

ML01 – Introduction to Machine Learning

Model Selection

Thierry Denœux

`tdenoeux@utc.fr`

`https://www.hds.utc.fr/~tdenoeux`

Université de technologie de Compiègne

Spring 2021

Overview

1 Introduction

2 Subset selection

- Best subset and stepwise procedures
- Choosing the optimal model

3 Regularization

- Ridge regression
- Lasso

Need for model selection

- Consider, for instance, a regression problem with a response variable Y and 3 predictors X_1, X_2, X_3 .
- We can consider many (an infinity of) models, such as

$$Y = \beta_0 + \beta_1 X_1 + \epsilon$$

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \epsilon$$

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \beta_4 X_1^2 + \beta_5 X_2^2 +$$

$$\beta_6 X_1 X_2 + \beta_7 X_3^2 + \beta_8 X_1 X_3 + \beta_9 X_2 X_3 + \epsilon$$

$$\vdots$$

Which model to choose?

Bias-variance trade-off

- We have seen that a more complex model will not always have a smaller error when applied to test data.
- This is due to the **bias-variance trade-off**: when the number of parameters increases, the bias of the model decreases, but the variance increases.
- Furthermore, a simpler model often has a distinct advantages in terms of its interpretability.
- In this chapter, we discuss some tools to select models that will be
 - Complex enough to fit the data, but
 - Not too complex to avoid overfitting and to be interpretable.
- We focus mainly on **linear regression**, but the tools can be adapted to classification.

Three classes of methods

Subset Selection. We identify a **subset** of the p predictors that we believe to be related to the response. We then fit a model using the reduced set of variables.

Regularization. We fit a model involving all p predictors, but the estimated coefficients are shrunk towards zero to obtain a smoother prediction function. This **regularization** (also known as **shrinkage**) has the effect of reducing variance and can also perform variable selection.

Dimension Reduction. We project the p predictors into a **q -dimensional subspace**, where $q < p$. This is achieved by computing q different linear combinations of the variables. Then these q new variables are used as predictors to fit a linear model. One such technique will be studied later in this course.

Overview

1 Introduction

2 Subset selection

- Best subset and stepwise procedures
- Choosing the optimal model

3 Regularization

- Ridge regression
- Lasso

Overview

1 Introduction

2 Subset selection

- Best subset and stepwise procedures
- Choosing the optimal model

3 Regularization

- Ridge regression
- Lasso

Best subset selection

- ① Let \mathcal{M}_0 denote the null model, which contains no predictors. This model simply predicts the sample mean for each observation.
- ② For $k = 1, 2, \dots, p$:
 - ① Fit all $\binom{p}{k} = \frac{p!}{(p-k)!k!}$ models that contain exactly k predictors.
 - ② Pick the best among these $\binom{p}{k}$ models, and call it \mathcal{M}_k . Here “best” is defined as having the smallest RSS, or equivalently the largest R^2 .
- ③ Select a single best model from among $\mathcal{M}_0, \dots, \mathcal{M}_p$. (How? to be seen later).

Example: air pollution and mortality

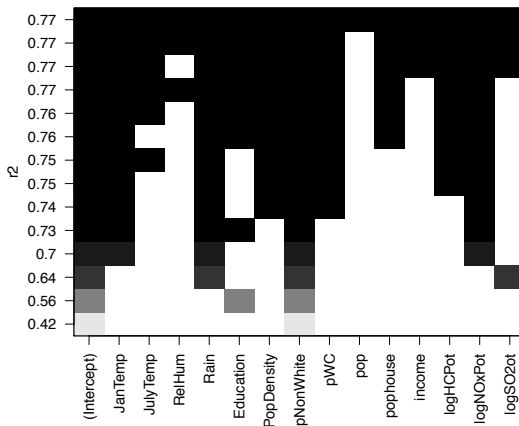
- Data are from McDonald and Schwing (1973), “Instabilities of Regression Estimates Relating Air Pollution to Mortality”, *Technometrics*, 15, 463-481.
- This data set of 15 predictors and a measure of mortality on 60 US metropolitan areas in 1959-1961.

Variables

- Response: Total Age Adjusted Mortality Rate
- Predictors:
 - ① Mean annual precipitation in inches
 - ② Mean January temperature in degrees Fahrenheit
 - ③ Mean July temperature in degrees Fahrenheit
 - ④ Percent of 1960 SMSA population that is 65 years of age or over
 - ⑤ Population per household, 1960 SMSA
 - ⑥ Median school years completed for those over 25 in 1960 SMSA
 - ⑦ Percent of housing units that are found with facilities
 - ⑧ Population per square mile in urbanized area in 1960
 - ⑨ % of 1960 urbanized area population that is non-white
 - ⑩ % employment in white-collar occupations in 1960 urbanized area
 - ⑪ % of families with income under 3,000 in 1960 urbanized area
 - ⑫ Relative population potential of hydrocarbons, HC
 - ⑬ Relative pollution potential of oxides of nitrogen, NO_x
 - ⑭ Relative pollution potential of sulfur dioxide, SO₂
 - ⑮ Percent relative humidity, annual average at 1 p.m.

