Ch3. Linear Regression

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Outline

1 Ordinary Least Square theory

2 Variables selection

3 Shrinkage methods

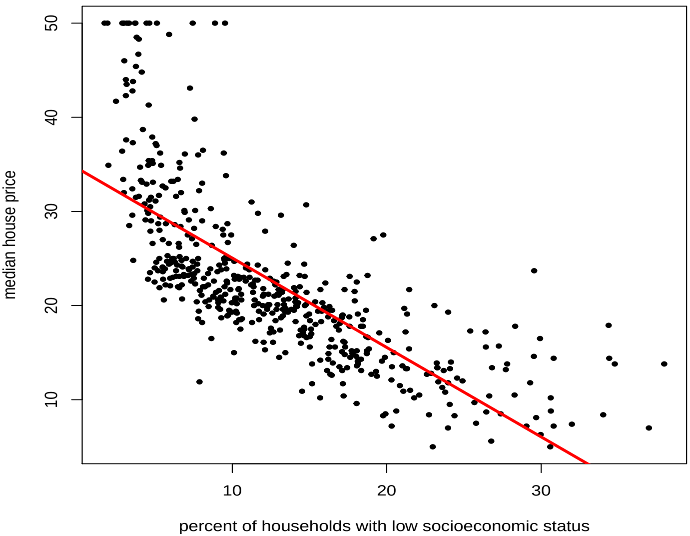
Linear Regression

- Response $y \in \mathbb{R}$
- Covariates (explanatory variables) $x = (x_0, x_1, \ldots, x_p) \in \mathbb{R}^p$
- Linear regression model

$$y = \beta_0 + \sum_{i=1}^{p} x_i\, \beta_i \ + \ (\text{noise})$$

- Training examples $\{(y_i, x_i)\}_{i=1}^n$ with $x_i = (x_{i,1}, \ldots, x_{i,p})$
- It is common to set $x_{i,0} = 1$ for the intercept β_0.

Linear Regression



One dimensional example

- Coefficients $\beta = (\beta_0, \beta_1)$ minimise

$$\textbf{RSS}(\beta_0, \beta_1) = \sum_{i=1}^{n} (y_i - [\beta_0 + \beta_1\, x_i])^2$$

- **[Exercise]** Setting the partial derivative of the function yields that

$$\begin{cases} \beta_0 + \beta_1\, \overline{x} & = \overline{y} \\ \beta_0\, \overline{x} + \beta_1\, \overline{xx} & = \overline{xy} \end{cases}$$

with $\overline{x} = n^{-1} \sum x_i$ and $\overline{y} = n^{-1} \sum y_i$ and $\overline{xx} = n^{-1} \sum x_i^2$ and $\overline{xy} = n^{-1} \sum x_i y_i$.

General case

- Training examples $\{(y_i, x_i)\}_{i=1}^{n}$.
- $\beta = (\beta_0, \beta_1, \ldots, \beta_p) \in \mathbb{R}^{p+1}$ minimises

$$\textbf{RSS}(\beta) = \sum_{i=1}^{n} \{y_i - [\beta_0 + \beta_1 \, x_{i,1} + \ldots + \beta_p \, x_{i,p}]\}^2 \, .$$

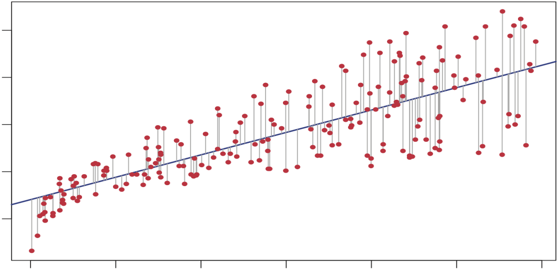
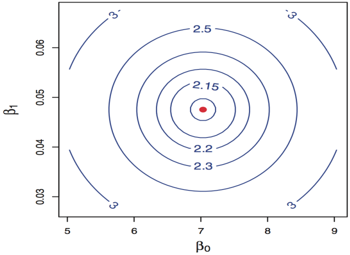
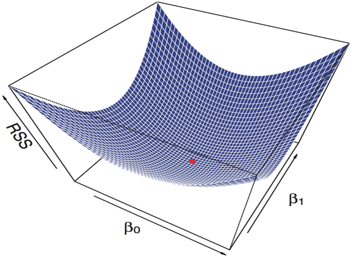


Figure : Residual Sum of Square (**RSS**)

- Ordinary Least Square (OLS) estimate $\widehat{\beta}$:

$$\widehat{\beta} = \mathbf{argmin} \left\{ \textbf{RSS}(\beta) \; : \; \beta \in \mathbb{R}^{p+1} \right\}. \qquad (1)$$





OLS: closed form expression

- One could numerically optimise **RSS**.

