Regression Techniques

Deepayan Sarkar

Regression

- Most of you should be familiar with Linear Regression / Least Squares
  - What is the purpose?
  - What are the model assumptions?
- Are there any other kinds of regression?

Course: Regression Techniques

- This course is **not** about linear regression!
- We will
  - Try to refine what we understand by the term "regression" *(linear regression is only a special case)*
  - Learn alternative approaches to solve the "regression" problem
  - Learn how to identify and address modeling errors
- Most techniques we will learn require non-trivial programming
  - We will learn and use the R language for computation
  - Room 11 (ground floor) is a computer lab (usually locked, but security guards at the main gate will open it when you ask them)
  - There are two more (smaller) computer labs in teh ground floor of the Faculty Building
  - You can use your own laptops as well

Evaluation scheme

- Midterm examination: 30%
- Final examination: 50%
- Assignments / Projects: 20%

What is Regression?

- Consider bivariate data (X, Y) with some distribution
- Interested in "predicting" Y for a fixed value of $X = x$
- In probability terms, want the *conditional distribution* of

$$Y | X = x$$

- In general
  - Y could be numeric or categorical
  - X could also be numeric or categorical
- The "Regression Problem": when Y is numeric
- The "Classification Problem": when Y is categorical
- A more modern approach is to view both as special cases of the "Learning Problem"

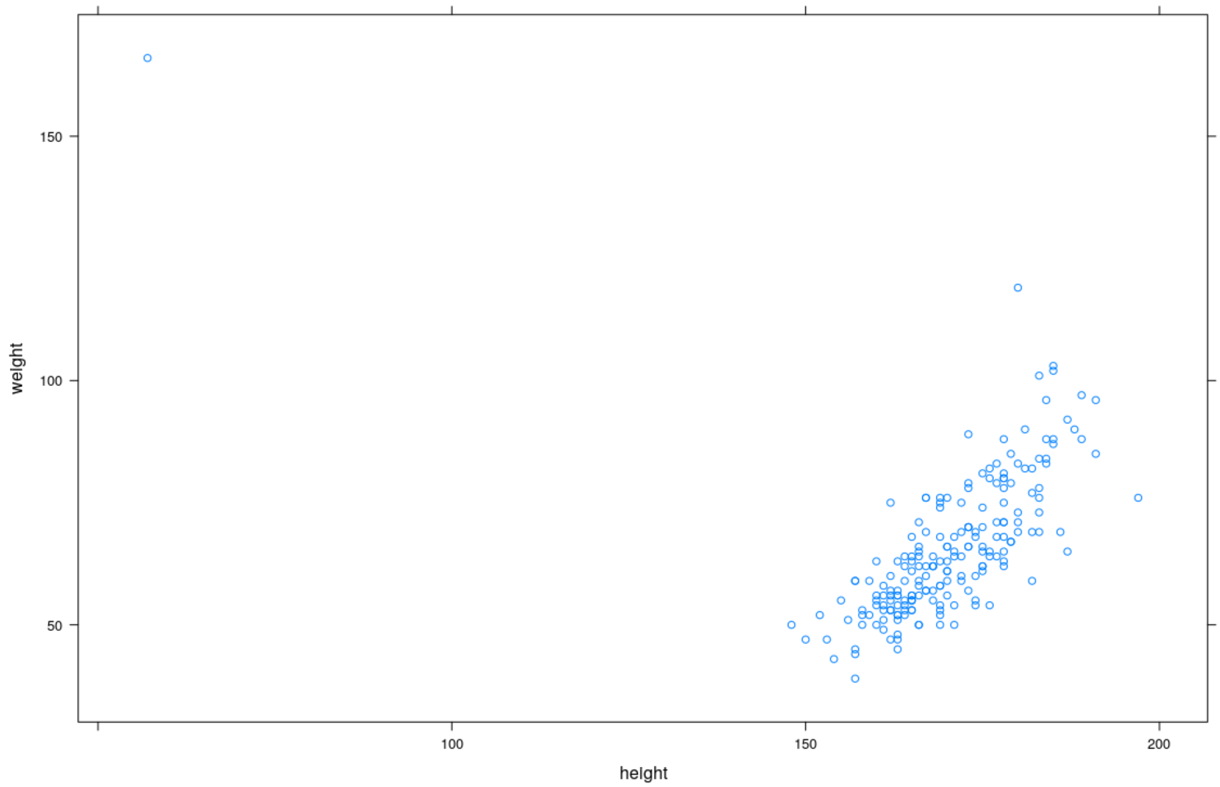
Example: Height and Weight Data

```
data(Davis, package = "carData")
Davis[1:20, ]
```

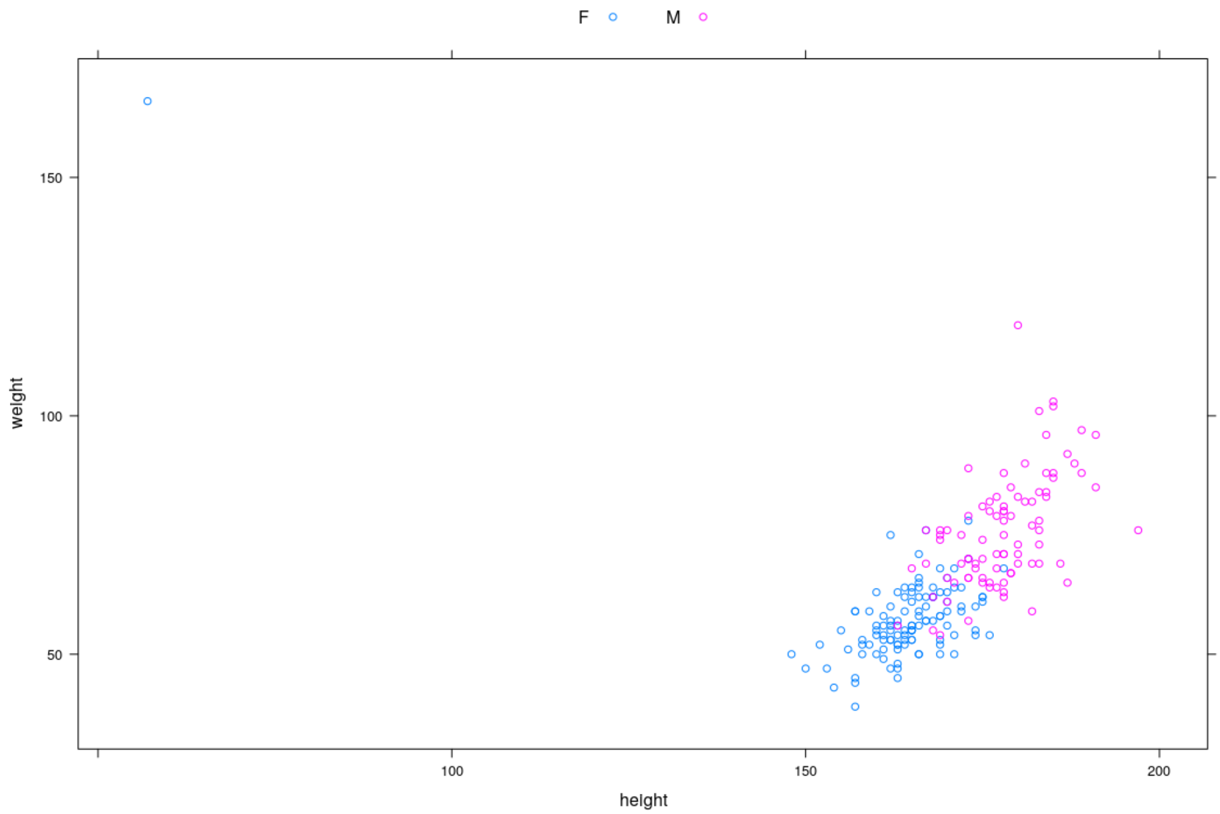
```
   sex weight height repwt repht
1    M     77    182    77   180
2    F     58    161    51   159
3    F     53    161    54   158
4    M     68    177    70   175
5    F     59    157    59   155
6    M     76    170    76   165
7    M     76    167    77   165
8    M     69    186    73   180
9    M     71    178    71   175
10   M     65    171    64   170
11   M     70    175    75   174
12   F    166     57    56   163
13   F     51    161    52   158
14   F     64    168    64   165
15   F     52    163    57   160
16   F     65    166    66   165
17   M     92    187   101   185
18   F     62    168    62   165
19   M     76    197    75   200
20   F     61    175    61   171
```

- Interested in predicting weight distribution as a function of height
- How should we proceed?

```
xyplot(weight ~ height, data = Davis)
```




```
xyplot(weight ~ height, data = Davis, groups = sex, auto.key = list(columns = 2))
```



Example: Survey of Labour and Income Dynamics

```
data(SLID, package = "carData")
str(SLID)
```

