Diagnostics

Subrata Paul
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What we need to check?

- Nonlinearity of regression function
- Nonconstancy of error variance
- Nonindependence of error terms
- Nonnromality of error terms
- Presence of outliers and influencial observations

Residual Plots

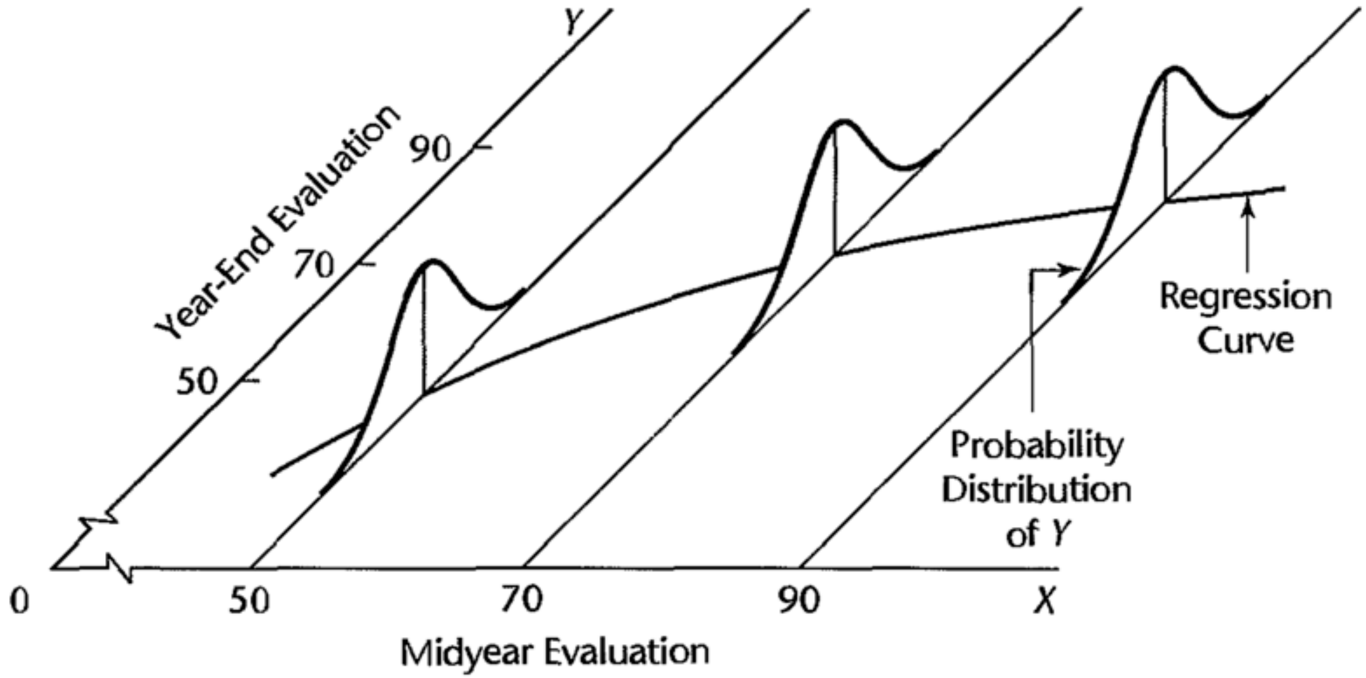
Importance

- Diagnostic plots of the response variable are not very useful
- Residual plots usually (indirectly) carries out diagnostics of the response variable
- Residuals gives us information about model structure and the nature of unobserved randomness.

