Lecture 3

Penalized Methods

Review of Linear Regression Model

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \ldots + \beta_{p-1} X_{i,p-1} + \varepsilon_i, \quad i = 1, \ldots n$$

- Y_i is the response for the ith subject
- $X_{i1}, X_{i2}, \ldots X_{i,p-1}$ are the values of the predictor variables for the ith subject. Some can be transformed predictors: $X_{i2}=\text{Log}(X_{i1})$ or interactions $X_{i3}= X_{i1}X_{i2}$ or polynomial expansion.
- $\beta_1, \beta_2, \ldots \beta_{p-1}$ are *unknown parameters* to be estimated from the data (they are also called *partial regression coefficients*)
- Regression (response) surface:

$$E(Y_i) = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \ldots + \beta_{p-1} X_{i,p-1}$$

- $E(\varepsilon_i)=0$, $\text{Cov}(\varepsilon_i, \varepsilon_j)=0$ for $i \neq j$, $\text{Var}(\varepsilon_i)=\sigma^2>0$

Linear Regression Model(Matrix form)

$$\underset{n\times 1}{Y} = \underset{n\times p}{X}\ \underset{p\times 1}{\beta} + \underset{n\times 1}{\varepsilon}$$

- Y – vector of responses
- β- vector of parameters
- X – matrix of constants (design matrix)
- $\varepsilon \sim \mathrm{N}(0,\sigma^2 I_p)$ and hence $Y \sim \mathrm{N}(X\beta,\sigma^2 I_p)$, where I_p is p-dimensional identity matrix.

Estimation of regression coefficients

- Least square estimates are obtained by minimizing the sum of distances from the points to the regression plane:

$$Q = \sum_{i=1}^{n} (Y_i - \beta_0 - \beta_1 X_{i1} - \beta_2 X_{i2} - \ldots - \beta_{p-1} X_{i,p-1})^2 \text{ ==> } \hat{\beta} = \underset{\beta}{\operatorname{argmin}} \| y - X\beta \|^2$$

- Denote the vector of the least squares estimated regression coefficients as $\hat{\beta}$:

$$\underset{p\times 1}{\hat{\beta}} = \begin{pmatrix} b_0 \\ b_1 \\ \ldots \\ b_{p-1} \end{pmatrix}$$

- Least squares normal equations:

$$X'Xb = X'Y$$

- Least squares estimates

$$\underset{p\times 1}{\hat{\beta}} = \underset{p\times p}{(X'X)^{-1}} \underset{p\times 1}{(X'Y)}$$

Maximum-likelihood estimates are the same

Fitted values and residuals

$$\underset{n\times 1}{\hat{Y}} = \begin{pmatrix} \hat{Y}_1 \\ \hat{Y}_2 \\ \dots \\ \hat{Y}_n \end{pmatrix} = \underset{n\times p}{X}\,\underset{p\times 1}{\hat{\beta}} = X(X'X)^{-1}X'Y = \underset{n\times n}{H}\,\underset{n\times 1}{Y}$$

$$H = X(X'X)^{-1}X'$$

(Hat matrix)

$$\underset{n\times 1}{e} = \begin{pmatrix} e_1 \\ e_2 \\ \dots \\ e_n \end{pmatrix} = \underset{n\times 1}{Y} - \underset{n\times 1}{\hat{Y}} = \underset{n\times 1}{Y} - \underset{n\times p}{X}\,\underset{p\times 1}{b} = (\underset{n\times n}{I} - \underset{n\times n}{H})\underset{n\times 1}{Y}$$

$$\sigma^2\{e\} = \sigma^2(I-H), \quad s^2\{e\} = MSE(I-H)$$

Geometric Interpretation

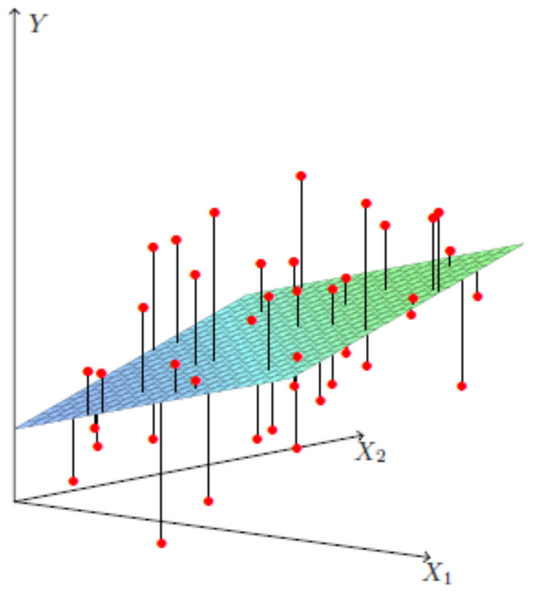


FIGURE 3.1. *Linear least squares fitting with $X \in \mathbb{R}^2$. We seek the linear function of X that minimizes the sum of squared residuals from Y.*

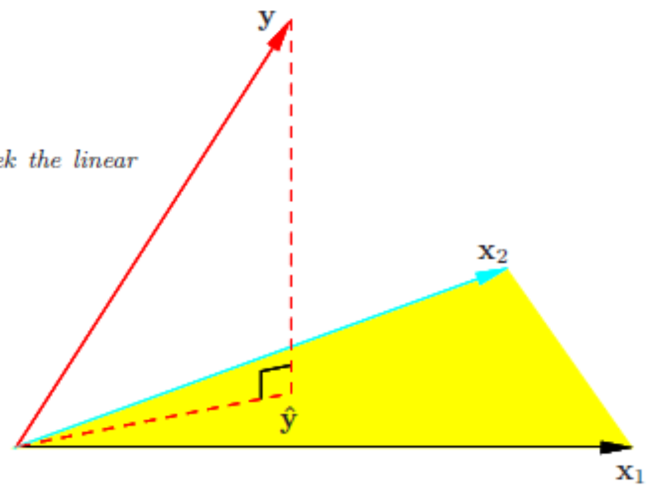


FIGURE 3.2. *The N-dimensional geometry of least squares regression with two predictors. The outcome vector $\mathbf{y}$ is orthogonally projected onto the hyperplane spanned by the input vectors $\mathbf{x}_1$ and $\mathbf{x}_2$. The projection $\hat{\mathbf{y}}$ represents the vector of the least squares predictions*

Sums of squares and mean squares

$$SSR = b'X'Y - \frac{1}{n}Y'JY = Y'[H - \frac{1}{n}J]Y$$

$$MSR = \frac{SSR}{p-1}$$

$$SSE = Y'Y - b'X'Y = Y'(I - H)Y$$

$$MSE = \frac{SSE}{n-p}$$

$$SSTO = Y'Y - \frac{1}{n}Y'JY = Y'[I - \frac{1}{n}J]Y$$

ANOVA table

Source of variation	df	SS	MS	F
Regression	p-1	SSR	MSR	MSR/MSE
Error	n-p	SSE	MSE	
Total	n-1	SSTO		

Gauss-Markov Theorem

Consider any linear combination of the β's: $\theta = a^T \beta$

The least squares estimate of θ is:

$$\hat{\theta} = a^T \hat{\beta} = a^T (X^T X)^{-1} X^T y$$

If the linear model is correct, this estimate is unbiased (*X* fixed):

$$E(\theta) = E(a^T (X^T X)^{-1} X^T y) = a^T (X^T X)^{-1} X^T X\beta = a^T \beta$$

