Lecture 12: Variable Selection (I)

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Outline

- Motivation for Variable Selection
- Classical Methods
  - best subset selection
  - forward selection
  - backward elimination
  - stepwise selection
- Modern Penalization Methods
  - L_q penalty, ridge
  - LASSO, adaptive LASSO, LARS
  - non-negative garotte, SCAD

Problems of Least Squares Methods

- Prediction Accuracy

$$\text{MSE} = \text{Bias}^2 + \text{Var}$$

  - Least square estimates with full models tend to have low bias and high variance.
  - It is possible to trade a little bias with the large reduction in variance, thus achieving higher prediction accuracy

- Interpretation
  - We would like to determine a small subset of variables with strong effects, without degrading the model fit

Variable Selection (VS)

A process of selecting a subset of predictors, fitting the selected model, and making inferences.

- include variables which are most predictive to the response
- exclude noisy/uninformative variables from the model

Advantages:

- to build more parsimonious and interpretable models
- to enhance the model prediction power
- to improve the precision of the estimates

Applications

VS is crucial to decision-making in many application and scientific areas:

- business: important factors to decide credit limit, insurance premium, mortgage terms
- medical and pharmaceutical industries:
  - select useful chemical compounds for drug-making
  - identify signature genes for cancer classification and diagnosis
  - find risk factors related to disease cause or survival time.
- information retrieval
  - Google search, classification of text documents, email/spam filter
  - speech recognition, image analysis
- more

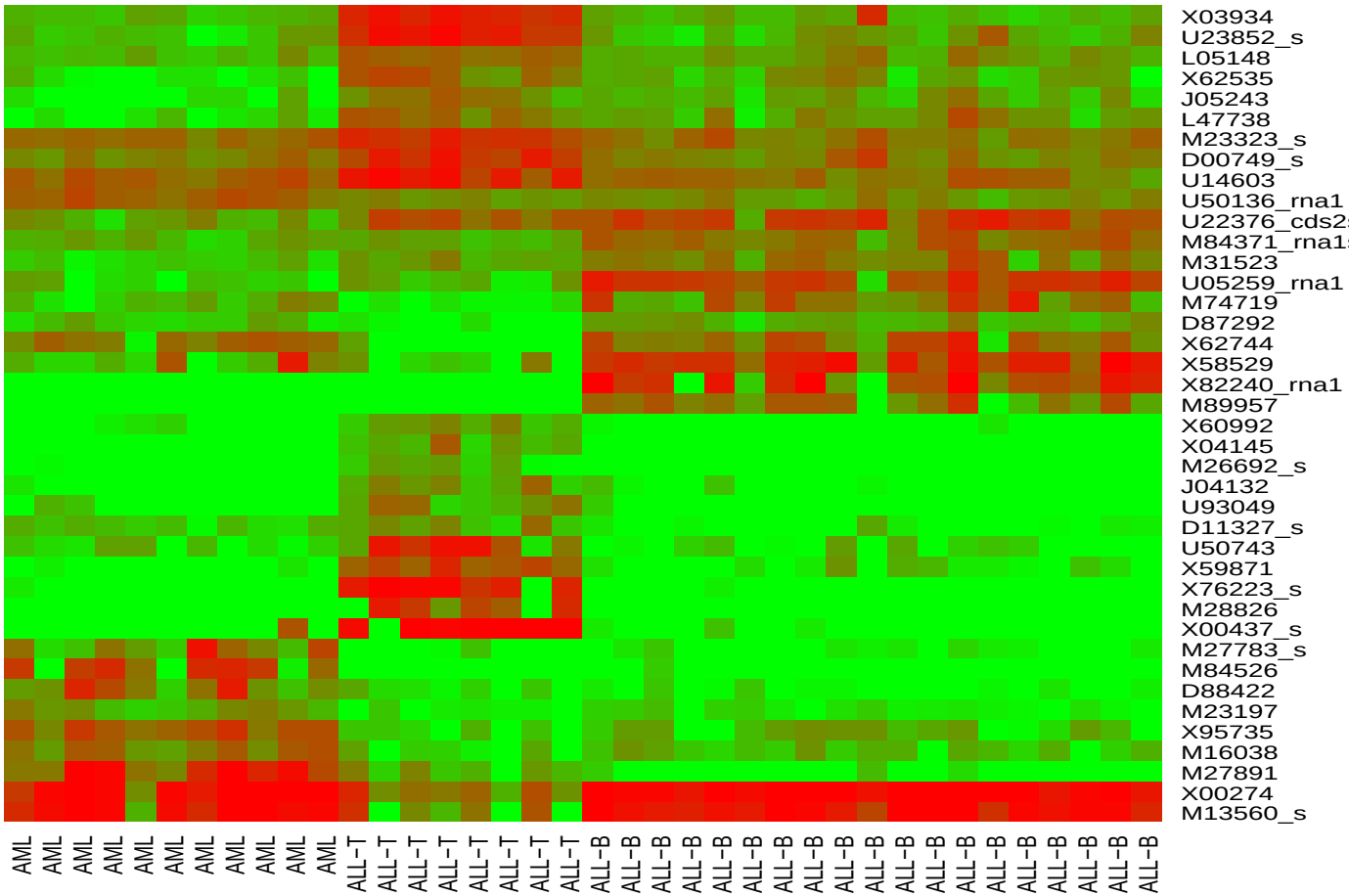
Example: Prostate Cancer Data (Stamey et al. 1989)