$$\mathbf{RSS}(\beta) = \|y - X\,\beta\|^2 = \langle y - X\,\beta, y - X\,\beta \rangle$$

- There is a closed form expression

$$\begin{aligned} \partial_\beta \mathbf{RSS} &= -2X^T\,(y - X\,\beta) \\ \partial^2_{\beta,\beta} \mathbf{RSS} &= 2\,X^T\,X. \end{aligned}$$

- **[Exercise]** the matrix $X^T\,X$ is positive semi-definite; if X has full rank, it is positive definite.
- **[Exercise]** if X has full rank,

$$\widehat{\beta} = (X^T\,X)^{-1}\,X^T\,y$$

the hat matrix

- we have **RSS** $= \sum_i (y_i - \widehat{y}_i)^2$ where the fitted values are

$$\widehat{y} = \widehat{H}\, y \qquad \text{with} \qquad \widehat{H} \equiv X\,(X^T\,X)^{-1}\,X^T.$$

- the hat matrix $\widehat{H}$ is a projection

$$\widehat{H}^2 = \widehat{H}.$$

- $\widehat{\beta}$ well defined only $X^T\,X \in \mathbb{R}^{p+1,p+1}$ is invertible
- $[\textbf{Exercise}]$ it is never the case if $n \le p$ i.e. when there is more covariates than observations

Some remarks

The OLS estimate is not necessarily a sensible thing to consider if:

- the relationship covariates / responses is not $\approx$ linear
- the covariates are highly correlated
- the variance of the noise is not (approximately) constant
- high correlation between the error terms
- presence of outliers (square loss is highly sensitive to outliers)

Properties of $\widehat{\beta}$

- Consider the Gaussian model

$$y_i = \beta_0 + \beta_1 x_{i,1} + \ldots + \beta_p\, x_{i,p} + \mathbf{N}\left(0, \sigma^2\right)$$

for unknown parameter $\beta_\star = (\beta_0, \ldots, \beta_p)$.

- $[\textbf{Exercise}]$ $\widehat{\beta}$ is an unbiased estimate of $\beta_\star$ and

$$\widehat{\beta} \sim \mathbf{N}\left(\beta_\star, \sigma^2\,(X^T X)^{-1}\right).$$

- if $(X^T X)$ is almost singular then the variance of $\widehat{\beta}$ is very high and thus $\widehat{\beta}$ is an unreliable estimate of β. This is for example the case if:
  - the covariates are highly correlated.
  - the number of covariate is if the same order as the number of observations.

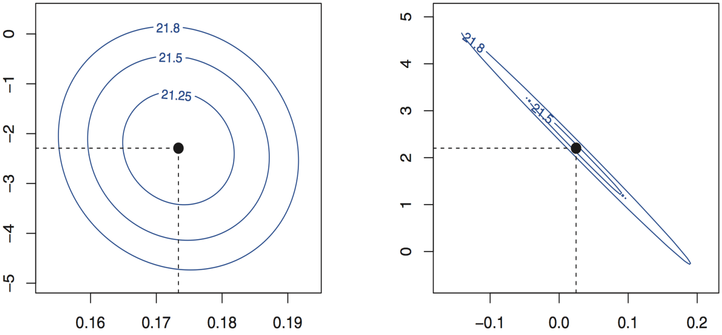


Figure : Left: no correlation. Right: high correlation

MLE connection

- Consider the Gaussian model

$$y_i = \beta_0 + \beta_1 x_{i,1} + \ldots + \beta_p \, x_{i,p} + \mathbf{N}\left(0, \sigma^2\right)$$

- the log-likelihood is given by

$$\ell(\beta) = -\frac{1}{2\sigma^2} \, \|y - X\beta\|^2 + (\text{irrelevant additive constants})$$

- [**Exercise**] the least square estimate is also the MLE.

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Issues with the OLS estimate

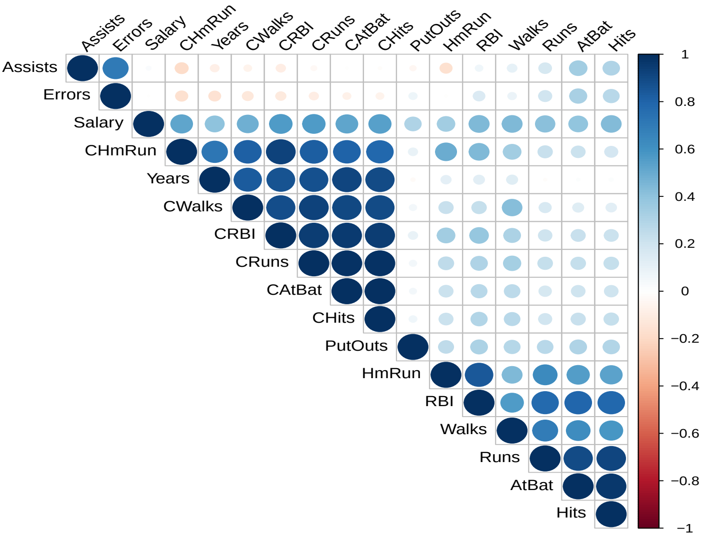
- If $p \geq n$ there is not unique solution for the minimisation of the **RSS** and the OLS estimate is not well defined.
- this large p small n situation is extremely important in practice.
- if $p \leq n-1$ but still large, even if the OLS is well-defined, it may be extremely unstable.
- When p is large, one may want to find a solution with as many zero coefficient as possible. Typically, all the coefficients of $\widehat{\beta}$ are non-zero.