Gauss-Markov states that for any other linear unbiased estimator $\tilde{\theta} = c^T y$

i.e., $E(c^T y) = E(a^T \beta)$,

$$\mathrm{Var}(a^T \hat{\beta}) \leq \mathrm{Var}(c^T y)$$

Of course, there might be a *biased* estimator with lower MSE…

bias-variance

For any estimator $\tilde{\theta}$:

$$
\begin{aligned}
\mathrm{MSE}(\tilde{\theta}) &= E(\tilde{\theta}-\theta)^2 \\
&= E(\tilde{\theta}-E(\tilde{\theta})+E(\tilde{\theta})-\theta)^2 \\
&= E(\tilde{\theta}-E(\tilde{\theta}))^2+E(E(\tilde{\theta})-\theta)^2 \\
&= Var(\tilde{\theta})+\underbrace{(E(\tilde{\theta})-\theta)}_{\text{bias}}{}^2
\end{aligned}
$$

Note MSE closely related to prediction error:

$$
E(Y_0-x_0^T\tilde{\beta})^2 = E(Y_0-x_0^T\beta)^2+E(x_0^T\tilde{\beta}-x_0^T\beta)^2 = \sigma^2+MSE(x_0^T\tilde{\beta})
$$

Modern procedures for model selection to avoid overfitting

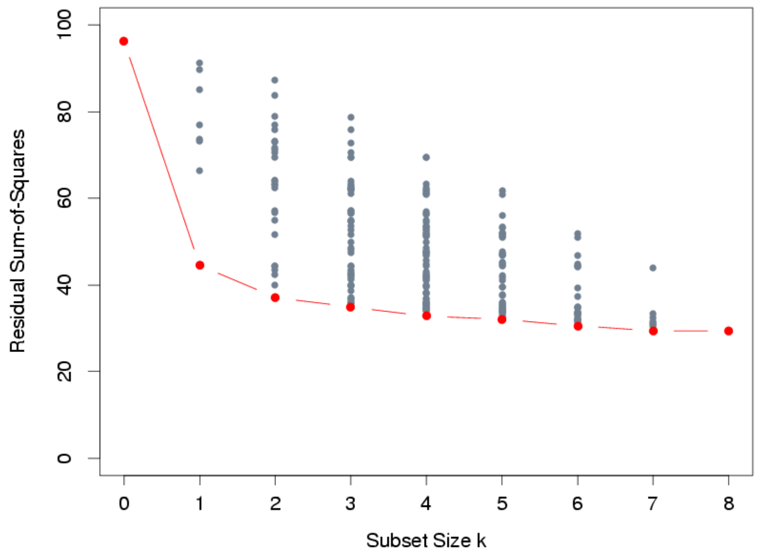
When there are too many *X*'s, noise X's can improve the fit just by chance. Overfitting causes bad prediction. Two avoid it we do:

1. Classical variable selection
   - Backward, Foreword, Stepwise methods,
   - All subsets
   - Best criteria: AIC, MAIC, BIC

2. Shrinkage Methods:
   Ridge Regression
   LASSO
   ELASTIC NET/GLM NET

Subset Selection

•Standard "all-subsets" finds the subset of size *k*, *k*=1,…,*p*, that minimizes RSS:



•In R function "leaps" will do it

•Choice of subset size requires tradeoff – AIC, BIC, marginal likelihood, cross-validation, etc.
•"Leaps and bounds" is an efficient algorithm to do all-subsets

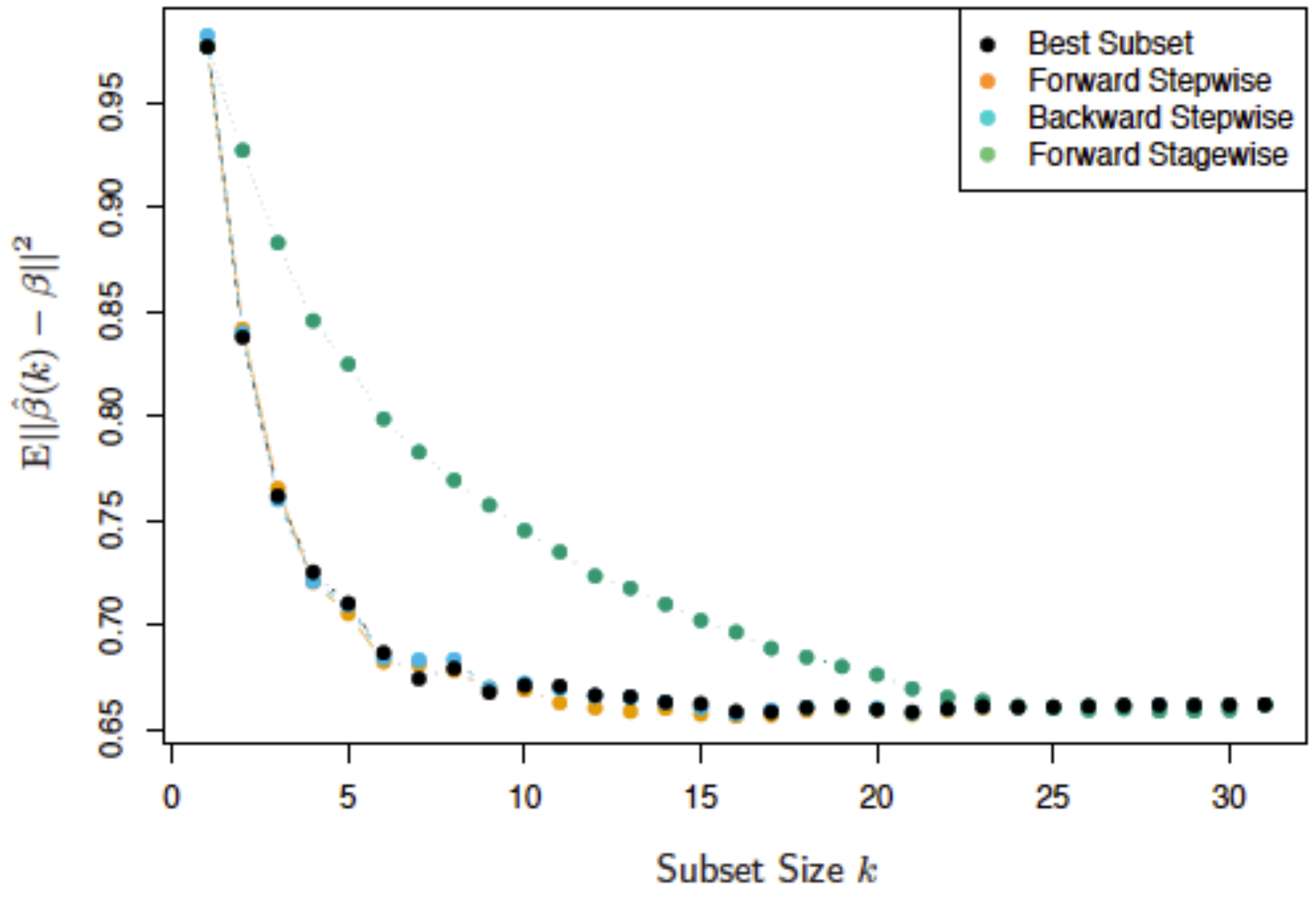
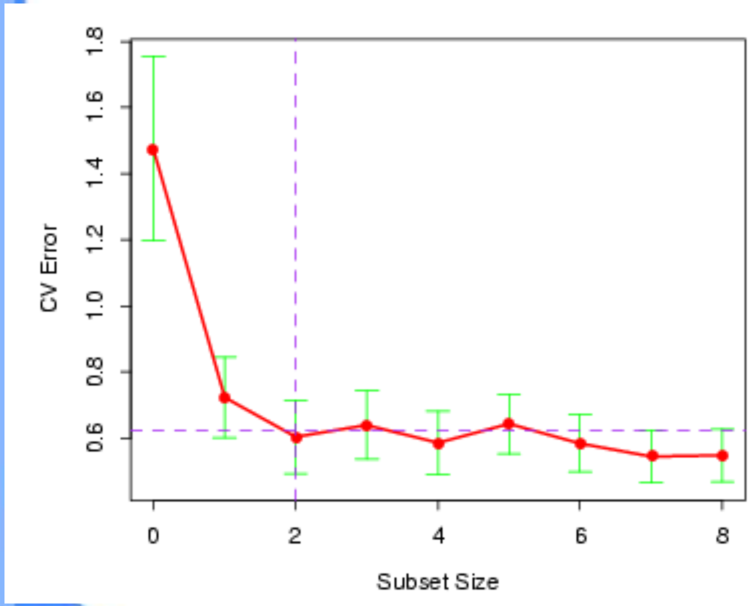


