Unusual and Influential Observations

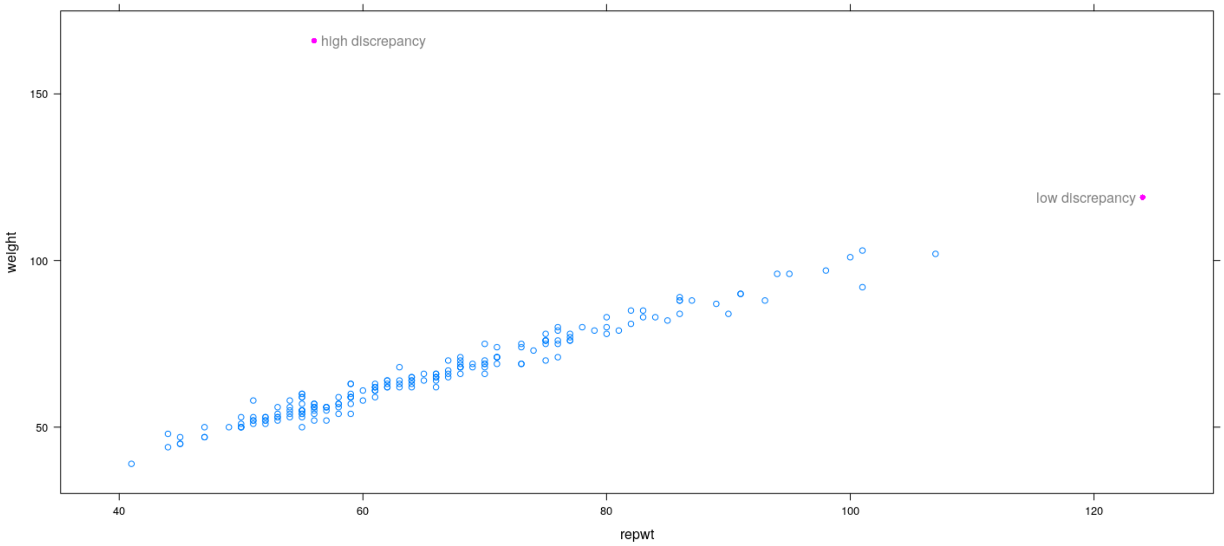
Deepayan Sarkar

Violation of assumptions in a linear regression model

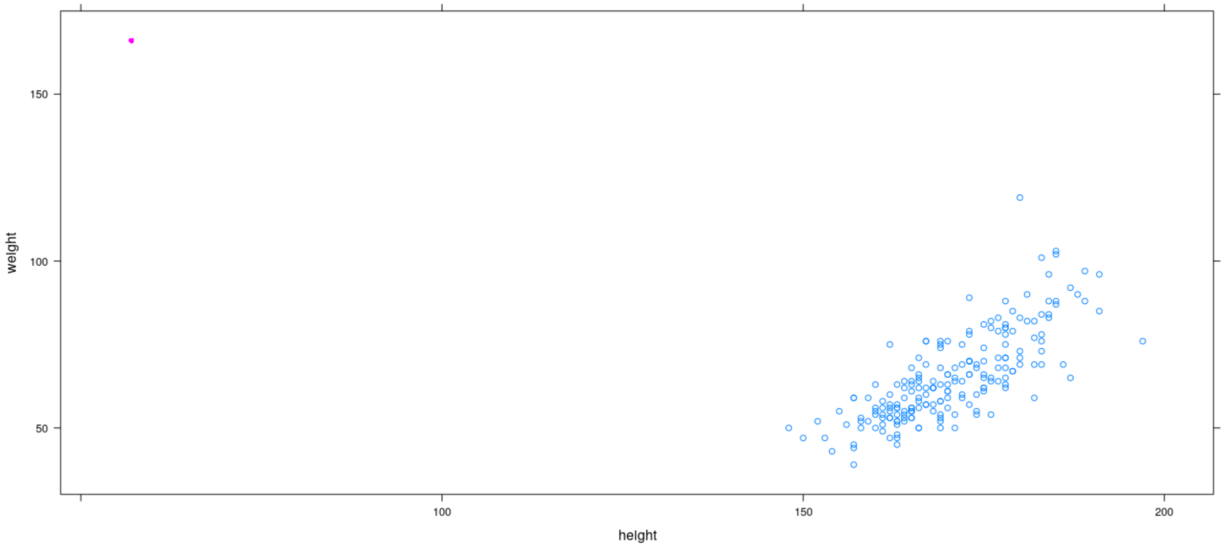
- Systematic violations
  - Non-normality of errors
  - Nonconstant error variance
  - Lack of fit (nonlinearity)
  - Autocorrelation in errors
- Discordant outliers and influential observations
- For now, we will focus on indentifying such observations
- Outline
  - Motivation and description of diagnostic measures
  - Cutoffs for diagnostics (mostly heuristic)
  - Mathematical details
- References
  - Cook and Weisberg (1982) *Residuals and influence in regression.*
  - Belsley, Kuh, Welsh (1980) *Regression diagnostics: Identifying influential data and sources of collinearity*
  - Chatterjee and Hadi (1988) *Sensitivity analysis in linear regression*

Important concepts

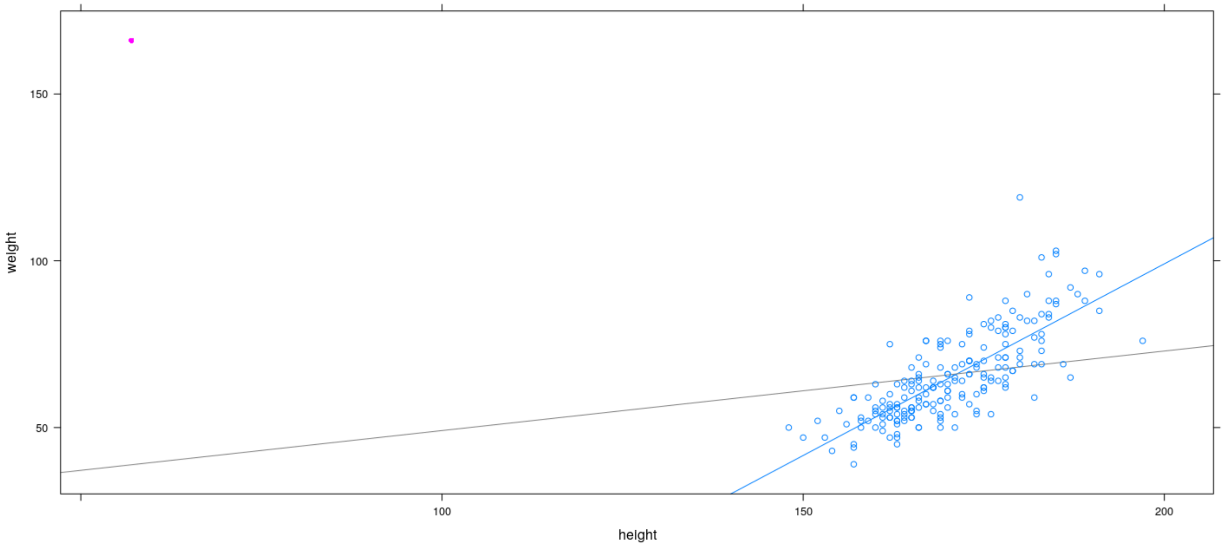
- *Regression Outlier* : Conditional distribution of $Y_i|X_i$ is unusual (*discrepancy*)



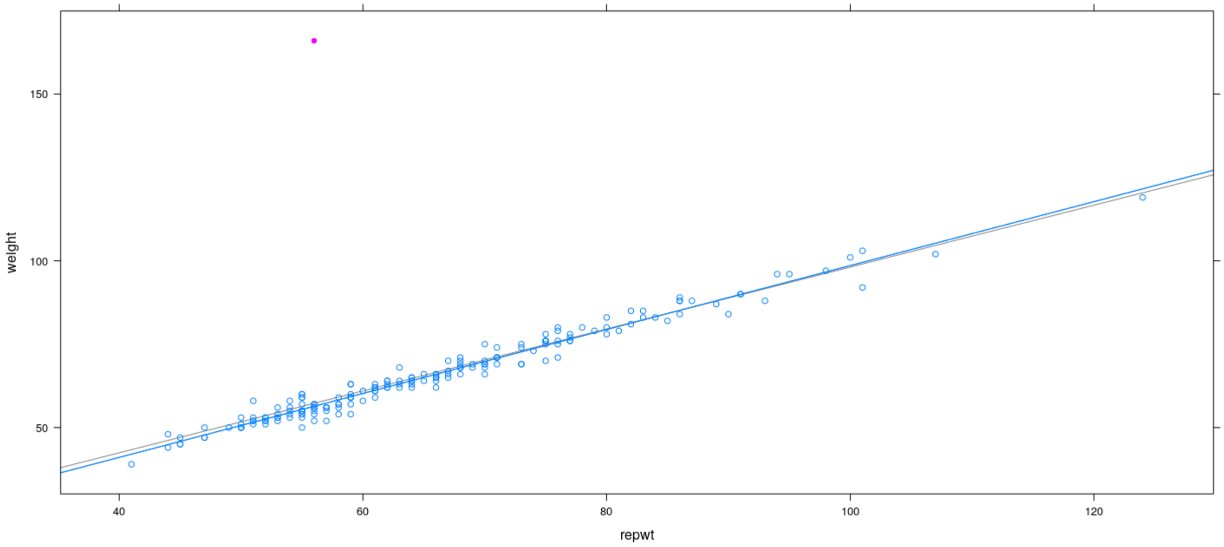
- *Covariate Outlier* : X_i value is unusual w.r.t. other values of X (may also be a regression outlier)



