MATH60026/MATH70026
Methods for Data Science
Lecture 1

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Department of Mathematics, Academic year 2024-2025

IMPERIAL

Learning from Data

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Multiplicity of data types, the main ones being:

1. categorical (or discrete): take on one of a limited (fixed) number of values, such as classes: name of a team, country, type of chemical etc.

Learning from Data

Data Science: an interdisciplinary field concerning methods and strategies to extract knowledge, insights, predictions from data

Multiplicity of data types, the main ones being:

1. categorical (or discrete): take on one of a limited (fixed) number of values, such as classes: name of a team, country, type of chemical etc.

2. quantitative (or continuous): the variable is numerical and represents a measurable quantity: height, speed, price, concentration of a chemical etc.

Learning from Data

Mathematically, we start from a set of data specified by:

Number of data points: measurements, individuals ...

$$\left\{ x_1^{(i)}, x_2^{(i)}, \ldots, x_p^{(i)} \right\}_{i=1}^{N}$$

Number of features (descriptors): the characteristics of each data point (variables measured, attributes of an individual …)

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We might want to carry out different analysis tasks:

Supervised learning: modelling an input – output mapping;
Unsupervised learning: discovering structure and properties.

Learning from Data

Supervised learning: we have pairs of input – output data

$$\{x_1^{(i)}, x_2^{(i)}, \ldots, x_p^{(i)}, \quad y^{(i)}\}_{i=1}^{N}$$

Input data, whose features are *predictors*

Output data (*outcomes*) to predict

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If *continuous*: the task is to predict its quantitative value (**regression**)

If *categorical*: the task is to predict (or assign to) the category (**classification**)

Linear Regression

We model the input – output mapping through a *linear* function:

$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_p x_p =: f_{\mathrm{LR}}(\mathbf{x}, \boldsymbol{\beta})$$

Why linear? A priori knowledge, data exploration, convenience.

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The vector of coefficients:

$$\boldsymbol{\beta} = \underbrace{\begin{pmatrix} \beta_0 \\ \vdots \\ \beta_p \end{pmatrix}}_{(p+1)\times 1} \in \mathbb{R}^{(p+1)}$$

contains the parameters of the models, that are *learnt* from data.

Linear Regression

We need the parameter values making the LR satisfied for all data:

$$\left\{\begin{array}{l} \hat{y}^{(1)} = \beta_0 + \beta_1 x_1^{(1)} + \cdots + \beta_p x_p^{(1)} \stackrel{?}{=} y^{(1)} \\ \hat{y}^{(2)} = \beta_0 + \beta_1 x_1^{(2)} + \cdots + \beta_p x_p^{(2)} \stackrel{?}{=} y^{(2)} \\ \quad \vdots \\ \hat{y}^{(N)} = \beta_0 + \beta_1 x_1^{(N)} + \cdots + \beta_p x_p^{(N)} \stackrel{?}{=} y^{(N)} \end{array}\right\}$$

Outcome *predicted by LR*

Outcome values *given, known*

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Outcome *predicted by LR*

Outcome values *given, known*

Problem: this linear system is over-determined: $N >> (p+1)$
There is *not* a solution (i.e., parameter values satisfying all eqs).

Least Squares Method

The solution comes from the Least Squares method: it learns optimal parameters making true and predicted outcomes *close*.

Let's first re-write everything in a convenient vector form:

Predictors

$$\mathbf{X} = \begin{bmatrix} 1 & x_1^{(1)} & \dots & x_p^{(1)} \\ 1 & x_1^{(2)} & \dots & x_p^{(2)} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(N)} & \dots & x_p^{(N)} \end{bmatrix}_{N \times (p+1)} \xrightarrow{?} \mathbf{y} = \begin{bmatrix} y^{(1)} \\ \vdots \\ y^{(N)} \end{bmatrix}_{N \times 1}$$

Outcome

We model this mapping assuming a linear relationship:

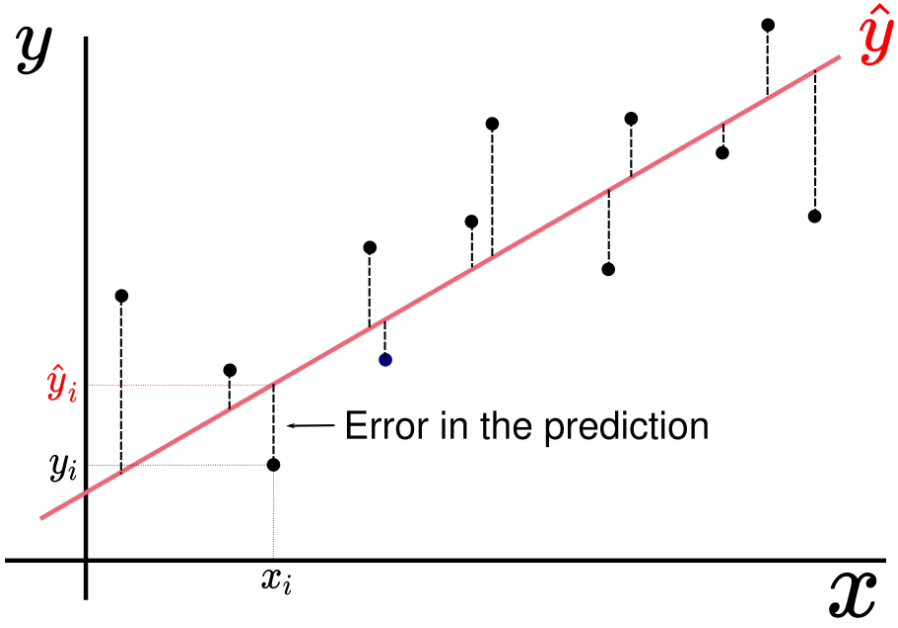
$$\hat{\mathbf{y}} = \mathbf{X}\boldsymbol{\beta}$$

With model parameters:

$$\boldsymbol{\beta} = \begin{pmatrix} \beta_0 \\ \vdots \\ \beta_p \end{pmatrix}_{(p+1)\times 1} \in \mathbb{R}^{(p+1)}$$

Least Squares Method

Main idea: look at the error between true and predicted outcomes.



