model selection in linear regression

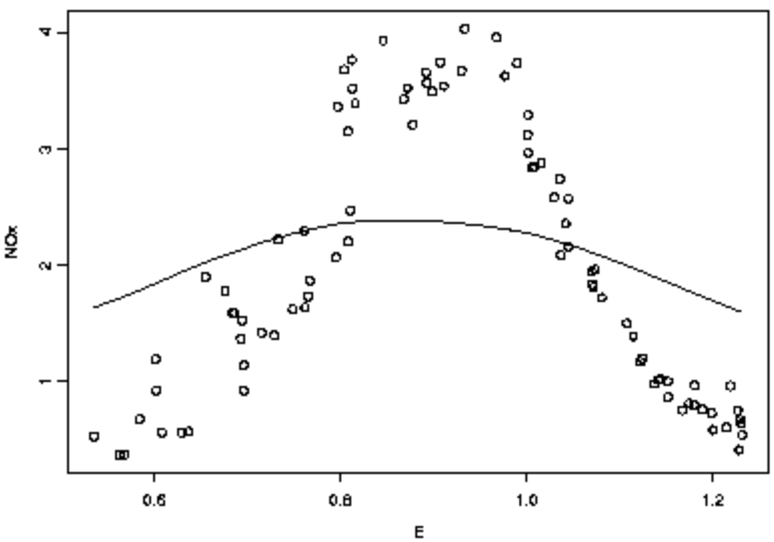
basic problem: how to choose between competing linear regression models

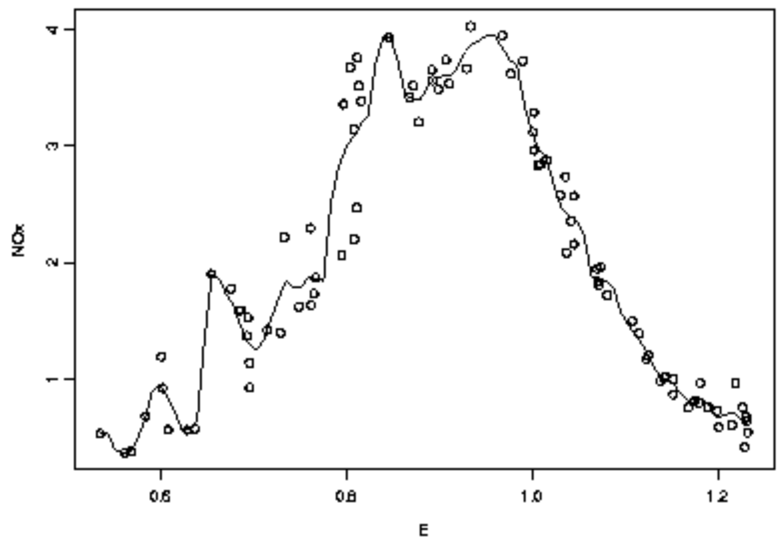
model too small: "underfit" the data; poor predictions;
high bias; low variance

model too big: "overfit" the data; poor predictions;
low bias; high variance

model just right: balance bias and variance to get
good predictions

Bias-Variance Tradeoff





High Bias - Low Variance

Low Bias - High Variance

"overfitting" - modeling the random component

Too Many Predictors?

When there are lots of X's, get models with high variance and prediction suffers. Three "solutions:"

1. Pick the "best" model

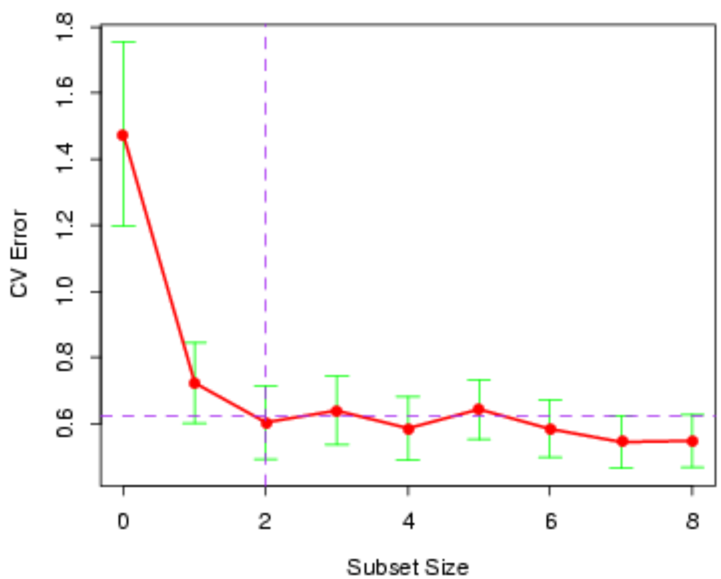
   Cross-validation
   Score: AIC, BIC
   All-subsets + leaps-and-bounds,
   Stepwise methods,