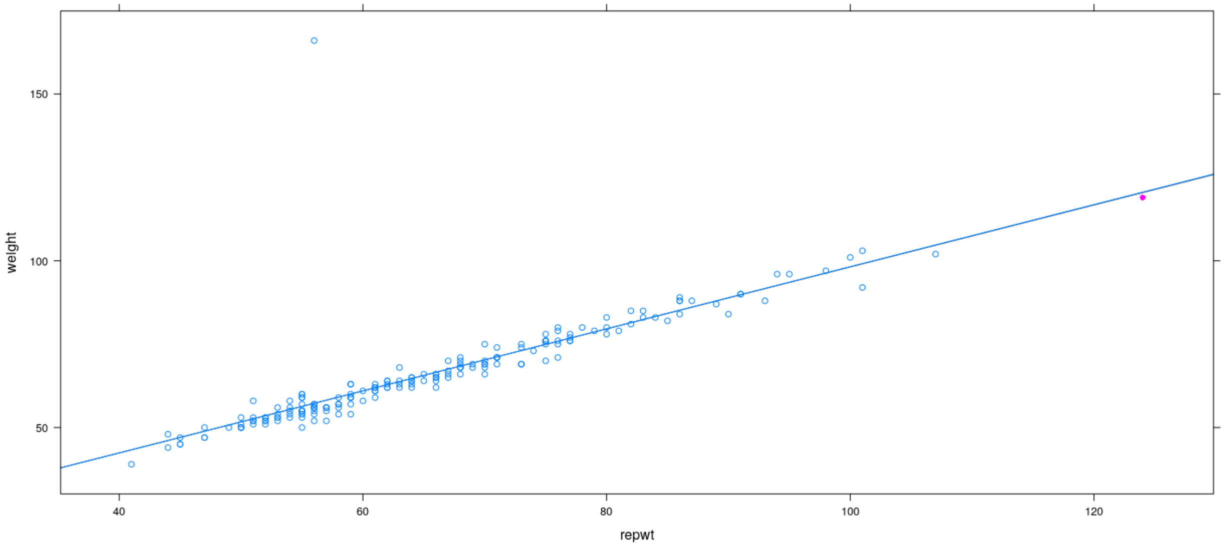
- *Leverage* : Potential ability of an observation to affect (*influence*) regression



- *Leverage* : Potential ability of an observation to affect (*influence*) regression



- *Leverage* : Potential ability of an observation to affect (*influence*) regression



General principle: outliers, leverage, and influence

- Covariate outliers have high leverage (potentially influential)
- Whether a discrepant observation (regression outlier) actually influences fit depends on whether it also has high leverage
- Roughly, influence = leverage × discrepancy
- We want to be able to identify high-leverage observations, regression outliers, and influential observations
- Relatively simple for single predictor, but want general methods that work with many predictors

Leverage: hat-values

In the linear model, $\hat{\beta}$ is a linear function of $\mathbf{y}$:

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

So is the vector of fitted values:

$$\hat{\mathbf{y}} = \mathbf{X}\hat{\beta} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} = \mathbf{H}\mathbf{y}$$

where $\mathbf{H} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$ is known as the "hat matrix"

In scalar notation,

$$\hat{y_j} = \sum_{i=1}^{n} h_{ji} y_i = \sum_{i=1}^{n} h_{ij} y_i$$

- h_{ij}-s depend on $\mathbf{X}$, not $\mathbf{y}$
- h_{ij} captures contribution of y_i on $\hat{y_j}$ (larger values means potentially larger impact)

- *Hat-values* (summarize leverage of y_i on *all* fitted values):

$$h_i \equiv h_{ii} = \sum_{j=1}^{n} h_{ij}^2$$

- The last result follows because $\mathbf{H}$ is symmetric and idempotent ($\mathbf{H}^2 = \mathbf{H}$)
- Corollary: $V(\hat{\mathbf{y}}) = \sigma^2 \mathbf{H}$ and $V(\hat{\mathbf{e}}) = \sigma^2(\mathbf{I} - \mathbf{H})$, where $e_i = y_i - \hat{y}_i$

Properties of hat-values h_i

- $0 \leq h_i \leq 1$
- In fact, $h_i \geq 1/n$ if the model includes the constant term
  - Easy to check if other columns are orthogonal to $\mathbf{1}$ (mean zero)
  - Enough to verify that $\mathbf{H}$ remains unchanged (exercise)
- $\bar{h} = p/n$ where p is the rank of $\mathbf{X}$
  - Proof follows from property of idempotent / projection matrices: rank = trace

For simple linear regression with one predictor, h_i simplifies to

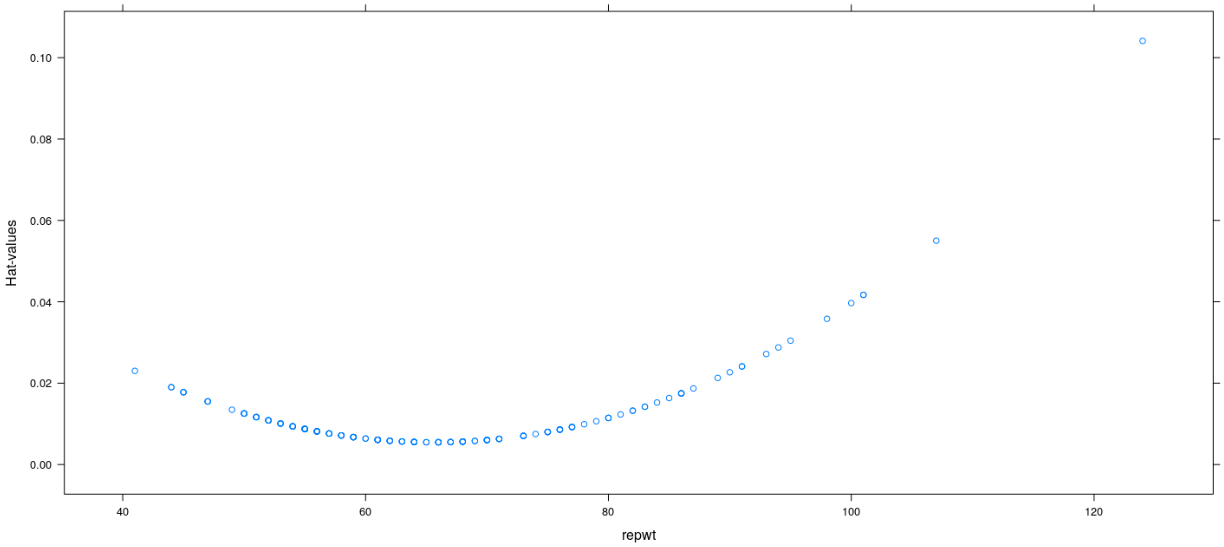
$$h_i = \frac{1}{n} + \frac{(x_i - \bar{x})^2}{\sum_j (x_j - \bar{x})^2}$$

In general, with $\tilde{\mathbf{X}}$ denoting "centered" $\mathbf{X}$ (mean zero columns),

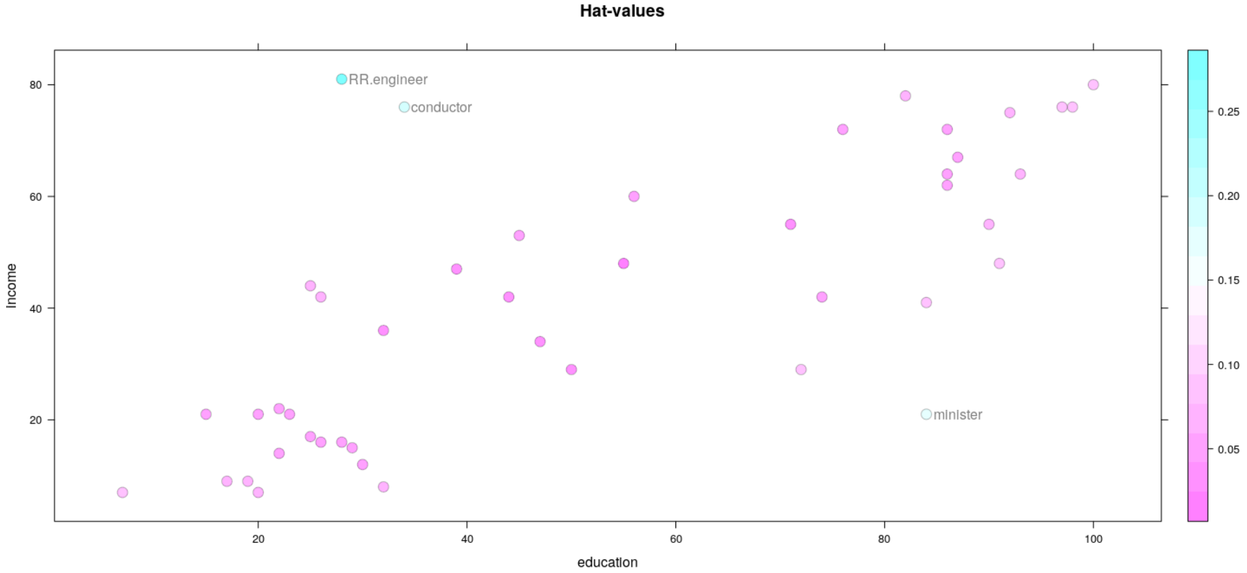
$$h_i = \frac{1}{n} + \tilde{\mathbf{x}}_i^T (\tilde{\mathbf{X}}^T \tilde{\mathbf{X}})^{-1} \tilde{\mathbf{x}}_i$$

