

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 Assessment and Selection for Prediction - Part 2 UC Irvine - ISI BUDS 2023

Presented July 26, 2023

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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 β 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



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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



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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



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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

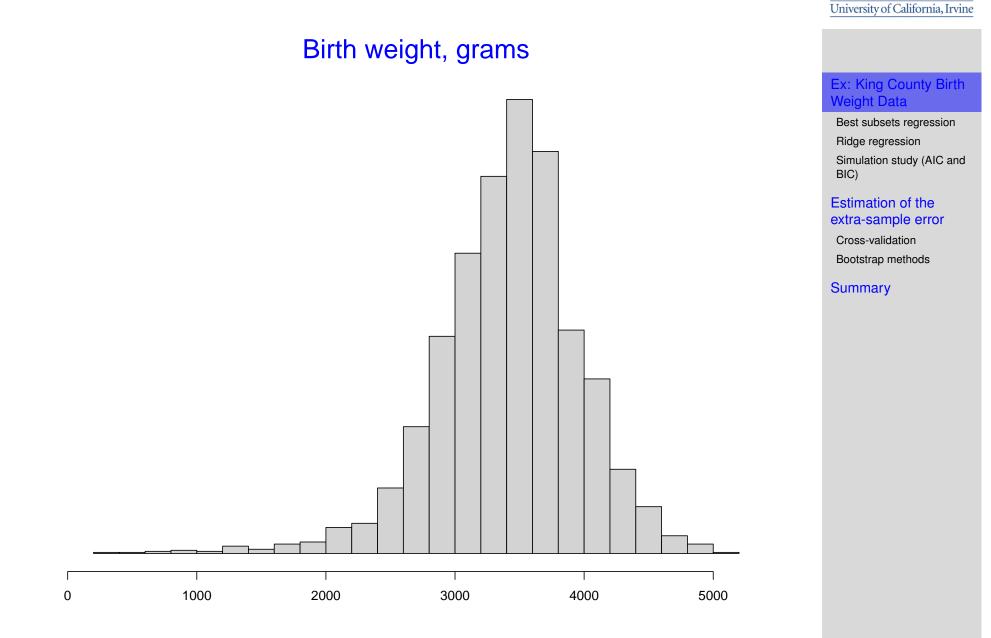
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Distribution of birth weights from the King County data

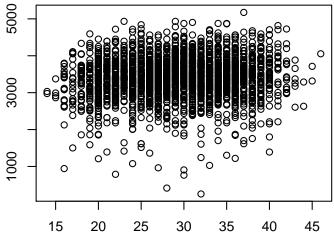


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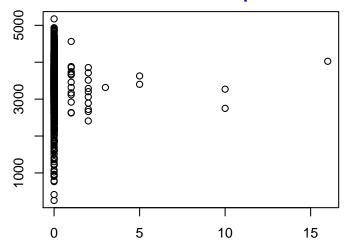
Selected scatterplots from the King County data



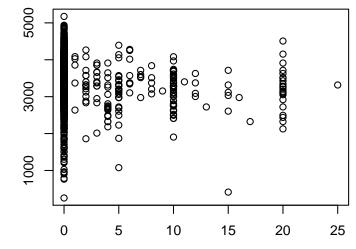
Mother's age, years



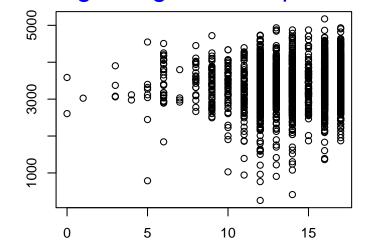
Alchoholic drinks per week



Cigarettes smoked per day



Highest grade completed



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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

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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



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Best subsets regression

Ridge regression Simulation study (AIC and BIC)

Estimation of the extra-sample error

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Bootstrap methods

Best subsets regression

- Suppose X consists of p components; X_1, \ldots, X_p
- For each k ∈ {1,..., 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



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Best subsets regression

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Bootstrap methods

Best subsets regression in R

library(leaps)

Model with only the intercept ## fit0 <- lm(bwt ~ 1, data=weight)</pre> ## Perform best subsets analysis ## ## maxModel: a model which includes all the variables you wish to ## entertain maximum number of variables for the subset selection ## nvmax: 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)