FIGURE 3.6. *Comparison of four subset-selection techniques on a simulated linear regression problem $Y = X^T\beta + \varepsilon$. There are $N = 300$ observations on $p = 31$ standard Gaussian variables, with pairwise correlations all equal to 0.85. For 10 of the variables, the coefficients are drawn at random from a $N(0, 0.4)$ distribution; the rest are zero. The noise $\varepsilon \sim N(0, 6.25)$, resulting in a signal-to-noise ratio of 0.64. Results are averaged over 50 simulations. Shown is the mean-squared error of the estimated coefficient $\hat{\beta}(k)$ at each step from the true β.*

Cross-Validation

- e.g. 10-fold cross-validation:
  - Randomly divide the data into ten parts
  - Train model using 9 tenths and compute prediction error on the remaining 1 tenth
  - Do these for each 1 tenth of the data
  - Average the 10 prediction error estimates



"One standard error rule"

pick the simplest model within one standard error of the minimum

Penalized methods (Shrinkage Methods)

- Stepwise or more generally Subset selection is a discrete process – individual variables are either in or out
- It can have high variability – a different dataset from the same source can result in a totally different model
- Overfitting is still a big problem with stepwise or subset selection
- Shrinkage methods allow a variable to be partly included in the model. That is, the variable is included but with a shrunken co-efficient.

Ridge Regression

$$\hat{\beta}^{\text{ridge}} = \arg\min_{\beta} \sum_{i=1}^{N} (y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j)^2 \quad \text{subject to: } \sum_{j=1}^{p} \beta_j^2 \le s$$

Equivalently:

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

$$Y'Y - 2Y'X\beta + \beta'(X'X + \lambda I)\beta$$

$$\text{Taking deriv w.r.t. } \beta: \ \text{-}2Y'X + 2(X'X + \lambda I)\beta = 0$$

This leads to: $$\hat{\beta}^{\text{ridge}} = (X'X + \lambda I)^{-1} X'Y$$

works even when $X'X$ is singular

Choose λ by cross-validation. Predictors should be centered.

Solution path for Ridge Regression

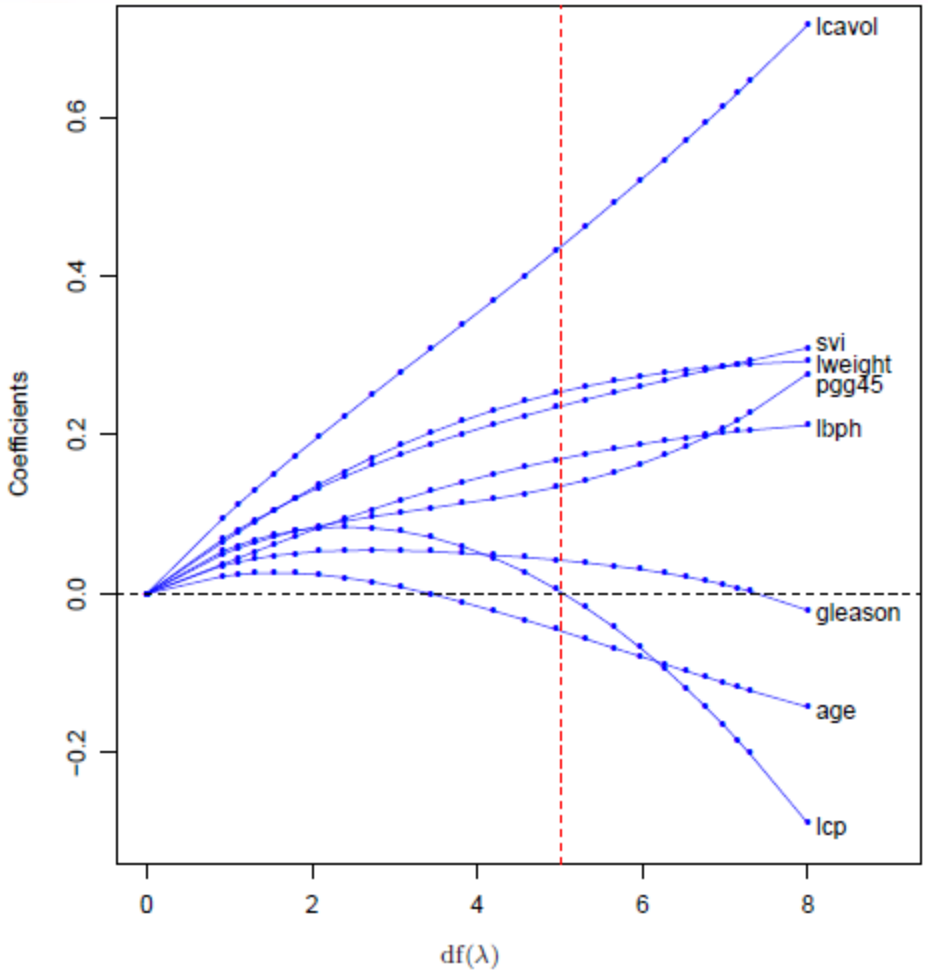


FIGURE 3.8. *Profiles of ridge coefficients for the prostate cancer example, as the tuning parameter λ is varied. Coefficients are plotted versus $\mathrm{df}(\lambda)$, the effective degrees of freedom. A vertical line is drawn at $\mathrm{df} = 5.0$, the value chosen by cross-validation.*

Ridge Regression = Bayesian Regression

$y_i \sim N(\beta_0 + x_i^T \beta, \sigma^2)$

$\beta_j \sim N(0, \tau^2)$

same as ridge with $\lambda = \sigma^2 / \tau^2$

The Lasso

Replace L_2 penalty by L_1 penalty => solution path eliminates variables

$$\hat{\beta}^{Lasso} = \arg\min_{\beta} \sum_{i=1}^{N} (y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j)^2$$