id	cv	wt	age	bph	svi	cp	gs	g45	psa
1	0.56	16.0	50	0.25	0	0.25	6	0	0.65
2	0.37	27.7	58	0.25	0	0.25	6	0	0.85
3	0.60	14.8	74	0.25	0	0.25	7	20	0.85
4	0.30	26.7	58	0.25	0	0.25	6	0	0.85
5	2.12	31.0	62	0.25	0	0.25	6	0	1.45
	....					...			

Response Y: prostate specific antigen (psa)

Predictors $\boldsymbol{X}$: cancer volume, prostate weight, age, benign prostatic hyperplasia amount, seminal vesicle invasion, capsular penetration, Gleason score, percent G-score 4 or 5.

Acute Leukemia Data (Golub et al. 1999)



Three types: AML (acute myeloid), ALL-B (acute lymphoblastic), ALL-T

Stanford Heart Transplant Data

start	stop	event	age	year	surg	plant	id
0	50	1	31	0.12	0	0	1
0	6	1	52	0.25	0	0	2
0	1	0	54	0.26	0	0	3
1	16	1	54	0.27	0	1	3
0	36	0	40	0.49	0	0	4
36	39	1	40	0.49	0	1	4
0	18	1	21	0.61	0	0	5
	....				...		

T_i: failure time; C_i: censoring time. Data $(\tilde{T}_i, \delta_i, \boldsymbol{X}_i)$, where $\tilde{T}_i = \min(T_i, C_i)$ and $\delta_i = I(T_i \leq C_i)$.

Notations

- data $(\boldsymbol{X}_i, Y_i), i = 1, \cdots, n$
- n: sample size
- d: the number of predictors, $\boldsymbol{X}_i \in R^d$.
- the full index set $\mathcal{S} = \{1, 2, \cdots, d\}$.
- the selected index set given by a procedure is $\hat{\mathcal{A}}$, its size is $|\hat{\mathcal{A}}|$.
- the linear coefficient vector $\boldsymbol{\beta} = (\beta_1, \cdots, \beta_d)^T$.
- the true linear coefficients $\boldsymbol{\beta}_0 = (\beta_{10}, \cdots, \beta_{d0})^T$.
- the true model $\mathcal{A}_0 = \{j : j = 1, \cdots, d, |\beta_{j0}| \neq 0\}$.

Variable Selection in Orthogonal Design

Assume that

- $\mathbf{y}, \mathbf{x}_1, ..., \mathbf{x}_d$ are centered
- $< \mathbf{x}_j, \mathbf{x}_k >= 0$ for $j \neq k$.