Different plots of residuals

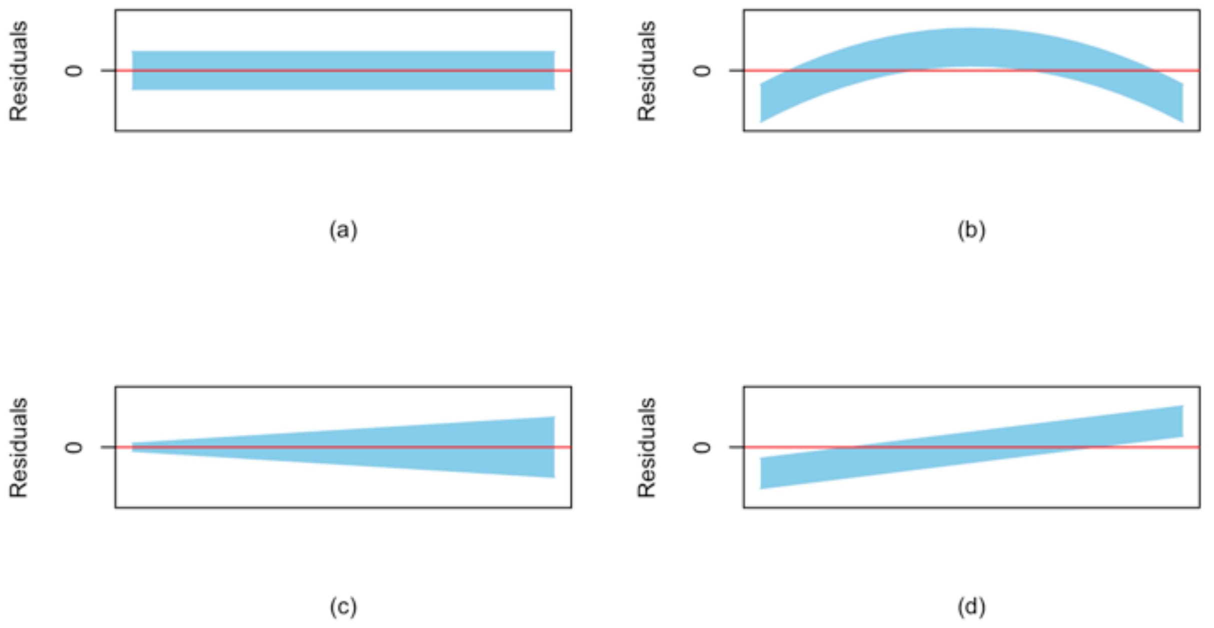
- Plots of residuals against predictor variables
- Plot of residuals against fitted values
- Plot of absolute or squared residuals against fitted values or predictor variables
- Plot of residuals against time or other sequence
- Plots of residuals against omited predictor variables
- Box plot and density plot of residuals
- Q-Q plot of residuals

Reminder

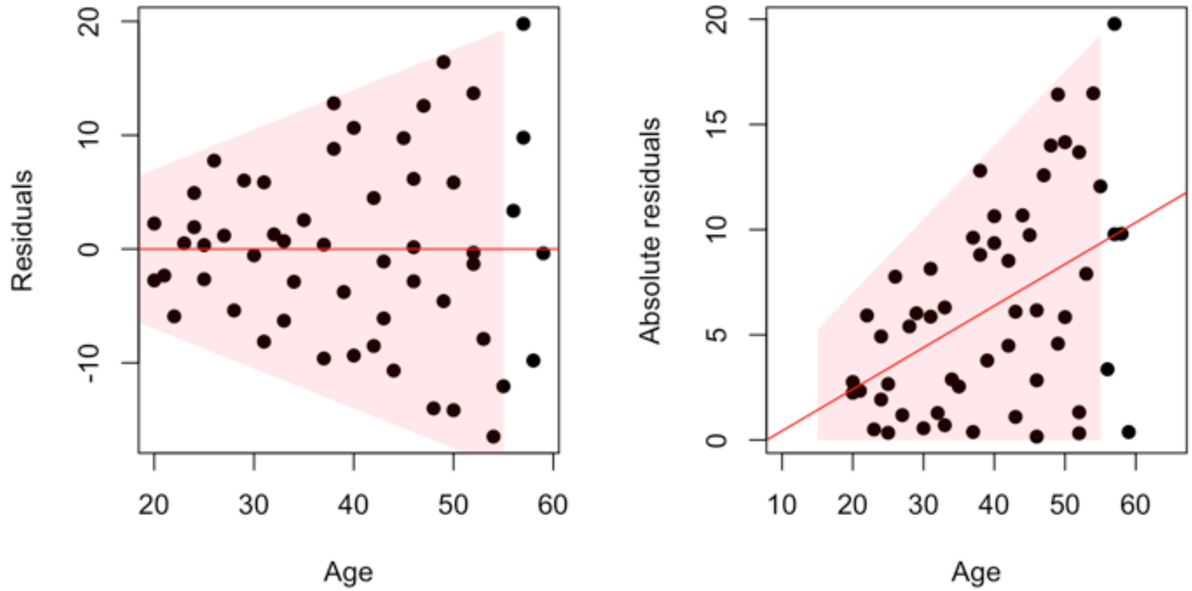


Y
Year-End Evaluation
90
70
50
0
50
70
90
X
Midyear Evaluation
Regression Curve
Probability Distribution of Y

Simulated scenarios



Example (Non-constant error variance)



Test for non-constatnt variance

- If the data is separable in some way then a F test works
- Brown_Forsythe test (a t-test)
- Breusch-Pegan test (also known as Cook-Weisberg score test)
  - It is a chi-squared test

Residual Plots

- It can be used to check
  - Nonlinear structure
  - Non-constant error variance
  - Non-zero error mean
- Though it is not used directly to detect unusual observations but gives us an overview of the observations.
- Though it indicates potential structural problem it does not clearly suggest transformation because it fails to distinguish between monotonic and non-monotonic transformation.
- Does not show the nature of the marginal effect of a predictor variable, given the other predictor variables in the model.

