Regression in high dimensions

STAT 471

October 7, 2021

Where we are

odds ⟷ probability

- ✓ **Unit 1:** Intro to modern data mining
- ✓ **Unit 2:** Tuning predictive models
- **Unit 3:** Regression-based methods
- **Unit 4:** Tree-based methods
- **Unit 5:** Deep learning

Lecture 1: Logistic regression

Lecture 2: Regression in high dimensions

Lecture 3: Ridge regression

[**Fall break:** No class]

Lecture 4: Lasso regression

Lecture 5: Unit review and quiz in class

Homework 1 due the following Sunday.

Midterm exam following Monday (7-9pm).

High-dimensional data

Recall: n is the number of training observations and p is the number of features.

↳ in this case ~4

Most datasets we've considered so far have n much larger than p.

In modern applications, can collect very many features for each observation, e.g.:

- Natural language processing
- Image processing
- Genetics/Genomics
- E-commerce

here, we are fitting 3 features on 1000+ data pts

High-dimensional data: Data with $p > n$ or $p \approx n$

what happens when $p \gg n$?

Challenges in high dimensions

in linear regression, p = df

number features = df

Let's consider fitting a linear regression with n observations and p features.

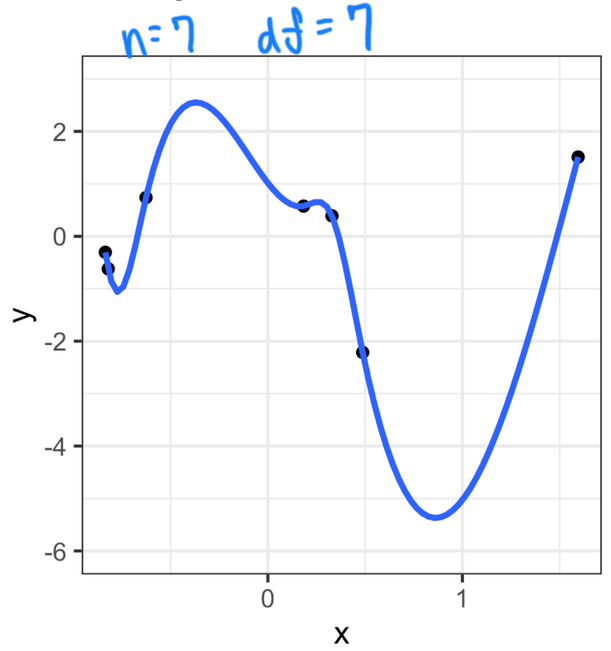
If $p > n$, the columns of the feature matrix X guaranteed to be multi-collinear, so the least squares linear regression estimate is not even defined.

If $p = n$, linear regression will perfectly fit training set, even with "junk" features.

If $p < n$, recall that linear regression variance is $\sigma^2 p/n$.
Therefore, if $p \approx n$ then variance will be very high.

