Statistical Machine Learning

Model Selection and Regularization

Three classes of methods

- Subset Selection. We identify a subset of the p predictors that we believe to be related to the response. We then fit a model using least squares on the reduced set of variables.
- Shrinkage. We fit a model involving all p predictors, but the estimated coefficients are shrunken towards zero relative to the least squares estimates. This shrinkage (also known as regularization) has the effect of reducing variance and can also perform variable selection.
- Dimension Reduction. We project the p predictors into a M-dimensional subspace ($M < p$). This is achieved by computing M different linear combinations, or projections, of the variables. Then these M projections are used as predictors to fit a linear regression model by least squares.

Subset Selection

- Best subset and stepwise model selection procedures
    - Best Subset Selection (global optimization)
        - Fit all 2^p models
    - Stepwise Selection (local optimization)
        - A greedy search

Shrinkage Methods

- Ridge regression, Lasso and Elastic net
- The subset selection methods use least squares to fit a linear model that contains a subset of the predictors.
- As an alternative, we can fit a model containing all p predictors using a technique that constrains or regularizes the coefficient estimates, or equivalently, that shrinks the coefficient estimates towards zero.
- It may not be immediately obvious why such a constraint should improve the fit, but it turns out that shrinking the coefficient estimates can significantly reduce their variance.

Ridge regression

- Ridge regression is like least squares but shrinks the estimated coefficients towards zero. Given a response vector y and a predictor matrix X, the ridge regression coefficients are defined as

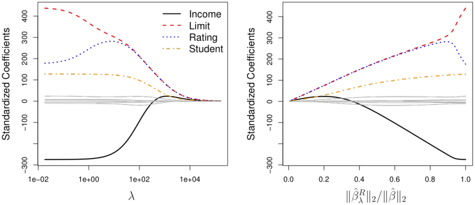
$$\hat{\beta}^{\text{ridge}} = \underset{\beta}{\text{argmin}} \sum_{i=1}^{n} (y_i - \beta_0 - x_{1i}\beta_1 - \ldots)^2 + \lambda \sum_{j=1}^{p} \beta_j^2$$

- Here $\lambda \geq 0$ is a turning parameter, which controls the strength of the penalty term.
- When $\lambda = 0$, we get the linear regression estimate
- WHen $\lambda = \infty$, we get $\hat{\beta}^{\text{ridge}} = 0$
- For λ in between, we are balancing two ideas: fitting a linear model of y on X, and shrinking the coefficients

Ridge regression: continue

- As with least squares, ridge regression seeks coefficient estimates that fit the data well, by making the RSS small.
- However, the second term, $\lambda \sum_{j=1}^{p} \beta_j^2$, called a shrinkage penalty, is small when β's are close to zero, and so it has the effect of shrinking the estimates of β's towards zero.
- The tuning parameter λ serves to control the relative impact of these two terms on the regression coefficient estimates.
- Selecting a good value for λ is critical; cross-validation is used for this.

Credit data example



- In the left-hand panel, each curve corresponds to the ridge regression coefficient estimate for one of the ten variables, plotted as a function of λ
- The right-hand panel displays the same ridge coefficient estimates as the left-hand panel, but instead of displaying λ on the x-axis, we now display

$$\|\hat{\beta}_\lambda^R\|_2/\|\hat{\beta}\|_2$$

- $\|\beta\|_2 = \sqrt{\sum_j \beta_j^2}$ is called the l_2 norm.

Ridge regression: scaling of predictors

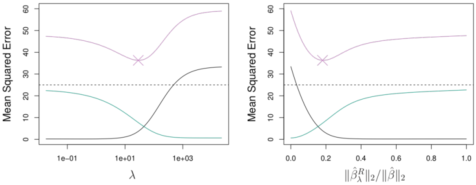
- The standard least squares coefficient estimates are scale equivariant: multipying x by a constant c simply leads to a scaling of the least squares coefficient estimates by a factor of $1/c$. In other words, regardless of how x is scaled, $\hat{\beta}x$ will reamin the same.
- In contrast, the ridge regression coefficient estimates can change substantially when multiplying a given predictor by a constant, due to the sum of squared coefficients term in the penalty part of the ridge regression objective function.
- Therefore, it is best to apply ridge regression after standardizing the predictors, for example,

$$\tilde{x} = x/sd_x$$

which makes sure that the s.d. of $\tilde{x}$ is 1.

Why Does Ridge Regression Improve Over Least Squares?