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Best subsets regression

Ridge regression Simulation study (AIC and BIC)

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Best subsets regression in R

##
minRSS <- tapply(results[,2], results[,1], FUN=min)</pre>



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Best subsets regression

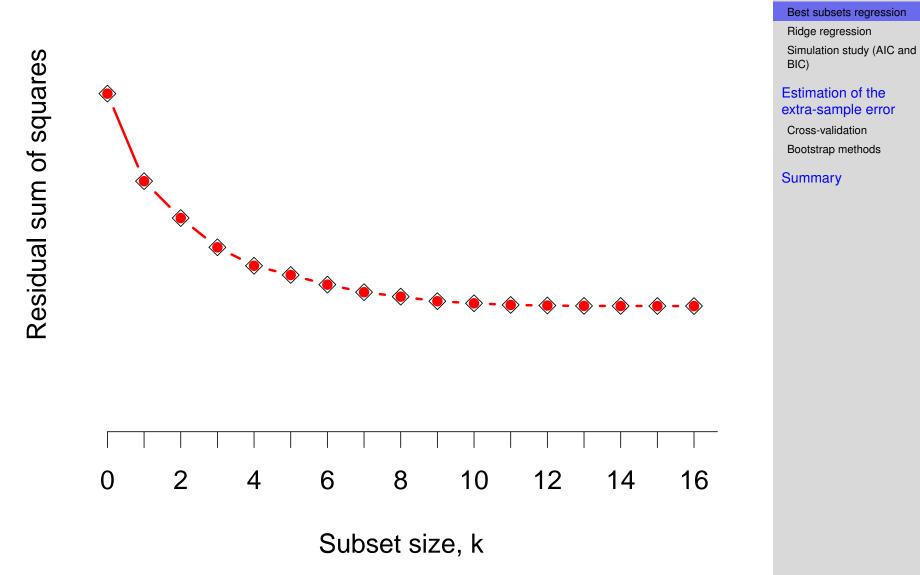
Ridge regression Simulation study (AIC and BIC)

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Bootstrap methods

Best subset selection for the King County 2001 birth weight data



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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)

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Best subsets regression in R

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



Ex: King County Birth Weight Data

Best subsets regression

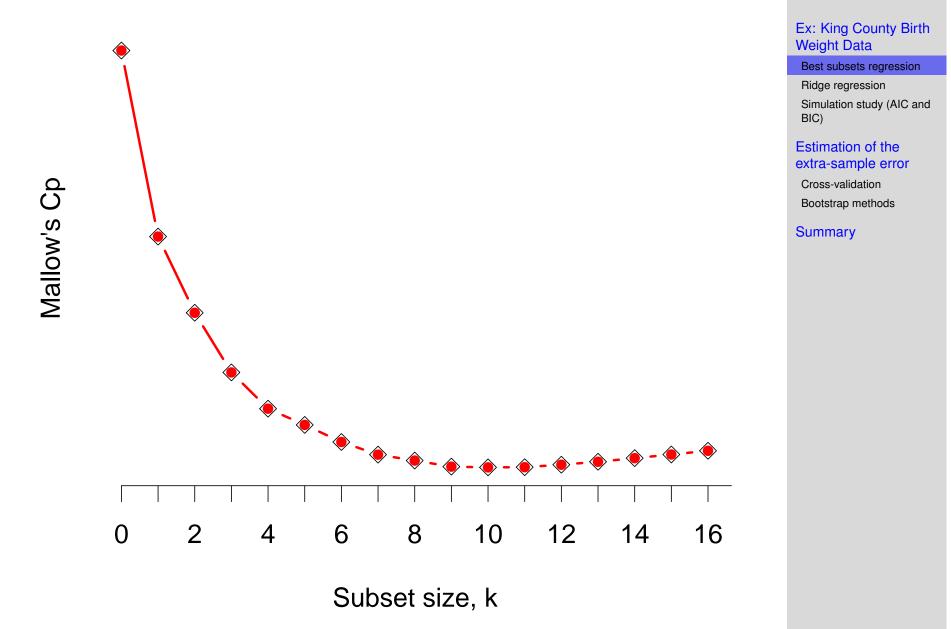
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Best subset selection for the King County 2001 birth weight data



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Best subsets regression in R