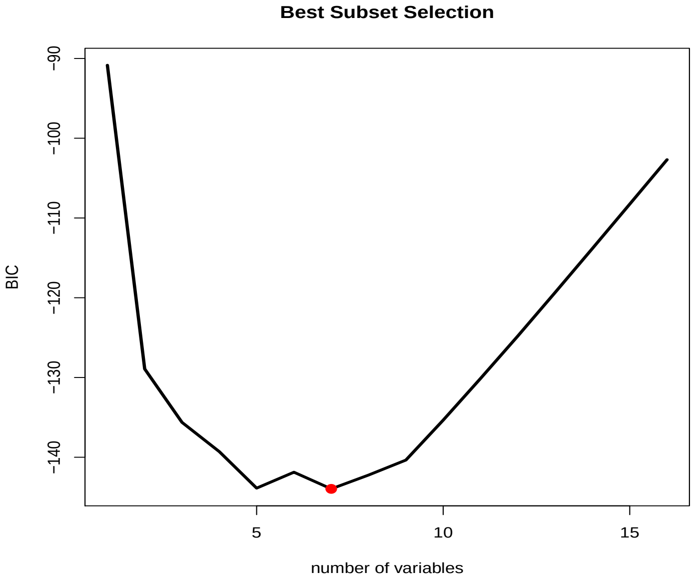
- Let $\mathcal{M}_0$ the *null* model that simply predicts the mean.
- More generally, let $\mathcal{M}_k$ the best model that uses only k covariates

$$\widehat{\beta}^{(k)} \equiv \mathbf{argmin} \Big\{ \textsf{\textbf{RSS}}(\beta) \ : \\ \beta \in \mathbb{R}^{p+1} \text{ has at most } (k+1) \text{ nonzero coordinate} \Big\}.$$

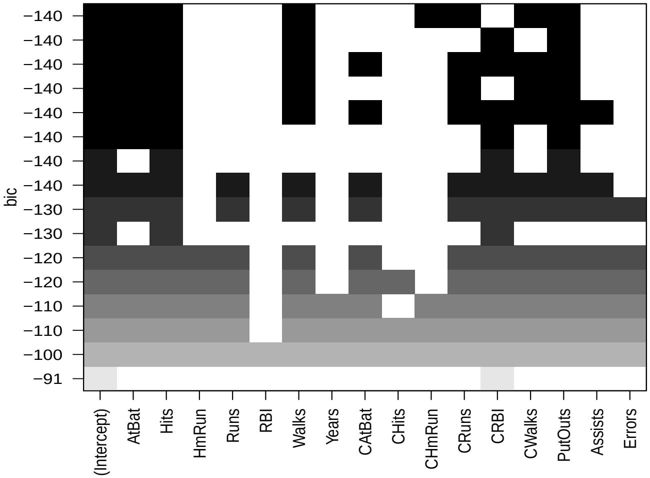
- Choose the best k_0 by optimising a measure of fit that takes into account the complexity of the model

$$\mathbf{AIC} = \frac{1}{n\,\widehat{\sigma}^2} \left(\textsf{\textbf{RSS}} + 2 \times (\text{dimension}) \times \widehat{\sigma}^2 \right)$$
$$\mathbf{BIC} = \frac{1}{n} \left(\textsf{\textbf{RSS}} + \log(n) \times (\text{dimension}) \times \widehat{\sigma}^2 \right)$$


Assists
Errors
Salary
CHmRun
Years
CWalks
CRBI
CRuns
CAtBat
CHits
PutOuts
HmRun
RBI
Walks
Runs
AtBat
Hits
1
0.8
0.6
0.4
0.2
0
−0.2
−0.4
−0.6
−0.8
−1


Best Subset Selection
BIC
−90
−100
−110
−120
−130
−140
5
10
15
number of variables

