Linear Model Selection & Validation

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Quiz questions on Wooclap

https://app.wooclap.com/SLWEEK5

Chapter 6: Linear Model Selection and Regularization

What if we have (too) many predictor variables?

Three classes of methods:

- Subset selection
- Regularization
  - Minimizing fit + penalty, a very powerful idea! Used in penalized regression, decision trees, tree ensembles, hierarchical models, smoothing splines / GAMs, ...
- Dimension reduction (ISLR section 6.3; next week)

Chapter 6: (Linear) Model Selection and Regularization

- Generalizations to other response variables types within the GLM (Poission, Binomial, etc.) are straightforward:
  - Instead of minimizing $\frac{\text{RSS}}{n} + \lambda \times$ penalty,
  - minimize $\frac{-2LL}{n} + \lambda \times$ penalty.
- In practical analyses, generally comes down to specifying different value for `family` argument.

Wooclap Questions

Best subset and stepwise selection (penalty on L0 norm)

- OLS coefficients $\hat{\beta}^{OLS}$ minimize:

$$RSS = \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)$$

- Best subset and stepwise selection (forward, backward or both) based on AIC $= -2LL + 2p$ or BIC $= -2LL + p \ln(n)$ also minimize a fit-plus-penalty criterion:

fixed λ L0范式 $I = \begin{cases} 1, & \beta_j \neq 0 \\ 0, & \beta_i = 0 \end{cases}$

$$\underline{\sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right) + \boxed{\lambda \sum_{j=1}^{p} I(\beta_j \neq 0)}}$$

- Right-most sum is often referred to as L0 norm: $||\beta||_0$, the number of non-zero coefficients.

Best subset selection

Trying 2^p combinations is computationally prohibitive.

- Many algorithms have been developed to speed up the search, allowing for (much) larger p.
- Best subset can work well in problems with high signal-to-noise ratio (i.e., low σ^2).

Stepwise selection (forward and/or backward)

Stepwise regression has a pretty bad name, because of widespread incorrect use of:

- Standard errors and p-values computed and reported as if no variable selection has taken place.
- Degrees of freedom used up by the model assumed to be equal to the number of selected variables.
- Fit measures like R^2 computed on data that was used for variable selection.

Solution: After selecting variables on the training data, perform inference or evaluate performance on new set of (test) data!

Shrinkage methods

Ridge regression coefficient estimates $\hat{\beta}^R$ minimize:

λ needs to be specified

L2范式

$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right) + \lambda\sum_{j=1}^{p}\beta_j^2$$

Shringe to similar value

- Right-most sum often referred to as squared L2 norm: $||\beta||_2^2$

unstable

Lasso regression coefficients estimates $\hat{\beta}^L$ minimize:

L1范式

$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right) + \lambda\sum_{j=1}^{p}|\beta_j|$$

- Right-most sum is often referred to as L1 norm: $||\beta||_1$

Wooclap Questions

Computational challenges

Even if optimal value of λ is known or given, minimizing the fit-plus-penalty criterion can be challenging:

- With L0 norm: Derivative of the fit-plus-penalty criterion w.r.t. β is zero in many places. But where it's interesting, it has jump discontinuities and is not differentiable.
- With L1 norm: Not differentiable with respect to a coordinate where that coordinate is zero. Elsewhere, the partial derivatives are just constants, ± 1 depending on the quadrant.
- With L2 norm: Differentiable, with squared L2 norm even at zero.

Ridge and degrees of freedom

OLS coefficients are given by:

$$\hat{\beta}^{OLS} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$$

$$\hat{y}^{OLS} = \mathbf{X}\hat{\beta}^{OLS} = \mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y} = \mathbf{P}\mathbf{y}$$

- **P** is the projection matrix, a.k.a. 'hat' matrix.
- Values on the diagonal of **P** quantify how much an observation contributes to its own predicted value.
- By definition, in OLS the trace (sum of diagonal elements) of **P** is equal to the rank of **X**, which equals the number of independent parameters.

Ridge solution and degrees of freedom

Ridge coefficients are given by:

$$\hat{\beta}^R = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^\top \mathbf{y}$$

n×n n×1

$$\hat{y}^R = \mathbf{X}\hat{\beta}^R = \mathbf{X}(\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^\top \mathbf{y} = \mathbf{P}_\lambda \mathbf{y}$$

- For ridge, the *effective* degrees of freedom are given by $\mathrm{tr}(\mathbf{P}_\lambda)$.
- Values on the diagonal $\mathbf{P}_\lambda$ are $\leq$ values on the diagonal of $\mathbf{P}$ from OLS: Predicted values are shrunken towards the mean (like coefficients are shrunken towards zero).