		[,]]
"(Intercept)"	"TRUE"	"TRUE"
"genderM"	"TRUE"	"TRUE"
"age"	"FALSE"	"FALSE"
"raceblack"	"FALSE"	"FALSE"
"racehispanic"	"TRUE"	"TRUE"
"raceother"	"FALSE"	"TRUE"
"racewhite"	"TRUE"	"TRUE"
"parity"	"TRUE"	"TRUE"
"married"	"TRUE"	"TRUE"
"smokeN"	"TRUE"	"TRUE"
"drinkN"	"FALSE"	"FALSE"
"firststep"	"FALSE"	"FALSE"
"welfare"	"TRUE"	"TRUE"
"smokerY"	"TRUE"	"TRUE"
"drinkerY"	"FALSE"	"FALSE"
"wpre"	"TRUE"	"TRUE"
"education"	"TRUE"	"TRUE"
	"(Intercept)" "genderM" "age" "raceblack" "racehispanic" "raceother" "racewhite" "parity" "married" "smokeN" "drinkN" "firststep" "welfare" "smokerY" "drinkerY"	"(Intercept)" "TRUE" "genderM" "TRUE" "age" "FALSE" "raceblack" "FALSE" "racehispanic" "TRUE" "raceother" "FALSE" "racewhite" "TRUE" "parity" "TRUE" "married" "TRUE" "smokeN" "TRUE" "drinkN" "FALSE" "welfare" "TRUE" "smokerY" "TRUE" "drinkerY" "FALSE" "wpre" "TRUE"



Ex: King County Birth Weight Data

Best subsets regression

Ridge regression Simulation study (AIC and BIC)