Best Subset Selection

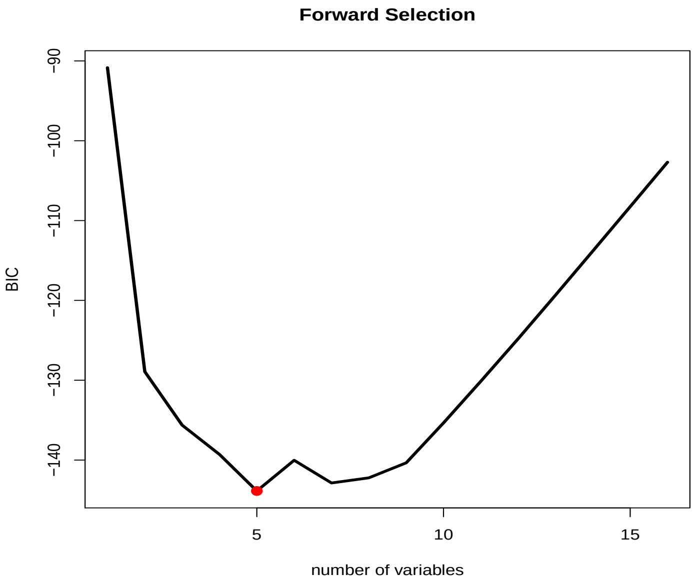


Greedy approach

- To find $\widehat{\beta}^{(k)}$, one has to run a $\binom{k+1}{p+1} = (p+1)!/[(k+1)!(p-k)!]$ regressions!
- This can quickly become prohibitively expensive if k is large.
- Instead, one can use a more greedy approach in order to only look at much less options

Forward Stepwise Selection

1. Let $\mathcal{M}_0$ be the *null* model
2. For $k = 0, \ldots, p-1$
   1. consider all the $(p-k)$ covariates that are not in $\mathcal{M}_k$
   2. choose the *best* among these $(p-k)$ models and call it $\mathcal{M}_{k+1}$
3. Finally, choose the best model among $\mathcal{M}_0, \ldots, \mathcal{M}_p$.



Forward Selection
BIC
−90
−100
−110
−120
−130
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5
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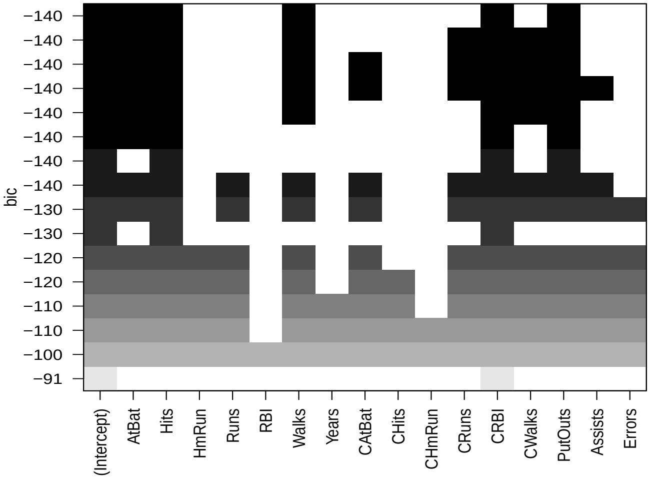
15
number of variables

Forward Selection



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Penalization

- Directly penalization of the size of the coefficients
- For a regularization parameter $\lambda > 0$

$$\widehat{\beta}(\lambda) \; = \; \mathbf{argmin} \left\{ \, \textsf{\textbf{RSS}}(\beta) + \lambda \times \Omega(\beta) \; : \; \beta \in \mathbb{R}^{p+1} \right\}.$$

  The quantity $\Omega(\beta)$ penalises large coefficients
- Estimate $\widehat{\beta}(\lambda)$ is similar to the OLS, with the important difference that a penalization term $\lambda \times \Omega(\beta)$ is added.
- $\lambda > 0$ is quantifies the amount of regularization.

LASSO and Ridge Penalization

$$\Omega_{\text{Ridge}}(\beta) \equiv \sum_{j=1}^{p} \beta_j^2 \equiv \|\beta\|_2^2$$
$$\Omega_{\text{Lasso}}(\beta) \equiv \sum_{j=1}^{p} |\beta_j| \equiv \|\beta\|_1.$$

- Recall the definition of the p-norm

$$\|v\|_p = \Big(|x_1|^p + \ldots + |x_n|^p\Big)^{1/p}$$

Normalization

- typically, the intercept coefficient β_0 is not penalized; this is because we do not want the procedures to be dependent on the location of the covariates
- shrinkage procedures do depend on the scale of the covariates
- In practice, the responses/covariates are centred/normalized

