ML extensions to OLS

Oxford Spring School in Advanced Research Methods, 2021

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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

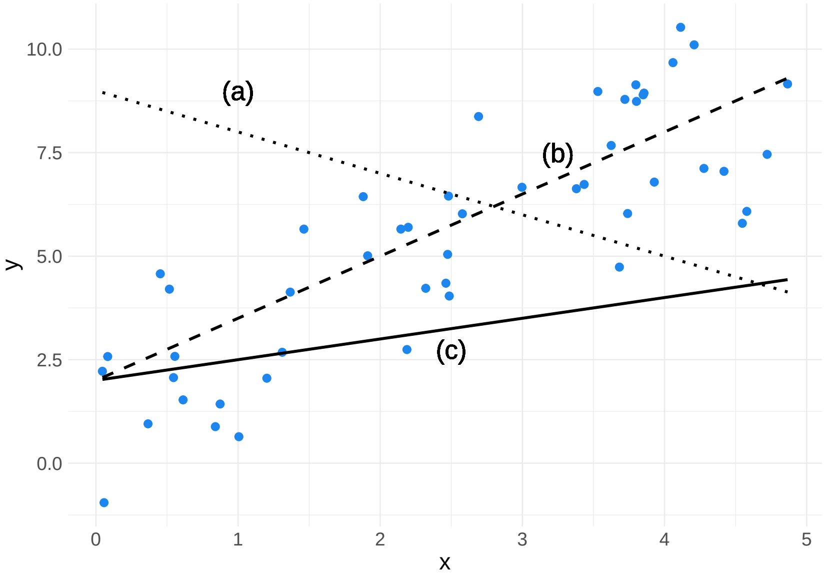
1. Recap OLS from prediction perspective
    - How does OLS work?
    - Optimisation criteria
    - Bias-variance trade-off
2. LASSO estimator
3. Hyperparameter tuning
4. Practical application

Key topics:

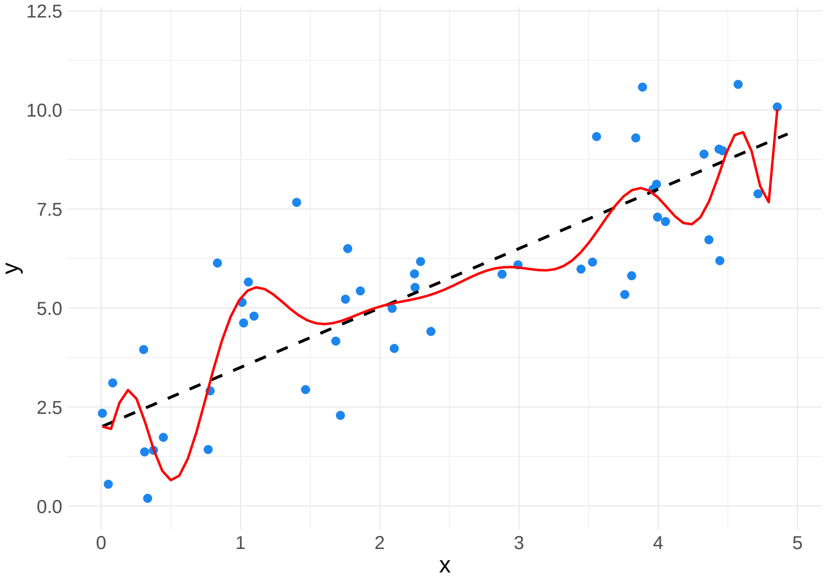
- Bias and variance
- Regularisation
- $K-$fold cross validation