2. Shrinkage/Ridge Regression

3. Derived Inputs

Cross-Validation

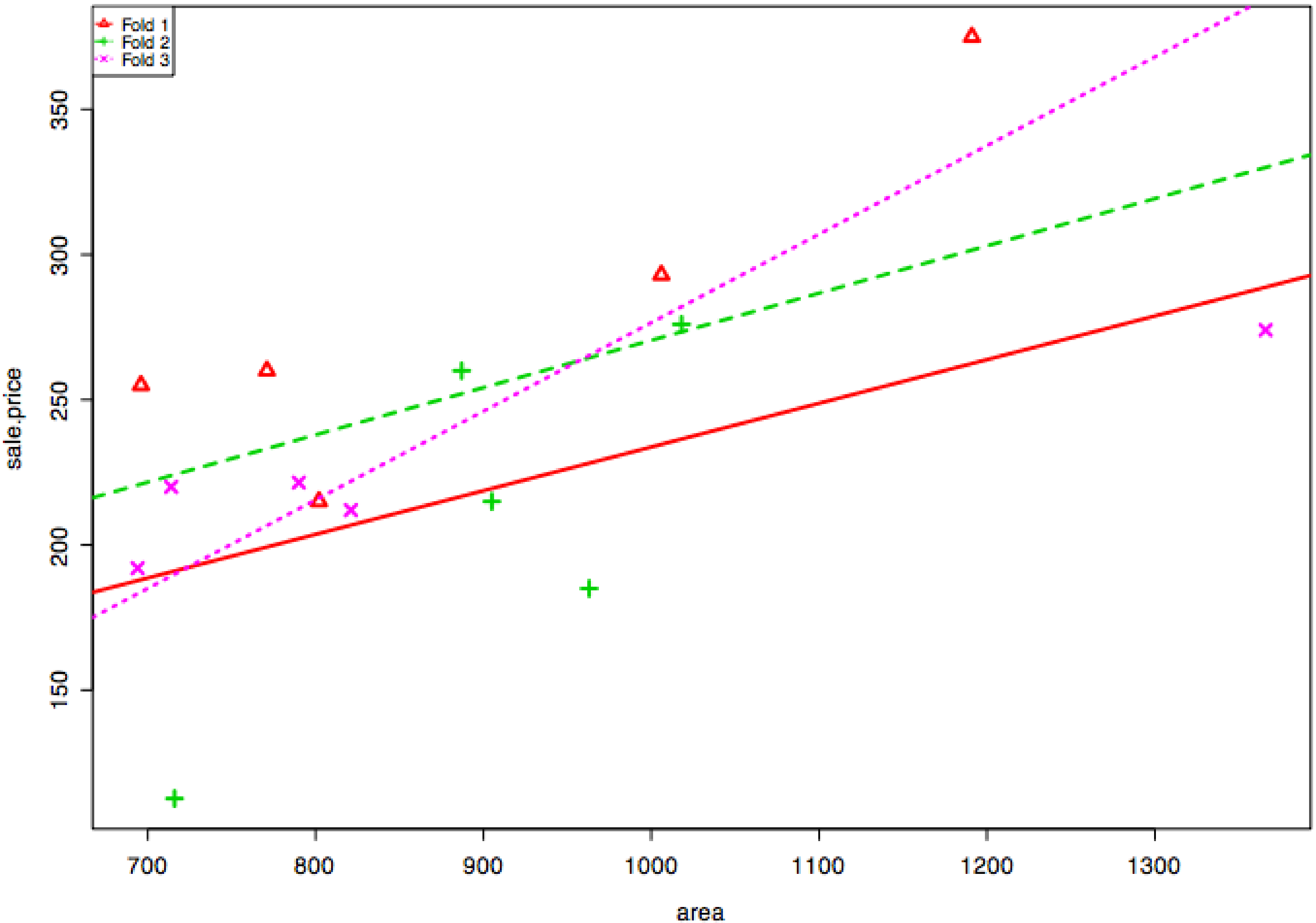
- e.g. 10-fold cross-validation:
  - Randomly divide the data into ten parts
  - Train model using 9 tenths and compute prediction error on the remaining 1 tenth
  - Do these for each 1 tenth of the data
  - Average the 10 prediction error estimates