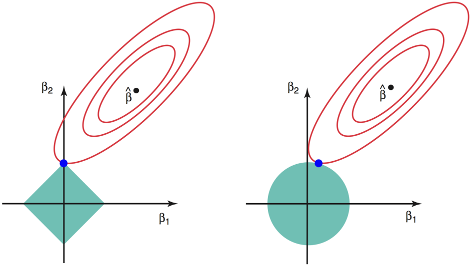
$$x_i \mapsto \frac{x_i - \bar{x}_i}{\widehat{\sigma}(x)} \qquad \text{and} \qquad y \mapsto y - \bar{y}$$

Dual view of regularisation

- One can show that $\widehat{\beta}(\lambda)$ is also solution of the following constrained optimization problem

$$\begin{cases} \text{Minimise} & \textsf{\textbf{RSS}}(\beta) \\ \text{Subject to} & \Omega(\beta) \leq T(\lambda) \end{cases} \tag{2}$$

for some threshold $T(\lambda)$ that depends on λ.



Ridge regression

- The coefficients are penalized by

$$\Omega_{\mathrm{Ridge}}(\beta) \equiv \sum_{j=1}^{p} \beta_j^2 .$$

- The ridge estimate $\beta_{\mathrm{Ridge}}(\lambda)$ is

$$\beta_{\mathrm{Ridge}}(\lambda) \;=\; \Big\{ \; \sum_{i=1}^{n} \big(y_i - [\beta_0 + \beta_1\, x_{i,1} + \ldots + \beta_p\, x_{i,p}]\big)^2 + \lambda \times \sum_{j=1}^{p} \beta_j^2 \;:\; \beta \in \mathbb{R}^{p+1} \Big\}$$

- In practice, the covariates are first normalized; one can thus suppose $\beta_0 = 0$. For $X \in \mathbb{R}^{n,p}$ and $\beta \in \mathbb{R}^p$ the estimate $\beta_{\mathrm{Ridge}}(\lambda)$ minimizes the function

$$\beta \mapsto \|y - X\,\beta\|^2 + \lambda\, \|\beta\|_2^2$$

Ridge regression

- The estimate $\beta_{\mathrm{Ridge}}(\lambda)$ minimizes the function

$$\beta \mapsto \|y - X\,\beta\|^2 + \lambda\,\|\beta\|_2^2$$

- **[Exercise]** The gradient of this function reads

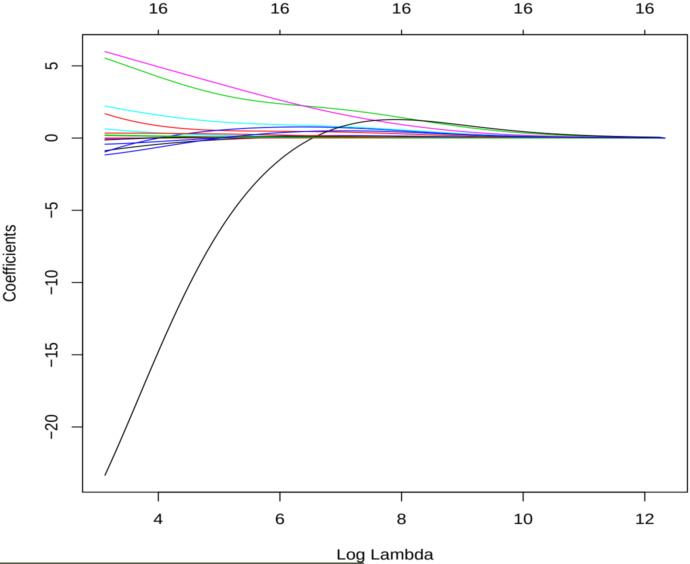
$$-2X^T\,(y - X\,\beta) + 2\lambda\,\beta$$

- **[Exercise]** Setting this gradient to zero yields that

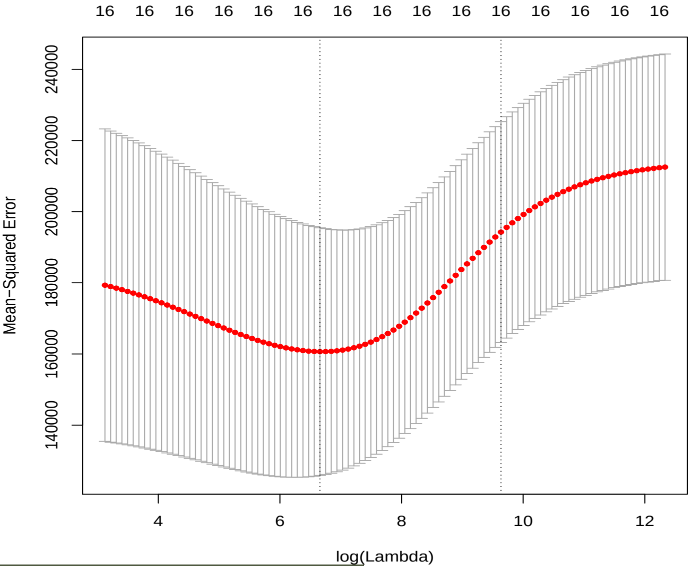
$$\widehat{\beta}(\lambda) = (X^T\,X + \lambda\,I)^{-1}\,X^T\,y.$$

- The matrix $(X^T\,X + \lambda\,I)$ is invertible if $\lambda > 0$.
- Ridge regression is well defined even for $p \geq n+1$.