Simulated data with $n = 50$ observations, $p = 45$ predictors, all having nonzero coefficients. Squared bias (black), variance (green), and test mean squared error (purple) for the ridge regression predictions on a simulated data set, as a function of λ and $\|\hat{\beta}_\lambda^R\|_2/\|\hat{\beta}\|_2$. The horizontal dashed lines indicate the minimum possible MSE. The purple crosses indicate the ridge regression models for which the MSE is smallest



The Lasso

- Ridge regression does have one obvious disadvantage: unlike subset selection, which will generally select models that involve just a subset of the variables, ridge regression will include all p predictors in the final model
- The Lasso is a relatively recent alternative to ridge regression that overcomes this disadvantage. The lasso coefficients, β_λ^L, minimize the quantity

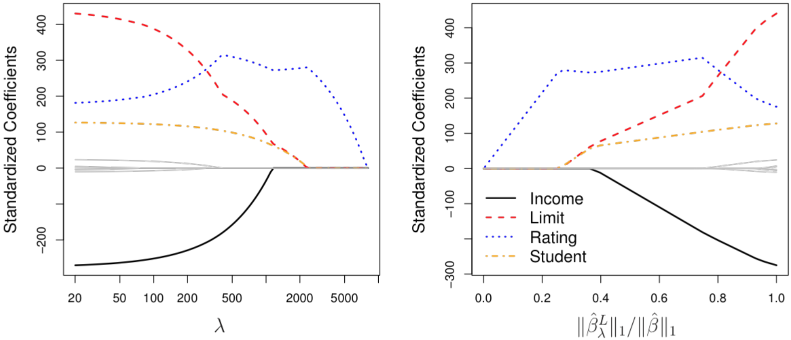
$$\hat{\beta}^{\mathrm{L}} = \underset{\beta}{\operatorname{argmin}} \sum_{i=1}^{n} (y_i - \beta_0 - x_{1i}\beta_1 - \dots)^2 + \lambda \sum_{j=1}^{p} |\beta_j|$$

In statistics language, the lasso uses an l_1 penalty instead of an l_2 penalty.

The Lasso: continued

- As with ridge regression, the lasso shrinks the coefficient estimates towards zero.
- However, in the case of the lasso, the l_1 penalty has the effect of forcing some of the coefficient estimates to be exactly equal to zero when the tuning parameter λ is sufficiently large.
- Hence, much like best subset selection, the lasso performs variable selection.
- We say that the lasso yields sparse models — that is, models that involve only a subset of the variables.
- As in ridge regression, selecting a good value of λ for the lasso is critical; cross-validation is again the method of choice.

Example: Credit dataset



The Variable Selection Property of the Lasso

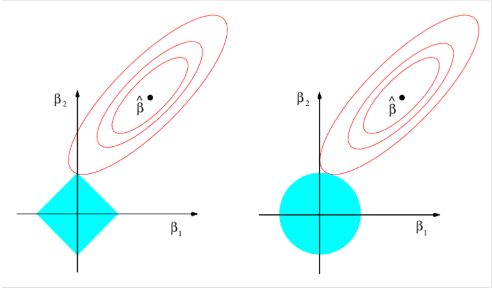
- Why is it that the lasso, unlike ridge regression, results in coefficient estimates that are exactly equal to zero?
- One can show that the lasso and ridge regression coefficient estimates solve the problems

$$\text{minimize} \sum_{i=1}^{n}(y_i - \beta_0 - x_{1i}\beta_1 - \ldots)^2 \quad \text{subject to} \sum_{j=1}^{p}|\beta_j| < s$$

$$\text{minimize} \sum_{i=1}^{n}(y_i - \beta_0 - x_{1i}\beta_1 - \ldots)^2 \quad \text{subject to} \sum_{j=1}^{p}\beta_j^2 < s$$

respectively.

The Variable Selection Property of the Lasso (continue)



Comparing the Lasso and Ridge Regression

- neither ridge regression nor the lasso would universally dominate the other
- In general, one might expect the lasso to perform better when the response is a function of only a relatively small number of predictors.
- However, the number of predictors that is related to the response is never known a priori for real data sets.
- A technique such as cross-validation can be used in order to determine which approach is better on a particular data set.

Elastic Net

- If $p > n$, the lasso selects at most n variables. The number of selected predictors is bounded by the number of samples.
- Grouped variables: the lasso fails to do grouped selection. It tends to select one variable from a group and ignore the others.

