Linear regression

Hastie, Tibshirani, Friedman Ch 6-7

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CS 6140
Machine Learning
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Generative vs discriminative models

- Goal: predict Y
  - Bayes rule:

$$p(Y|\mathbf{X}) = \frac{p(Y) \cdot p(\mathbf{X}|Y)}{p(\mathbf{X})}$$

- Generative classifiers
  - Specify prior probability of $p(Y)$
  - Assume conditional distribution $p(\mathbf{X}|Y)$
  - Use Bayes rule to derive the posterior $p(Y|\mathbf{X})$
  - **Example:** Linear discriminant analysis

- Discriminative classifiers
  - Estimate the posterior the posterior $p(Y|\mathbf{X})$
  - Do not assume the distribution on $\mathbf{X}$
  - **Example:** Y continuous: linear regression

Linear regression with two predictors

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \varepsilon_i; \qquad i = 1, \ldots, n$$

- β_0 is the intercept
- β_1 and β_2 are the regression coefficients
- Meaning of regression coefficients
  - β_1 describes change in mean response per unit increase in X_1 when X_2 is held constant
  - β_2 describes change in mean response per unit increase in X_2 when X_1 is held constant
- Variables X_1 and X_2 are **additive**.
- Same change in X_1 for all X_2.
- The response surface is a plane.

Interaction model

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \beta_3 X_{i1} X_{i2} + \varepsilon_i$$

- Meaning of parameters:
  - Change in X_1 when $X_2 = x_2$

$$\begin{aligned} \Delta Y &= (\beta_0 + \beta_1(X_1 + 1) + \beta_2 x_2 + \beta_3(X_1 + 1)x_2) - \\ &\quad (\beta_0 + \beta_1 X_1 + \beta_2 x_2 + \beta_3 X_1 x_2) \\ &= \beta_1 + \beta_3 x_2 \end{aligned}$$

  - Change in X_2 when $X_1 = x_1$

$$\Delta Y = \beta_2 + \beta_3 x_1$$

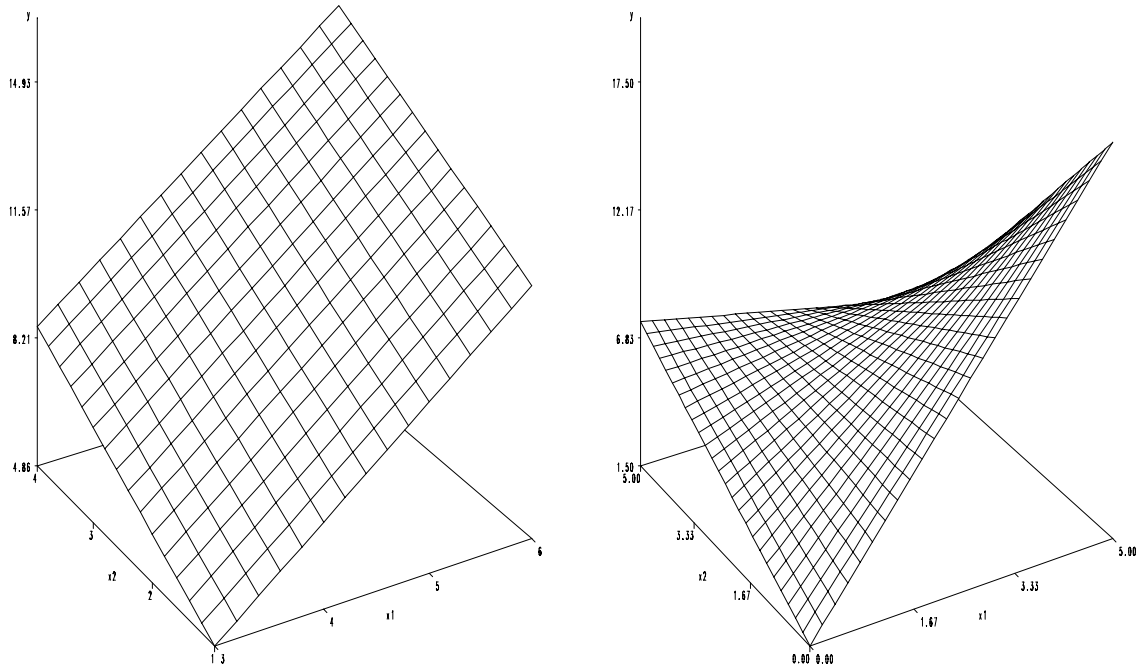
- Rate of change due to one variable affected by the other

Additive vs interaction model

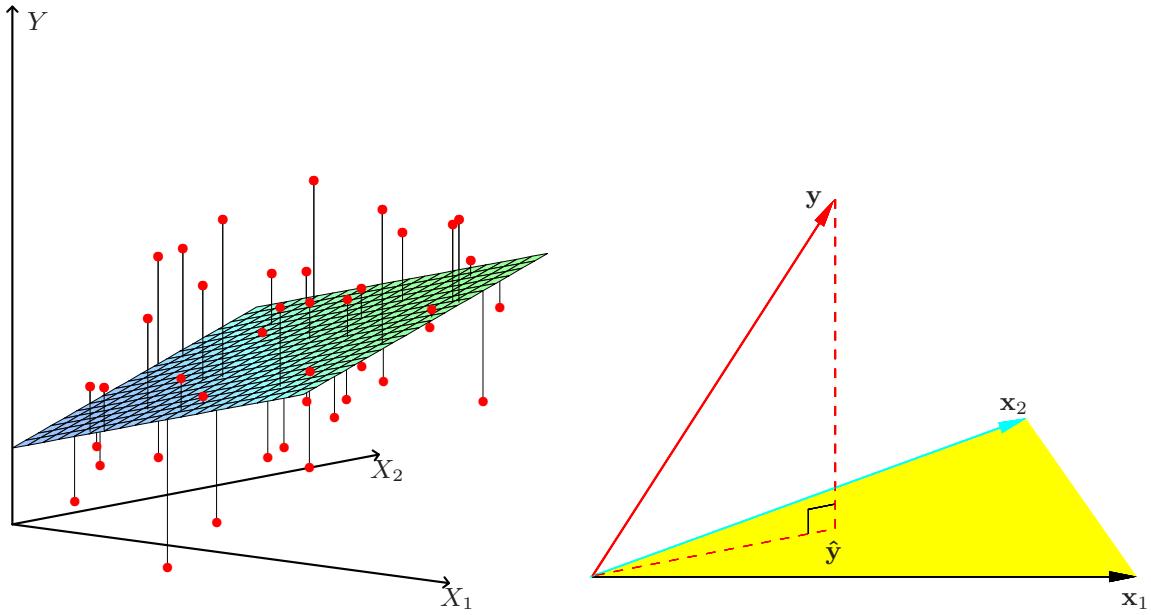
$$\widehat{Y}_i = -2.79 + 2.14X_{i1} + 1.21X_{i2}$$

versus

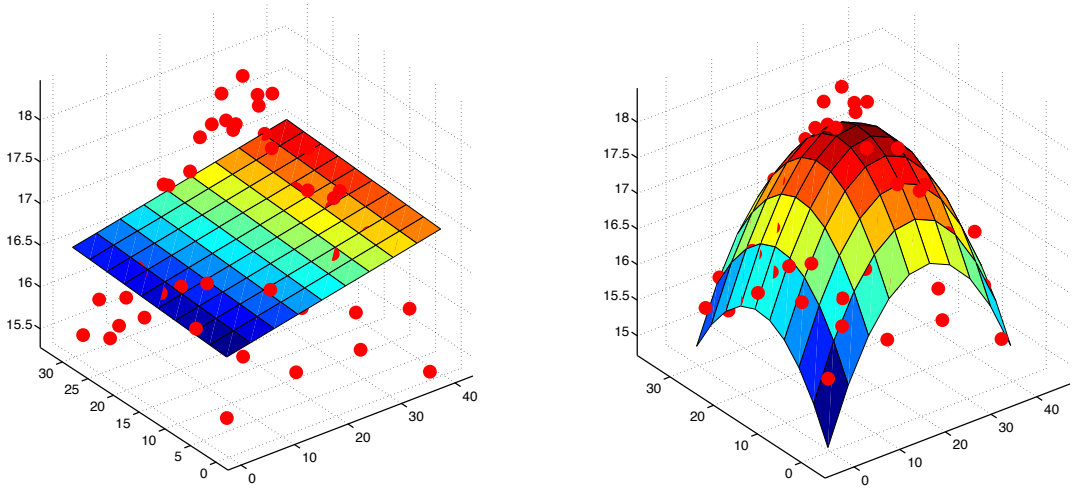
$$\widehat{Y}_i = 1.5 + 3.2X_{i1} + 1.2X_{i2} - .75X_{i1}X_{i2}$$



Linear regression with two predictors



Hastie, Tibshirani, Friedman, Fig 3.1 and 3.2



K. Murphy, Fig 7.1

Polynomial regression and transformations

- Polynomial regression:

$$\begin{aligned} Y_i &= \beta_0 + \beta_1 X_i + \beta_2 X_i^2 + \varepsilon_i \\ &= \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \varepsilon_i \end{aligned}$$

where $X_{i2} = X_i^2$.

  - this is a linear model because it is a linear function of parameters β

- Transformations

$$log(Y_i) = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \varepsilon_i$$

$$Y_i = \frac{1}{\beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \varepsilon_i}$$

  - this is a linear model on the $log(Y_i)$ scale

General linear regression in matrix terms

- As an equation

$$Y_i = \beta_0 + \beta_1 X_{i1} + \cdots + \beta_{p-1} X_{i,p-1} + \varepsilon_i$$

- As an array

$$\begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} = \begin{bmatrix} 1 & X_{11} & X_{12} & \cdots & X_{1\ p-1} \\ 1 & X_{21} & X_{22} & \cdots & X_{2\ p-1} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & X_{n1} & X_{n2} & \cdots & X_{n\ p-1} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \cdots \\ \beta_{p-1} \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix}$$