Best subset selection in R

```
library('leaps')
reg.fit<-regsubsets(Mortality~.-logNOx,data=pollution,method='exhaustive',nvmax=15)
plot(reg.fit,scale="r2")
```



Extension to other models

- Although we have presented best subset selection here for least squares regression, the same ideas apply to other types of models, such as logistic regression.
- The **deviance**, $-2\ell(\hat{\theta})$, plays the role of RSS for a broader class of models.

Stepwise selection

- For computational reasons, best subset selection cannot be applied with very large p .
- Best subset selection may also suffer from statistical problems when p is large: larger the search space, the higher the chance of finding models that look good on the training data, even though they might not have any predictive power on future data.
- Thus an enormous search space can lead to overfitting and high variance of the coefficient estimates.
- For both of these reasons, **stepwise methods**, which explore a far more restricted set of models, are attractive alternatives to best subset selection.

Forward stepwise selection

- **Forward stepwise selection** begins with a model containing no predictors, and then adds predictors to the model, one-at-a-time, until all of the predictors are in the model.
- In particular, at each step the variable that gives the greatest additional improvement to the fit is added to the model.

Forward stepwise selection in detail

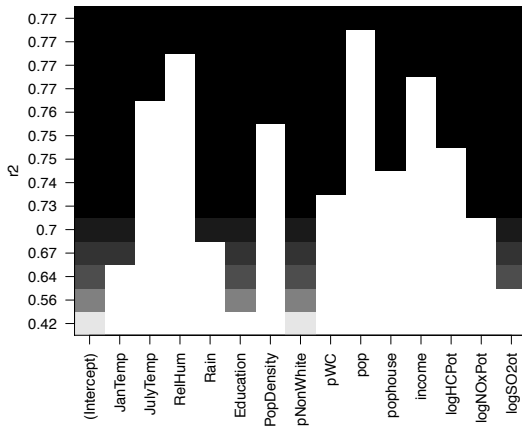
- ① Let \mathcal{M}_0 denote the null model, which contains no predictors.
- ② For $k = 0, \dots, p - 1$:
 - ① Consider all $p - k$ models that augment the predictors in \mathcal{M}_k with one additional predictor.
 - ② Choose the best among these $p - k$ models, and call it \mathcal{M}_{k+1} . Here “best” is defined as having highest R^2 .
- ③ Select a single best model from among $\mathcal{M}_0, \dots, \mathcal{M}_p$.

More on forward stepwise selection

- Computational advantage over best subset selection is clear.
- It is not guaranteed to find the best possible model out of all 2^p models containing subsets of the p predictors.

Forward stepwise selection in R

```
reg.fit<-regsubsets(Mortality~.-logNOx,data=pollution,method='forward',nvmax=15)
plot(reg.fit,scale="r2")
```



Backward stepwise selection

- Like forward stepwise selection, **backward stepwise selection** provides an efficient alternative to best subset selection.
- However, unlike forward stepwise selection, it begins with the full least squares model containing all p predictors, and then iteratively removes the least useful predictor, one-at-a-time.

Backward stepwise selection in detail

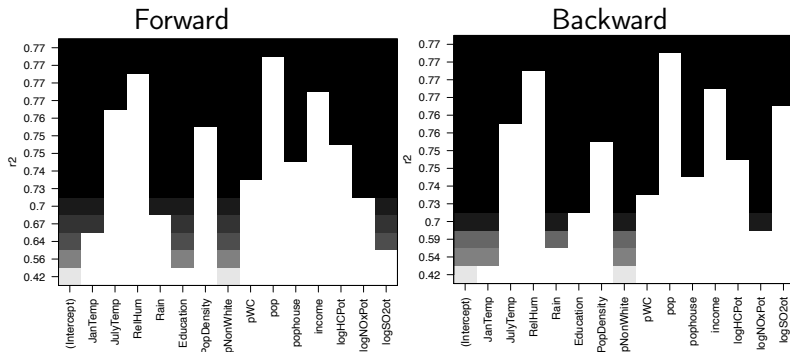
- ① Let \mathcal{M}_p denote the full model, which contains all p predictors.
- ② For $k = p, p - 1, \dots, 1$:
 - ① Consider all k models that contain all but one of the predictors in \mathcal{M}_k , for a total of $k - 1$ predictors.
 - ② Choose the best among these k models, and call it \mathcal{M}_{k-1} . Here “best” is defined as having highest R^2 .
- ③ Select a single best model from among $\mathcal{M}_0, \dots, \mathcal{M}_p$.

More on backward stepwise selection

- Like forward stepwise selection, the backward selection approach searches through only $1 + p(p+1)/2$ models, and so can be applied in settings where p is too large to apply best subset selection
- Like forward stepwise selection, backward stepwise selection is **not guaranteed to yield the best model** containing a subset of the p predictors.
- Backward selection requires that the number of samples n is larger than the number of variables p (so that the full model can be fit). In contrast, forward stepwise can be used even when $n < p$, and so is the only viable subset method when p is very large.