"One standard error rule"

pick the simplest model within one standard error of the minimum

```
Library(DAAG)
houseprices.lm <- lm(sale.price ~ area, data=houseprices)
CVlm(houseprices,houseprices.lm,m=3)

    fold 1
    Observations in test set: 3 12 13 14 15
                 X11 X20   X21    X22  X23
    x=area     802.0 696 771.0 1006.0 1191
    Predicted  204.0 188 199.3  234.7  262
    sale.price 215.0 255 260.0  293.0  375
    Residual    11.0  67  60.7   58.3  113

    Sum of squares = 24000    Mean square = 4900    n = 5

    fold 2
    Observations in test set: 2 5 6 9 10
               X10  X13   X14     X17    X18
    x=area     905  716 963.0 1018.00 887.00
    Predicted  255  224 264.4  273.38 252.06
    sale.price 215  113 185.0  276.00 260.00
    Residual   -40 -112 -79.4    2.62   7.94

    Sum of squares = 20000    Mean square = 4100    n = 5
```


Fold 1
Fold 2
Fold 3
350
300
250
200
150
sale.price
700
800
900
1000
1100
1200
1300
area

```
fold 3
Observations in test set: 1 4 7 8 11
              X9  X12    X15   X16    X19
x=area     694.0 1366 821.00 714.0 790.00
Predicted  183.2  388 221.94 189.3 212.49
sale.price 192.0  274 212.00 220.0 221.50
Residual     8.8 -114  -9.94  30.7   9.01

Sum of squares = 14000    Mean square = 2800    n = 5
Overall ms
      3934
```

```
> summary(houseprices.lm)$sigma^2
[1] 2321
```

```
> CVlm(houseprices,houseprices.lm,m=15)
```

```
Overall ms
      3247
```

Quicker solutions

- AIC and BIC try to mimic what cross-validation does
- AIC(MyModel)
- Smaller is better

Quicker solutions

- If have 15 predictors there are 2^{15} different models (even before considering interactions, transformations, etc.)

- "Leaps and bounds" is an efficient algorithm to do all-subsets

```
# All Subsets Regression
library(leaps)

leaps <- regsubsets(newAccounts~.,data=bank,nbest=1,nvmax=15)
summary(leaps)

MySummary <- summary(leaps)
MySummary$bic

# plot a table of models showing variables in each model
# models are ordered by the selection statistic.
# plot(leaps)

# plot statistic by subset size
library(car)
subsets(leaps, statistic="rsq")
```

Variable selection with pure noise using leaps

```
y <- rnorm(100)
xx <- matrix(rnorm(4000),ncol=40)
dimnames(xx) <- list(NULL,paste("X",1:40,sep=""))
```

```
library(leaps)
xx.subsets <- regsubsets(xx, y, method="exhaustive",
nvmax=3, nbest=1)
subvar <- summary(xx.subsets)$which[3,-1]
best3.lm <- lm(y ~ -1 + xx[, subvar])
print(summary(best3.lm, corr=FALSE))
```

```
or…bestsetNoise(m=100,n=40)
```

run this experiment ten times:

-all three significant at $p<0.01$	1
-all three significant at $p<0.05$	3
-two out of three significant at $p<0.05$	3
-one out of three significant at $p<0.05$	1

- Stepwise methods are very popular but can perform badly

```
library(MASS)
fit <- lm(newAccounts~.,data=bank)
step <- stepAIC(fit, direction="both")
step$anova # display results
```

