

# ML extensions to OLS

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Day 2/5

# Introduction

Yesterday we explored how a familiar estimator (logistic regression) incorporates some fundamental aspects of ML

- ▶ ML is not some entirely new, alien type of doing statistics
- ▶ ML is typically focused on prediction problems
- ▶ Lots of really useful ML models are extensions of regression framework

So how should we understand OLS within a prediction context?

How do other popular forms of ML come out of it?

# Today's session

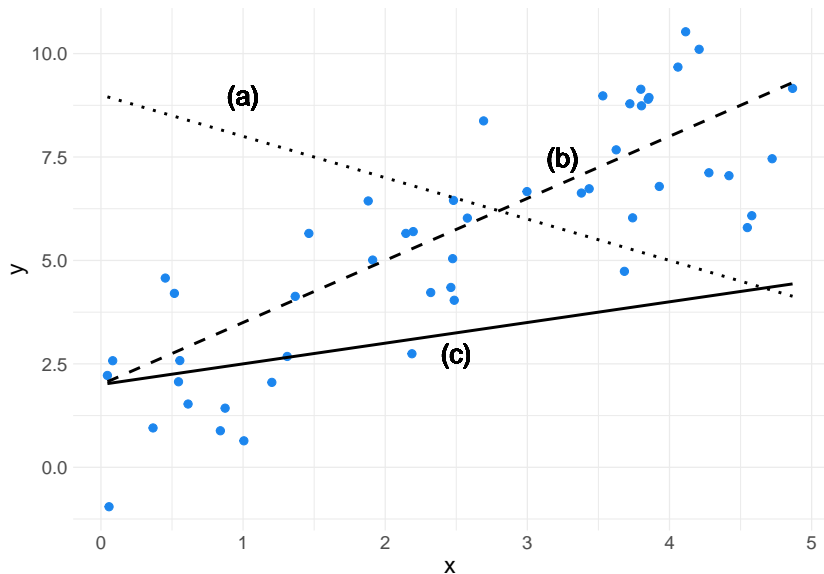
1. Recap OLS from prediction perspective
  - ▶ How does OLS work?
  - ▶ Optimisation criteria
  - ▶ Bias-variance trade-off
2. LASSO estimator
3. Hyperparameter tuning
4. Practical application

Key topics:

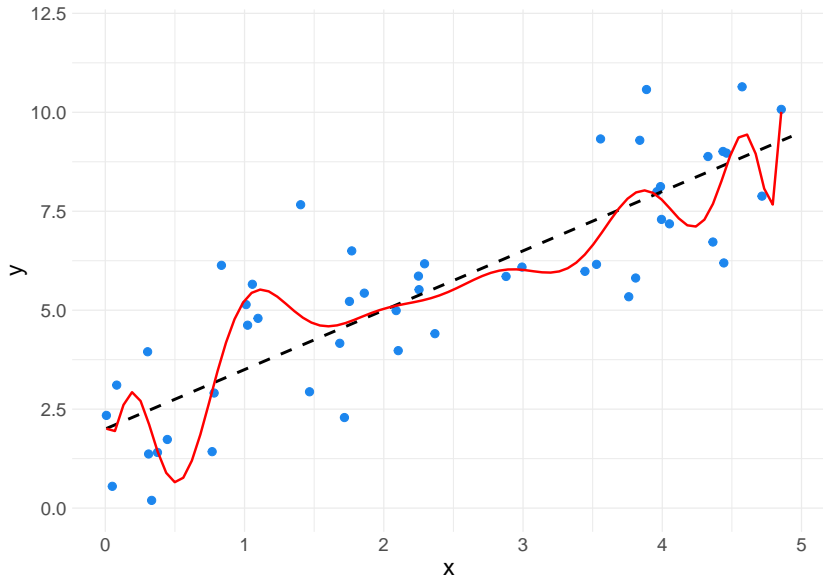
- ▶ Bias and variance
- ▶ Regularisation
- ▶  $K$ -fold cross validation