Backward stepwise selection in R

```
reg.fit<-regsubsets(Mortality~.-logNOx,data=pollution,method='backward',nvmax=15)
plot(reg.fit,scale="r2")
```



Overview

1 Introduction

2 Subset selection

- Best subset and stepwise procedures
- Choosing the optimal model

3 Regularization

- Ridge regression
- Lasso

Choosing the optimal model

- The model containing all of the predictors will always have the smallest RSS and the largest R^2 , since these quantities are related to the training error.
- We wish to **choose a model with low test error**, not a model with low training error. Recall that training error is usually a poor estimate of test error.
- Therefore, RSS and R^2 are not suitable for selecting the best model among a collection of models with different numbers of predictors.

Estimating test error: two approaches

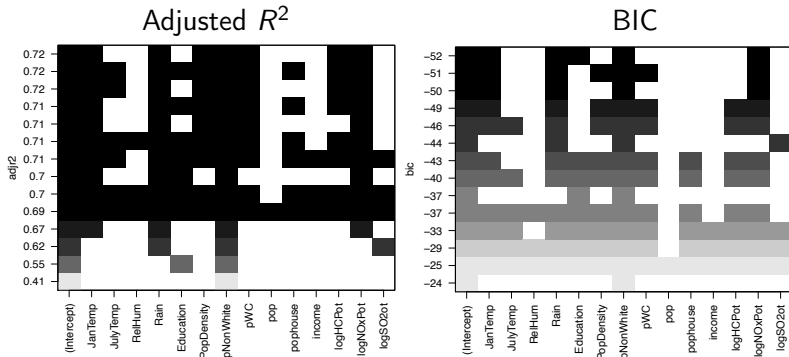
- We can
 - ① Indirectly estimate test error by making an **adjustment** to the training error to account for the bias due to overfitting, or
 - ② Directly estimate the test error, using either a **hold-out** approach or a **cross-validation** approach.
- We illustrate both approaches next.

Training error adjustment techniques

- These techniques **adjust the training error for the model size**, and can be used to select among a set of models with different numbers of variables.
- Three criteria:
 - 1 Adjusted R^2
 - 2 Akaike information criterion (AIC)
 - 3 Bayesian information criterion (BIC)
- The next figure displays BIC, and adjusted R^2 for the best model of each size produced by best subset selection on the pollution data set.

Example

```
reg.fit<-regsubsets(Mortality~.-logNOx,data=pollution,method='exhaustive',nvmax=15)
plot(reg.fit,scale="adjr2") plot(reg.fit,scale="bic")
```



Adjusted R -squared

- Idea: introduce the “population R^2 ” as

$$R_{pop}^2 = 1 - \frac{\sigma^2}{\text{Var}(Y)}$$

- The usual R^2 is

$$R^2 = 1 - \frac{RSS/n}{TSS/n}$$

It is based on biased estimates of the residual and total variances.

- The **adjusted R^2** is based on unbiased estimates:

$$\bar{R}^2 = 1 - \frac{RSS/(n - p - 1)}{TSS/(n - 1)}$$

where p is the number of predictors used.

- This criterion is specific to regression.

AIC

- The **AIC criterion** is defined for a large class of models fit by maximum likelihood:

$$AIC = -2\ell(\hat{\theta}) + 2r$$

where $\ell(\hat{\theta})$ is the maximized value of the log-likelihood function for the estimated model, and r is the number of parameters.

- The best model has the smallest AIC value.
- For linear regression with p variables and a constant term, $r = p + 1$.

BIC

- Definition:

$$BIC = -2\ell(\hat{\theta}) + r \log(n)$$

where r is the number of parameters.

- Like AIC, BIC will tend to take on a small value for a model with a low test error, and so generally we select the model that has the lowest BIC value.
- Notice that BIC replaces the $2r$ used by AIC with a $r \log(n)$ term, where n is the number of observations.
- Since $\log n > 2$ for any $n > 7$, the BIC statistic generally places a heavier penalty on models with many variables, and hence results in the selection of smaller models than AIC.

Direct estimation of the prediction error

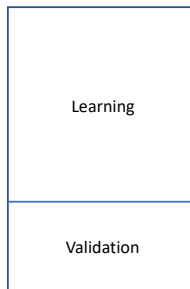
- Each of the subset selection procedures returns a sequence of models \mathcal{M}_k indexed by model size $k = 0, 1, 2, \dots, p$. Our job here is to select \hat{k} . Once selected, we will return model $\mathcal{M}_{\hat{k}}$.
- We compute an **estimate of the prediction error** for each model \mathcal{M}_k under consideration, and then select the k for which the resulting estimated prediction error is smallest.
- This procedure has an advantage relative to AIC, BIC, and adjusted R^2 , in that it provides a **direct estimate of the prediction error**.
- It can also be used in a wider range of model selection tasks, even in cases where it is hard to define the model degrees of freedom.

