

Lesson 08 Regularization

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April 06 (Monday), 2020

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Linear Regression (Reminder)

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- When we have a lot of observations we can be fairly confident that the Least Squares line accurately reflects the relationship between y and x .

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- In practice, some of the assumptions of linear regression are violated.
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- Number of observations is much larger than the number of variables ($n \gg p$)
- Absence of multicollinearity.

Problems

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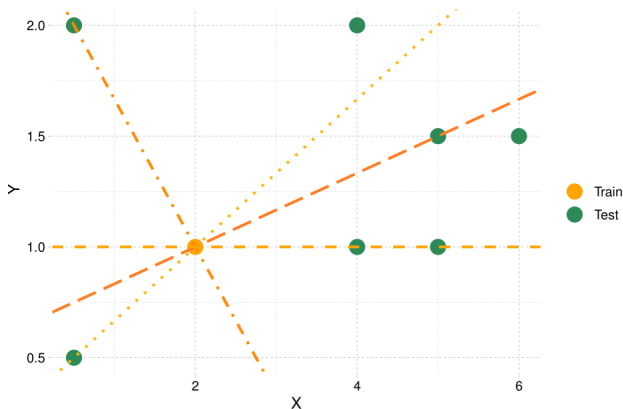
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- Multicollinearity problem:
- With perfect collinearity $\text{rank}(X) < m \Rightarrow (X^T X)^{-1}$ does not exist.
- With multicollinearity: $\text{rank}(X) = m$, but there are high correlation, thus standard error for $\hat{\beta}_j$ will be large.

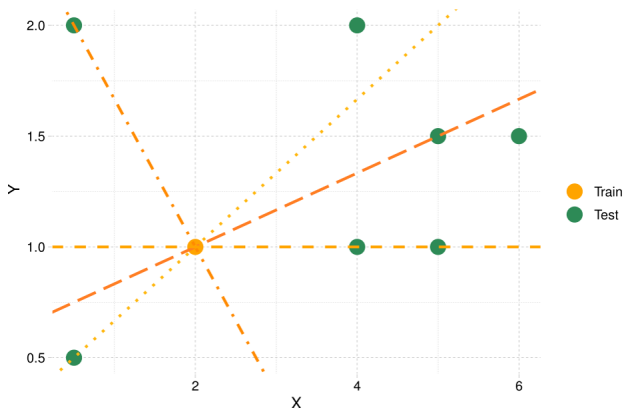
Problem with number of variables and observations

- Suppose train data consists of 1 observation and 1 variable



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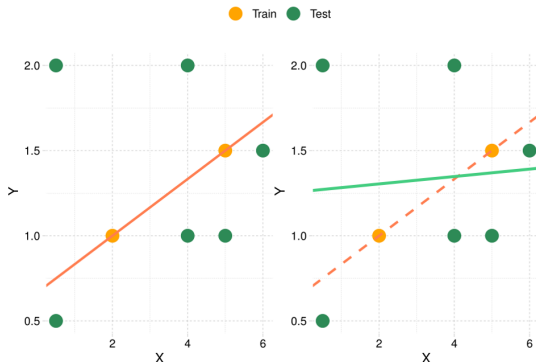
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- All regressions has $RSS = 0$ for train data.

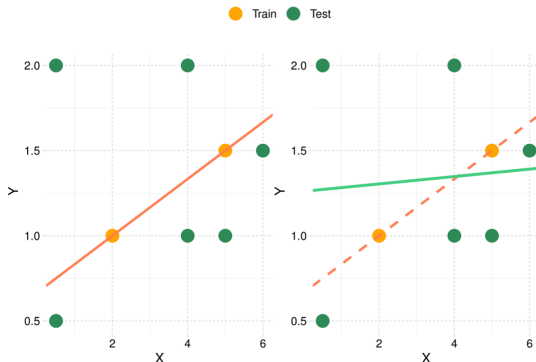
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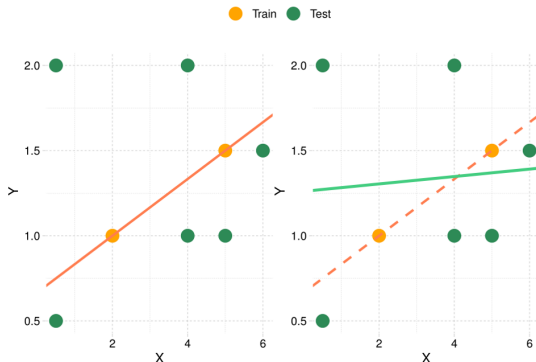
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- The regression has high variance and zero bias.