# Ordinary Least Squares Regression

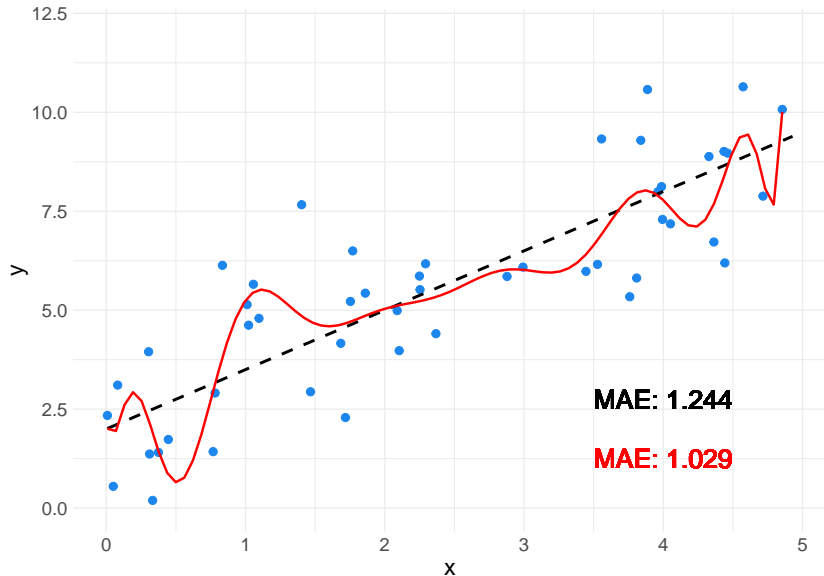
## Refresher: which is the best line?



## Refresher: which is the best line? 2



## Refresher: which is the best line? 2



# OLS as a tool for inference

In inference terms, OLS estimates  $\hat{\beta}$  that:

- ▶ Captures the linear relationship between  $\mathbf{X}$  and  $\mathbf{y}$
- ▶ Yields individual estimates of the “effects” of  $\mathbf{X}$  on  $\mathbf{y}$
- ▶ Allows us to understand the uncertainty over  $\hat{\beta}$ 
  - ▶ E.g., how confident are we that there is +/- effect of  $x_1$  on  $\mathbf{y}$



# OLS: Optimisation

OLS regression minimises the **sum of the squared error** between the regression line ( $\mathbf{X}\beta$ ) and the observed outcome ( $\mathbf{y}$ ):

$$\arg \min_{\beta} \sum_{i=1}^N (y_i - \mathbf{x}_i \beta)^2,$$

where  $\mathbf{x}_i \beta$  is the linear regression function.

*How might we solve this?*

- ▶ Calculus – there is a closed form solution (unlike logistic regression)
- ▶ Maximum likelihood estimation

# Why do we like OLS?

Not only does OLS have a closed form solution, we also know that, under the Gauss Markov (GM) assumptions, OLS is:

- ▶ **B**est
- ▶ **L**inear (Hansen 2021)
- ▶ **U**nbiased
- ▶ **E**stimator

## GM Assumptions

In other words, in terms of estimating the parameters  $\beta$ , you won't find a linear model that is unbiased with a lower variance

OLS is fantastic for inference:

- ▶ Typically concerned with generating **unbiased** estimate of  $\hat{\beta}$
- ▶ So we can perform valid significance testing

# Bias

Bias is a feature of the estimator:

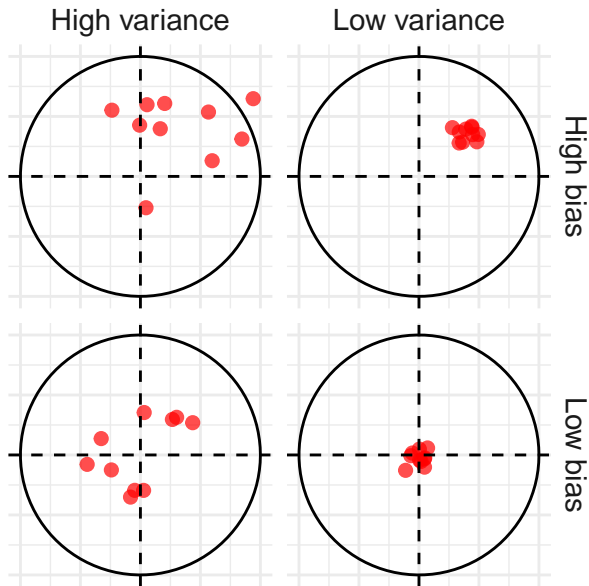
- ▶  $\text{Bias}_\beta = (\mathbb{E}[\hat{\beta}] - \beta)$
- ▶ On average, the estimated parameters are equal to the true parameters
- ▶ Under GM, we know that  $(\mathbb{E}[\hat{\beta}] - \beta) = 0$

# Variance

As we sample new (GM-satisfying) data, the parameters of our model will shift:

- ▶ Hence, there will be variance over our parameter estimates
- ▶  $\mathbb{V}_{\hat{\beta}} = \mathbb{E}[(\mathbb{E}[\hat{\beta}] - \hat{\beta})^2]$
- ▶ The average distance between a particular parameter estimate and the mean of parameter estimates over multiple samples

## Visualising bias and variance



# Predicting *new* values

In the remainder of today's session, we are going to consider the following generic supervised learning problem:

- ▶ We observe  $(\mathbf{y}, \mathbf{X}) \in \mathcal{D}$ 
  - ▶ A training sample that is taken from a wider possible set of data
  - ▶ I.e. we can think, counterfactually, of resampling to get a new sample  $(\mathbf{y}_{\text{New}}, \mathbf{X}_{\text{New}})$
- ▶ We also observe a “test” dataset  $\mathbf{X}'$

The goal is to estimate  $\mathbf{y}'$  by training a model  $\hat{f}$

- ▶ The outcomes that correspond to  $\mathbf{X}'$

# OLS as a tool for prediction

When we run OLS, we also get a “trained model”:

- ▶  $\hat{f}$  – that has parameters equal to  $\hat{\beta}$
- ▶ Can be applied to a new “test” dataset  $\mathbf{X}'$
- ▶ To generate new predictions  $\mathbf{y}'$

# Bias and variance of predictions

We can also think of bias in terms of the predictions:

- ▶  $\text{Bias}_y = (\mathbb{E}[\hat{y}] - y)$
- ▶ We ideally want low bias
- ▶ High bias suggests the model is not sensitive enough

And we can think about the variance of the prediction:

- ▶  $\mathbb{V}_{\hat{y}} = \mathbb{E}[(\mathbb{E}[\hat{y}] - \hat{y})^2]$

High variance means that the model is very sensitive to  $\mathbf{X}$  – the training data – but will perform poorly on new samples of data

- ▶ With the new data, and high variance, we would expect quite different predictions



## Bias-variance trade off

So can't we just choose a low-variance, low-bias modeling strategy?  
Not quite!

Assume we could calculate the mean squared error of some new data  $\mathbf{X}'$  given a trained model  $\hat{f}$ :

$$\text{MSE} = \mathbb{E}[(\hat{f}(\mathbf{X}') - \mathbf{y}')^2].$$

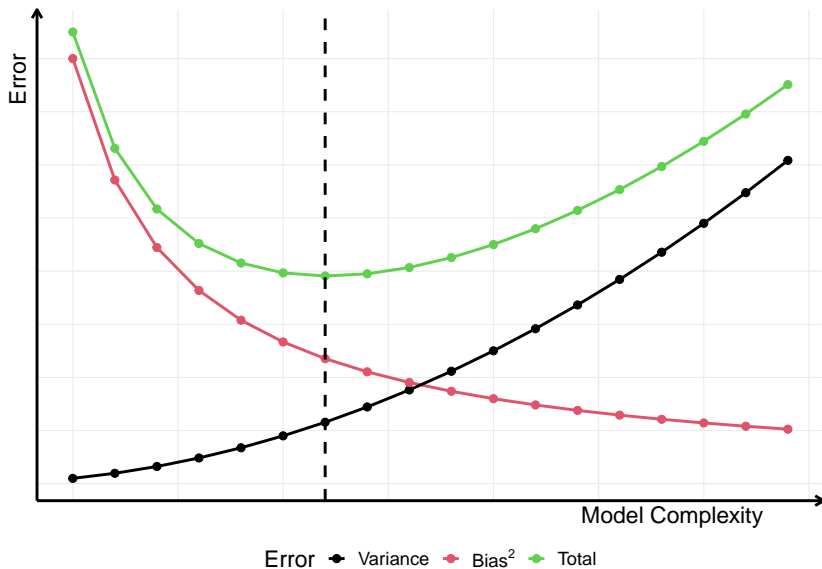
We can decompose this further:

$$\text{MSE} = \underbrace{\mathbb{E}[(\hat{f}(\mathbf{X}') - \mathbb{E}[\hat{\mathbf{y}}])^2]}_{\text{Variance}} + \underbrace{(\mathbb{E}[\hat{\mathbf{y}}] - \mathbf{y}')^2}_{\text{Bias}^2}$$