So h_i essentially measures (up to scaling) the Mahalanobis distance of $\mathbf{x}_i$ from the centroid (mean vector) of the covariates (taking their correlation structure into account)

```
fm <- lm(weight ~ repwt, Davis, na.action = na.exclude)
xyplot(hatvalues(fm) ~ repwt, Davis, ylab = "Hat-values")
```



```
fm <- lm(prestige ~ education + income, Duncan, na.action = na.exclude)
id <- which(hatvalues(fm) > 0.15)
levelplot(hatvalues(fm) ~ education + income, Duncan, main = "Hat-values", cex = 1.5,
          panel = panel.levelplot.points, prepanel = prepanel.default.xyplot) +
    layer(panel.text(x[id], y[id], labels = rownames(Duncan)[id], pos = 4, col = "grey50"))
```



Detecting outliers: standardized and Studentized residuals

- Regression outliers have high discrepancy, i.e., high ε_i
- Unfortunately, corresponding $\hat{\varepsilon}_i$ may not be large
- As noted earlier, $V(e_i) = \sigma^2(1 - h_i)$
- Define *standardized residual* :

$$r_i = \frac{e_i}{\hat{\sigma}\sqrt{1 - h_i}}$$

Unfortunately, numerator and denominator are not independent.

Deletion models

- Natural fix: estimate σ from model fitted without observation (deletion model)
- Define *Studentized residual*

$$t_i = \frac{e_i}{\hat{\sigma}_{(-i)}\sqrt{1 - h_i}}$$

- May be more natural to define the *deleted Studentized residual*

$$\tilde{t}_i = \frac{e_{i(-i)}}{\hat{V}(e_{i(-i)})}$$

- $\hat{V}(e_{i(-i)})$ needs to be computed, but involves unknown σ, which is replaced by $\hat{\sigma}_{(-i)}$
- In fact, even though this is not immediately obvious,
  - $\tilde{t}_i$ and t_i are actually the same
  - Under null hypothesis (no outliers), each t_i has a t_{n-p-1} distribution

More formal approach: the mean-shift outlier model

- Consider a model that allows the ith observation to be fit separately
- Additional "predictor" $\mathbf{u}_k$ — k-th unit vector in $\mathbb{R}^n$

$$u_{ki} = \begin{cases} 1 & \text{if } i = k \\ 0 & \text{otherwise} \end{cases}$$

- Model

$$\mathbf{y} = \mathbf{X}\beta + \mathbf{u}_k\delta + \varepsilon$$

- Can test for $H_0 : \delta = 0$ (k-th observation not outlier)

Easy to see that for this model, $e_k = 0, \hat{y}_k = y_k$

More importantly,

- $\hat{\beta}$ is same as $\hat{\beta}_{(-k)}$ for original model
- $\hat{\delta}$ is same as $e_{k(-k)}$ for original model
- RSS is same as $\text{RSS}_{(-k)}$ for original model; so
- $\hat{\sigma}^2 = \frac{\text{RSS}}{n-p-1}$ is same as $\hat{\sigma}^2_{(-k)} = \frac{\text{RSS}_{(-k)}}{(n-1)-p}$
- Test statistic for $H_0 : \delta = 0$:

$$T_k = \frac{\hat{\delta}}{s.e.(\hat{\delta})}$$

- Claim: $V(\hat{\delta}) = \frac{\sigma^2}{1-h_k}$
- It easily follows that

$$T_k = \frac{e_{k(-k)}\sqrt{1-h_k}}{\hat{\sigma}_{(-k)}} = \tilde{t}_k \text{ (by definition)}$$

Proof of claim requires a basic inversion formula for symmetric partitioned matrices:

$$\begin{bmatrix} A & B \\ B^T & D \end{bmatrix}^{-1} = \begin{bmatrix} A^{-1} + FE^{-1}F^T & -FE^{-1} \\ -E^{-1}F^T & E^{-1} \end{bmatrix}$$

where $E = D - B^T A^{-1} B$ and $F = A^{-1}B$ (we only need to compute E^{-1})

- It turns out that it is also true that

- The equality $t_i = \tilde{t}_i$ follows because

$$e_k = e_{k(-k)}(1 - h_k)$$

- Proof: exercise. Possibly useful matrix result: For u, v column vectors

$$(A + uv^T)^{-1} = A^{-1} - \frac{A^{-1}uv^T A^{-1}}{1 + v^T A^{-1} u}$$

Testing for outliers in linear models

- t_i can be used to test if observation i is an outlier
- Makes sense if we suspected that the ith observation was an outlier
- Usually we don't know in advance, and want to test for all i
- This leads to a multiple testing situation
- Expect αn tests to be rejected even if no outliers (assuming independent tests)

Testing for outliers in linear models: usual strategies

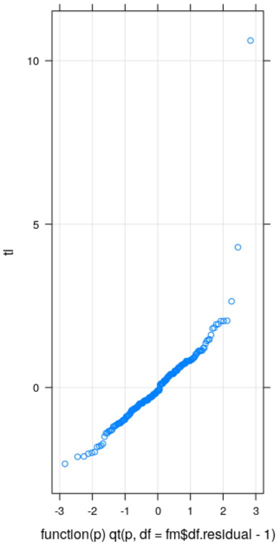
- Examine graphically (Q-Q plot comparing to t_{n-p-1})
- Simulate the largest (absolute) t_i from the null model (distribution does not depend on β or σ^2 — exercise)
- If we assume independence, the smallest p-value has a Beta distribution
  - p-values are all independent $U(0, 1)$ under null
  - Interested in the distribution of the smallest of these, follows Beta$(1, n)$
  - CDF easily computed as $F(u) = 1 - (1 - u)^n$
- Another solution (without assuming independence): Bonferroni adjustment
  - Boole's inequality: $P(\cup A_i) \leq \sum P(A_i)$
  - Bonferroni correction: $H_0 : p_i \sim U(0, 1)$ is rejected if $np_i < \alpha$, for $i = 1, \ldots, n$
  - Then, under the combined null hypothesis where all $p_i \sim U(0, 1)$,

$$P(\text{at least one rejection}) = P\left(\cup\{np_i < \alpha\}\right) \leq \sum P\left(p_i < \frac{\alpha}{n}\right) \leq \sum \frac{\alpha}{n} = n\frac{\alpha}{n} = \alpha$$

- Both these procedures can be viewed as an *adjustment* to the original p-values
- Test i is rejected if the adjusted p_i is less than α
- The Bonferroni adjustment is $p_i' = np_i$
- Adjustment with independent tests is $p_i' = 1 - (1 - p_i)^n$
- `p.adjust()` implements various p-value adjustment procedures in R

Testing for outliers: examples

```
fm <- lm(weight ~ height * sex, Davis)
ri <- rstandard(fm)
ti <- rstudent(fm)
pi <- 2 * pt(-abs(ti), df = fm$df.residual - 1)
qqmath(ti, distribution = function(p) qt(p, df = fm$df.residual - 1), grid = TRUE, aspect = "iso")
```



```
n <- with(fm, rank + df.residual)
names(which(ti > 4))
```

```
[1] "12" "21"
```