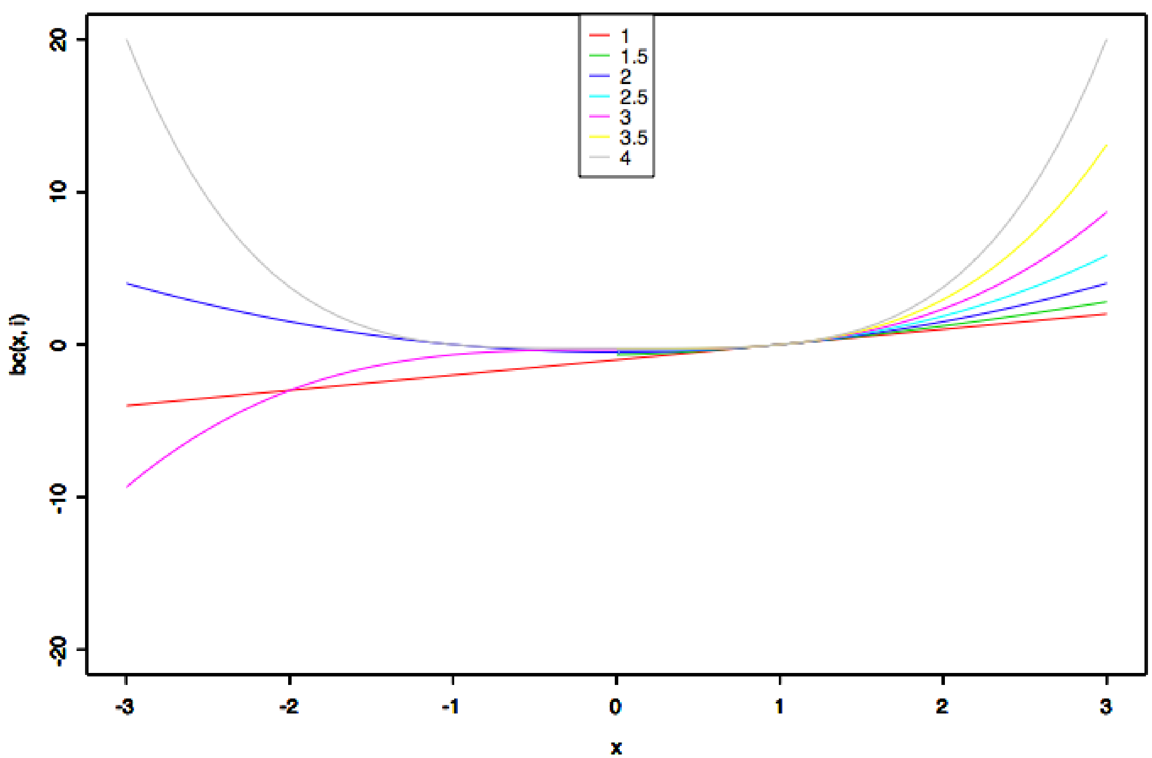
Transformations

log, exp, sqrt, sqr, cube root, cube, etc.

box-cox:

$$y^{(\lambda)} = \begin{cases} (y^{\lambda} - 1)/\lambda, & \lambda \neq 0 \\ \log y, & \lambda = 0 \end{cases}$$

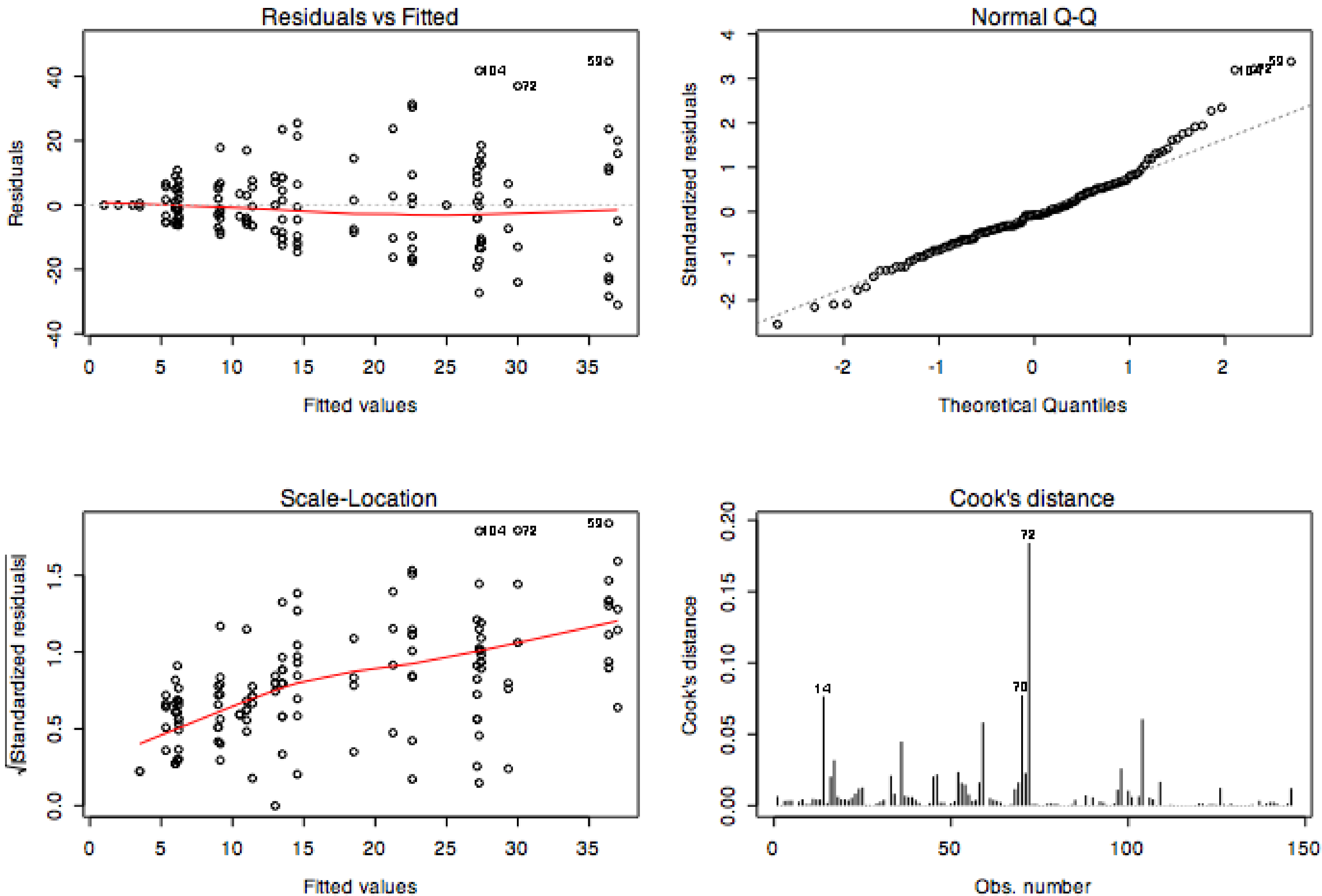
```
bc <- function(x,l) {(x^l-1)/l}
l<-seq(1,4,0.5)
x<-seq(-3,3,0.1)
par(new=FALSE)
for (i in l) {
       plot(x,bc(x,i),type="l",ylim=c(-20,20),col=2*i);
      par(new=TRUE)
}
legend("top",paste(l),col=2*l,lty=rep(1,length(l)))
```



