Regression and Regularization: Part I

Prof. Gustavo Nonato

NYU / CUSP - GX 5006

February 7, 2017

Basic Concepts

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Properly estimating the parameters β_j is the main goal of a linear regression.

Residual Sum of Squares

The **least squares** method computes the parameters $\boldsymbol{\beta} = (\beta_0, \beta_1, \ldots, \beta_d)^\top$ so as to minimize the **residual sum of squares**

$$RSS(\boldsymbol{\beta}) = \sum_{i=1}^{n} (y_i - f(\mathbf{x}_i))^2 = \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{d} x_{ij}\beta_j \right)^2$$

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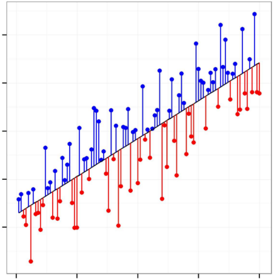

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$$\boxed{RSS(\boldsymbol{\beta}) = (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^\top (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})}$$

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Differentiating $RSS(\boldsymbol{\beta}) = (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^\top(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$ with respect to $\boldsymbol{\beta}$ and setting the derivative to zero

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In practice $\hat{\boldsymbol{\beta}}$ is computed solving the system $(\mathbf{X}^\top\mathbf{X})\boldsymbol{\beta} = \mathbf{X}^\top\mathbf{y}$ (using QR factorization).

Linear Model as the Mean

Lets assume that the linear model is the correct model for the mean behavior of the data and that the deviations of Y around its expectation is Gaussian, that is,

$$Y = \beta_0 + \sum_{j=1}^{p} X_j \beta_j + \epsilon, \quad \epsilon \sim N(0, \sigma^2)$$

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PS. In practice $\hat{\boldsymbol{\beta}} \pm 2\, se(\hat{\boldsymbol{\beta}})$, where $se(\hat{\boldsymbol{\beta}}) = \frac{\sigma^2}{n}$, is used to approximate 95% confidence interval.

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$$MSE(\hat{\boldsymbol{\beta}}) = E(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})^2 = \underbrace{Var(\hat{\boldsymbol{\beta}})}_{variance} + \underbrace{\left[E(\hat{\boldsymbol{\beta}}) - \boldsymbol{\beta}\right]^2}_{\substack{bias \\ (=0\, for\ least\ squares)}}$$

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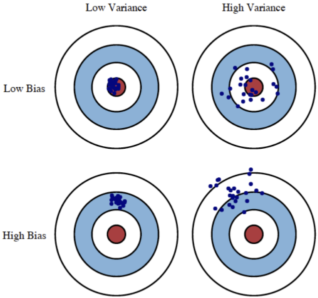

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There are several ways to obtain such biased estimates, for example *subset selection* and *regularized optimization schemes*.

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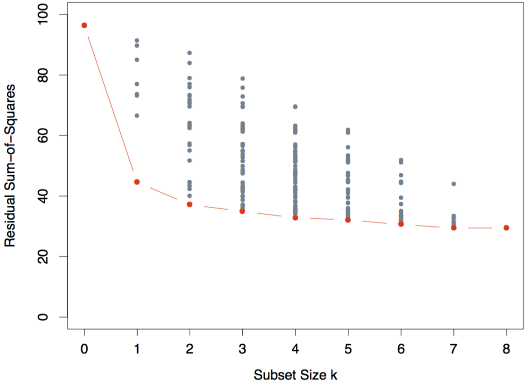

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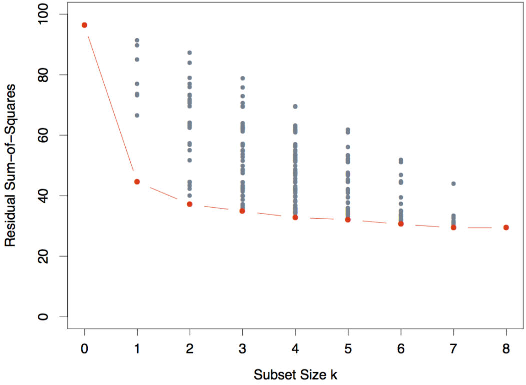

Computationally unfeasible for large values of d !!

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Greedy-like alternatives to reduce the computational burden !!

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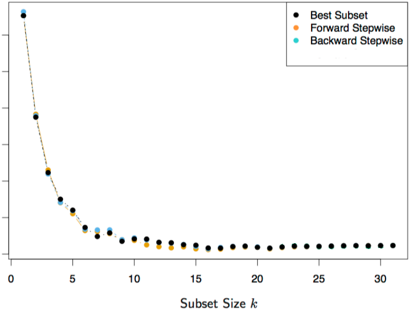

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However, in contrast to the discrete nature of subset selection, shrinkage methods are continuous, resulting in lower variance parameter estimation.

The idea is play with the full model, but imposing penalties to the parameters so as to shrink them to zero.

Ridge Regression

$$\hat{\boldsymbol{\beta}} = \text{argmin}_{\beta} \left\{ \sum_{i=1}^{n} (y_i - \beta_0 - \sum_{j=1}^{d} x_{ij}\beta_j)^2 + \lambda \sum_{j=1}^{d} \beta_j^2 \right\}$$

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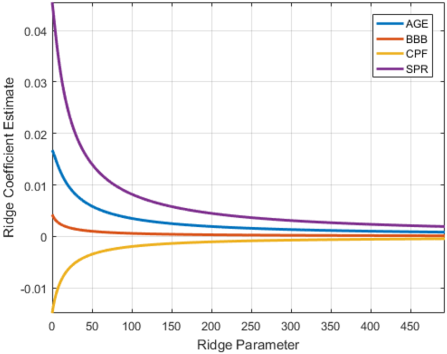

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Without β_0 we can write the residual sum of squares as:

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Since small d_j are related to noise (remember PCA lesson !), rigde regression is making a “soft” selection of the main components, removing noise and writing data back in the original coordinate system.

Lasso

Lasso is similar to ridge regression,

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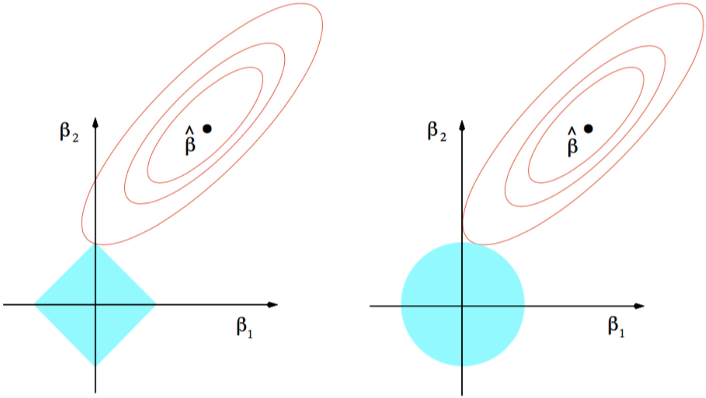
Unfortunately there is no closed form expression for the solution of the Lasso regression, thus a quadratic optimization procedure has to be employed to compute $\hat{\boldsymbol{\beta}}$.

Lasso

An import aspect of Lasso is that, tuning λ properly, non-relevant parameters are quickly truncated to zero.



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