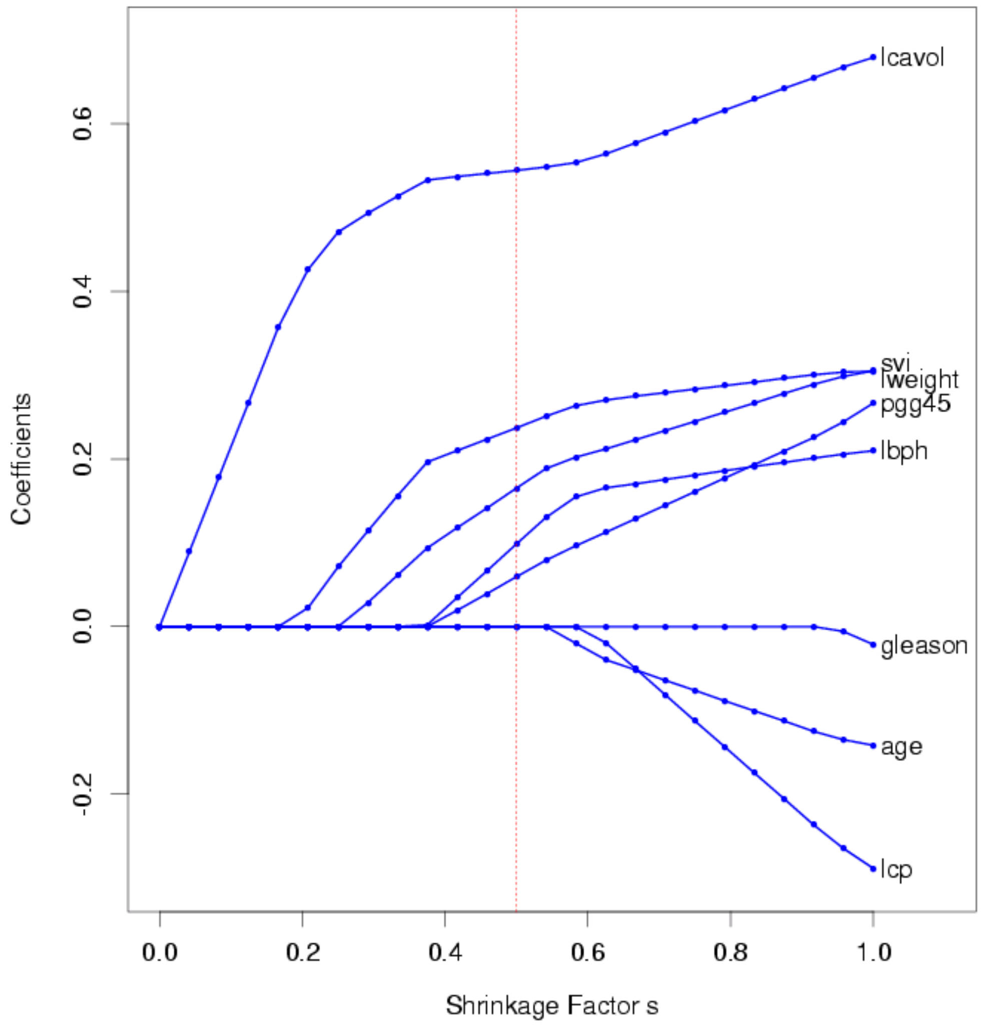
subject to: $$\sum_{j=1}^{p} \left|\beta_j\right| \leq s$$

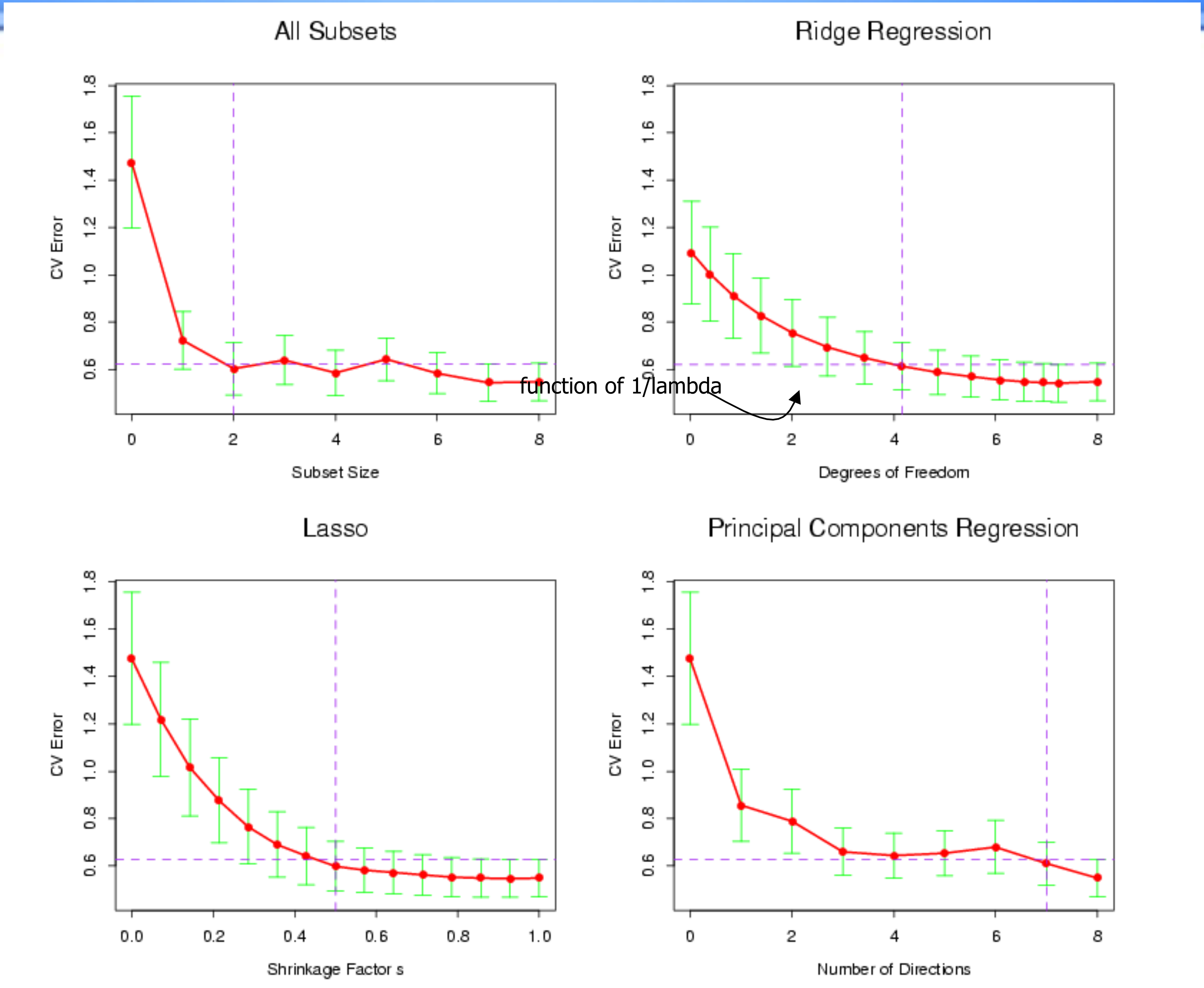
Quadratic programming algorithm needed to solve for the parameter estimates. Choose *s* via cross-validation.

$$\tilde{\beta} = \arg\min_{\beta} \left(\sum_{i=1}^{N} (y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j)^2 + \lambda \sum_{j=1}^{p} \left|\beta_j\right|^q \right)$$

q=0: var. sel.
q=1: lasso
q=2: ridge
Learn *q*?

