Model Assessment and Selection for Prediction - Part 2

UC Irvine - ISI BUDS 2022

Presented July 20, 2022

Daniel L. Gillen
Chancellor's Professor and Chair
Department of Statistics
University of California, Irvine

Ex: King County Birth Weight Data
- Best subsets regression
- Ridge regression
- Simulation study (AIC and BIC)

Estimation of the extra-sample error
- Cross-validation
- Bootstrap methods

Summary

Ex: King County birth weight data

Model selection and coefficient shrinkage

- In many prediction situations there are a large number of inputs, X
- While it may be the case that $f(X) = X^T\beta$ appropriately describes the underlying mechanisms, it is always the case that we have a finite training sample size, n
- Prediction accuracy:
  - least squares estimates may have low bias, but in 'small'-sample settings can exhibit large variability
  - we could sacrifice a little bias to reduce variation and achieve better overall predictive accuracy

Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

Ex: King County birth weight data

Model selection and coefficient shrinkage

- Another issue is interpretation:
  - with a large number of predictors, it may be hard conceptualize ‘holding everything else constant’
  - may be desirable to restrict attention to a smaller subset of variables which exhibit the strongest effects

Ex: King County birth weight data

King County birth data

- As an example, let's consider data on child birth weights for children born in King County, WA in 2001
- The dataset contains information on a sample of n=2,500 births from 2001
- The data was originally obtained to determine if a new state program ('First Steps') to educate women on proper nutrition during pregnancy was associated with greater birth weight
- The key outcome variable of interest is birth weight
  - Birth weight ranges from 255g to 5,175g
  - 5.1% of babies (127) were born at *low birth weight* ($<$ 2,500g)
- A total of 15 potential predictor variables are available for investigation

Ex: King County birth weight data

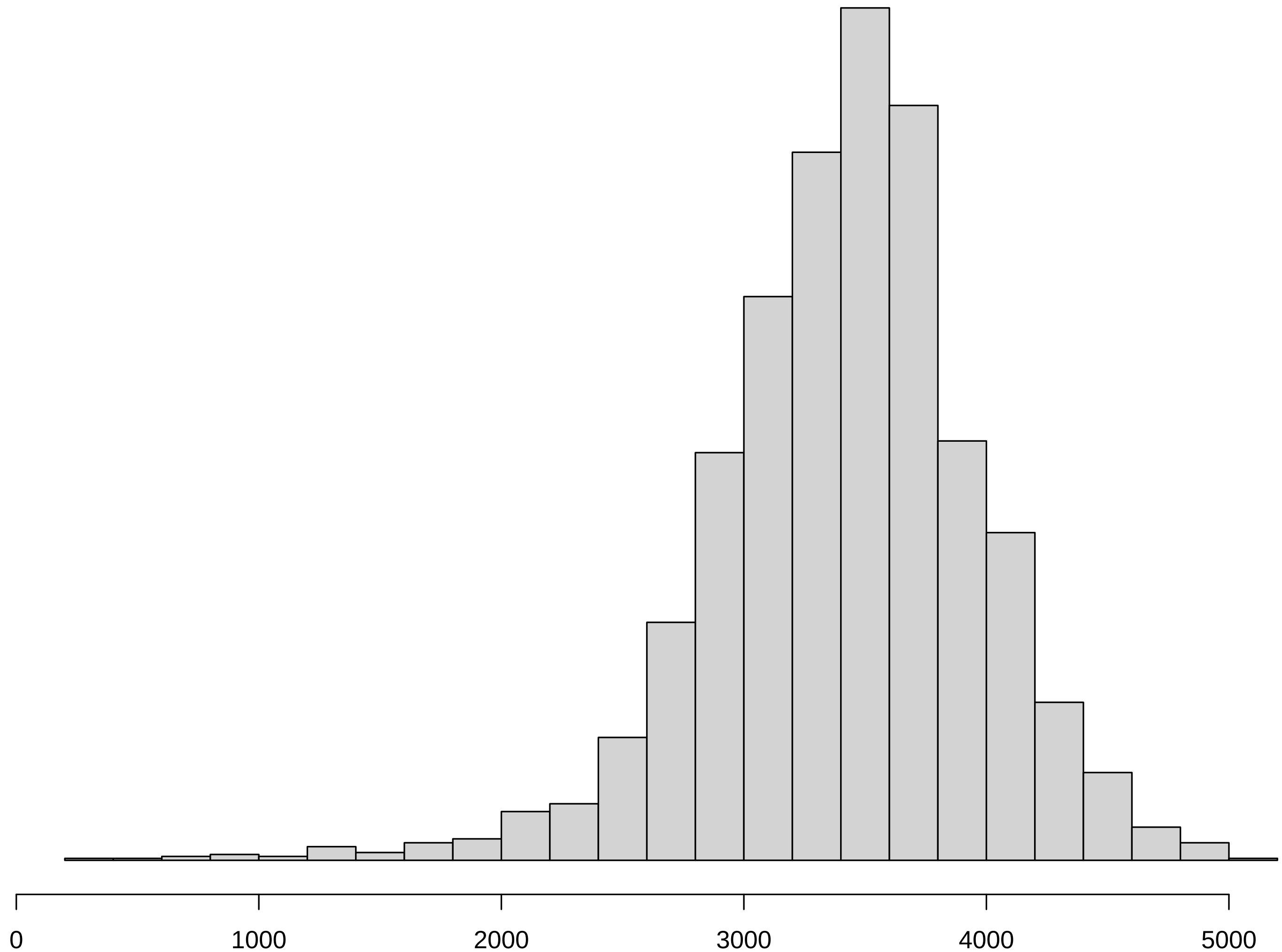
Complete variable listing

```
"gender"        M = male, F = female baby
"plural"        1 = singleton, 2 = twin, 3 = triplet
"age"           mother's age in years
"race"          race categories (for mother)
"parity"        number of previous live born infants
"married"       Y = yes, N = no
"bwt"           birth weight in grams
"smokeN"        number of cigarettes smoked per day during pregnancy
"drinkN"        number of alcoholic drinks per week during pregnancy
"firstep"       1 = participant in program; 0 = did not participate
"welfare"       1 = participant in public assistance program; 0 = did not
"smoker"        Y = yes, N = no, U = unknown
"drinker"       Y = yes, N = no, U = unknown
"wpre"          mother's weight in pounds prior to pregnancy
"wgain"         mother's weight gain in pounds during pregnancy
"education"     highest grade completed (add 12 + 1 / year of college)
"gestation"     weeks from last menses to birth of child
```


Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

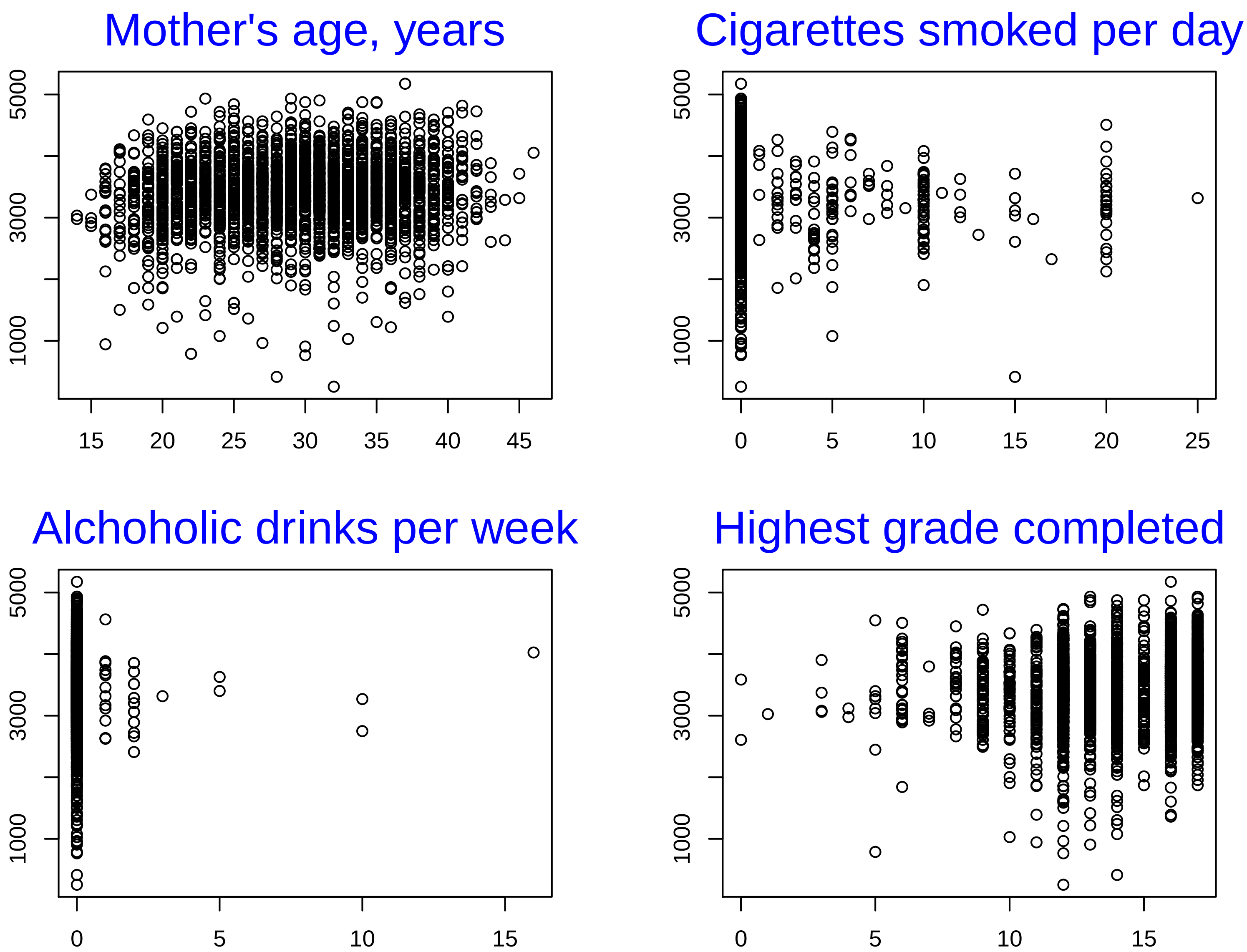
Distribution of birth weights from the King County data

Birth weight, grams



Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

Selected scatterplots from the King County data



Ex: King County birth weight data

Subset selection vs. shrinkage

- Rather than attempting to fit and report a model which includes all the potential predictors, we can consider two strategies
  - subset selection
  - shrinkage methods

Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

Ex: King County birth weight data

Subset selection

- Here we retain only a subset of variables
  - the remaining variables essentially have their β coefficients set to zero
- Various strategies exist for ‘choosing’ the variables to keep (or throw out)
  - best subset selection
  - stepwise strategies

Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

Ex: King County birth weight data

Best subsets regression

- Suppose X consists of p components; $X_1, \ldots, X_p$
- For each $k \in \{1, \ldots, p\}$, find the subset of k variables which results in the smallest residual sums of squares
  - other criteria include Mallow's C_p, R^2 and adjusted R^2
- Can quickly become computationally intensive when p gets large
- In `R`, code is implemented in the `leaps` package

Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

Ex: King County birth weight data

Best subsets regression in R

```
library(leaps)

## Model with only the intercept
##
fit0 <- lm(bwt ~ 1, data=weight)

## Perform best subsets analysis
##
##  maxModel: a model which includes all the variables you wish to
##            entertain
##  nvmax:    maximum number of variables for the subset selection
##  nbest:    specify, for any given k, the number of the best models
##            are to be returned
##
maxModel <- as.formula(bwt ~ gender + age + race + parity + married
                             + smokeN + drinkN + firststep + welfare
                             + smoker + drinker + wpre + education )

bestSub  <- summary(regsubsets(maxModel, data=weight,
                         nvmax=17, nbest=10))
```

Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

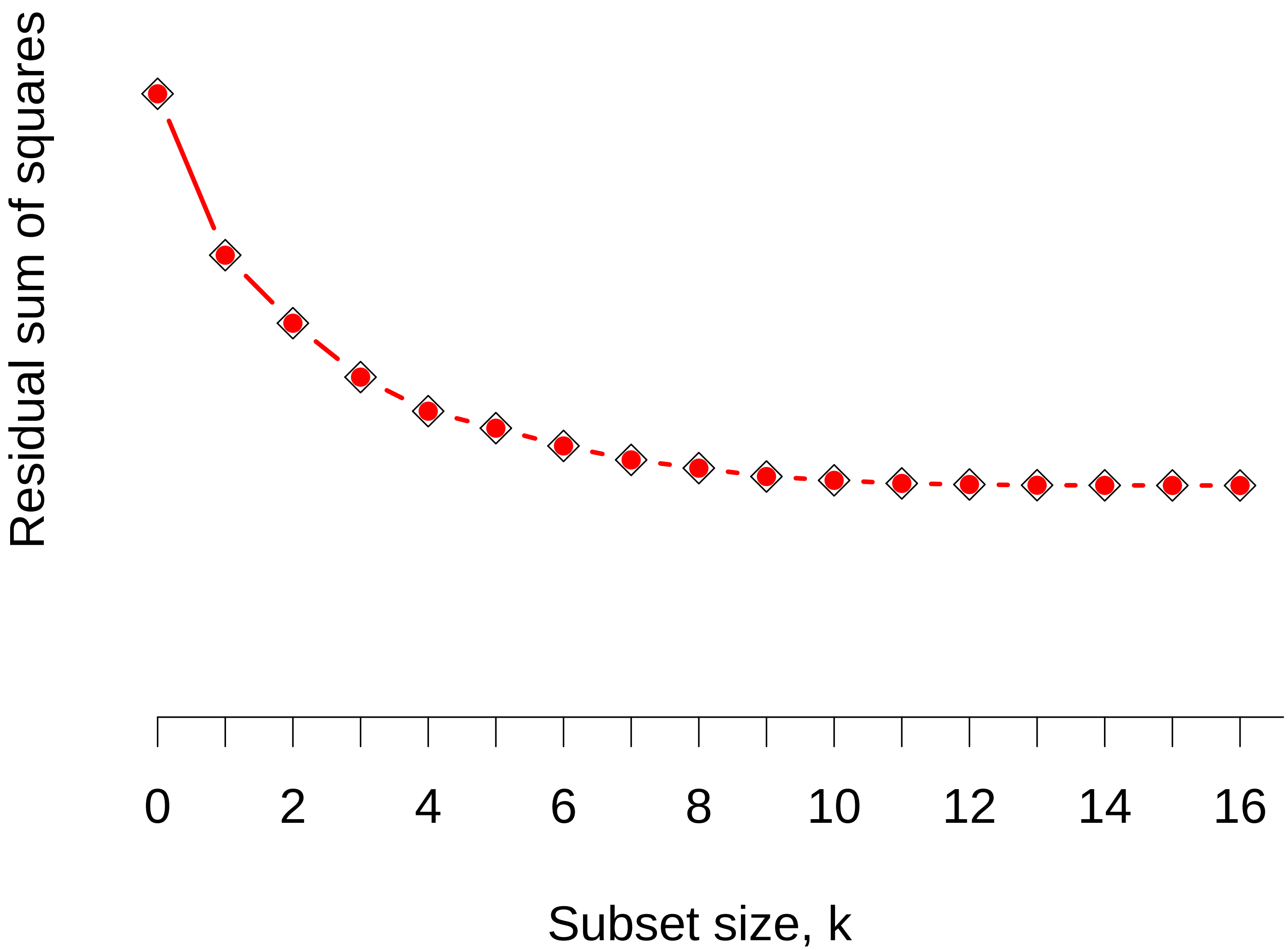
Ex: King County birth weight data

Best subsets regression in R

```
names(bestSub)
[1] "which"  "rsq"    "rss"    "adjr2"  "cp"     "bic"
    "outmat" "obj"

## 'results' contains the subset size, k, and the residual
## sum of squares

results <- c(0, sum((weight$bwt- fitted(fit0))^2))
results <- rbind(results,
                 cbind(apply(bestSub$which, 1, sum)-1, bestSub$rss))

##
##### Look at minimum residual sums of squares
##
minRSS <- tapply(results[,2], results[,1], FUN=min)
```


Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

Best subset selection for the King County 2001 birth weight data



Ex: King County birth weight data

Best subsets regression

- The best-subset curve is necessarily decreasing, so it cannot be used as a criteria for choosing k
- Typically choose a model which minimizes an estimate of the EPE
  - Mallow's C_p, AIC, BIC, cross-validation

Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

Ex: King County birth weight data

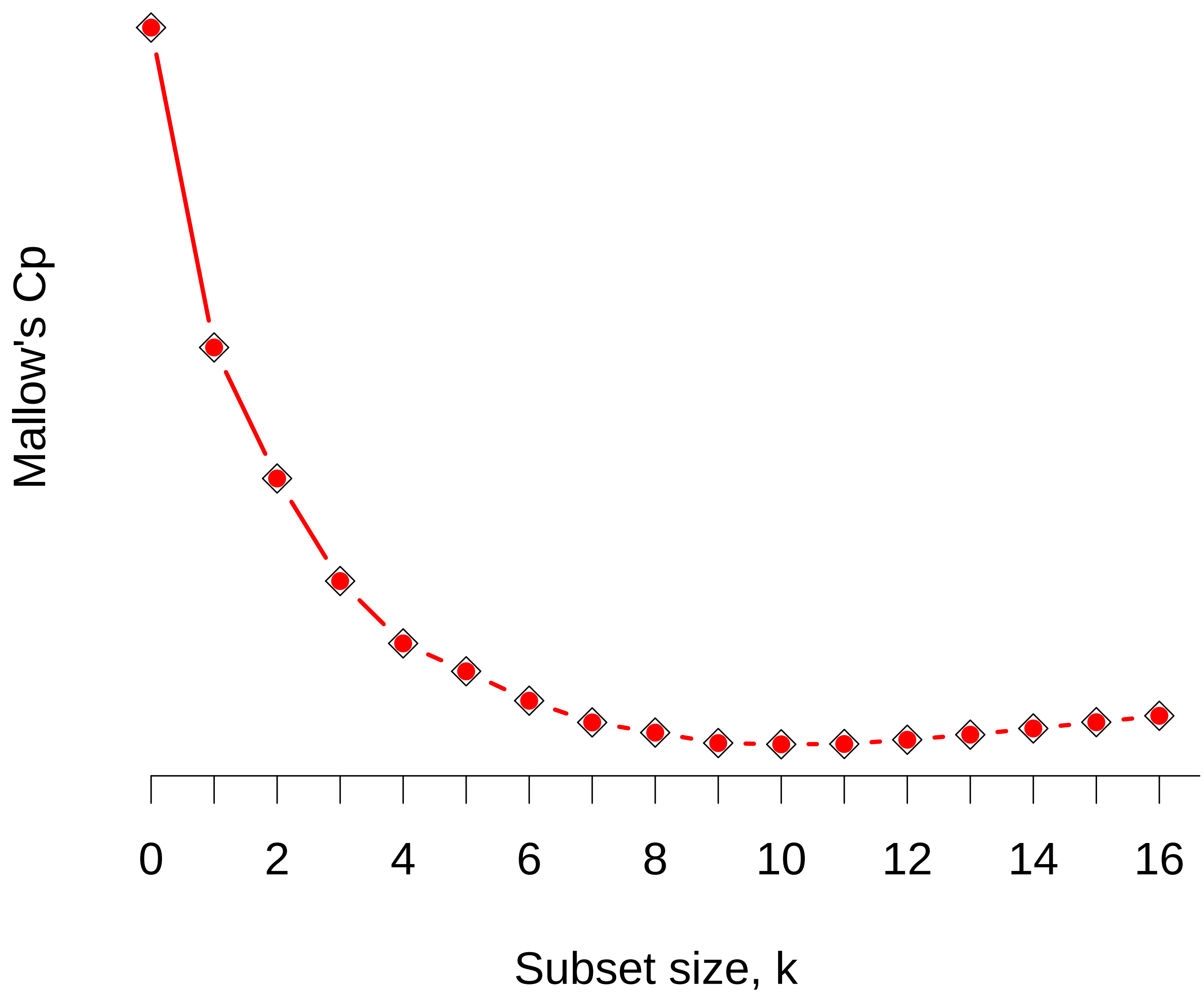
Best subsets regression in R

```
##
#####
#####        Now let's do best subsets with Cp as the criteria
#####
##
bestSubCp  <- leaps(x=model.matrix(fitF),
                        y=weight$bwt, int=FALSE,
                        nbest=1, method="Cp")
## 'results' contains the subset size, k, and the Cp value
##
results <- NULL
results <- rbind(results, cbind(apply(bestSubCp$which, 1, sum)-1,
                                        bestSubCp$Cp))

##
minCp<- tapply(results[,2], results[,1], FUN=min)
```