Ordinary Least Squares Regression

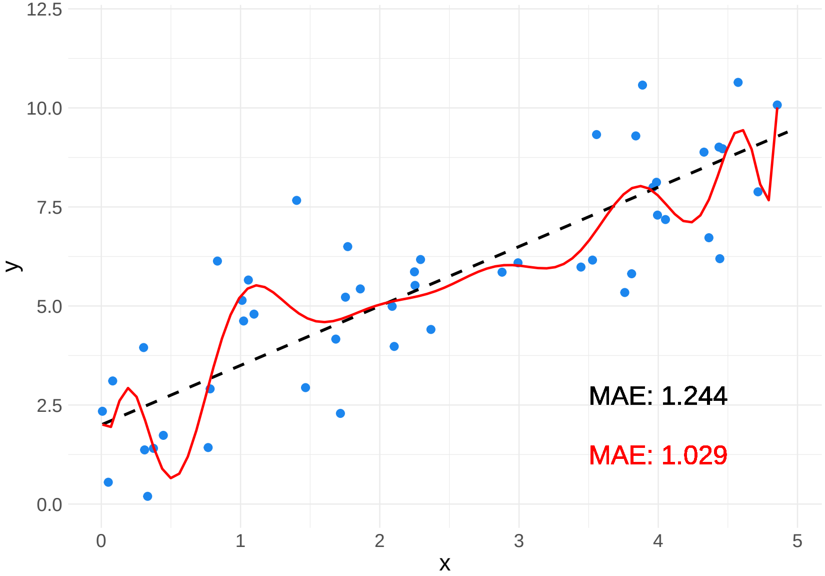
Refresher: which is the best line?



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 $\boldsymbol{X}$ on $\boldsymbol{y}$
- Allows us to understand the uncertainty over $\hat{\beta}$
  - E.g., how confident are we that there is $+/$- effect of $\boldsymbol{x_1}$ on $\boldsymbol{y}$

OLS: Optimisation

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

$$\arg\min_{\boldsymbol{\beta}} \sum_{i=1}^{N} (y_i - \boldsymbol{x_i}\boldsymbol{\beta})^2,$$

where $\boldsymbol{x_i}\boldsymbol{\beta}$ 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
- ~~Linear~~ (Hansen 2021)
- **U**nbiased
- **E**stimator

GM Assumptions

In other words, in terms of estimating the parameters β, 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:

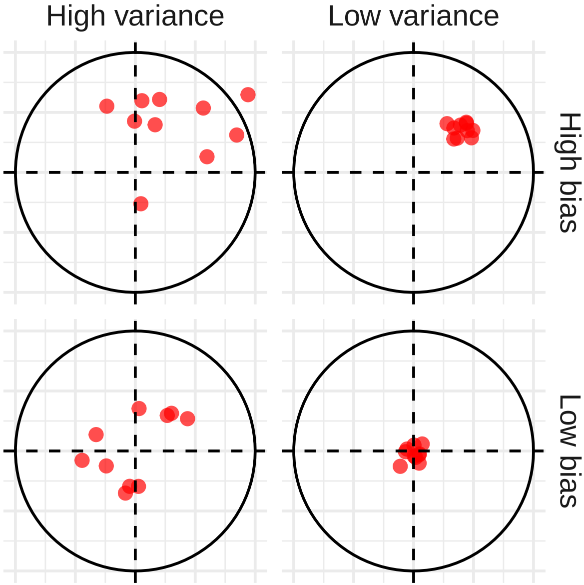
- $\text{Bias}_{\boldsymbol{\beta}} = (\mathbb{E}[\hat{\boldsymbol{\beta}}] - \boldsymbol{\beta})$
- On average, the estimated parameters are equal to the true parameters
- Under GM, we know that $(\mathbb{E}[\hat{\boldsymbol{\beta}}] - \boldsymbol{\beta}) = 0$

Variance

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

- Hence, there will be variance over our parameter estimates
- $\mathbb{V}_{\hat{\boldsymbol{\beta}}} = \mathbb{E}\big[(\mathbb{E}[\hat{\boldsymbol{\beta}}] - \hat{\boldsymbol{\beta}})^2\big]$
- 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 $(\boldsymbol{y}, \boldsymbol{X}) \in \mathcal{D}$
  - 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 $(\boldsymbol{y}_{\text{New}}, \boldsymbol{X}_{\text{New}})$
- We also observe a "test" dataset $\boldsymbol{X'}$

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

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

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 $\boldsymbol{X'}$
- To generate new predictions $\boldsymbol{y'}$