Estimation of the extra-sample error

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Bootstrap methods

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



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Best subsets regression

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Stepwise AIC in R

```
library(MASS)
##
#####
#####
             Stepwise selection using AIC
#####
##
fitStepAIC <- stepAIC( fit0, scope=maxModel, direction="forward" )</pre>
>Step: AIC=31425
bwt ~ wpre + smoker + gender + married + race + parity + welfare +
    education + smokeN
            Df Sum of Sq
                              RSS
                                       AIC
                         7.12e+08 3.14e+04
<none>
+ 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



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Best subsets regression

Ridge regression Simulation study (AIC and BIC)

Estimation of the extra-sample error

Cross-validation

Bootstrap methods

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 β are subject to bias
 - results often don't suffer as much in terms of variability
- Ridge regression imposes an L₂-type penalty
 - the solution is give by

$$\hat{oldsymbol{eta}}^{\mathsf{ridge}} \ = \ \mathsf{argmin}_{oldsymbol{eta}} \ \mathsf{RSS}(oldsymbol{eta})$$

subject to the constraint:

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



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Best subsets regression

Ridge regression

Simulation study (AIC and BIC)

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Shrinkage methods

An alternative way of writing the problem is

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

• Here, $\lambda \ge 0$ 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

$$\hat{oldsymbol{eta}}^{\mathsf{ridge}} \ = \ (\mathbf{X}^{\mathcal{T}}\mathbf{X} \ + \ \lambda \mathbf{I})^{-1}\mathbf{X}^{\mathcal{T}}\mathbf{y}$$

Could allow \(\lambda\) to be a vector, and ensure no shrinkage among certain coefficients



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Best subsets regression

Ridge regression

Simulation study (AIC and BIC)

Estimation of the extra-sample error

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Shrinkage methods

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

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

- depends on the complexity/smoothing parameter λ
- Ridge regression for the linear model is implemented in R

library(MASS)



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Best subsets regression

Ridge regression

Simulation study (AIC and BIC)

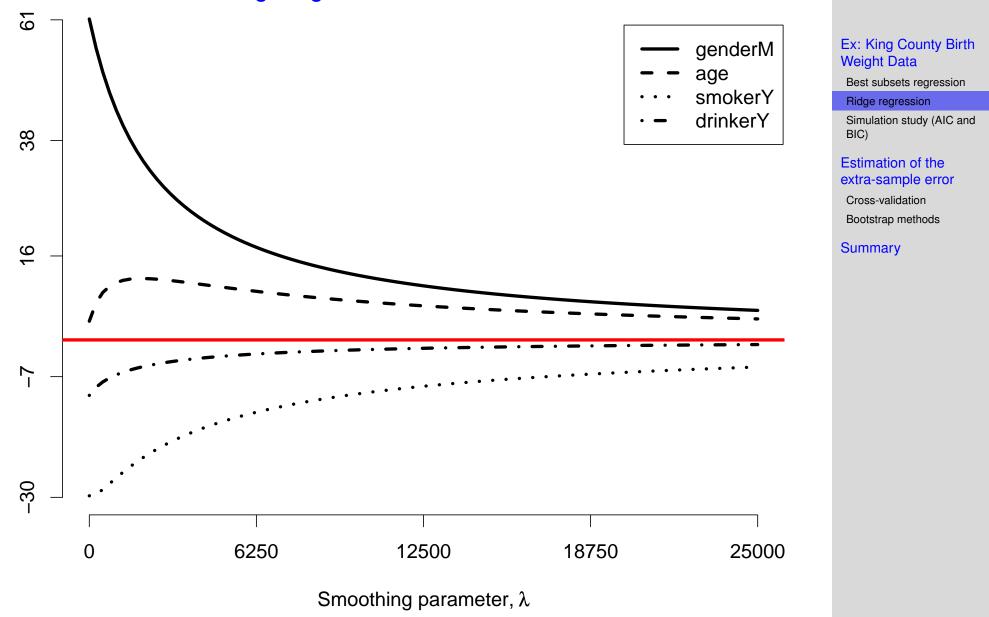
Estimation of the extra-sample error

Cross-validation

Bootstrap methods

Ridge regression for the King County Birth data

Ridge regression coefficient estimates



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 $\lambda = 1,000$



Ex: King County Birth Weight Data

Best subsets regression

Ridge regression

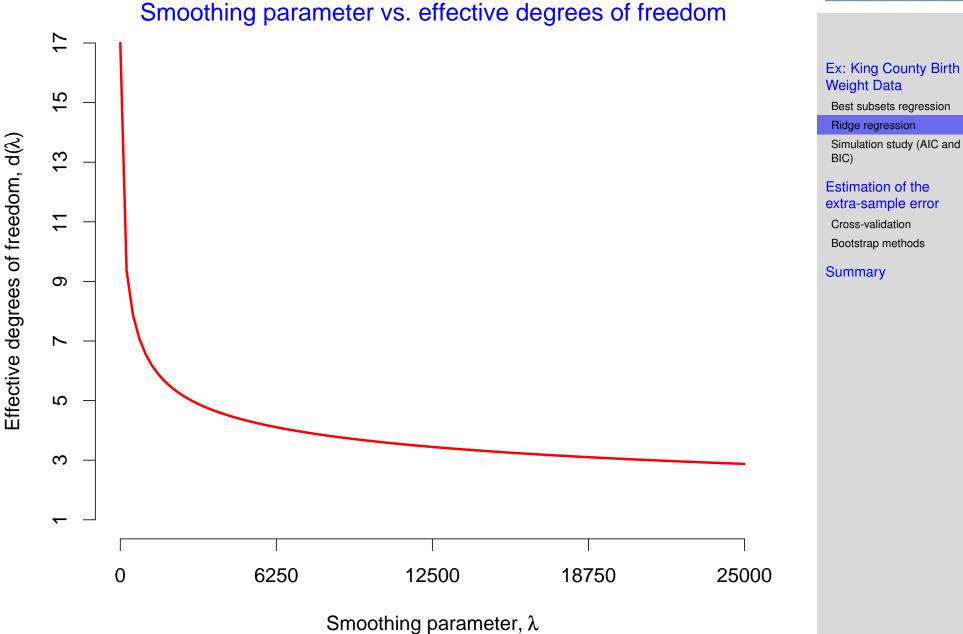
Simulation study (AIC and BIC)

Estimation of the extra-sample error

Cross-validation

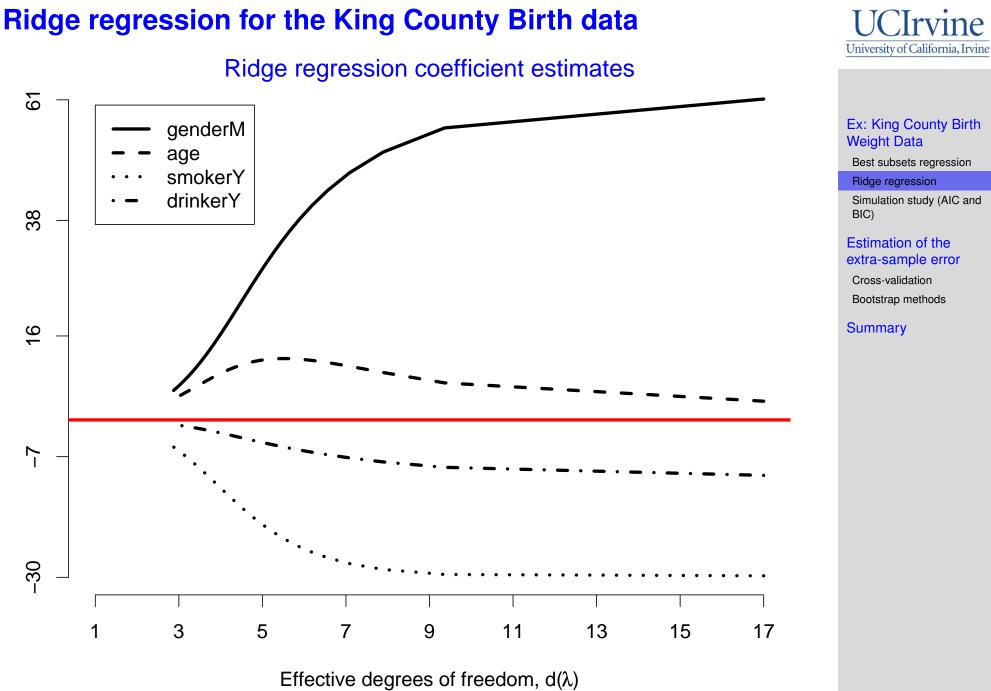
Bootstrap methods

Ridge regression for the King County Birth data



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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

 $\begin{array}{l} \mathsf{AIC} \ \Rightarrow \ 2p \\ \mathsf{BIC} \ \Rightarrow \ (\log n)p \end{array}$

- 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

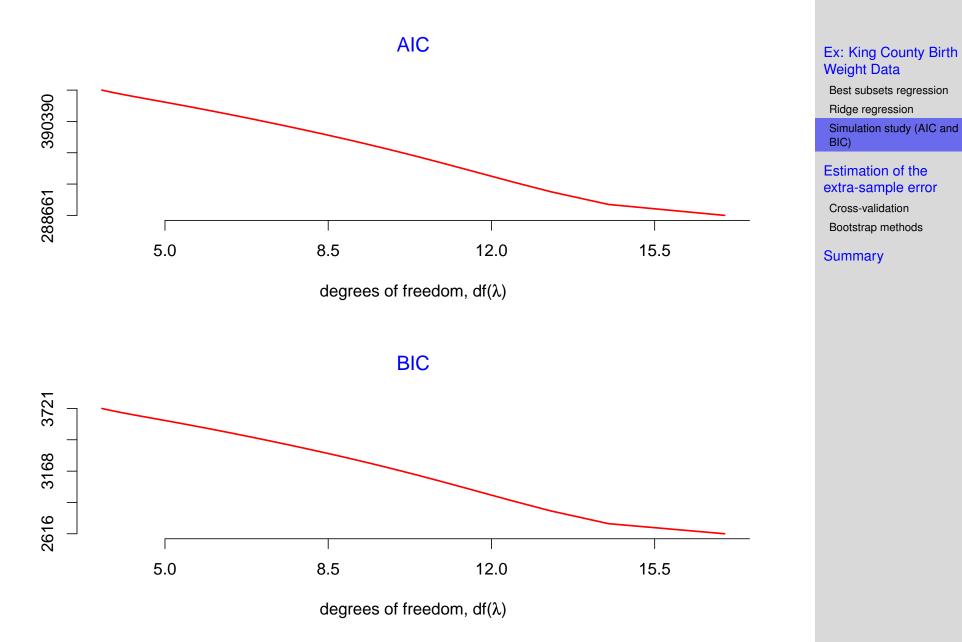
Simulation study (AIC and BIC)

Estimation of the extra-sample error

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Bootstrap methods

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



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Model selection for 'complexity'

AIC vs. BIC

- It seems that both AIC and BIC choose the optimal value of \(\lambda\) 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...



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Best subsets regression

Ridge regression

Simulation study (AIC and BIC)

Estimation of the extra-sample error

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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,

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

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



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Best subsets regression Ridge regression Simulation study (AIC and BIC)

