

Linear Regression Models

Segment 5 – Model Selection

Topic 3 - Regularization Approaches Using glmnet

Sudarsan N.S. Acharya (sudarsan.acharya@manipal.edu)

Topics



- 1. Regularization Overview
- 2. Regularization: Ridge, Lasso, & Elastic-net
- 3. The glmnet Package
- 4. Some Remarks on Ridge and Lasso Regularization





• The stepwise methods for model selection involved building several models using subsets of predictors.



- The stepwise methods for model selection involved building several models using subsets of predictors.
- An alternative approach for model selection is to build a model using all predictors while *shrinking* the coefficient estimates towards zero.



- The stepwise methods for model selection involved building several models using subsets of predictors.
- An alternative approach for model selection is to build a model using all predictors while *shrinking* the coefficient estimates towards zero.
- Shrinking the coefficient estimates can significantly reduce their variance.



- The stepwise methods for model selection involved building several models using subsets of predictors.
- An alternative approach for model selection is to build a model using all predictors while *shrinking* the coefficient estimates towards zero.
- Shrinking the coefficient estimates can significantly reduce their variance.
- Such shrinkage approaches are referred to as *regularization methods* which can also be used for feature selection.







$$\underbrace{\sum_{i=1}^{n} \left(y^{(i)} - \left(\beta_0 + \beta_1 x_1^{(i)} + \dots + \beta_p x_p^{(i)} \right) \right)^2}_{RSS}$$



$$\underbrace{\sum_{i=1}^{n} \left(y^{(i)} - \left(\beta_0 + \beta_1 x_1^{(i)} + \dots + \beta_p x_p^{(i)} \right) \right)^2}_{RSS} + \left\{$$



$$\underbrace{\sum_{i=1}^{n} \left(y^{(i)} - \left(\beta_0 + \beta_1 x_1^{(i)} + \dots + \beta_p x_p^{(i)} \right) \right)^2}_{RSS} + \begin{cases} \lambda \sum_{j=1}^{p} |\beta_j|^2 \\ (\mathsf{ridge}) \end{cases}$$



$$\underbrace{\sum_{i=1}^{n} \left(y^{(i)} - \left(\beta_0 + \beta_1 x_1^{(i)} + \dots + \beta_p x_p^{(i)}\right)\right)^2}_{RSS} + \begin{cases} (\mathsf{ridge}) \\ \mathsf{or} \end{cases}$$



coefficient estimates:
$$\underbrace{\sum_{i=1}^{n} \left(y^{(i)} - \left(\beta_0 + \beta_1 x_1^{(i)} + \dots + \beta_p x_p^{(i)}\right)\right)^2}_{RSS} + \begin{cases} \lambda \sum_{j=1}^{p} |\beta_j|^2 \\ (\text{ridge}) \\ \text{or} \\ \lambda \sum_{j=1}^{p} |\beta_j| \\ (\text{lasso}) \end{cases}$$



coefficient estimates:
$$\underbrace{\sum_{i=1}^n \left(y^{(i)} - \left(\beta_0 + \beta_1 x_1^{(i)} + \dots + \beta_p x_p^{(i)}\right)\right)^2}_{RSS} + \begin{cases} \lambda \sum_{j=1}^p |\beta_j|^2 \\ (\mathsf{ridge}) \\ \mathsf{or} \\ \lambda \sum_{j=1}^p |\beta_j| \\ (\mathsf{lasso}) \\ \mathsf{or} \end{cases}$$



Elastic-net

Regularization is achieved by adding to the
$$RSS$$
 constraints on the coefficient estimates:

$$\sum_{i=1}^{n} \left(y^{(i)} - \left(\beta_0 + \beta_1 x_1^{(i)} + \dots + \beta_p x_p^{(i)}\right)\right)^2 + \begin{cases} \lambda \sum_{j=1}^{p} |\beta_j|^2 \\ (\text{ridge}) \\ \text{or} \\ \lambda \sum_{j=1}^{p} |\beta_j| \\ (\text{lasso}) \\ \text{or} \\ \lambda \left[\alpha \sum_{j=1}^{p} |\beta_j| + (1-\alpha) \sum_{j=1}^{p} |\beta_j|^2 \right] \\ (\text{elastic-net}), \end{cases}$$

Linear Regression Models | Segment 5 | Topic 3



Regularization is achieved by adding to the RSS constraints on the

Regularization is achieved by adding to the
$$RSS$$
 constraints on the coefficient estimates:
$$\sum_{i=1}^n \left(y^{(i)} - \left(\beta_0 + \beta_1 x_1^{(i)} + \dots + \beta_p x_p^{(i)}\right)\right)^2 + \begin{cases} \lambda \sum_{j=1}^p |\beta_j|^2 \\ (\text{ridge}) \\ \text{or} \\ \lambda \sum_{j=1}^p |\beta_j| \\ (\text{lasso}) \\ \text{or} \\ \lambda \left[\alpha \sum_{j=1}^p |\beta_j| + (1-\alpha) \sum_{j=1}^p |\beta_j|^2\right] \end{cases}$$
 where $\lambda > 0$ is the strength of regularization. Linear Regression Models | Segment 5 | Topic 3





 glmnet is a powerful R package for building generalized linear models with regularization



 glmnet is a powerful R package for building generalized linear models with regularization (linear,



 glmnet is a powerful R package for building generalized linear models with regularization (linear, logistic,



• glmnet is a powerful R package for building generalized linear models with regularization (linear, logistic, multinomial etc.)