Direct estimation of the test error

Two methods:

- 1 Validation-set (hold-out) approach
- 2 Cross-validation

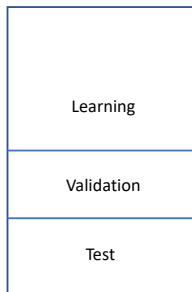
Validation-set approach



- Here we randomly divide the available set of samples into two parts:
 - 1 a training set and
 - 2 a **validation** set
- The model is fit on the training set, and the fitted model is used to predict the responses for the observations in the validation set.
- The resulting **validation error** provides an estimate of the prediction error. This is typically assessed using MSE in the case of regression and misclassification rate in the case of classification.

Hold-out approach (continued)

- After the best model has been selected, it is usually **fit on the whole data (training+validation)**.
- The validation error for the best model is biased (optimistic).



- The error of the best model has to be estimated using an independent **test set**.

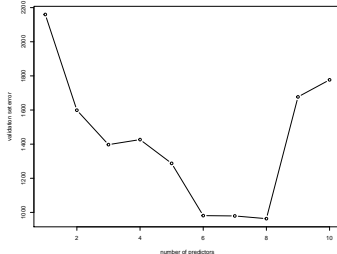
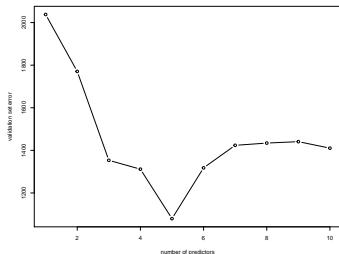
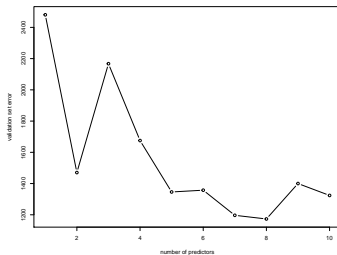
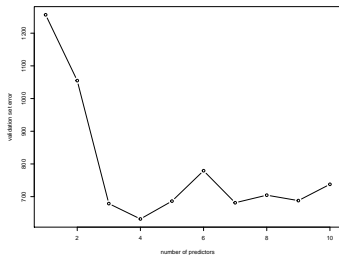
Example

```
n<-nrow(pollution)
napp=45
ntst=n-napp
train<-sample(1:n,napp)
pollution.train<-pollution[train,]
pollution.test<-pollution[-train,]

Formula<-c(Mortality ~ pNonWhite,
Mortality ~ Education + pNonWhite,
Mortality ~ Rain + pNonWhite + logSO2ot,
Mortality ~ JanTemp+ Rain +pNonWhite +logNOxPot,
...
)

for(i in 1:10){
reg<-lm(Formula[[i]],data=pollution.train)
pred<-predict(reg,newdata=pollution.test)
err[i]<-mean((pollution.test$Mortality-pred)^2)
}
```

Results with 4 different splits (Air pollution data)



Limitations of the hold-out approach

- The validation estimate of the test error can be **highly variable**, depending on precisely which observations are included in the training set and which observations are included in the validation set.
- In the hold-out approach, only a subset of the observations – those that are included in the training set rather than in the validation set – are used to fit the model.
- This suggests that the validation-set error may tend to **overestimate the test error** for the model fit on the entire data set.

K-fold cross-validation

- Widely used approach for estimating test error.
- Estimates can be used to select best model, and to give an idea of the test error of the final chosen model.
- Idea is to randomly divide the data into K equal-sized subsets. We leave out subset k , fit the model to the other $K - 1$ subsets (combined), and then obtain predictions for the left-out k -th subset.
- This is done in turn for each subset $k = 1, 2, \dots, K$, and then the results are combined.

1	2	3	4	5
Validation	Train	Train	Train	Train

K-fold cross-validation in detail

- Let the K subsets be C_1, C_2, \dots, C_K , where C_k denotes the indices of the observations in subset k . There are n_k observations in subset k : if n is a multiple of K , then $n_k = n/K$.
- Compute

$$CV_{(K)} = \frac{1}{n} \sum_{k=1}^K n_k \times \text{MSE}_k,$$

where

$$\text{MSE}_k = \frac{1}{n_k} \sum_{i \in C_k} \left(y_i - \hat{y}_i^{(-k)} \right)^2$$

and $\hat{y}_i^{(-k)}$ is the fit for observation i , obtained from the data with subset k removed.

- Setting $K = n$ yields n -fold or **leave-one-out** cross-validation (LOOCV).

Special case

- With least-squares linear or polynomial regression, a shortcut makes the cost of LOOCV the same as that of a single model fit!
- The following formula holds:

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

where \hat{y}_i is the i th fitted value from the original least squares fit, and h_i is the **leverage** (diagonal term of the “hat” matrix). (Reminder: $\mathbf{H} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$, and $\hat{\mathbf{y}} = \mathbf{H}\mathbf{y}$).

