Lecture 11: Model and Variable Selection

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Training versus Test Performance

Given $n \times p$ matrix X and response Y, we obtain a fitted model:

$$\hat{Y} = \hat{f}_{X,Y}(X).$$

For example, in the linear regression models we have been studying,

$$\hat{f}_{X,Y}(X) = X\hat{\beta}_{X,Y} = X(X'X)^{-1}X'Y.$$

The predicted values for Y are based on regression parameters that were fit using X, Y.

How would the model perform on unseen data?

$$EPE \equiv E[Y_{\text{new}} - \hat{Y}_{\text{new}}]^2 \quad ?$$

The expectation is taken over everything that is random:

$$X, Y, X_{\text{new}}, Y_{\text{new}}.$$

Good training performance does not imply good test performance.

Bias-Variance Trade-off

X, Y used to fit the model are called “training data”, and “unseen” data used to estimate prediction error are called '“test data”.

$$\text{Truth:} \quad y = f(x) + \epsilon, \quad Var(\epsilon) = \sigma^2.$$

$$\text{Estimate } f(\cdot) \text{ using } \hat{f}_{X,Y}.$$

$$\begin{aligned}
EPE &\equiv E[Y_{\text{new}} - \hat{Y}_{\text{new}}]^2 \\
&= E[Y_{\text{new}} - \hat{f}_{X,Y}(X_{\text{new}})]^2 \\
&= E[(Y_{\text{new}} - f(X_{\text{new}})) + (f(X_{\text{new}}) - E\hat{f}_{X,Y}(X_{\text{new}})) + (E\hat{f}_{X,Y}(X_{\text{new}}) - \hat{f}_{X,Y}(X_{\text{new}}))]^2 \\
&= E[Y_{\text{new}} - f(X_{\text{new}})]^2 + E[f(X_{\text{new}}) - E\hat{f}_{X,Y}(X_{\text{new}})]^2 \\
&\quad + E[E\hat{f}_{X,Y}(X_{\text{new}}) - \hat{f}_{X,Y}(X_{\text{new}})]^2 \\
&= \sigma^2 + (\text{Model bias})^2 + \text{Model variance}
\end{aligned}$$

As model complexity increases, bias *decreases* while variance *increases*. How to achieve a balance?

Bias-Variance Trade-off

If you care more about $\hat{\beta}$:

$$\begin{aligned} MSE \equiv E[\beta - \hat{\beta}]^2 &= [E(\hat{\beta}) - \beta]^2 + E[\hat{\beta} - E(\hat{\beta})]^2 \\ &= Bias(\hat{\beta})^2 + Var(\hat{\beta}). \end{aligned}$$

For linear regression, assuming that you've got the correct model, the least squares estimates had 0 bias:

$$E[\hat{\beta}] = \beta,$$

so

$$MSE = Var(\hat{\beta}).$$

In a multiple regression, for any $\hat{\beta}_i$:

$$MSE(\hat{\beta}_i) = Var(\hat{\beta}_i) = \frac{\sigma^2}{\|r_{i,\ i}\|^2},$$

where $r_{i,\ i}$ are the residuals of regression X_i on all other predictors.

Estimating the prediction error

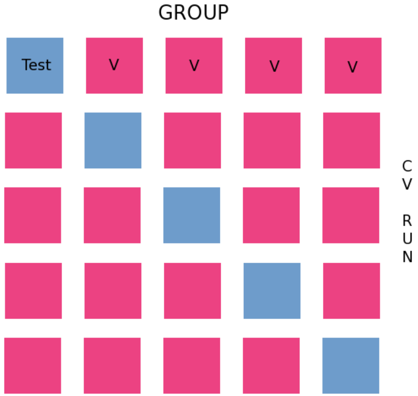
1. Asymptotic approximations
    - Mallows C_p:
      $$C_p = SSE + 2p\hat{\sigma}^2,$$
      where p is the number of predictors. This is an unbiased estimate for EPE.
    - Akaike's Information Criterion:
      $$AIC = -2loglik + 2p.$$
      Reduces to C_p for linear models. Will be useful later for non-linear models.
2. Cross-validation (next slide)

Select the model that *minimizes* the C_p or AIC.

The BIC is another useful model selection criterion, but is *not* based on prediction error (more later).

Cross-Validation

Idea: Use a part of the data for training, the other part for testing.



More on the C_p

$$C_p = SSE + 2p\hat{\sigma}^2.$$

Sometimes also written as:

$$C_p = SSE + 2p\hat{\sigma}^2 - n\hat{\sigma}^2,$$

but the last term doesn't change across models.

1. $\hat{\sigma}^2$ is usually estimated from the largest model.
2. Usual practice: plot C_p versus p, choose model with minimum.