So holding the MSE fixed, if we reduce the variance we must increase the bias

- I.e. there is a **bias-variance trade-off**

## Visualising the trade-off

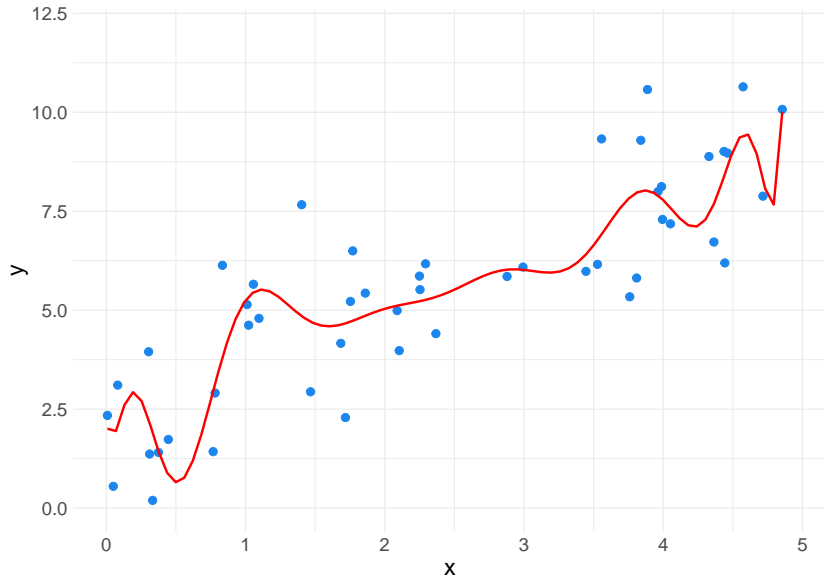


# Out of sample performance of OLS

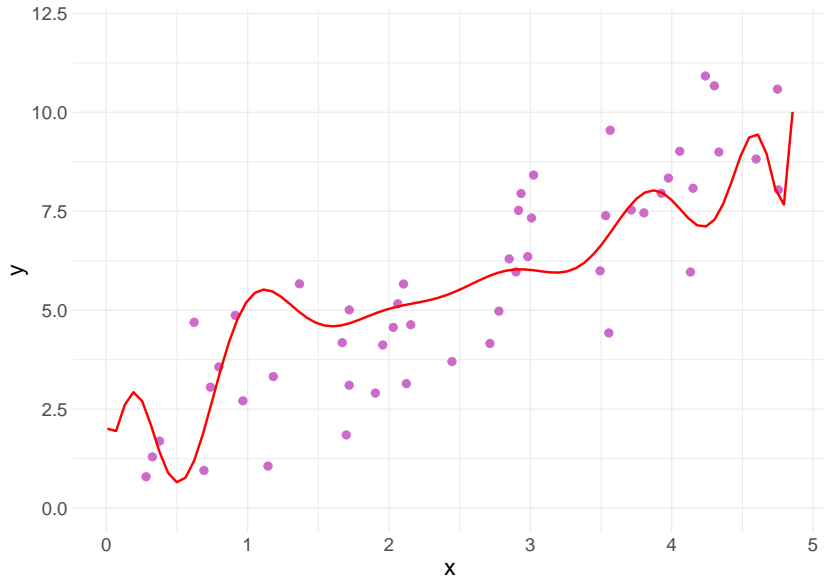
This trade-off explains why we might not want to use OLS for prediction tasks:

- ▶ By virtue of GM assumptions and BLUE, MSE is explained entirely by variance
  - ▶ Averaging across models, the model parameters are centred on the true values (an unbiased estimator)
- ▶ So we cannot tweak the model to get slightly better out-of-sample predictions at the expense of some added bias
  - ▶ In other words, we cannot leverage the bias-variance trade-off

