Lecture 12: Ridge Regression, LARS, Logistic Regression

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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*

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

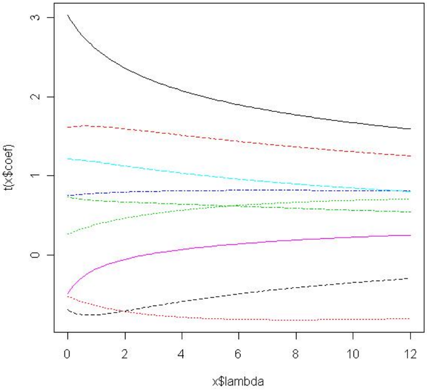
2. However, at the cost of bias, Ridge reduces the variance, and thus might reduce MSE.

$$MSE = Bias^2 + Variance$$

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?

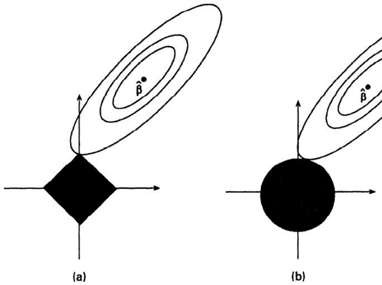
$$\text{Minimize:} \quad \sum_{i=1}^{n} \left(Y_i - \beta_0 - \sum_{j=1}^{p} X_{ij}\beta_j \right)^2$$

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

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:

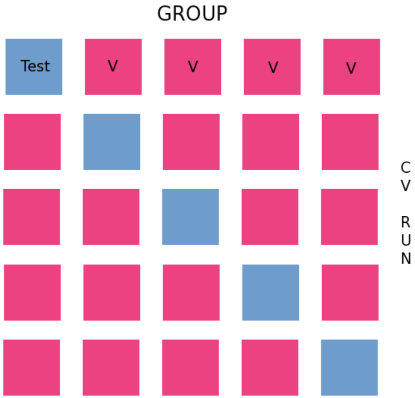
$$\text{Minimize:} \quad \sum_{i=1}^{n} \left(Y_i - \beta_0 - \sum_{j=1}^{p} X_{ij}\beta_j \right)^2 + \lambda \sum_{j=1}^{p} |\beta_j|.$$

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.

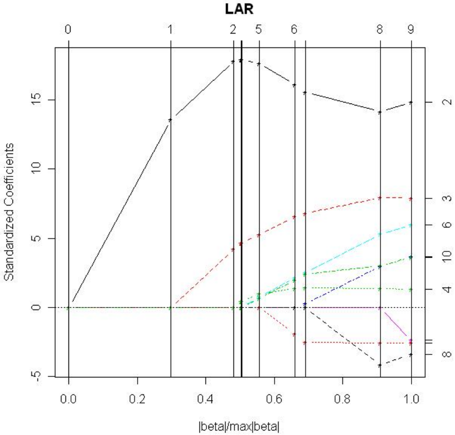
Selecting the shrinkage parameter λ

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`).

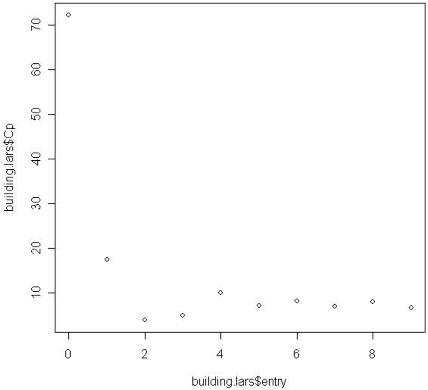


Lars output



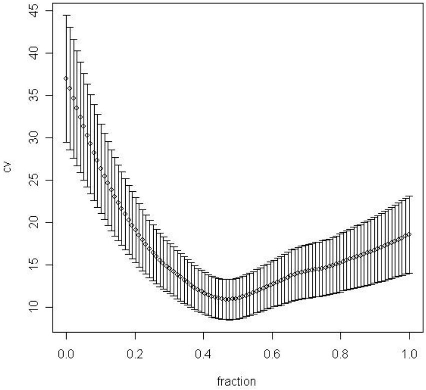
LAR
0
1
2
5
6
8
9
Standardized Coefficients
15
10
5
0
-5
0.0
0.2
0.4
0.6
0.8
1.0
|beta|/max|beta|
2
3
6
10
4
8

Lars C_p

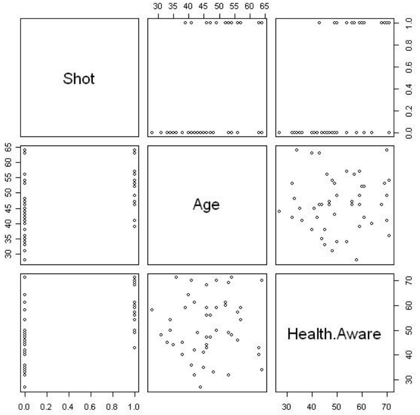


building.lars$Cp
70
60
50
40
30
20
10
0
2
4
6
8
building.lars$entry

Lars cross validation prediction error



Binary Response - Flu Shot Example



A clinic sent fliers to its clients to encourage everyone, but especially older persons, to get a flu shot in time for protection against an expected flu epidemic.