Bayes Information Criterion

Asymptotic approximation for

$$-2\log P(\text{Model}|\text{Data}) \propto -2\log\left\{P(\text{Model})\int_{\theta\in\Theta} P(\text{Data}|\theta)f(\theta)d\theta\right\}$$

$$\text{BIC} = -2l(\hat{\theta}) + p\log n,$$

where

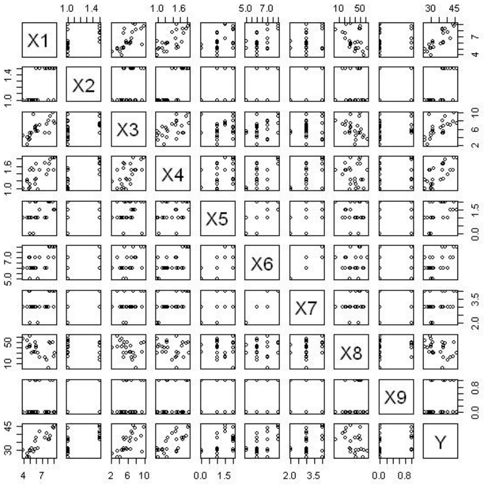
- $l(\cdot)$ is the log likelihood function. For linear regressions assuming Gaussian errors,

$$BIC \approx SSE/\hat{\sigma}^2 + p\log n.$$

- $\hat{\theta}$ is the likelihood maximizing value, for linear regressions this is the least squares estimate.
- p is the number of parameters in the model.

Pick the model that minimizes the BIC.

Exploring the model space



Property values data:

Y: Sales price
X_1: Local taxes
X_2: # bathrooms
X_3: Lot size
X_4: Living space
X_5: Garage
X_6: # rooms
X_7: # bedrooms
X_8: Property age
X_9: # fireplaces

$2^9 = 512$ possible models!

Exploring the model space

1. Forward selection:
    1. Start with null model.
    2. Repeat: add variable with the most significant F-test.
    3. End when no variable has F-test p-value < α.
2. Backward elimination:
    1. Start with full model.
    2. Repeat: delete variable with the least significant F-test.
    3. End when all variables have F-test p-value < α.
3. Forward + Backward: Same as forward procedure, with option of deleting a variable at each step.
4. All subsets: possible when number of possible predictors is small ($<$ 20).

Model Shrinkage Methods

1. Bias variance trade off:

$$EPE = \sigma^2 + (\text{Model bias})^2 + \text{Model variance}$$

$$MSE \equiv E[\beta - \hat{\beta}]^2 = Bias(\hat{\beta}) + Var(\hat{\beta}).$$

2. Mallows C_p statistic:

$$C_p = SSE + 2p\hat{\sigma}^2.$$

   The second term is a “penalty” for model size.

3. Today: penalties based on $\hat{\beta}$.
   1. Ridge regression
   2. LASSO

Ridge Regression

Ridge was developed first. It is based on the idea of constrained minimization:

$$\text{Minimize:} \quad \sum_{i=1}^{n} \left(Y_i - \beta_0 - \sum_{j=1}^{p} X_{ij}\beta_j \right)^2$$

$$\text{Subject to:} \quad \sum_{j=1}^{p} \beta_j^2 < C.$$

By the Lagrange multiplier method, this is equivalent to:

$$\text{Minimize:} \quad \sum_{i=1}^{n} \left(Y_i - \beta_0 - \sum_{j=1}^{p} X_{ij}\beta_j \right)^2 + \lambda_C \sum_{j=1}^{p} \beta_j^2.$$

The second term is a penalty that depends on $\|\beta\|^2$.

Ridge Regression

Ridge regression:

$$\text{Minimize:} \quad \sum_{i=1}^{n} \left(Y_i - \beta_0 - \sum_{j=1}^{p} X_{ij}\beta_j \right)^2 + \lambda \sum_{j=1}^{p} \beta_j^2.$$

1. In statistics this is also called "shrinkage": you are shrinking $\|\beta\|^2$ towards 0.
2. λ is a shrinkage parameter that you have to choose.
3. The Ridge solution $\hat{\beta}_{\text{ridge}}$ is easy to solve, because the above is still a quadratic function in β.

Ridge Solutions

Ridge loss function:

$$f(\beta) = \sum_{i=1}^{n} \left(Y_i - \beta_0 - \sum_{j=1}^{p} X_{ij}\beta_j \right)^2 + \lambda \sum_{j=1}^{p} \beta_j^2.$$

In matrix notation:

$$\begin{aligned} f(\beta) &= (Y - X\beta)'(Y - X\beta) + \lambda\beta'\beta \\ &= \beta'[X'X + \lambda I]\beta - \beta'X'Y - Y'X\beta + Y'Y \end{aligned}$$