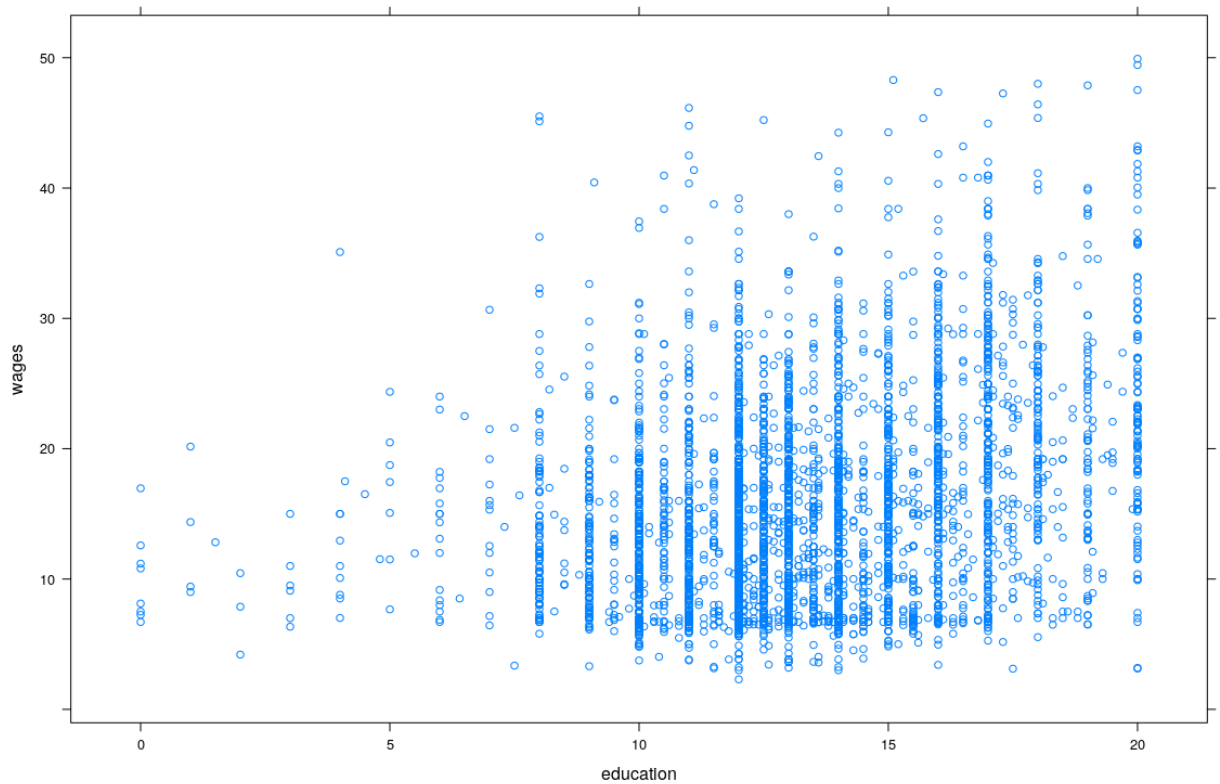
```
'data.frame':   7425 obs. of  5 variables:
 $ wages    : num  10.6 11 NA 17.8 NA ...
 $ education: num  15 13.2 16 14 8 16 12 14.5 15 10 ...
 $ age      : int  40 19 49 46 71 50 70 42 31 56 ...
 $ sex      : Factor w/ 2 levels "Female","Male": 2 2 2 2 2 1 1 1 2 1 ...
 $ language : Factor w/ 3 levels "English","French",..: 1 1 3 3 1 1 1 1 1 1 ...
```

```
head(SLID, 10)
```

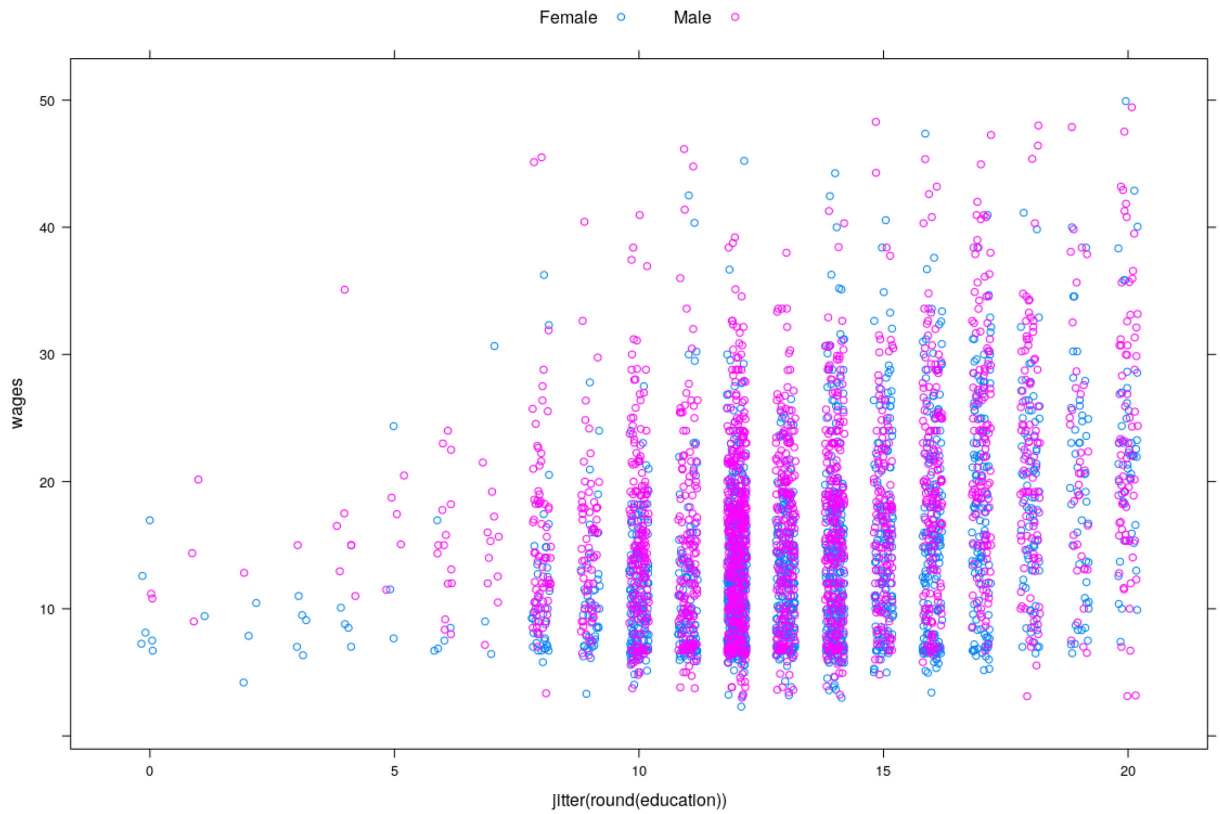
```
   wages education age    sex language
1  10.56      15.0  40   Male  English
2  11.00      13.2  19   Male  English
3     NA      16.0  49   Male    Other
4  17.76      14.0  46   Male    Other
5     NA       8.0  71   Male  English
6  14.00      16.0  50 Female  English
7     NA      12.0  70 Female  English
8     NA      14.5  42 Female  English
9   8.20      15.0  31   Male  English
10    NA      10.0  56 Female  English
```

- Interested in predicting wage

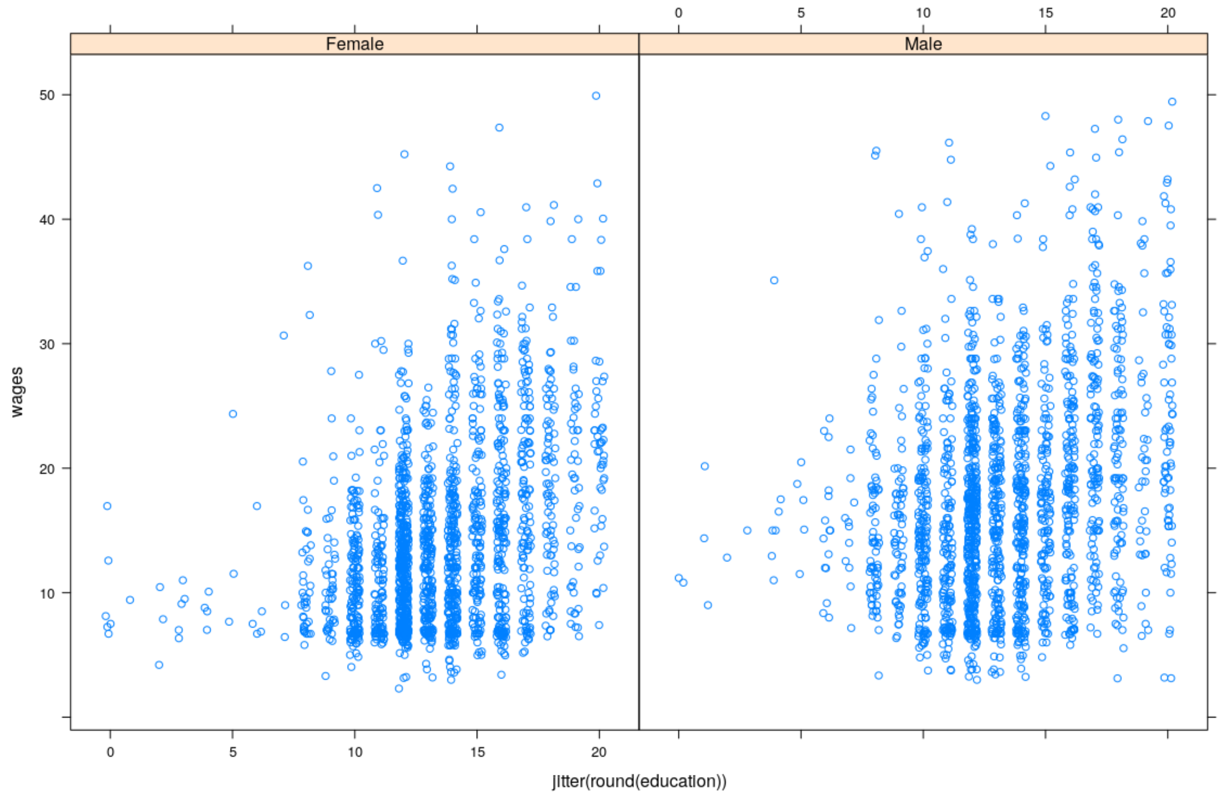
```
xyplot(wages ~ education, data = SLID)
```