- In matrix notation

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

Estimation of regression coefficients

- Objective function: least squares
  - find $\hat{\beta}$ to minimize

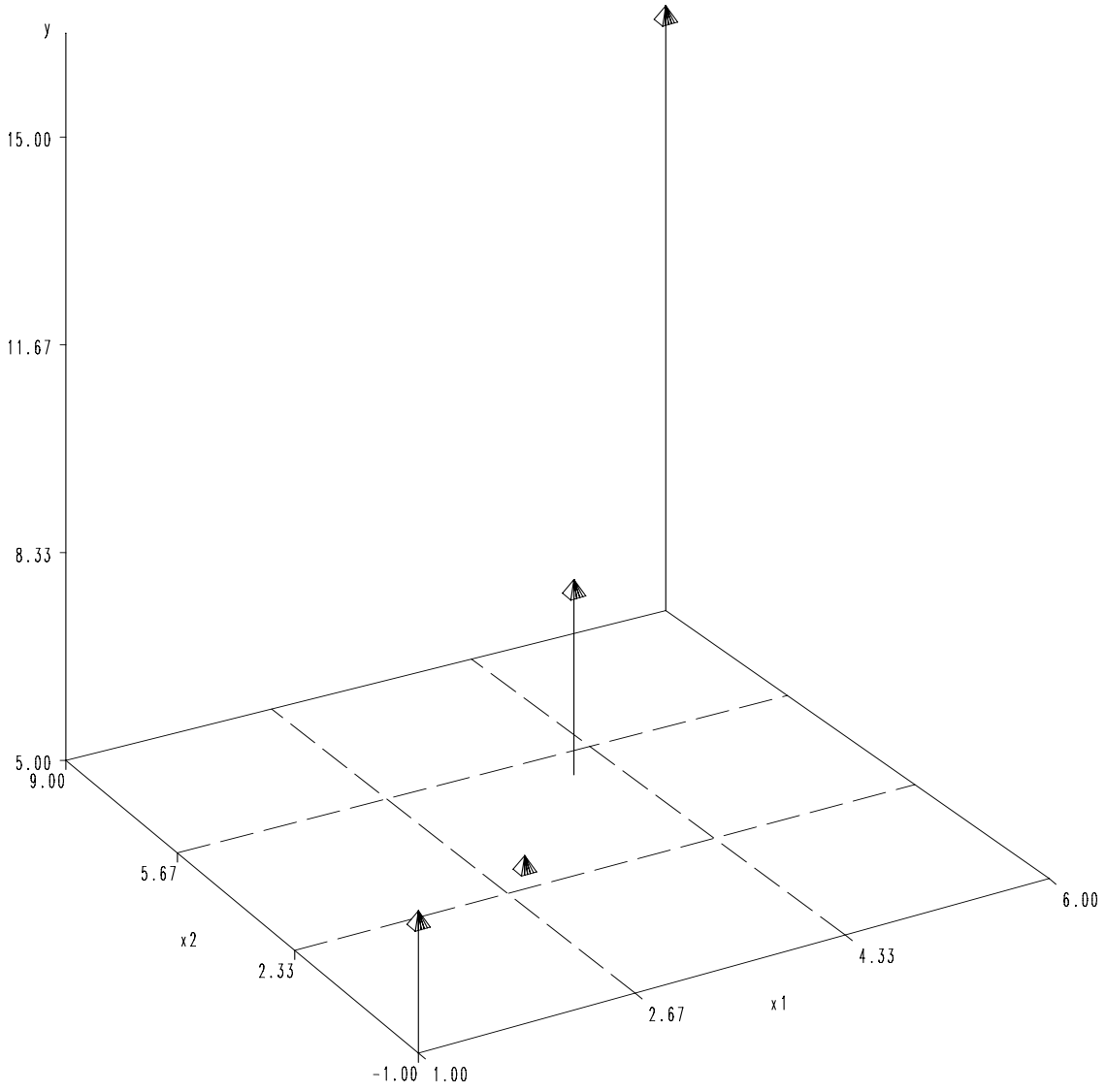
    $$\sum_{i=1}^{N}(y_i - x_i'\beta)^2 = (\mathbf{Y} - \mathbf{X}\hat{\beta})'(\mathbf{Y} - \mathbf{X}\hat{\beta})$$

  - Quadratic objective function $\Rightarrow$
    its minimum always exists, but may not be unique

- Finding estimates
  - Differentiating wrt β:
  - Normal equations $\mathbf{X}'(y - \mathbf{X}\beta) = 0 \Rightarrow \hat{\beta} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$

- Fitted values define a (hyper)plane
  - $\hat{\mathbf{Y}} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y} = \mathbf{H}\mathbf{Y}$
  - Residuals: $\mathbf{e} = \mathbf{Y} - \hat{\mathbf{Y}} = (\mathbf{I} - \mathbf{H})\mathbf{Y}$

Multicollinearity



Qualitative predictors

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \beta_3 X_{i1} X_{i2} + \varepsilon_i$$

- Let $X_2 = 1$ if case from Massachusetts

- Meaning of parameters:
  - Case from Massachusetts ($X_2 = 1$):

$$\begin{aligned} Y &= \beta_0 + \beta_1 X_1 + \beta_2 1 + \beta_3 X_1 (1) \\ &= (\beta_0 + \beta_2) + (\beta_1 + \beta_3) X_1 \end{aligned}$$

  - Case from other location ($X_2 = 0$)

$$\begin{aligned} Y &= \beta_0 + \beta_1 X_1 + \beta_2 0 + \beta_3 X_1 (0) \\ &= \beta_0 + \beta_1 X_1 \end{aligned}$$

- Have <u>two</u> regression lines

- β_2 and β_3 quantify the differences

Two groups: Wrong coding

- Assume an additive model with two groups

- Wrong approach: add both indicators

$$X_2 = \begin{cases} 1 \text{ , if stock firm} \\ 0 \text{ , otherwise} \end{cases} \quad X_3 = \begin{cases} 1 \text{ , if mutual fund} \\ 0 \text{ , otherwise} \end{cases}$$

  - the model below is wrong

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \beta_3 X_{i3} + \varepsilon_i$$

- The corresponding design matrix

  - 4 data points (first 2 from stock firm, last 2 from mutual fund)

$$\mathbf{X} = \begin{pmatrix} 1 & X_{11} & 1 & 0 \\ 1 & X_{21} & 1 & 0 \\ 1 & X_{31} & 0 & 1 \\ 1 & X_{41} & 0 & 1 \end{pmatrix}$$

  - this model creates fully collinear columns in the design matrix $\mathbf{X}$ (R will drop the first)

Two groups: Correct coding

- Correct approach 1:

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \varepsilon_i$$

  - interpretation:

$$\begin{aligned} E\{Y_i\} &= \beta_0 + \beta_1 X_{i1} && \text{if mutual fund} \\ E\{Y_i\} &= (\beta_0 + \beta_2) + \beta_1 X_{i1} && \text{if stock firm} \end{aligned}$$

  - Mutual fund is the reference group
  - β_2: the deviation of the intercept of the stock firm from the reference

- The corresponding design matrix:

  - 4 data points (first 2 from stock firm, last 2 from mutual fund)

$$\mathbf{X} = \begin{pmatrix} 1 & X_{11} & 1 \\ 1 & X_{21} & 1 \\ 1 & X_{31} & 0 \\ 1 & X_{41} & 0 \end{pmatrix}$$

Three groups: Wrong coding

- Extend the indicator

$$X_2 = \begin{cases} 0 \text{ , if mutual fund} \\ 1 \text{ , if stock firm} \\ 2 \text{ , if foreign firm} \end{cases}$$

- The model below is still appropriate

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \varepsilon_i$$

  - interpretation: enforces an equal change in $E\{Y\}$ for each extra indicator

$$\begin{aligned} E\{Y_i\} &= \beta_0 + \beta_1 X_{i1} && \text{if mutual fund} \\ E\{Y_i\} &= (\beta_0 + \beta_2) + \beta_1 X_{i1} && \text{if stock firm} \\ E\{Y_i\} &= (\beta_0 + 2\beta_2) + \beta_1 X_{i1} && \text{if foreign firm} \end{aligned}$$

- The corresponding design matrix:

  - 6 data points (first 2 from mutual fund, 2 from stock, 2 foreign)

$$\mathbf{X} = \begin{pmatrix} 1 & X_{11} & 0 \\ 1 & X_{21} & 0 \\ 1 & X_{31} & 1 \\ 1 & X_{41} & 1 \\ 1 & X_{41} & 2 \\ 1 & X_{41} & 2 \end{pmatrix}$$

Three groups: Correct coding

- First option:

$$X_2 = \begin{cases} 1 \text{ , if stock firm} \\ 0 \text{ , otherwise} \end{cases} \qquad X_3 = \begin{cases} 1 \text{ , if foreign firm} \\ 0 \text{ , otherwise} \end{cases}$$

- The model below contains two indicators

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \beta_3 X_{i3} + \varepsilon_i$$

  - interpretation:

$$\begin{aligned} E\{Y_i\} &= \beta_0 + \beta_1 X_{i1} && \text{if mutual fund} \\ E\{Y_i\} &= (\beta_0 + \beta_2) + \beta_1 X_{i1} && \text{if stock firm} \\ E\{Y_i\} &= (\beta_0 + \beta_3) + \beta_1 X_{i1} && \text{if foreign firm} \end{aligned}$$

  - mutual fund is the reference
  - β_2 and β_3 are deviations of the intercepts from the reference
  - also more flexibility in presence of interactions X_1X_2 and X_1X_3
  - the number of indicators is always one less than the number of groups

Normal Error Model

- **The least square estimates of the parameters do not require the assumption of Normality**

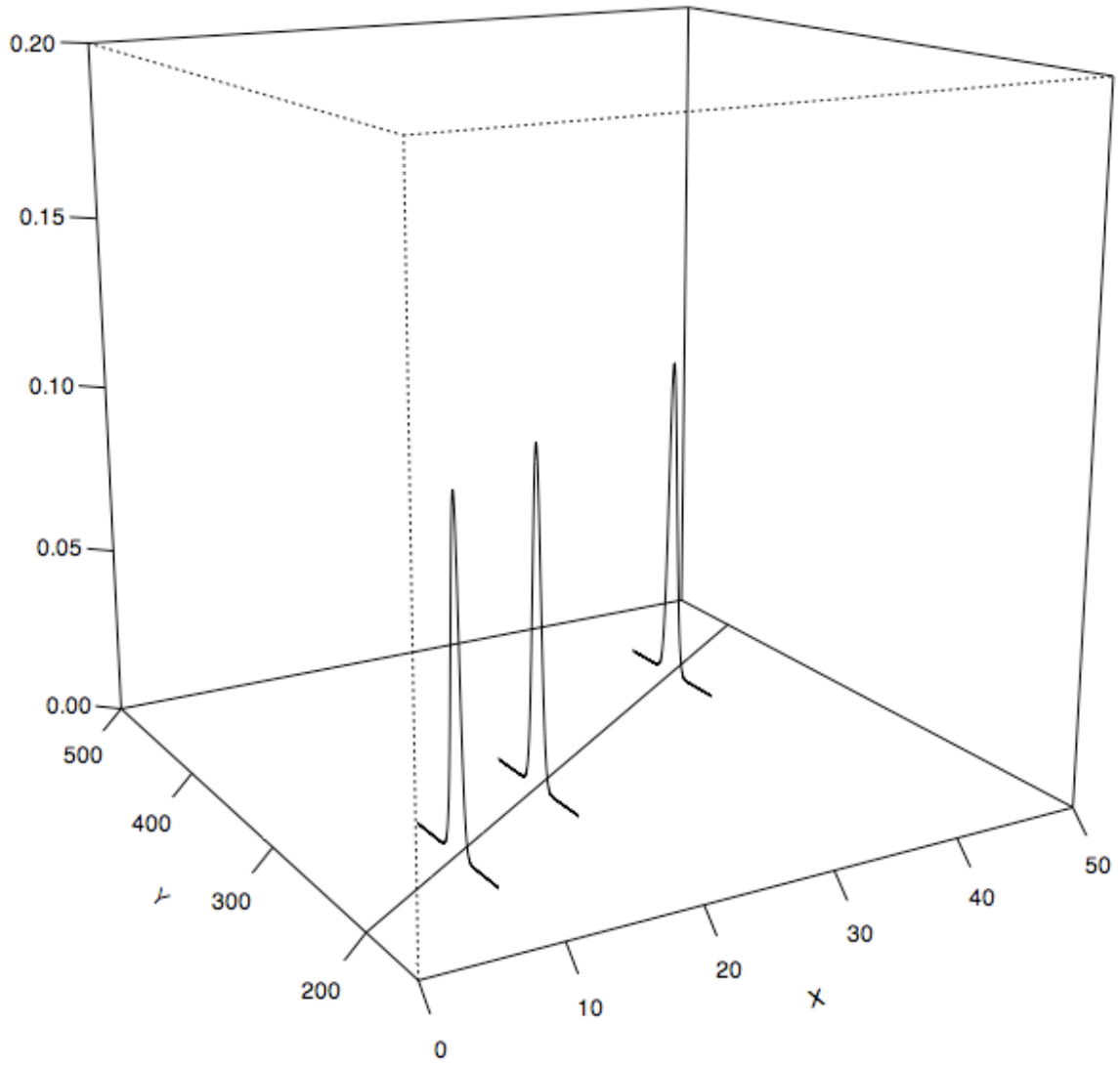
- Normal error assumption greatly simplifies the theory of analysis

- Normality is used to construct confidence intervals / perform hypothesis tests follow known distributions (e.g., t, F)

- While not always true in practice, most inference only sensitive to large departures from normality