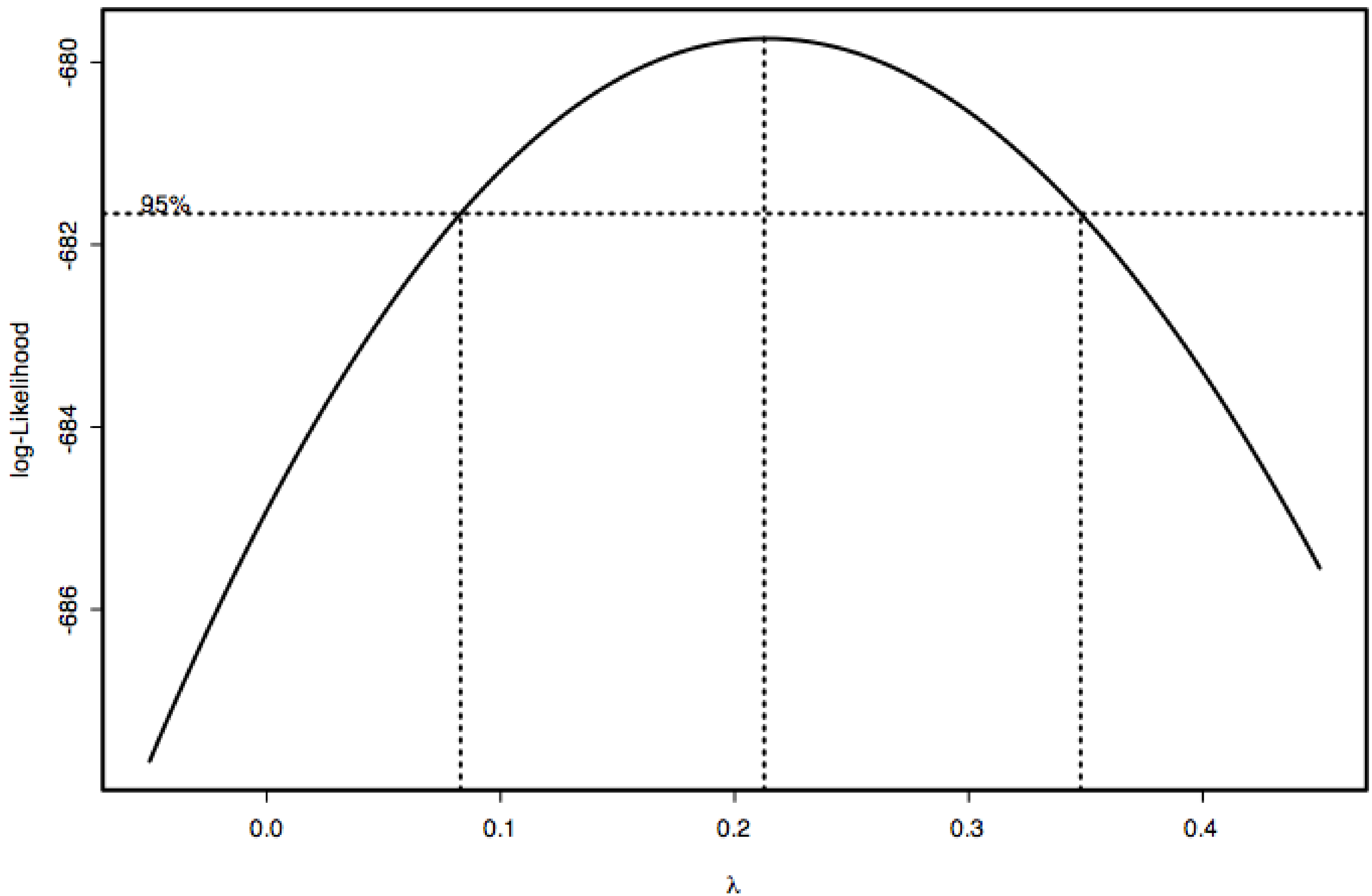
y=number of days absent from school in Quine, Australia

```
> attach(quine)
> table(Lrn,Age,Sex,Eth)
, , Sex = F, Eth = A

    Age
Lrn  F0 F1 F2 F3
  AL  4  5  1  9
  SL  1 10  8  0

, , Sex = M, Eth = A

    Age
Lrn  F0 F1 F2 F3
  AL  5  2  7  7
  SL  3  3  4  0

, , Sex = F, Eth = N

    Age
Lrn  F0 F1 F2 F3
  AL  4  6  1 10
  SL  1 11  9  0

, , Sex = M, Eth = N

    Age
Lrn  F0 F1 F2 F3
  AL  6  2  7  7
  SL  3  7  3  0
```

