Regularization and Penalized Regression

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Review

Consider the basic linear regression model:

$$Y = w_o + w_1 X_1 + w_2 X_2 + \ldots + w_p X_p + \epsilon$$

We've previously estimated $\mathbf{w}$, the vector of weights, by optimizing the following cost function:

$$\text{Cost} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 = \frac{1}{n}(\mathbf{y} - \mathbf{X}\hat{\mathbf{w}})^T(\mathbf{y} - \mathbf{X}\hat{\mathbf{w}})$$

Regularized Regression

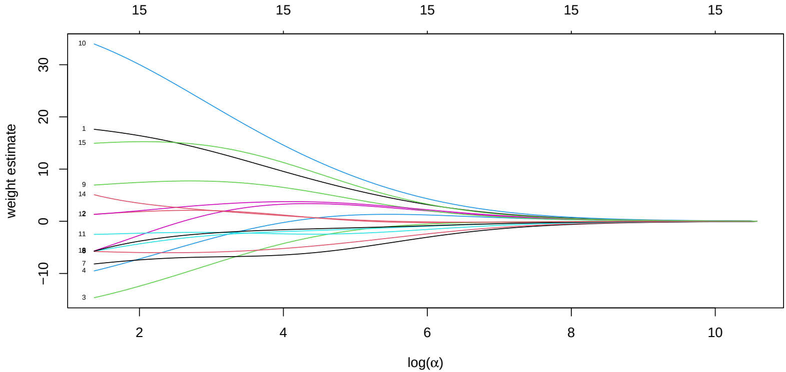
Regularized regression adds a penalty term to the cost function that shrinks weight estimates towards zero:

$$\text{Cost} = \frac{1}{n}(\mathbf{y} - \mathbf{X}\hat{\mathbf{w}})^T(\mathbf{y} - \mathbf{X}\hat{\mathbf{w}}) + P_\alpha(\hat{\mathbf{w}})$$

- $P()$ is a *penalty function* involving α, a **regularization parameter** that controls the trade-off between each term in the cost function

Example

When the regularization parameter, α, is large, the penalty term dominates the cost function and weights are estimated to be zero. When *alpha* is zero, cost function reduces to squared error loss.

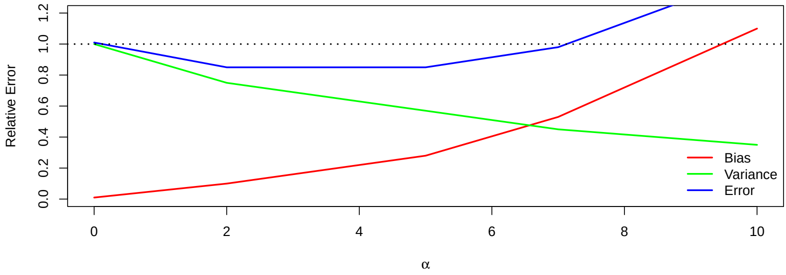


Benefits of Regularization

- Intuitively, the premise behind regularization is that small weights should occur more frequently than large weights when many predictors are considered
  - Thus, using penalization to discourage larger estimated weights can prevent overfitting
- In 1970, Hoerl and Kennard proved that *ridge regression* (a type of regularized regression) can *always* produce a lower out-of-sample *RMSE* than ordinary (unpenalized) regression

Benefits of Regularization

Mathematically, it's possible to decompose mean-squared error (MSE) into bias and variance terms. Here's a heuristic look at how these components might look as α is varied:



Ridge Regression

Ridge regression uses the penalty function: $P_\alpha(\mathbf{w}) = \alpha \sum_{j=1}^{p} w_i^2$

In matrix form, the Ridge regression cost function looks like:

$$\text{Cost} = \frac{1}{n}(\mathbf{y} - \mathbf{X}\hat{\mathbf{w}})^T(\mathbf{y} - \mathbf{X}\hat{\mathbf{w}}) + \alpha \hat{\mathbf{w}}^T \hat{\mathbf{w}}$$