Bias and variance of predictions

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

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

And we can think about the variance of the prediction:

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

High variance means that the model is very sensitive to $\boldsymbol{X}$ – 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 calculate the mean squared error of some new data $\boldsymbol{X'}$ given a trained model $\hat{f}$:

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

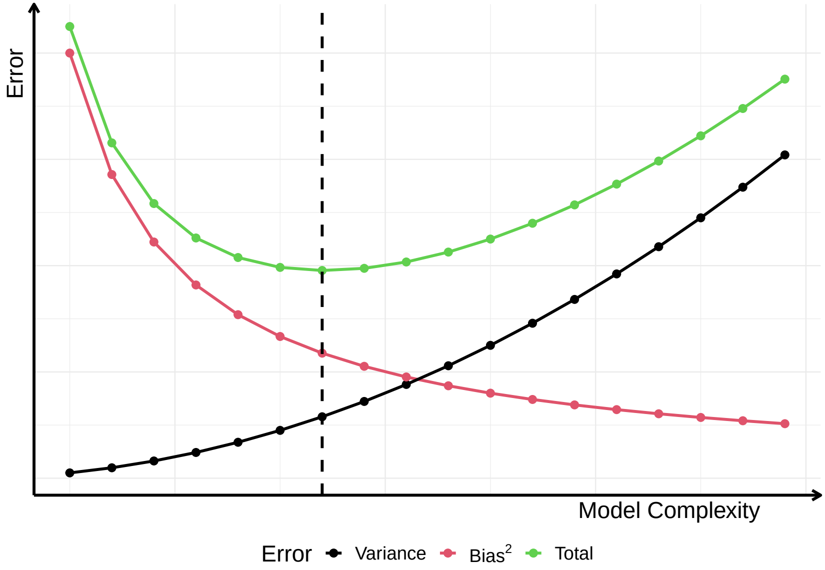
We can decompose this further:

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

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

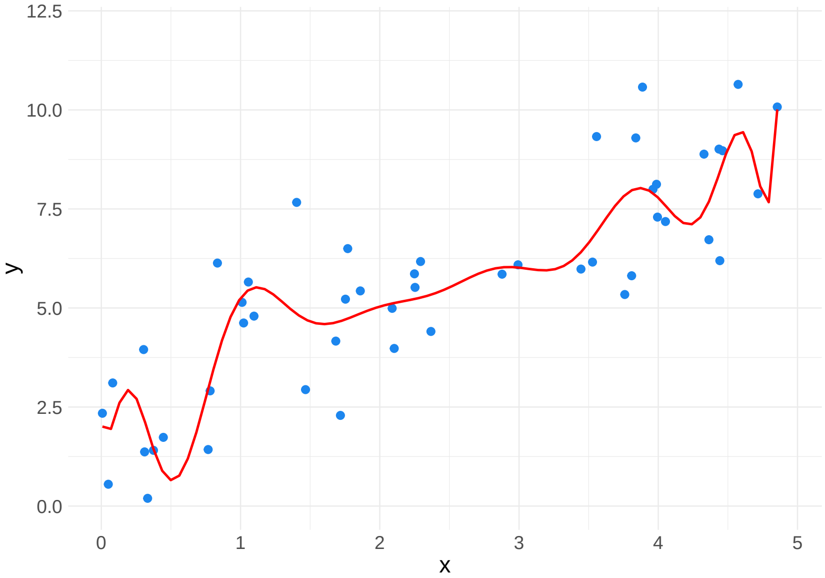


Out of sample performance of OLS

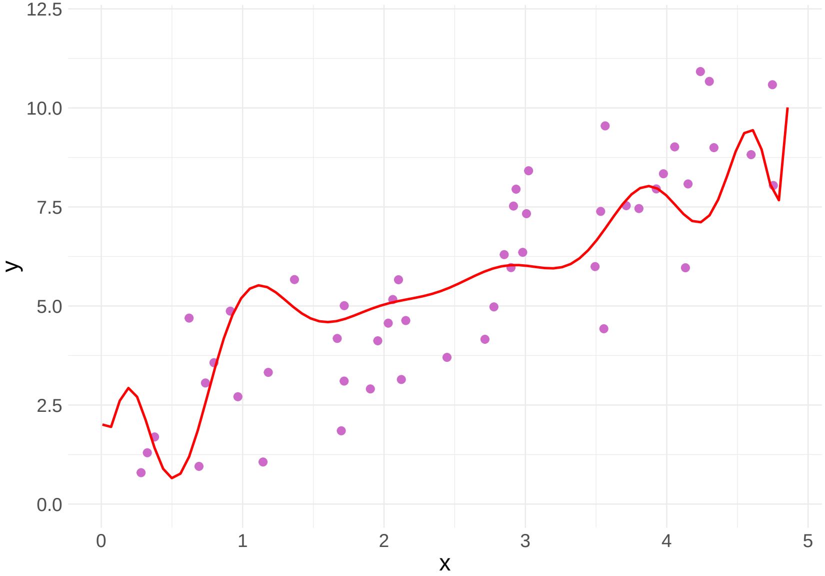
This trade-off explains why we might not want to use OLS for prediction tasks:

- 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

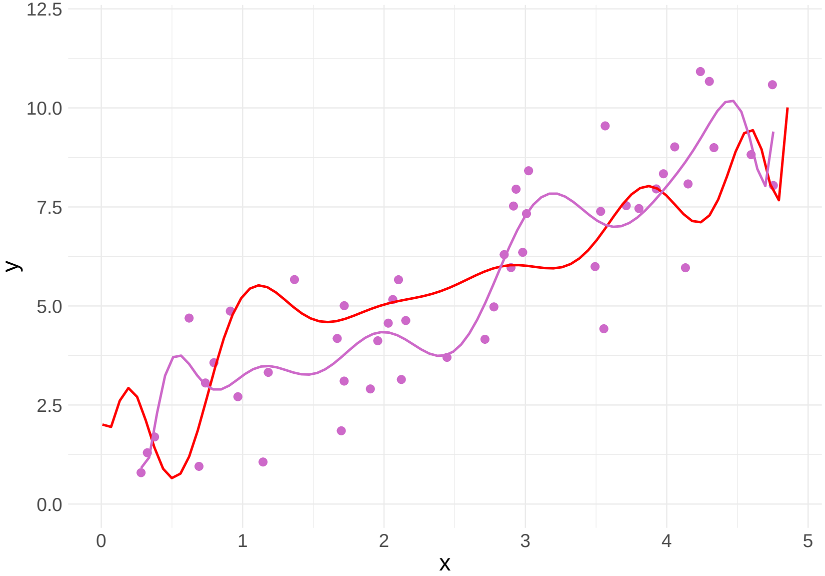
OLS: Complex OLS model trained on $\mathbf{X}$



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



OLS: Variance in model predictions over $\mathbf{X}$



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 ($\boldsymbol{X'}$)

- 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 $\boldsymbol{X'}$

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 $\boldsymbol{X'}$

Generalising OLS with regularization

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

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

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 λ – 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:

$$||\boldsymbol{\beta}||_1 = \sum_j |\beta_j|$$

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

$$||\boldsymbol{\beta}||_1 \leq t$$

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

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

This final optimisation constraint is equivalent to:

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

LASSO

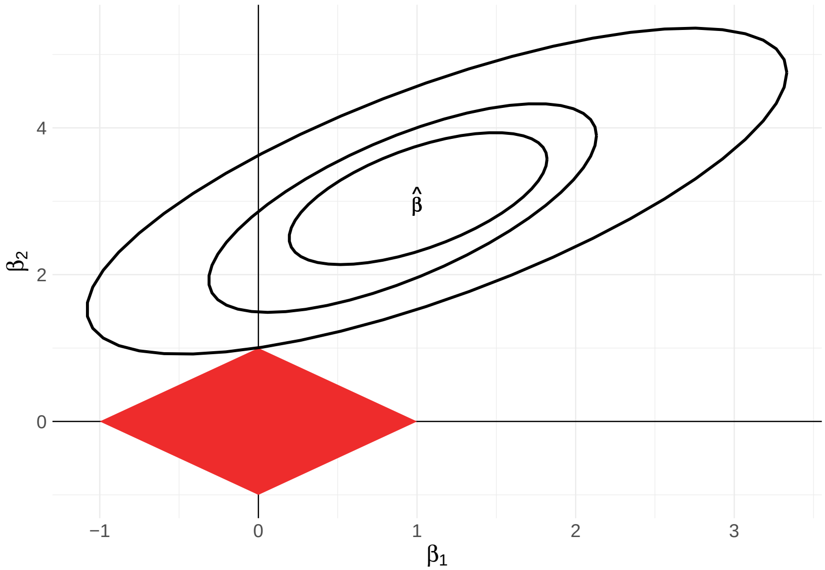
Hence, the LASSO estimator conforms to the generalised loss function introduced earlier

- $R(f) = ||\hat{\boldsymbol{\beta}}||_1$

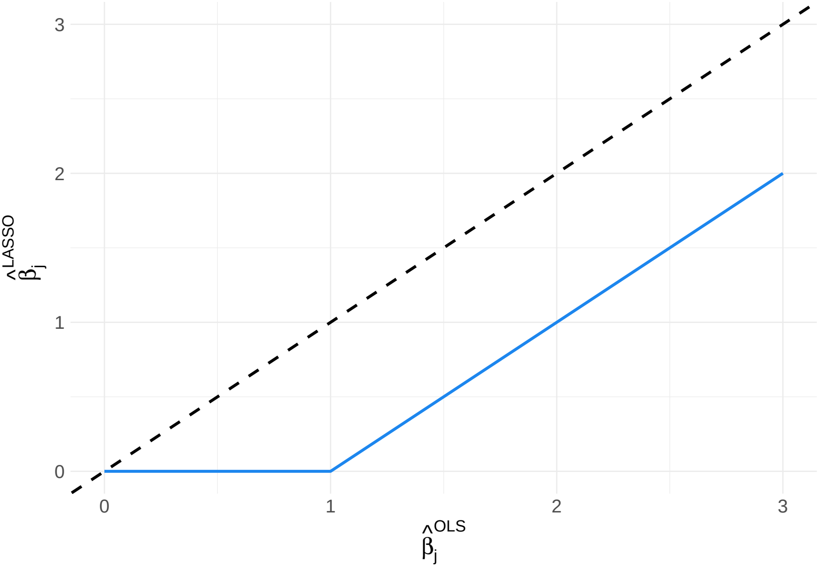
LASSO often yields coefficient estimates of exactly zero:

- Think about varying the true value of some coefficient β_j:
  - When β_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 λ

The final part of the estimation problem is setting λ. Recall that:

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

λ 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 λ 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 $\boldsymbol{X}$ into $\{\boldsymbol{X}^{\text{Train}}, \boldsymbol{X}^{\text{Holdout}}\}$
- Train our model for each value of λ on $\boldsymbol{X}^{\text{Train}}$
- Then test the predictive accuracy on $\boldsymbol{X}^{\text{Holdout}}$
- 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 λ we want to test

Choose λ 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 $\boldsymbol{y}$, a treatment $\boldsymbol{d}$, covariates $\boldsymbol{X}$, and an “effect moderator” $\boldsymbol{v}$

- 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. $y_i = \beta_0 + \beta_1 d_i + \beta_2 v_i + \beta_3 d_i v_i + \boldsymbol{\beta' X_i}$

What’s wrong with this model?