Error of the model:

$$\mathbf{y} - \hat{\mathbf{y}} = \mathbf{y} - \mathbf{X}\boldsymbol{\beta}$$

Least Squares Method

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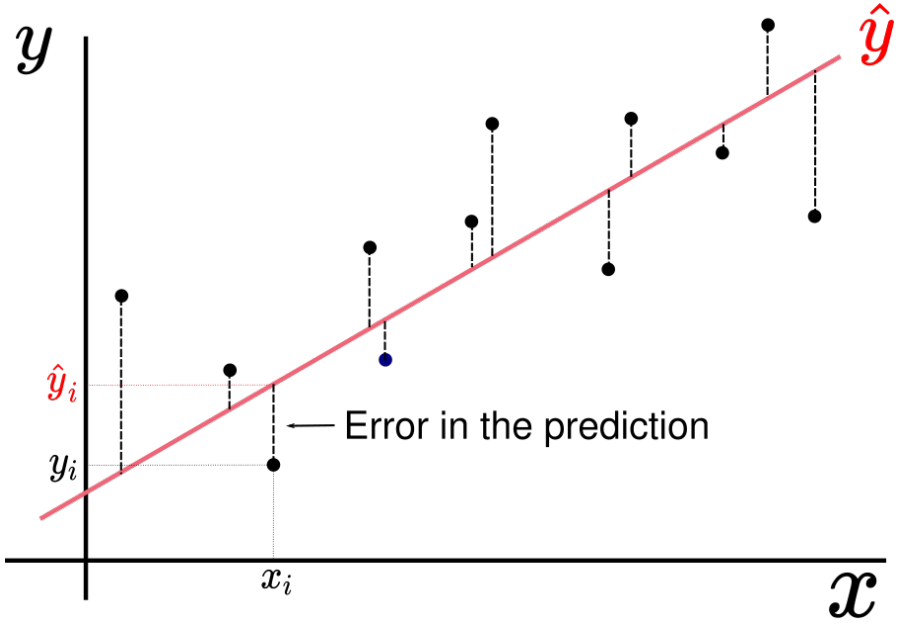

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Least Squares solution: learn the parameters by minimising the squared errors of prediction across data points:

$$\min_{\boldsymbol{\beta}} \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2$$

Some terminology

In general, a supervised learning task is carried out by minimising a **Loss Function,** here the **Mean Squared Error**:

$$L_{MSE}\big(y, f(x)\big) = \frac{1}{N}\sum_{i=1}^{N}\big(y^{(i)} - f(x^{(i)})\big)^2$$

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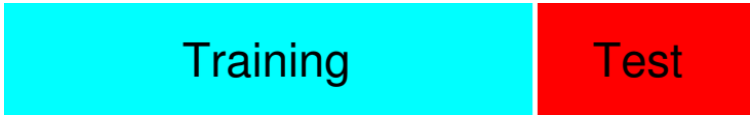
Once the model is trained, it can be evaluated on *new, unseen* data for which we don't have any given outcome variables. **Generalisability**: ability to perform well on unseen data. To measure it, we need a **Test Set:**

Divide data into:



$$\mathbb{E}\left[L\left(f(\{x^{(k)}\}), \{y^{(k)}\}\right)\right]_{k \in \text{test}}$$

should be small too

Least Squares solution: learn the parameters by minimising the squared errors of prediction across data points:

$$\min_{\boldsymbol{\beta}} \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2$$

1. Analytical, Exact Solution:

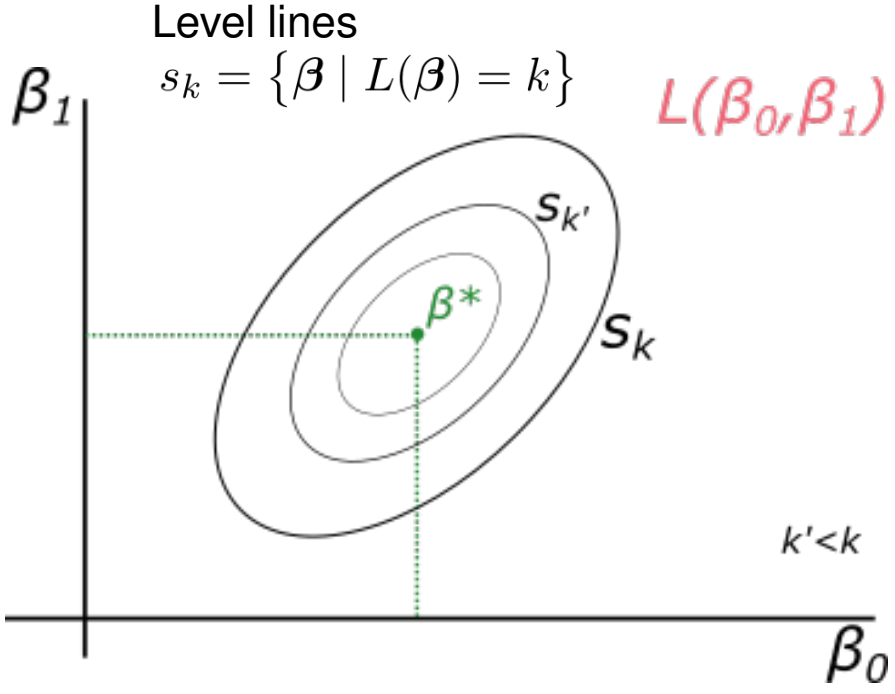
$$\boldsymbol{\beta}^\star = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} = \mathbf{X}^+\mathbf{y}$$

Moore-Penrose Pseudo-inverse

Found by carrying out explicitly the minimisation (see notes).

Minimum = Hessian positive definite

$$\nabla_{\boldsymbol{\beta}}(\nabla_{\boldsymbol{\beta}} L) = \frac{2}{N}\mathbf{X}^T\mathbf{X} = H$$



It's a multidimensional parabola, a **convex loss function**: guarantee that we have a global, unique minimum

Least Squares solution: learn the parameters by minimising the squared errors of prediction across data points:

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2. Numerical Solution: via Gradient Descent

Iteration by iteration, we update parameters:

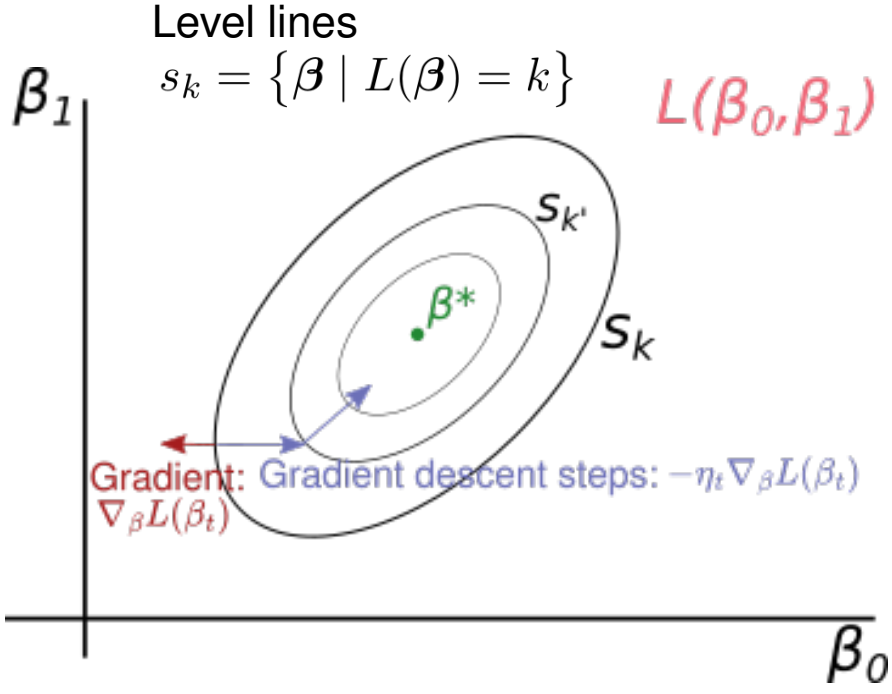
$$\boldsymbol{\beta}_{t+1} = \boldsymbol{\beta}_t - \eta_t \nabla_{\boldsymbol{\beta}} L(\boldsymbol{\beta}_t)$$

Iteration index

Step size

MSE loss:

$$L(\boldsymbol{\beta}) = \frac{1}{N}(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^T(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$



Simple idea: the gradient gives the direction of maximal variation; following the opposite of this direction leads to a minimum.

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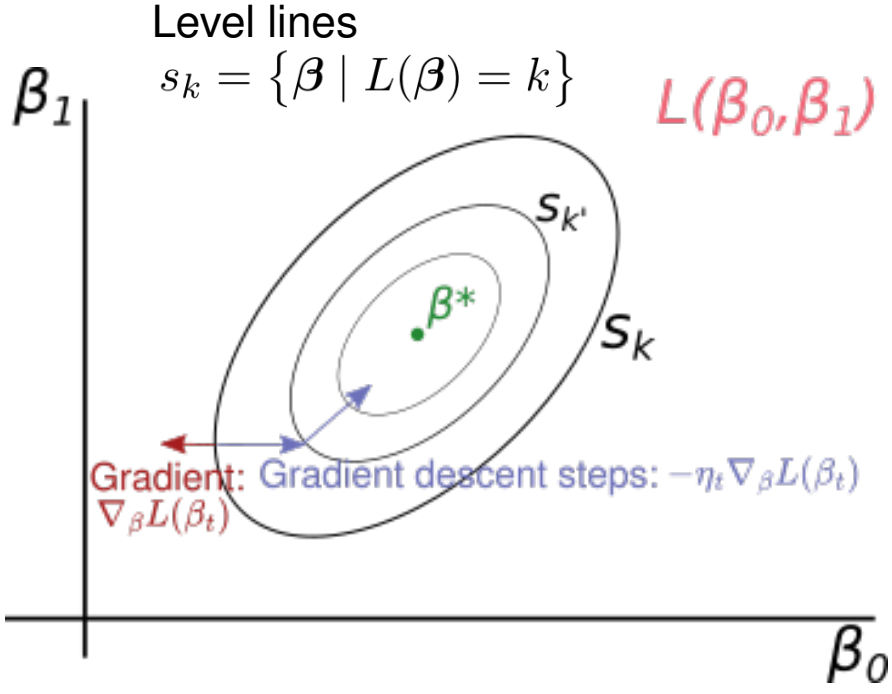

Not necessary for LR, but the only viable strategy for non-convex cases

Simple idea: the gradient gives the direction of maximal variation; following the opposite of this direction leads to a minimum.

Statistical Interpretation

The Least Squares solution is **equivalent** to assuming that deviations from the line across data are Gaussian distributed.

$$y^{(i)} = \beta_0 + \beta_1 x_1^{(i)} + \varepsilon^{(i)}$$

i.i.d, Gaussian: $\varepsilon \sim \mathcal{N}(0, \sigma^2)$

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I can write a likelihood of the data under the model:

$$\underset{\text{tot}}{\text{Lik}}(\mathbf{y} \mid \boldsymbol{\beta}) = \prod_{i=1}^{N} \text{Lik}(y^{(i)} \mid \boldsymbol{\beta})$$

with: $\text{Lik}(y^{(i)} \mid \boldsymbol{\beta}) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp \frac{-\left(y^{(i)} - (\beta_0 + \beta_1 x_1^{(i)})\right)^2}{2\sigma^2}$

and find the best model parameters by maximum likelihood:

$$\underbrace{-\frac{d\mathcal{L}_{\text{tot}}}{d\boldsymbol{\beta}}}_{\text{maximum likelihood}} \longleftrightarrow \underbrace{\frac{dL_{\text{MSE}}}{d\boldsymbol{\beta}}}_{\text{minimal loss (MSE)}}$$

Same solution!

Bias-Variance trade-off

Let's look at the learning problem from a statistical perspective.

$\boldsymbol{\beta}$: True parameter $\boldsymbol{\beta}^\star$: LS estimate from data

Many realisations of data sample = many $\boldsymbol{\beta}^\star$ with a distribution

Two key quantities to analyse the performance of an *estimator*:

$$\text{Bias: } \|\mathbb{E}[\boldsymbol{\beta}^\star] - \boldsymbol{\beta}\|$$

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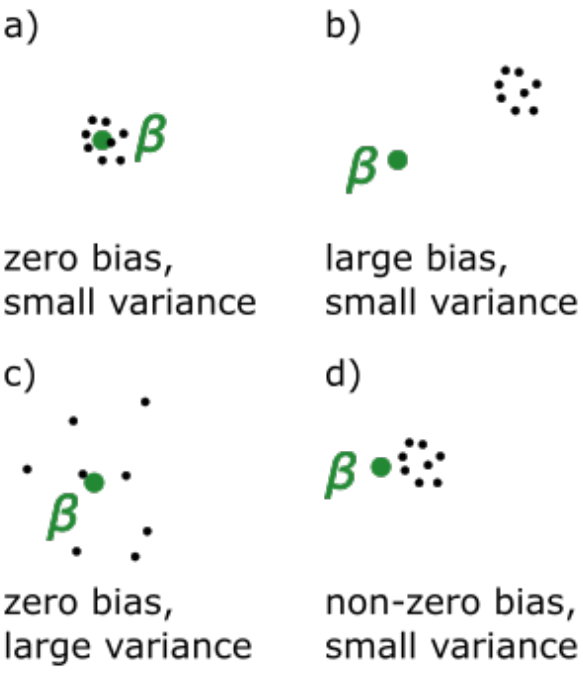
Related to the expected error of the estimate