Elastic Net regularization

- The Naive Elastic net estimate is defined as

$$\hat{\beta}^{\text{naive}} = \underset{\beta}{\operatorname{argmin}} \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_{1i} - \ldots)^2 + \lambda_2 \sum_{j=1}^{p} \beta_j^2 + \lambda_1 \sum_{j=1}^{p} |\beta_j|$$

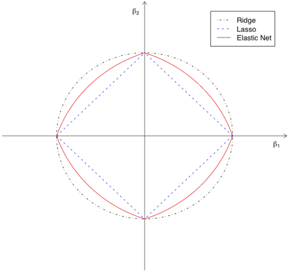
- The l_1 part of the penalty generates a sparse model
- The quadratic part of the penalty
    - Removes the limitation on the number of selected variables
    - Encourages grouping effect
    - Stabilizes the l_1 regularization path
- Rewrite elastic net

$$\hat{\beta}^{\text{naive}} = \underset{\beta}{\operatorname{argmin}} \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_{1i} - \ldots)^2 + \lambda \left[\alpha \sum_{j=1}^{p} \beta_j^2 + (1 - \alpha) \sum_{j=1}^{p} |\beta_j| \right]$$

Geometry of the elastic net

- The elastic net penalty: $\alpha \sum_{j=1}^{p} \beta_j^2 + (1-\alpha) \sum_{j=1}^{p} |\beta_j|$
- Singularities at the vertexes (necessary for sparsity)
- Strict convex edges. The strength of convexity varies with α (grouping)

2-dimensional illustration $\alpha = 0.5$



A simple illustration: elastic net vs. lasso

- Two independent 'hidden' factors z_1 and z_2

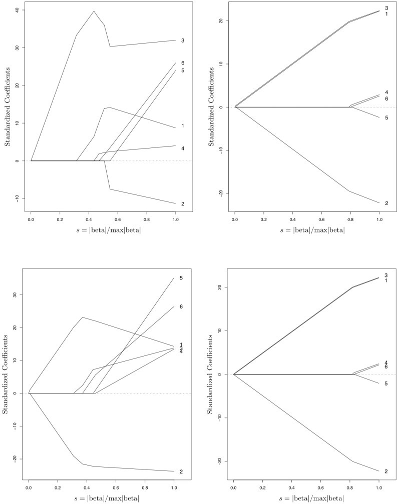
$$z_1 \sim U(0,20), \quad z_2 \sim U(0,20)$$

- Generate the response vector $y = z_1 + 0.1 \times z_2 + \varepsilon$, $\varepsilon \sim N(0,1)$
- Suppose only observe predictors

$$x_1 = z_1 + \varepsilon_1, \quad x_2 = -z_1 + \varepsilon_2, \quad x_3 = z_1 + \varepsilon_3$$
$$x_4 = z_2 + \varepsilon_4, \quad x_5 = -z_2 + \varepsilon_5, \quad x_6 = z_2 + \varepsilon_6$$

- Fit y on $x_1, \ldots, x_6$
- An 'oracle' would identify x_1, x_2 and x_3 (the z_1 group) as the most important variables.

A simple illustration: elastic net vs. lasso (cont)



Left: Lasso; Right: Elastic Net with $\alpha = 0.5$

Deficiency of the 'naive' elastic net

- Empirical evidence shows the naive elastic net does not perform satisfactorily unless it is very close to either ridge or the lasso $\alpha = 0$ or $\alpha = 1$
- The naive elastic net estimator is a two-stage procedure: for each fixed λ_2 we first find the ridge regression coefficients, and then we do the lasso type shrinkage along the lasso coefficient solution paths.
- the coefficients are doubly penalized
- $$\hat{\beta}^{\mathrm{enet}} = (1 + \lambda_2)\hat{\beta}^{\mathrm{naive}}$$

Dimension Reduction Methods

- The methods that we have discussed so far in this chapter have involved fitting linear regression models, via least squares or a shrunken approach, using the original predictors
- We now explore a class of approaches that transform the predictors and then fit a least squares model using the transformed variables. We will refer to these techniques as dimension reduction methods.

Dimension Reduction Methods: details

- Let $Z_1, Z_2, \ldots, Z_M$ represent $M < p$ linear combinations of our original p predictors. That is,

$$Z_m = \sum_{j=1}^{p} \phi_{mj} X_j$$

for some constants $\phi_{m1}, \ldots, \phi_{mp}$

- We can then fit the linear regression model,

$$y_i = \theta_0 + \sum_{m=1}^{M} \theta_m z_{im} + \varepsilon, \quad i = 1, \ldots, n$$

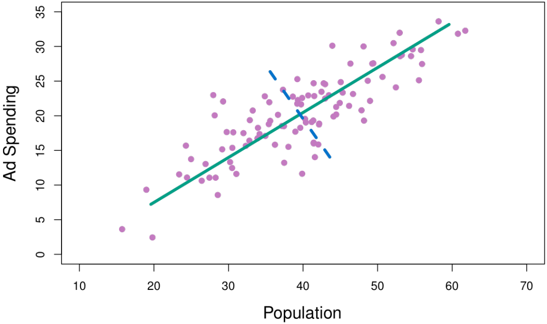
  using ordinary least squares.