The way of solving these problems

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- **Shrinkage (Regularization).** Fitting a model involving all p predictors and then shrinking coefficients towards zero relative to OLS estimates.
- **Dimension Reduction.** Projecting the p predictors into a m -dimensional subspace by computing m ($m < p$) linear combinations of p variables.

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- $\lambda \sum_{j=1}^p \hat{\beta}_j^2$ is a shrinkage penalty
- $\lambda \geq 0$ is the **tuning** parameter

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- Ridge shrinks the estimated association of each variable with the response.
- There is no need to shrink the intercept, which is simply a measure of the mean value of the response when $x_{i1} = x_{i2} = \dots = x_{ip} = 0$.

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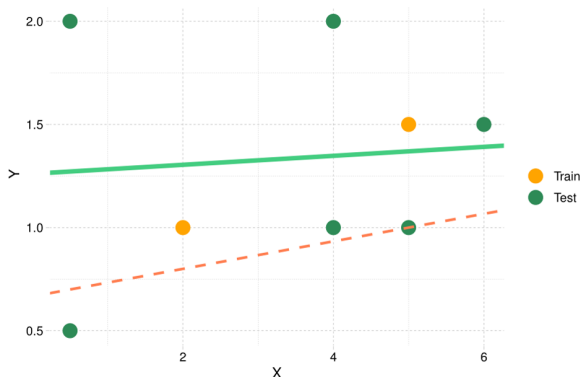
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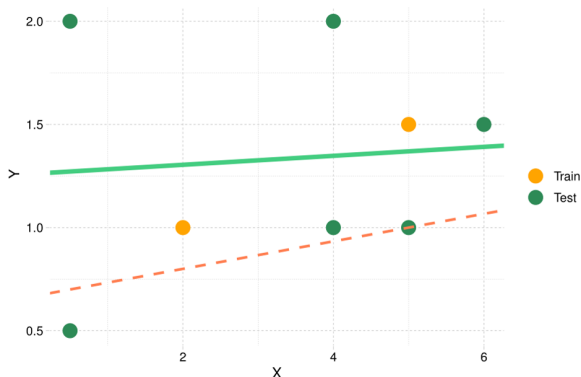
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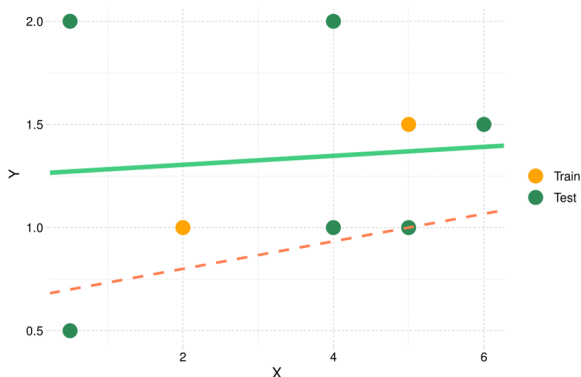
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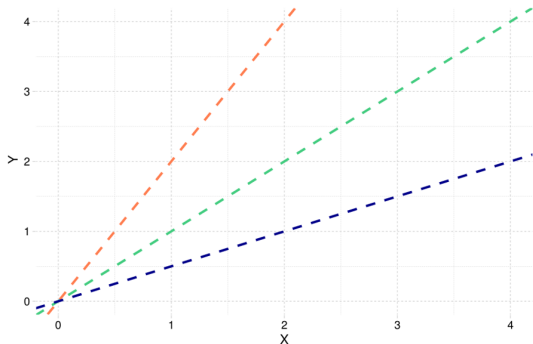
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- Shrinking the coefficient estimates can significantly reduce their

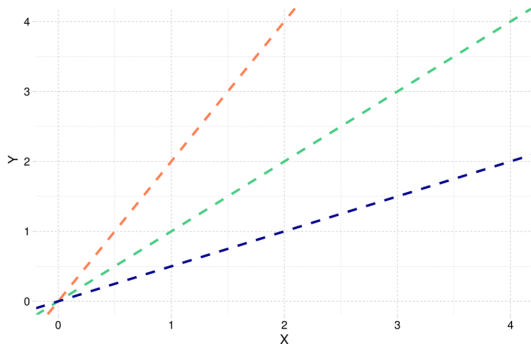
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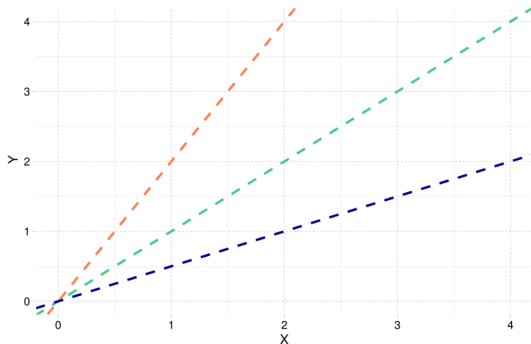
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- $\lambda \rightarrow \infty, \hat{\beta}_{ridge} \rightarrow 0$
- Less and less sensitive to x variable