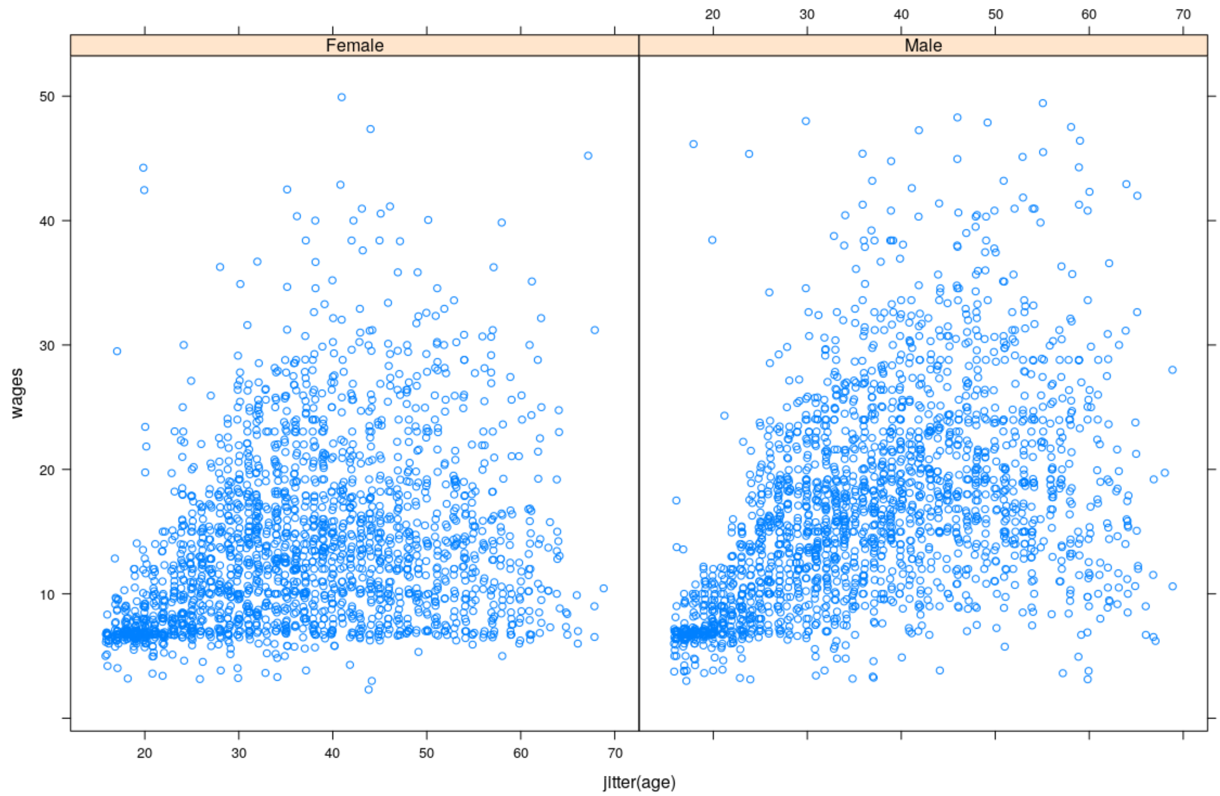

```
xyplot(wages ~ jitter(round(education)), data = SLID, groups = sex, auto.key = list(columns = 2))
```




```
xyplot(wages ~ jitter(round(education)) | sex, data = SLID)
```




```
xyplot(wages ~ jitter(age) | sex, data = SLID, subset = !is.na(wages))
```



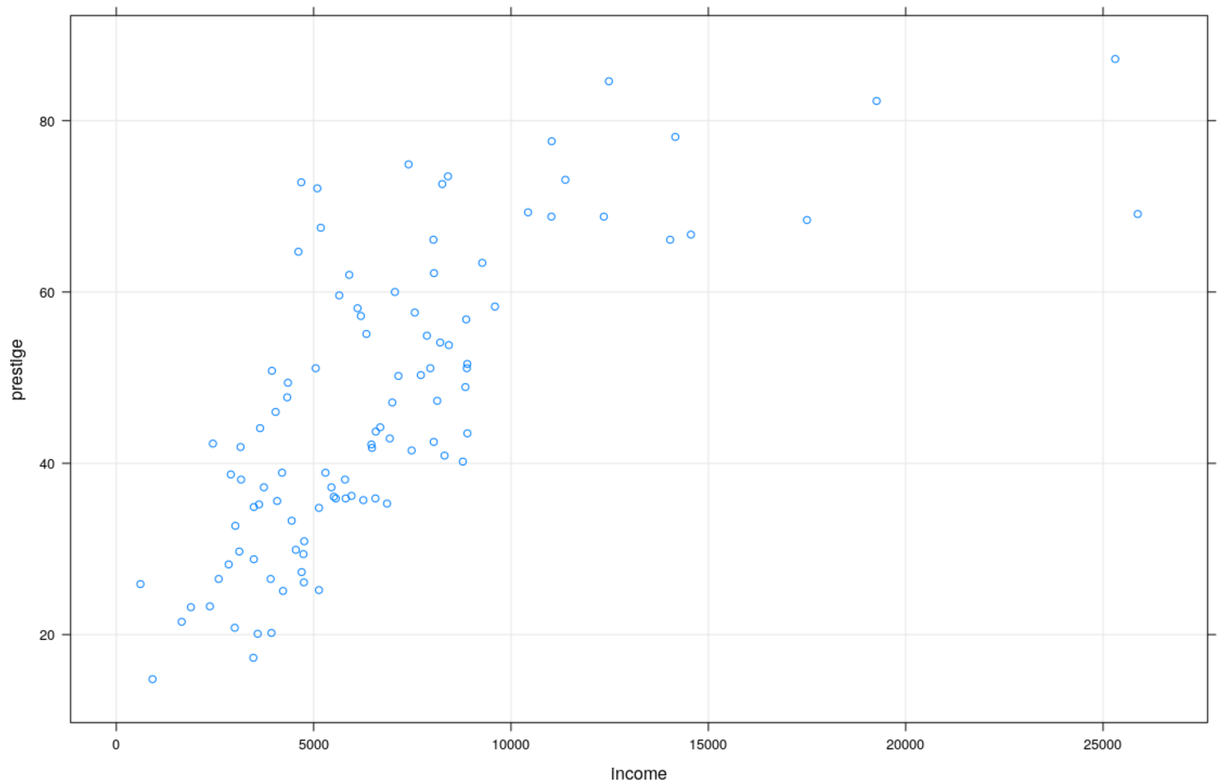
Example: Prestige vs Average income (Canada, 1971)

```
data(Prestige, package = "carData")
Prestige[1:20, ]
```

```
                        education income women prestige census type
gov.administrators          13.11  12351 11.16     68.8   1113 prof
general.managers            12.26  25879  4.02     69.1   1130 prof
accountants                 12.77   9271 15.70     63.4   1171 prof
purchasing.officers         11.42   8865  9.11     56.8   1175 prof
chemists                    14.62   8403 11.68     73.5   2111 prof
physicists                  15.64  11030  5.13     77.6   2113 prof
biologists                  15.09   8258 25.65     72.6   2133 prof
architects                  15.44  14163  2.69     78.1   2141 prof
civil.engineers             14.52  11377  1.03     73.1   2143 prof
mining.engineers            14.64  11023  0.94     68.8   2153 prof
surveyors                   12.39   5902  1.91     62.0   2161 prof
draughtsmen                 12.30   7059  7.83     60.0   2163 prof
computer.programers         13.83   8425 15.33     53.8   2183 prof
economists                  14.44   8049 57.31     62.2   2311 prof
psychologists               14.36   7405 48.28     74.9   2315 prof
social.workers              14.21   6336 54.77     55.1   2331 prof
lawyers                     15.77  19263  5.13     82.3   2343 prof
librarians                  14.15   6112 77.10     58.1   2351 prof
vocational.counsellors      15.22   9593 34.89     58.3   2391 prof
```

```
ministers                    14.50    4686   4.14      72.8    2511 prof
```

```r
xyplot(prestige ~ income, Prestige, grid = TRUE)
```



Example: UN National Statistics

```r
data(UN, package = "carData")
UN[1:20, ]
```

