

Linear Model Selection & Validation

Marjolein Fokkema

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 (Poisson, Binomial, etc.) are straightforward:
 - ▶ Instead of minimizing $\frac{RSS}{n} + \lambda \times \text{penalty}$,
 - ▶ minimize $\frac{-2LL}{n} + \lambda \times \text{penalty}$.
- ▶ 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:

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

- ▶ 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:

$$\sum_{i=1}^n \left(y_i - \beta_0 - \sum_{j=1}^p \beta_j x_{ij} \right)^2 + \lambda \sum_{j=1}^p I(\beta_j \neq 0)$$

- ▶ 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:

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

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

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

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

- ▶ 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:

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

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

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

Useful extensions: Elastic Net

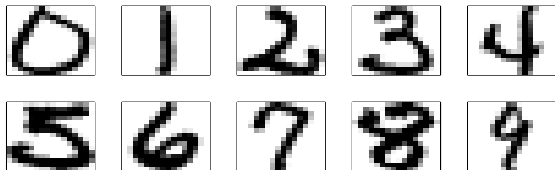
Both Ridge and Lasso penalties are added to the criterion:

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

- ▶ 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 $\alpha = 1$?

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)



- ▶ 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", alpha = 1)
```

```
##
```

```
## 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

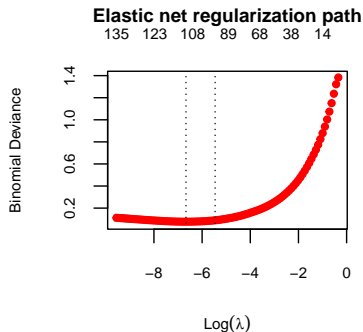
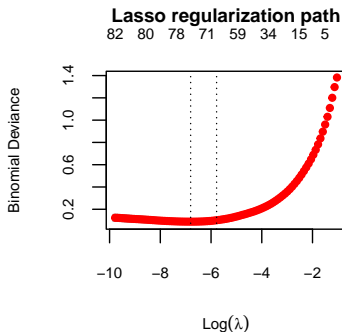
Elastic net: Digit recognition example

```
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", alpha = .5)
##
## 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

```
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

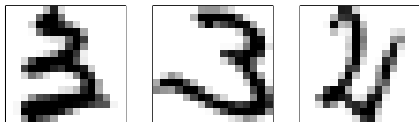
Correct classification rates on training data:

- ▶ 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 shrunk 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:

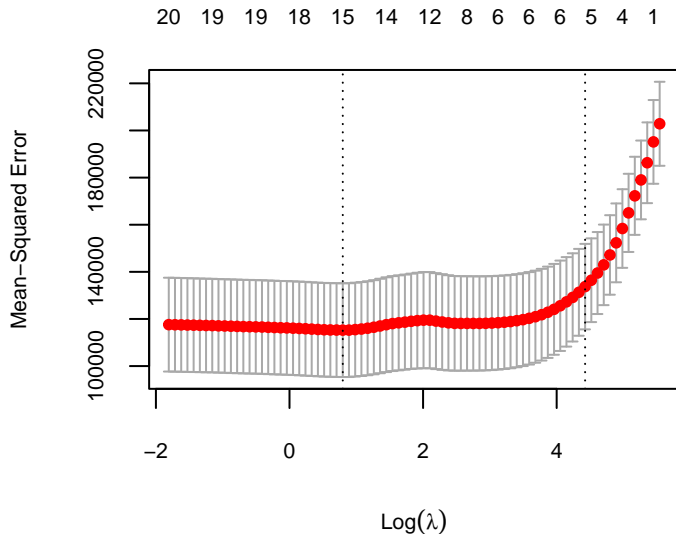
$$\hat{\beta}_{\text{relaxed}} = (1 - \gamma)\hat{\beta}_{\text{OLS}} + \gamma\hat{\beta}_{\text{Lasso}}$$

Relaxed Lasso: Predicting baseball player's salaries

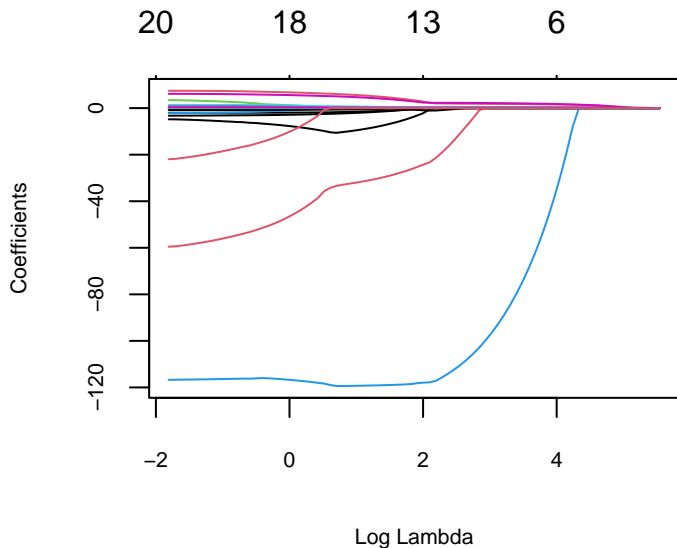
- ▶ “Hitters” data: Major League Baseball data (from 1986-1987), $N = 263$.
- ▶ Task: Predict player's salary.
- ▶ 19 predictors: Times at bat, number of homeruns, number of walks, for many variable in '86 and '87 season.

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

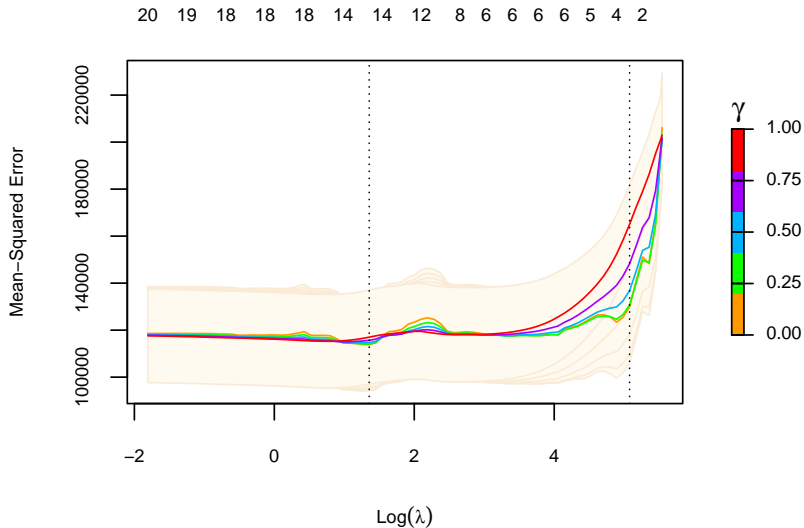
Standard Lasso: Predicting baseball player's salaries



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.