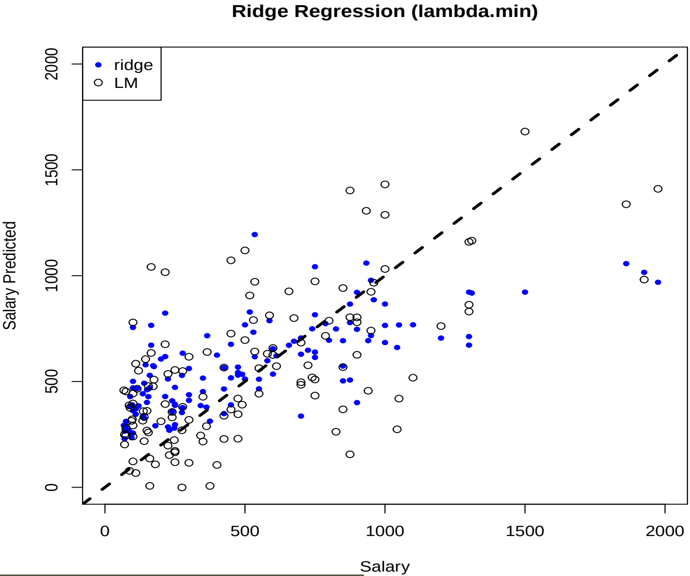
Ridge path



Ridge Cross Validation

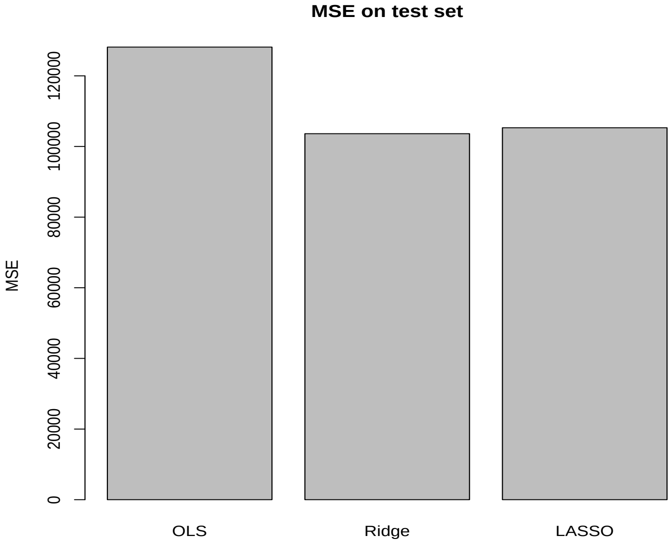


Ridge v.s. OLS



Ridge Regression (lambda.min)
ridge
LM
Salary Predicted
Salary
0
500
1000
1500
2000

Is it worth it?



Least Absolute Shrinkage and Selection Operator (LASSO)

- The coefficients are penalized by

$$\Omega_{\text{Lasso}}(\beta) \equiv \sum_{j=1}^{p} |\beta_j|.$$

- The LASSO estimate $\beta_{\text{Lasso}}(\lambda)$ is

$$\beta_{\text{Lasso}}(\lambda) \;=\; \Big\{ \;\sum_{i=1}^{n} \big(y_i - [\beta_0 + \beta_1\, x_{i,1} + \ldots + \beta_p\, x_{i,p}]\big)^2 \\ + \lambda \times \sum_{j=1}^{p} |\beta_j| \;:\; \beta \in \mathbb{R}^{p+1} \Big\}$$

- In practice, the covariates are first normalized; one can thus suppose $\beta_0 = 0$. For $X \in \mathbb{R}^{n,p}$ and $\beta \in \mathbb{R}^{p}$ the estimate $\beta_{\text{Ridge}}(\lambda)$ minimizes the function