UCIrvine
University of California, Irvine

Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

Best subset selection for the King County 2001 birth weight data



Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

UCIrvine
University of California, Irvine

Best subsets regression in R

```
##
#####
#####        Compare which were selected in the k=10 models...
#####
##
> cbind( dimnames( model.matrix(fitF) )[[2]],
                 bestSubCp$which[11,],
                 bestSubRSS$which[11,] )

  [,1]            [,2]    [,3]
1 "(Intercept)"   "TRUE"  "TRUE"
2 "genderM"       "TRUE"  "TRUE"
3 "age"           "FALSE" "FALSE"
4 "raceblack"     "FALSE" "FALSE"
5 "racehispanic"  "TRUE"  "TRUE"
6 "raceother"     "FALSE" "TRUE"
7 "racewhite"     "TRUE"  "TRUE"
8 "parity"        "TRUE"  "TRUE"
9 "married"       "TRUE"  "TRUE"
A "smokeN"        "TRUE"  "TRUE"
B "drinkN"        "FALSE" "FALSE"
C "firststep"     "FALSE" "FALSE"
D "welfare"       "TRUE"  "TRUE"
E "smokerY"       "TRUE"  "TRUE"
F "drinkerY"      "FALSE" "FALSE"
G "wpre"          "TRUE"  "TRUE"
H "education"     "TRUE"  "TRUE"
```

Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

Ex: King County birth weight data

Stepwise procedures

- Instead of performing an exhaustive enumeration for each value for k, we can search for a 'good path'
- Forward selection
  - start with an 'intercept-only' model and build up the model
- Backward selection
  - start with a 'full' model and reduce the model
- In R, see `stepAIC` in the `MASS` library

Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

Ex: King County birth weight data

Stepwise AIC in R

```
library(MASS)
##
#####
#####        Stepwise selection using AIC
#####
##
fitStepAIC <- stepAIC( fit0, scope=maxModel, direction="forward" )
.
.
.
>Step:  AIC=31425
bwt ~ wpre + smoker + gender + married + race + parity + welfare +
    education + smokeN

            Df Sum of Sq      RSS      AIC
<none>                   7.12e+08 3.14e+04
+ drinker    1  1.96e+05 7.12e+08 3.14e+04
+ drinkN     1  4.37e+04 7.12e+08 3.14e+04
+ firststep  1  2.41e+04 7.12e+08 3.14e+04
+ age        1  1.88e+04 7.12e+08 3.14e+04
```

Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

Ex: King County birth weight data

Shrinkage methods

- Rather retaining some variables and discarding the rest, an alternative is to keep all the variables but impose restrictions on the size of the coefficients
  - the point esitmates for $\boldsymbol{\beta}$ are subject to bias
  - results often don't suffer as much in terms of variability

- Ridge regression imposes an L_2-type penalty
  - the solution is give by

$$\hat{\boldsymbol{\beta}}^{\text{ridge}} = \text{argmin}_{\boldsymbol{\beta}} \, \text{RSS}(\boldsymbol{\beta})$$

subject to the constraint:

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

  - value of s influences how large the components of $\boldsymbol{\beta}$ can get

Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

Ex: King County birth weight data

Shrinkage methods

- An alternative way of writing the problem is

$$\hat{\beta}^{\text{ridge}} = \text{argmin}_{\beta} \left\{ \text{RSS}(\beta) + \lambda \sum_{j=1}^{p} \beta_j^2 \right\}$$

- Here, $\lambda \geq 0$ controls the amount of shrinkage
  - when $\lambda = 0$, we are performing ordinary least squares estimation
  - for large λ, minimizing the penalized RSS requires the components of β to be small
  - there is a one-to-one relationship between λ and s

- Minimization yields the solution

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

- Could allow λ to be a vector, and ensure no shrinkage among certain coefficients

Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

Ex: King County birth weight data

Shrinkage methods

- The solution is linear, and we can therefore obtain the effective degrees of freedom as

$$\text{df}(\lambda) = \text{tr}\{\mathbf{X}(\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\}$$

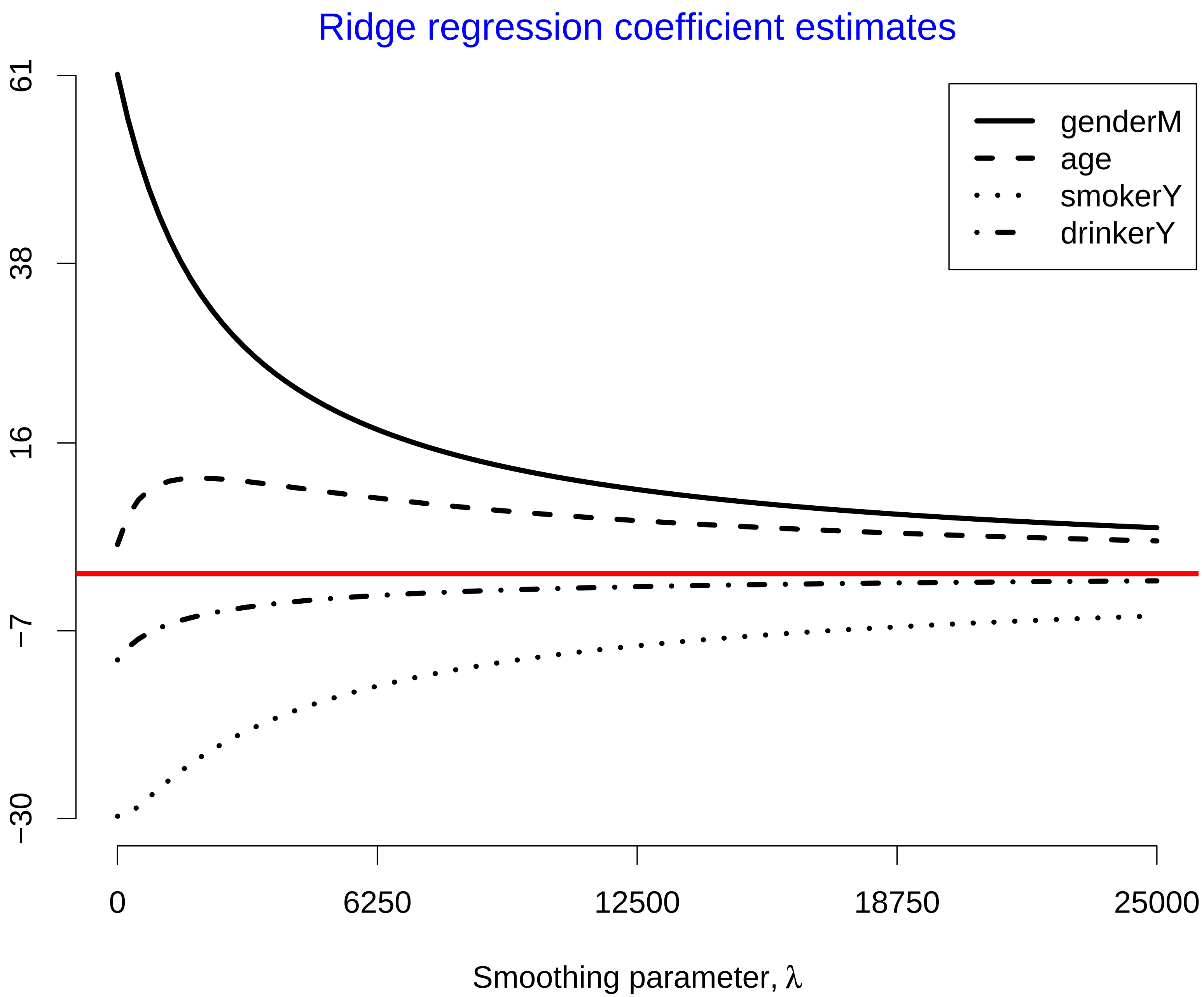
  - depends on the complexity/smoothing parameter λ