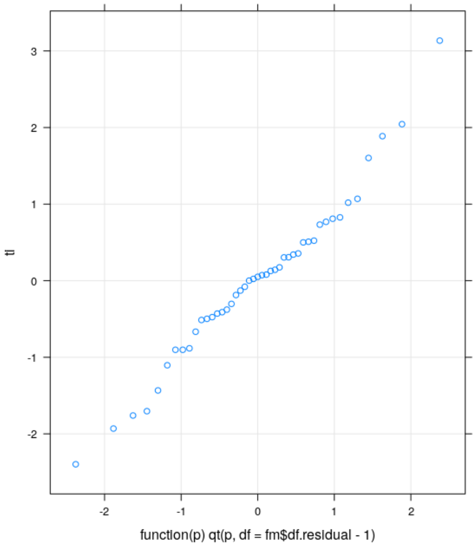
```
names(which(1 - (1-pi)^n < 0.05))
```

```
[1] "12" "21"
```

```
names(which(n * pi < 0.05))
```

```
[1] "12" "21"
```

```
fm <- lm(prestige ~ education + income, Duncan)
ri <- rstandard(fm)
ti <- rstudent(fm)
pi <- 2 * pt(-abs(ti), df = fm$df.residual - 1)
qqmath(ti, distribution = function(p) qt(p, df = fm$df.residual - 1), grid = TRUE, aspect = "iso")
```



```
n <- with(fm, rank + df.residual)
names(which(ti > 4))
```

```
character(0)
```

```
names(which(1 - (1-pi)^n < 0.05))
```

```
character(0)
```

```
names(which(n * pi < 0.05))
```

```
character(0)
```

```
head(sort(pi))
```

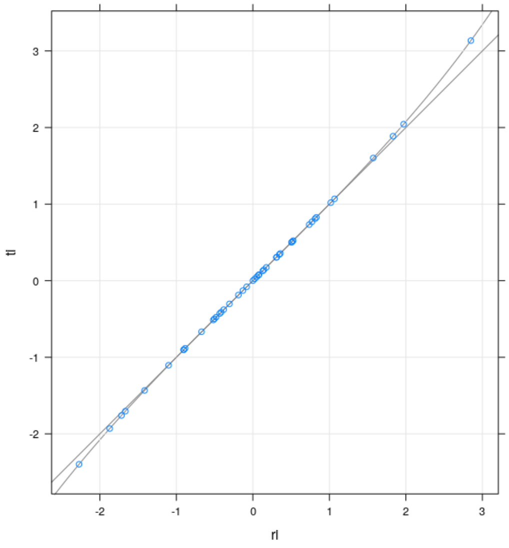
```
       minister        reporter      contractor insurance.agent       machinist     store.clerk 
    0.003177202     0.021170298     0.047432955     0.060427645     0.066248120     0.085783008 
```

A useful relationship

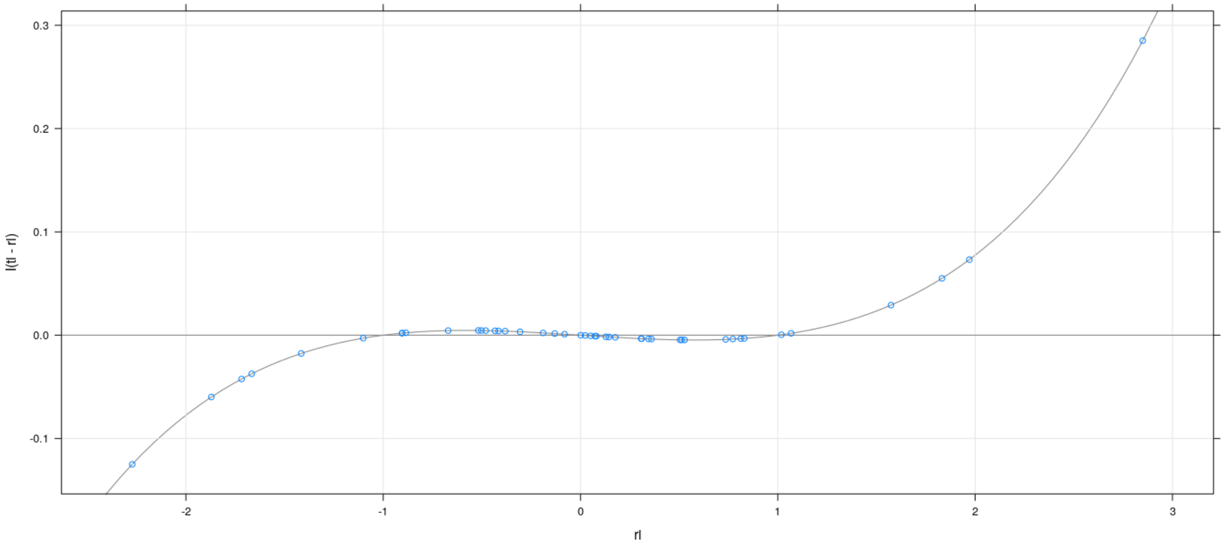
- As already noted, $e_{i(-i)} = e_i/(1 - h_i)$
- This means that to compute $e_{i(-i)}$, we do not actually need to re-fit model
- In particular, leave-one-out cross-validation SSE can be calculated without actually re-fitting models
- There is a similar exact relationship between r_i and t_i

$$t_i = r_i \sqrt{\frac{n-p-1}{n-p-r_i^2}}$$

```
p <- fm$rank
tfun <- function(r) r * sqrt((n-p-1) / (n-p-r^2))
xyplot(ti ~ ri, grid = TRUE, aspect = "iso", abline = list(c(0, 1), col = "grey50")) +
    layer_(panel.curve(expr = tfun(x), col = "grey50"))
```



```
xyplot(I(ti - ri) ~ ri, grid = TRUE, abline = list(h = 0, col = "grey50")) +
    layer_(panel.curve(expr = tfun(x) - x, col = "grey50"))
```



Measures of influence

- We are typically more interested in *influential* observations
- Direct measure of the influence of objervation i on coefficient β_j is (for $i = 1, \ldots, n; j = 1, \ldots, p$)

$$DFBETA_{ij} = d_{ij} = \hat{\beta}_j - \hat{\beta}_{j(-i)}$$

- It is common to standardize this:

$$DFBETAS_{ij} = d^*_{ij} = \frac{d_{ij}}{SE_{(-i)}(\hat{\beta}_j)}$$

- Drawback: there can be many of them (np in total).
- When p is small, it is useful to plot $DFBETA_{ij}$ (or $DFBETAS_{ij}$) against i separately for each j.
- It is also common to look at a summary influence measure for each observation.

Cook's distance

- Think of testing the "hypothesis" that $\beta = \hat{\beta}_{(-i)}$
- Consider the "F-statistic" for this test, recalculated for each i (though not really meaningful)
- This is known as Cook's distance D_i. It can be shown that

$$D_i = \frac{{r_i}^2}{p} \times \frac{h_i}{1 - h_i}$$

- D_i can be viewed as a combination of discrepancy and leverage.
- Observations with high values of D_i are considered influential

DFFITS

- A similar measure is

$$DFFITS_i = t_i \times \sqrt{\frac{h_i}{1 - h_i}}$$

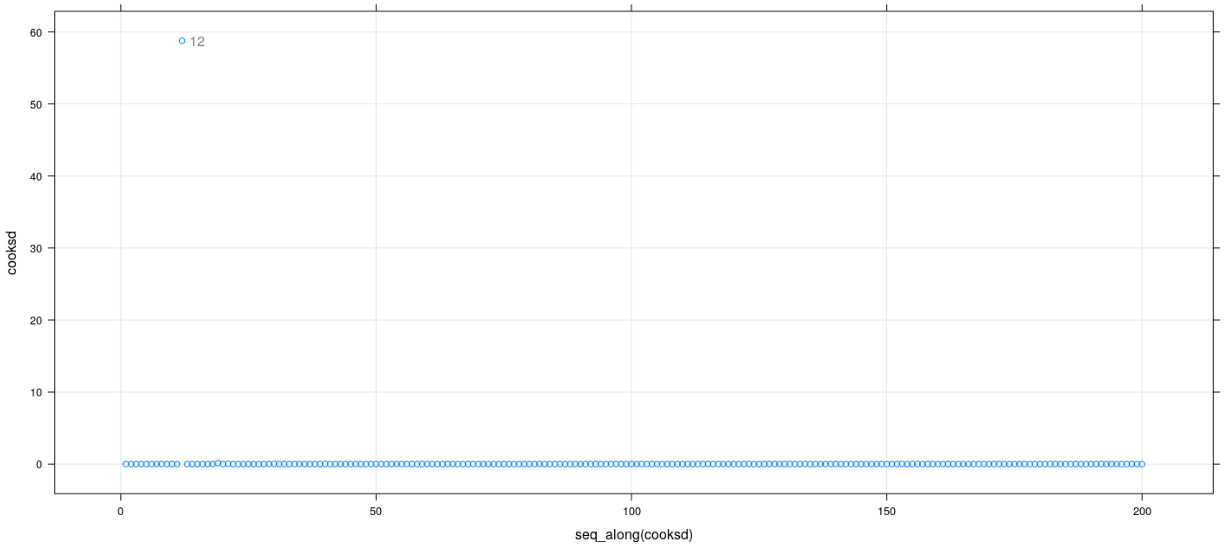
- In most cases (since $t_i \approx r_i$)