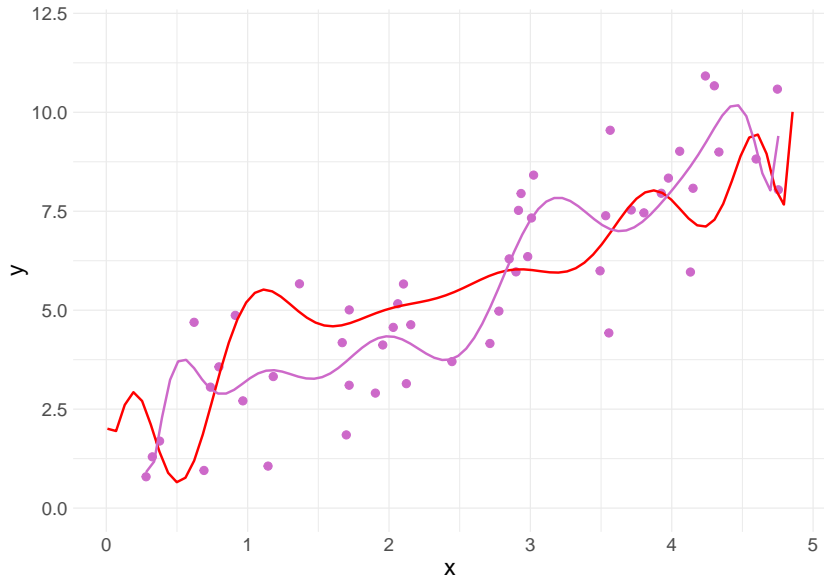
## OLS: Complex OLS model trained on $\mathbf{X}$



## OLS: Compare models' predictions to $\mathbf{X}'$



## OLS: Variance in model predictions over $X$



## The LASSO estimator

## Regularisation and overfitting

In the previous examples, an overly complicated model yields poor out-of-sample predictions. To ensure our model does not have too much variance, we can *penalise* overly-complicated models that will perform poorly on new test data ( $\mathbf{X}'$ )

- ▶ This may introduce bias into the model
- ▶ But, if done correctly, we can reduce the total MSE by offsetting overly-high variance
- ▶ And therefore yield better predictions on  $\mathbf{X}'$

This is a generalisable feature of ML:

- ▶ Regularisation constrains model complexity to prevent overfitting
- ▶ Especially important for the models we consider in the remainder of the week that are very powerful



# Regularisation of OLS

If we want to continue using a linear predictor we need to modify the loss function  $L$ :

- ▶  $L_{OLS}$  is known to be unbiased
- ▶ So adding a term that is non-zero to  $L$  will *add* bias...
- ▶ ... and hopefully improve out-of-sample prediction

In other words:

- ▶ We sacrifice some variance in order to improve the predictive performance of the model on  $\mathbf{X}'$

# Generalising OLS with regularization

We can state this problem using the following general linear optimisation problem:

$$\arg \min_f \underbrace{\sum_{i=1}^N (y_i - f(\mathbf{x}_i))^2}_{\text{Sum of squared error}} + \underbrace{\lambda R(f)}_{\text{Regularisation}}$$

For OLS:

- ▶  $f \in \mathcal{F}_{\text{linear}}$
- ▶  $\lambda = \frac{1}{\infty} = 0$

But what if  $\lambda \neq 0$ ?

- ▶ Then we must decide what  $R(\cdot)$  is
- ▶ And decide on a value of  $\lambda$  – a hyperparameter

## $R(\cdot)$ as shrinkage

Consider an OLS model with  $k$  parameters:

- ▶ The model estimates coefficients for each parameter
- ▶ Regardless of how large or small that coefficient is
- ▶ In a sense, with non-zero estimates for each parameter these models can be considered “complex”

We can reduce the complexity of the regression model by setting some parameters to zero

- ▶ I.e. we **shrink** the coefficient estimates
- ▶ Aim to reduce the variance error by more than the increase in bias error

In the linear framework, we need some way to penalize non-zero coefficients

## Least absolute shrinkage and selection operator (LASSO)

We can calculate the total magnitude (or **L1 Norm**) of the coefficients in a model as:

$$||\beta||_1 = \sum_j |\beta_j|$$

Next, we can think about restricting the size of this norm:

$$||\beta||_1 \leq t$$

And finally we want to include this in our loss function:

$$\arg \min_{\beta} \sum_{i=1}^N (y_i - \mathbf{x}_i \beta)^2 \text{ subject to } ||\beta||_1 \leq t$$

This final optimisation constraint is equivalent to:

$$\arg \min_{\beta} \sum_{i=1}^N (y_i - \mathbf{x}_i \beta)^2 + \lambda ||\beta||_1.$$