Solution path for Lasso




All Subsets
Ridge Regression
Lasso
Principal Components Regression
CV Error
Subset Size
Degrees of Freedom
Shrinkage Factor s
Number of Directions
function of 1/lambda

Elastic Net

$$\hat{\beta}^{Enet} = \underset{\beta}{\arg\min}\left(\frac{1}{2N}\sum_{i=1}^{N}(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j)^2 + \lambda(\frac{1-\alpha}{2}\sum_{j=1}^{p}\beta_j^2 + \alpha\sum_{j=1}^{p}|\beta_j|) \right)$$

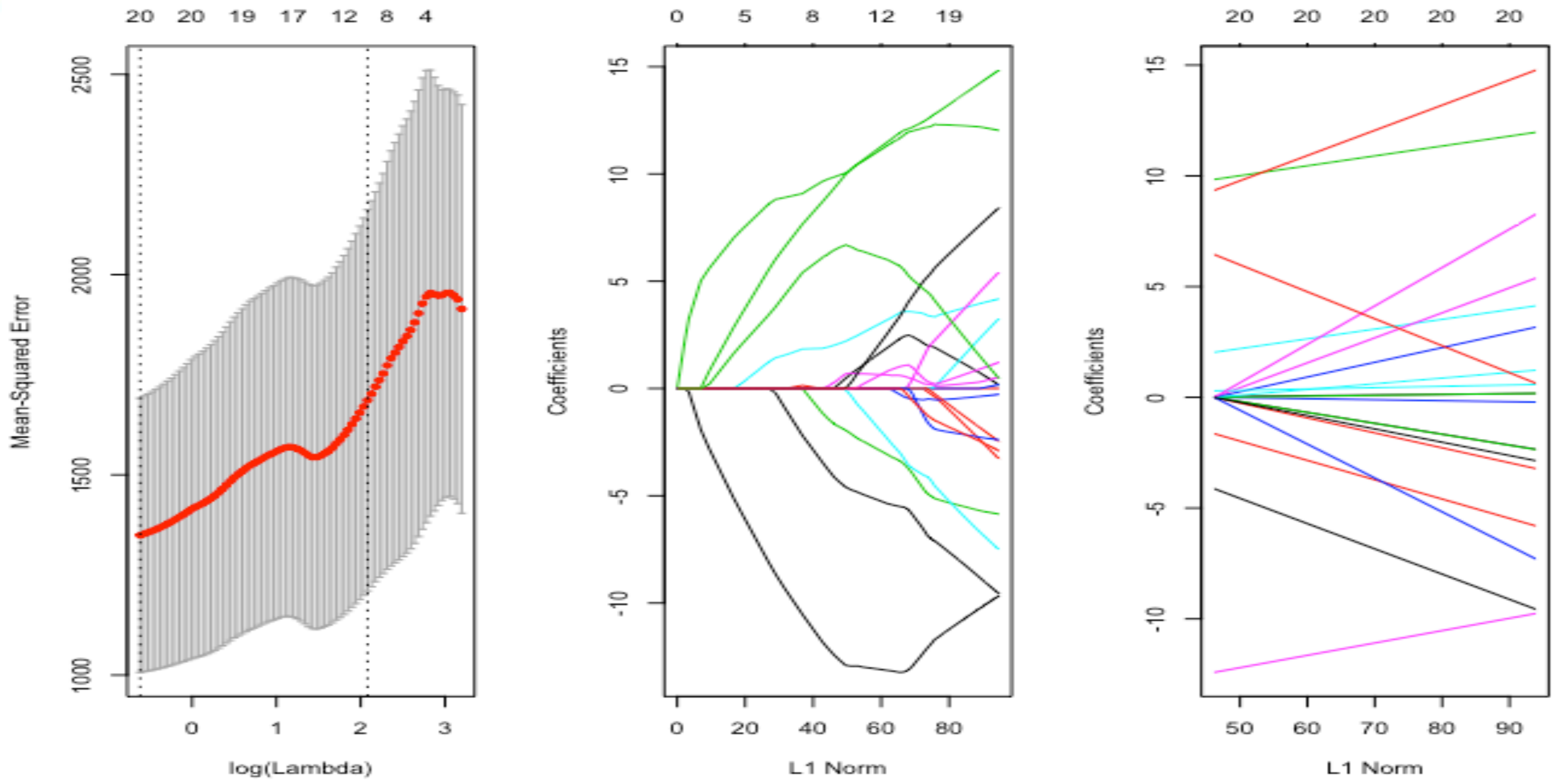
FOR NORMAL MODEL: $\frac{1}{2}$ RSS/N + λ PENALTY

FOR OTHER MODELS: $-\mathit{Loglik}$/N + λ PENALTY

R Code for Ridge(a=0), Lasso(a=1) and Enet (a=any) using GLM net

```
myglmnet = function(z, y, a=0.5) {
# Center and scale variables
z = as.matrix(t((t(z)-apply(z,2,mean))/apply(z,2,sd)))
# Find lambda by CV
plot(u<-cv.glmnet(z,y,alpha=a))
# Plot full solution path
plot(glmnet(z,y,alpha=a ))
lam=c(u$lambda.1se,u$lambda.min)
v <- glmnet(z,y,alpha=a,lambda=lam)
# Plot Lambda path
plot(v)
# Output lambda and estimates
list(lambda=lam,beta=v$beta)
}
library(glmnet) ; set.seed(2016)
n=20; p=60; k=4
x=matrix(rnorm(n*p),n,p)
b= rt(k,20)*5 ; y=x[,1:k] %*% b+rnorm(n)*2
par(mfrow=c(1,3))
myglmnet(x,y,a=1)
```

