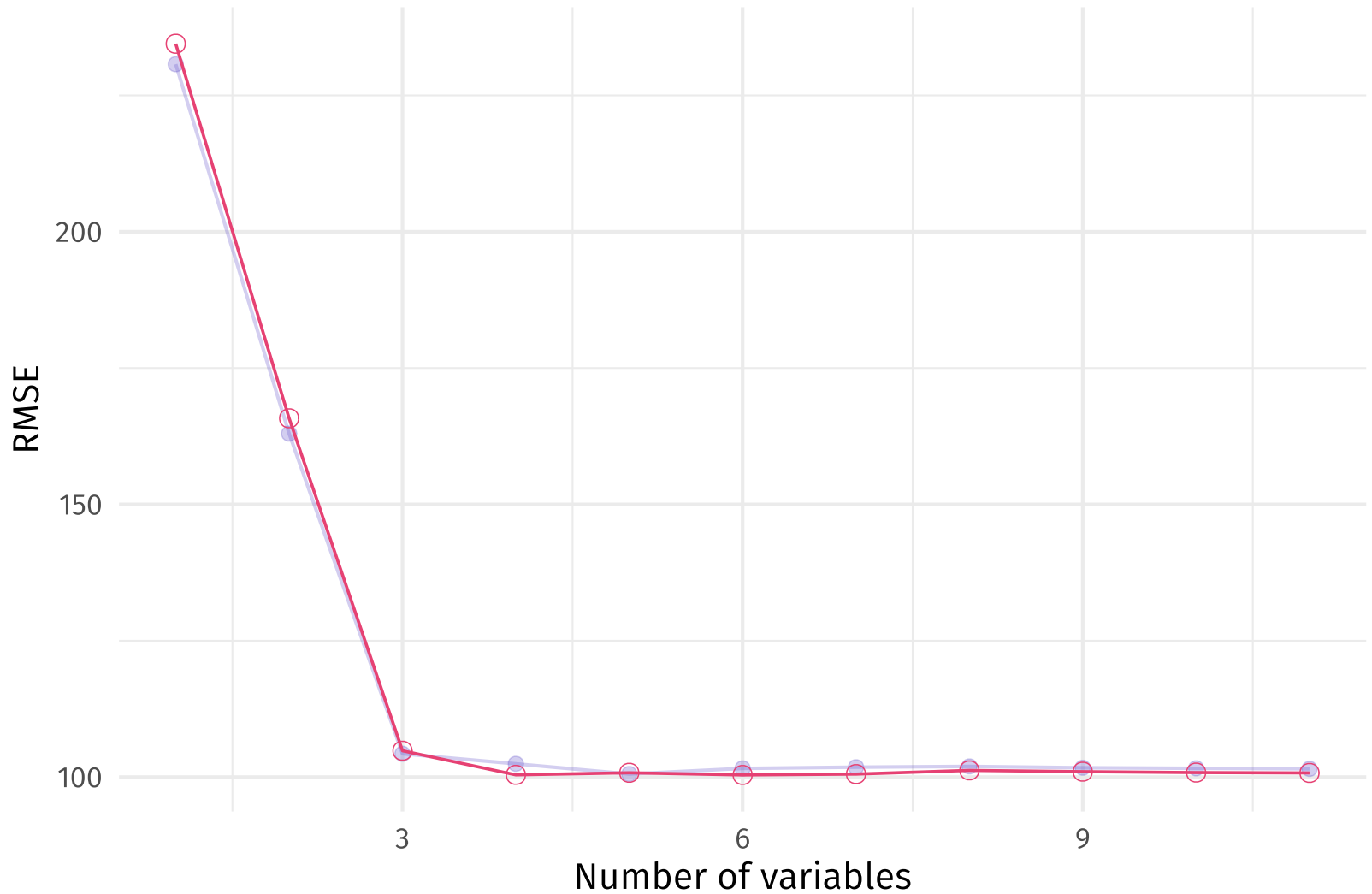
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4	100.41	0.954	80.1
5	100.79	0.954	80.6
6	100.39	0.954	80.2
7	100.55	0.954	80.1
8	101.23	0.954	80.6
9	100.99	0.954	80.4
10	100.83	0.954	80.3



Note: **forward** and **backward** step. selection can choose different models.



# Model selection

## Stepwise selection

Notes on stepwise selection

- **Less computationally intensive** (relative to best subset selection)
  - With  $p = 20$ , BSS fits 1,048,576 models.
  - With  $p = 20$ , forward/backward selection fits 211 models.
- There is **no guarantee** that stepwise selection finds the best model.
- **Best** is defined by your fit criterion (as always).
- Again, **cross validation is key** to avoiding overfitting.

# Model selection

## Criteria

Which model you choose is a function of **how you define "best"**.

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## Criteria

Which model you choose is a function of **how you define "best"**.

And we have many options... We've seen RSS, (R)MSE, RSE, MA,  $R^2$ , Adj.  $R^2$ .

Of course, there's more. Each **penalizes** the  $d$  predictors differently.

$$C_p = \frac{1}{n} \left( \text{RSS} + 2d\hat{\sigma}^2 \right)$$

$$\text{AIC} = \frac{1}{n\hat{\sigma}^2} \left( \text{RSS} + 2d\hat{\sigma}^2 \right)$$

$$\text{BIC} = \frac{1}{n\hat{\sigma}^2} \left( \text{RSS} + \log(n)d\hat{\sigma}^2 \right)$$

# Model selection

## Criteria

$C_p$ ,  $AIC$ , and  $BIC$  all have rigorous theoretical justifications...  
the adjusted  $R^2$  is not as well motivated in statistical theory

*ISL, p. 213*

In general, we will stick with cross-validated criteria, but you still need to choose a selection criterion.

# Sources

These notes draw upon

- [An Introduction to Statistical Learning \(ISL\)](#)  
James, Witten, Hastie, and Tibshirani

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