Useful extensions: Elastic Net

Both Ridge and Lasso penalties are added to the criterion:

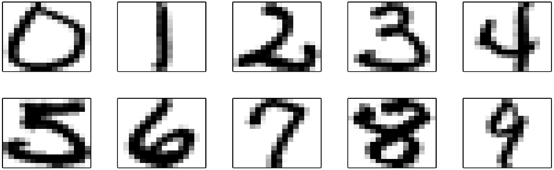
$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right) + \lambda\left(\frac{1-\alpha}{2}\sum_{j=1}^{p}\beta_j^2 + \alpha\sum_{j=1}^{p}|\beta_j|\right)$$

- Where α determines the weight of the Lasso and Ridge penalties.
- Note that now two hyperparameters need to be optimized!
- What penalties result when we set $\alpha = 0$? And $\alpha = 1$?

Ridge Lasso

Elastic net: Digit recognition example

- Task: Recognize hand-written digits from 16x16 grayscale images.
- Data: 7291 training samples, 2007 test samples.
- Predictor variables: 256 grayscale values (one for each pixel).
- 10-class response (digits 0-9)



low irreducable error

- What do you expect for signal-to-noise ratio (low or high)? Multicollinearity (low or high)?
- In this example, we perform binary classification of digits 2 ($y = 0$) and 3 ($y = 1$).

Elastic net: Digit recognition example

```
library("glmnet")
set.seed(42)
L_mod <- cv.glmnet(x = x, y = y, family = "binomial",
                   alpha = 1)
L_mod
```

```
##
## Call:  cv.glmnet(x = x, y = y, family = "binomial", alph
##
## Measure: Binomial Deviance
##
##       Lambda Index Measure      SE Nonzero
## min 0.001109    63 0.08893 0.01356      74
## 1se 0.003086    52 0.10145 0.01076      66
```

min CV error

1 standard error

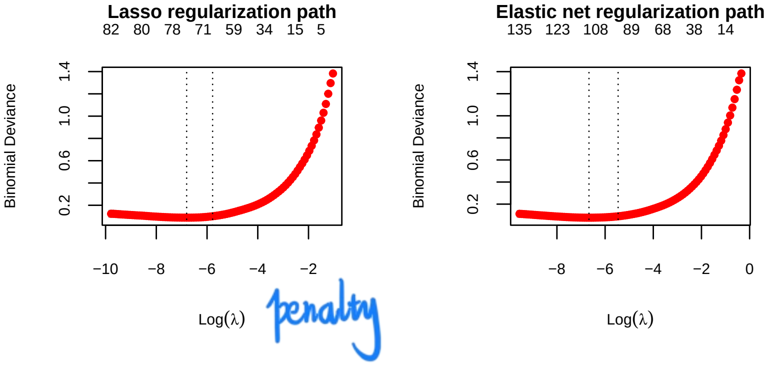
Elastic net: Digit recognition example

```r
set.seed(42)
EN_mod <- cv.glmnet(x = x, y = y, family = "binomial",
                    alpha = .5)
EN_mod
```

```
##
## Call:  cv.glmnet(x = x, y = y, family = "binomial", alph
##
## Measure: Binomial Deviance
##
##        Lambda Index Measure      SE Nonzero
## min 0.001269    69 0.07701 0.01388     112
## 1se 0.004255    56 0.08950 0.00994     101
```

Elastic net: Digit recognition example

```r
par(mfrow = c(1, 2))
plot(L_mod, main = "Lasso regularization path")
plot(EN_mod, main = "Elastic net regularization path")
```



Elastic net: Digit recognition example

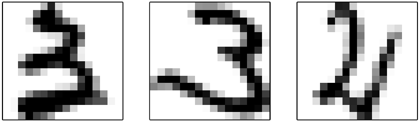
Correct classification rates on training data:

- Lasso: 0.9985601
- Elastic Net: 0.9985601

Correct classification rates on test data:

- Lasso: 0.956044
- Elastic Net: 0.9642857

Misclassified by Lasso, correctly classified by Elastic Net:



(Lasso predicted 2, 2, 3; Elastic Net predicted 3, 3, 2)

Useful extensions: Relaxed Lasso

- Lasso performs shrinkage and selection. Both strength and weakness!
- λ optimized for *variable selection* will likely not be optimal for *prediction*, vice versa.
  - In order to shrink many coefficients to zero, large λ is needed, large coefficients will be shrunken too much to predict well.
- Relaxed Lasso:
  1) Use Lasso for variable selection
  2) Refit OLS on *selected predictors* only.
  3) Compute relaxed-lasso coefficients as a weighted sum:

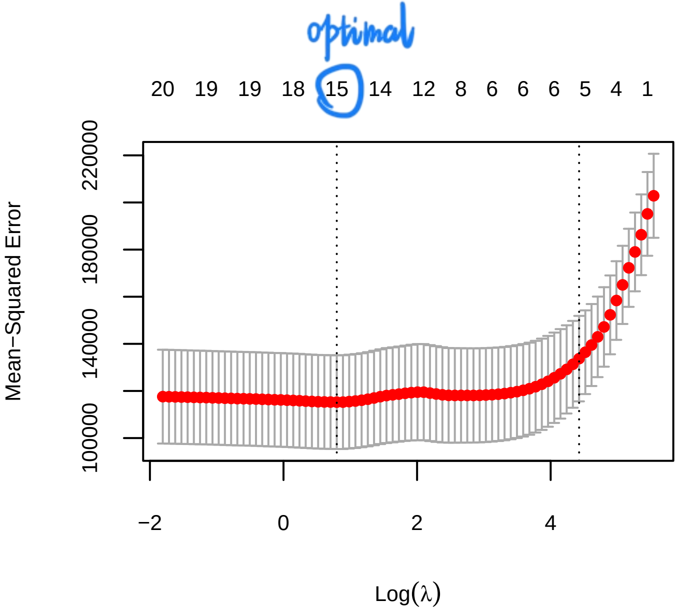
$$\hat{\beta}_{\text{relaxed}} = (1-\gamma)\hat{\beta}_{\text{OLS}} + \gamma\hat{\beta}_{Lasso}$$

Relaxed Lasso: Predicting baseball player's salaries

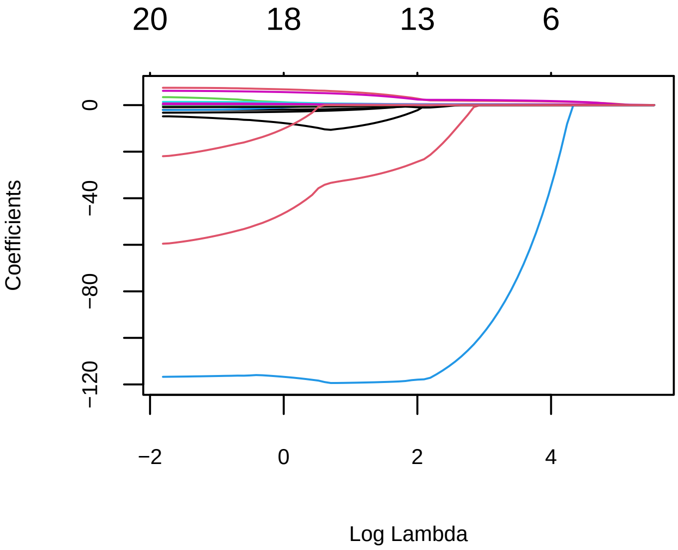
- "Hitters" data: Major League Baseball data (from 1986-1987), $N = 263$.
- Task: Predict player's salary.
- 19 predictors: Times at bat, number of homeruns, number of walks, for many variable in '86 and '87 season.

```
library("glmnet")
set.seed(42)
cv_lasso <- cv.glmnet(x, y) ## 'standard' lasso
plot(cv_lasso)
```

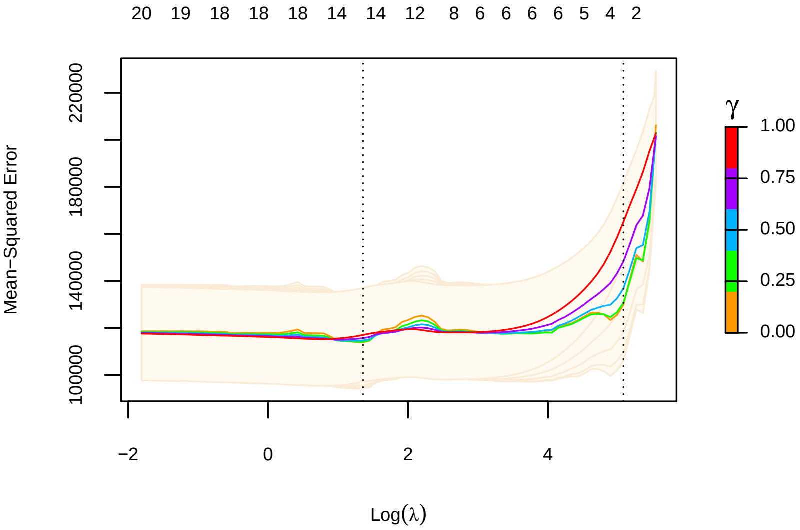
Standard Lasso: Predicting baseball player's salaries



Standard Lasso: Predicting baseball player's salaries



Relaxed Lasso: Predicting baseball player's salaries



Relaxed Lasso: Predicting baseball player's salaries

Lasso coefficients:

(Intercept)	Hits	Walks	CRuns	CRBI	PutOuts
167.912	1.293	1.398	0.142	0.322	0.047

Relaxed lasso coefficients:

(Intercept)	Hits	Walks	CRuns	CRBI
41.765	1.921	2.339	0.15	0.413

Reading materials

What to focus on in the book (ISLR chapter 6):

- Lasso and Ridge penalties as Bayesian priors.
- Penalties as a "spending budget"
  - We'll meet regularization with a penalty again with decision trees and smoothing splines.
  - We'll meet regularization with a budget again with support vector machines.

What to focus on in the paper (Hastie et al., 2020):

- Which method works best in which situation? Best subset, forward stepwise, lasso, relaxed lasso.