Estimation of the extra-sample error

Cross-validation

Bootstrap methods

Cross-validation

One possibility for choosing \u03c6 could be to attempt to to minimize the observed mean squared error:

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

- 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 ŷ_i = 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 ith case



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Bootstrap methods

Cross-validation

If we denote the resulting prediction as ŷ_(i), then the corresponding sum of squared residuals is referred to as the predicted residual sum of squares

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

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



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Simulation study (AIC and BIC)

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- 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

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



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Generalized cross-validation

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

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

For the case of penalized regression, we replace trace(H) with the effective degrees of freedom



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Cross-validation

Bootstrap methods

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</p>
 - (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, ..., 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

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



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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

$$CV_{K} = \frac{1}{n} \sum_{i=1}^{n} L(y_{i}, \hat{f}^{-k(i)}(x_{i}))$$

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



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Summary

BIC)

Cross-validation

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

> [1] 9.3619

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



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Estimation of the extra-sample error

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Bootstrap methods

Bootstrap estimates of prediction error

- Let *f*^b(·) denote the estimate of *f*(·) obtained from the *b*th bootstrap replicate, *b* = 1, ..., *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

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



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Estimation of the extra-sample error

Cross-validation

Bootstrap methods

Leave-one-out bootstrap

- Typically EPE_{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



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Bootstrap methods

Leave-one-out bootstrap

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

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

- 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



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Best subsets regression Ridge regression Simulation study (AIC and BIC)

Estimation of the extra-sample error

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Bootstrap methods

.632 bootstrap estimator

- While the leave-one-out bootstrap estimator resolves the overfitting associated with EPE_{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

Pr(observation $i \in \text{bootstrap sample } b) = 1 - \left(1 - \frac{1}{n}\right)^n$

$$\approx 1 - e^{-1}$$

= 0.632

 so ÊPÊ⁽¹⁾ behaves roughly in the same way as two-fold cross-validation



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.632 bootstrap estimator

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

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

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



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Ex: King County birth weight data

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 +</pre>
                          married + smokeN + drinkN +
+
                           firststep + welfare + smoker +
^{+}
+
                          drinker + wpre + education)
> ridgeFit <- lm.ridge(maxModel, data=weight, lambda=252.53)</pre>
> ridge.predcrit( ridgeFit, formula=maxModel, data=weight,
                  K=10, B=500, boot=TRUE, sigmaSq="calculate" )
     df
           mse aic bic
                                cv bs.mse bs.lout bs.632
 9.3619 284974 38514 38568 287171 286657 290600 289149
```