Normal Error regression model

- $Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i$



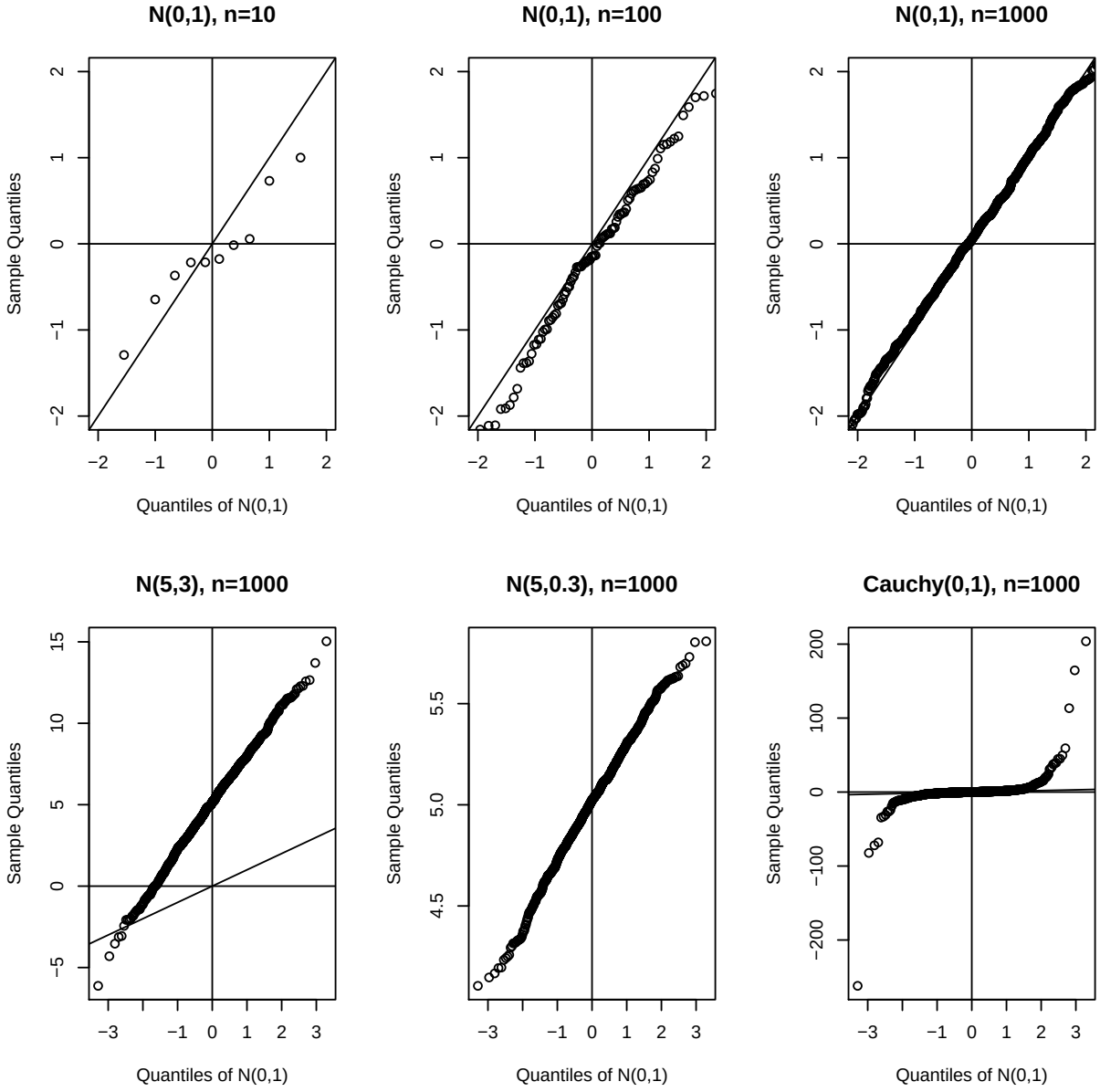
Normal Error regression model

$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i$$

- β_0 is the intercept
- β_1 in the slope
- ε_i is the i^{th} random error term
  - $\varepsilon_i \sim \mathsf{N}(0, \sigma^2) \longleftarrow$ **NEW**
  - Uncorrelated $\longrightarrow$ independent error terms
- Defines distribution of Y: $p(Y|\mathbf{X})$

$$Y_i \sim \mathsf{N}(\beta_0 + \beta_1 X_i, \sigma^2)$$

Assessing Normality: Quantile-quantile plot



Can be used with any other distribution

Example

Height of 11 women

i	Observed height	Adj. percentile $100(i-\frac{1}{2})/11)$	z	Sample quantiles
1	61.0	4.55	-1.69	60.6
2	62.5	13.64	-1.10	62.3
3	63.0	22.73	-0.75	63.4
4	64.0	31.82	-0.47	64.1
5	64.5	40.91	-0.23	64.8
6	65.0	50.00	0.00	65.5
7	66.5	59.09	0.23	66.2
8	67.0	68.18	0.47	66.9
9	68. 0	77.27	0.75	67.6
10	68.5	86.36	1.10	68.7
11	70.5	95.45	1.69	70.4

QQplot: plot Observed height vs sample quantiles

Sample quantiles $= x + Z \cdot \hat{\sigma} + \hat{\mu}$

```
> ?qqplot
> ?qqnorm
```

Maximum Likelihood Estimation

- Assumption of Normality gives us more choices of methods for parameter estimation

$$Y_i \sim \mathsf{N}(\beta_0 + \beta_1 X_i, \sigma^2)$$

$$\downarrow$$

$$f_i = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{1}{2\sigma^2}(Y_i - \beta_0 - \beta_1 X_i)^2\right\}$$

- Likelihood function $L = f_1 \times f_2 \times \cdots \times f_n$ (i.e. the joint probability distribution of the observations, viewed as function of parameters)

- Find β_0, β_1 and σ^2 which maximizes L

- Obtain same estimators $\widehat{\beta}_0$ and $\widehat{\beta}_1$

- A slightly smaller estimate of σ^2
  - See KM 7.3 for derivation in vector notation

Partitioning sums of squares

- Organizes results arithmetically
- Total sums of squares in Y is defined

$$\text{SSTO} = \sum (Y_i - \overline{Y})^2$$

- Can partition sum of squares into
  - Model (explained by regression)
  - Error (unexplained / residual)
- Rewrite the total sum of squares as

$$\sum (Y_i - \overline{Y})^2 = \sum (Y_i - \hat{Y}_i + \hat{Y}_i - \overline{Y})^2$$

$$\begin{aligned} \sum (Y_i - \overline{Y})^2 &= \sum (\hat{Y}_i - \overline{Y})^2 + \sum (Y_i - \hat{Y}_i)^2 \\ &= b_1^2 \sum (X_i - \overline{X})^2 + \sum (Y_i - \hat{Y}_i)^2 \\ \text{SSTO} &= \text{SSR} + \text{SSE} \end{aligned}$$

Coefficient of multiple determination

- Coefficient of Determination R^2 describes proportionate reduction in total variation associated with the **full set** of X variables

$$R^2 = \frac{SSR}{SSTO} = 1 - \frac{SSE}{SSTO},\ 0 \leq R^2 \leq 1$$

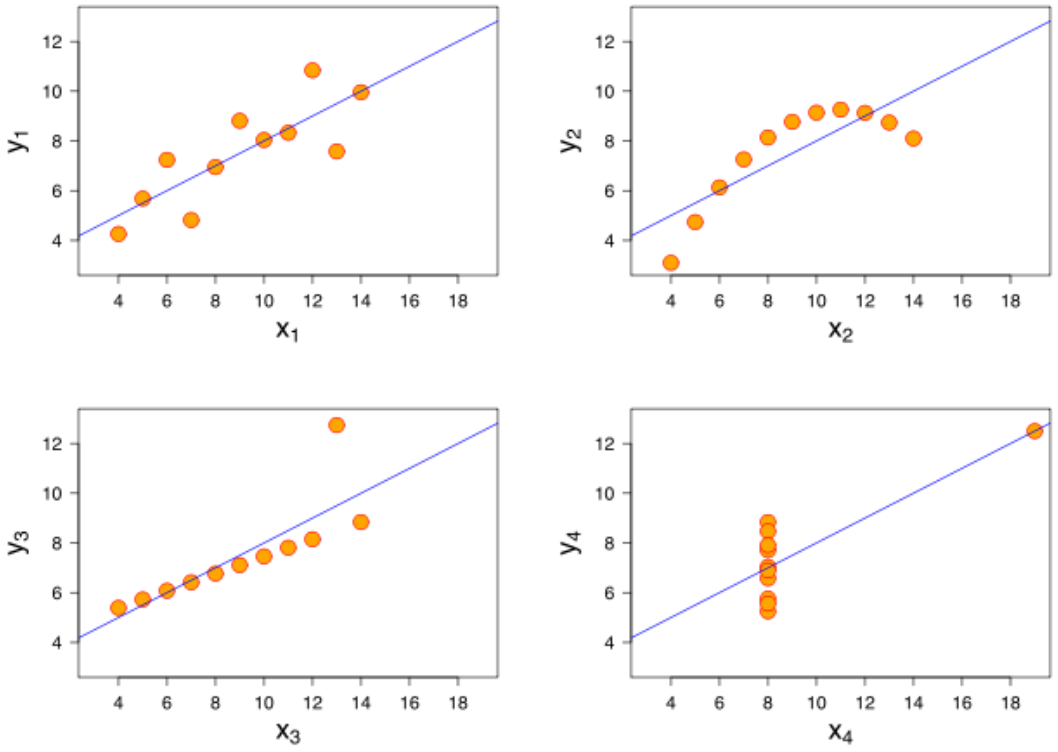
- R^2 usually increases with the increasing p
  - Adjusted R_a^2 attempts to account for p

$$R_a^2 = 1 - \frac{SSE/n-p}{SSTO/n-1},\ 0 \leq R_a^2 \leq 1$$

  - The adjustment is often insufficient

Anscombe's quartet

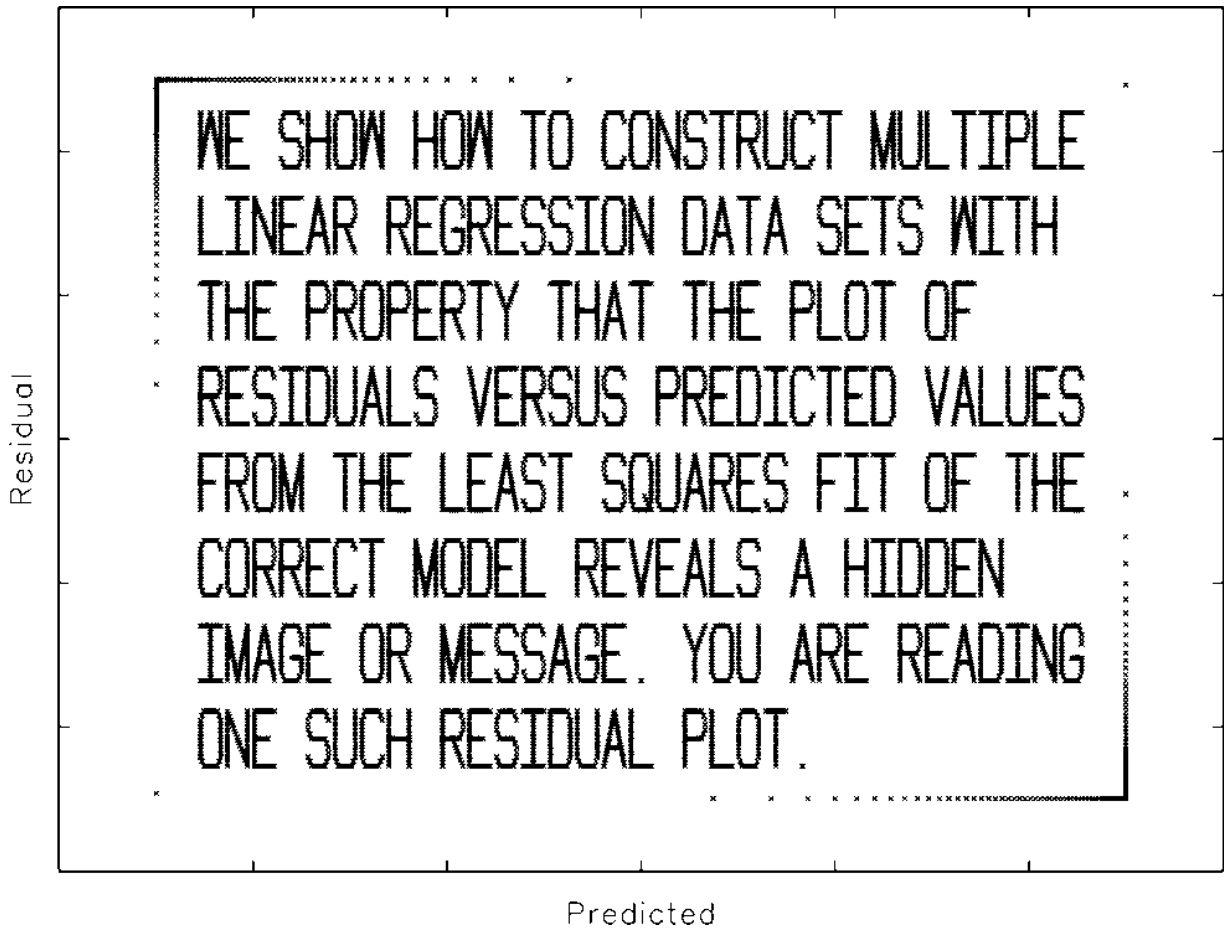
- Constructed in 1973 by Francis Anscombe
- All four datasets share properties
  - $n = 1$, $\bar{x} = 9$, $\bar{y} = 7.50$
  - $Var\{x\} = 11$, $Var\{y\} = 4.12$
  - $Corr(x, y) = 0.816$, $\hat{y} = 0.5x + 3$