# LASSO

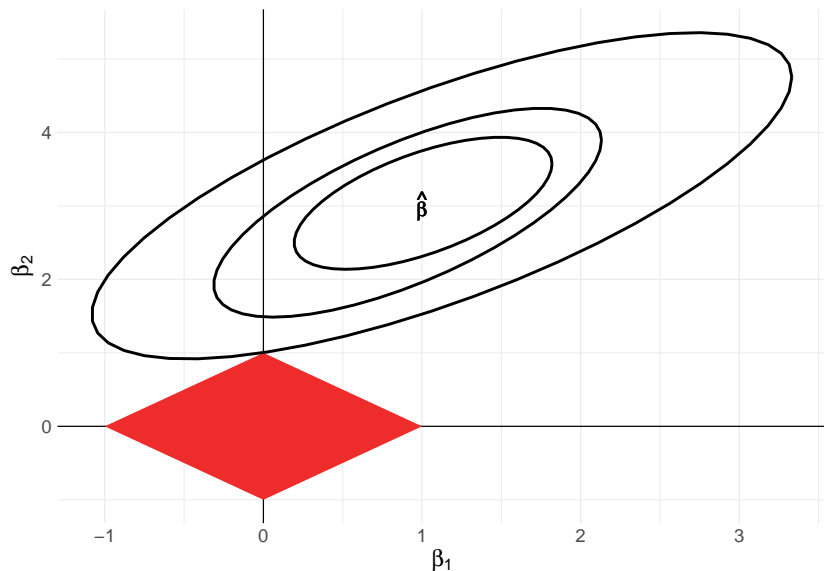
Hence, the LASSO estimator conforms to the generalised loss function introduced earlier

- ▶  $R(f) = ||\hat{\beta}||_1$

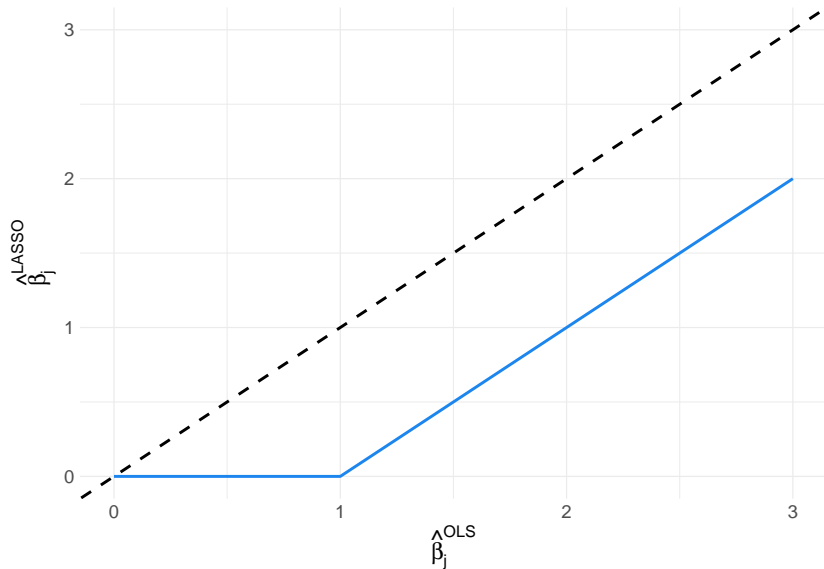
LASSO often yields coefficient estimates of exactly zero:

- ▶ Think about varying the true value of some coefficient  $\beta_j$ :
  - ▶ When  $\beta_j$  is large, we might shrink it (relative to OLS) but the importance of this predictor is sufficient to entail a non-zero coefficient
  - ▶ But for some small enough value  $b$ , the cost of including  $b$  in L1-norm is greater than the reduction in squared error
- ▶ In other words, the L1 norm constraint can lead to “corner solutions”

Example of LASSO corner solution ( $||\beta||_1 \leq 1$ )



# Comparison of $\hat{\beta}_j^{\text{OLS}}$ to $\hat{\beta}_j^{\text{LASSO}}$



# Two helpful properties of LASSO

## 1. Prediction accuracy

- ▶ We trade off an amount of bias for a (hopefully) greater reduction in variance, improving out-of-sample prediction
- ▶ Cf. a non-zero *true* coefficient estimated with a large confidence interval

## 2. Selection of relevant variables

- ▶ The possibility of corner-solutions acts as a useful variable selection mechanism
- ▶ LASSO essentially selects the most important variables for us



## Hyperparameter tuning

## Choosing $\lambda$

The final part of the estimation problem is setting  $\lambda$ . Recall that:

$$\mathcal{L} = \sum_{i=1}^N (y_i - f(x_i))^2 + \lambda \|\hat{\beta}\|_1$$

$\lambda$  regulates how much bias we add to the model:

- ▶ Too large a value = overly constricted model, large MSE
- ▶ Too small a value = overly complex model, large MSE

We need to find a value that helps us get near the bottom of the total-error curve!