Bias-variance trade-off

$$\text{Expected squared error} = \text{Variance} + \text{Bias}^2$$

Bias: difference between average estimated parameter and its true value

Variance: variation of estimated parameters on different data sets (i.e., sensitivity to the particular set, compromises stability, generalisability)



Bias-Variance trade-off

How can we improve the performance of the Least Squares estimator? We have:

$$\mathbb{E}\big[(\boldsymbol{\beta} - \boldsymbol{\beta}^\star)(\boldsymbol{\beta} - \boldsymbol{\beta}^\star)^T\big] = \mathbb{E}\big[(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T \underbrace{\boldsymbol{\varepsilon}\boldsymbol{\varepsilon}^T}_{\mathbb{E}[\boldsymbol{\varepsilon}\boldsymbol{\varepsilon}^T]=\sigma^2\mathbf{I}} \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\big] = (\mathbf{X}^T\mathbf{X})^{-1}\sigma^2$$

$(\mathbf{X}^T\mathbf{X})$ can be badly conditioned due to dependencies among features, poor sampling

LS is unbiased!

$$\|\mathbb{E}[\boldsymbol{\beta}^\star] - \boldsymbol{\beta}\| = 0$$

For improvements, one needs to reduce the variance

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Strategies:

1. **Best-subset regression**: finds the subset of size k<p with the smallest regression error. The model has a reduced number of features, i.e. it's sparser.

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→ For improvements, one needs to reduce the variance

Strategies:

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2. **Shrinkage methods**: Ridge and LASSO regression.
Main idea: modify the loss function to make the size of learnt parameters small.

Gain: one has an estimator at lower variance, but biased;
one enforces a continuous version of spasity.

Ridge Regression

In Ridge regression, one adds a term penalising large values of the parameters

$$L_{\text{RIDGE}}(\boldsymbol{\beta}) = \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2 + \lambda\|\boldsymbol{\beta}\|^2$$

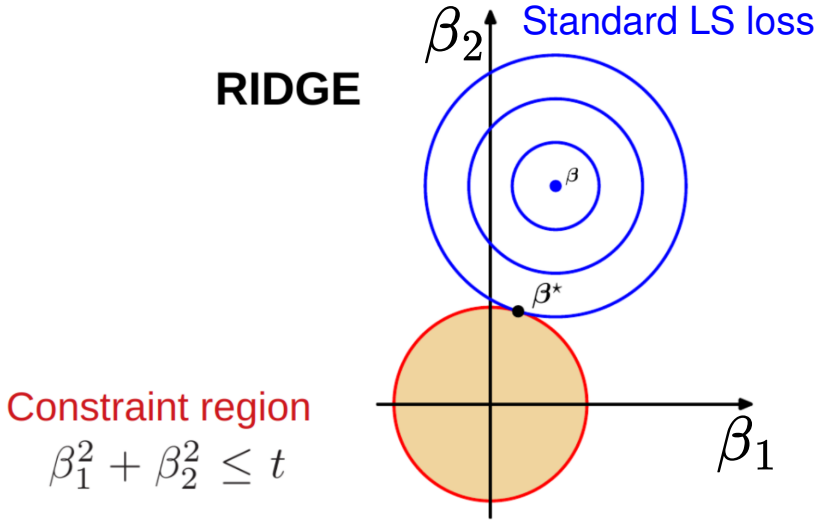
$\lambda > 0$ is the *penalty term*

$\|\boldsymbol{\beta}\|^2 = \sum_{i=1}^{p} |\beta_i|^2$

The solution is found by:

$$\min_{\boldsymbol{\beta}} \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2 + \lambda\|\boldsymbol{\beta}\|^2 \quad \Leftrightarrow \quad \min_{\boldsymbol{\beta}} \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2 \text{ subject to } \|\boldsymbol{\beta}\|^2 \leq t$$

This equivalence allows us to rationalise a bit more geometrically the solution:



It can be obtained analytically:

$$\boldsymbol{\beta}^\star_{\text{RIDGE}} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y}$$

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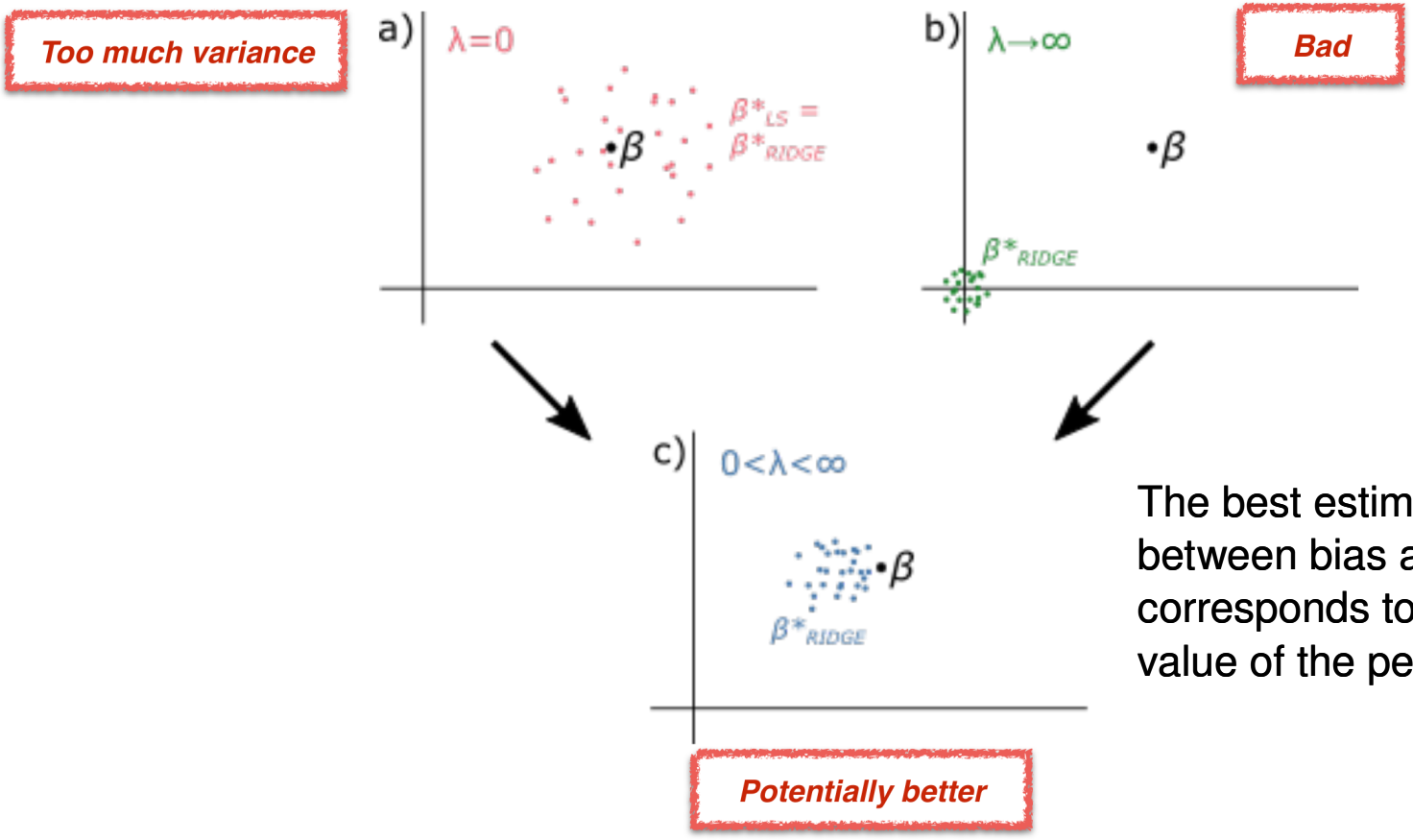