https://en.wikipedia.org/wiki/Anscombe's_quartet

Residual (Sur)Realism

- Algorithm for creating multi-variable linear regressions with arbitrary residuals



L. Stefanski, Residual (Sur)Realism. *The American Statistician*, vol. 61, p.163, 2007.

Properties of sampling distribution of $\widehat{\beta}$

- Consistent estimators $\widehat{\beta} \to \beta$ as $n \to \infty$
- Unbiased estimators $E\{\widehat{\beta}\} = \beta$
- Minimum variance estimators: min $Var\{\widehat{\beta}\}$
- Gauss-Markov theorem: $\widehat{\beta}$ least squares
  - Are unbiased
  - Have **minimum variance** among all unbiased linear estimators
  - i.e., are the most precise of any estimators where

    b_l is of the form $\sum k_i Y_i$ and $E(b_l) = \beta_l$

- See KM 6.4 and HTF 3.2.2 for details

Bias-variance decomposition

- Mean Squared Error (MSE):

$$\begin{aligned} MSE &= E\{\widehat{\beta} - \beta\}^2 \\ &= E\left\{\widehat{\beta} - E\{\widehat{\beta}\} + E\{\widehat{\beta}\} - \beta\right\}^2 \\ &= E\left\{\widehat{\beta} - E\{\widehat{\beta}\}\right\}^2 + E\left\{\{\widehat{\beta}\} - \beta\right\}^2 \\ &= \text{Var}\{\widehat{\beta}\} + \text{Bias}\{\widehat{\beta}\}^2 \end{aligned}$$

- For unbiased estimators, MSE=Var$\{\widehat{\beta}\}$

- Biased estimators can $\downarrow$ MSE if Var$\{\widehat{\beta}\}$ $\downarrow$

Empirical risk minimization

- Consider loss function $L\left(Y, f(\mathbf{X})\right)$
  - y is true but unknown response
  - $f(\mathbf{X})$ is function (e.g., linear combination) of observed predictors
- The risk (of making incorrect decision) is
  - $R = E\{L\left(Y, f(\mathbf{X})\right)\} = \sum_x \sum_y L\left(Y, f(\mathbf{X})\right) \cdot p(\mathbf{X}, Y)$
  - When $L\left(Y, f(\mathbf{X})\right)$ is 0-1- function: misclassification rate
  - When $L\left(Y, f(\mathbf{X})\right) = (Y - \delta(\mathbf{X}))^2$: mean squared error
- The estimated (i.e. empirical) risk is
  - $R = \frac{1}{N} \sum_{i=1}^{N}, L\left(Y, f(\mathbf{X})\right)$
  - If validation set is not available: use cross-validation (see KM 6.5.3)

Model selection and bias-variance tradeoff

- Consider polynomial regression, fixed X

  $Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \ldots + \beta_k X^k = f_k(X) + \epsilon$

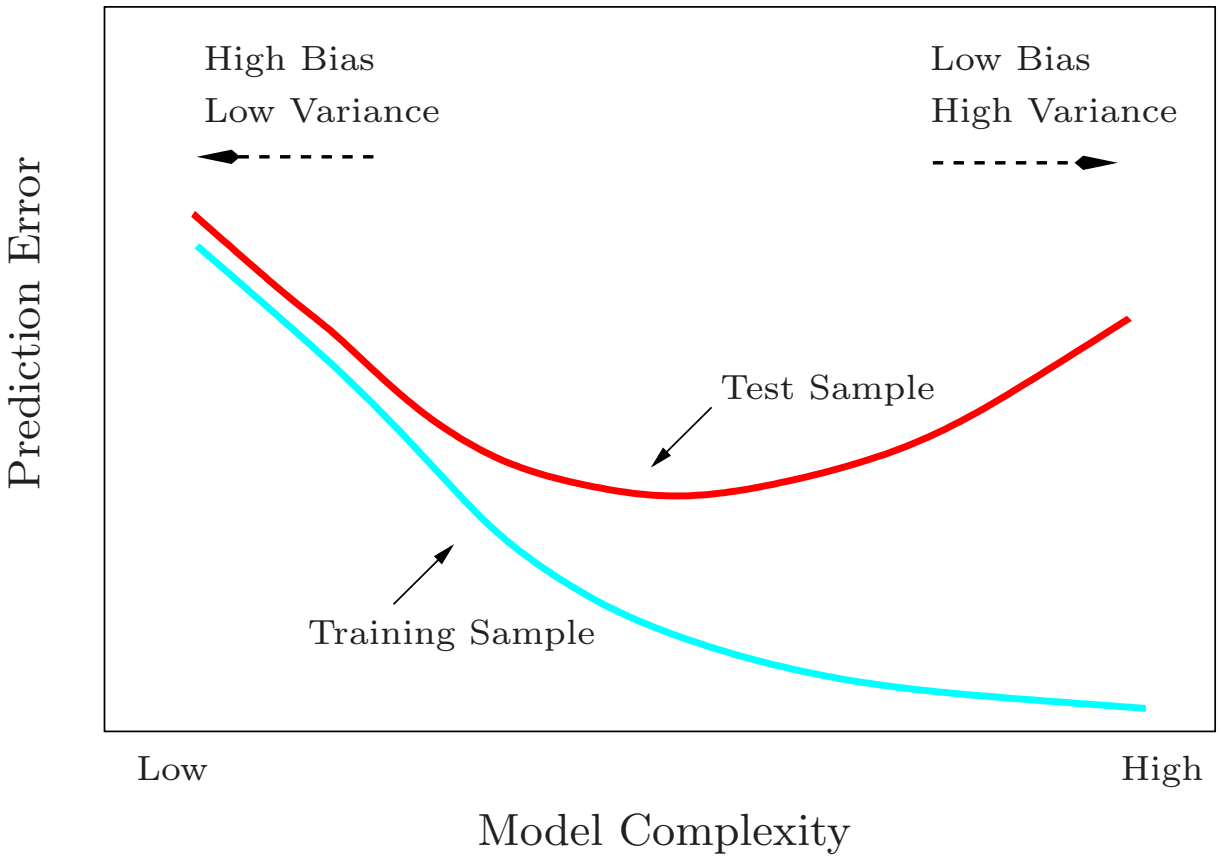
- When $L\left(Y, f_k(X)\right) = (Y - \delta(X))^2$
  - The expected loss for a fixed $X = x$ $L\left(Y, f(x)\right)$ is

$$
\begin{aligned}
& E\left\{(Y - f_k(x)^2 | X = x)\right\} \\
= \;& \sigma^2 + \left[f(x) - \frac{1}{k}\sum_{l=1}^{k} f(x_l)\right]^2 + \frac{\sigma^2}{k} \\
= \;& \text{irreducible error} + \text{Bias}^2\{\widehat{f}_k(x)\} + Var\{\widehat{f}_k(x)\}
\end{aligned}
$$

See Hastie, Friedman, Tibshirani Section 2.9 for details

Model selection and bias-variance tradeoff

- Select k that minimizes the loss



Hastie, Friedman, Tibshirani Section 2.9

AIC and BIC

- In Normal linear regression, the likelihood:

$$L_p = \frac{1}{(2\pi\sigma^2)^{\frac{n}{2}}} e^{-\frac{1}{2\sigma^2}\sum_{i=1}^{n}(Y_i-\beta_0-\beta_1 X_{1i}-\ldots-\beta_{p-1}X_{p-1,i})^2}$$

$$-2logL_p \propto \frac{1}{\sigma^2}\sum_{i=1}^{n}(Y_i-\beta_0-\beta_1 X_{1i}-\ldots\beta_{p-1}X_{p-1,i})^2$$

- Min -2log(likelihood), while penalizing p

- AIC - Akaike's information criterion

$$AIC = \frac{\text{SSE}_\text{p}}{MSE_P} + 2p \text{ (proportional to } C_p\text{)}$$

also written as $AIC = n\log\left(\frac{\text{SSE}_p}{n}\right) + 2p$

- SBC - Schwarz Bayesian Criterion

$$BIC = \frac{\text{SSE}_\text{p}}{MSE_P} + p\,log(n) \text{ (heavier penalty for } p\text{)}$$

also written as $BIC = n\log\left(\frac{\text{SSE}_p}{n}\right) + p\log(n)$

- Can use to compare non-nested models

Steps of Model Building (1)

- Data examination
  - outliers? errors? missing data?
  - correct records; complete missings; remove unreliable predictors
- Preliminary model investigation
  - scatterplots; correlations between Xs and between Xs and Y; normality of errors
  - potential transformations of Y
  - remove redundant or uninformative variables
  - identify potentially important predictors that are not part of the dataset
    - in designed experiments, randomization helps avoid the bias due to important unobserved predictors

Steps of Model Building (2)

- Further reduction of potential predictors
  - domain knowledge
  - (semi-)automated subset selection techniques
- Model refinement
  - higher-order terms (curvature, interactions)
  - consider influential or atypical observations
  - a small number of competing models can be kept at this stage
- Model validation
  - stability of estimated coefficients on new dataset
  - predictive ability on new dataset
    - one model can be better at estimation, but another better at prediction

Surgical Unit Example, p. 350

- Random sample of 54 patients undergoing a liver operation

- Response `surv` or `lsurv` post-operation survival (or log-survival) time

- Predictor variables
  - `blood` blood clotting score
  - `prog` prognostic index
  - `enz` enzyme function score
  - `liver` liver function score
  - `age` in years
  - `female` gender, 0=male, 1=female
  - `modAlc` and `heavyAlc` alcool use

Getting to know the data

```
> require(RCurl)
> ch09ta01.file <- getURL("[...]", ssl.verifypeer=FALSE)
>
> X <- read.table(textConnection(ch09ta01.file), sep='')
> dimnames(X)[[2]] <- c('blood', 'prog', 'enz', 'liver',
+  'age', 'female', 'modAlc', 'heavyAlc', 'surv', 'lsurv')

> dim(X)
[1] 54 10


> head(X)
 blood prog enz liver age female modAlc heavyAlc surv lsurv
1  6.7   62  81  2.59  50      0      1        0  695 6.544
2  5.1   59  66  1.70  39      0      0        0  403 5.999
3  7.4   57  83  2.16  55      0      0        0  710 6.565
4  6.5   73  41  2.01  48      0      0        0  349 5.854
5  7.8   65 115  4.30  45      0      0        1 2343 7.759
6  5.8   38  72  1.42  65      1      1        0  348 5.852


> sum(is.na(X))
[1] 0
```