- We assume that the interactive effect β_3 is constant across covariates
- This introduces bias into the model if $\boldsymbol{vX}$ is related either to $\boldsymbol{dv}$ or $\boldsymbol{y}$

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 $\boldsymbol{X}, \boldsymbol{v}, \boldsymbol{d}$, and $\boldsymbol{y}$?
- **Prediction problem**: Which interactions within $\boldsymbol{vX}$ 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 $\boldsymbol{\beta}$

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

Stage 2

- Regress $\boldsymbol{y}$ on $\boldsymbol{d}, \boldsymbol{dv}$ and $\boldsymbol{Z*}$

Blackwell and Olson also suggest adding all "base-terms" (i.e $\boldsymbol{X}$) 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 $||\boldsymbol{\beta}||_2$:

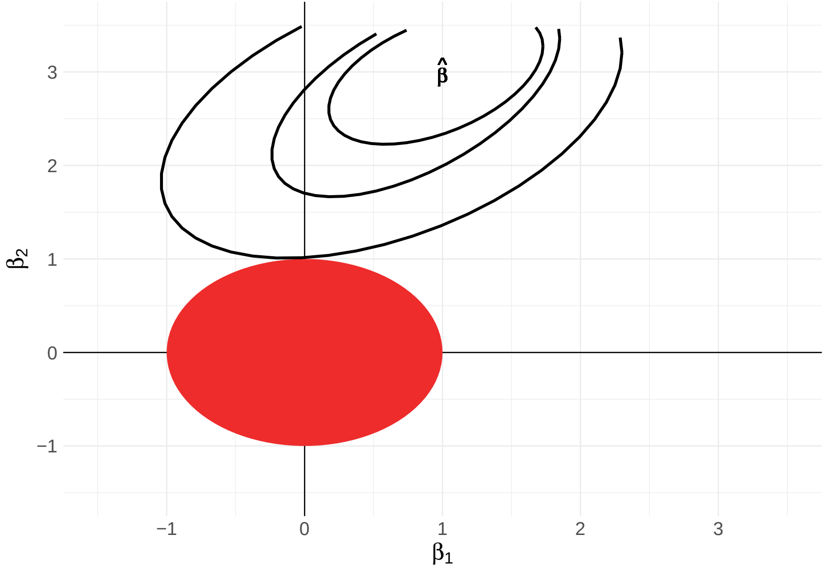
$$\sqrt{\sum_j |\beta_j|^2}$$

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

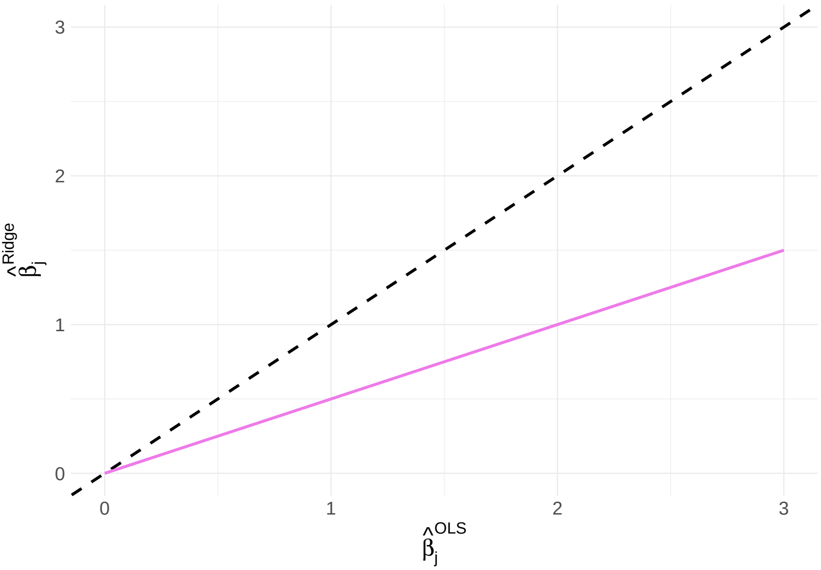
$$\arg\min_{\boldsymbol{\beta}} \sum_{i=1}^{N} (y_i - \boldsymbol{x_i}\boldsymbol{\beta})^2 + \lambda||\boldsymbol{\beta}||_2$$

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. $\boldsymbol{y}$ is a linear function of $\boldsymbol{\beta}$
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. $Cov(\boldsymbol{x_i}, \epsilon_i) = 0$