Solving $f'(\beta) = 0$ gives you:

$$\hat{\beta}_{\text{ridge}} = (X'X + \lambda I)^{-1} X'Y.$$

Ridge Solutions

1. Whereas the least squares solutions $\hat{\beta} = (X'X)^{-1}X'Y$ are unbiased if model is correctly specified, ridge solutions are *biased*

$$E[\hat{\beta}_{\text{ridge}}] \neq \beta.$$

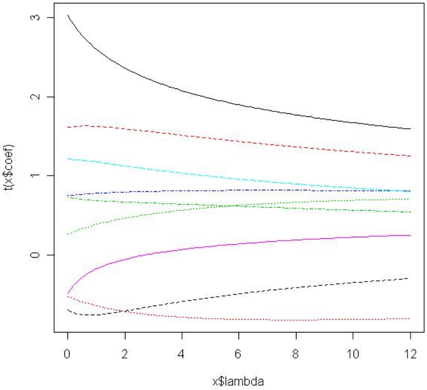
2. However, at the cost of bias, Ridge reduces the variance, and thus might reduce MSE.

$$MSE = Bias^2 + Variance$$

3. Ridge solutions are hard to interpret, because it is not sparse.

Sparse: some β_j's are set exactly to 0.

Ridge solutions versus lambda



L_1 penaties

What if we constrain the L_1 norm instead of the Euclidean norm?

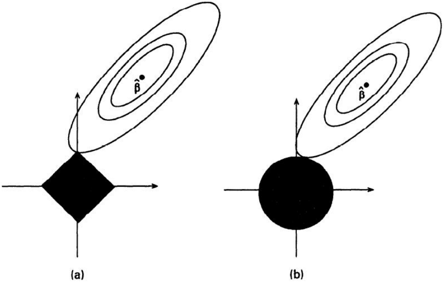
$$\text{Minimize:} \quad \sum_{i=1}^{n} \left(Y_i - \beta_0 - \sum_{j=1}^{p} X_{ij}\beta_j \right)^2$$

$$\text{Subject to:} \quad \sum_{j=1}^{p} |\beta_j| < C.$$

This is a subtle, but important change.

$$\text{Minimize:} \quad \sum_{i=1}^{n} \left(Y_i - \beta_0 - \sum_{j=1}^{p} X_{ij}\beta_j \right)^2 + \lambda_C \sum_{j=1}^{p} |\beta_j|.$$

The above is termed Lasso regression (Tibshirani, 1996).



Comparing Lasso and Ridge, from Tibshirani (1996).

Lasso

Lasso loss function is no longer quadratic, but is still convex:

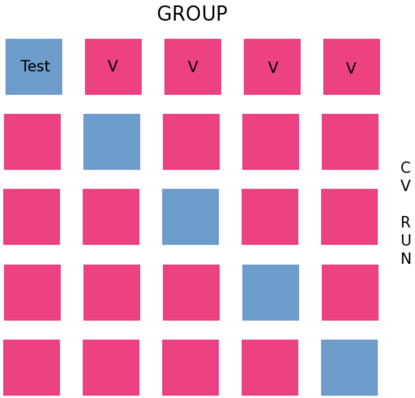
$$\text{Minimize:} \quad \sum_{i=1}^{n} \left(Y_i - \beta_0 - \sum_{j=1}^{p} X_{ij}\beta_j \right)^2 + \lambda \sum_{j=1}^{p} |\beta_j|.$$

1. Unlike Ridge, there is no analytic solution for the LASSO.
2. Efron et al. (2002) gave an efficient algorithm `lars` to solve the Lasso.
3. Lasso solutions are sparse.

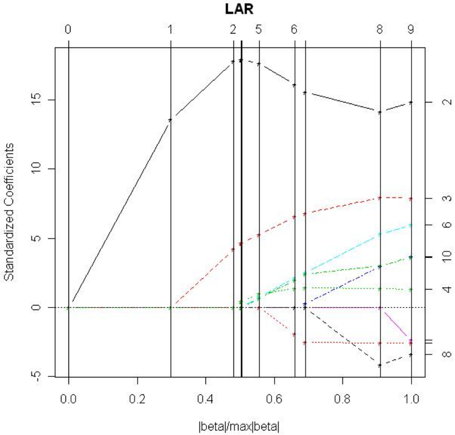
Selecting the shrinkage parameter λ

λ can be selected based on any of the model selection criterions we have discussed.

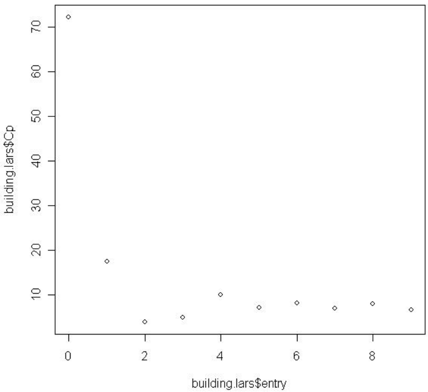
1. C_p included in the output of `lars`.
2. Cross-validation (`cv.lars`).



Lars output


LAR
0
1
2
5
6
8
9
Standardized Coefficients
-5
0
5
10
15
0.0
0.2
0.4
0.6
0.8
1.0
|beta|/max|beta|
2
3
6
10
4
8

Lars C_p



building.lars$Cp
70
60
50
40
30
20
10
0
2
4
6
8
building.lars$entry

Lars cross validation prediction error