1. 50 clients randomly sampled
2. Y: did they get flu shot?
3. Predictor variables: Age, health awareness.

Binary outcomes

Previously, we have dealt only with Gaussian models:

1. Continuous response.
2. Errors assumed to be approximately Gaussian

$$Y \sim N(\mu, \sigma^2), \quad \mu = X\beta.$$

3. Variance of errors don't depend on mean.

$$\sigma^2 \quad \text{constant.}$$

Binary outcomes:

1. Reponse is 0 or 1.
2. E(Response) is restricted in $[0, 1]$ iterval.
3. The concept of "Gaussian error" does not apply here.

Logistic Regression Model

Suppose we have an increasing function $g : (0,1) \rightarrow (-\infty, \infty)$. It seems reasonable to model the binary responses as follows:

$$P(Y = 1|X_1, \ldots, X_p) = g^{-1}(\beta_1 X_1 + \beta_2 X_2 + \ldots \beta_p X_p).$$

A popular choice for g is the logit transform:

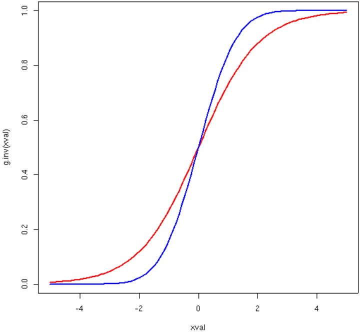
$$g(\pi) = \log\left(\frac{\pi}{1-\pi}\right).$$

The inverse g^{-1} is

$$g^{-1}(z) = \frac{e^z}{1+e^z}.$$

Logit link function

$$P(Y = 1|X) = \frac{e^{X\beta}}{1 + e^{X\beta}}$$



Logistic Regression Model

So far, we've given a model for the relationship between the mean of Y and X:

$$\pi(X) = P(Y = 1|X) = \frac{e^{X\beta}}{1 + e^{X\beta}}.$$

Or, equivalently,

$$logit[P(Y = 1|X)] = \beta X.$$

What about the variance of Y? Since Y is bernoulli 0-1,

$$Var(Y) = \pi(X)[1 - \pi(X)].$$

Note that the variance is a function of the mean.

Interpretation of Logistic Model

A commonly used quantity to quantify binary data is the *odds*

$$odds = \frac{P(Y = 1|X)}{P(Y = 0|X)}.$$

What are the odds of

1. rain?
2. winning the match?

In the logistic regression model,

$$\log(odds) = \beta X.$$

The parameter β is the contribution of unit increase in X to the odds.

Maximum likelihood estimation of β

- Data: $\mathbf{X}_i$, $Y_i \in \{0, 1\}$, $i = 1, \ldots, n$.
- Model: $P(Y_i = 1) = \frac{e^{\mathbf{X}_i \beta}}{1+e^{\mathbf{X}_i \beta}}$.
- Goal: estimate β, compute confidence intervals, hypothesis testing.

Log-likelihood:

$$
\begin{aligned}
l(\beta) &= \log \left[\prod_{i=1}^{n} \left(\frac{e^{\mathbf{X}_i \beta}}{1 + e^{\mathbf{X}_i \beta}} \right)^{Y_i} \left(\frac{1}{1 + e^{\mathbf{X}_i \beta}} \right)^{1-Y_i} \right] \\
&= \left(\sum_{i=1}^{n} Y_i \mathbf{X}_i \right) \beta - \sum_{i=1}^{n} \log(1 + e^{\mathbf{X}_i \beta})
\end{aligned}
$$

Goal: solve for $\hat{\beta} = \text{argmax}_{\beta} l(\beta)$.

Review - Model fitting (i.e. solving for $\hat{\beta}$)

Fitting can be done by Newton-Raphson:

1. Let $u' = (\frac{\delta l(\beta)}{\delta \beta_i})_{i=1,\ldots,p}$ be the gradient vector.
2. Let H be the Hessian matrix $h_{i,j} = \frac{\delta^2 l(\beta)}{\delta\beta_i \delta\beta_j}$.
3. Start with an initial $\beta^{(0)}$, then iterate $\beta^{(t+1)} = \beta^{(t)} - (H^{(t)})^{-1} u^{(t)}$.

The idea is, for each iteration t, to approximate $l(\beta)$ locally by a quadratic:

$$l(\beta) = l(\beta^{(t)}) + u^{(t)'}(\beta - \beta^{(t)}) + \frac{1}{2}(\beta - \beta^{(t)})' H^{(t)} (\beta - \beta^{(t)}),$$

and solve for $\delta l(\beta)/\delta\beta \approx u^{(t)} + H^{(t)}(\beta - \beta^{(t)}) = 0$.