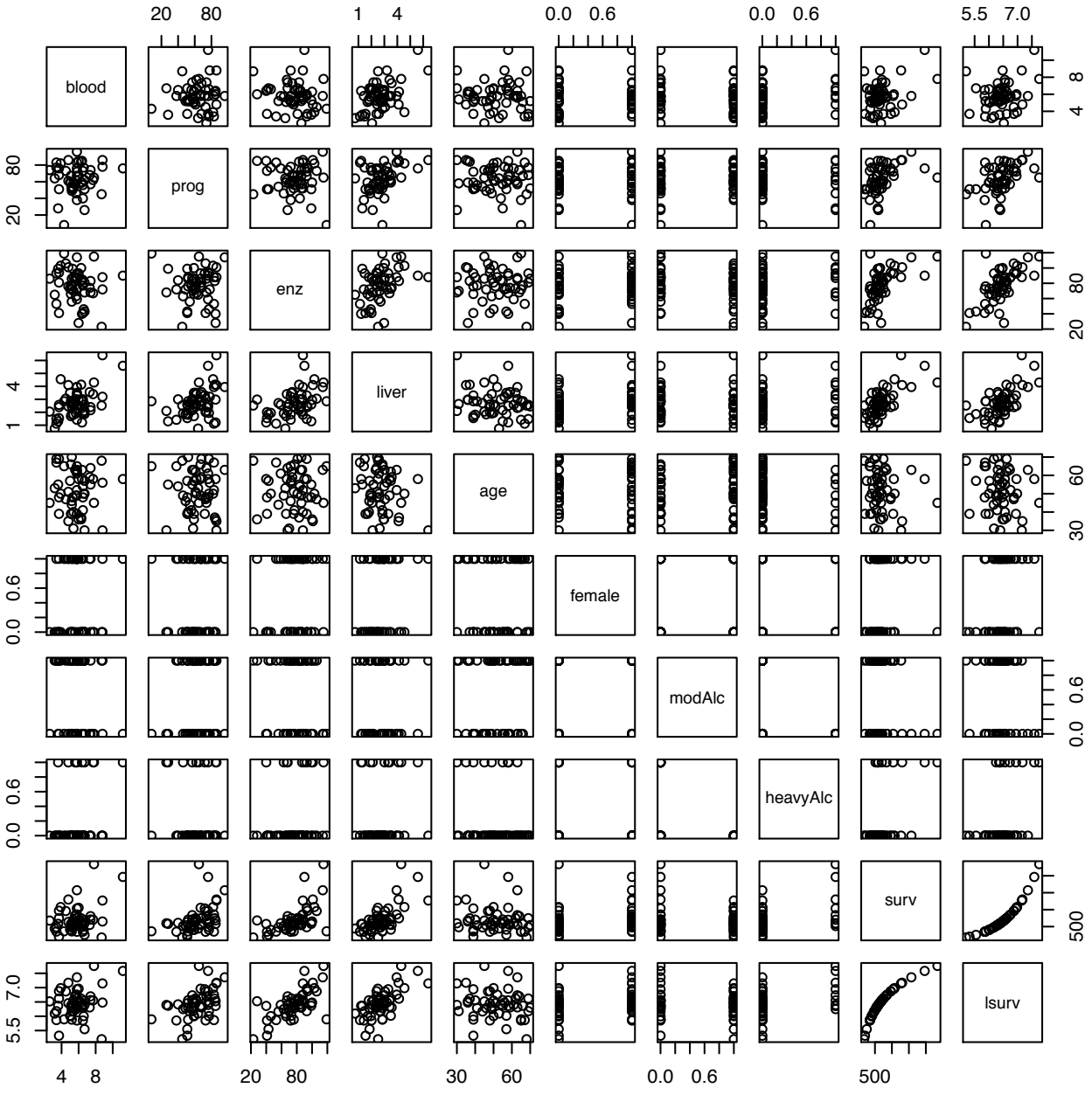
Getting to know the data

Pairwise correlation of predictors:

```
> round(cor(X[,-c(9:10)]), digits=1)
         blood prog  enz liver  age female modAlc heavyAlc
blood      1.0  0.1 -0.1   0.5  0.0    0.0   -0.1      0.2
prog       0.1  1.0  0.0   0.4  0.0    0.1    0.1     -0.1
enz       -0.1  0.0  1.0   0.4  0.0    0.1   -0.1      0.1
liver      0.5  0.4  0.4   1.0 -0.2    0.3    0.0      0.1
age        0.0  0.0  0.0  -0.2  1.0    0.0    0.1     -0.1
female     0.0  0.1  0.1   0.3  0.0    1.0    0.0     -0.1
modAlc    -0.1  0.1 -0.1   0.0  0.1    0.0    1.0     -0.5
heavyAlc   0.2 -0.1  0.1   0.1 -0.1   -0.1   -0.5      1.0
```

```
> pairs(X)
```

Pairwise plots



Exhaustive subset selection

```
> library(leaps)
> # By default - exhaustive search
> regfit.full <- regsubsets(lsurv ~ ., data=X[,-9])
> reg.summary <- summary(regfit.full)
> reg.summary

....

1 subsets of each size up to 8
Selection Algorithm: exhaustive
         blood prog enz liver age female modAlc heavyAlc
1  ( 1 ) " "   " "  "*" " "   " " " "    " "    " "
2  ( 1 ) " "   "*"  "*" " "   " " " "    " "    " "
3  ( 1 ) " "   "*"  "*" " "   " " " "    " "    "*"
4  ( 1 ) "*"   "*"  "*" " "   " " " "    " "    "*"
5  ( 1 ) "*"   "*"  "*" " "   " " "*"    " "    "*"
6  ( 1 ) "*"   "*"  "*" " "   "*" "*"    " "    "*"
7  ( 1 ) "*"   "*"  "*" " "   "*" "*"    "*"    "*"
8  ( 1 ) "*"   "*"  "*" "*"   "*" "*"    "*"    "*"

> names(reg.summary)
[1] "which" "rsq" "rss" "adjr2" "cp" "bic" "outmat" "obj"
```

The `leaps` library uses an efficient branch and bound algorithm

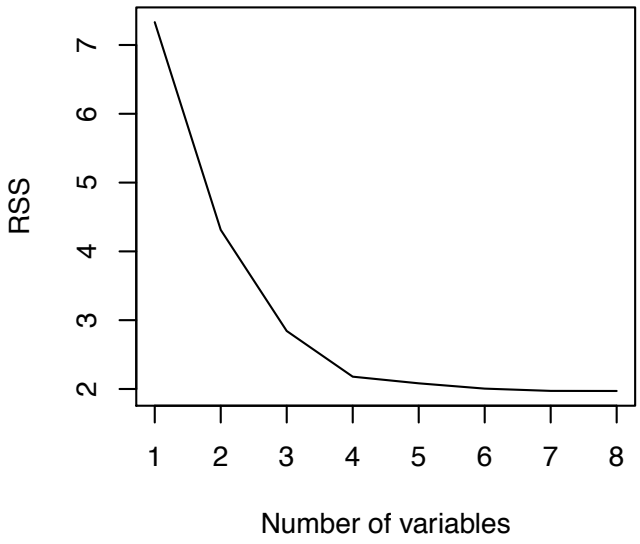
Exhaustive subset selection

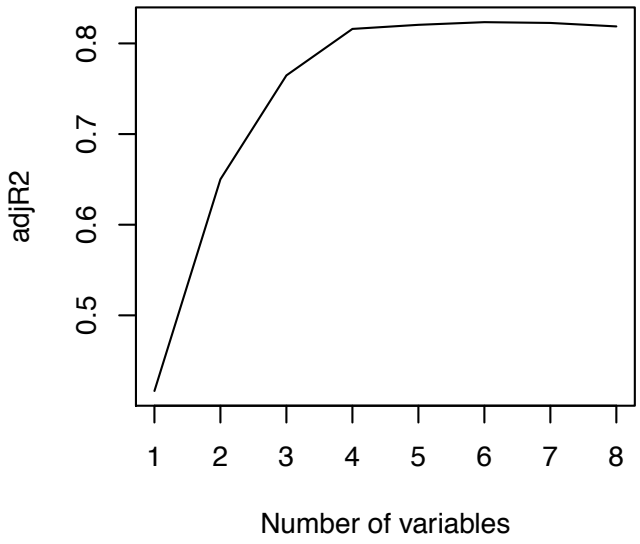
```
> par(mfrow=c(2,2))
> plot(reg.summary$rss, xlab='Number of variables',
+        ylab='RSS', type='l')
> plot(reg.summary$adjr2, xlab='Number of variables',
+        ylab='adjR2', type='l')
> plot(reg.summary$cp, xlab='Number of variables',
+        ylab='Cp', type='l')
> abline(a=0,b=1, lty=3, lwd=2)
> plot(reg.summary$bic, xlab='Number of variables',
+        ylab='BIC', type='l')
```

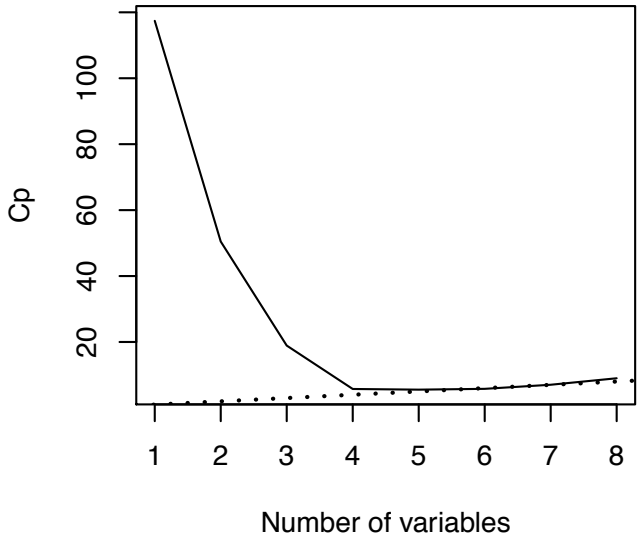
```
> which.min(reg.summary$bic)
[1] 4

> coef(regfit.full, 4)
(Intercept)      blood        prog         enz    heavyAlc
 3.85241856 0.07332263  0.01418507 0.01545270  0.35296762
```

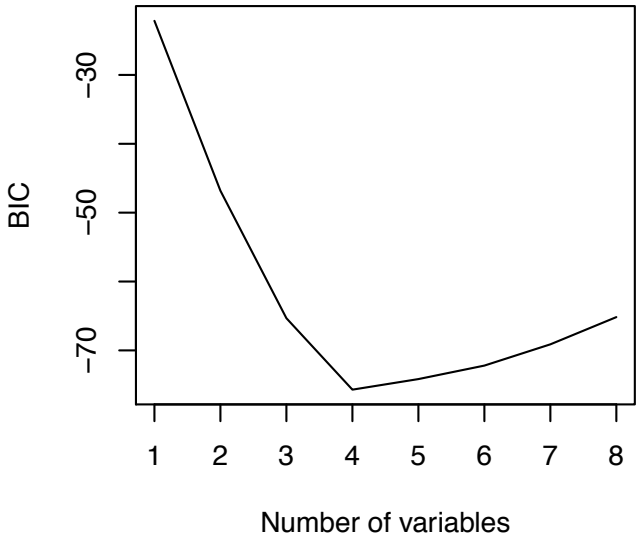
Conclusion: Model with 4 predictors appears best

Best model visualization









Note: BIC has a heavier penalty than C_p

Data-rich situation: independent validation

Randomly partition the dataset into 3 parts

1 Training set
  - predictive ability of any model is too optimistic (model fit caters to the training set)

2 Independent variable selection set
  - select predictors that minimize predictive error on this independent set
  - predictive ability of the "best" model is still too optimistic (variable selection caters to the variable selection set)