$$D_i \approx \frac{DFFITS_i^2}{p}$$

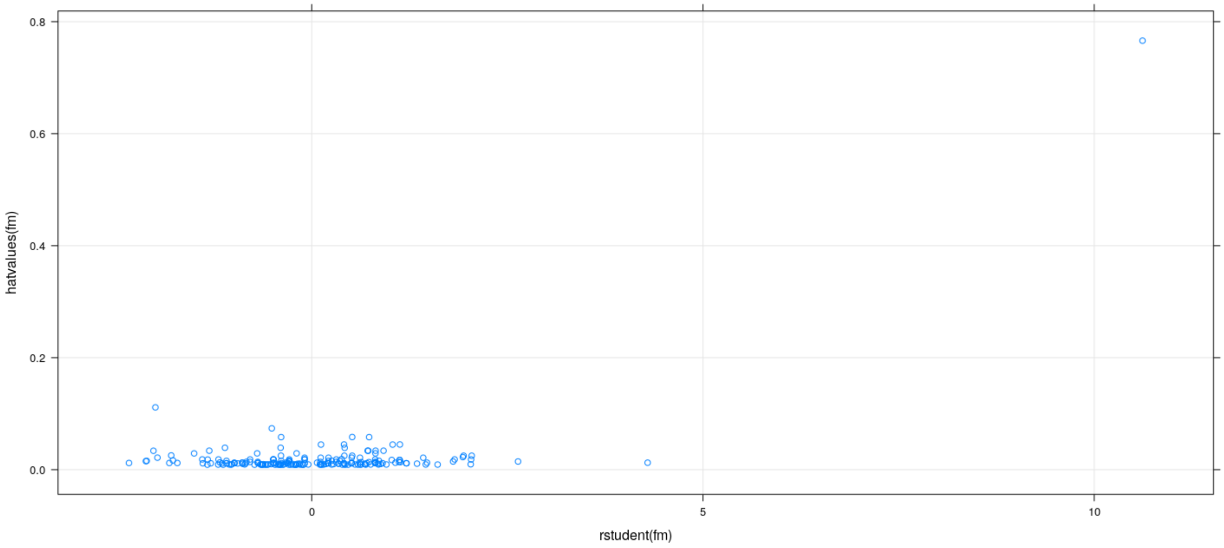
- A graphical alternative is to plot h_i vs t_i and look for unusual extreme values.

Measures of influence: examples

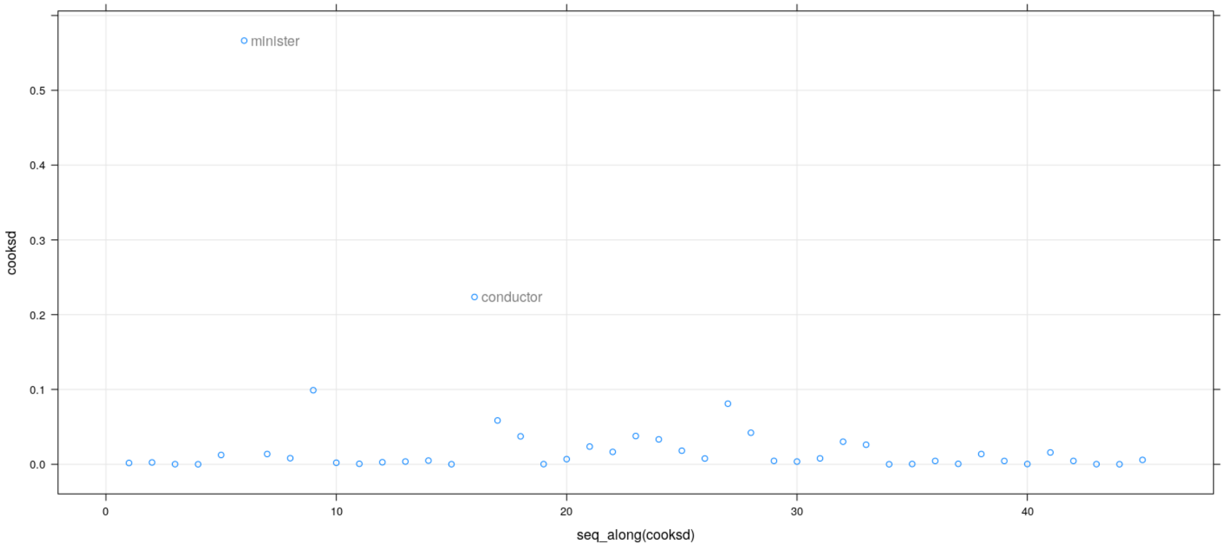
```
fm <- lm(weight ~ height * sex, Davis)
dfb <- dfbetas(fm); cooksd <- cooks.distance(fm)
id <- cooksd > 10
xyplot(cooksd ~ seq_along(cooksd), grid = TRUE) +
    layer(panel.text(x[id], y[id], labels = rownames(Davis)[id], pos = 4, col = "grey50"))
```



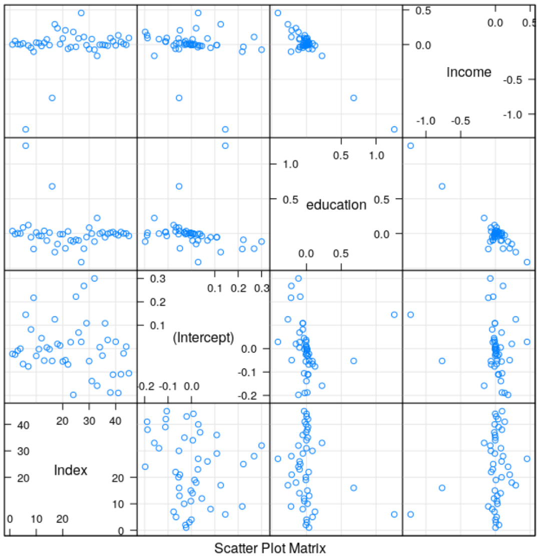
```
xyplot(hatvalues(fm) ~ rstudent(fm), grid = TRUE)
```



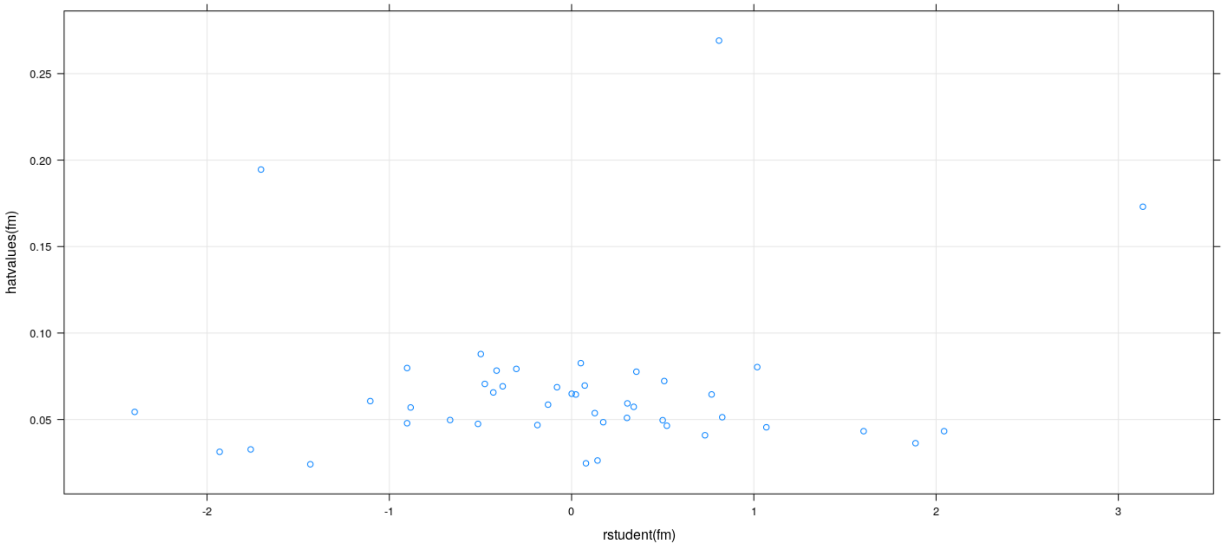
```
fm <- lm(prestige ~ education + income, Duncan, na.action = na.exclude)
dfb <- dfbetas(fm); cooksd <- cooks.distance(fm)
id <- cooksd > 0.1
xyplot(cooksd ~ seq_along(cooksd), grid = TRUE) +
    layer(panel.text(x[id], y[id], labels = rownames(Duncan)[id], pos = 4, col = "grey50"))
```



```
splom(cbind(Index = seq_along(cooksd), dfb), grid = TRUE)
```



```
xyplot(hatvalues(fm) ~ rstudent(fm), grid = TRUE)
```