Then

$$\hat{\beta}_j = \frac{< \mathbf{x}_j, \mathbf{y} >}{< \mathbf{x}_j, \mathbf{x}_j >}, \quad j = 1, \cdots, d.$$

Define $t_j = \hat{\beta}_j \|\mathbf{x}_j\|^{1/2} / \hat{\sigma} = \hat{\beta}_j / [\|\mathbf{x}_j\|^{-1/2} \hat{\sigma}]$ for $j = 1, \cdots, d$, then

$$\begin{aligned} SSR &= < X\hat{\boldsymbol{\beta}}, X\hat{\boldsymbol{\beta}} >= \sum_{j=1}^{d} \hat{\beta}_j^2 \|\mathbf{x}_j\|^2 \\ &= \sum_{j=1}^{d} \hat{\sigma}^2 t_j^2 = \sum_{j=1}^{d} R_j^2. \end{aligned}$$

Ranking Variables in Orthogonal Design

The coefficient of determination

$$R^2 = \frac{\text{SSR}}{S_{yy}} = \frac{1}{S_{yy}} \sum_{j=1}^{d} R_j^2$$

- Each $\mathbf{x}_j$ contributes to R^2 regardless other variables
- One can use R_j^2, or t_j^2, or $|t_j|$ to rank the importance of variables.

Variable Selection in Non-orthogonal Design

More practical and difficult cases: variables are correlated.

- There are no natural orderings of importance for the input variables
- The role of a variable can only be measured relative to the other variables in the model.
  - Example: highly correlated variables
- It is essential to check all possible combinations.

Best Subset Selection

For each $k \in \{0, 1, ..., d\}$, find the subset of size k that gives smallest residual sum of squares

- Search through all (2^d) possible subsets:
  - When $d = 10$, we check 1024 combinations.
  - When $d = 20$, more than one million combinations.
- The larger k, the smaller RSS. (see the following picture)

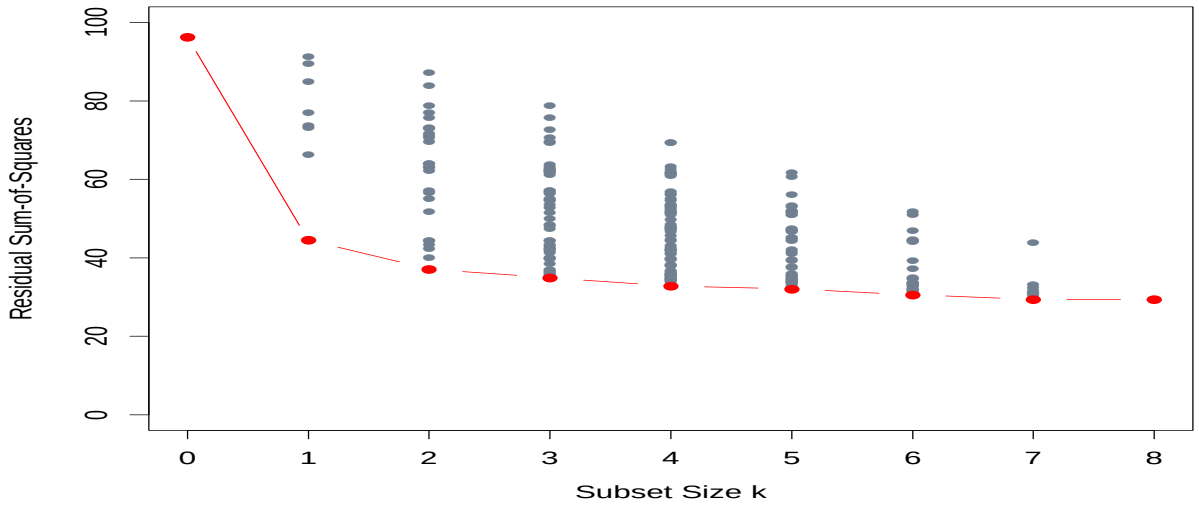


Figure 3.5: *All possible subset models for the prostate cancer example. At each subset size is shown the residual sum-of-squares for each model of that size.*

How to Choose the best k

This question involves

- the tradeoff between bias and variance,
- the more subjective desire for parsimony

In practice, we can use a number of model selection criteria

- cross validation; prediction error on the test set
- Mallow's C_p, F-statistic
- Generalized Information Criteria (GIC):

$$\text{GIC(model)} = -2 \cdot \text{loglik} + \alpha \cdot \text{ df},$$

df is the model size (or the number of effective parameters).

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About Best Subset Selection

Advantages:

- Based on exhaustive search
- Check and compare all (2^d) models

Computation Limitations:

- The computation is infeasible for $d \geq 40$.
- Leaps and bounds procedure (Furnival and Wilson 1974) is efficient for $d \leq 40$
- There is a contributed package *leaps* in R.