- Independent validation set
  - predictive ability of the model on independent data

$$MSPR = \frac{\sum_{i=1}^{n^*} (Y_i - \hat{Y}_i)^2}{n^*}$$

  - n^* = # of observations in validation set

Data-poor situation: cross-validation

- If # of observations is relatively small, but larger than # of variables, randomly partition the dataset into three parts
  - (1) training, (2) var. selection, (3) validation
- Iteratively use each part for training / variable selection / validation
  - each observation will play each role once
  - a value of predictive error for each observation
  - better use of the resources
  - may have a different model at different iteration of cross-validation
- See JWHT Sec. 6.5.3 for R code
  - Or, use `library(DAAG)`
    Maindonald, J.H. and Braun, W.J. (3rd Ed., 2010) *Data Analysis and Graphics Using R*

Cross-validation: full model

```
> library(DAAG)
> lm.full <- lm(lsurv ~ ., data=X[,-9])
> CVlm(X[,-9], lm.full)

[...]

fold 1
Observations in test set: 18
                1     3    5     12    16     20   [...]
Predicted   6.455 6.387 7.44  5.708 6.503 6.6898
cvpred      6.372 6.227 7.29  5.660 6.541 6.6539
lsurv       6.544 6.565 7.76  5.549 6.695 6.7310
CV residual 0.172 0.338 0.47 -0.111 0.154 0.0771

Sum of squares = 1.25    Mean square = 0.07    n = 18


fold 2
Observations in test set: 18
                  2      7     9     24     25    27  [...]
Predicted    6.0551  6.315 6.625  6.630  6.809 6.220
cvpred       6.0634  6.516 6.600  6.733  7.026 6.166
lsurv        5.9990  6.250 6.962  6.332  6.478 6.302
CV residual -0.0644 -0.266 0.362 -0.401 -0.548 0.136

Sum of squares = 1.3    Mean square = 0.07    n = 18
```

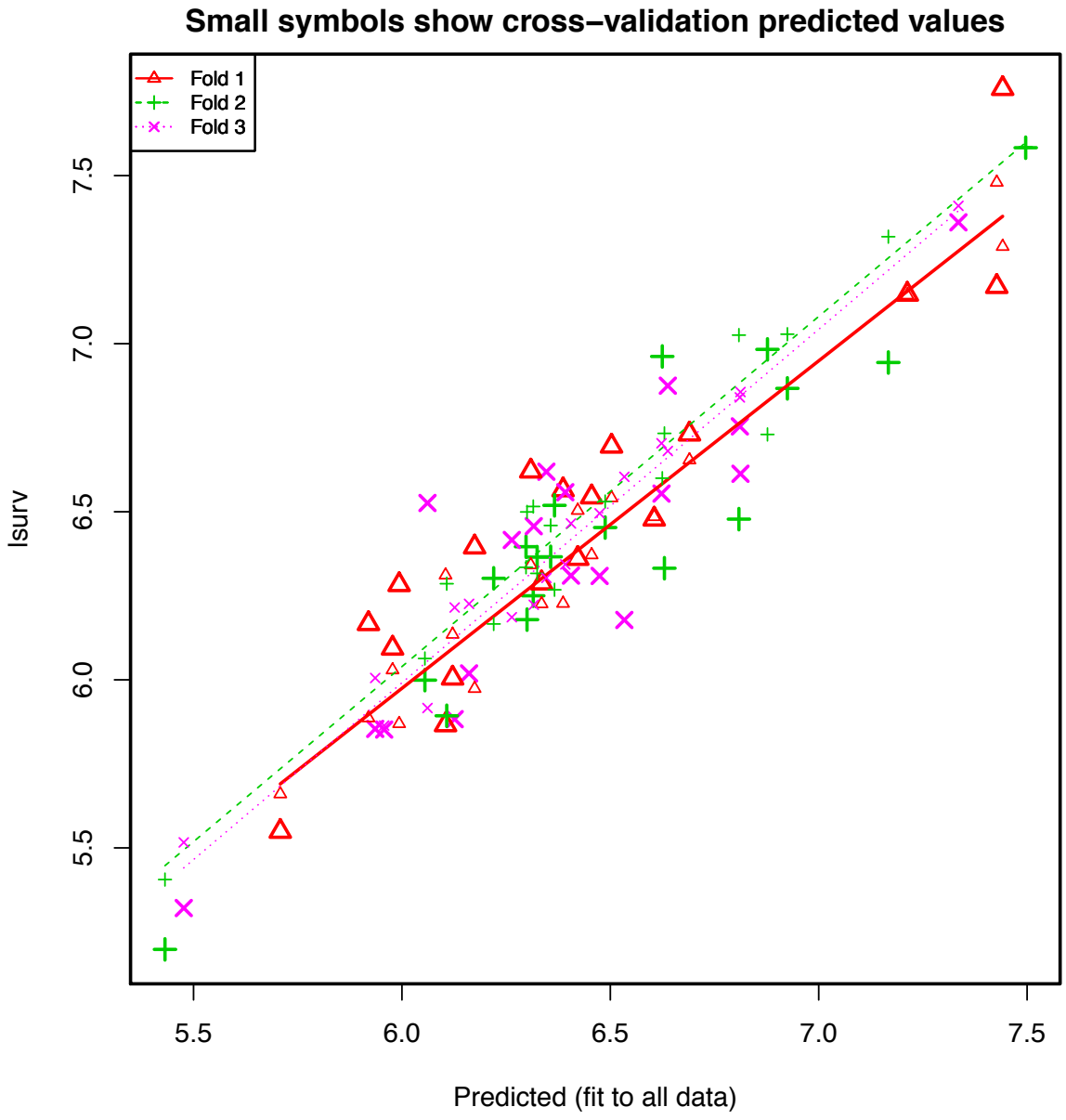
Cross-validation: full model

```
fold 3
Observations in test set: 18
                    4       6     8    10     11      13
Predicted       5.936  5.9574 6.347 6.638  6.812  7.3352
cvpred          6.005  5.8639 6.303 6.681  6.856  7.4101
lsurv           5.854  5.8520 6.619 6.875  6.613  7.3610
CV residual -0.151 -0.0119 0.316 0.194 -0.243

Sum of squares = 1.21    Mean square = 0.07    n = 18

Overall (Sum over all 18 folds)
    ms
0.0696
```

Note: Cross-validation should be done as part of variable selection.

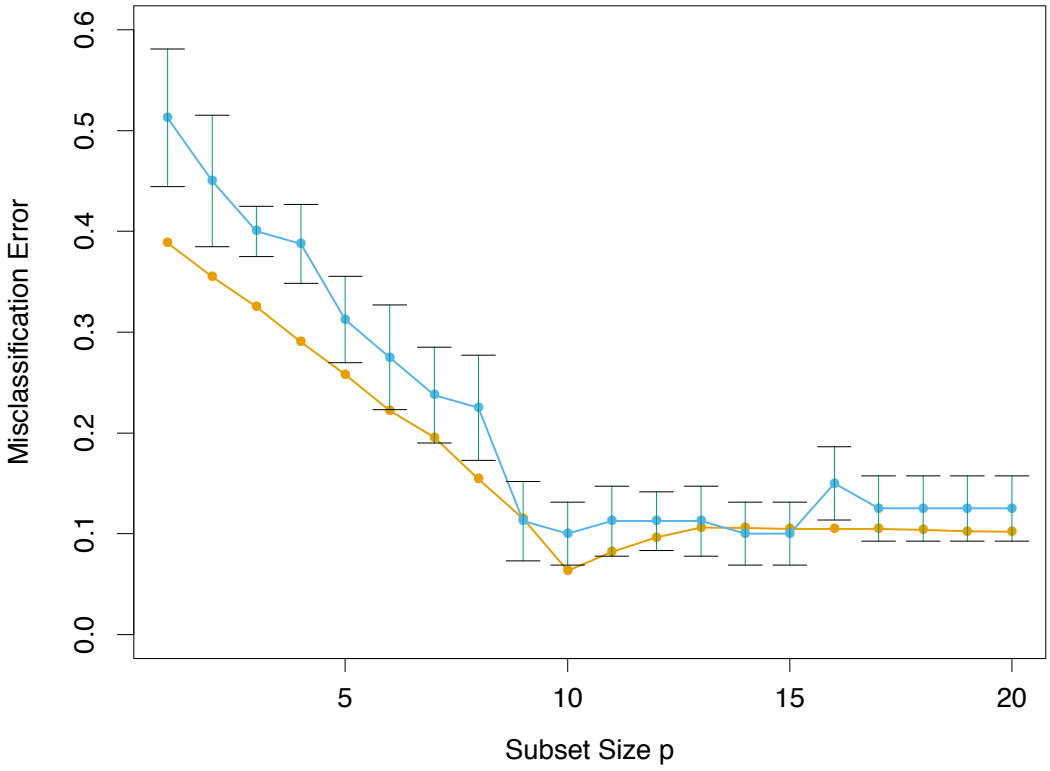
- Selecting the model on the full dataset, and then using cross-validation to evaluate the predictive accuracy, will yield biased results.

Visualization of cross-validation: fit



Cross-validation as part of variable selection

- Orange line: in-sample prediction error
- Blue line: cross-validated prediction error
  - Error bars are obtained over each fold (alternatively, by repeatedly partitioning data into folds)



From Hastie, Tibshirani, Friedman *The elements of Statistical Learning*, 2nd Ed., Springer

Small n large p situation: Variable selection by regularization.

Ridge, Lasso and Elastic Net

Linear Regression: Ridge

- Consider linear model
  $\mathbf{Y} = \mathbf{X}\beta + \varepsilon,\ \varepsilon \sim \mathcal{MVN}(0, \sigma^2\mathbf{I})$

- Properties of least squares estimates
  - $\widehat{\beta} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$
  - unbiased: $\mathrm{E}\{\widehat{\beta}\} = \beta$
  - minimal $\mathrm{Var}\{\widehat{\beta}\}$ among all unbiased estimates

- In problems with many predictors and few replicates, $\mathrm{Var}\{\widehat{\beta}\} = \sigma^2(\mathbf{X}'\mathbf{X})^{-1}$ is large

- Solution by ridge regression: introduce a bias to reduce the variance
  - reduce the overall mean squared error
    $\mathrm{MSE} = \mathrm{E}\{(\widehat{\beta} - \beta)^2\} = \mathrm{Bias}^2\{\widehat{\beta}\} + \mathrm{Var}\{\widehat{\beta}\}$

Parameter Estimation in Ridge Regression

- Ordinary least squares estimates
  - Standardize the predictors $\mathbf{X}^*$
  - All β are comparable after standardization
  - $\widehat{\beta} = (\mathbf{X}^{*\prime}\mathbf{X})^{-1}\mathbf{X}^{*\prime}\mathbf{Y}^*$ (standardized regression)
  - $\text{Var}\{\widehat{\beta}\} = \sigma^2(\mathbf{X}^{*\prime}\mathbf{X}^*)^{-1}$
  - Difficulty inverting $\mathbf{X}^{*\prime}\mathbf{X}^*$ when multicollinearity
- Ridge regression estimates
  - $\widehat{\beta} = (\mathbf{X}^{*\prime}\mathbf{X}^* + \lambda\mathbf{I})^{-1}\mathbf{X}^{*\prime}\mathbf{Y}^*$
  - Biased estimates $\widehat{\beta}$, but stable $(\mathbf{X}^{*\prime}\mathbf{X}^* + \lambda\mathbf{I})^{-1}$
- Difficulty: choice of λ
  - λ varies between datasets, subjective choice
- Difficulty: approximate inference only

