Model Selection & Regularization

Lecture 7

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Recall: Linear Models and Least Squares

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p + \epsilon$$

$$\text{RSS} = \sum_{i=1}^{n} (y_i - \hat{\beta}_0 - \sum_{j=1}^{p} \hat{\beta}_{j_1} x_{ij})^2$$

Model with all available predictor variables is commonly referred to as **the full model**

Issues:

- predictive accuracy
- model interpretability

Solutions:

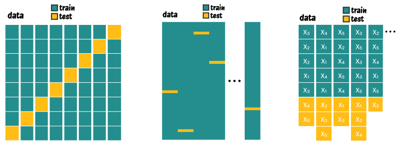
- select subset of predictors
- consider extension to the least squares solution of full model

Part I - Variable Subset Selection

Model Selection Criteria: Validation by Prediction Error

Last week: how to use cross validation to choose a set of predictors
by directly estimate prediction error using cross-validation techniques

e.g. $\text{MSE} = \frac{\text{RSS}}{n}$ $\quad \text{RMSE} = \sqrt{\frac{\text{RSS}}{n}}$ $\quad R^2 = 1 - \frac{\text{RSS}}{\text{TSS}}$



Now: indirectly estimating test performance using an approximation

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Model Selection Criteria

Four ways to estimate test performance using an approximation

Full model has p predictors
RSS is the residual sum of squares for model with d predictors
$\hat{\sigma}^2 = \text{RSS}_p/(n-p-1)$ is an estimate of the error variance for full model

1. Mallow's C_p criterion:

For a given model with d (out of the p available) predictors

$$C_p = \frac{1}{n}\left(\text{RSS} + 2d\hat{\sigma}^2\right)$$

we are penalizing models of higher dimensionality (larger d, greater penalty)
$\implies$ choose the model which has **minimum** C_p

Model Selection Criteria

Four ways to estimate test performance using an approximation

Full model has p predictors
RSS is the residual sum of squares for model with d predictors
$\hat{\sigma}^2 = \text{RSS}_p/(n-p-1)$ is an estimate of the error variance for full model

2. Akaike Information Criterion (AIC)

For linear models: equivalent to Mallow's C_p (proportional to)

$$AIC = \frac{1}{n\hat{\sigma}^2}\left(\text{RSS} + 2d\hat{\sigma}^2\right)$$

we are penalizing models of higher dimensionality (larger d, greater penalty)
$\implies$ choose the model which has **minimum** AIC

Model Selection Criteria

Four ways to estimate test performance using an approximation

Full model has p predictors

RSS is the residual sum of squares for model with d predictors

$\hat{\sigma}^2 = \text{RSS}_p/(n-p-1)$ is an estimate of the error variance for full model

3. Bayesian Information Criterion (BIC)

$$BIC = \frac{1}{n\hat{\sigma}^2}\left(\text{RSS} + \underbrace{\log(n)}_{\textit{heavier penalty}} d\hat{\sigma}^2\right)$$

we are penalizing models of higher dimensionality (larger d, greater penalty)

$\implies$ choose the model which has **minimum** BIC

Model Selection Criteria

Four ways to estimate test performance using an approximation

Full model has p predictors

RSS is the residual sum of squares for model with d predictors

$\hat{\sigma}^2 = \text{RSS}_p/(n-p-1)$ is an estimate of the error variance for full model

4. Adjusted R-squared value

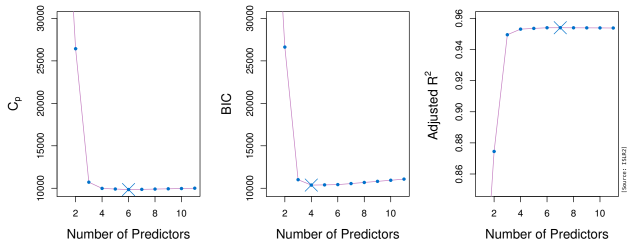
Adjust the regular R^2 by taking into account number of predictors

$$\text{Adjusted-}R^2 = 1 - \frac{\text{RSS}/(n-d-1)}{\text{TSS}/(n-1)}$$

$\implies$ choose the model which has **maximum** Adjusted-R^2

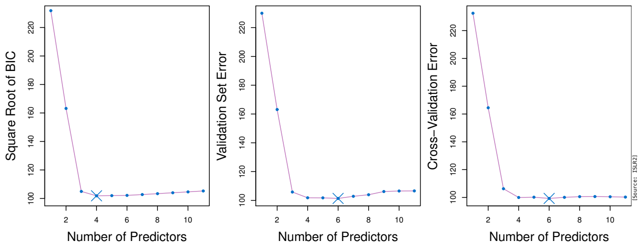
Model Selection Criteria

Four ways to estimate test performance using an approximation



Model Selection Criteria

...and compared to cross validation



Model Search Methods

Best Subset Selection

1. Let M_0 denote null model which contains no predictors. This model simply predicts the response for each observation.
2. For $k = 1, 2, \ldots, p$
   - Fit all $\binom{p}{k}$ models that contain exactly p predictors
   - Pick the best among these $\binom{p}{k}$ models and call it M_k.