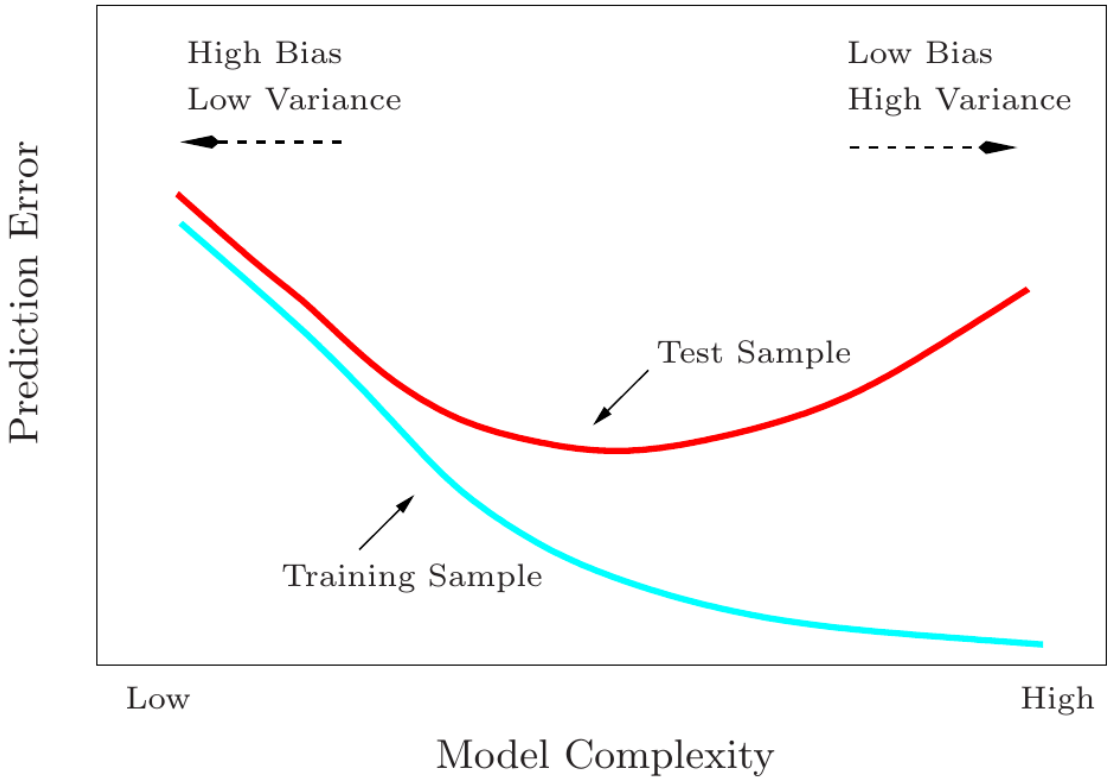
The best estimator strikes a balance between bias and variance, and corresponds to an intermediate value of the penalty term.

How do we set the right value of λ ?

λ is a hyper-parameter - we need a hyperparametric search

Region of underfitting

Region of overfitting



or 'Model capacity' (from flexible parametrization)

Large $\longleftarrow \lambda \longrightarrow$ Small

Plays the role of regularisation
(control overfitting via a penalty)

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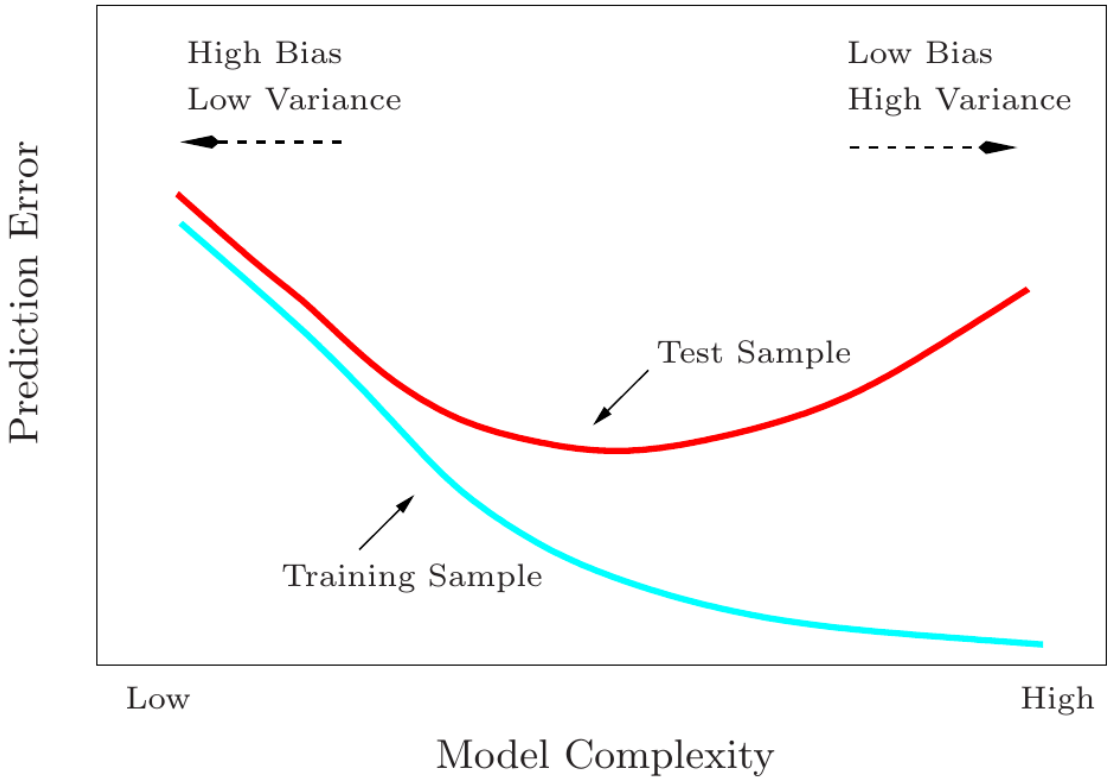