$$\beta \mapsto \|y - X\,\beta\|^2 + \lambda\;\|\beta\|_1$$

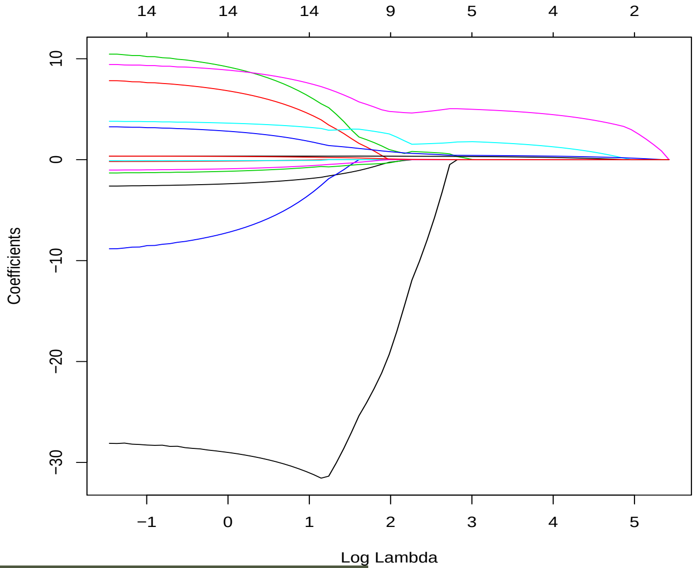
Least Absolute Shrinkage and Selection Operator (LASSO)

- The estimate $\beta_{\mathrm{Lasso}}(\lambda)$ minimizes the function

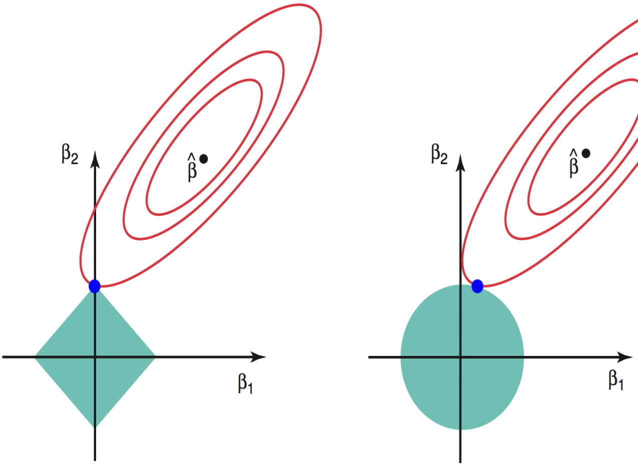
$$\beta \mapsto \|y - X\,\beta\|^2 + \lambda\,\|\beta\|_1$$

- there is no closed form
- the objective function is not differentiable
- **[Exercise]** the objective function is convex
- LASSO regression is well defined even for $p \geq n + 1$.