For logistic regression model,

$$\beta^{(t+1)} = \beta^{(t)} + \{X' diag[\pi_i^{(t)}(1 - \pi_i^{(t)})]X\}^{(-1)} X'(y - \pi^{(t)}).$$

This is equivalent to doing a weighted linear regression at each step.

Inference for β

In Gaussian case:

$$\hat{\beta} = (X'X)^{-1}X'Y, \quad Y \sim N(X\beta, \sigma^2 I).$$

Since Gaussian vectors remain Gaussian under linear transforms,

$$\hat{\beta} \sim N(\beta, (X'X)^{-1}\sigma^2).$$

For logistic regression, $\hat{\beta}$ is no longer linear in Y. However, *asymptotically* (i.e. n large), it is Gaussian. It's covariance can be estimated by

$$\widehat{cov(\hat{\beta})} = (X' diag[\hat{\pi}_i(1 - \hat{\pi}_i^{(t)})]X)^{-1}.$$

From the square root of the diagonal elements of the above matrix you can get $\widehat{s.e.(\hat{\beta})}$.

Wald tests for β

1. Confidence intervals for β:

$$[\hat{\beta} - z_{\alpha/2}\widehat{s.e.(\hat{\beta})}, \quad \hat{\beta} + z_{\alpha/2}\widehat{s.e.(\hat{\beta})}]$$

2. Two sided test $H_0 : \beta = 0$, reject if

$$\left| \frac{\hat{\beta}}{\widehat{s.e.(\hat{\beta})}} \right| > z_{\alpha/2}$$

3. Test of constraint $H_0 : C_{j\times p}\beta_{p\times 1} = h_{j\times 1}$, reject if

$$(C\hat{\beta} - h)'(C\widehat{cov(\hat{\beta})}C')^{-1}(C\hat{\beta} - h)$$

is larger than $\chi^2_{j,1-\alpha}$.

Assessment of model fit

In linear regression, we used the F-test:

$$F = \frac{[SSE(RM) - SSE(FM)]/[\Delta df]}{SSE(FM)/[n - df(FM)]}.$$

$$F \sim F_{\Delta df, n-df(FM)}.$$

The analogous quantity of SSE for non-linear models is *deviance*:

$$Deviance(\hat{\beta}) = -2[l(\tilde{\beta}, Y) - l(\hat{\beta}, Y)],$$

where

$$l(\cdot, Y) \quad \text{is log-likelihood,}$$

$$\tilde{\beta} \quad \text{is fit of data using saturated model (n predictors).}$$

Assessment of model fit

For Gaussian model,

$$Deviance(\hat{\beta}) = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2.$$

For Logistic model,

$$Deviance(\hat{\beta}) = 2 \sum_{i=1}^{n} \left[Y_i \log \frac{Y_i}{\hat{\pi}_i} + (1 - Y_i) \log \frac{1 - Y_i}{1 - \hat{\pi}_i} \right]$$

Convention: $0 \times \log 0 = 0.$

Nested Chi-squared tests of model fit

As for SSE, the greater the deviance, the poorer the fit. If reduced model (RM) were true, then

$$Deviance(RM) - Deviance(FM) \to \chi^2_{df(FM)-df(RM)}.$$

Thus, reject *RM* at asymptotic level *alpha* if

$$Deviance(RM) - Deviance(FM) > \chi^2_{df(FM)-df(RM),1-\alpha}.$$

Model diagnosis

In linear regression, the standardized residuals were used to diagnose model fit.

$$r_i = y_i - \hat{y}_i, \quad r_i^* = \frac{r_i}{\widehat{\sigma}_{r_i}} = \frac{r_i}{\sqrt{1 - p_{ii}}}.$$

The analogous quantity here is the Pearson residual,

$$r_i = \frac{y_i - \hat{\pi}_i}{\sqrt{\hat{\pi}_i(1 - \hat{\pi}_i)}},$$

$$r_i^* = \frac{r_i}{\sqrt{1 - \hat{h}_{ii}}}.$$

where $\hat{h}_{ii}$ are diagonals of

$$Hat = W^{1/2} X (X' W X)^{-1} X' W^{1/2}.$$

$$W = diag[\pi_i (1 - \pi_i)].$$

Model diagnosis

Another quantity you can use is the deviance residuals:

$$\begin{aligned} \mathit{Deviance}(\hat{\beta}) &= 2\sum_{i=1}^{n}\left[Y_i \log \frac{Y_i}{\hat{\pi}_i} + (1-Y_i)\log \frac{1-Y_i}{1-\hat{\pi}_i}\right] \\ &= 2\sum \text{observed} \times \log \frac{\mathit{observed}}{\mathit{fitted}}. \end{aligned}$$

So let d_i be the contribution of data point i to the above measure of mis-fit:

$$d_i = Y_i \log \frac{Y_i}{\hat{\pi}_i} + (1-Y_i)\log \frac{1-Y_i}{1-\hat{\pi}_i}$$

$$\text{Deviance residual:} \quad \sqrt{d_i} \times \text{sign}(y_i - \hat{\pi}_i).$$