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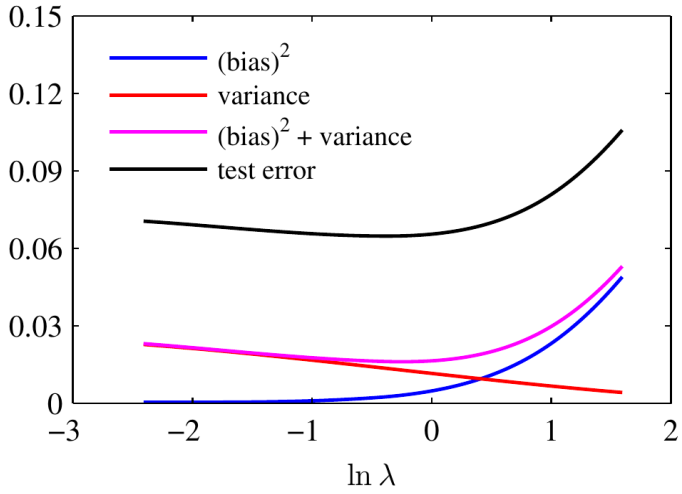

Example on RIDGE regression (from Bishop, Pattern Recognition and Machine Learning, chap. 3)

Large

Small

λ

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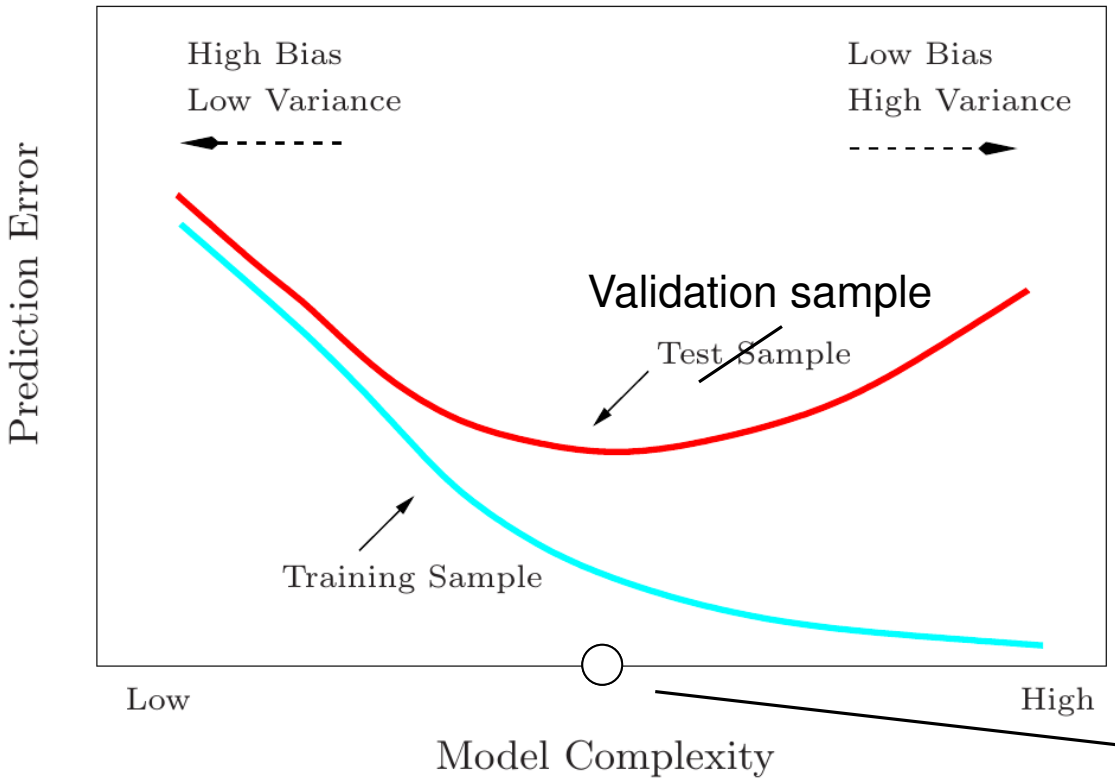


Optimal value

or 'Model capacity' (from flexible parametrization)

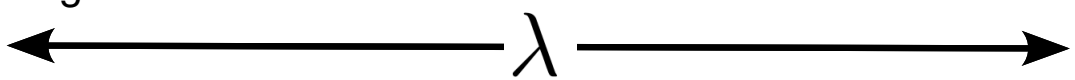
Cross-validation (next lecture)

Model selection
(hyperparametric search)

Model assessment
(out-of-sample performance)

Large

Small



LASSO Regression

Also in Lasso regression, one adds a term penalising large values of the parameters

$$L_{\text{LASSO}}(\boldsymbol{\beta}) = \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2 + \lambda\|\boldsymbol{\beta}\|_1$$

$\lambda > 0$ is the *penalty term*

$$\|\boldsymbol{\beta}\|_1 = \sum_{i=1}^{p} |\beta_i|$$

Compared to ridge, it does **not** have an analytical solution, but it is solvable numerically with standard convex optimisation techniques (you will see one in the coding notebook)