- This is like the ordinary MSE, except the i -th residual is divided by $1 - h_i$.

Choice of K

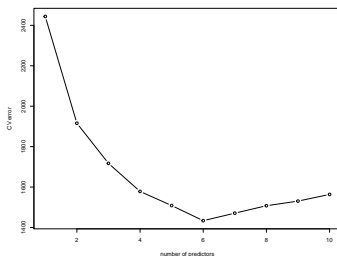
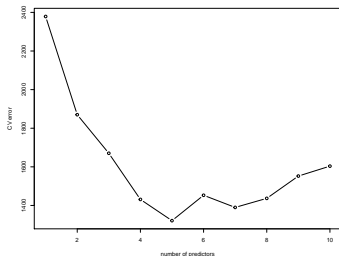
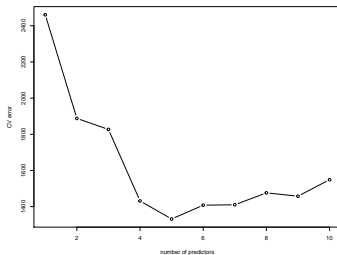
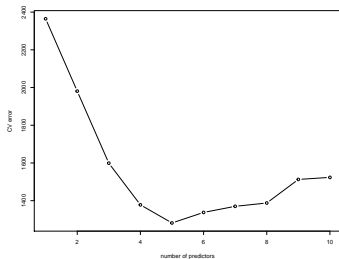
- Since each training set is only $(K - 1)/K$ as big as the original training set, the estimates of prediction error will typically be **biased upward**.
- This bias is minimized when $K = n$ (LOOCV), but this estimate has high variance, because the estimates from each fold are highly correlated.
- $K = 5$ or 10 provides a good compromise for this bias-variance tradeoff.

Example of 10-fold cross-validation

```
K<-10
folds=sample(1:K,n,replace=TRUE)
CV<-rep(0,10)

for(i in (1:10)){
  for(k in (1:K)){
    reg<-lm(Formula[[i]],data=pollution[folds!=k,])
    pred<-predict(reg,newdata=pollution[folds==k,])
    CV[i]<-CV[i]+ sum((pollution$Mortality[folds==k]-pred)^2)
  }
  CV[i]<-CV[i]/n
}
```

Result (4 trials)



Final remarks on cross-validation

- The CV error rates can be averaged over r repetitions of K -fold cross-validation with different random partitions, to reduce the variance of the CV error estimates.
- After the best model has been selected, we usually re-estimate the model parameters using the whole training set.
- To obtain an unbiased estimate of the best model's error, we need an **independent test set**.

Overview

- 1 Introduction
- 2 Subset selection
 - Best subset and stepwise procedures
 - Choosing the optimal model
- 3 Regularization
 - Ridge regression
 - Lasso

Shrinkage methods

- By retaining only a subset of the predictors, subset selection produces a model that is interpretable and has possibly lower prediction error than the full model.
- However, because it is a discrete process – variables are either retained or discarded – it often exhibits high variance, and so does not always reduce the prediction error of the full model.
- **Shrinkage methods** are more continuous, and do not suffer as much from high variability.
- Two main methods:
 - 1 Ridge regression
 - 2 Lasso

Overview

- 1 Introduction
- 2 Subset selection
 - Best subset and stepwise procedures
 - Choosing the optimal model
- 3 Regularization
 - Ridge regression
 - Lasso

Ridge regression

- **Ridge regression** shrinks the regression coefficients by imposing a penalty on their size. The ridge coefficients minimize a penalized residual sum of squares:

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

- Here $\lambda \geq 0$ is a **complexity parameter** that controls the amount of shrinkage: the larger the value of λ , the greater the amount of shrinkage. The coefficients are shrunk toward zero (and each other), i.e., to the simplest model (with only the constant term).
- Selecting a good value for λ is critical; cross-validation can be used for this.

Equivalent form

- An equivalent way to write the ridge problem is

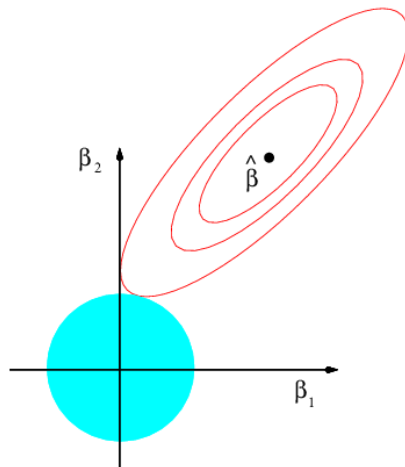
$$\hat{\beta}^{\text{ridge}} = \arg \min_{\beta} \left\{ \sum_{i=1}^n \left(y_i - \beta_0 - \sum_{j=1}^p x_{ij} \beta_j \right)^2 \right\}$$