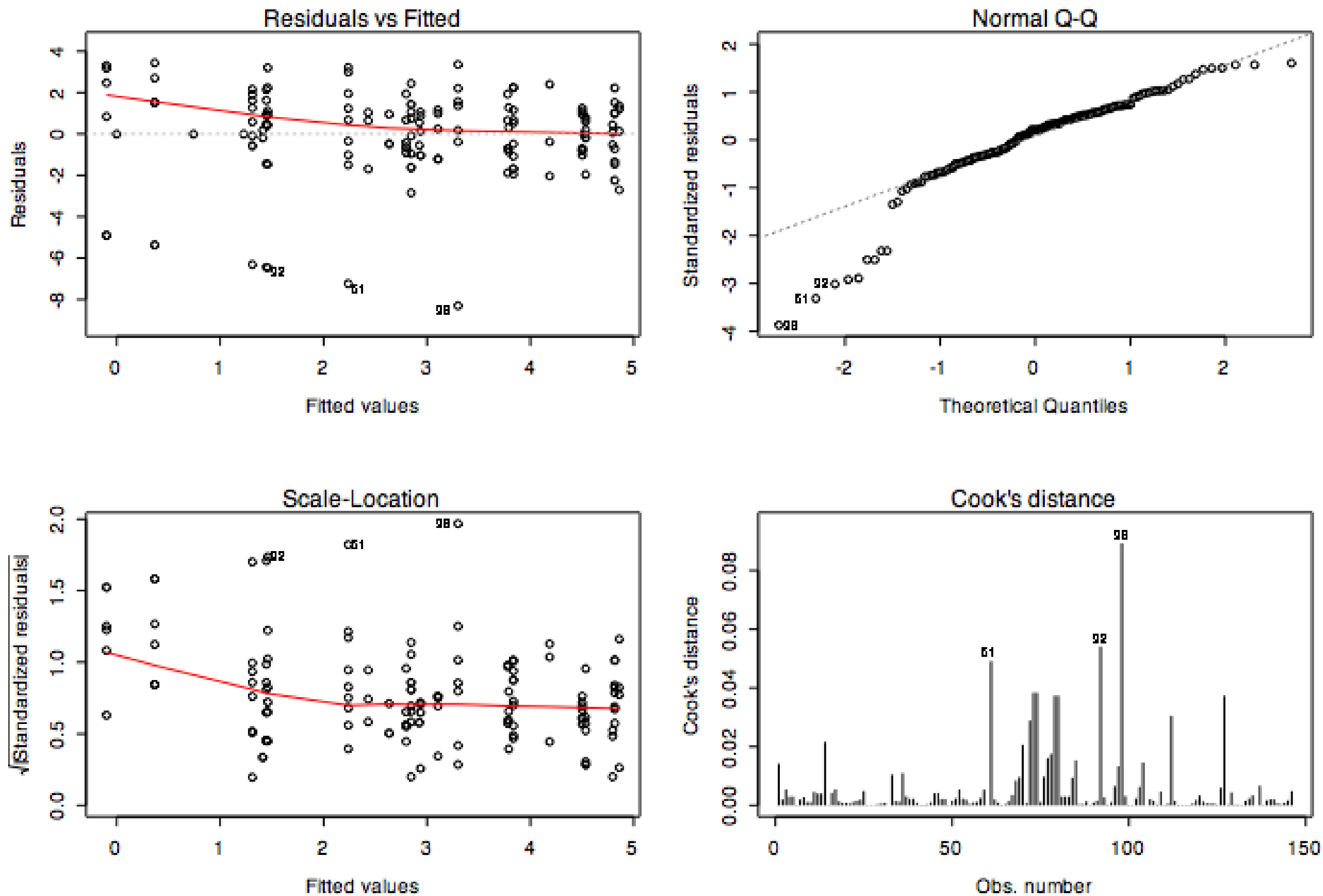
```
plot(lm(Days ~ Eth*Sex*Age*Lrn, data=quine),which=1:4)
```



```
> boxcox(Days+1 ~ Eth*Sex*Age*Lrn, data = quine,
         lambda = seq(-0.05, 0.45, len = 20))
```



```
quineBC <- quine
quineBC$Days <- (quineBC$Days^0.2 - 1)/0.2
plot(lm(Days ~ Eth*Sex*Age*Lrn, data=quineBC),which=1:4)
```