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Bootstrap methods

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
######
##
> fit.lm <- lm(bwt ~ wpre + age + gender + smokeN, data=weight)
> lm.predcrit(fit.lm, data=weight, K=10, boot=TRUE, B=100)

 > Im.predcrit(IIt.Im, data=weight, K=10, boot=IROE, B=100)

 df
 mse
 Cp
 aic
 bic
 cv
 cv.k bs.mse
 bs.lout
 bs.632

 5
 291265
 292432
 38560
 38589
 292487
 292512
 291927
 293132
 292689



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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

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

- 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



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Estimation of the extra-sample error

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Possibilities for estimating EPE

Might consider training error

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

Negatively biased....Overly optimistic

Analytically, focus on *in-sample* error

$$\operatorname{Err} = \frac{1}{n} \sum_{i=1}^{n} \operatorname{E}_{\mathcal{Y}} \left[\operatorname{E}_{\mathcal{Y}} \operatorname{new} \left[L(\mathcal{Y}_{i}^{\operatorname{new}}, \hat{f}(x_{i}) \right] \right]$$



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Estimation of the extra-sample error

Cross-validation

Bootstrap methods

Possibilities for estimating ERR

- ► <u>AIC</u>
 - Consider (-2 times) the log-likelihood to be a loss function

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

► <u>BIC</u>

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

$$BIC = -2loglike + (log n)p$$



Ex: King County Birth Weight Data

Best subsets regression Ridge regression Simulation study (AIC and BIC)

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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

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

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



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Resampling estimates EPE

Bootstrapping

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

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



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