$$\text{subject to } \sum_{j=1}^p \beta_j^2 \leq t,$$

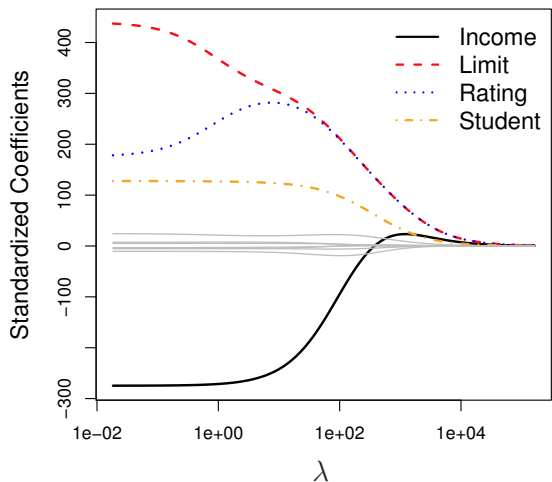
which makes explicit the size constraint on the parameters. (See next slide).

- There is a one-to-one correspondence between parameters t and λ in the previous formulation.

Ridge regression as a constrained optimization problem



The effect of ridge regression



Derivation of the ridge regression estimates

- We can show that $\hat{\beta}^{\text{ridge}}$ can be found by separating the minimization problem into two parts, after centering the inputs (replacing x_{ij} by $x_{ij} - \bar{x}_j$):
 - ① We estimate β_0 by $\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i$
 - ② The remaining coefficients get estimated by a ridge regression without intercept, using the centered x_{ij} and the centered y_i .
- We assume that both the inputs and the output have been centered, so that the input matrix \mathbf{X} has p (rather than $p + 1$) columns, and \mathbf{y} is the n -vector of centered outputs.
- The criterion can be written in matrix form

$$\text{RSS}_{\lambda}(\beta) = (\mathbf{y} - \mathbf{X}\beta)^T(\mathbf{y} - \mathbf{X}\beta) + \lambda\beta^T\beta.$$

Derivation of the ridge regression estimates (continued)

- The criterion can be rewritten as

$$\text{RSS}_\lambda(\beta) = \mathbf{y}^T \mathbf{y} - 2\beta^T \mathbf{X}^T \mathbf{y} + \beta^T (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_p) \beta$$

- Differentiating with respect to β we obtain

$$\frac{\partial \text{RSS}_\lambda(\beta)}{\partial \beta} = -2\mathbf{X}^T \mathbf{y} + 2(\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_p) \beta$$

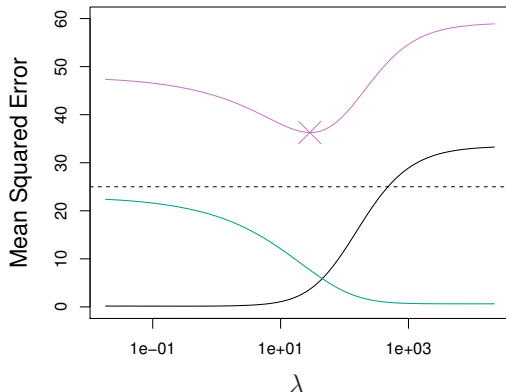
- The solution of the equation $\frac{\partial \text{RSS}_\lambda(\beta)}{\partial \beta} = 0$ is

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

Ridge regression: scaling of predictors

- The standard least squares coefficient estimates are scale **equivariant**: multiplying X_j by a constant c simply leads to a scaling of the least squares coefficient estimates by a factor of $1/c$. In other words, regardless of how the j th predictor is scaled, $X_j\hat{\beta}_j$ will remain the same.
- In contrast, the ridge regression coefficient estimates can change substantially when multiplying a given predictor by a constant, due to the sum of squared coefficients term in the penalty part of the ridge regression objective function.
- Therefore, it is best to apply ridge regression after **standardizing the predictors** (dividing each centered variable by its standard deviation).

Why does ridge regression improve over least squares?



Simulated data with $n = 50$ observations, $p = 45$ predictors, all having nonzero coefficients. Squared bias (black), variance (green), and test MSE (purple) for the ridge regression predictions, as a function of λ . The horizontal dashed lines indicate the minimum possible MSE.