- ▶ This process is called hyperparameter tuning
- ▶ It is a recurrent feature of ML methods

## Simple tuning

Simplest way is to simply try a few values:

- ▶ In the case of LASSO, we might try  $\lambda = \{0.1, 1, 10\}$
- ▶ Choose  $\lambda$  that yields lowest MSE from  $MSE_{\lambda=0.1}, MSE_{\lambda=1}, MSE_{\lambda=10}$
- ▶ Use this value in the final model

But there are some limitations:

- ▶ You are “testing” your model on the same data that it was trained upon
- ▶ So this will inflate the actual accuracy of your model
- ▶ Goes against the train-test ethos of ML prediction

# Holdout sample

As an alternative, we could create a holdout sample:

- ▶ Split our training data  $\mathbf{X}$  into  $\{\mathbf{X}^{\text{Train}}, \mathbf{X}^{\text{Holdout}}\}$
- ▶ Train our model for each value of  $\lambda$  on  $\mathbf{X}^{\text{Train}}$
- ▶ Then test the predictive accuracy on  $\mathbf{X}^{\text{Holdout}}$
- ▶ In other words, create a miniature version of the train-test split within our training data

But again, there are limitations:

- ▶ By leaving out some observations, we lose predictive power
- ▶ Even if observations are randomised across the two datasets, the model can never learn from the fixed holdout data

## $K$ -fold cross validation

We can generalise holdout sampling to incorporate all of our training data:

1. Randomly assign each *training* observation to one of  $k$  **folds**
2. Estimate the model  $k$  times, omitting one “fold” from training at a time
3. Calculate the prediction error using the fold not included in the data
4. Average the prediction errors across  $k - folds$
5. Repeat 2-4 for each value of  $\lambda$  we want to test

Choose  $\lambda$  where the average cross-validated MSE is lowest

The choice of  $k$  will depend on:

- ▶ The time it takes to train the model
- ▶ The size of your training data

## Application

## Blackwell and Olsen (2021)

Suppose we have an outcome  $y$ , a treatment  $d$ , covariates  $X$ , and an “effect moderator”  $v$

- ▶ We want to estimate an *inference* model
- ▶ Understand how the treatment effect is moderated

Naive suggestion:

- ▶ Include an interaction term to model the differential effect of treatment
  - ▶ I.e.  $y_i = \beta_0 + \beta_1 d_i + \beta_2 v_i + \beta_3 d_i v_i + \beta' X_i$

What's wrong with this model?

- ▶ We assume that the interactive effect  $\beta_3$  is constant across covariates
- ▶ This introduces bias into the model if  $vX$  is related either to  $dv$  or  $y$

# Prediction and inference problem

Therefore the researcher faces a prediction problem *and* an inference problem:

- ▶ **Inference problem:** How do we control for potential bias introduced between  $X, v, d$ , and  $y$ ?
- ▶ **Prediction problem:** Which interactions within  $vX$  are most likely to confound the results?
  - ▶ Let us denote the true non-zero predictors  $\mathcal{P}$
  - ▶ Inverting a  $\hat{y}$  problem – which variables are useful to predict new data?

From today's session we know that:

- ▶ Bias can be useful to offset variance when making out-of-sample predictions
- ▶ Bias inherently distorts our estimate of  $\beta$



# Combining LASSO and OLS

Blackwell and Olsen propose splitting the problem of interaction estimation into two stages:

## 1. **Variable selection**

- ▶ Use LASSO to estimate a series of variable selection models
- ▶ Attempt to find interaction terms that correlate with either outcome, treatment, or treatment-moderated interaction

## 2. **Inference**

- ▶ Use OLS to estimate an inference model
- ▶ Using only non-zero interaction terms in LASSO models

What makes this strategy so useful (and informative!) is that:

- ▶ We leverage bias to make better predictions in Stage 1
- ▶ We de-bias inference in Stage 2 using OLS + Stage 1 results

# Post-double selection method

## Stage 1

- ▶ Estimate LASSO models for:
  1.  $y$  on  $\{v, X, vX\}$
  2.  $d$  on  $\{v, X, vX\}$
  3.  $dv$  on  $\{v, X, vX\}$
- ▶ Let  $Z^*$  index all variables with non-zero coefficients in any of models 1-3

## Stage 2

- ▶ Regress  $y$  on  $d, dv$  and  $Z^*$

Blackwell and Olson also suggest adding all “base-terms” (i.e  $X$ ) regardless of LASSO coefficient