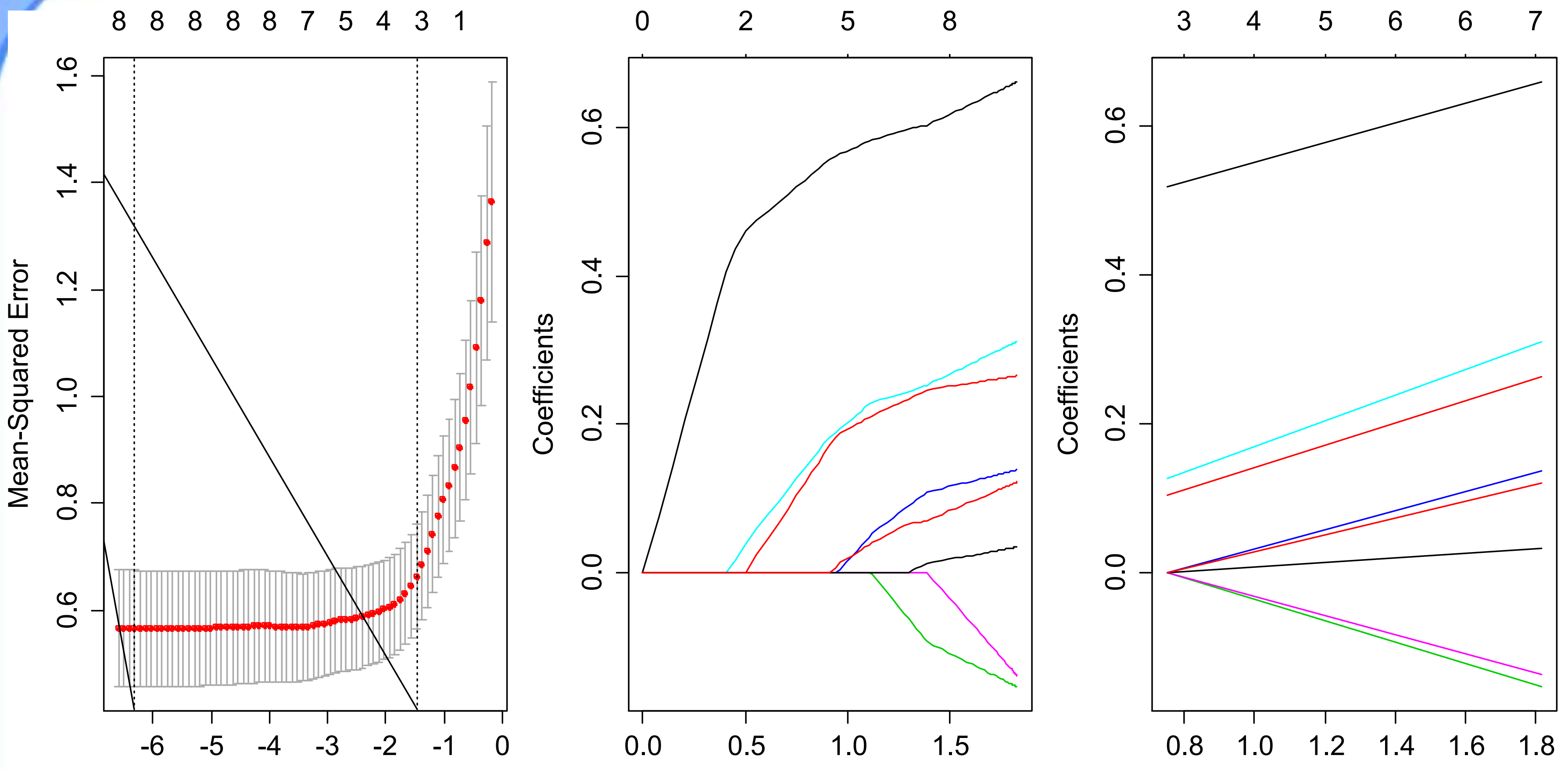
Ridge Output from GLM net



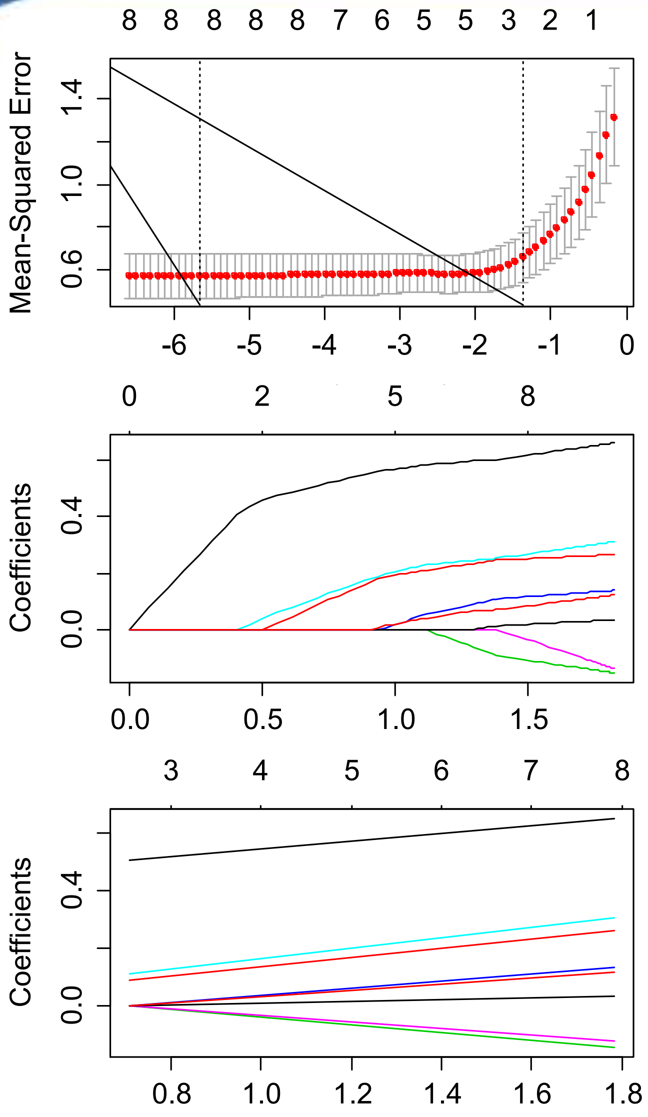
Lasso Output from GLM net

```
#prost=url("http://www-stat.stanford.edu/~tibs/
ElemStatLearn/datasets/prostate.data")
> prost=read.table("prost.txt",head=T)
> myglmnet(prost[,1:8],prost[,9],a=0)
$lambda
[1] 0.86327415 0.08434274
$beta
8 x 2 sparse Matrix of class "dgCMatrix"
                 s0          s1
lcavol    0.32398301  0.58020370
lweight   0.18612911  0.25875483
age      -0.02308884 -0.12450751
lbph      0.07491161  0.12456784
svi       0.19230986  0.28396396
lcp       0.10308122 -0.05559908
gleason   0.06022965  0.04594414
pgg45     0.07370693  0.09625296
```