Ridge regression in R

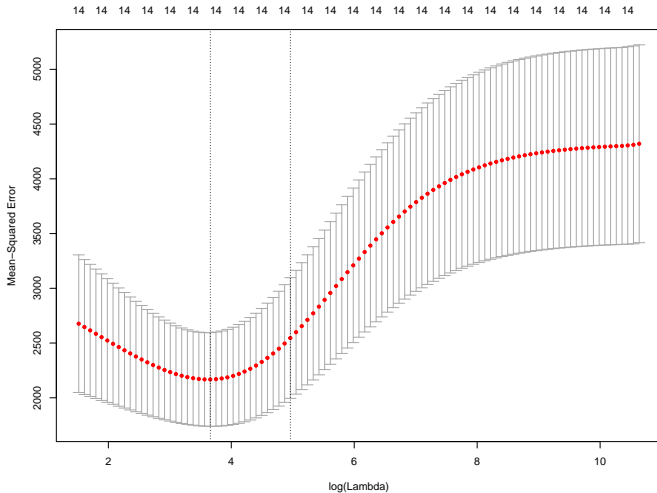
```
library(glmnet)

x<-model.matrix(Mortality~.-logNOx,pollution)
y<-pollution$Mortality[-21] # obs 21 has 2 missing values
n<-nrow(x)
napp=45
ntst=n-45
train<-sample(1:n,napp)
xapp<-x[train,]
yapp<-y[train]
xtst<-x[-train,]
ytst<-y[-train]

cv.out<-cv.glmnet(xapp,yapp,alpha=0)
plot(cv.out)

fit<-glmnet(xapp,yapp,lambda=cv.out$lambda.min,alpha=0)
ridge.pred<-predict(fit,s=cv.out$lambda.min,newx=xtst)
print(mean((ytst-ridge.pred)^2))
2421.136
```

CV error as a function of λ



Coefficients

```
fit$beta
s0
(Intercept) .
JanTemp -2.641635e-01
JulyTemp 7.231499e-01
RelHum -1.443636e-01
Rain 9.618201e-01
Education -1.154417e+01
PopDensity 2.066547e-03
pNonWhite 1.478269e+00
pWC -1.105875e+00
pop 2.629839e-06
pophouse 3.057905e+01
income -1.008305e-03
logHCPot 2.311552e+00
logNOxPot 6.616369e+00
logSO2ot 3.966114e+00
```

Overview

- 1 Introduction
- 2 Subset selection
 - Best subset and stepwise procedures
 - Choosing the optimal model
- 3 Regularization
 - Ridge regression
 - Lasso

The lasso

- Ridge regression has one obvious disadvantage: unlike subset selection, it includes all p predictors in the final model
- The **lasso** is a relatively recent alternative to ridge regression that overcomes this disadvantage. The lasso coefficients, $\hat{\beta}^{\text{lasso}}$ minimize the quantity

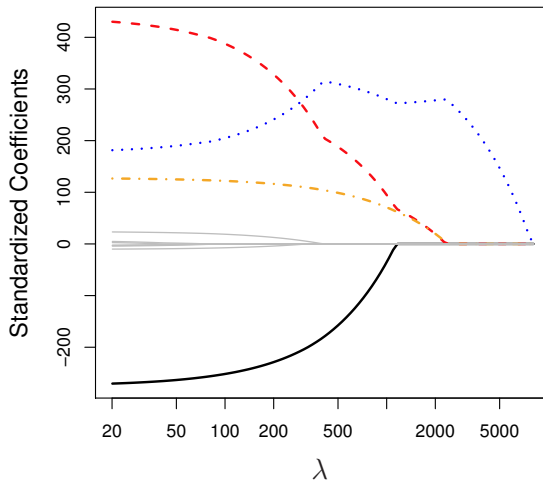
$$\hat{\beta}^{\text{lasso}} = \arg \min_{\beta} \left\{ \sum_{i=1}^n \left(y_i - \beta_0 - \sum_{j=1}^p x_{ij} \beta_j \right)^2 + \lambda \sum_{j=1}^p |\beta_j| \right\},$$

i.e., the L_2 norm is replaced by the L_1 norm in the penalty term.
(Reminder: the L_p norm is defined as $\|\beta\|_p = \left(\sum_j |\beta_j|^p \right)^{1/p}$).

The lasso (continued)

- As with ridge regression, the lasso **shrinks the coefficient estimates towards zero**.
- However, in the case of the lasso, the L_1 penalty has the effect of forcing some of the coefficient estimates to be **exactly equal to zero** when the tuning parameter λ is sufficiently large.
- Hence, much like best subset selection, the lasso performs **variable selection**.
- We say that the lasso yields **sparse models** – that is, models that involve only a subset of the variables.
- As in ridge regression, selecting a good value of λ for the lasso is critical; cross-validation is again the method of choice.

Example



Equivalent form

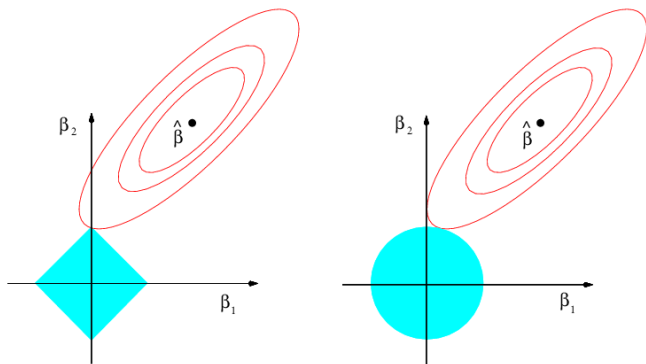
- As in the case of ridge problem, the previous unconstrained optimization problem is equivalent to the following constrained one:

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

subject to $\sum_{j=1}^p |\beta_j| \leq t,$

- This problem can be solved using a quadratic programming algorithm.