- Ridge regression for the linear model is implemented in R

```
library(MASS)

ridgeFit  <- lm.ridge(maxModel, data=weight,
                      lambda=c(0, 100, 1000, 10000))
```

Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

Ridge regression for the King County Birth data



Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

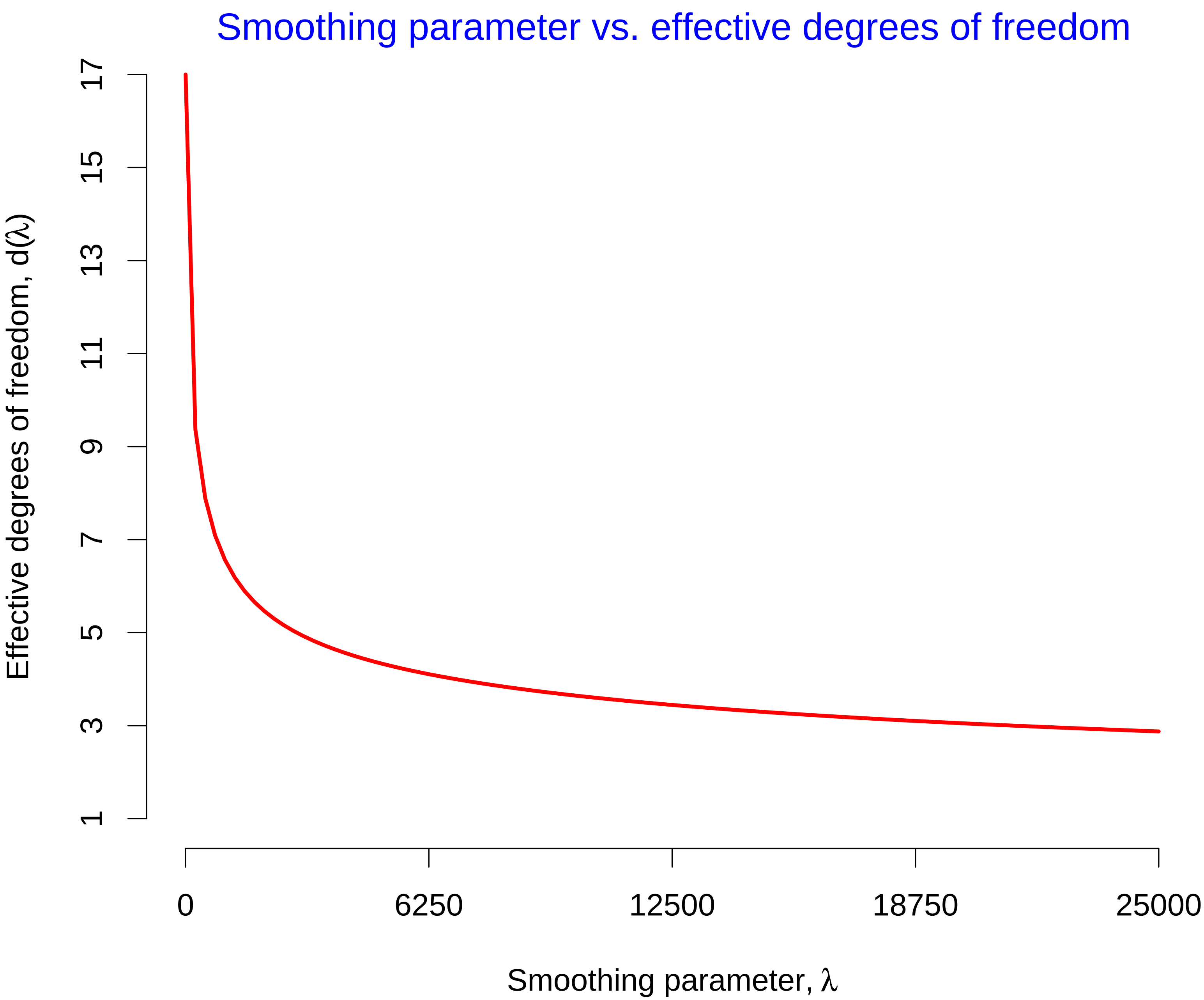
Ex: King County birth weight data

Ridge regression results for King County data

- Relationship between λ and df(λ) is non-linear
- For these data, there is a dramatic reduction in 'complexity' of the model up to about λ = 1,000