- $\hat{\mathbf{w}}^T \hat{\mathbf{w}}$ is the squared *L2 Norm* of the weight vector (or $||\hat{\mathbf{w}}||_2^2$), so the ridge penalty is often called *L2 regularization*
- The meaning of α is entirely relative, so sometimes you'll see the cost written using $P_\alpha(\mathbf{w}) = \frac{1}{2n}\alpha \sum_{j=1}^{p} w_i^2$

Ridge Regression

Similar to ordinary linear regression, minimizing the ridge regression cost function has a closed-form solution:

$$\hat{\mathbf{w}} = (\mathbf{X}^T\mathbf{X} + \alpha\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y}$$

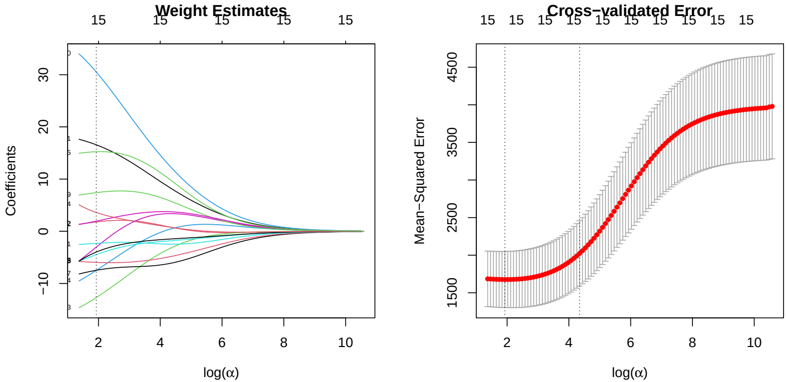
The method gets its name from the “ridge” added to the diagonal of $\mathbf{X}^T\mathbf{X}$ prior to inversion

Choosing α

- In penalized regression, α is a tuning parameter, with different values leading to different weight estimates
  - Larger values of α shrink the weights closer to zero (introducing more bias while reducing variance)
  - When $\alpha = 0$, the ridge regression estimates are the same those of ordinary linear regression
- Because penalization is proportional to the magnitude of w_j, it is important to *standardize* each variable as a pre-processing step when using regularization

Choosing α (example)

Below are results for data that uses pollution and demographic variables of 60 US metro areas to their predict age-adjusted mortality:



Lasso

- The ridge penalty provides *stability* (ie: reduces variance) at the expense of adding *bias*
  - However, it doesn't truly reduce the complexity of the model (the number of non-zero weights is the same, regardless of the amount of penalization)

Lasso

- The ridge penalty provides *stability* (ie: reduces variance) at the expense of adding *bias*
  - However, it doesn't truly reduce the complexity of the model (the number of non-zero weights is the same, regardless of the amount of penalization)
- The lasso (least absolute shrinkage and selection operator) addresses this shortcoming by promoting *sparsity* in the estimated weight vector
  - The lasso penalty function is: $P_\alpha(\mathbf{w}) = \alpha \sum_{j=1}^{p} |w_i|$
- Recognize that the absolute value function is not strictly differentiable at its minimum
  - This promotes weight estimates of exactly zero (sparsity)

Lasso

- To better understand why the lasso penalty promotes sparse weight estimates, we can view minimizing the lasso cost function as a constrained optimization problem
  - That is, the lasso's estimate of $\mathbf{w}$ minimizes $\frac{1}{n}\sum_{i=1}^{n}(y_i - \mathbf{x}_i^T\mathbf{w})^2$ subject to the constraint $\sum_{j=1}^{p}|w_j| < c$ where c describes a fixed amount of penalization (a function of α)
  - For comparison, the ridge estimate is similar but with the constraint $\sum_{j=1}^{p} w_j^2 < c$
- The next slide provides a geometric illustration of why the lasso constraint promotes sparsity, but the ridge constraint does not

Lasso vs. Ridge

Estimates satisfying $\sum_{j=1}^{p} |w_j| < c$ exist within a diamond, while those satisfying $\sum_{j=1}^{p} w_j^2 < c$ exist within an ellipse.

