Models

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Problem Setting

- Data: Observe for each case i (Y_i, X_i)
- Response or dependent variable Y_i
- Predictor(s) or **independent** variable X_i

Goals:

- Exploring distribution of $p(y|X = x)$ as a function of x
- Understanding the mean in Y as a function of x :
  $E(Y \mid X = x) = f(X)$

Special cases:

- regression (normal Y) or additive error model
- classification (binary or Bernoulli Y where probability $p(Y = 1 \mid X)$ depends on x)
- exponential family models
  - Poisson regression (counts)
  - Gamma regression (continous, positive)
- Survival models

Additive Error Model

- Assume $E[\epsilon_i] = 0$ for $i = 1, \ldots, n$,

$$Y_i = f(X_i) + \epsilon_i$$

- Regression function $E(Y \mid x) = f(x)$
- ideal or optimal predictor of Y given $X = x$
- minimizes $E[(Y - g(x))^2 \mid X = x]$ over all functions $g(x)$ at all points $X = x$
- for prediction $\epsilon = Y - f(x)$ is *irreducible error* as even if we know $f(x)$ there are still errors in predicting Y
- for any estimator $\hat{f}(x)$ we have

$$E[(Y - \hat{f}(x))^2 \mid X = x] = \underbrace{(f(x) - \hat{f}(x)))^2}_{\textit{Reducible}} + \underbrace{\mathrm{Var}(\epsilon)}_{\textit{Irreducible}}$$

Linear Regression

- Taylors series expansion of regression function about point x_0

$$f(x_i) = f(x_0) + f'(x_0)(x_i - x_0) + \text{ Remainder}$$

  leads to locally linear approximation

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

- ε_i : errors (sampling/measurement errors ϵ, lack of fit)

Regression in Matrix Notation

Simple Linear Regression:

$$Y_i = \beta_0 + x_i\beta_1 + \epsilon_i \text{ for } i = 1, \ldots, n$$

Rewrite in vectors:

$$\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix} \beta_0 + \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} \beta_1 + \begin{bmatrix} \epsilon_1 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

$$\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

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

Big Picture:

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon} \overset{iid}{\sim} N(0, \sigma^2)$$

- Estimate parameters (β, σ)
- interpretation of parameters: β, σ
- assess model fit — adequate? good? if inadequate, how?
- move to more complicated model?
- predict new ("future") responses at new $x_{n+1}, \ldots$
- how much variability does x explain?
- how important is X is predicting Y

Body Fat Data

- For a group of 252 male subjects, various body measurements were obtained
- An accurate measurement of the percentage of body fat is recorded for each
- Goal is to use the other body measurements as a proxy for predicting body fat
- Understand how changing one measurement may lead to changes in Bodyfat

Data

```
library(BAS)
data(bodyfat)  #from BAS   help(bodyfat)
dim(bodyfat)
```

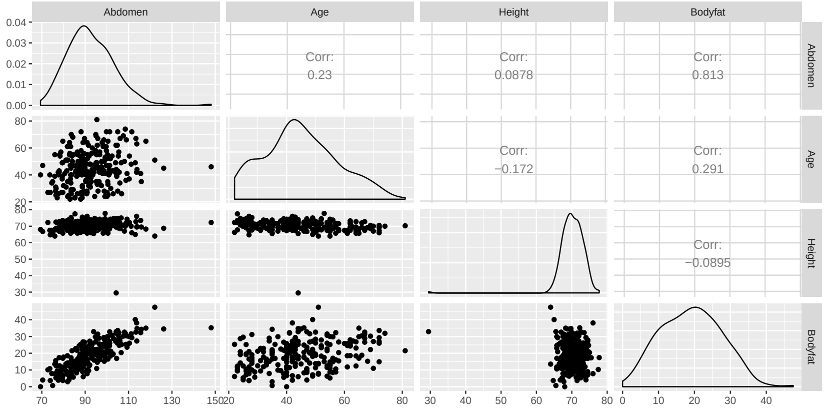
```
## [1] 252  15
```

```
summary(bodyfat)  # anything strange ?
```

```
##     Density          Bodyfat           Age             We
##  Min.   :0.995   Min.   : 0.00   Min.   :22.00   Min.
##  1st Qu.:1.041   1st Qu.:12.47   1st Qu.:35.75   1st Qu
##  Median :1.055   Median :19.20   Median :43.00   Median
##  Mean   :1.056   Mean   :19.15   Mean   :44.88   Mean
##  3rd Qu.:1.070   3rd Qu.:25.30   3rd Qu.:54.00   3rd Qu
##  Max.   :1.109   Max.   :47.50   Max.   :81.00   Max.
##      Height            Neck            Chest            Abd
##  Min.   :29.50   Min.   :31.10   Min.   : 79.30   Min.
##  1st Qu.:68.25   1st Qu.:36.40   1st Qu.: 94.35   1st Qu
```