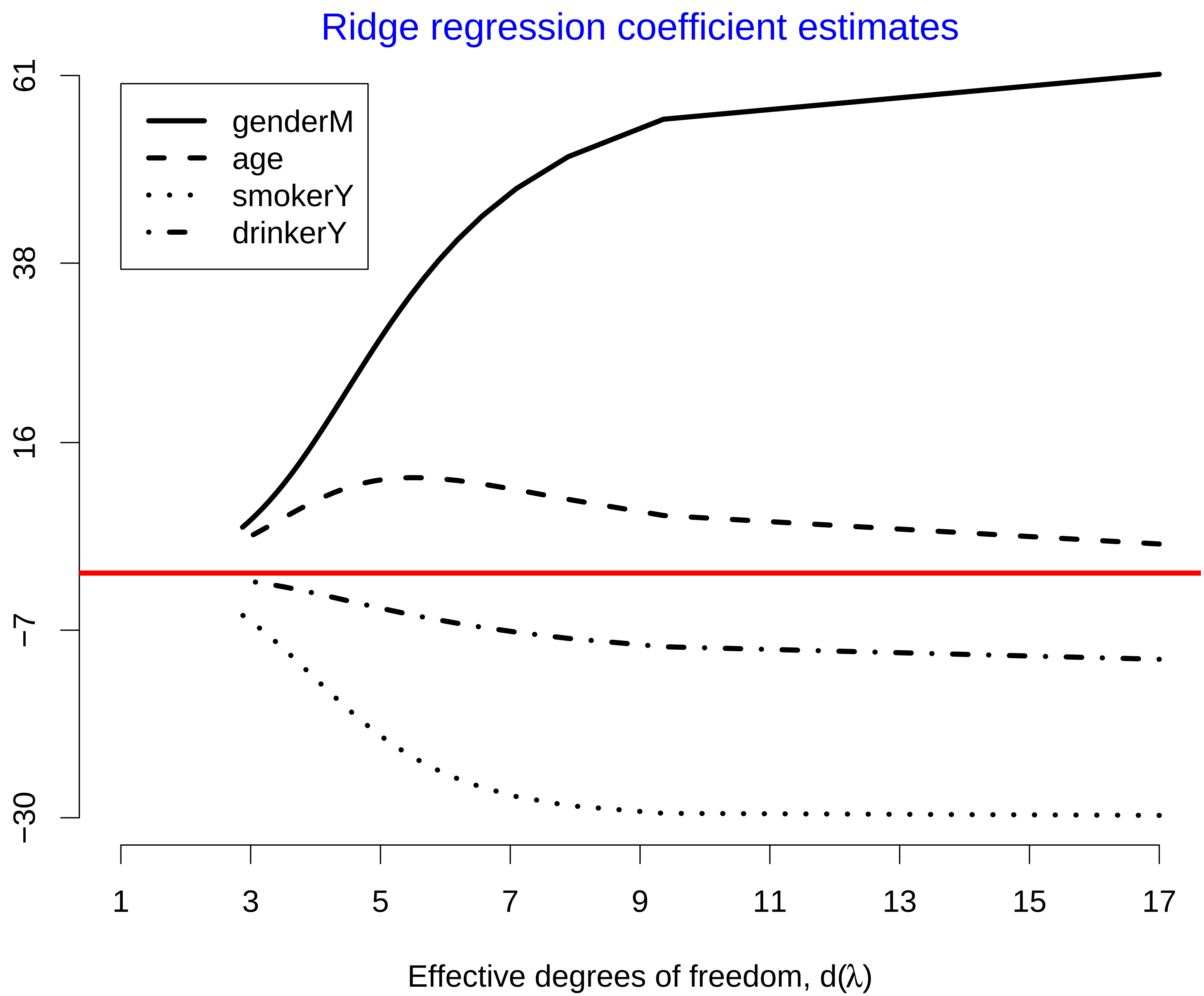
Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

Ridge regression for the King County Birth data



Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

Ridge regression for the King County Birth data



Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

Model selection for 'complexity'

AIC vs. BIC

- Up to a constant of proportionality, AIC and BIC differ in terms of the penalty imposed on increasing complexity

$$\begin{aligned} \text{AIC} &\Rightarrow 2p \\ \text{BIC} &\Rightarrow (\log n)p \end{aligned}$$

  - for reasonable sample sizes, BIC imposes a heavier penalty

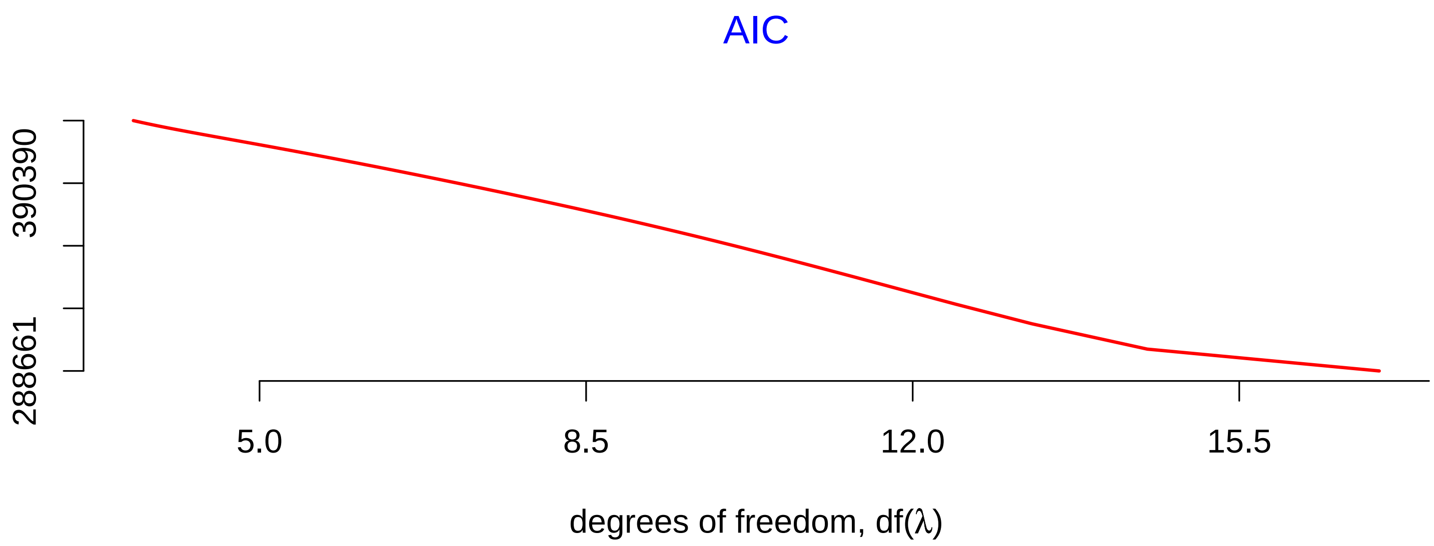
- Unfortunately, in practice, there isn't a clear choice between the two