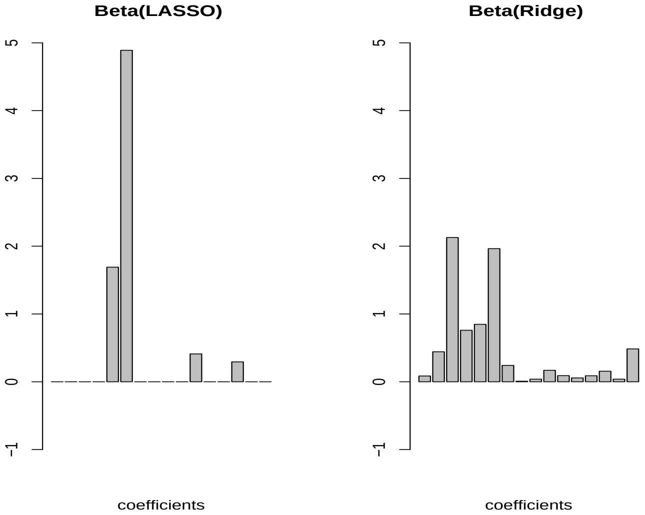
LASSO path



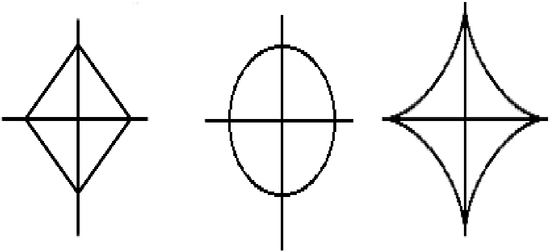
LASSO and sparsity



LASSO and sparsity

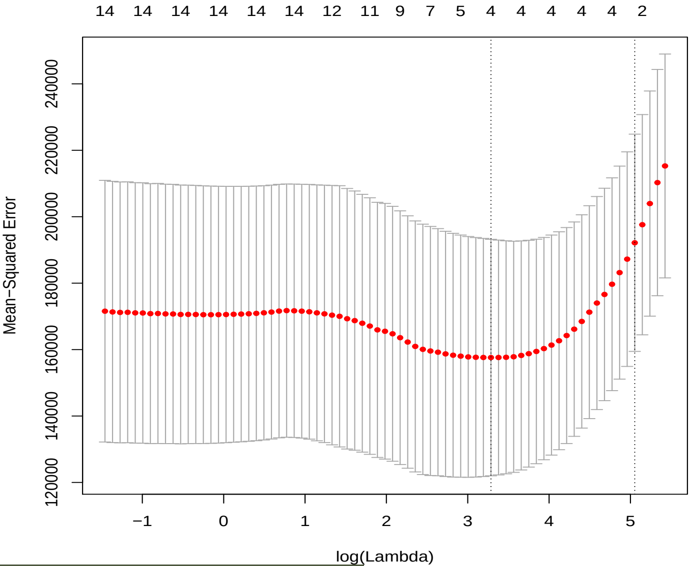


Why not a p-norm with $p < 1$?

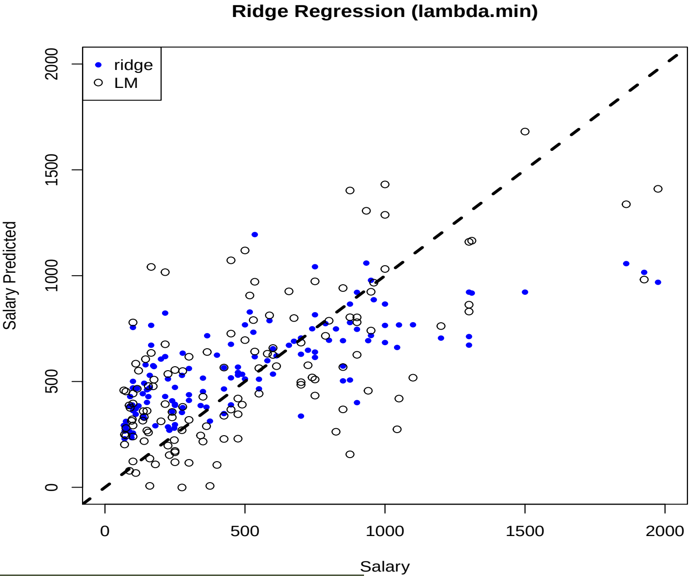


$$\beta \mapsto \|y - X\beta\|^2 + \lambda \, \|\beta\|_p^p$$

Ridge Cross Validation



Ridge v.s. OLS



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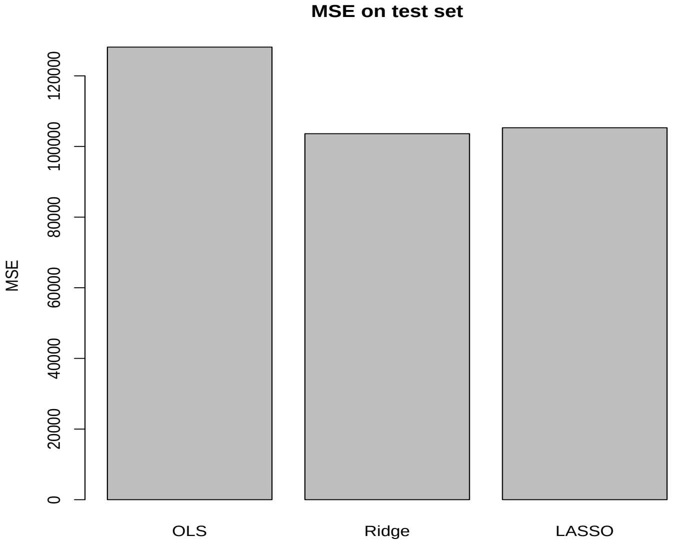
Is it worth it?



Case of orthogonal design

- observation $y = X\beta_\star + \varepsilon$
- after normalisation: $1^T y = 0$ and $\sum_j X_{i,j} = 0$ and $\sum_j X_{i,j}^2 = 1$
- one can assume that $\beta_0 = 0$ and forget about the intercept
- for tractability, let us assume that $X^T X = I_p$
- [**Exercise**] we have $\beta_{\mathrm{OLS}} = X^T y$

- **[Exercise]** ridge regression estimate $\beta_{\mathrm{Ridge}}(\lambda)$ minimises

$$\beta \mapsto \|\beta\|^2 - 2\,\langle \beta_{\mathrm{OLS}}, \beta \rangle + \lambda\,\|\beta\|_2^2$$

- **[Exercise]** the ridge estimate is given by

$$\beta_{\mathrm{Ridge}} = \beta_{\mathrm{OLS}}/(1+\lambda).$$

- one can show that the LASSO estimate is

$$\beta_{\mathrm{Lasso}} = T(\beta_{\mathrm{OLS}}, \lambda/2)$$

  with the soft thresholding operator

$$T(x,\lambda) = \mathrm{sign}(x)\ (|x| - \lambda)^{+}$$

Case of orthogonal design