- glmnet is a powerful R package for building generalized linear models with regularization (linear, logistic, multinomial etc.)
- The glmnet object contains all relevant information of the fitted model for further use.





- glmnet is a powerful R package for building generalized linear models with regularization (linear, logistic, multinomial etc.)
- The glmnet object contains all relevant information of the fitted model for further use.
- Additional methods for visualizing coefficients, prediction on new data, cross validation for selecting optimal regularization strength λ are available.



- glmnet is a powerful R package for building generalized linear models with regularization (linear, logistic, multinomial etc.)
- The glmnet object contains all relevant information of the fitted model for further use.
- Additional methods for visualizing coefficients, prediction on new data, cross validation for selecting optimal regularization strength λ are available.
- It is important to scale the predictors and response variable before running regularized regression using glmnet.





 Both ridge and lasso approaches for regularization shrink the coefficient estimates towards zero but lasso typically yields a much smaller subset of nonzero coefficient estimates.



- Both ridge and lasso approaches for regularization shrink the coefficient estimates towards zero but lasso typically yields a much smaller subset of nonzero coefficient estimates.
- Thus, lasso regularization can be used for feature selection.



- Both ridge and lasso approaches for regularization shrink the coefficient estimates towards zero but lasso typically yields a much smaller subset of nonzero coefficient estimates.
- Thus, lasso regularization can be used for feature selection.
- The drop in the magnitude of the coefficients in lasso regularization is not monotone.



- Both ridge and lasso approaches for regularization shrink the coefficient estimates towards zero but lasso typically yields a much smaller subset of nonzero coefficient estimates.
- Thus, lasso regularization can be used for feature selection.
- The drop in the magnitude of the coefficients in lasso regularization is not monotone.
- By modifying the values of the regularization strength λ increases, we can trade-off the bias and variance of the model:



- Both ridge and lasso approaches for regularization shrink the coefficient estimates towards zero but lasso typically yields a much smaller subset of nonzero coefficient estimates.
- Thus, lasso regularization can be used for feature selection.
- The drop in the magnitude of the coefficients in lasso regularization is not monotone.
- By modifying the values of the regularization strength λ increases, we can trade-off the bias and variance of the model: $\lambda=0\Rightarrow$ low bias, high variance, and



- Both ridge and lasso approaches for regularization shrink the coefficient estimates towards zero but lasso typically yields a much smaller subset of nonzero coefficient estimates.
- Thus, lasso regularization can be used for feature selection.
- The drop in the magnitude of the coefficients in lasso regularization is not monotone.
- By modifying the values of the regularization strength λ increases, we can trade-off the bias and variance of the model: $\lambda=0\Rightarrow$ low bias, high variance, and $\lambda\to\infty\Rightarrow$ high bias, low variance.



- Both ridge and lasso approaches for regularization shrink the coefficient estimates towards zero but lasso typically yields a much smaller subset of nonzero coefficient estimates.
- Thus, lasso regularization can be used for feature selection.
- The drop in the magnitude of the coefficients in lasso regularization is not monotone.
- By modifying the values of the regularization strength λ increases, we can trade-off the bias and variance of the model: $\lambda = 0 \Rightarrow$ low bias. high variance, and $\lambda \to \infty \Rightarrow$ high bias, low variance.
- Ridge regression has a unique OLS solution $\hat{\beta} = (\mathbf{X}^T\mathbf{X} + \lambda \mathbf{I})^{-1}\mathbf{X}^T\mathbf{y}$.



- Both ridge and lasso approaches for regularization shrink the coefficient estimates towards zero but lasso typically yields a much smaller subset of nonzero coefficient estimates.
- Thus, lasso regularization can be used for feature selection.
- The drop in the magnitude of the coefficients in lasso regularization is not monotone.
- By modifying the values of the regularization strength λ increases, we can trade-off the bias and variance of the model: $\lambda=0\Rightarrow$ low bias, high variance, and $\lambda\to\infty\Rightarrow$ high bias, low variance.
- Ridge regression has a unique OLS solution $\hat{\boldsymbol{\beta}} = \left(\mathbf{X}^{\mathrm{T}}\mathbf{X} + \lambda \mathbf{I}\right)^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{y}$.
- Optimal λ for ridge and lasso are typically not the same.

Summary



- Importance of regularization in model building
- Different regularization approaches
- glmnet package