Influence on standard errors

- Individual observations can also influence standard errors
- For example, standard error for estimated slope in simple linear regression $y = \alpha + \beta x + \varepsilon$

$$s.e.(\hat{\beta}) = \frac{\hat{\sigma}}{\sqrt{\sum_i (x_i - \bar{x})^2}}$$

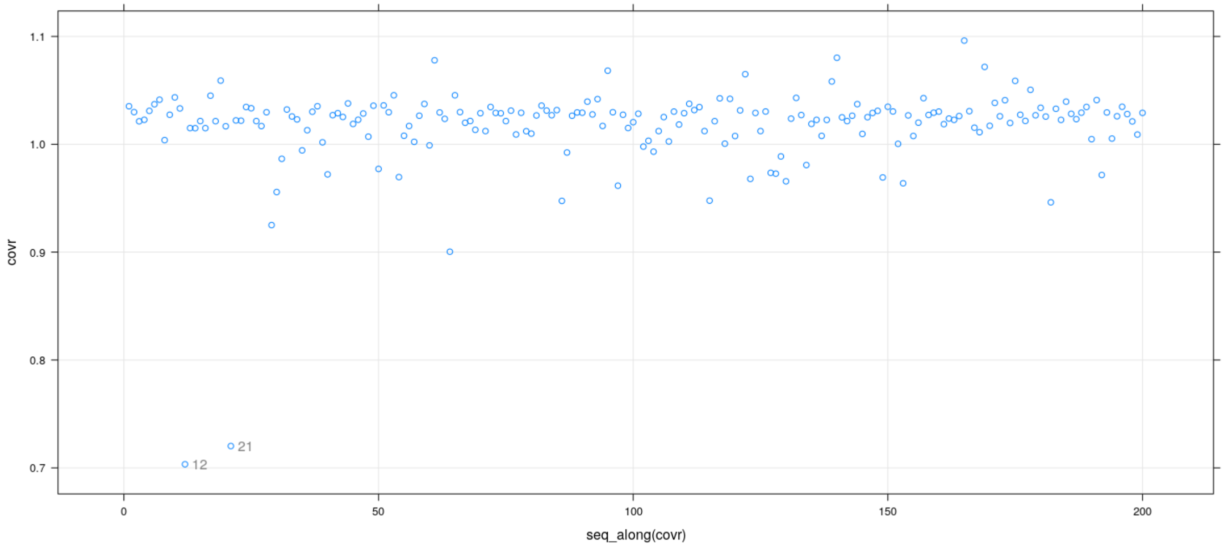
- High leverage + low discrepancy: may decrease standard error without influencing estimated coefficients
- Generally, we could measure influence by effect on size of joint confidence region of $\hat{\beta}$
- Measure proposed by Belsley et al (1980)

$$\begin{aligned} COVRATIO_i &= \frac{|\hat{\sigma}^2_{(-i)}(\mathbf{X}^T\mathbf{X})^{-1}_{(-i)}|}{|\hat{\sigma}^2(\mathbf{X}^T\mathbf{X})^{-1}|} \\ &= \frac{1}{(1-h_i)} \times \left(\frac{\hat{\sigma}^2_{(-i)}}{\hat{\sigma}^2}\right)^p = \frac{1}{(1-h_i)\left(\frac{n-p-1+t_i^2}{n-p}\right)^p} \end{aligned}$$

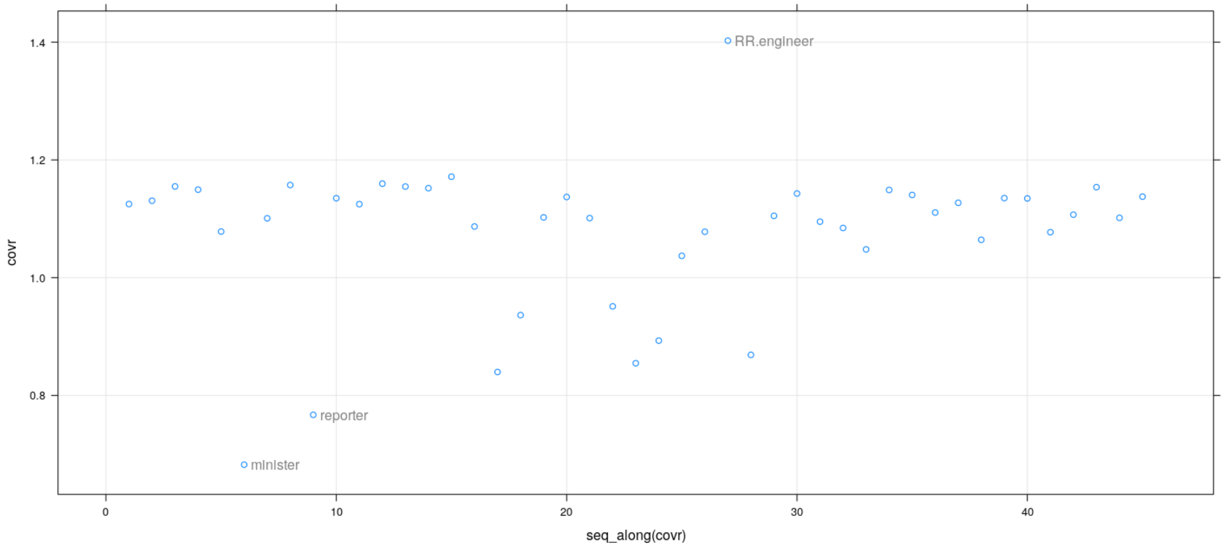
- Observations that increase precision have $COVRATIO_i > 1$
- Observations that decrease precision have $COVRATIO_i < 1$
- Look for values that differ from 1

Measures of influence: examples

```
fm <- lm(weight ~ height * sex, Davis)
covr <- covratio(fm)
id <- which(abs(covr-1) > 0.2)
xyplot(covr ~ seq_along(covr), grid = TRUE) +
    layer(panel.text(x[id], y[id], labels = rownames(Davis)[id], pos = 4, col = "grey50"))
```



```
fm <- lm(prestige ~ education + income, Duncan, na.action = na.exclude)
covr <- covratio(fm)
id <- which(abs(covr-1) > 0.2)
xyplot(covr ~ seq_along(covr), grid = TRUE) +
    layer(panel.text(x[id], y[id], labels = rownames(Duncan)[id], pos = 4, col = "grey50"))
```



Numerical cutoffs

- Blindly following numerical cutoffs is not recommended
- Most regression diagnostics are designed for graphical examination
- Still, numerical cutoffs can be a useful complement
- Particularly useful to indicate a "cutoff line" on a graph

- Hat values: $2 \times \frac{p}{n}$ or $3 \times \frac{p}{n}$ for small samples
- Studentized residuals: ± 2 (adjusted p-value for more formal test)
- $DFBETAS_{ij}$
  - As these are standardized, an absolute cutoff of 1 or 2 is reasonable
  - For large n, a size adjusted cutoff $2/\sqrt{n}$ is suggested by Belsley et al
- Cook's distance D: analogy with F-test gives a natural cutoff (Chatterjee and Hadi, 1988)