Pairs Plots

```r
library(GGally)
ggpairs(bodyfat, columns=c(8,3,5,2))
```



Ordinary Least Squares

- OLS estimates of parameters β_0 and β minimize sum of squared errors

$$\sum_{i=1}^{n}(Y_i - (\beta_0 + X_i\beta_1))^2$$

$$L(\boldsymbol{\beta}) = (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})^T(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})$$

- OLS estimate of $\boldsymbol{\beta}$

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$$

- Ad Hoc
- Equivalent to Maximum Likelihood Estimates with assumption that errors are iid Normal (Model based)

Summarizing Model Fit

- Fitted values

$$\hat{Y}_i = x_i^T \hat{\beta}$$

- Residuals (estimates of errors)

$$e_i = Y_i - \hat{Y}_i = \hat{\epsilon}_i$$

- Sum of Squared Errors

$$\mathrm{SSE} = \sum e_i^2$$

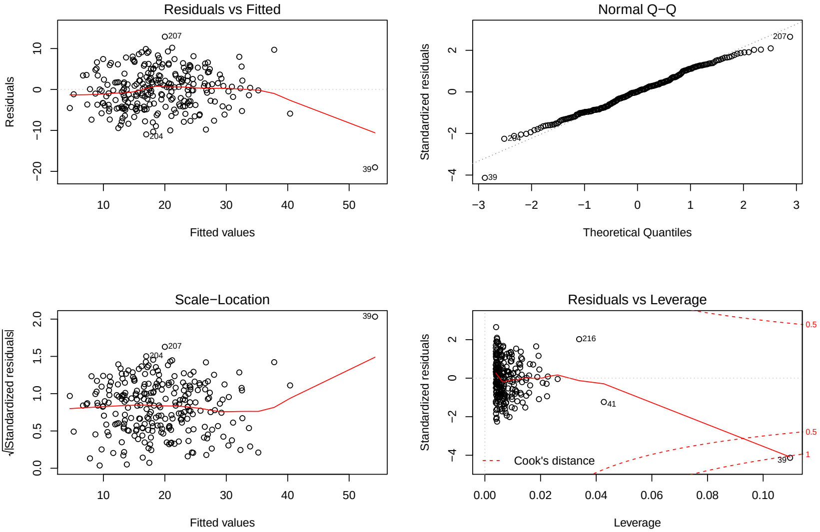
- measures remaining residual variation in response
- MSE = SSE/(n -2) (or more generally $n - p$) is an estimate of σ^2
- degrees of freedom n-p

Fitting Models in R

```
bodyfat.lm = lm(Bodyfat ~ Abdomen, data=bodyfat)
summary(bodyfat.lm)   #summary of regression output
```

```
##
## Call:
## lm(formula = Bodyfat ~ Abdomen, data = bodyfat)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -19.0160  -3.7557   0.0554   3.4215  12.9007
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept) -39.28018    2.66034  -14.77   <2e-16 ***
## Abdomen       0.63130    0.02855   22.11   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1
##
```

Residual Plots



Diagnostic Plots

- Residuals versus fitted values
- Normal Quantil: check normality of residuals or look for heavier tails than normal where observed quantiles are larger than expected under normality
- Scale-Location plot:
  Detect if the spread of the residuals is constant over the range of fitted values. (Constant variance with mean)
- standardized residuals versus leverage with contours of Cook's distance: shows influential points where points greater than 1 or 4/n are considered influential

Case 39 appears to be influential!

Hat Matrix

- predictions

$$\hat{Y} = X\hat{\beta} = X(X^TX)^{-1}X^TY$$

$$H = X(X^TX)^{-1}X^T$$

- Hat Matrix or Projection Matrix
  - idempotent $HH = H$
  - symmetric
  - leverage values are the diagonal elements h_{ii}

$$Y_i = h_{ii}Y_i + \sum_{i \neq j} h_{ij}Y_j$$

- leverage values near 1 imply $\hat{Y}_i = Y_i$
- potentially influential
- measure of how far x_i is from center of data

Residual Analysis

- residuals
$$e = Y - \hat{Y} = (I - H)Y$$
$$\mathrm{var}(e_i) = \hat{\sigma}^2(1 - h_{ii})$$
- Standardize:
$$r_i = e_i / \sqrt{\mathrm{var}(e_i)}$$
- if leverage is near 1 then residual is near 0 and variance is near 0 and r_i is approximately 0 (may not be helpful)

Cook's Distance

Measure of influence of case i on predictions

$$D_i = \frac{\| Y - \hat{Y}_{(i)} \|^2}{\hat{\sigma}^2 \, p}$$

after removing the ith case

Easier way to calculate

$$D_i = \frac{e_i^2}{\hat{\sigma}^2 p} \left[\frac{h_{ii}}{(1 - h_{ii})^2} \right],$$

$$D_i = \frac{r_{ii}}{p} \frac{h_{ii}}{1 - h_{ii}}$$

Model Assessment

- Always look at residual plots!
- Check constant variance, outliers, influence, normality assumption
- Treat e_i as ‘`new data'' -- look at structure, other predictorsavplots`‘
- Case 39 looks influential!

How should we proceed?