Connection to Penalized Least Squares

- Can show that ridge parameter estimates can be obtained by minimizing

$$\sum_{i=1}^{n}\left[Y_i^* - (\beta_0^* + \beta_1^* X_{i1}^* + \ldots + \beta_{p-1}^* X_{ip}^*)\right]^2 + \lambda \cdot \left[\sum_{j=1}^{p-1} \beta_j^{*2}\right]$$
$$= (\mathbf{Y}^* - \mathbf{X}^*\boldsymbol{\beta}^*)'(\mathbf{Y}^* - \mathbf{X}^*\boldsymbol{\beta}^*) + \lambda \cdot \boldsymbol{\beta}^{*\prime}\boldsymbol{\beta}^*$$

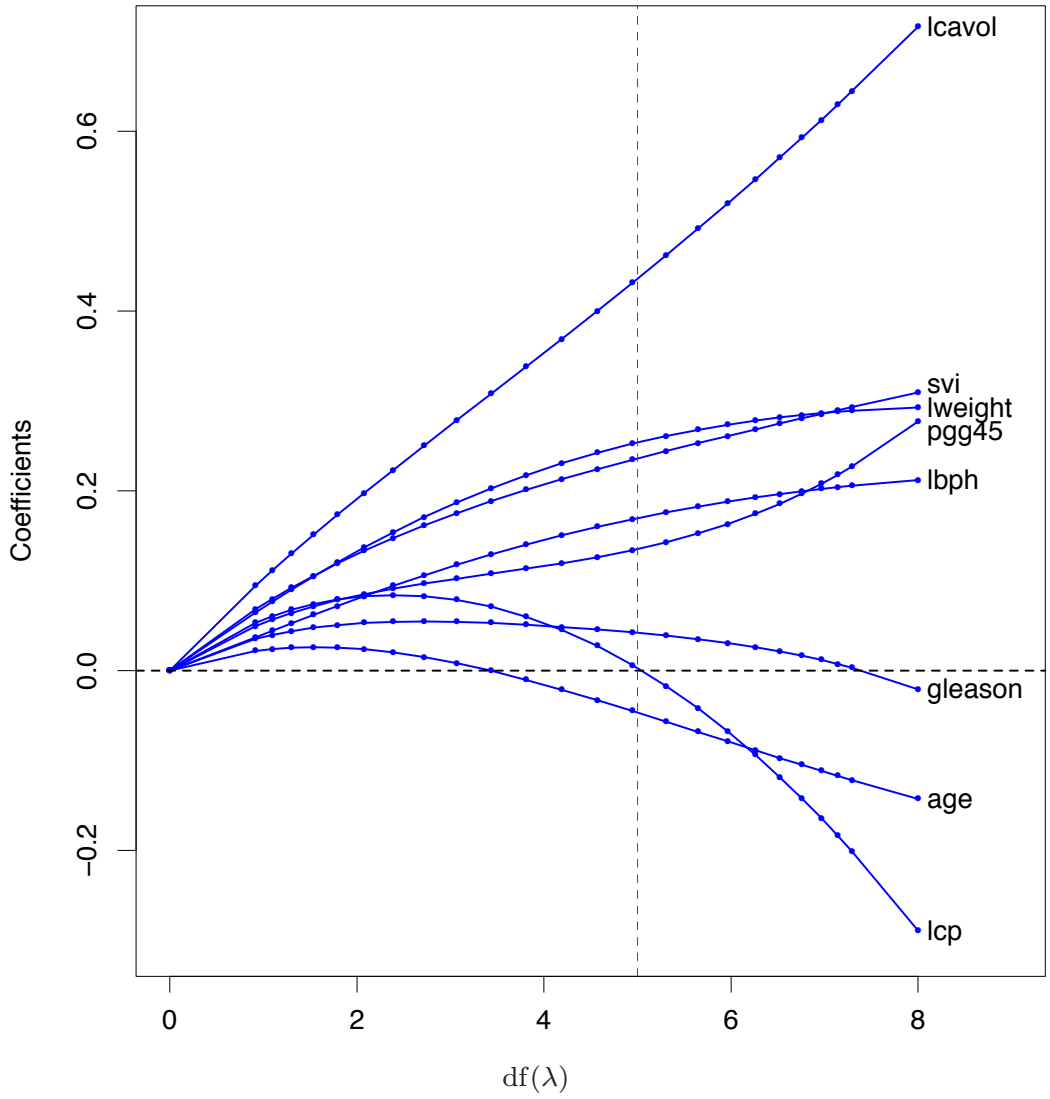
- Or by minimizing

$$\sum_{i=1}^{n}\left[Y_i^* - (\beta_0^* + \beta_1^* X_{i1}^* + \ldots + \beta_{p-1}^* X_{ip}^*)\right]^2 s.t. \sum_{j=1}^{p-1} \beta_j^{*2} \leq t$$

  λ and t have a one-to-one correspondence

- Or as the mean or mode of a posterior distribution, with a suitably chosen prior

Example: Ridge



X axis: 'effective degrees of freedom'

$$df(\lambda) = \text{tr}\left[\mathbf{X}(\mathbf{X}'\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}'\right] = \sum_{j=1}^{p} \frac{d_j^2}{d_j^2 + \lambda}$$

Hastie, Tibshirani, Friedman, *The Elements of Statistical Learning* 2008

Adaptive choice of λ: Ridge Trace

- Ridge trace:
  - Simultaneous plot of all parameter estimates for different values of $\lambda \geq 0$.
  - Curves may fluctuate widely when $\lambda \approx 0$
  - Eventually stabilize and converge to $\hat{\beta} = 0$ for large λ.

- Choose λ
  - Where things tend to "stabilize"
  - Better yet, use cross-validation

- λ determines the amount of penalty
  - Large λ is associated with smaller $|\beta_j^*|$
  - Therefore these are *shrinkage* estimators

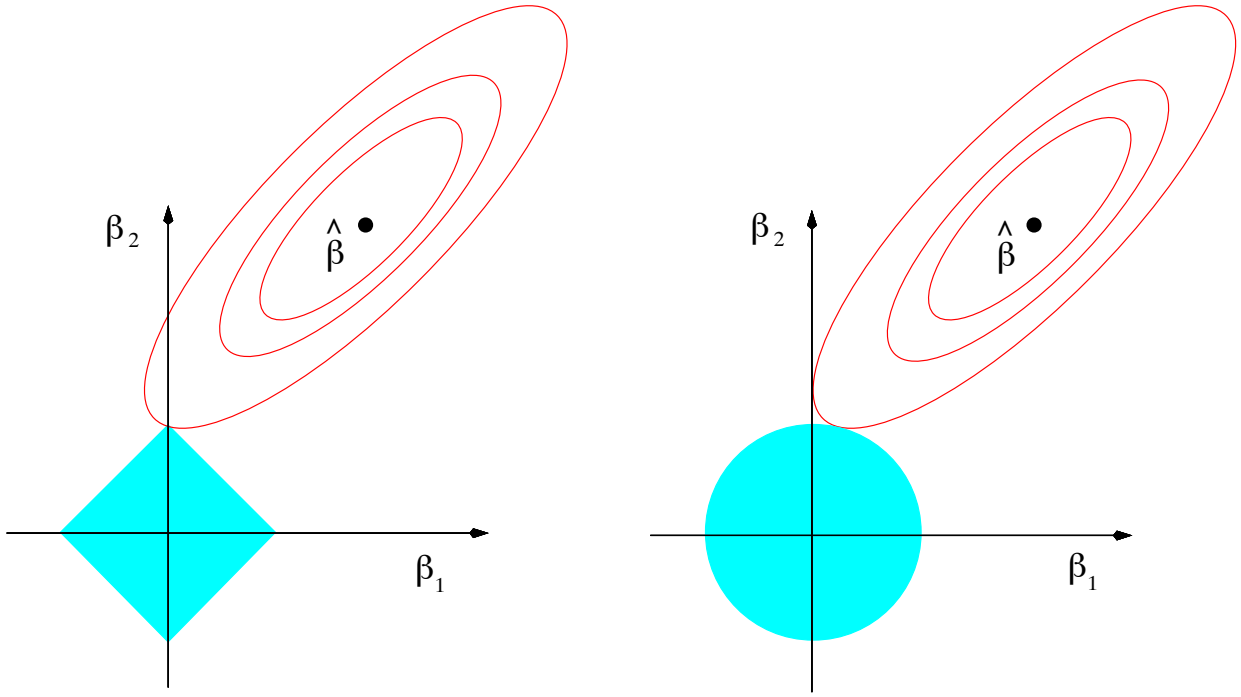
Modifications to Penalized Least Squares: LASSO

- Least absolute shrinkage and selection operator (LASSO): minimize

$$\sum_{i=1}^{n}\left[Y_i^* - (\beta_0^* + \beta_1^* X_{i1}^* + \ldots + \beta_{p-1}^* X_{ip}^*)\right]^2 + \lambda \cdot \left[\sum_{j=1}^{p-1} |\beta^*|_j\right]$$

- Weaker penalty on β than Ridge
  - Solution is non-linear in y_i.
  - Efron et al. (2004) derived an algorithm to obtain a sequence of solutions for discrete λ
  - A subset of parameters in the solutions = 0
  - It can be viewed as a stepwise procedure with a single addition to or deletion from the set of nonzero regression coefficients at any step.
  - Usually estimate $\widehat{\beta}_{LS}$ for the selected predictors

Graphical illustration of regularized estimation

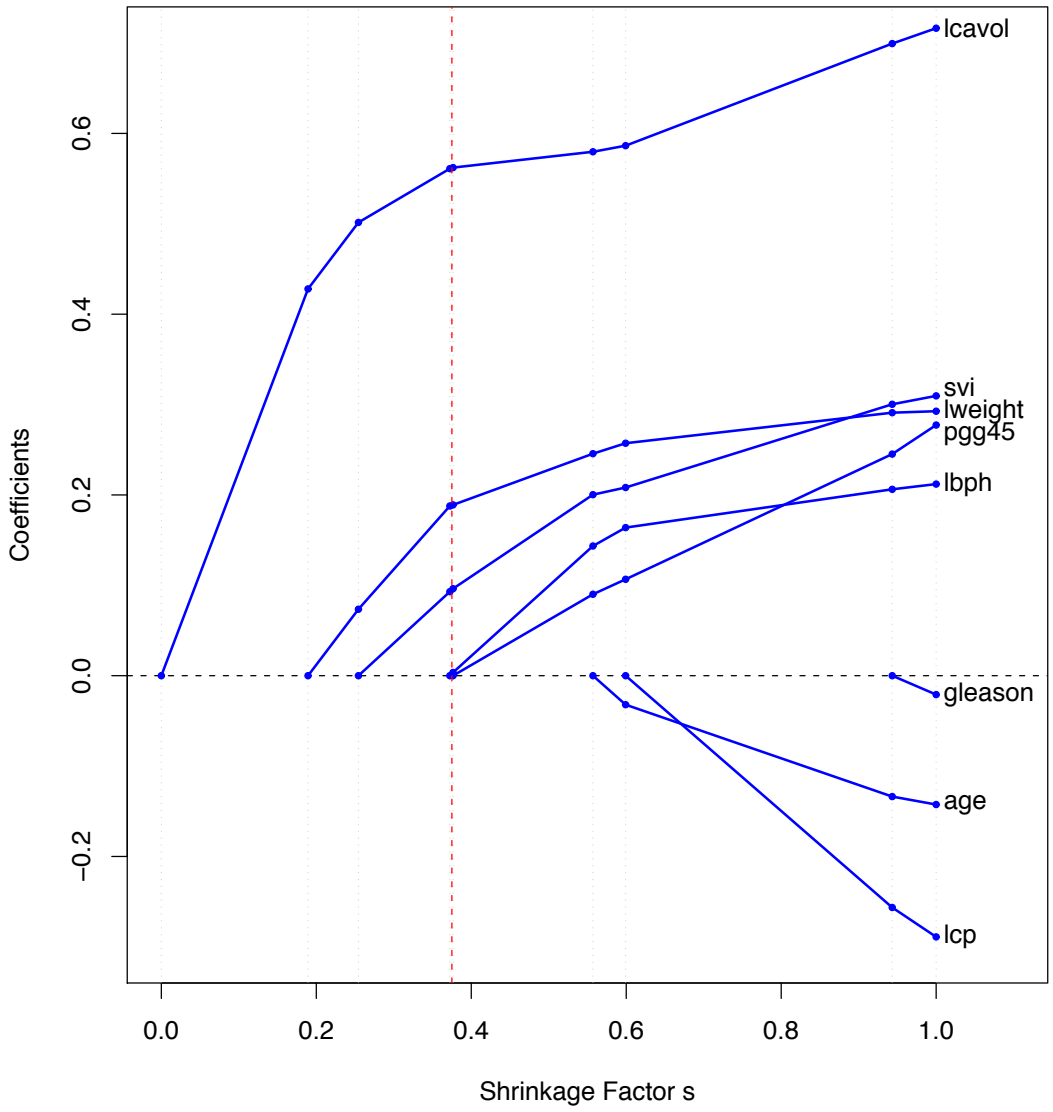


Iterative optimization for each parameter, in order of least steep descent

For LASSO, the optimum is always on the intersection with some axes, while for ridge it is not. Therefore LASSO is more effective for feature selection.