Decrease in the slope: example

- Suppose we have $y_i = \beta x_i + \varepsilon_i$ and we have the following data:

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- $\hat{\beta}_{OLS} = \frac{\sum_{i=1}^n y_i x_i}{\sum_{i=1}^n x_i^2} = \frac{10 + 20 + 60}{1^2 + 1^2 + 2^2} = \frac{90}{6} = 15$

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- Suppose $\lambda = 240$
- $\hat{\beta}_{ridge} \frac{90}{6+240} = \frac{90}{6+246} = 0.37 < 15$

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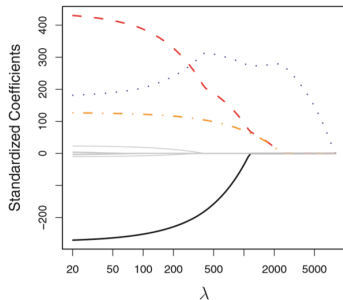
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- $\text{rank}(X) < m \Rightarrow (X^T X)^{-1}$ does **NOT** exist, but $(X^T X + \lambda I)^{-1}$ does exist.

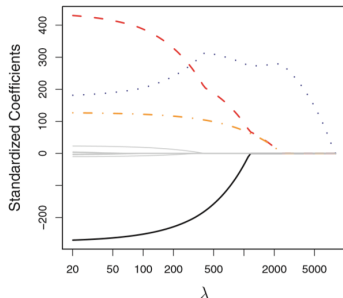
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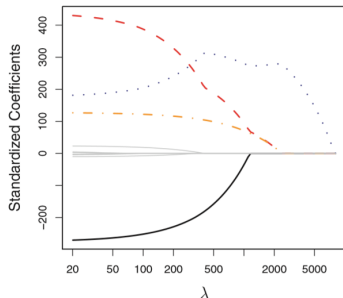
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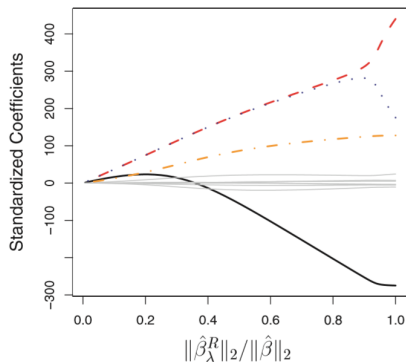
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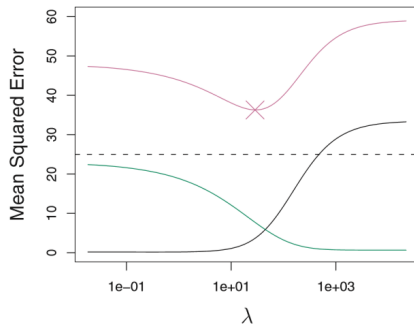
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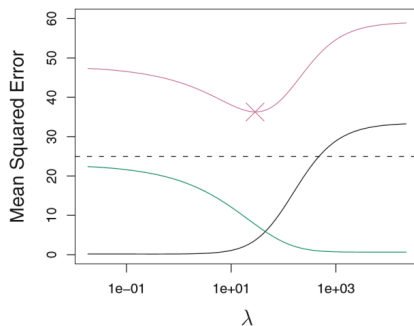
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Bias-variance trade-off as a function of lambda



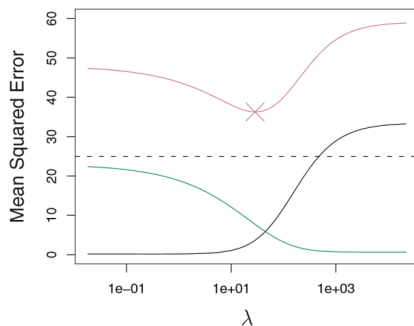
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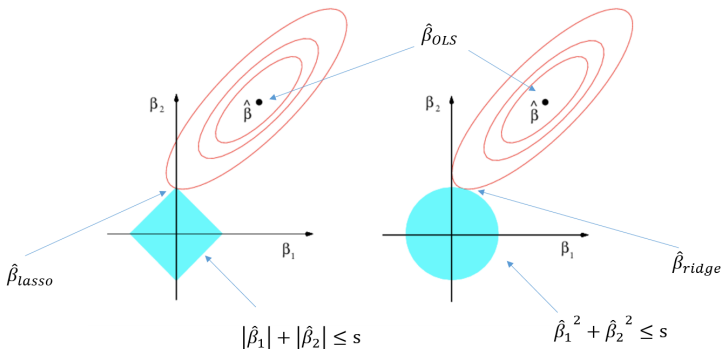
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- If s is sufficiently large, then the constraint regions will contain $\hat{\beta}$, and so the ridge regression and lasso estimates will be the same as the least squares estimates.