Shrinkage Methods

- Subset selection is a discrete process – individual variables are either in or out
- This method can have high variance – a different dataset from the same source can result in a totally different model
- 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

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

subject to: $$\sum_{j=1}^{p} \beta_j^2 \leq s$$

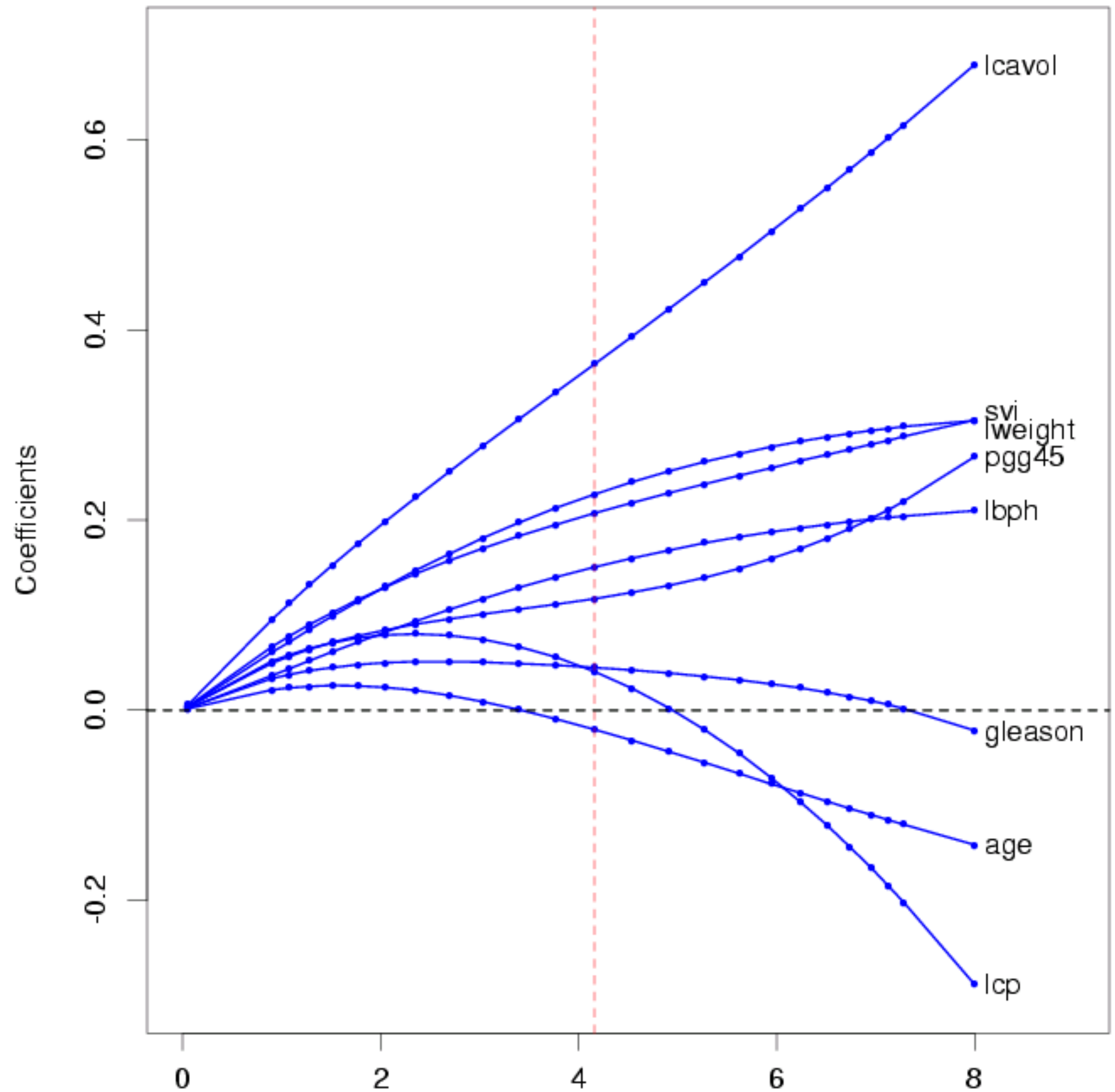
Equivalently:

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

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

works even when $X^T X$ is singular

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



$\mathrm{df}(\lambda)$ ← effective number of X' s

The Lasso

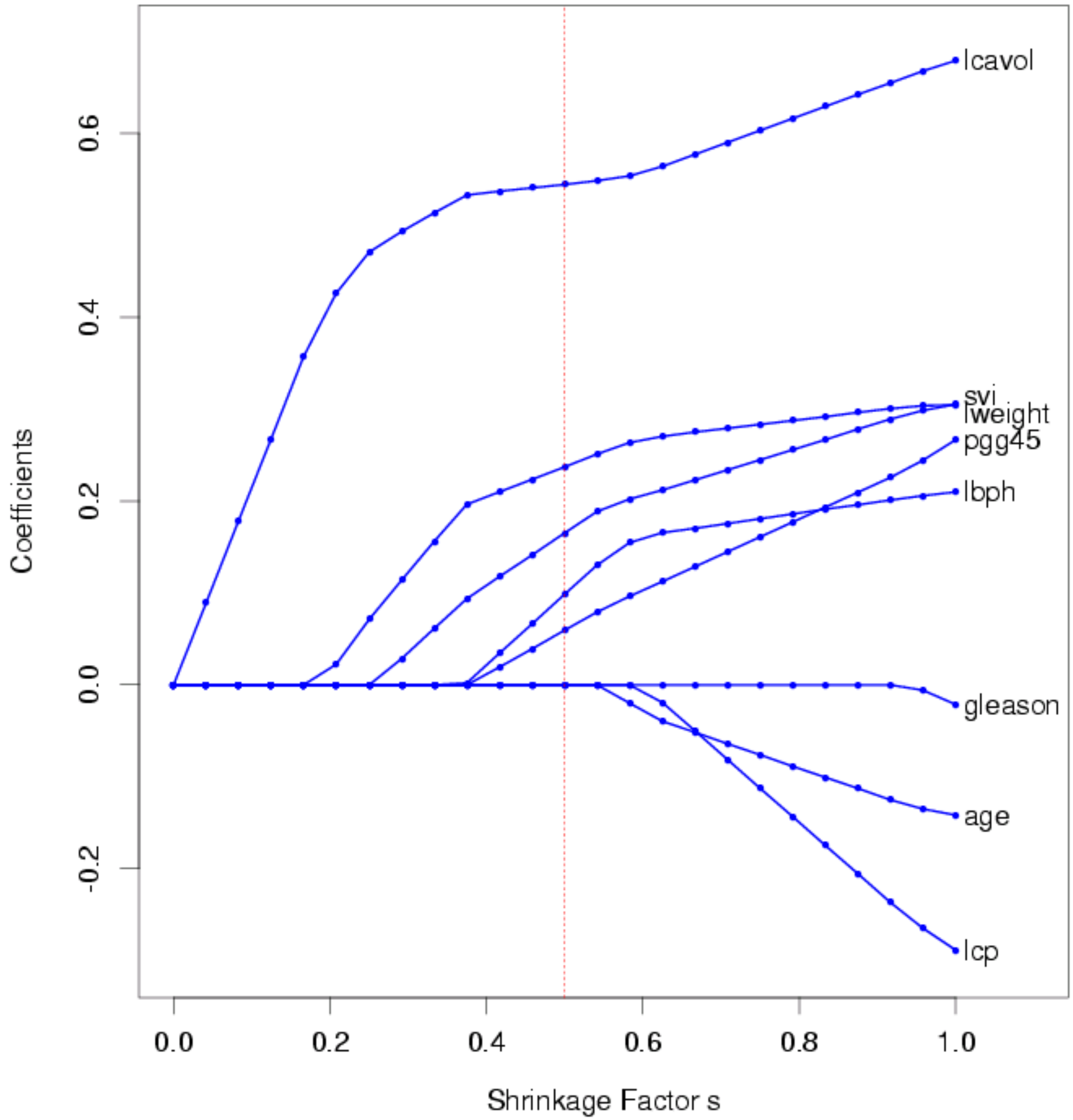
$$\hat{\beta}^{\text{ridge}} = \arg\min_{\beta} \sum_{i=1}^{N} (y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j)^2$$

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

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

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

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


lcavol
svi
lweight
pgg45
lbph
gleason
age
lcp
Coefficients
0.6
0.4
0.2
0.0
-0.2
0.0
0.2
0.4
0.6
0.8
1.0
Shrinkage Factor s

```
library(glmnet)
bank <- read.table("/Users/dbm/Documents/W2025/
BankSortedMissing.TXT",header=TRUE)
names(bank)
bank <- as.matrix(bank)
x <- bank[1:200,-1]
y <- bank[1:200,1]
fit1 <- glmnet(x,y)

xTest <- bank[201:233,-1]
predict(fit1,newx=xTest,s=c(0.01,0.005))

predict(fit1,type="coef")

plot(fit1,xvar="lambda")

MyCV <- cv.glmnet(x,y)
```