Searching Methods

Basic Idea: seeking a good path through all the possible subsets

- forward selection
- backward elimination
- stepwise selection

Forward Selection

- Starting with the intercept, sequentially add one variable that most improves the model fit
  - If there are k variables in the model and the parameter estimate is $\hat{\beta}$, and we add in one variable, resulting in the estimate $\tilde{\beta}$.
  - The improvement in fit is often based on the F statistic

$$F = \frac{\text{RSS}(\hat{\beta}) - \text{RSS}(\tilde{\beta})}{\text{RSS}(\tilde{\beta})/(n-k-2)}.$$

    Typical add the variable which produces the largest value of F.
- Stops when no variable produces an F-ratio greater than the 90th or 95th percentile of the $F_{1,n-k-2}$ distribution

Forward Selection for Prostate Cancer Data

The *leaps* function in R produces the sequence:

	cv	wt	age	bph	svi	cp	gs	g45
step1	x							
step2	x	x						
step3	x	x			x			
step4	x	x		x	x			
step5	x	x	x	x	x			
step6	x	x	x	x	x			x
step7	x	x	x	x	x	x		x
step8	x	x	x	x	x	x	x	x

Forward selection for prostate cancer data: $\hat{\mathcal{A}}_{AIC} = \{1, 2, 3, 4, 5\}$, $\hat{\mathcal{A}}_{BIC} = \{1, 2, 5\}$.

Backward Elimination

- Starting with the full model, sequentially drop one variable that produces the smallest F value
- Stops when each variable in the model produces an F-ratio greater than the 90th or 95th percentile of the $F_{1,n-k-2}$.
- Can only be used when $n > d$.

Stepwise Selection

- In each step, consider both forward and backward moves and make the "best" move
- A thresholding parameter is used to decide "add" or "drop" move.

It allows previously added/removed variables to be removed/added later.

Pros and Cons

Advantages:

- intuitive; simple to implement; work well in practice
- May have lower prediction error than the full model

Limitations:

- Greedy-search type algorithms are fast, but locally optimal
- Highly variable due to discreteness (Breiman, 1996; Fan and Li, 2001)
- Hard to establish asymptotic theory and make inferences.

R code

You need to install the package "leaps" first.

The function "regsubsets()" can be used to conduct model selection by exhaustive search, forward or backward stepwise,

```
library(leaps)
help(regsubsets)
```

```
## Default S3 method:
regsubsets(x=, y=, weights=rep(1, length(y)), nbest=1,
nvmax=8, force.in=NULL, force.out=NULL, intercept=TRUE,
method=c("exhaustive", "backward", "forward", "seqrep"),
really.big=FALSE)
```

Details

Arguments:

- x: design matrix
- y: response vector
- weights: weight vector
- nbest: number of subsets of each size to record
- nvmax: maximum size of subsets to examine
- force.in: index to columns of design matrix that should be in all models
- force.out: index to columns of design matrix that should be in no models
- intercept: Add an intercept?
- method: Use exhaustive search, forward selection, backward selection or sequential re- placement to search.

Fit Sequential Selection Methods in R

```
library(leaps)

# sample size
n = 50
# data dimension
p = 4

# generate design matrix
set.seed(2015)
x <- matrix(rnorm(n*p),ncol=p)
# true regression model
y <- x[,1]+x[,2]+rnorm(n)*0.5

## forward selection
for1 <- regsubsets(x,y,method="forward")
```

```
## backward elimination
back1 <- regsubsets(x,y,method="forward")
summary(back1)
coef(back1, id=1:4)

## exhaustive search
ex1 <- regsubsets(x,y,method="exhaustive")
summary(ex1)
coef(ex1,id=1:4)
```

Two Information Criteria: AIC and BIC

These are based on the maximum likelihood estimates of the model parameters. Assume that

- the training data are $(\mathbf{x}_i, y_i), i = 1, \cdots, n$.
- a fitted linear regression model is $\hat{f}(\mathbf{x})$.