- If the constants $\phi_{m1}, \ldots, \phi_{mp}$ are chosen wisely, then such dimension reduction approaches can often outperform OLS regression

Principal Components Regression

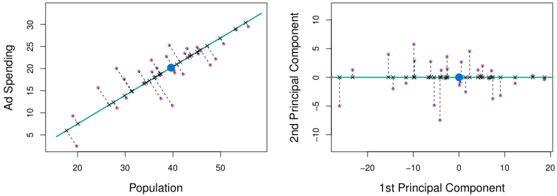
- The first principal component is that (normalized) linear combination of the variables with the largest variance.
- The second principal component has largest variance, subject to being uncorrelated with the first.
- And so on
- Hence with many correlated original variables, we replace them with a small set of principal components that capture their joint variation.

Pictures of PCA



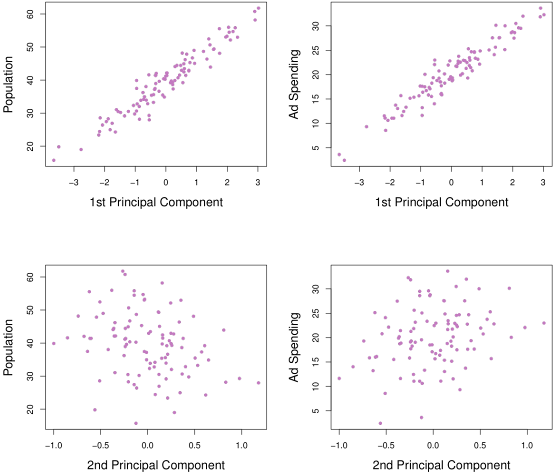
The population size (pop) and ad spending (ad) for 100 different cities are shown as purple circles. The green solid line indicates the first principal component, and the blue dashed line indicates the second principal component.

Pictures of PCA: continued

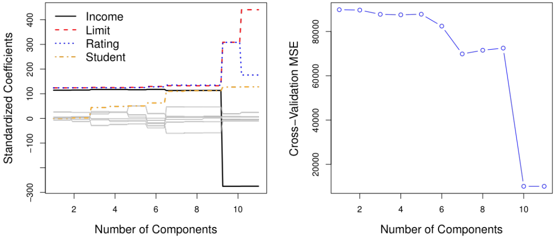


A subset of the advertising data. Left: The first principal component, chosen to minimize the sum of the squared perpendicular distances to each point, is shown in green. These distances are represented using the black dashed line segments. Right: The left-hand panel has been rotated so that the first principal component lies on the x-axis.

Pictures of PCA: continued



Choosing the number of directions M



Left: PCR standardized coefficient estimates on the Credit data set for different values of M. Right: The 10-fold cross validation MSE obtained using PCR, as a function of M.

Partial Least Squares

- PCR identifies linear combinations, or directions, that best represent the predictors $X_1, \ldots, X_p$
- These directions are identified in an unsupervised way, since the response Y is not used to help determine the principal component directions.
- That is, the response does not supervise the identification of the principal components.
- Consequently, PCR suffers from a potentially serious drawback: there is no guarantee that the directions that best explain the predictors will also be the best directions to use for predicting the respons

Partial Least Squares: continued

- Like PCR, PLS is a dimension reduction method, which first identifies a new set of features $Z_1, \ldots, Z_M$ that are linear combinations of the original features, and then fits a linear model via OLS using these M new features.
- But unlike PCR, PLS identifies these new features in a supervised way – that is, it makes use of the response Y in order to identify new features that not only approximate the old features well, but also that are related to the response.
- Roughly speaking, the PLS approach attempts to find directions that help explain both the response and the predictors.

Details of Partial Least Squares

- After standardizing the p predictors, PLS computes the first direction Z_1 by setting each ϕ_{1j} equal to the coefficient from the simple linear regression of Y onto X_j.
- One can show that this coefficient is proportional to the correlation between Y and X_j.
- Hence, in computing $Z_1 = \sum_{j=1}^{p} \phi_{1j} X_j$, PLS places the highest weight on the variables that are most strongly related to the response.
- Subsequent directions are found by taking residuals and then repeating the above prescription.