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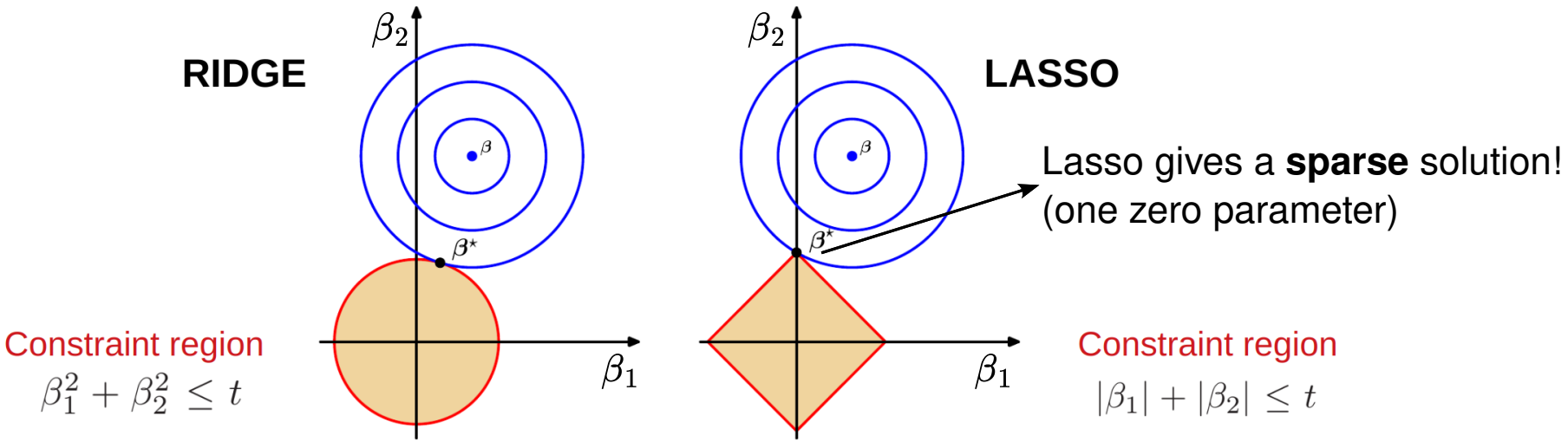
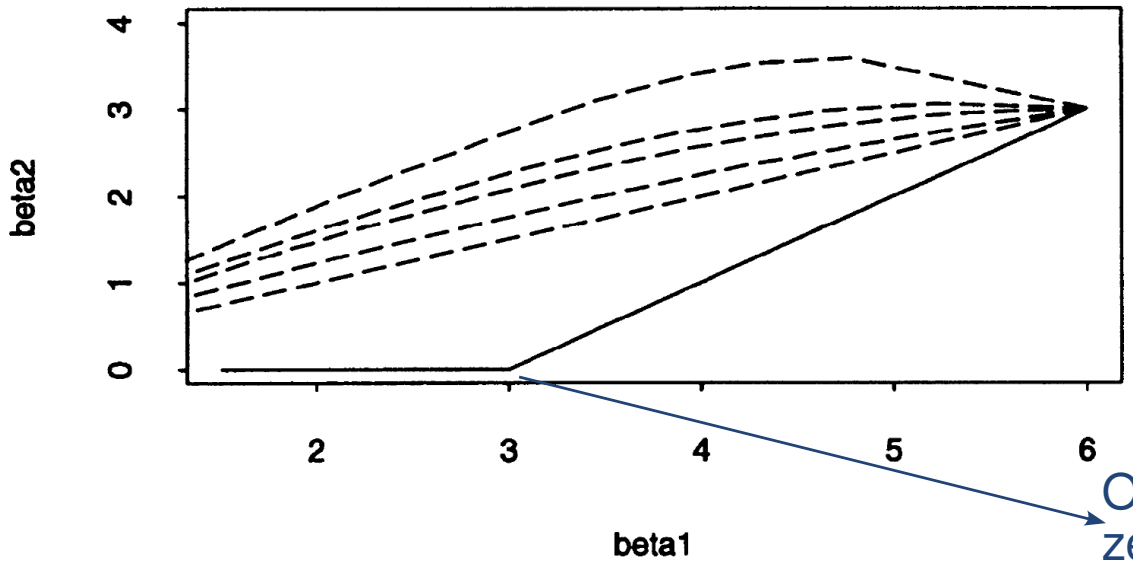


Figure adapted from Bishop, Pattern Recognition and Machine Learning, chap. 3

LASSO Regression

Compared to ridge, **LASSO induces a stronger sparsity**,
as was illustrated already in the original article introducing it:

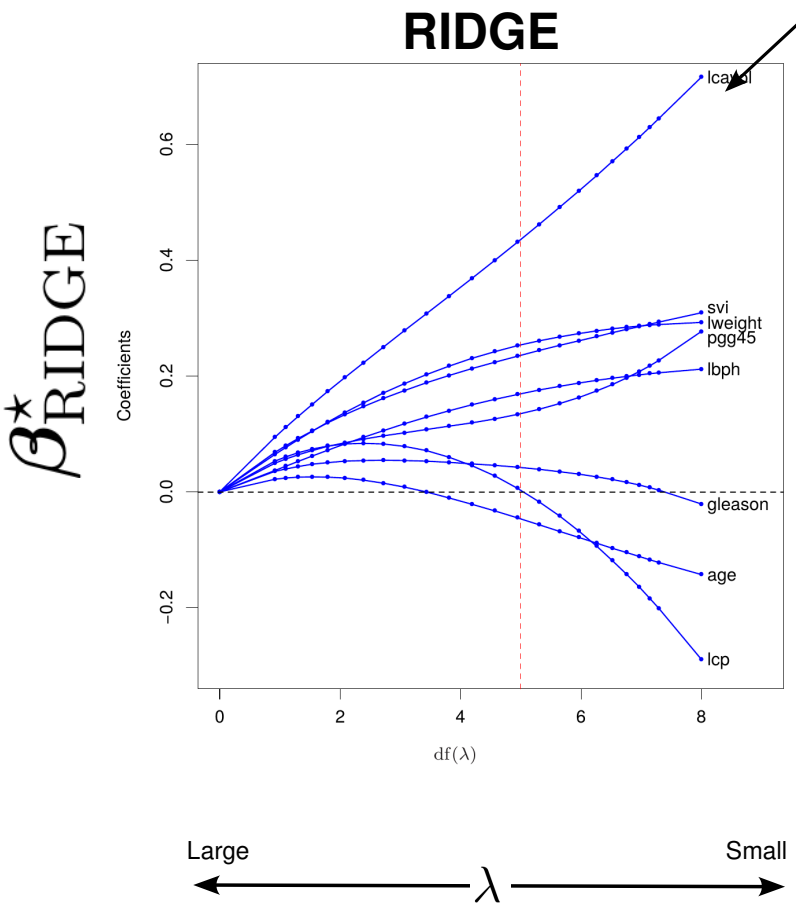


From Tibshirani R,
J. R. Statistic. Soc. B (1996),
see additional reading

Fig. 4. Lasso (———) and ridge regression (– – – –) for the two-predictor example: the curves show the (β_1, β_2) pairs as the bound on the lasso or ridge parameters is varied; starting with the bottom broken curve and moving upwards, the correlation ρ is 0, 0.23, 0.45, 0.68 and 0.90

Example of linear regression on a clinical dataset: the outcome is a marker of prostate cancer, the predictors are patients' clinical characteristics (from Hastie, Tibshirani, Friedman, Elements of statistical learning, chap. 3

One coefficient per predictor (clinical charactertistic)



