

THE Winter School

Predictive Machine Learning

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References

- ▶ James, Witten, Hastie, and Tibshirani (2013): "An Introduction to Statistical Learning", Springer, [download](#).
- ▶ Hastie, Tibshirani, and Friedman (2009): "Elements of Statistical Learning", 2nd ed., Springer, [download](#).

Ridge

Summation notation:

$$\min_{\beta} \left\{ \sum_{i=1}^N \left(y_i - \beta_0 - \sum_{j=1}^p x_{ij} \beta_j \right)^2 + \lambda \sum_{j=1}^p \beta_j^2 \right\}$$

where $\lambda \geq 0$ is the penalty parameter and the number of covariates p can be high-dimensional ($p \gg N$).

- Note that coefficient size depends on the scaling of x_j . It is best practice to standardise non-binary x_j . In the following, we assume that all covariates are standardized.

Closed-Form Solution

Matrix notation:

$$\min_{\beta} \{ (Y - X\beta)'(Y - X\beta) + \lambda \|\beta\|_2^2 \}$$

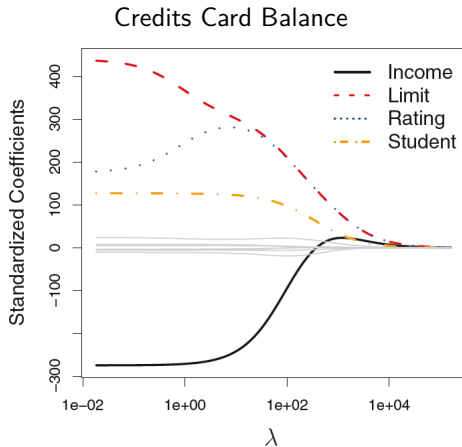
where $\beta = (\beta_1, \beta_2, \dots, \beta_p)'$ does not include the constant term $\beta_0 = \frac{1}{N} \sum_{i=1}^N y_i$. The squared l_2 -norm is $\|\beta\|_2^2 = \beta' \beta = \sum_{j=1}^p \beta_j^2$.

Closed-form solution:

$$\hat{\beta} = (X'X + \lambda I)^{-1} X'Y$$

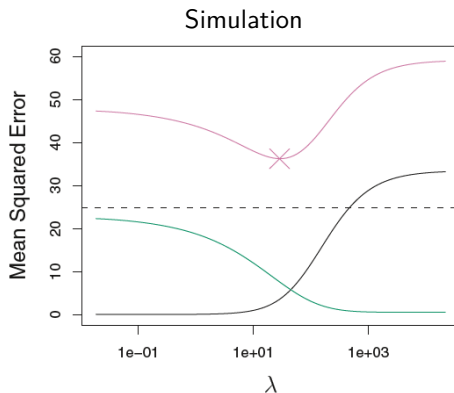
with $(X'X + \lambda I)$ being positive definite.

Ridge Coefficients



Source: James et al. (2013), p. 216

Ridge: Variance-Bias Trade-Off



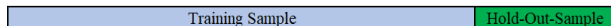
Note: squared bias (black), variance (green), MSE (red)

Source: James et al. (2013), p. 218

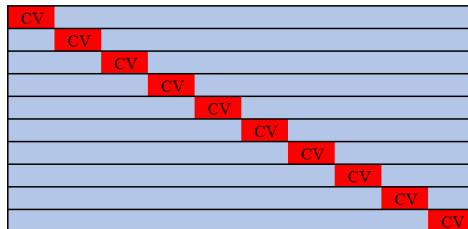
Selection of Optimal Penalty Parameter

Cross-Validation (CV) Algorithm

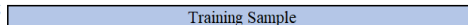
Sample Split



CV Complexity



Estimate Model Using
Optimal Complexity



Extrapolate Fitted
Values and Evaluate
Prediction Power



Summation notation:

$$\min_{\beta} \left\{ \sum_{i=1}^N \left(y_i - \beta_0 - \sum_{j=1}^p x_{ij} \beta_j \right)^2 + \lambda \sum_{j=1}^p |\beta_j| \right\}$$