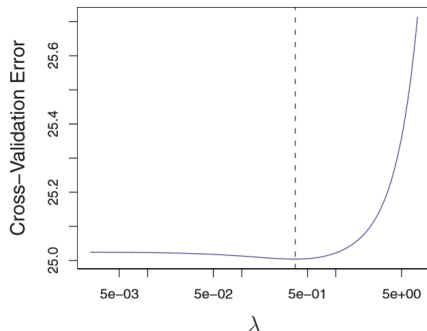
Another Formulation for Ridge Regression and the Lasso



- Since ridge regression has a circular constraint with no sharp points, this intersection will not generally occur on an axis, and so the ridge regression coefficient estimates will be exclusively non-zero.

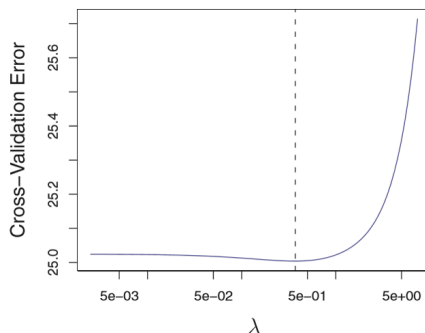
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- Finally, the model is re-fit using all of the available observations and the selected value of the tuning parameter.

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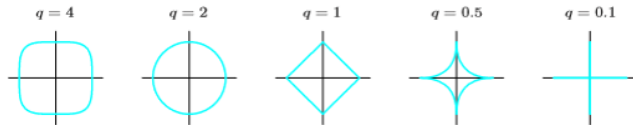
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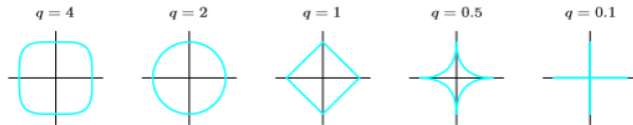
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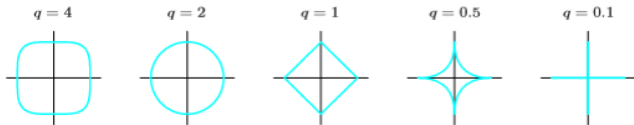
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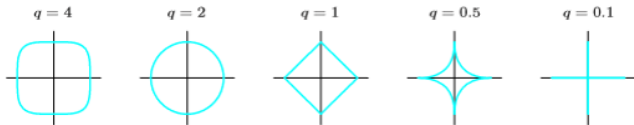
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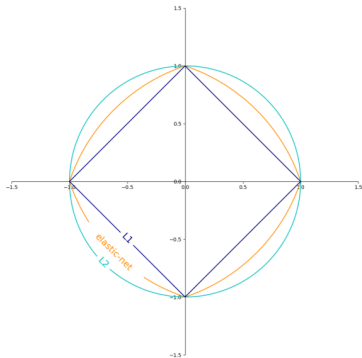
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- The most popular combination is **Elastic Net Regression**.

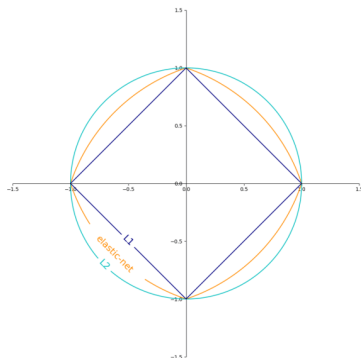
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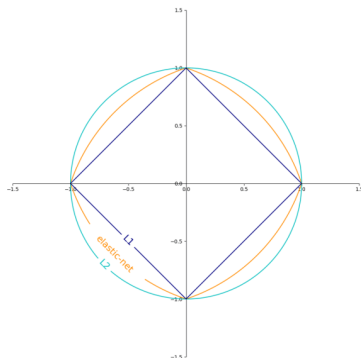
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- $\lambda = 0 \Rightarrow OLS$
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- $\{\alpha, \lambda\} \neq 0 \Rightarrow Elastic Net$

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- **Elastic Net regression** is useful if the knowledge about data is not available.