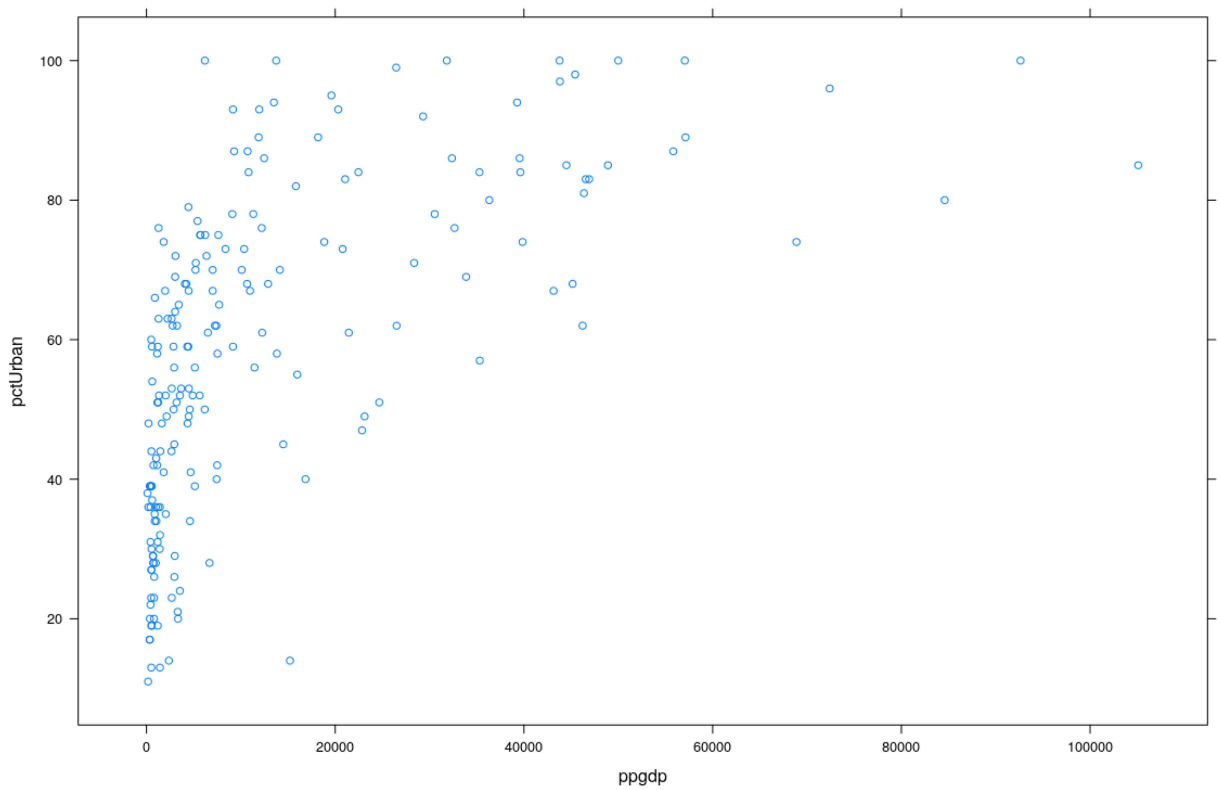
```
                   region  group fertility   ppgdp lifeExpF pctUrban infantMortality
Afghanistan          Asia  other     5.968   499.0    49.49       23       124.53500
Albania            Europe  other     1.525  3677.2    80.40       53        16.56100
Algeria            Africa africa     2.142  4473.0    75.00       67        21.45800
American Samoa       <NA>   <NA>        NA      NA       NA       NA        11.29389
Angola             Africa africa     5.135  4321.9    53.17       59        96.19100
Anguilla        Caribbean  other     2.000 13750.1    81.10      100              NA
Argentina      Latin Amer  other     2.172  9162.1    79.89       93        12.33700
Armenia              Asia  other     1.735  3030.7    77.33       64        24.27200
Aruba           Caribbean  other     1.671 22851.5    77.75       47        14.68700
Australia         Oceania   oecd     1.949 57118.9    84.27       89         4.45500
Austria            Europe   oecd     1.346 45158.8    83.55       68         3.71300
Azerbaijan           Asia  other     2.148  5637.6    73.66       52        37.56600
Bahamas         Caribbean  other     1.877 22461.6    78.85       84        14.13500
Bahrain              Asia  other     2.430 18184.1    76.06       89         6.66300
Bangladesh           Asia  other     2.157   670.4    70.23       29        41.78600
Barbados        Caribbean  other     1.575 14497.3    80.26       45        12.28400
```

```
Belarus            Europe  other    1.479  5702.0    76.37       75          6.49400
Belgium            Europe   oecd    1.835 43814.8    82.81       97          3.73900
Belize         Latin Amer  other    2.679  4495.8    77.81       53         16.20000
Benin              Africa africa    5.078   741.1    58.66       42         76.67400
```

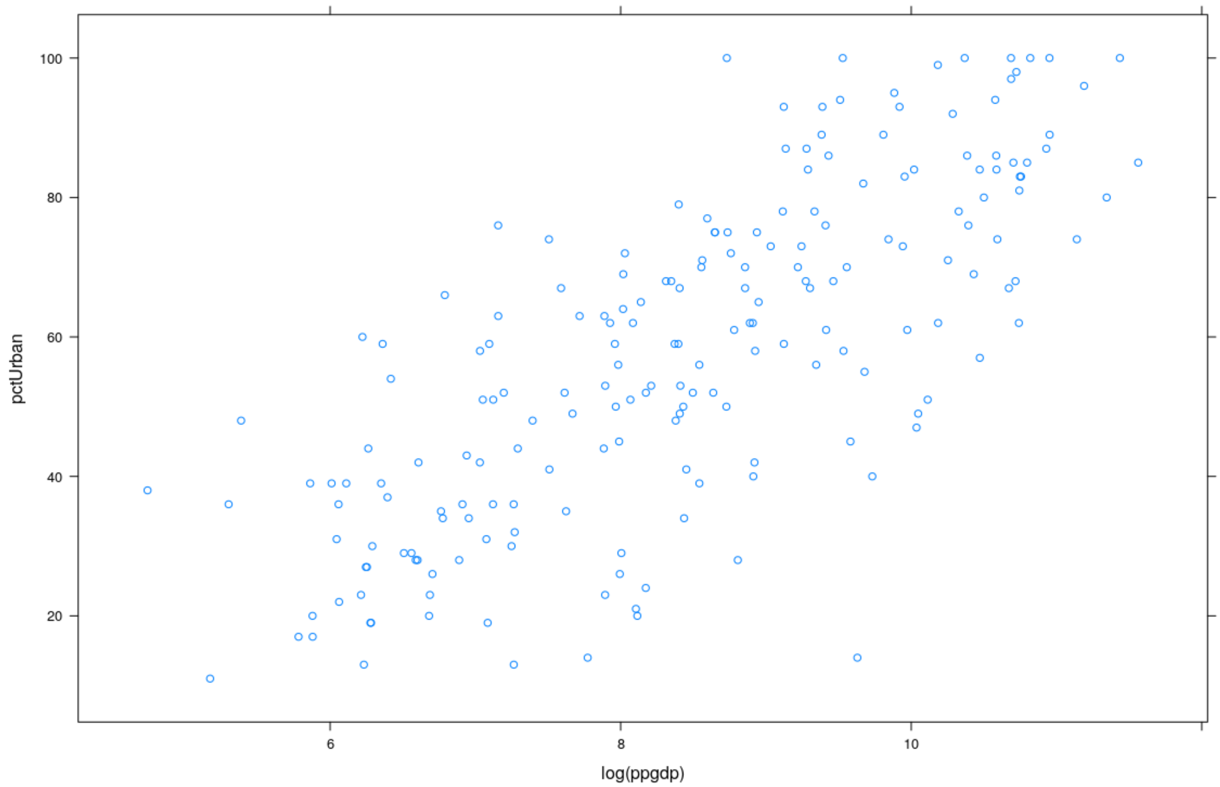
- Interested in predicting `pctUrban` using `ppgdp`

Example: UN Data

```
xyplot(pctUrban ~ ppgdp, data = UN)
```




```
xyplot(pctUrban ~ log(ppgdp), data = UN)
```



Review of Linear Regression

- Interested in "predicting" Y for a fixed value of $X = x$
- In probability terms, want the *conditional distribution* of

$$Y|X = x$$

- Important special case: *linear regression*
  - Appropriate under certain model assumptions
  - Essential component in more general procedures
  - You will learn theory in *Linear Model* course
  - We will review basics

Conditional distribution

$$Y|X = x$$

- In general, the conditional distribution can be anything
- If (X, Y) is jointly Normal, then

$$Y|X = x \sim N(\alpha + \beta x, \sigma^2)$$

  for some α, β, σ^2

- This is the motivation for *Linear Regression*

Correlation: Measuring linear dependence

- Suppose $E(X) = \mu_X$ and $E(Y) = \mu_Y$
- The *covariance* of X and Y is defined by

$$Cov\,(X, Y) = E\big((X - \mu_X)(Y - \mu_Y)\big) = E(XY) - \mu_X\,\mu_Y$$

- The *correlation coefficient* $\rho\,(X, Y)$ of X and Y is defined by

$$\rho(X, Y) = \frac{Cov\,(X, Y)}{\sqrt{Var\,(X)\,Var\,(Y)}}$$

Properties of Correlation Coefficient

- $-1 \leq \rho \leq 1$
- $\rho = -1$: perfect decreasing linear relation
- $\rho = 1$: perfect increasing linear relation
- $\rho = 0$: no linear relation