Extra Slides

## Alternative $R(f)$ to the L1 norm

Following a similar logic to the shrinkage used by LASSO, we can define other measures of magnitude, like the L2 norm  $||\beta||_2$ :

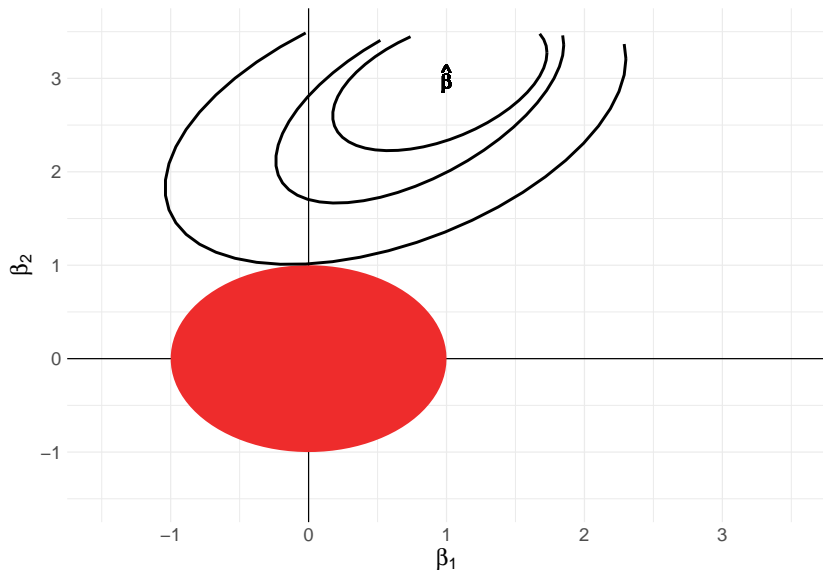
$$\sqrt{\sum_j |\beta_j|^2}$$

When we plug in the L2 norm into the loss function, we get the **ridge regression** estimator:

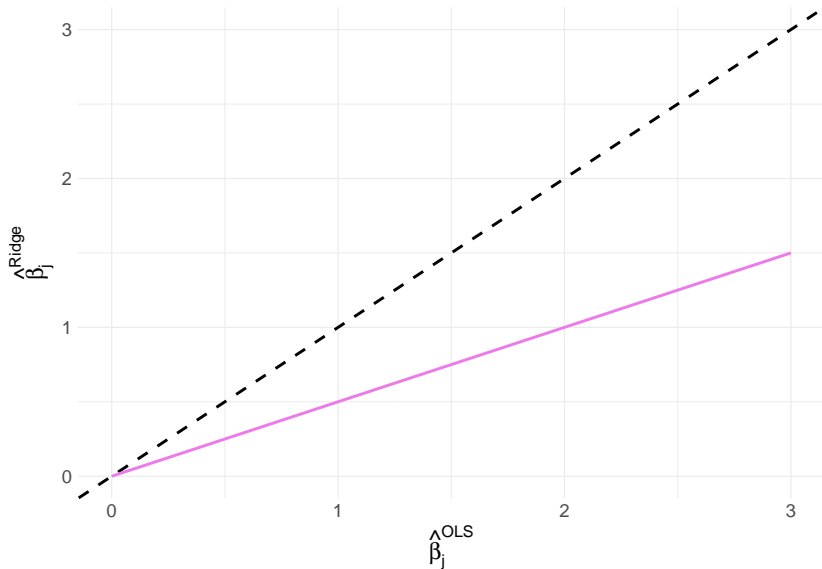
$$\arg \min_{\beta} \sum_{i=1}^N (y_i - \mathbf{x}_i \beta)^2 + \lambda ||\beta||_2$$

Unlike the LASSO estimator, ridge regression does not have a sharp cut-off, but rather scales the size of all coefficients in the model

## Ridge regression – no corner solutions



## Ridge regression – constant scaling of coefficients



# Gauss Markov Assumptions

Five assumptions need to hold:

1.  $\mathbf{y}$  is a linear function of  $\beta$
2.  $\mathbb{E}[\epsilon_i] = 0$
3.  $\mathbb{V}[\epsilon_i] = \sigma_i^2, \forall i$
4.  $Cov(\epsilon_i, \epsilon_j) = 0, \forall i \neq j$
5.  $Cov(\mathbf{x}_i, \epsilon_i) = 0$