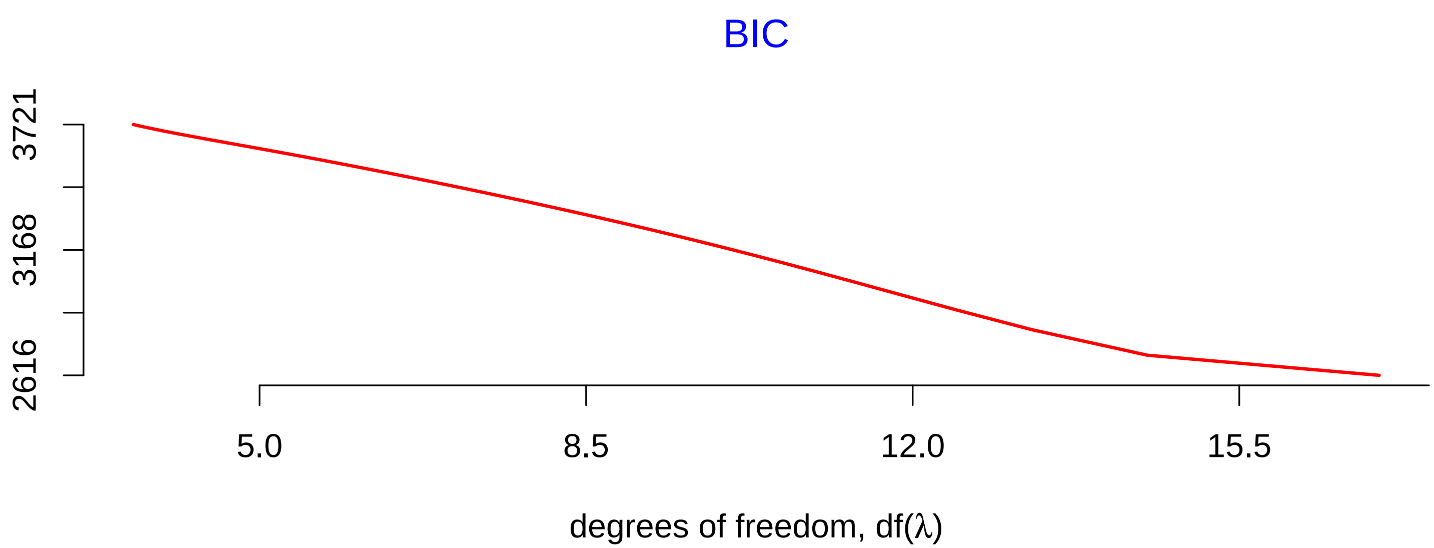
- We can investigate their relative merits using the King county birth weight data

  - consider determining the value of λ in a ridge regression analysis which includes all 13 predictors

Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

AIC and BIC for a ridge regression analysis of the King county birth weight data





Model selection for 'complexity'

AIC vs. BIC

- It seems that both AIC and BIC choose the optimal value of λ to be zero
  - degrees of freedom = 17
- They both favor the most complex models
  - neither penalty seems to offset the reduction in RSS by increasing the complexity of the model
- Even though we are estimating 17 parameters with 2500 observations, seems that there should still be room for improvement in the model...

Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

Estimation of the extra-sample error

Extra-sample error

- While AIC and BIC permit an analytic treatment of assessing the predictive ability of a given model, their focus on the in-sample error, Err, is somewhat of a drawback

- Here we return to estimation of the extra-sample error,

$$\text{EPE} \;=\; \mathrm{E}_{X,Y}\left[L(Y,\hat{f}(X))\right],$$

  interpreted as the generalization error when the prediction rule $\hat{f}(\cdot)$ is applied to an independent test sample, from the joint distribution of X and Y

- Both approaches we consider here involve the clever use and re-use of the training data

Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

Cross-validation

Cross-validation

- One possibility for choosing λ could be to attempt to to minimize the observed mean squared error:

$$err = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

- However, this is typically a poor estimate of mean squared prediction error (or out-of-sample prediction error)
- One aspect of the problem is that the estimate $\hat{y}_i = \hat{f}(x_i)$ uses the observed outcome y_i, as well as the others, to predict y_i
- One solution to this would be to predict y_i using all the observations *except* the i^{th} case

Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

UCIrvine
University of California, Irvine

Cross-validation

- If we denote the resulting prediction as $\hat{y}_{(i)}$, then the corresponding sum of squared residuals is referred to as the *predicted residual sum of squares*

$$\text{PRESS} = \sum_{i=1}^{n} \left(y_i - \hat{y}_{(i)}\right)^2$$

- PRESS is also referred to as the *cross-validation* statistic
  - *leave-one-out cross-validation*
  - denote with CV
- In general situation the computational burden can be substantial
  - requires n fits of the model

Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

Cross-validation

Cross-validation

- However, calculation of the CV statistic is fairly straightforward for linear models
  - leave-one-out, or deleted, residuals are obtained from the residuals of the model based on all the data as well as the hat matrix, **H**

$$y_i - \hat{y}_{(i)} = \frac{y_i - \hat{y}_i}{1 - H_{ii}}$$

where H_{ii} denote the i^{th} diagonal element of **H**

- We therefore have

$$\text{CV} = \frac{1}{n} \sum_{i=1}^{n} \left[\frac{y_i - \hat{y}_i}{1 - H_{ii}} \right]^2$$

Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

Cross-validation

Generalized cross-validation

- The generalized cross-validation statistic arises when we approximate the H_{ii} by their average

$$\text{GCV} = \frac{1}{n}\sum_{i=1}^{n}\left[\frac{y_i - \hat{y}_i}{1 - \text{trace}(\mathbf{H})/n}\right]^2$$

- For the case of penalized regression, we replace trace($\mathbf{H}$) with the effective degrees of freedom

Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

Cross-validation

K-fold cross-validation

- Leave-one-out cross-validation involves splitting the data into n parts
- The approach can be generalized somewhat by splitting the data into $K < n$ parts as follows

(1) Split the data into K roughly equal parts, and denote the collection of indexes for the k^{th} part as C_k, $k = 1, \ldots, K$

(2) For each part, fit a model using all the remaining data,

$$\mathbf{y}^{(k)} = \{y_i \mid i \notin C_k\},$$

and denote the fitted model as $\hat{f}^k(x)$

(3) For all i such that $i \in C_k$, obtain a prediction via

$$\hat{y}_i = \hat{f}^k(x_i)$$

UCIrvine University of California, Irvine

Cross-validation

K-fold cross-validation

- Let $k(i)$ denote the part in which y_i resides
- The K-fold cross validation statistic, for a general loss function, is given by

$$\mathrm{CV}_K = \frac{1}{n}\sum_{i=1}^{n} L(y_i, \hat{f}^{-k(i)}(x_i))$$

where L denotes a *loss function*. (We have been considering squared error loss so that

$$L(y_i, \hat{f}^{-k(i)}(x_i)) = (y_i - \hat{f}^{-k(i)}(x_i))^2$$

- As we decrease K, however, the bias of CV_K as an estimate of MS[P]E increases
  - CV_K is biased upward
  - extent depends on the sample size

Cross-validation

Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

Cross-validation for ridge regression

- The `select()` in the `MASS` library minimizes the generalized cross validation statistic for ridge regression
- Let's compare the complexity of the model when GCV is used as opposed to AIC and BIC

```
##
#####
##### How does AIC/BIC compare with GCV???
#####
##
maxLambda <- 25000
lambdaVal <- seq(from=0, to=maxLambda, length=100)
select(lm.ridge(maxModel, data=weight, lambda=lambdaVal))
Xmat       <- model.matrix(lm(maxModel, data=weight))

calcDF(Xmat, lambda=252.53)
> [1] 9.3619
```

So, the effective degrees of freedom using cross validation are 9.36, as compared to 17 for AIC and BIC