Sample Correlation

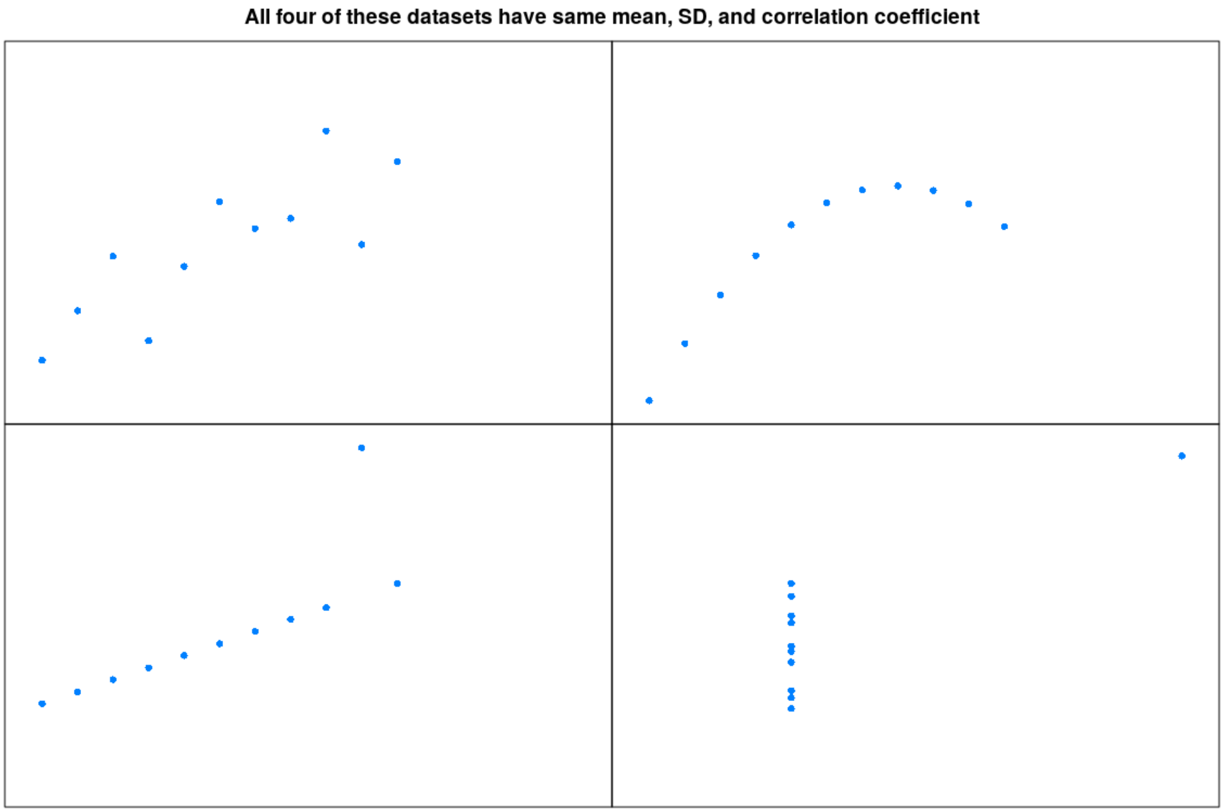
- Sample analog of correlation

$$r(X, Y) = \frac{\sum_i (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_i (x_i - \bar{x})^2 \sum_i (y_i - \bar{y})^2}}$$

- Closely related with regression
- Correlation between height and weight (`Davis` data): 0.19
- Correlation between reported height and weight (`Davis` data): 0.762
- Correlations in labour dynamics data

	wages	education	age
wages	1.000	0.307	0.361
education	0.307	1.000	-0.298
age	0.361	-0.298	1.000

Warning! Correlation only measures *linear* relation!



(Multiple) Linear Regression

In general form, the regression model assumes

$$E(Y|X_1 = x_1, X_2 = x_2, \ldots, X_p = x_p) = \beta_0 + \sum_{j=1}^{p} \beta_j x_j$$

$$Var(Y|X_1 = x_1, X_2 = x_2, \ldots, X_p = x_p) = \sigma^2$$

where

- $\beta_0, \beta_1, \ldots, \beta_p, \sigma^2 > 0$ are unknown parameters
- $X_1, X_2, \ldots, X_p$ are *(conditionally) fixed* covariates
- $X_1, X_2, \ldots, X_p$ may be *derived* from a smaller set of *predictors*, e.g.,
  - $X_2 = Z_1$ (linear term for Z_1)
  - $X_3 = Z_2$ (linear term for Z_2)
  - $X_4 = Z_1^2$ (quadratic term for Z_1)
  - $X_5 = Z_2^2$ (quadratic term for Z_2)
  - $X_6 = Z_1 Z_2$ (interaction term)

- In vector notation (incorporating intercept term in $\mathbf{X}$)

$$E(Y|\mathbf{X} = \mathbf{x}) = \mathbf{x}^T\beta$$
$$Var(Y|\mathbf{X} = \mathbf{x}) = \sigma^2$$

- Alternatively

$$Y = \mathbf{x}^T\beta + \varepsilon \text{ where}$$
$$E(\varepsilon) = 0, Var(\varepsilon) = \sigma^2$$

Sample version: n independent observations from this model

- For ith sample point, let
  - Y_i = response
  - $\mathbf{x}_i$ = p-dimensional vector of predictors
- We assume that

$$Y_i = \mathbf{x}_i^T\beta + \varepsilon_i,$$

where ε_i are independent and

$$E(\varepsilon_i) = 0, Var(\varepsilon_i) = \sigma^2$$

In matrix notation

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

- where

$$\mathbf{Y} = \begin{pmatrix} Y_1 \\ \vdots \\ Y_n \end{pmatrix}, \mathbf{X} = \begin{pmatrix} \mathbf{x}_1^T \\ \vdots \\ \mathbf{x}_n^T \end{pmatrix}, \varepsilon = \begin{pmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_n \end{pmatrix}$$

- $\mathbf{Y}$ and ε are $n \times 1$
- $\mathbf{X}$ is $n \times p$
- Columns of $\mathbf{X}$ are assumed to be linearly independent (rank($\mathbf{X}$) = p)
- $\beta_{p\times 1}$ and $\sigma^2 > 0$ are unknown parameters

Problem: How to estimate β and σ^2

- Least squares approach: minimize sum of squared errors

$$\widehat{\beta} = \arg\min_{\beta} q(\beta)$$

where

$$q(\beta) = \sum (Y_i - \mathbf{x}_i^T\beta)^2 = (\mathbf{Y} - \mathbf{X}\beta)^T(\mathbf{Y} - \mathbf{X}\beta)$$

- Set gradient with respect to β to $\mathbf{0}$.

$$\nabla q(\beta) = 2\mathbf{X}^T(\mathbf{Y} - \mathbf{X}\beta) = 2(\mathbf{X}^T\mathbf{Y} - \mathbf{X}^T\mathbf{X}\beta) = \mathbf{0}$$

- This leads to Normal Equations:

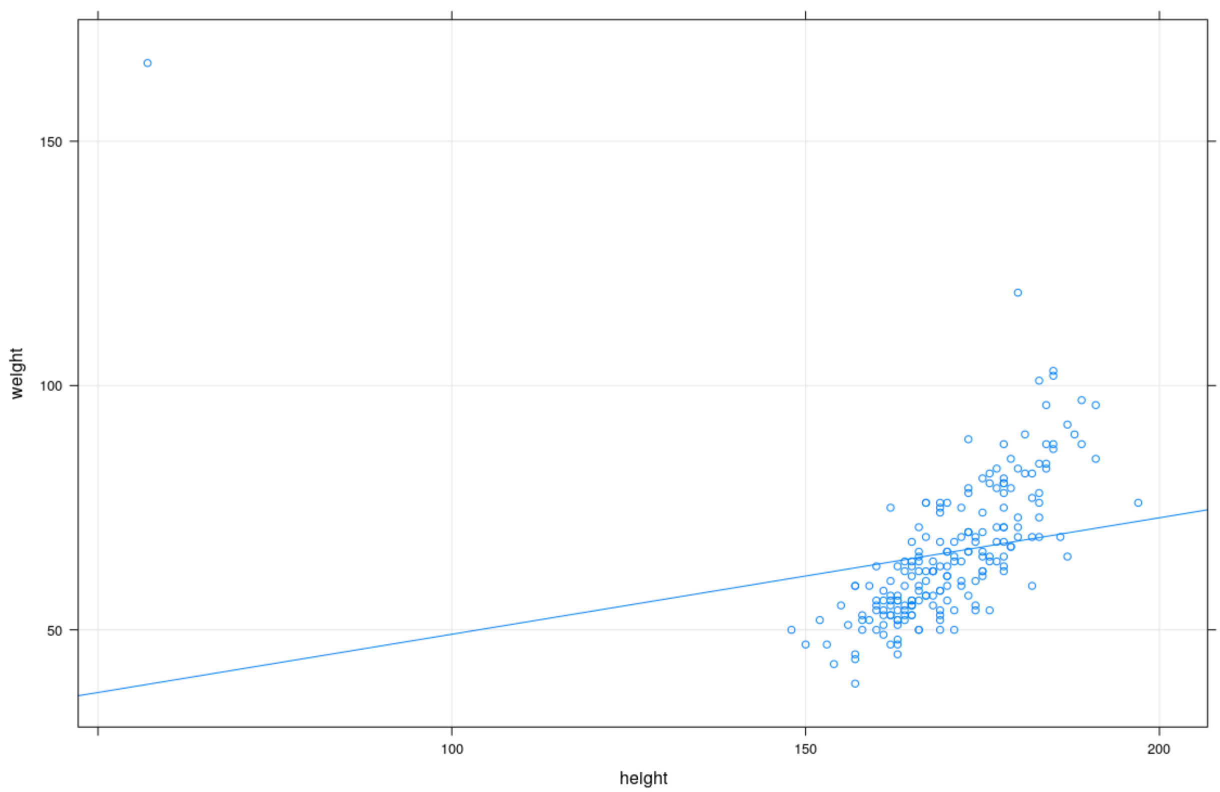
$$\mathbf{X}^T\mathbf{X}\beta = \mathbf{X}^T\mathbf{Y}$$