Define

- The degree of freedom (df) of $\hat{f}$ as the number of effective parameters of the model, or the model size
- The residual sum of squares as $\text{RSS} = \sum_{i=1}^{n}[y_i - \hat{f}(\mathbf{x}_i)]^2$

Then

$$\begin{aligned} AIC &= n\log(\text{RSS}/n) + 2 \cdot \text{df}, \\ BIC &= n\log(\text{RSS}/n) + \log(n) \cdot \text{df}, \end{aligned}$$

We choose the model which gives the smallest AIC or BIC.

AIC and BIC for Linear Rgression Models

Assume that

- the training data are $(\mathbf{x}_i, y_i), i = 1, \cdots, n$.
- a fitted linear regression model is $\hat{f}(\mathbf{x}) = \hat{\beta}^T \mathbf{x}$.
- For example, $\hat{\beta}$ can be the regression coefficients given by the OLS, Lasso, forward selection.

Define

- The degree of freedom (df) of $\hat{\beta}$ as the number of nonzero elements in β (model size), including the intercept
- The residual sum of squares as RSS $= \sum_{i=1}^{n} (y_i - \hat{\beta}^T \mathbf{x}_i)^2$

$$\begin{aligned} \text{AIC} &= n \log(\text{RSS}/n) + 2 \cdot \text{df}, \\ \text{BIC} &= n \log(\text{RSS}/n) + \log(n) \cdot \text{df}, \end{aligned}$$

We choose the model which gives the smallest AIC or BIC.

How To Derive BIC

By definition, the BIC for the model M is formally defined as

$$BIC = -2 \log \hat{L} + \log(n) \cdot \text{df},$$

where

- L is the likelihood function of the model parameters;
- $\hat{L}$ is the maximumized value of the likelihood function of the model M.

Special example: Consider the regression model:

$$Y_i = \mathbf{X}_i^T \beta + \epsilon_i, \quad \epsilon_i \sim N(0, \sigma^2).$$

The observations $Y_i \sim N(\mathbf{X}_i^T \beta, \sigma^2), i = 1, \cdots, n$ are independent.

Example: BIC in Regression Case

For model M, the design matrix $X_M = \{X_{ij} : i = 1, \cdots, n; j \in M\}$. The likelihood

$$L(\beta|\mathbf{y}, X_M) = (2\pi\sigma^2)^{-n/2} \exp\{-\frac{(\mathbf{y} - X_M\beta)^T(\mathbf{y} - X_M\beta)}{2\sigma^2}\},$$

and the log likelihood is

$$\log L(\mathbf{y}|\mathbf{x}_1, \cdots, \mathbf{x}_n) = -\frac{n}{2}\log(2\pi) - \frac{n}{2}\log(\sigma^2) - \frac{(\mathbf{y} - X_M\beta)^T(\mathbf{y} - X_M\beta)}{2\sigma^2}.$$

The MLE is given by

$$\widehat{\beta}_{MLE} = (X_M^T X_M)^{-1} X_M^T \mathbf{y}, \quad \hat{\sigma}^2_{MLE} = \frac{RSS}{n},$$

where $\text{RSS} = (\mathbf{y} - X_M\widehat{\beta})^T(\mathbf{y} - X_M\widehat{\beta})$.

Derivation of BIC (continued)

Then

$$-2\log\hat{L} = n\log(2\pi) + n\log(\hat{\sigma}^2) + n = n\log(2\pi) + n\log(\frac{\text{RSS}}{n}) + n.$$

Removing the constant, we get

$$BIC = n\log(\frac{RSS}{n}) + \log(n)\cdot|M|.$$

Compute AIC and BIC for Forward Selection

```
# four candidate models
m1 <- lm(y~x[,1])
m2 <- lm(y~x[,1]+x[,2])
m3 <- lm(y~x[,1]+x[,2]+x[,4])
m4 <- lm(y~x)

# compute RSS for the four models
rss <- rep(0,4)
rss[1] <- sum((y-predict(m1))^2)
rss[2] <- sum((y-predict(m2))^2)
rss[3] <- sum((y-predict(m3))^2)
rss[4] <- sum((y-predict(m4))^2)
```

Compute AIC and BIC for Forward Selection

```
# compute AIC and BIC
bic <- rep(0,4)
aic <- rep(0,4)

for (i in 1:4){
bic[i] = n*log(rss[i]/n)+log(n)*(1+i)
aic[i] =  n*log(rss[i]/n)+2*(1+i)
}

# find the optimal model
which.min(bic)
which.min(aic)
```