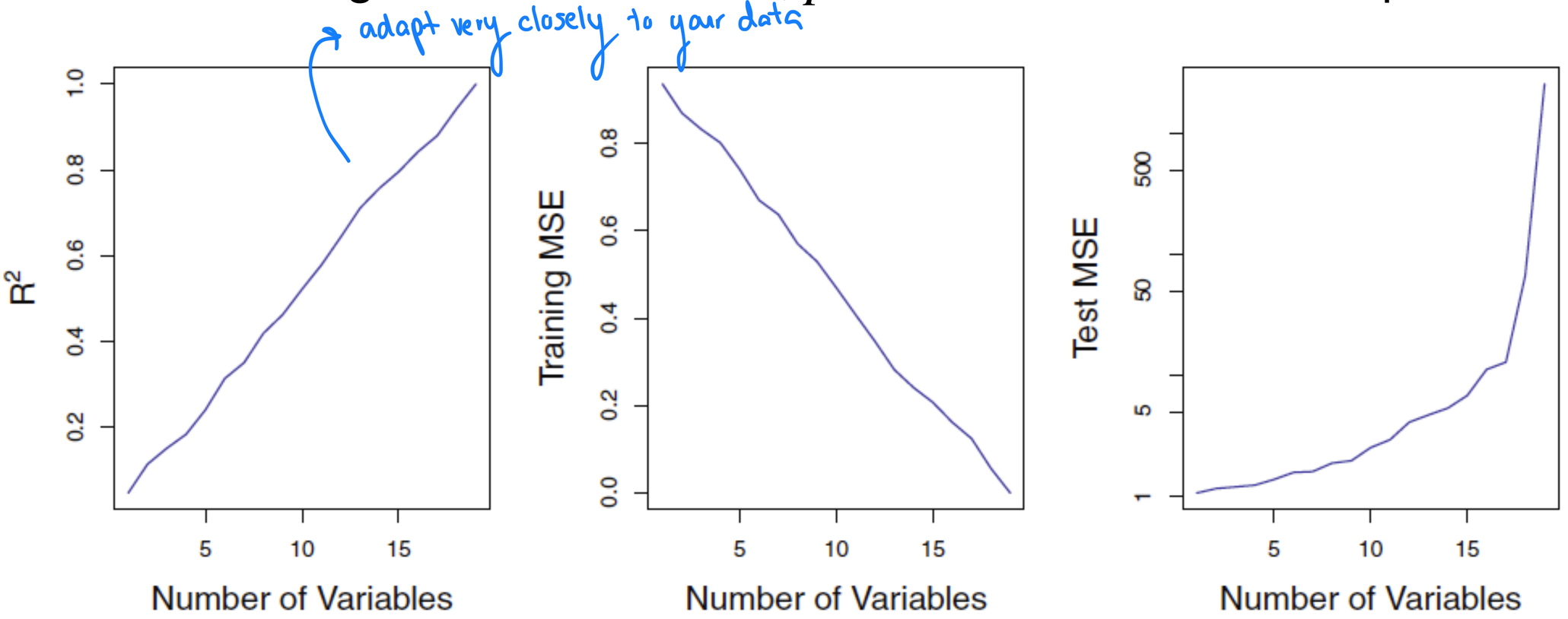
even if no trend in data, overfit = high variance

Linear models fit using too many features (i.e. too many degrees of freedom) perform poorly due to high variance.



Challenges in high dimensions (illustration)

Linear regression for $n = 20$; p features unrelated to response



The solution

The solution is to constrain the fitted coefficients in some way, e.g.:

1. Make sure fitted coefficients are not too large (ridge regression).
2. Make sure fitted coefficients are mostly equal to zero (lasso regression).

These constraints reduce the degrees of freedom of the fit, reducing variance.

We are still fitting p coefficients, but using fewer than p degrees of freedom.

Penalization: A way of constraining the fit

penalty is applied during optimization

Recall least squares solution: set up incentives to keep coefficients from getting out of hand

$$\widehat{\beta} = \underset{\beta_0,\beta_1,\ldots,\beta_{p-1}}{\arg\min} \sum_{i=1}^{n} (y_i - (\beta_0 + \beta_1 X_{i1} + \cdots + \beta_{p-1} X_{i,p-1}))^2.$$

Here we let $\widehat{\beta}$ fit the data as close as possible, putting no constraints.

Penalization: Add a term $P(\beta)$ that measures how "wild" β is, to incentivize β not to be too wild:

cost & cost to ↑ df

how important is penalty vs. fit

$$\widehat{\beta}' = \underset{\beta_0,\beta_1,\ldots,\beta_{p-1}}{\arg\min} \sum_{i=1}^{n} (y_i - (\beta_0 + \beta_1 X_{i1} + \cdots + \beta_{p-1} X_{i,p-1}))^2 + \lambda \cdot P(\beta).$$

how well β fits the data ← compromise → how wild β is

Example: L0-penalized regression

Consider the penalized regression

$$\widehat{\beta}' = \underset{\beta_0,\beta_1,\ldots,\beta_{p-1}}{\arg\min} \sum_{i=1}^{n} (y_i - (\beta_0 + \beta_1 X_{i1} + \cdots + \beta_{p-1} X_{i,p-1}))^2 + \lambda \cdot P(\beta),$$

$$\text{with } P(\beta) = |\{j : \beta_j \neq 0\}|.$$

The L0 penalty P counts the number of nonzero entries in β, and creates sparse solutions $\widehat{\beta}$.