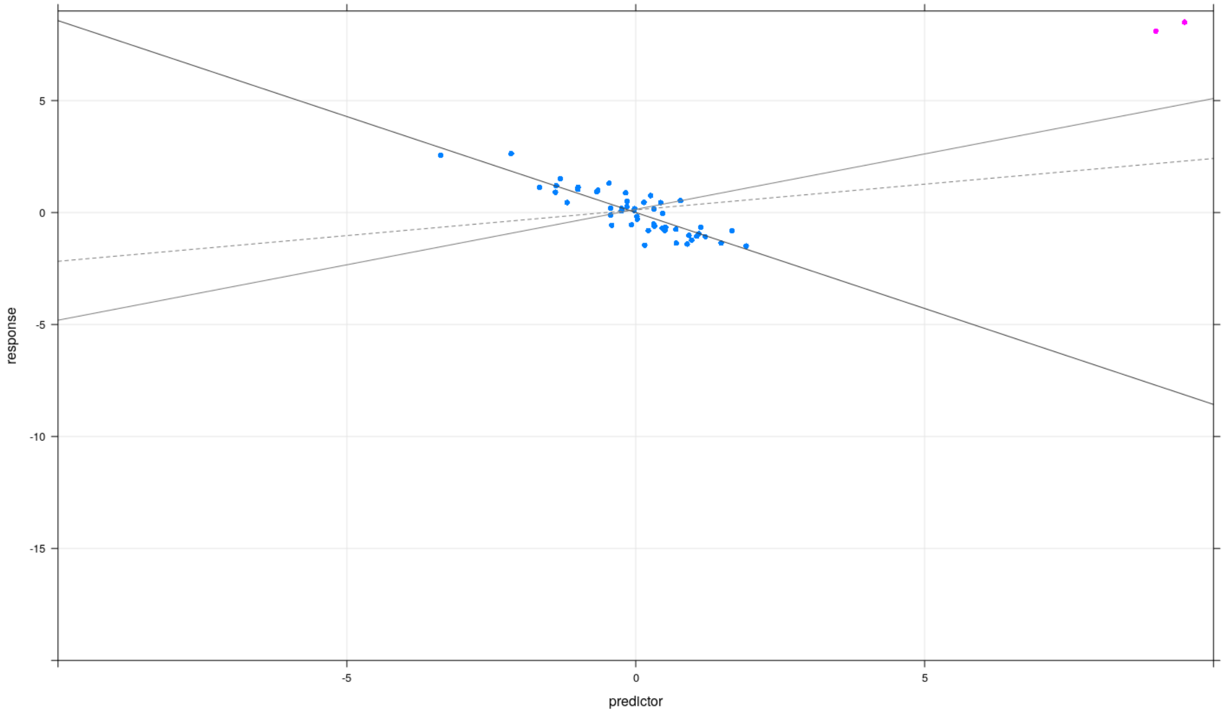
$$D_i > \frac{4}{n-p}$$

- Translates to cutoff for $DFFITS$ using approximate relation with D_i

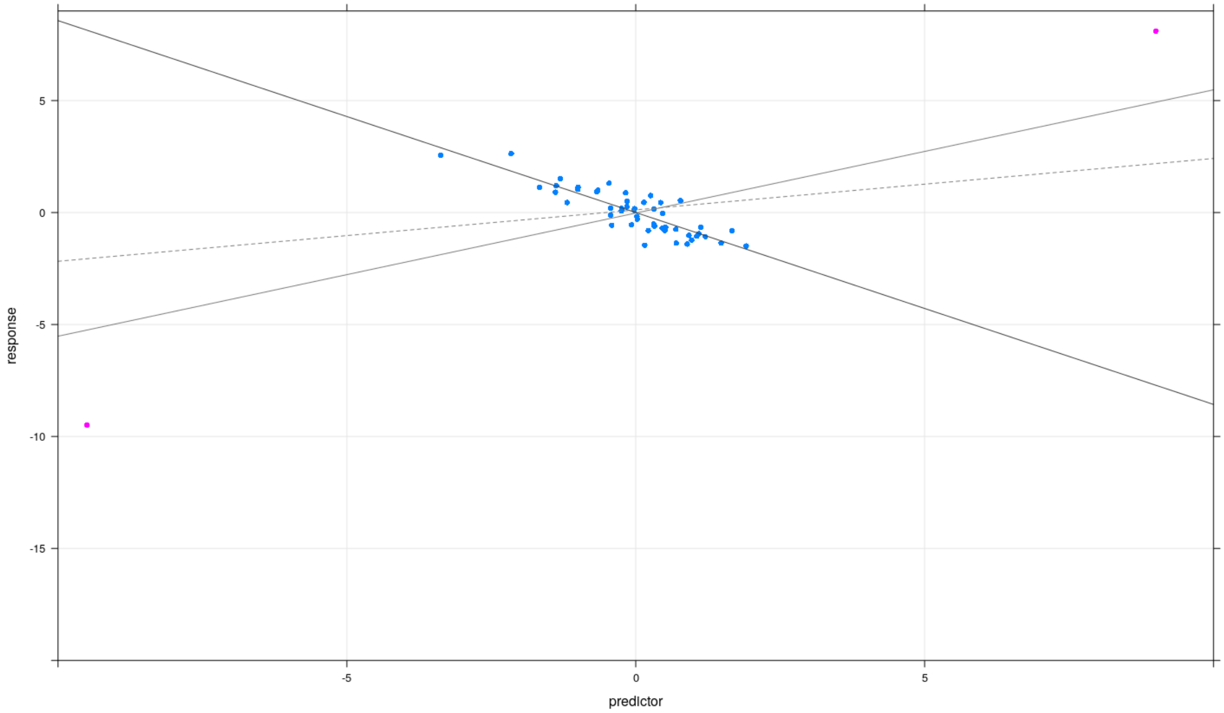
$$DFFITS_i > 2\sqrt{\frac{p}{n-p}}$$

Jointly influential observations

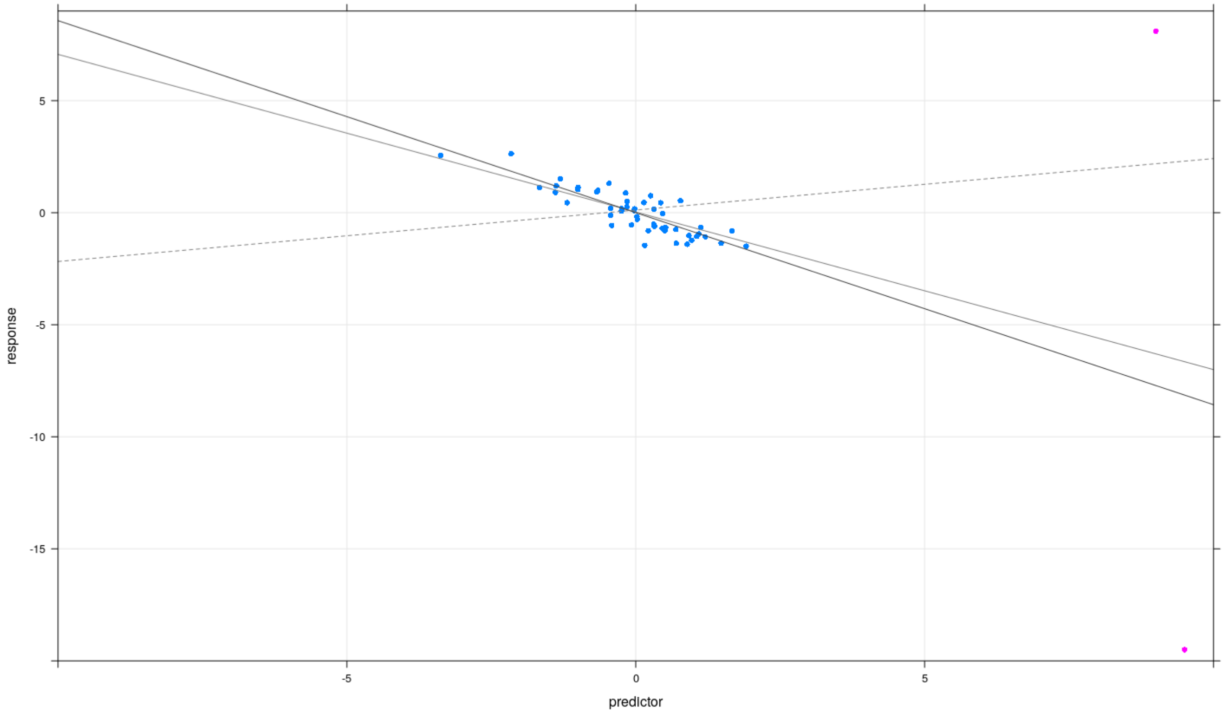
- Subsets of observations can be jointly influential, or can offset each other



- Subsets of observations can be jointly influential, or can offset each other



- Subsets of observations can be jointly influential, or can offset each other



Jointly influential observations: possible strategies

- Find most influential observation
- If considered unusual, remove, re-fit model, and consider next most influential observation
- Can often work, but is not always successful
- Alternatively, extend Cook's distance to subsets of observations
- Number of possible subsets can become large

Graphical alternative: partial regression / added variable plots

- Insight: Jointly influential observations easy to detect visually for single covariate
- Can we reduce multiple regression to simple regression?
- Partial regression plots can do this, provided we focus on influence on one coefficient at a time

Partial regression

Question: What is the interpretation of β_j in the Mutiple regression model

$$\mathbf{y} = \beta_0 \mathbf{1} + \beta_1 \mathbf{x}^{(1)} + \cdots + \beta_j \mathbf{x}^{(j)} + \cdots + \beta_p \mathbf{x}^{(p)}$$

(where $\mathbf{x}^{(j)}$ represents j-th column of $\mathbf{X}$)

- β_j is effect of j-th covariate $x^{(j)}$ on response y
- t-test for $\beta_j = 0$ tests significance of β_j *in the presence of* other covariates
- Significance determined by amount of reduction in total sum of squares

Partial regression: example

```
Davis$dsex <- ifelse(Davis$sex == "M", 1, 0)
fm.full <- lm(weight ~ 1 + height + dsex, Davis)
fm.partial <- lm(weight ~ 1 + height, Davis)
sum(residuals(fm.full)^2)
```

```
[1] 27493.32
```

```
coef(fm.full)
```

```
(Intercept)      height        dsex 
109.1141967  -0.3129827  22.4980107 
```

```
coef(fm.partial)
```

```
(Intercept)      height 
 25.2662278   0.2384059 
```

Can we recover the additional effect of β_j from the partial model?

```
e.partial <- residuals(fm.partial)
fm.marginal <- lm(e.partial ~ dsex, Davis)
sum(residuals(fm.marginal)^2)
```

```
[1] 33166.05
```

```
coef(fm.marginal)
```

```
(Intercept)        dsex 
  -6.436995   14.629534 
```

Can we recover the additional effect of β_j from the partial model?

```
e.partial <- residuals(fm.partial)
fm.marginal <- lm(e.partial ~ 0 + residuals(lm(dsex ~ 1 + height)), Davis)
sum(residuals(fm.marginal)^2)
```

```
[1] 27493.32
```

```
coef(fm.marginal)
```