Lasso Output from GLM net



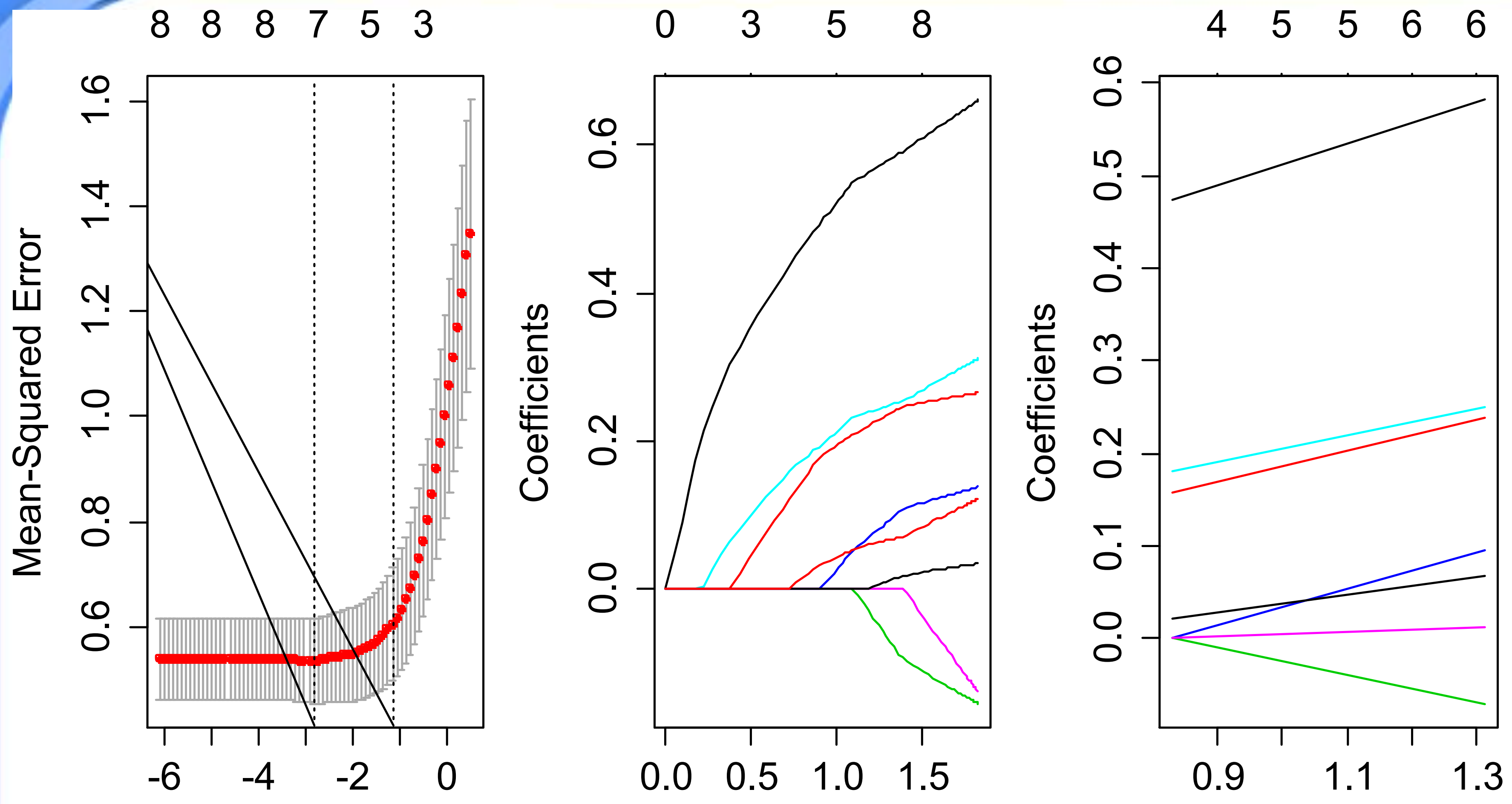
Ridge Output from GLM net



```
> myglmnet(prost[,1:8],prost[,9],a=1)
$lambda
[1] 0.22929319 0.02961435

$beta
8 x 2 sparse Matrix of class
"dgCMatrix"
               s0          s1
lcavol  0.5197469  0.599935919
lweight 0.1041996  0.239353146
age     .         -0.076377704
lbph    .          0.097817827
svi     0.1268638  0.248051507
lcp     .          .
gleason .          0.006135243
pgg45   .          0.067144999
```

ENET a=0.5 Output from GLM net



ENET a=0.5 Output from GLM net

```
> myglmnet(prost[,1:8],prost[,9],a=0.5)
$lambda
[1] 0.31608581 0.05922871
$beta
8 x 2 sparse Matrix of class "dgCMatrix"
               s0          s1
lcavol  0.4733168  0.58093039
lweight 0.1566415  0.23748890
age     .         -0.07015625
lbph    .          0.09417850
svi     0.1808864  0.24915717
lcp     .          .
gleason .          0.01241265
pgg45   0.0208983  0.06719576
```

ENET Output from GLM net

Iterate twice

```
myglmnet(prost[,c(1:5,7:8)],prost[,9],a=0.5)
$lambda
[1] 0.26241999 0.01939473
$beta
s0           s1
lcavol  0.49281146  0.60105347
lweight 0.17661952  0.25678221
age     .          -0.11896632
lbph    .           0.12304168
svi     0.19240422  0.26050966
gleason .           0.02448453
pgg45   0.03130061  0.07446277

myglmnet(prost[,c(1:5,7:8)],prost[,9],a=0.5)
$lambda
[1] 0.38072647 0.02813844
$beta
s0           s1
lcavol  0.450558382  0.59661837
lweight 0.133438442  0.25247009
age     .           -0.10798982
lbph    .            0.11658586
svi     0.167118111  0.25803568
gleason .            0.02175753
pgg45   0.008532863  0.07284914
```

ENET a=0.5 Output from GLM net

```
CV leave one out

myglmnet(prost[,c(1:5,7:8)],prost[,9],a=0.5)
$lambda
[1] 0.34690378 0.01610185
$beta
7 x 2 sparse Matrix of class "dgCMatrix"
                s0          s1
lcavol  0.46238264  0.60281372
lweight 0.14546563  0.25837993
age     .          -0.12309295
lbph    .           0.12552973
svi     0.17430576  0.26152330
gleason .           0.02553766
pgg45   0.01497629  0.07497455
```

Principal Component Regression

Consider a an eigen-decomposition of X^TX (and hence the covariance matrix of X):

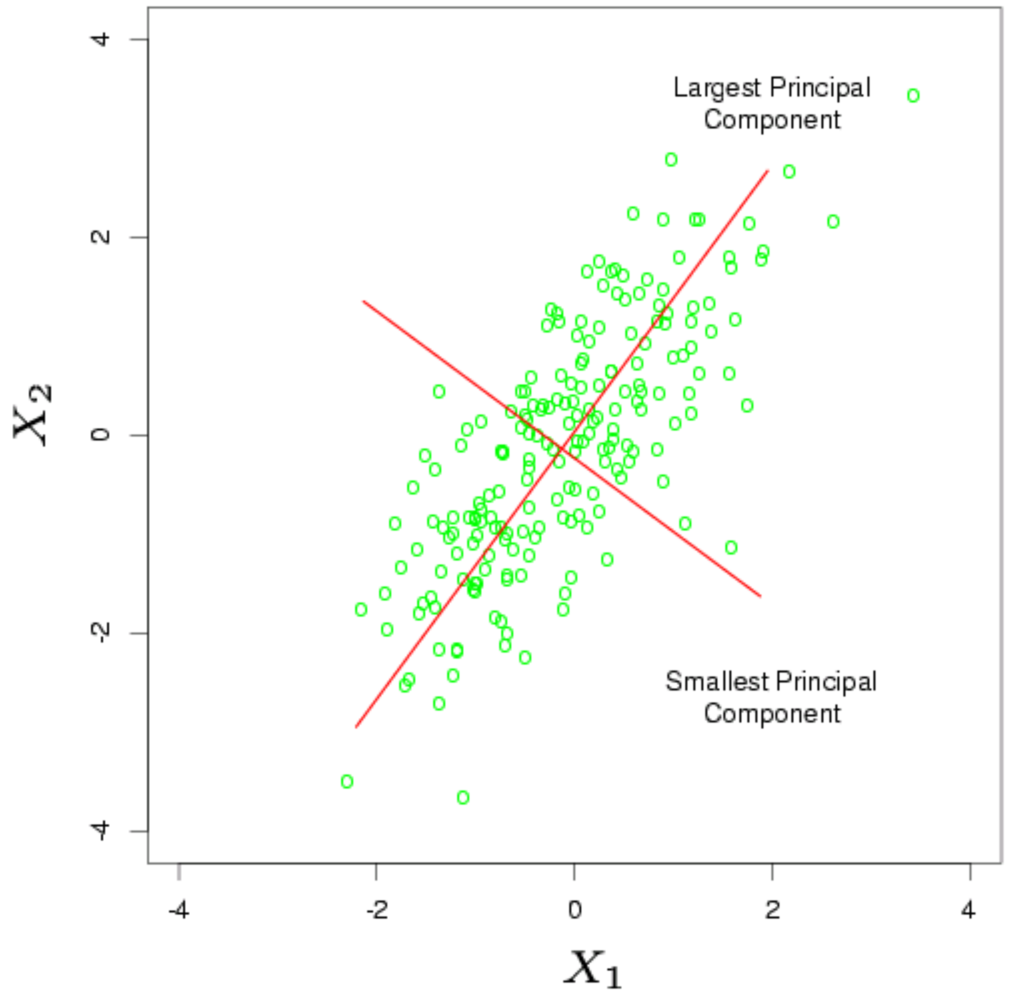
$$X^T X = VD^2V^T$$

The eigenvectors v_j are called the *principal components* of X
D is diagonal with entries $d_1 \geq d_2 \geq \ldots \geq d_p$