     Here, *best* is defined as having the smallest RSS or largest R^2
3. Select a single best model from among $M_0, M_1, \ldots, M_p$ using cross validated prediction error, C_p (AIC), BIC, or Adjusted-R^2

requires training 2^p models

Example

$p = 3$

M_0 : intercept only (null)

C_1: X_1 X_2 X_3

lowest training RSS within C_1 $\Longrightarrow M_1$

C_2: X_1, X_2 X_1, X_3 X_2, X_3

lowest training RSS within C_2 $\Longrightarrow M_2$

M_3 : full model with X_1 X_2 X_3

Model Search Methods

Forward Stepwise Selection

1. Let M_0 denote null model which contains no predictors.
2. For $k = 1, 2, \ldots, p - 1$
   - Consider all $p - k$ models that augment the predictors in M_k with one additional predictor
   - Choose the best among these $p - k$ models and call it M_{k+1}. Here, *best* is defined as having the smallest RSS or largest R^2
3. Select a single best model from among $M_0, M_1, \ldots, M_p$ using cross validated prediction error, C_p (AIC), BIC, or Adjusted-R^2

requires training $1 + \dfrac{p(p+1)}{2}$ models

Example

$p = 3$

M_0 : intercept only (null)

C_1: X_1 X_2 X_3

lowest training RSS within C_1 $\Longrightarrow M_1$

C_2: X_1, X_2 X_2, X_3

lowest training RSS within C_2 $\Longrightarrow M_2$

M_3 : full model with X_1 X_2 X_3

Model Search Methods

Backward Stepwise Selection

1. Let M_p denote full model which all predictors.
2. For $k = p,\ p-1,\ p-2, \ldots, 1$
   - Consider all k models that contain all but one of the predictors in M_k , for a total of $k-1$ predictors
   - Choose the best among these k models and call it M_{k-1}. Here, *best* is defined as having the smallest RSS or largest R^2
3. Select a single best model from among $M_0, M_1, \ldots, M_p$ using cross validated prediction error, C_p (AIC), BIC, or Adjusted-R^2

requires training $1 + \dfrac{p(p+1)}{2}$ models

Example

$p = 3$

M_3 : full mode X_1 X_2 X_3

C_2: X_1, X_2 X_1, X_3 X_2, X_3

lowest training RSS within C_1 $\Longrightarrow M_2$

C_1: X_1 X_2

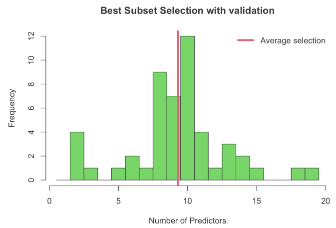
lowest training RSS within C_2 $\Longrightarrow M_1$

M_0 : intercept only (null)

Model Search Methods

Best Subset Selection

validation approach based on 50 different seeds and storing number of predictors in selected model each time



[plot is made based on the 'hitters' data se used in this week's practical in ISLR2]

Part II - Shrinkage

Shrinkage Methods

Before: **Discrete model search methods**

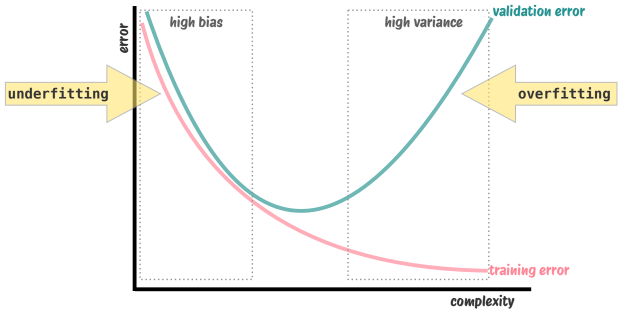
$$\underbrace{\text{model fit}}_{\text{RSS}} + \text{penalty on model dimensionality}$$

Now: **Continuous model search method** (also faster)