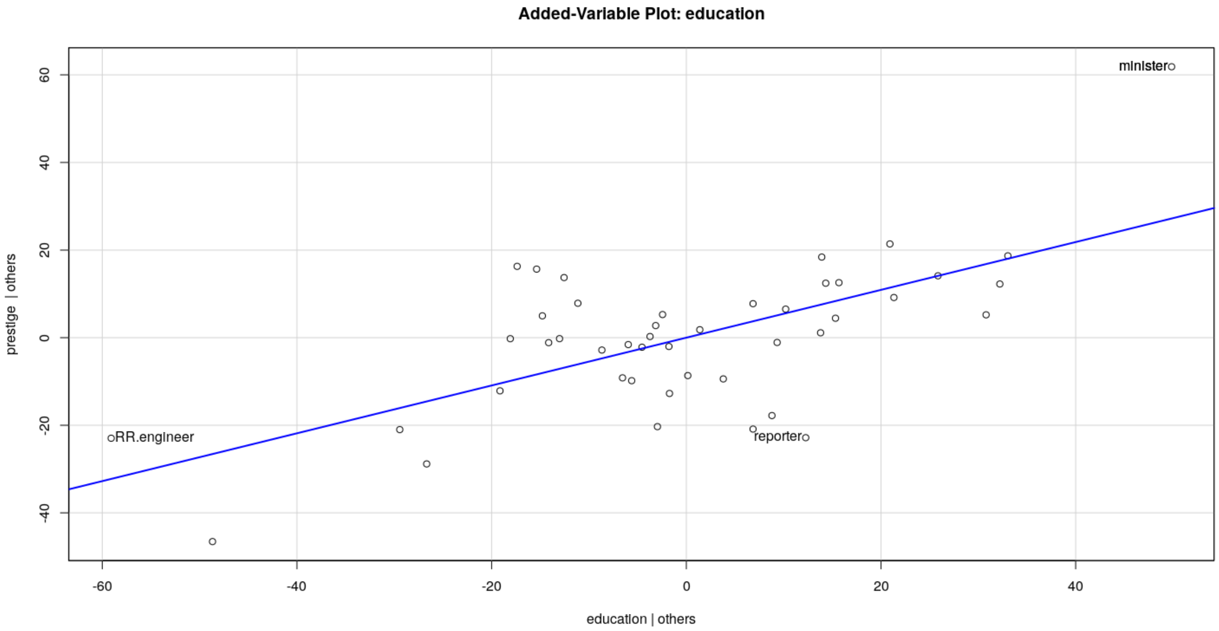
```
residuals(lm(dsex ~ 1 + height)) 
                        22.49801 
```

Partial regression / added variable plot for β_j

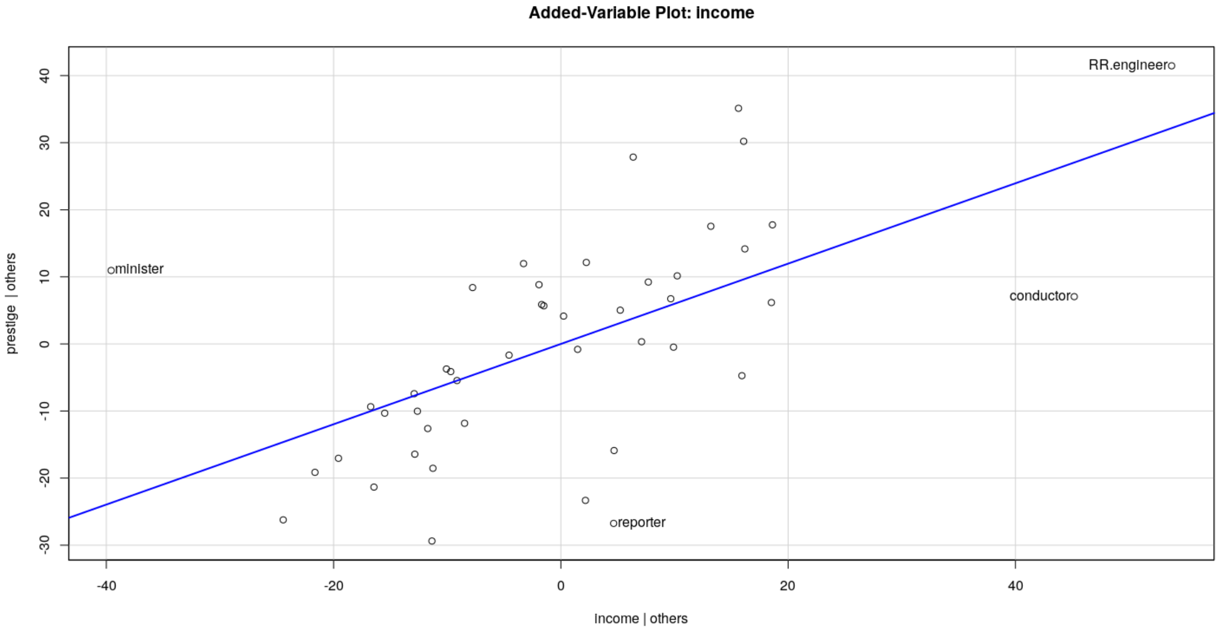
- Denote $\mathbf{X}$ excluding its j-th column by $\mathbf{X}^{(-j)}$
- Regress $\mathbf{y}$ on $\mathbf{X}^{(-j)}$, denote residual vector by $\mathbf{y}^{(j)}$
- Regress j-th column of $\mathbf{X}$ on $\mathbf{X}^{(-j)}$, denote residual vector by $\mathbf{X}^{(j)}$
- In other words
  - $\mathbf{y}^{(j)} = (\mathbf{I} - \mathbf{H}_{\mathbf{X}^{(-j)}})\mathbf{y}$
  - $\mathbf{X}^{(j)} = (\mathbf{I} - \mathbf{H}_{\mathbf{X}^{(-j)}})\mathbf{X}_{*j}$
- Plot $\mathbf{y}^{(j)}$ against $\mathbf{X}^{(j)}$
- This is useful because the coefficient of this regression is the same as $\hat{\beta}_j$

Example: Duncan data

```
library(car)
fm <- lm(prestige ~ education + income, Duncan)
avPlot(fm, "education")
```

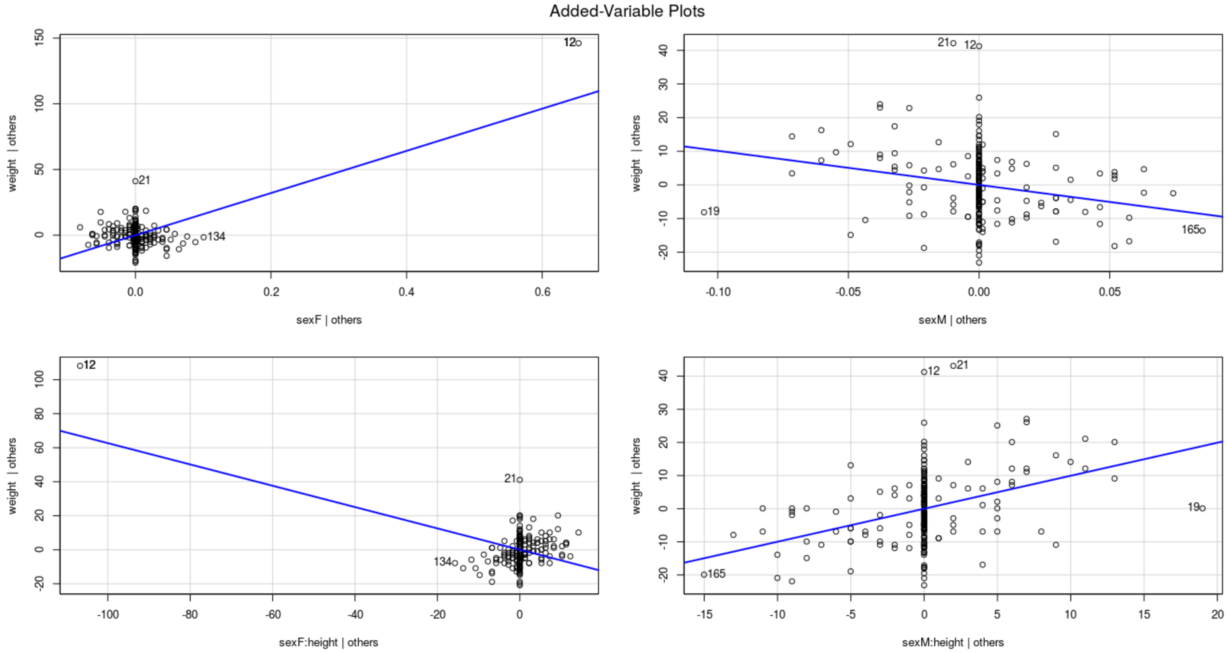


```
library(car)
fm <- lm(prestige ~ education + income, Duncan)
avPlot(fm, "income")
```



Example: Davis data

```
fm <- lm(weight ~ 0 + sex + height:sex, Davis)
avPlots(fm)
```



What should we do with unusual data?

- Easy solution: discard
- This is sometimes the right thing to do, but should not be done automatically
- Unusual data may provide insight (e.g., Duncan's prestige data)
- It may indicate data recording errors (e.g., Davis data has values switched)

```
   sex weight height repwt repht
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
```

- Finally, can try alternatives to least squares: robust regression