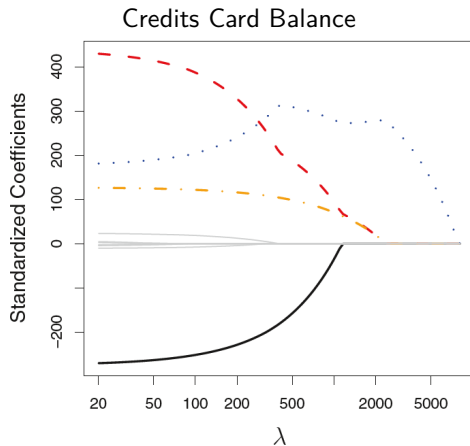
where $\lambda \geq 0$ is the penalty parameter.

Matrix notation:

$$\min_{\beta} \{ (Y - X\beta)'(Y - X\beta) + \lambda \|\beta\|_1 \}$$

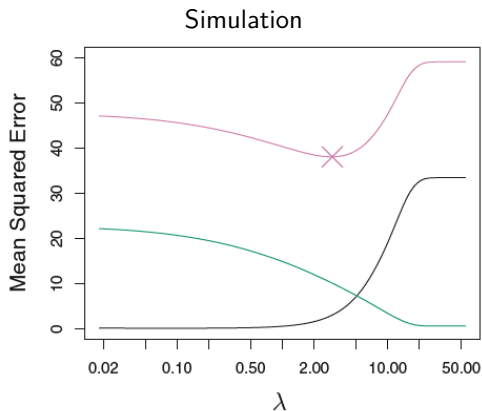
with $\|\beta\|_1 = \sum_{j=1}^p |\beta_j|$ (l_1 -norm).

Lasso Coefficients



Source: James et al. (2013), p. 220

Lasso: Variance-Bias Trade-Off



Note: squared bias (black), variance (green), MSE (red)

Source: James et al. (2013), p. 223

Constrained Regression

- ▶ OLS residual sum of squares (RSS):

$$RSS = \sum_{i=1}^N (y_i - \beta_0 - \sum_{j=1}^p x_{ij}\beta_j)^2$$

- ▶ Penalized regression:
 - ▶ Lagrangian operator

$$\min_{\beta} \{RSS + \lambda \sum_{j=1}^p p(\beta_j)\}$$

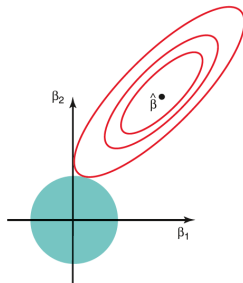
- ▶ Constrained regression

$$\min_{\beta} \{RSS\} \text{ s.t. } \sum_{j=1}^p p(\beta_j) \leq c$$

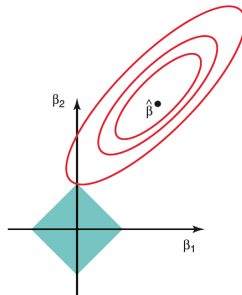
where $p(\beta_j) = \beta_j^2$ for Ridge and $p(\beta_j) = |\beta_j|$ for Lasso.

Constraint Regions

Ridge Penalty



Lasso Penalty



Source: James et al. (2013), p. 222

Simple Example

- ▶ Consider $X = I$ with dimension $p = N$.

- ▶ OLS model

$$\sum_{j=1}^p (y_j - \beta_j)^2,$$

such that the estimated OLS coefficients are $\hat{\beta}_j = y_j$.

- ▶ Ridge model

$$\sum_{j=1}^p (y_j - \beta_j)^2 + \lambda \sum_{j=1}^p \beta_j^2,$$

such that the estimated Ridge coefficients are $\hat{\beta}_j^R = \hat{\beta}_j / (1 + \lambda)$.

Simple Example (cont.)