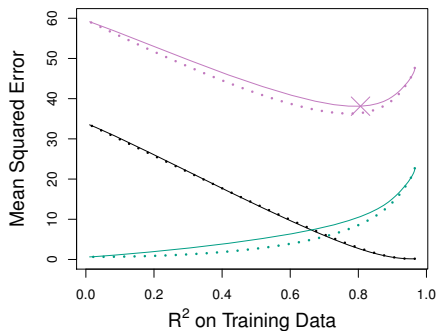
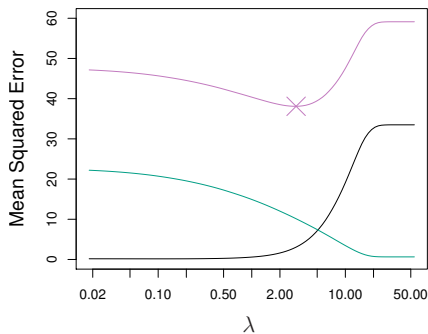
Why does the lasso eliminate variables?



When $p = 2$, the feasibility region is a diamond, which has corners; if the solution occurs at a corner, then it has one parameter β_j equal to zero.

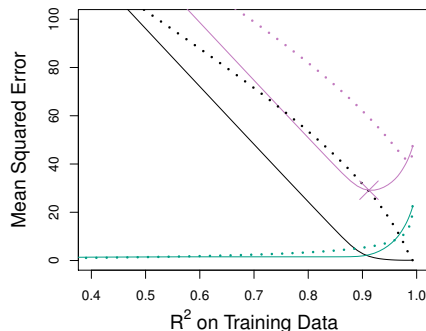
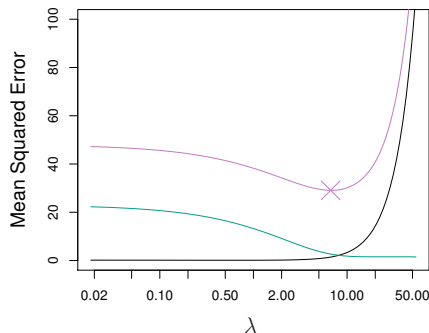
When $p > 2$, the feasibility region has many corners, flat edges and faces; there are many more opportunities for the estimated parameters to be zero.

Comparing the lasso and ridge regression



Left: Plots of squared bias (black), variance (green), and test MSE (purple) for the lasso on simulated data set of Slide 54. Right: Comparison of squared bias, variance and test MSE between lasso (solid) and ridge (dashed). Both are plotted against their R^2 on the training data, as a common form of indexing.

Comparing the lasso and ridge regression (continued)



Left: Plots of squared bias (black), variance (green), and test MSE (purple) for the lasso. The simulated data are similar to those in the previous slide, except that now **only two predictors are related to the response**. Right: Comparison of squared bias, variance and test MSE between lasso (solid) and ridge (dashed). Both are plotted against their R^2 on the training data, as a common form indexing.

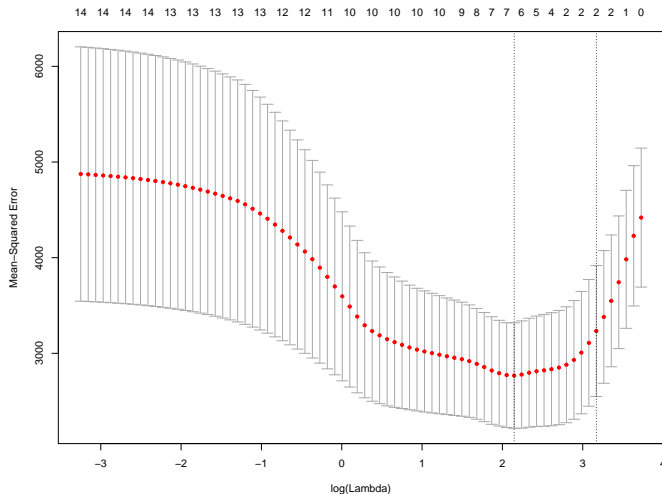
The lasso in R

```
cv.out<-cv.glmnet(xapp,yapp,alpha=1)
plot(cv.out)

fit.lasso<-glmnet(xapp,yapp,lambda=cv.out$lambda.min,alpha=1)

lasso.pred<-predict(fit.lasso,s=cv.out$lambda.min,newx=xtst)
print(mean((ytst-lasso.pred)^2))
1946.667
```

CV error as a function of λ (lasso)



Coefficients

```
> print(fit.lasso$beta)
s0
(Intercept) .
JanTemp -1.157095e+00
JulyTemp .
RelHum .
Rain 1.404239e+00
Education -1.796084e+01
PopDensity .
pNonWhite 2.880287e+00
pWC -9.421496e-01
pop 2.141275e-06
pophouse .
income -4.655832e-04
logHCPot .
logNOxPot 1.392387e+01
logSO2ot 3.461564e-01
```