- Estimate of β assuming that $\mathbf{X}^T\mathbf{X}$ has full rank (OLS estimator):

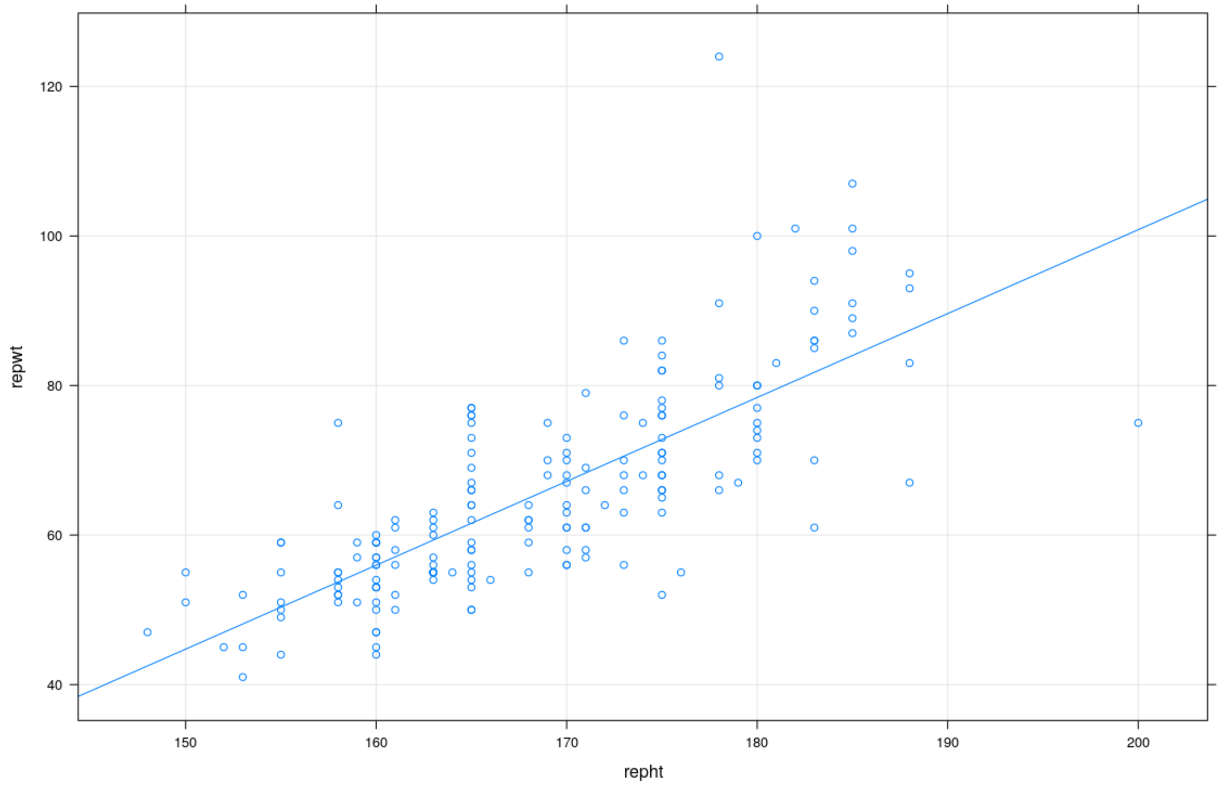
$$\widehat{\beta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$$

The OLS estimator in practice

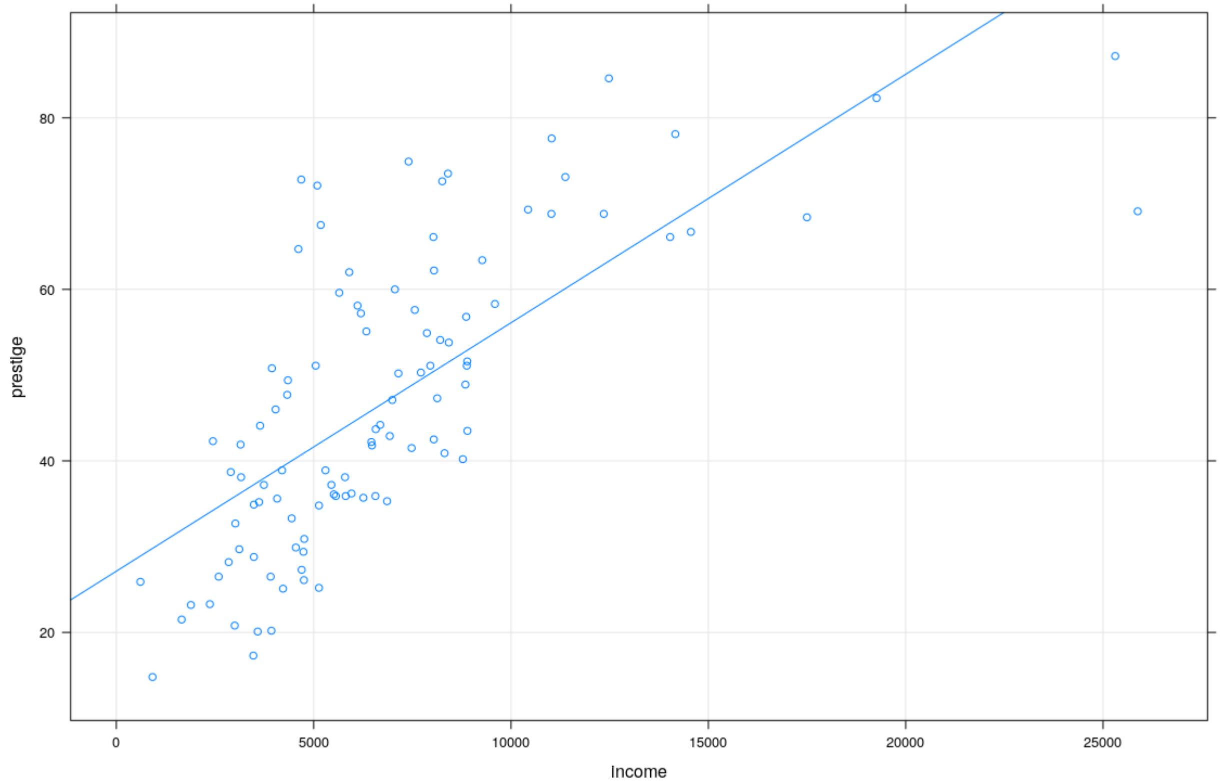
```
fm1 <- lm(weight ~ height, data = Davis)
xyplot(weight ~ height, data = Davis, grid = TRUE, type = c("p", "r"))
```



