Machine Learning for Economists and Business Analysts

Regularized Regression

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Literature

- ▶ James, Witten, Hastie, and Tibshirani (2023): "An Introduction to Statistical Learning", Springer, Chapter 6.2, <u>download</u>.
- ► Hastie, Tibshirani, and Friedman (2009): "Elements of Statistical Learning", 2nd ed., Springer, Chapter 3.4, download.

Best Subset Selection

- Consider we want to predict Y with a linear model including a constant and k predictors. Overall the data includes p covariates (excluding the constant). For the shake of illustration, assume p=100.
- ► The number of possible models depends on *k*:
 - ▶ If k = 0, there is only one possible model.
 - ▶ If k = 1, there are 100 possible models.
 - ▶ If k = 2, there are 4,950 possible models.
 - ▶ If k = 3, there are 161,700 possible models.
 - If k = 4, there are 3,921,225 possible models.
- ► In general, the number of possible models for any *k* is (binomial expansion)

$$\left(\begin{array}{c}p\\k\end{array}\right)=\frac{p!}{k!(p-k)!},$$

or 2^p models across all possibel k's.

► Select optimal *k* using cross-validation.

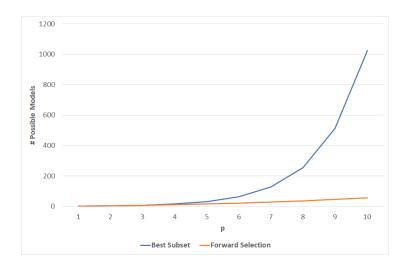
Forward Stepwise Selection

- ▶ Impose a bottom-up hierarchical structure on the covariates:
 - ▶ The first model (k = 0) contains only a constant.
 - ▶ The second model (k = 1) adds to the constant one out of p possible covariates.
 - The third model (k = 2) equals the second model, but adds one out of p 1 possible covariates.
 - ▶ The fourth model (k = 3) equals the third model, but adds one out of p 2 possible covariates.
- In general, the number of possible models is

$$1+\frac{p(p+1)}{2}.$$

► Select optimal *k* using cross-validation.

Number of Possible Models



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 ($p \gg N$).

 \rightarrow 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.

Matrix notation:

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

where $\beta=(\beta_1,\beta_2,\cdots\beta_p)'$ does not include the constant term $\beta_0=\frac{1}{N}\sum_{i=1}^N y_i$. The squared I_2 -norm is $\|\beta\|_2^2=\beta'\beta=\sum_{i=1}^p \beta_i^2$.

First Order Condition

Partial derivative w.r.t. β :

$$-2X'(Y-X\beta)+2\lambda I\beta=0$$

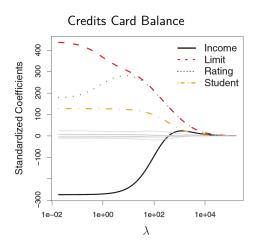
where I is a $p \times p$ identity matrix.

Closed-form solution:

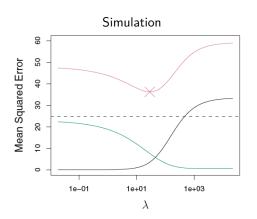
$$\widehat{\beta} = (X'X + \lambda I)^{-1}X'Y$$

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

Ridge Coefficients



Ridge: Variance-Bias Trade-Off



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

Selection of Optimal Penalty Parameter

Cross-Validation (CV) Algorithm



Firewall Principle

Why do we use the hold-out-sample to evaluate the prediction power?

- ▶ If we try many tuning parameter values, we may end up overfitting even in cross-validation samples.
- ► The cross-validation performance is an aggregation over multiple different prediction functions, which differs from the single prediction function we finally estimate.

Lasso

Summation notation:

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

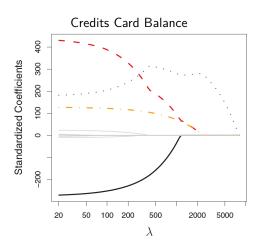
where $\lambda \geq 0$ is the penalty parameter.

Matrix notation:

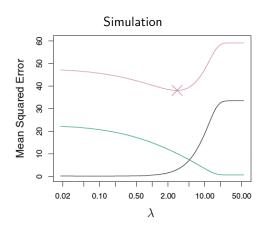
$$\min_{\beta} \left\{ (Y - X\beta)'(Y - X\beta) + \lambda \|\beta\|_1 \right\}$$

with $\|\beta\|_1 = \sum_{j=1}^{p} |\beta_j|$ (I₁-norm).

Lasso Coefficients



Lasso: Variance-Bias Trade-Off



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

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

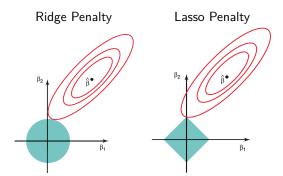
$$\min_{\beta} \{RSS + \lambda \sum_{j=1}^{p} p(\beta_j)\}$$

Constrained regression

$$\min_{\beta} \{RSS\} \text{ s.t. } \sum_{i=1}^{p} p(\beta_i) \le c$$

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

Constraint Regions



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 $\widehat{\beta}_j = y_j$.

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 $\widehat{\beta}_j^R = \widehat{\beta}_j/(1+\lambda).$

Simple Example (cont.)

► LASSO model

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

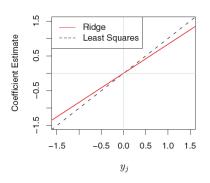
such that the estimated LASSO coefficients are

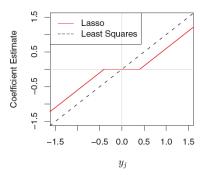
$$\widehat{\beta}_{j}^{L} = \begin{cases} \widehat{\beta}_{j} - \lambda/2 & \text{if } \widehat{\beta}_{j} > \lambda/2, \\ \widehat{\beta}_{j} + \lambda/2 & \text{if } \widehat{\beta}_{j} < -\lambda/2, \\ 0 & \text{if } |\widehat{\beta}_{j}| \leq \lambda/2, \end{cases}$$

which corresponds to the soft-thresholding operator

$$\widehat{eta}_{j}^{L} = \mathit{sign}(\widehat{eta}_{j})(|\widehat{eta}_{j}| - \lambda/2)_{+}$$

Simple Example (cont.)





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

$$\beta_{j} = sign(\tilde{\beta}_{j})(|\tilde{\beta}_{j}| - \lambda_{s})_{+}$$

(4) Repeat (3) for s = 1, ..., S

Note: Standardisation of x is required

Post-Lasso

- ightharpoonup Coefficients of LASSO $\widehat{\beta}_j$ are biased when $\lambda > 0$, because the penalty terms shrinks the coefficients towards zero.
- Post-LASSO enables an easy interpretation.

► Idea:

- Estimate a Lasso model with the cross-validated optimal penalty.
- 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:

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