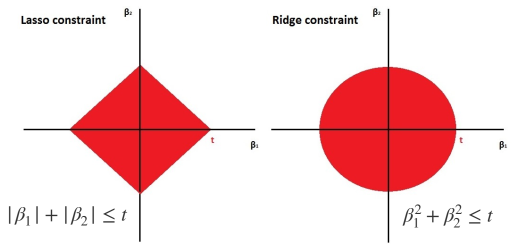
$$\underbrace{\text{model fit}}_{\text{RSS}} + \text{penalty on size of coefficients}$$

this is called **penalized** or **regularized regression**

Bias Variance Trade-Off



Ridge and Lasso Regression: The Constraints



Ridge Regression

Least Squares produces estimates by minimizing

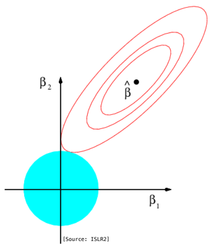
$$\text{RSS} = \sum_{i=1}^{n} (y_i - \hat{\beta}_0 - \sum_{j-1}^{p} \hat{\beta}_{j_1} x_{ij})^2$$

Ridge regression instead minimizes

$$\underbrace{\sum_{i=1}^{n} (y_i - \hat{\beta}_0 - \sum_{j-1}^{p} \hat{\beta}_{j_1} x_{ij})^2}_{\text{model fit}} + \underbrace{\lambda \sum_{j=1}^{p} \beta_j^2}_{\text{penalty}} = \text{RSS} + \lambda \sum_{j=1}^{p} \beta_j^2$$

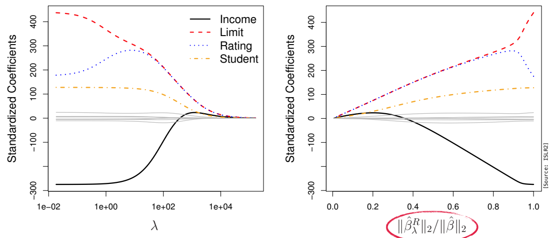
where $\lambda \geq 0$ is the tuning parameter controlling trade off between model fit and size of coefficients ($\lambda \to \infty, \hat{\beta}_j \to 0$)

ridge uses ℓ_2 penalty



Ridge Regression

Regularization Paths

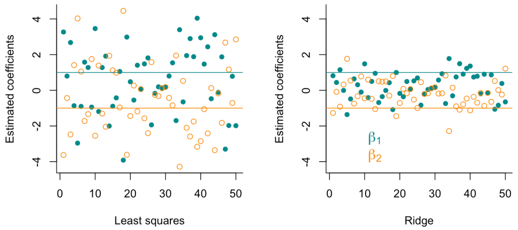


$\|\hat{\beta}_\lambda^R\|_2 / \|\hat{\beta}\|_2$

ℓ_2 norm $= \|\beta\|_2 = \sqrt{\sum_{j=1}^{p} \beta_j^2}$

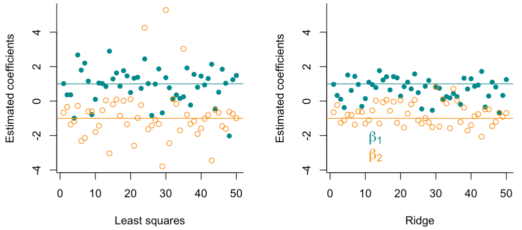
Ridge Regression

Advantage 1: Multicollinearity (a simulation study)



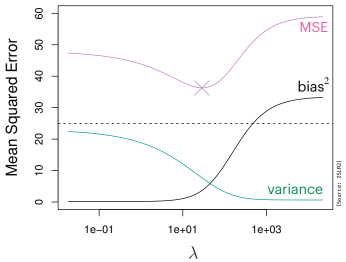
Ridge Regression

Advantage 2: When p is close to n (a simulation study)



Ridge Regression

Bias-Variance Trade Off



Lasso Regression

Least Absolute Shrinkage and Selection Operator

Least Squares produces estimates by minimizing

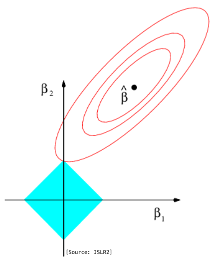
$$\text{RSS} = \sum_{i=1}^{n} (y_i - \hat{\beta}_0 - \sum_{j-1}^{p} \hat{\beta}_{j_1} x_{ij})^2$$