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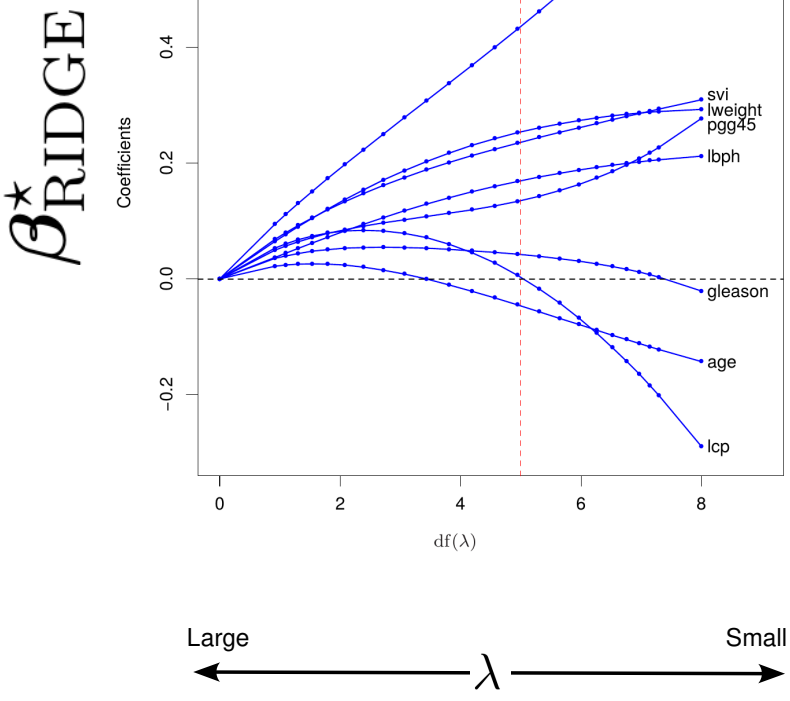
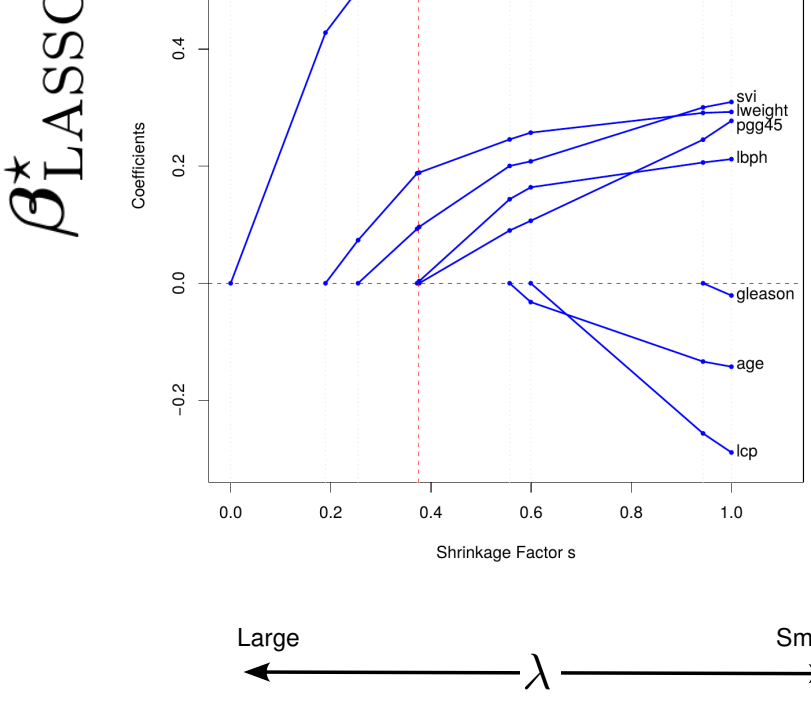
One coefficient per predictor (clinical charactertistic)

RIDGE



Large ← λ → Small

LASSO



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Effective subset selection

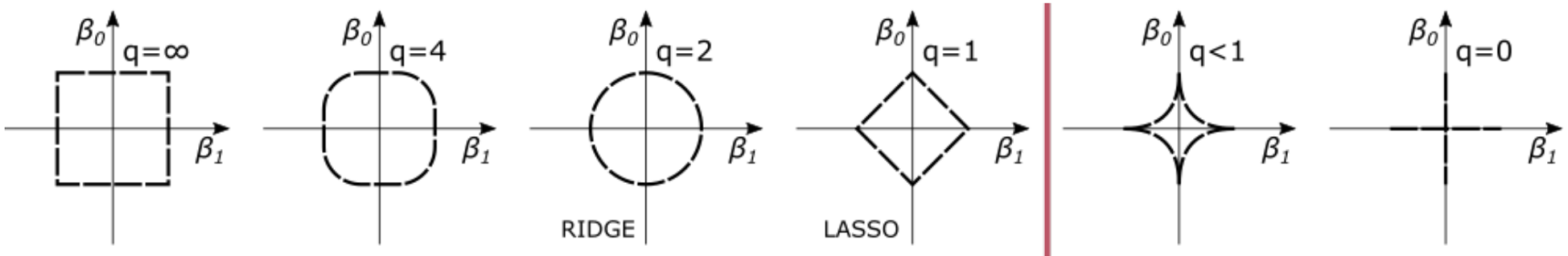
Generalisations

Elastic nets: combine benefits of both, but have an additional hyperparameter

$$L_{\text{EN}}(\boldsymbol{\beta}) = \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2 + \lambda\left[\alpha\|\boldsymbol{\beta}\|_1 + (1-\alpha)\|\boldsymbol{\beta}\|^2\right]$$

General variations involve regularisation terms containing the l_q-norm:

$$L_q(\boldsymbol{\beta}) = \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2 + \lambda\|\boldsymbol{\beta}\|_q^q \qquad \|\boldsymbol{\beta}\|_q^q = \sum_{i=1}^{p} |\beta_i|^q$$



Convex sets

Non-convex sets

Optimisation is doable

Optimisation is difficult

Summary I: regression & LS

Supervised learning: the basic process schematically is

(1) Start with data $(x^{(i)}, y^{(i)}), \quad i = 1, \ldots, N.$

(2) Decide: Classification or regression?

(3) Define a *loss function* $L(y, f(x))$

(4) Minimise the *mean sample loss*: $E(L) = \frac{1}{N} \sum_{i=1}^{N} L(y^{(i)}, f(x^{(i)}))$

(5) Try to also achieve a reasonable *expected test loss*: $E\big(L(y^{\text{in}}, f(x^{\text{in}}))\big)$

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3. The LS estimator is unbiased, but can have large variance.

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Regularisations, bias-variance trade-off, hyperparametric search are more general than linear models and regression (e.g. k-NN, deep neural networks)!