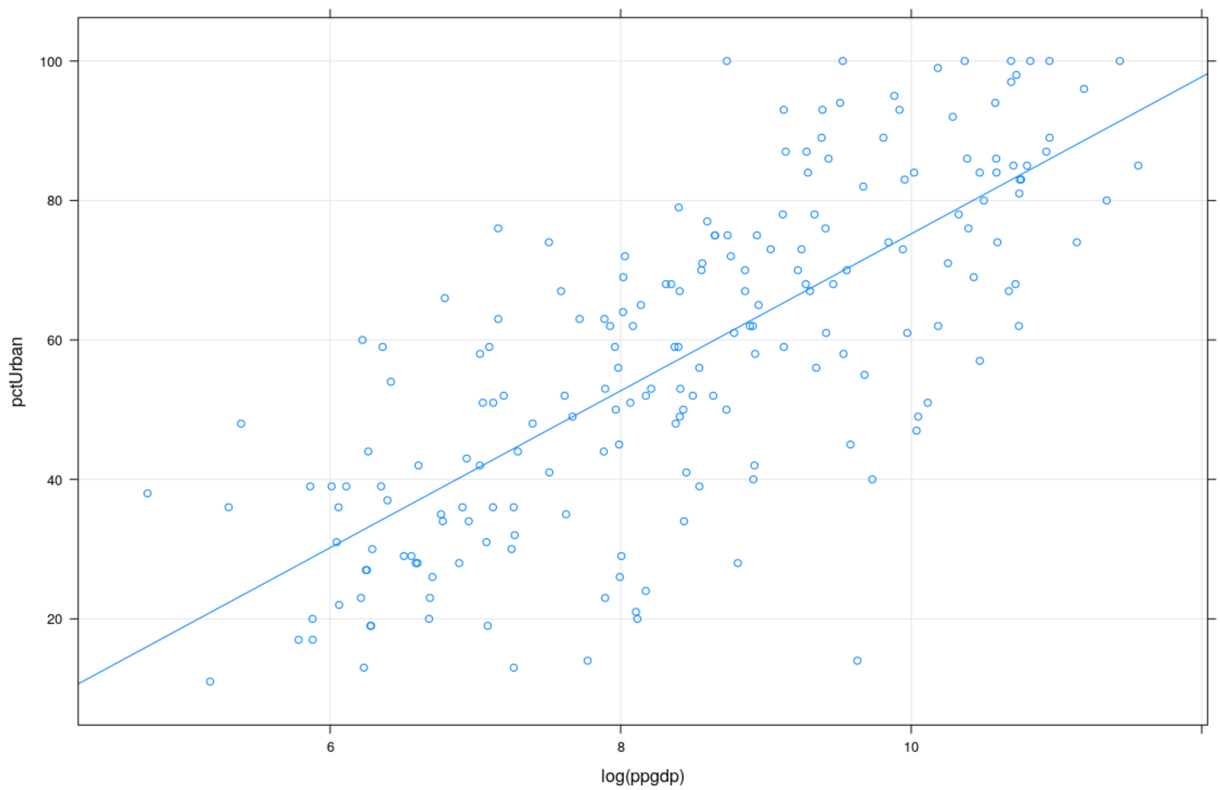

```
fm1 <- lm(repwt ~ repht, data = Davis)
xyplot(repwt ~ repht, data = Davis, grid = TRUE, type = c("p", "r"))
```




```r
xyplot(prestige ~ income, Prestige, grid = TRUE, type = c("p", "r"))
```




```
xyplot(pctUrban ~ log(ppgdp), data = UN, grid = TRUE, type = c("p", "r"))
```



Alternative approach: maximum likelihood

- Less arbitrary, but needs model assumption: **Multivariate Normality**
- To indicate that $\mathbf{Y}$ follows n-dimensional Multivariate Normal Distribution with mean vector μ and covariance matrix Σ, we write

$$\mathbf{Y} \sim N_n(\mu, \Sigma)$$

- When Σ has full rank (positive definite), $\mathbf{Y}$ has joint density function (pdf)

$$f(\mathbf{y}) = (2\pi)^{-n/2} |\Sigma|^{-1/2} \exp\left\{-\frac{1}{2}(\mathbf{y}-\mu)^T \Sigma^{-1}(\mathbf{y}-\mu)\right\}$$

- Note that this function has the two worst things in matrices, the determinant and the inverse of a matrix.
- Fortunately, the situation is simpler for the regression model

$$\mathbf{Y} \sim N_n(\mathbf{X}\beta, \sigma^2\mathbf{I})$$

with probability density function

$$f(\mathbf{y}) = (2\pi)^{-n/2} \left(\sigma^2\right)^{-n/2} \exp\left\{-\frac{1}{2\sigma^2} \|\mathbf{y}-\mathbf{X}\beta\|^2\right\}$$

- Therefore the likelihood for this model is

$$L\left(\beta,\sigma^2\right) = (2\pi)^{-n/2}\left(\sigma^2\right)^{-n/2}\exp\left\{-\frac{1}{2\sigma^2}\left\|\mathbf{Y}-\mathbf{X}\beta\right\|^2\right\}$$

- Maximizing $L\left(\beta,\sigma^2\right)$ w.r.t. β is equivalent to minimizing $\left\|\mathbf{Y}-\mathbf{X}\beta\right\|^2$

Is this a good estimator?

- To answer this, we need some more tools
- Mean and Covariance of a random vector $\mathbf{Y}$

$$\mu = \begin{pmatrix} \mu_1 \\ \vdots \\ \mu_n \end{pmatrix},\ \Sigma = \begin{pmatrix} \Sigma_{11} & \cdots & \Sigma_{1n} \\ \vdots & \ddots & \vdots \\ \Sigma_{n1} & \cdots & \Sigma_{nn} \end{pmatrix}$$

  where

$$\mu_i = EY_i,$$

  and

$$\Sigma_{ij} = \begin{cases} Var(Y_i) & \text{for } i = j \\ Cov(Y_i, Y_j) & \text{for } i \neq j \end{cases}$$

Properties of mean and covariance

- The covariance matrix is symmetric
- For any $n \times n$ matrix $\mathbf{A}$ and $n \times 1$ vector $\mathbf{b}$

$$E\left(\mathbf{A}\mathbf{Y}+\mathbf{b}\right) = \mathbf{A}E(\mathbf{Y})+\mathbf{b},$$

$$Cov(\mathbf{A}\mathbf{Y}+\mathbf{b}) = \mathbf{A}Cov(\mathbf{Y})\mathbf{A}^T$$

- Variance of a linear combination

$$0 \leq Var(\mathbf{a}^T\mathbf{Y}) = \mathbf{a}^T Cov(\mathbf{Y})\mathbf{a}$$

  which implies that the covariance matrix is non-negative definite.

Properties of the OLS estimator $\widehat{\beta}$

- Mean:

$$E\widehat{\beta} = \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T E\mathbf{Y} = \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{X}\beta = \beta$$

- Covariance:

$$Cov(\widehat{\beta}) = \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\sigma^2\mathbf{I}\mathbf{X}\left(\mathbf{X}^T\mathbf{X}\right)^{-1} = \sigma^2\left(\mathbf{X}^T\mathbf{X}\right)^{-1} = \sigma^2\mathbf{M}$$

- Property of Multivariate Normal:

  If $\mathbf{Y} \sim N_n(\mu, \Sigma)$, then

$$\mathbf{A}\mathbf{Y}+\mathbf{b} \sim N(\mathbf{A}\mu+\mathbf{b}, \mathbf{A}\Sigma\mathbf{A}^T)$$

- Therefore

$$\widehat{\beta} \sim N_p\left(\beta, \sigma^2 \mathbf{M}\right)$$

- For the normal model, the OLS is the *best unbiased estimator*, i.e., it has smaller variance than any other unbiased estimator.
- More precisely, $\ell^T \widehat{\beta}$ is the best unbiased estimator of $\ell^T \beta$ for any linear combination $\ell^T \beta$.
  - $E(\ell^T \widehat{\beta}) = \ell^T \beta$
  - $Var(\ell^T \widehat{\beta}) = \sigma^2 \ell^T \left(\mathbf{X}^T \mathbf{X}\right)^{-1} \ell$
  - Note that this *conditional* variance depends on $\mathbf{X}$ — does distribution of $\mathbf{X}$ matter?
- Prediction: Put $\ell = \mathbf{x}$ for some future covariates $\mathbf{x}$
- Even without assuming normality, the OLS estimator has smaller variance than any other *linear* unbiased estimator.
- The OLS estimator is consistent (as long as $\mathbf{X}$ grows reasonably), i.e., $\widehat{\beta} \to \beta$ as $n \to \infty$.

The unbiased estimator of σ^2

- We typically estimate σ^2 by

$$\widehat{\sigma}^2 = \left\| \mathbf{Y} - \mathbf{X}\widehat{\beta} \right\|^2 / (n-p)$$

  which is called the unbiased estimator of σ^2
- Distribution of $\widehat{\sigma}^2$:

$$\frac{(n-p)\,\widehat{\sigma}^2}{\sigma^2} \sim \chi^2_{n-p}$$

  independently of $\widehat{\beta}$

Properties of $\widehat{\sigma}^2$

- For the normal model $\widehat{\sigma}^2$ is the best unbiased estimator.
- Even without normality, $\widehat{\sigma}^2$ is unbiased.
- $\widehat{\sigma}^2$ is consistent

The maximum likelihood estimator (MLE)

- To find MLE of σ^2, differentiate $\log L(\widehat{\beta}, \sigma^2)$ with respect to σ
- Easy to show that this gives

$$\widehat{\sigma}^2_{MLE} = \frac{1}{n} \left\| \mathbf{Y} - \mathbf{X}\widehat{\beta} \right\|^2$$

- Note that the MLE is not unbiased, but is consistent.
- In general, neither the OLS estimator nor the MLE of σ^2 minimize mean squared error (MSE)

Testing

- We are often interested in coefficients β_j
- Note that by properties given above

$$\widehat{\beta}_j \sim N(\beta_j, \sigma^2 M_{jj})$$

- "Standard error" of $\widehat{\beta}_j$

$$\widehat{\sigma}_{\widehat{\beta}_j} = \widehat{\sigma}\sqrt{M_{jj}}$$

Testing: t-statistic

- Testing the null hypothesis $H_0 : \beta_j = c$

$$t = \frac{\widehat{\beta}_j - c}{\widehat{\sigma}_{\widehat{\beta}_j}} \sim t_{n-p}.$$