Lasso regression instead minimizes

$$\underbrace{\sum_{i=1}^{n} (y_i - \hat{\beta}_0 - \sum_{j-1}^{p} \hat{\beta}_{j_1} x_{ij})^2}_{\text{model fit}} + \lambda \underbrace{\sum_{j=1}^{p} |\beta_j|}_{\text{penalty}} = \text{RSS} + \lambda \sum_{j=1}^{p} |\beta_j|$$

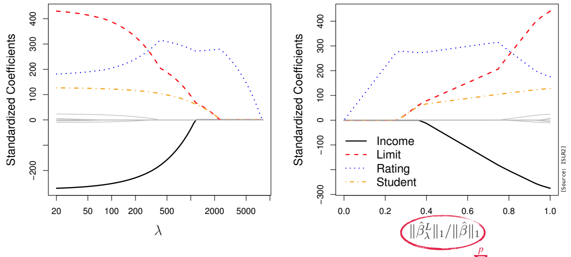
where $\lambda \geq 0$ is the tuning parameter controlling trade off between model fit and size of coefficients ($\lambda \to \infty$, $\hat{\beta}_j = 0$)

lasso uses ℓ_1 penalty



Lasso Regression

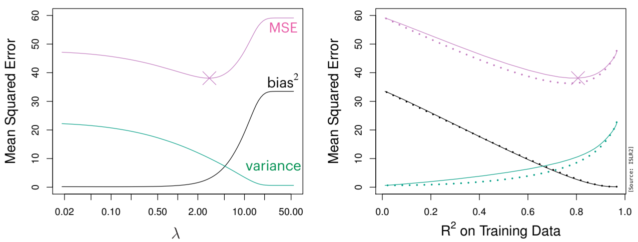
Regularization Paths



ℓ_1 norm $= \|\beta\|_1 = \sum_{j=1}^{p} |\beta_j|$

Lasso Regression

Bias-Variance Trade Off



Ridge vs. Lasso Regression

- Both ridge and lasso are convex optimization
- The ridge solution exists in closed form
- Lasso does not have closed form solution, but very efficient optimization algorithms exist

When to choose which?

- When the actual data-generating mechanism is **sparse** lasso has the advantage
- When the actual data-generating mechanism is **dense** ridge has the advantage

Sparse mechanisms: Few predictors are relevant to the response → good setting for lasso regression
Dense mechanisms: A lot of predictors are relevant to the response → good setting for ridge regression

- Also depends on:
  - Signal strength (the magnitude of the effects of the relevant variables)
  - The correlation structure among predictors
  - Sample size n vs. number of predictors p

Ridge vs. Lasso Regression

Ridge

+ Reduces Multicollinearity
+ Continuous Shrinking
+ Stable Solutions
+ Computationally Efficient

- No variable selection
- Interpretability
- Sensitive to scale

Lasso

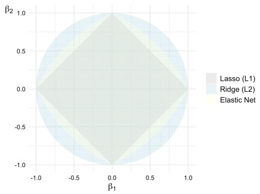
+ Variable selection
+ Sparse models
+ Improves interpretability
+ Particularly useful for when $p > n$

- Collinearity issues
- Bias in coefficients (ℓ_1 penalty is harsher)
- Computationally intensive

λ Tuning

- *K*-fold Cross Validation
  1. Choose the number of folds *K*
  2. Split the data accordingly into training and testing sets.
  3. Define a grid of values for λ
  4. For each λ, calculate the validation MSE within each fold
  5. For each λ, calculate the overall cross-validation MSE
  6. Locate under which λ cross-validation MSE is minimized, i.e. minimum_cv λ
- Packages such as will `glmnet` do this automatically

Hybrid Approach: Elastic Nets



$$\text{RSS} + \underbrace{\lambda_1 \sum_{j=1}^{p} \beta_j^2}_{\text{“ridge”}} + \underbrace{\lambda_2 \sum_{j=1}^{p} |\beta_j|}_{\text{“lasso”}}$$

λ_1 and λ_2 are regularization parameters controlling the strength of the penalties

- Helps stabilize the solution when predictors are correlated
- Shrinks some coefficients to zero, enabling feature selection
- Particularly useful for high-dimensional datasets with correlated predictors

Part III- Dimensionality Reduction

another strategy which aims to reduce dimensionality before applying LS

create q transformed variables which are linear combinations of the original predictors ($q < p$)

we return to this during our PCA lecture…

Part IV- Transformations: next week!

extensions to the regression model when the best straight line doesn't quite work!

This Week's Practical

Hands on discrete and continuous model search!