Xv_1 has largest sample variance amongst all normalized linear combinations of the columns of X

$$(\mathrm{var}(Xv_1) = \frac{d_1^2}{N})$$

Xv_k has largest sample variance amongst all normalized linear combinations of the columns of X subject to being orthogonal to all the earlier ones


Largest Principal Component
Smallest Principal Component
X_1
X_2
-4
-2
0
2
4

Principal Component Regression

PC Regression regresses on the first M principal components where $M<p$

Similar to ridge regression in some respects –

Partial Least Squares Regression

Y Centered, X_i has mean(X_i)=0, Var(X_i)=1 for all i.

1. $\hat{\varphi}_{1j} = \langle \mathbf{x}_j, \mathbf{y} \rangle$:   regressing **y** on each $\mathbf{x}_j$
2. $z_1 = \sum \hat{\varphi}_{1j} \mathbf{x}_j$
3. $\hat{\theta}_1 = \langle \mathbf{z}_1, \mathbf{y} \rangle / \langle \mathbf{z}_1, \mathbf{z}_1 \rangle$ coefficient of regressing **y** on $\mathbf{z}_1$,
4. Update the $\mathbf{x}_\mathrm{i}$'s by orthogonalizing them w/r $\mathbf{z}_1$.
5. Update **y** by the residuals of the previous linear fit.

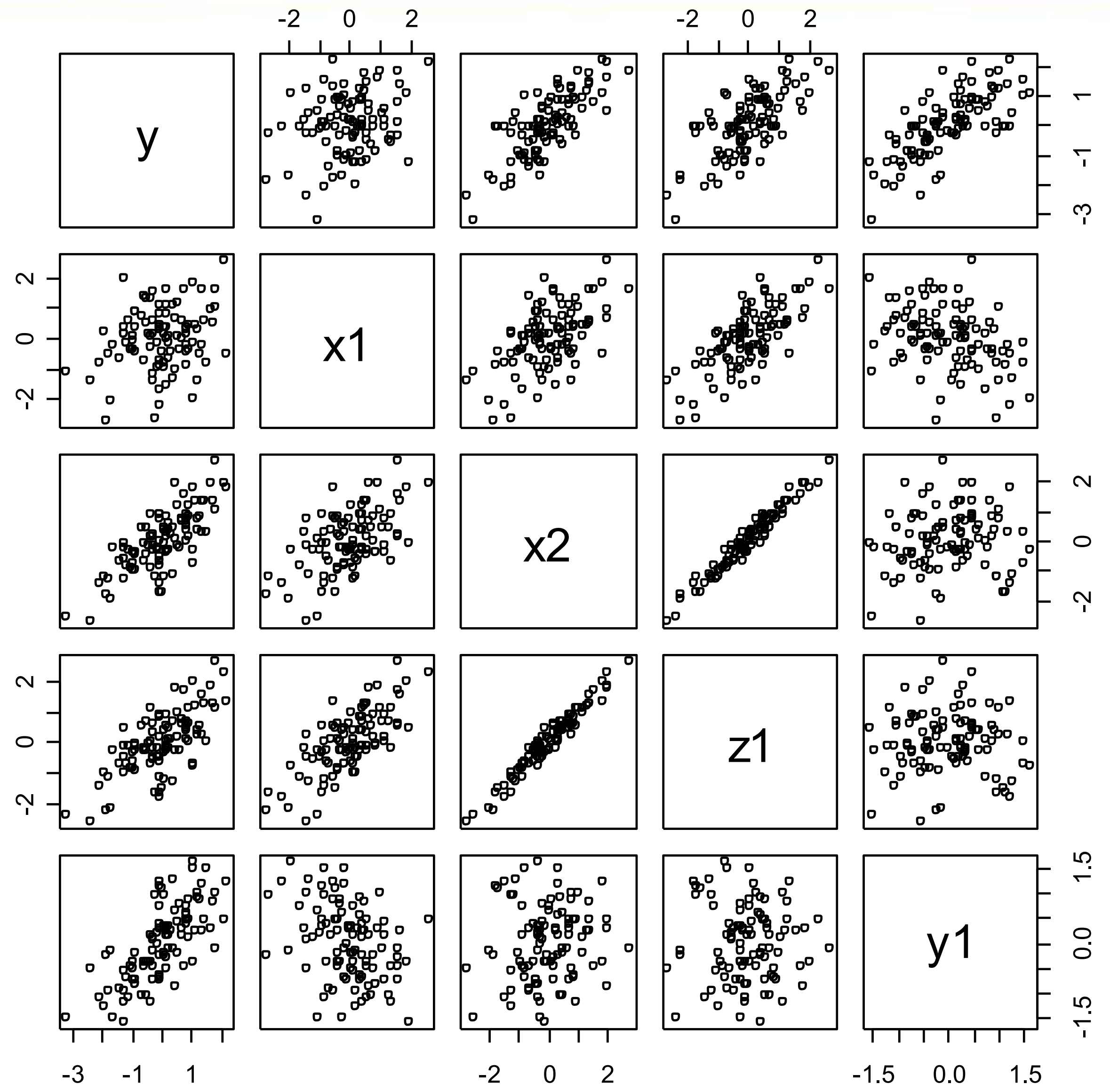
Iterate these 5 steps

This produces a sequence of orthogonal vectors $\{\mathbf{z}_i\}$ and a sequence of estimators $\hat{\beta}_j^{PLS}$

Simple R program

```
# Generate some data
y = rnorm(100)
y = y -mean(y)
x1 = rnorm(100)
x1 = (x1 - mean(x1))/sd(x1)
x2 = y+x1+rnorm(100)
x2 = (x2 - mean(x2))/sd(x2)
#
pi1 = sum(y*x1)
pi2 = sum(y*x2)
z1 = pi1*x1 + pi2*x2
z1 = (z1 - mean(z1))/sd(z1)
th1 = lsfit(z1,y,int=F)$coef
y1 = y - th1*z1
pairs(cbind(y,x1,x2,z1,y1))
```

Scatter Matrix of intermediate vars



Simple R program (cont.)

```
# Now we do the second iteration.
x11 = x1 - sum(x1*z1)*z1/sum(z1*z1)
x21 = x2 - sum(x2*z1)*z1/sum(z1*z1)
phi1 = sum(y1*x1)
phi2 = sum(y1*x2)
z2 = phi1*x11 + phi2*x21
z2 = (z2 - mean(z2))/sd(z2)
th2 = lsfit(z2,y1,int=F)$coef
y2 = y1 - th2*z2
#another way to calculate z2:
z2 = (x11-mean(x11))/sd(x11)
pairs(cbind(y1,x11,x21,z1,z2))
```