lots of entries equal to zero

The optimization above is computationally infeasible, so in practice we use a different penalty (called the lasso) to achieve sparsity (stay tuned for Lecture 4).

How and when penalization works

if you are looking for a sparse solution, but the solution is not sparse, you are out of luck

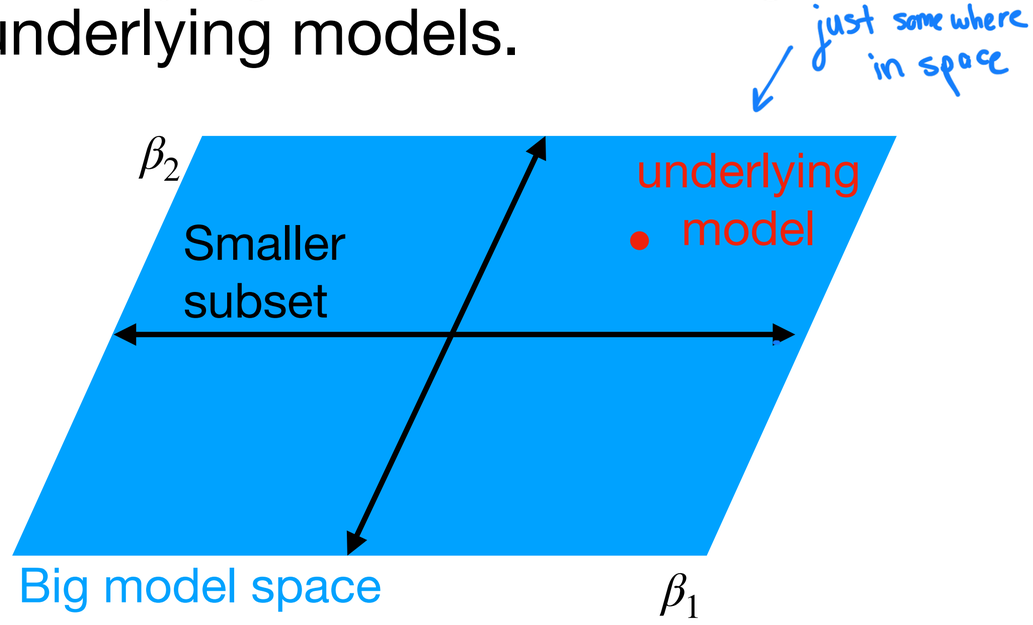
Penalization reduces the variance, but increases the bias of the predictions.

⇒ Reduces test error when reduction in variance outweighs increase in bias.

The bias is a function of the complexity of the underlying model, and in high dimensions, we can have some very complex underlying models.

Penalization: a bet on the model being close to a smaller subset of the big model space:

- If so, overall win (the bias is not too big);
- If not, out of luck (the bias is too big).



Statistical significance in high dimensions

We can quantify statistical significance based on linear or logistic regression (using p-values and confidence intervals).

In high-dimensions, the theory underlying statistical significance breaks.

It is a topic of current research (including my own!) how to quantify statistical significance in high-dimensional problems.

For now: There is no standard way to get p-values or confidence intervals from a penalized regression. We mainly use penalized regression for prediction.

Looking ahead to lectures 3 and 4

Lecture 3: Ridge regression (constraining coefficients not to be too large)

Lecture 4: Lasso regression (constraining coefficients to be sparse)

We'll learn about the theory and practice of these penalized regression methods.