- LASSO model

$$\sum_{j=1}^p (y_j - \beta_j)^2 + \lambda \sum_{j=1}^p |\beta_j|,$$

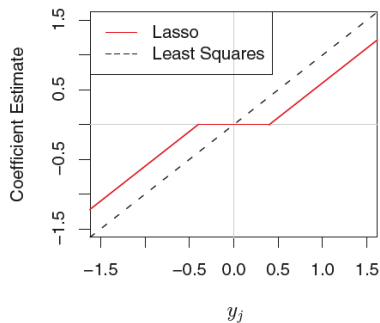
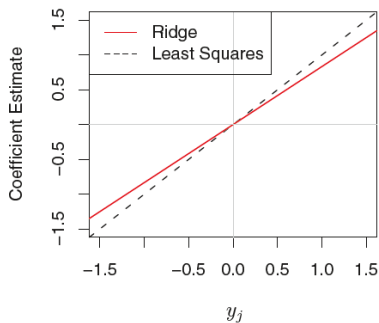
such that the estimated LASSO coefficients are

$$\hat{\beta}_j^L = \begin{cases} \hat{\beta}_j - \lambda/2 & \text{if } \hat{\beta}_j > \lambda/2, \\ \hat{\beta}_j + \lambda/2 & \text{if } \hat{\beta}_j < -\lambda/2, \\ 0 & \text{if } |\hat{\beta}_j| \leq \lambda/2, \end{cases}$$

which corresponds to the soft-thresholding operator

$$\hat{\beta}_j^L = \text{sign}(\hat{\beta}_j)(|\hat{\beta}_j| - \lambda/2)_+$$

Simple Example (cont.)



Source: James et al. (2013), p. 226

Coordinate Descent Algorithm for Lasso

$$\min_{\beta} \left\{ \frac{1}{2N} \sum_{i=1}^N (y_i - \beta_0 - \sum_{j=1}^p x_{ij} \beta_j)^2 + \lambda_s \sum_{j=1}^p |\beta_j| \right\}$$

- (1) Specify a grid of $s = 1, \dots, S$ tuning parameters $\lambda_s \in \{\lambda_1, \lambda_2, \dots, \lambda_S\}$
- (2) Take residuals $y_i^* = y_i - \frac{1}{N} \sum_{i=1}^N y_i$ and initialise $\beta_j = 0$
- (3) Circulate repeatedly over all $j = 1, \dots, p$ until convergence:
 - (a) Compute the partial residuals by $r_{ij} = y_i^* - \sum_{k \neq j} x_{ik} \beta_k$
 - (b) Calculate the simple univariate OLS coefficient
$$\tilde{\beta}_j = \frac{1}{N} \sum_{i=1}^N x_{ij} r_{ij}$$
 - (c) Update β_j with the soft-thresholding operator:

$$\beta_j = \text{sign}(\tilde{\beta}_j)(|\tilde{\beta}_j| - \lambda_s)_+$$

- (4) Repeat (3) for $s = 1, \dots, S$

Note: Standardisation of x is required

Post-Lasso

- ▶ Coefficients of Lasso $\hat{\beta}_j$ are biased when $\lambda > 0$, because the penalty terms shrinks the coefficients.
- ▶ **Idea of Post-Lasso:**
 1. Estimate a Lasso model with the cross-validated optimal penalty.
 2. Estimate an OLS model (called Post-Lasso) which includes all variables with non-zero coefficients from the first-step Lasso model.
- ▶ **Problems:**
 - ▶ Post-Lasso coefficients are also biased in the presence of omitted variable bias.
 - ▶ The first-step model selection of the Lasso is often unstable.

Other Extensions

Elastic Net:

$$\min_{\beta} \left\{ \sum_{i=1}^N \left(y_i - \beta_0 - \sum_{j=1}^p x_{ij} \beta_j \right)^2 + \lambda \sum_{j=1}^p (\alpha |\beta_j| + (1 - \alpha) \beta_j^2) \right\}$$

Best Subset Selection:

$$\min_{\beta} \left\{ \sum_{i=1}^N \left(y_i - \beta_0 - \sum_{j=1}^p x_{ij} \beta_j \right)^2 + \lambda \sum_{j=1}^p 1\{\beta_j \neq 0\} \right\}$$

Other Supervised Machine Learning Methods

- ▶ Forward Selection, Backward Selection
- ▶ Trees and Forests
- ▶ Neural Networks
- ▶ Boosting
- ▶ Ensemble Methods
- ▶ etc.