- Can be generalized to:
  - any linear combination of β_j
  - more than one simultaneous restrictions (F-test)

t-tests in practice

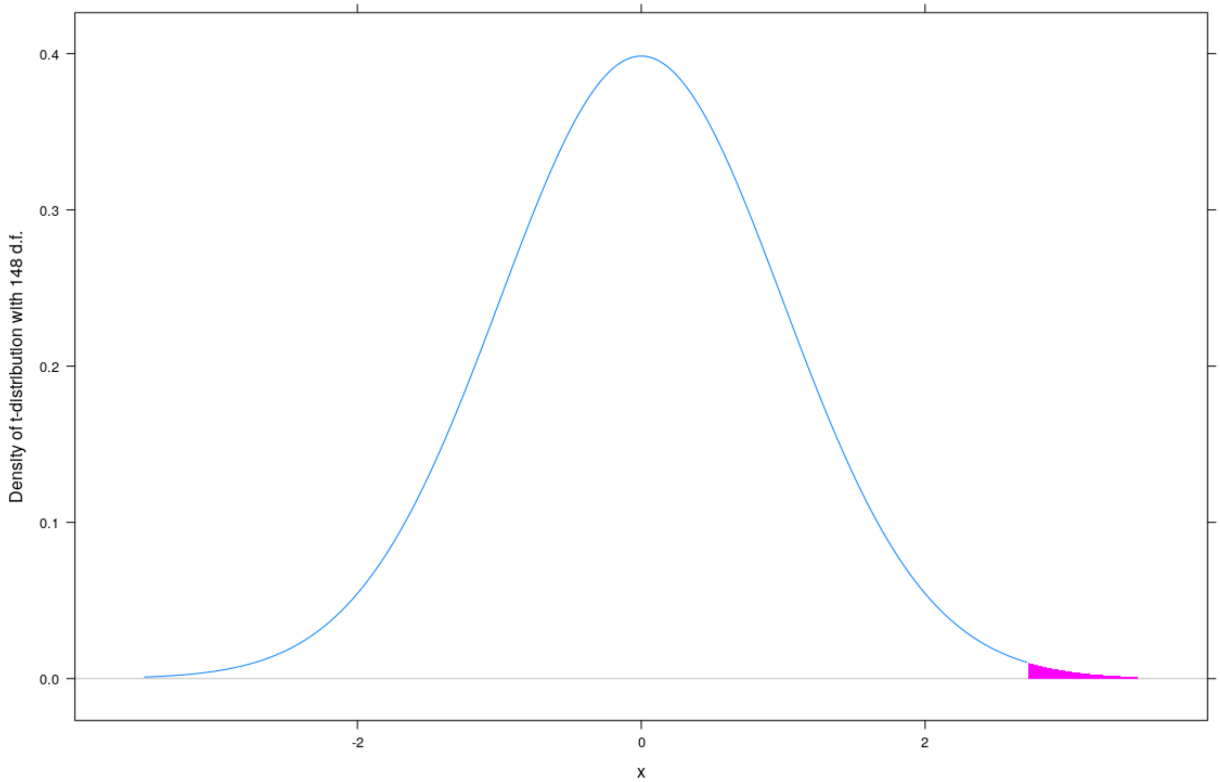
```
fm1 <- lm(weight ~ height, data = Davis)
print(summary(fm1), signif.stars = FALSE)
```

```

Call:
lm(formula = weight ~ height, data = Davis)

Residuals:
    Min      1Q  Median      3Q     Max 
-23.696  -9.506  -2.818   6.372 127.145 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 25.26623   14.95042   1.690  0.09260
height       0.23841    0.08772   2.718  0.00715

Residual standard error: 14.86 on 198 degrees of freedom
Multiple R-squared:  0.03597,	Adjusted R-squared:  0.0311 
F-statistic: 7.387 on 1 and 198 DF,  p-value: 0.007152
```

t-tests - computing p-values in R

```
2 * pt(2.718, df = 198, lower.tail = FALSE)
```

```
[1] 0.007150357
```



Testing: F-statistic

Loosely speaking,

- Suppose we are interested in testing H_0 vs H_1, where H_0 is a sub-model of H_1

$$H_0 \subset H_1 \quad (H_m : \mathbf{Y} \sim N_n(\mathbf{X}_m \beta_m, \sigma^2 \mathbf{I}))$$

- Let the sum of squared errors for the two models be S_0^2 and S_1^2

$$S_m^2 = \left\| \mathbf{Y} - \mathbf{X}_m \widehat{\beta}_m \right\|^2, m = 0, 1$$

- Let the number of parameters (length of β) in the two models be p_0 and p_1
- Then the test statistic

$$F = \frac{\frac{S_0^2 - S_1^2}{p_1 - p_0}}{\frac{S_1^2}{n - p_1}} \text{ follows } F_{p_1 - p_0, n - p_1} \text{ under } H_0$$

(Cochran's theorem, Linear Models course)

F-tests in practice

```r
fm2 <- lm(weight ~ height * sex, data = Davis)
summary(fm2)
```

```

Call:
lm(formula = weight ~ height * sex, data = Davis)

Residuals:
    Min      1Q  Median      3Q     Max 
-23.091  -6.331  -0.995   6.207  41.230 

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)  160.49748   13.45954  11.924  < 2e-16
height        -0.62679    0.08199  -7.644 9.17e-13
sexM        -261.82753   32.72161  -8.002 1.05e-13
height:sexM    1.62239    0.18644   8.702 1.33e-15

Residual standard error: 10.06 on 196 degrees of freedom
Multiple R-squared:  0.5626,    Adjusted R-squared:  0.556 
F-statistic: 84.05 on 3 and 196 DF,  p-value: < 2.2e-16
```

```r
anova(fm1, fm2)
```

```
Analysis of Variance Table

Model 1: weight ~ height
Model 2: weight ~ height * sex
  Res.Df   RSS Df Sum of Sq      F    Pr(>F)
1    198 43713
2    196 19831  2     23882 118.02 < 2.2e-16
```

Measuring Goodness of Fit: Coefficient of Determination

- Consider residual sum of squared errors

  $$T^2 = \sum \left(Y_i - \bar{Y}\right)^2$$

  and

  $$S^2 = \sum \left(Y_i - \mathbf{x}_i^T \widehat{\beta}\right)^2 = \left\| \mathbf{Y} - \mathbf{X}\widehat{\beta} \right\|^2$$

  for intercept-only model and regression model
- We can think of these as measuring the "unexplained variation" in $\mathbf{Y}$ under these two models.
- Then the coefficient of determination R^2 is defined by

  $$R^2 = \frac{T^2 - S^2}{T^2} = 1 - \frac{S^2}{T^2}$$

  Note that

  $$0 \leq R^2 \leq 1$$

R^2

- $T^2 - S^2$ is the amount of variation in the intercept-only model which has been explained by including the extra predictors of the regression model and
- R^2 is the proportion of the variation left in the intercept-only model which has been explained by including the additional predictors.
- Link with correlation: It can be shown that for one predictor,

$$R^2 = r^2(X, Y)$$

Adjusted R^2

- Note that

$$R^2 = \frac{\frac{T^2}{n} - \frac{S^2}{n}}{\frac{T^2}{n}}$$

- Possible alternative: substitute unbiased estimators
- Adjusted R^2:

$$R_a^2 = \frac{\frac{T^2}{n-1} - \frac{S^2}{n-p}}{\frac{T^2}{n-1}} = 1 - \frac{n-1}{n-p}(1 - R^2)$$

Predictive R^2: Leave-One-Out Cross-validation

- Disadvantage of R^2 and adjusted R^2
  - Evaluates fit based on same data that is used to obtain fit
  - Adding more covariates will always improve R^2
- A better procedure is based on *cross-validation*.
- Delete the ith observation and compute $\widehat{\beta}_{(-i)}$ after excluding ith observation.
- Also compute the sample mean excluding the ith observation

$$\bar{Y}_{(-i)} = \frac{1}{n-1} \sum_{j \neq i} Y_j$$

- Do this for all i.
- Define

$$T_p^2 = \sum \left(Y_i - \bar{Y}_{(-i)} \right)^2$$

  and

$$S_p^2 = \sum \left(Y_i - \mathbf{x}_i^T \widehat{\beta}_{(-i)} \right)^2$$

- The predictive R^2 is defined as

$$R_p^2 = \frac{T_p^2 - S_p^2}{T_p^2}$$

- This computes the fit to the ith observation without using that observation
- Better measure of goodness of model fit than R^2 or adjusted R^2

Beyond linear regression (topics of this course)

- Identifying violations of linear model assumptions
  - Lack of fit (linearity)
  - Heteroscedasticity
  - Autocorrelation in errors
  - Collinearity (not a violation, but still problematic)
  - Discordant outliers and influential observations
  - Non-normality of errors
- Possible solutions
  - Nonparametric regression
  - More flexible "linear" regression models (e.g., splines)
  - Transformations
  - Modeling heteroscedasticity
  - Regularization (constrain parameters)
  - Variable selection
  - Robust Regression

First, get familiar with R

- Overview of R
- R Tutorials
- Many other online resources available