Hastie, Tibshirani, Friedman, *The Elements of Statistical Learning* 2008

Example: Lasso

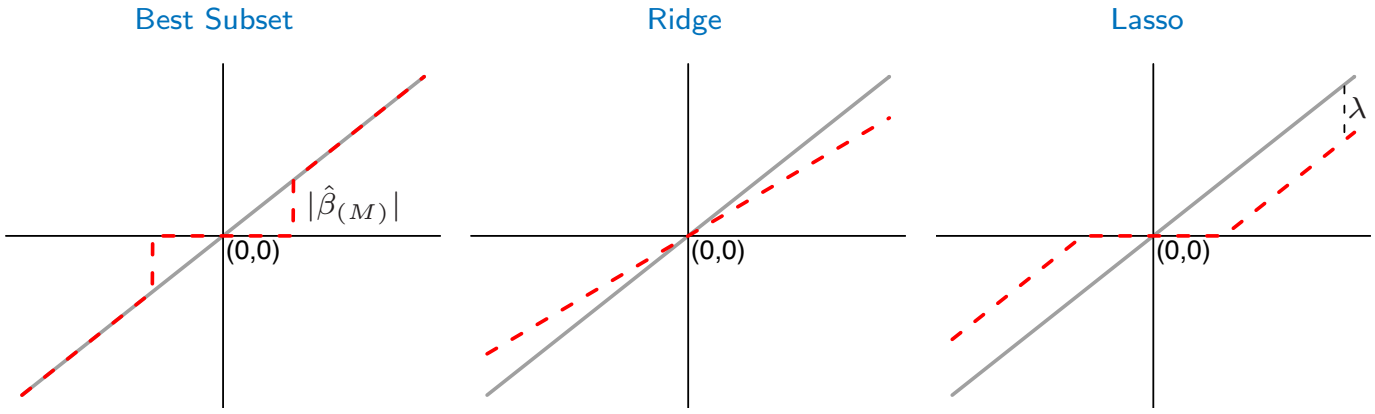


Shrinkage factor $s = t / \sum_{j=1}^{P} |\beta_j^*|$

Hastie, Tibshirani, Friedman, *The Elements of Statistical Learning* 2008

Estimators in case of orthonormal columns

Estimator	Formula
Best subset (size M)	$\hat{\beta}_j \cdot I(\lvert\hat{\beta}_j\rvert \geq \lvert\hat{\beta}_{(M)}\rvert)$
Ridge	$\hat{\beta}_j/(1+\lambda)$
Lasso	$\text{sign}(\hat{\beta}_j)(\lvert\hat{\beta}_j\rvert - \lambda)_+$



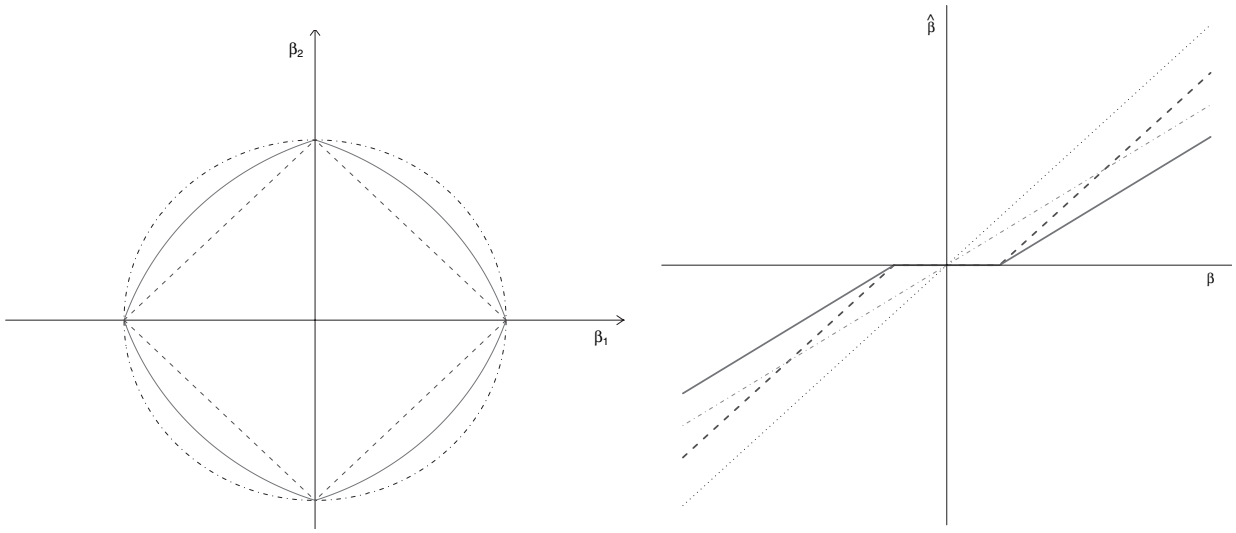
- Best subset: least squares estimates, if selected
- Ridge: Scaled least squares estimates
- Lasso: soft thresholding

Hastie, Tibshirani, Friedman, *The Elements of Statistical Learning* 2008

More extensions

- Elastic net penalty

$$\lambda \cdot \sum_{j=1}^{p-1} \left[\alpha \beta_j^{*2} + (1-\alpha) |\beta^*|_j \right]$$



- LASSO, Ridge, Elastic Net

Zoe and Hastie,
Journal of the Royal Statistical Society, Series B 2005

Ridge selection

```
library(glmnet)
grid=10^seq(10,-2,length=100)
ridge.mod <- glmnet(x=as.matrix(X[,-c(9:10)]), y=X[,10],
+       alpha=0, lambda=grid)
plot(ridge.mod$lambda, ridge.mod$beta)

> ridge.mod$lambda[20]
[1] 49770236
> coef(ridge.mod)[,20]
  (Intercept)        blood         prog          enz
 6.430481e+00 7.387398e-10  1.337399e-10 1.479902e-10 [...]

> ridge.mod$lambda[80]
[1] 2.656088
> coef(ridge.mod)[,80]
  (Intercept)        blood         prog          enz
 5.9968742835 0.0093395444  0.0019819344 0.0021961768 [...]
```

- α is a mixing parameter in elastic net penalty

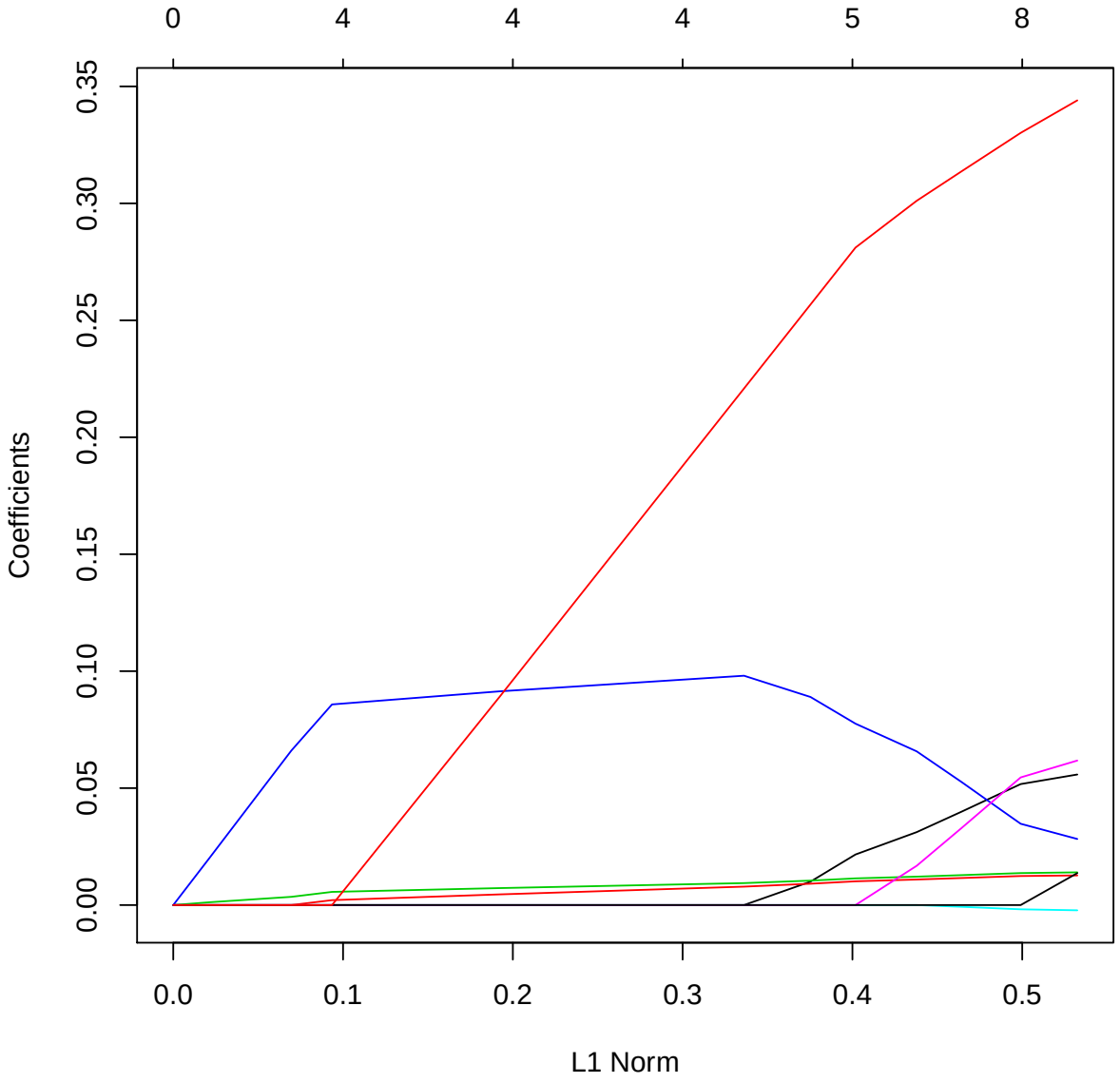
$$(1-\alpha)/2||\beta||_2^2 + \alpha||\beta||_1$$

- By default, $\mathbf{X}$ is standardized but Y is not
- Smaller λ corresponds to larger coefficients

Lasso fit

```
> # Fit lasso for a pre-specified (set of) lambda
> #-----------------------------------------------
> lasso.mod  <- glmnet(x=as.matrix(X[,-c(9:10)]),
+       y=X[,10], alpha=1, lambda=grid)
> plot(lasso.mod)
>

> # Select optimal lambda by cross-validation
> #-----------------------------------------------
> cv.out <- cv.glmnet(x=as.matrix(X[,-c(9:10)]),
+      y=X[,10], alpha=1)
> plot(cv.out)
> bestlam <- cv.out$lambda.min
> bestlam
[1] 0.00144
```

Lasso model fit



Cross-validation to help select λ