UCIrvine
University of California, Irvine

Bootstrap estimates of prediction error

- Let $\hat{f}^b(\cdot)$ denote the estimate of $f(\cdot)$ obtained from the b^{th} bootstrap replicate, $b = 1, \ldots, B$
- For each fit, keep a track of how well it predicts the original training data
  - evaluate the training error for each fit
- We could average across the B replicates to get an estimate of EPE

$$\widehat{\text{EPE}}_{\text{boot}} = \frac{1}{B}\sum_{b=1}^{B}\left[\frac{1}{n}\sum_{i=1}^{n} L(y_i, \hat{f}^b(x_i))\right]$$

Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

Bootstrap methods

Leave-one-out bootstrap

- Typically $\widehat{\text{EPE}}_{\text{boot}}$ is not a good estimate of EPE since there is too much overlap between the bootstrap samples (which act as training data) and the training data (which acts as the test data)
- Cross-validation worked by averaging across replications where the training (sub-)data and test (sub-)data were explicitly separated
- We could mimic this by only evaluating the predictions for the i^{th} observation from bootstrap datasets in which it was not sampled

Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

Bootstrap methods

Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

Leave-one-out bootstrap

- The *leave-one-out bootstrap* is defined by

$$\widehat{\text{EPE}}^{(1)} = \frac{1}{n}\sum_{i=1}^{n}\left[\frac{1}{|C_i|}\sum_{b\in C_i} L(y_i, \hat{f}^b(x_i))\right]$$

  - the set C_i denotes the indices of the bootstrap samples b that do *not* contain observation i
  - $|C_i|$ is the number of such samples

.632 bootstrap estimator

- While the leave-one-out bootstrap estimator resolves the overfitting associated with $\widehat{\text{EPE}}_{\text{boot}}$, it can suffer in terms of bias analogous to that suffered by K-fold cross-validation when $K > 1$

- The average number of distinct observations in each bootstrap sample is $0.632n$

$$\begin{aligned} \Pr(\text{observation } i \in \text{bootstrap sample } b) &= 1 - \left(1 - \frac{1}{n}\right)^n \\ &\approx 1 - e^{-1} \\ &= 0.632 \end{aligned}$$

  - so $\widehat{\text{EPE}}^{(1)}$ behaves roughly in the same way as two-fold cross-validation

Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

.632 bootstrap estimator

- The '.632 estimator' is design to alleviate the 'training-set-size' bias, and is defined by

$$\widehat{\text{EPE}}^{(.632)} = 0.368\text{err} + 0.632\widehat{\text{EPE}}^{(1)}$$

  - intuitively, the estimator pulls the leave-one-out bootstrap estimator down towards the training error rate, and hence reduces its upward bias

Ex: King County birth weight data

Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

Computation of prediction criteria for ridge regression models

- The function `ridge.predcrit()` on the course webpage will compute all of our commonly used estimates of prediction error for ridge regression models...

```
> set.seed(12345)
> source( "http://www.ics.uci.edu/~dgillen/
                      Stat211/Code/ridgePredCrit.q" )
> maxModel <- as.formula(bwt ~  gender + age + race + parity +
+                        married + smokeN + drinkN +
+                        firststep + welfare + smoker +
+                        drinker + wpre + education)

> ridgeFit  <- lm.ridge(maxModel, data=weight, lambda=252.53)
> ridge.predcrit( ridgeFit, formula=maxModel, data=weight,
                K=10, B=500, boot=TRUE, sigmaSq="calculate" )
    df    mse   aic   bic     cv bs.mse bs.1out bs.632
 9.3619 284974 38514 38568 287171 286657  290600 289149
```

Obtaining prediction criteria for an OLS fit in R

Obtaining prediction criteria for an OLS fit in R

- Similarly, the function `lm.predcrit()` will compute all of our commonly used estimates of prediction error for a standard OLS regression model...

```
##
#####
#####        Fit a standard liner regression model adjusting for
#####        wpre, age, gender, and smokeN
#####
##
 > fit.lm <- lm( bwt ~ wpre + age + gender + smokeN, data=weight )

 > lm.predcrit( fit.lm, data=weight, K=10, boot=TRUE, B=100 )
 df     mse      Cp    aic    bic      cv    cv.k bs.mse bs.1out bs.632
  5 291265 292432 38560 38589 292487 292512 291927  293132 292689
```


Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

Summary

Criteria to assess predictive accuracy

- Decision theoretic approach
- We measure errors between Y and $\hat{f}(X)$ by specifying a loss function $L(Y, \hat{f}(X))$
- The *test* or *generalization* error is the expected prediction error over an *independent* test sample

$$\text{EPE} = \text{E}_{X,Y}\left[L(Y, \hat{f}(X))\right]$$

  - the expectation is taken over the joint distribution of X and Y
  - the average error, were the prediction model to be applied to an independent sample from the population

Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

Criteria

Possibilities for estimating EPE

- Might consider *training error*

$$\text{err} = \frac{1}{n}\sum_{i=1}^{n} L(y_i, \hat{f}(x_i))$$

  - Negatively biased....Overly optimistic

- Analytically, focus on *in-sample* error

$$\text{Err} = \frac{1}{n}\sum_{i=1}^{n} \mathrm{E}_y\left[\mathrm{E}_{Y^{\text{new}}}\left[L(Y_i^{\text{new}}, \hat{f}(x_i))\right]\right]$$

Criteria

Possibilities for estimating ERR

- AIC
  - Consider (-2 times) the log-likelihood to be a loss function

$$\text{AIC} = -\frac{2}{n}\text{loglike} + 2\frac{p}{n}$$

- BIC
  - Motivated by the Bayes factor in model selection

$$\Pr(\text{Data}|\,\mathcal{M}_m) \approx \log \Pr(\text{Data}|\,\mathcal{M}_m, \hat{\theta}_m) - (\log n)\frac{p_m}{2}$$

  - Computed in practice as

$$\text{BIC} = -2\text{loglike} + (\log n)p$$

Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

Criteria

Resampling estimates EPE

- Using resampling to change the support of the observed predictors...
- General strategies that can be applied to any estimation technique (some quicker than others!)
- Cross-validation
  - Focus on the *predicted residual sum of squares*

$$\text{PRESS} = \sum_{i=1}^{n} \left(y_i - \hat{y}_{(i)} \right)^2$$

  - Easily computed for OLS fits
  - Can be computationally intensive for more complicated regression models
  - In this case, could focus on K-fold cross-validation

Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary

Criteria

Resampling estimates EPE

- Bootstrapping
  - Basic bootstrap is biased downwards
  - Leave-one-out bootstrap is generally biased upwards
  - Compromise is the .632 bootstrap

$$\widehat{\mathrm{EPE}}^{(.632)} = 0.368\mathrm{err} + 0.632\widehat{\mathrm{EPE}}^{(1)}$$

Ex: King County Birth Weight Data
Best subsets regression
Ridge regression
Simulation study (AIC and BIC)
Estimation of the extra-sample error
Cross-validation
Bootstrap methods
Summary