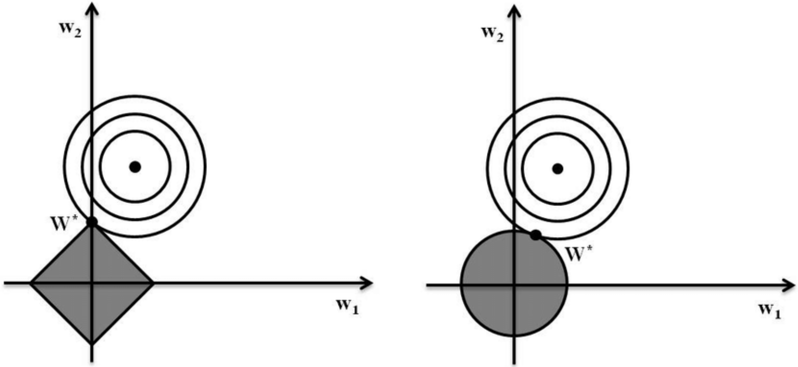
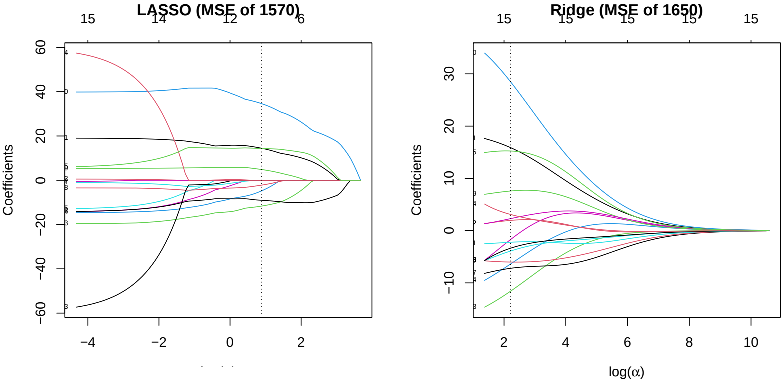


image credit: https://www.researchgate.net/figure/Plot-demonstrating-the-Sparsity-caused-by-the-LASSO-Penalty-The-plot-shows-the_fig1_317357840

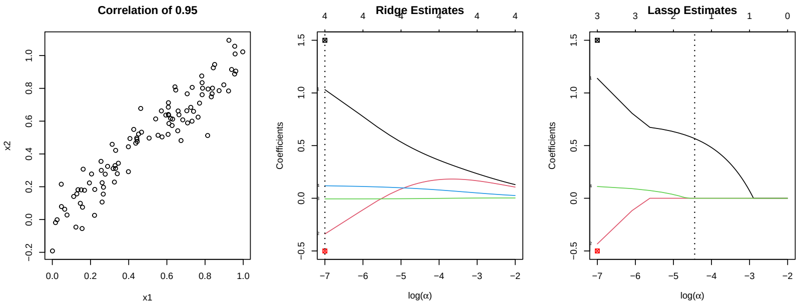
Lasso

For pollution example, lasso achieves a minimum cross-validated mean-squared error of around 1570, while ridge regression's minimum error (shown in an earlier slide) is around 1650 for these data.



Ridge Regression and Multicollinearity

- Consider data where $y_i = 1.5 * x_{i,1} - 0.75 * x_{i,2} + \epsilon$ where X_1 and X_2 have a correlation of 0.95
  - lasso favors a single representative, while ridge will distribute the weight estimates in a more balanced manner:



Final Remarks on Regularization

- L1 (lasso) and L2 (ridge) regularization can be used in many different machine learning models to help balance the bias-variance trade-off
- By default, the implementation of logistic regression in `sklearn` includes L2 regularization to promote stable weight estimates
  - In this regard, regularization can be used to address the "perfect separation" issue that arose in our previous lab