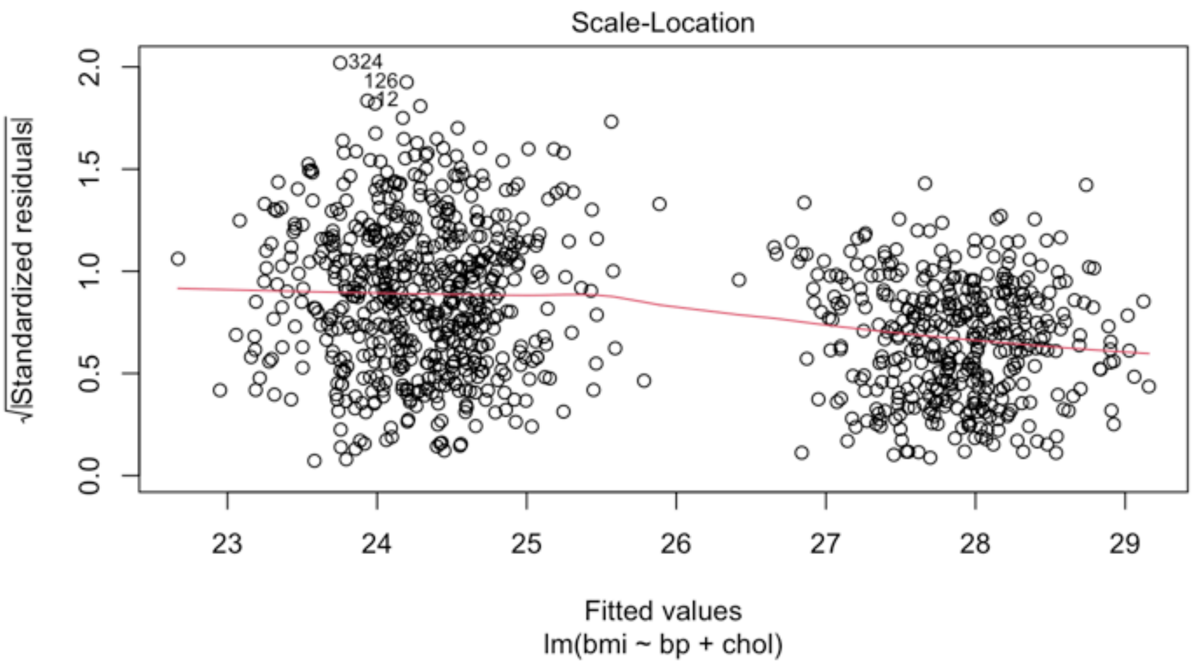
Interesting Extreme Example

```r
library(faraway)
set.seed(123)
male = 600
female = 400

bp = c(rnorm(male, 85, 2), rnorm(female, 75, 1))
bmi = c(rnorm(male, 24, 4), rnorm(female, 28, 2))
chol = c(rnorm(male, 200, 10), rnorm(female, 150, 15))
gender = c(rep(1, male), rep(0, female))
dat = data.frame(bp = bp, bmi= bmi ,chol = chol, gender = gender)
lmod = lm(bmi ~ bp + chol, data = dat)
sumary(lmod)
```

```
##               Estimate Std. Error t value  Pr(>|t|)
## (Intercept) 48.4499279  2.1428433 22.6101 < 2.2e-16
## bp          -0.2169564  0.0388197 -5.5888  2.95e-08
## chol        -0.0286526  0.0074002 -3.8719  0.000115
##
## n = 1000, p = 3, Residual SE = 3.38723, R-Squared = 0.23
```

Interesting Extreme Example (Residual Plot)



What does the residual plot suggests?

```
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept) 9.7006468  7.8100284  1.2421  0.21470
## bp          0.1604810  0.0823442  1.9489  0.05177
## chol        0.0038192  0.0168418  0.2268  0.82068
##
## n = 600, p = 3, Residual SE = 3.89664, R-Squared = 0.01
```

```
##               Estimate Std. Error t value Pr(>|t|)
## (Intercept) 12.0170106  7.8054019  1.5396  0.12446
## bp           0.2005841  0.1027723  1.9517  0.05167
## chol         0.0071092  0.0068681  1.0351  0.30125
##
## n = 400, p = 3, Residual SE = 2.11171, R-Squared = 0.01
```

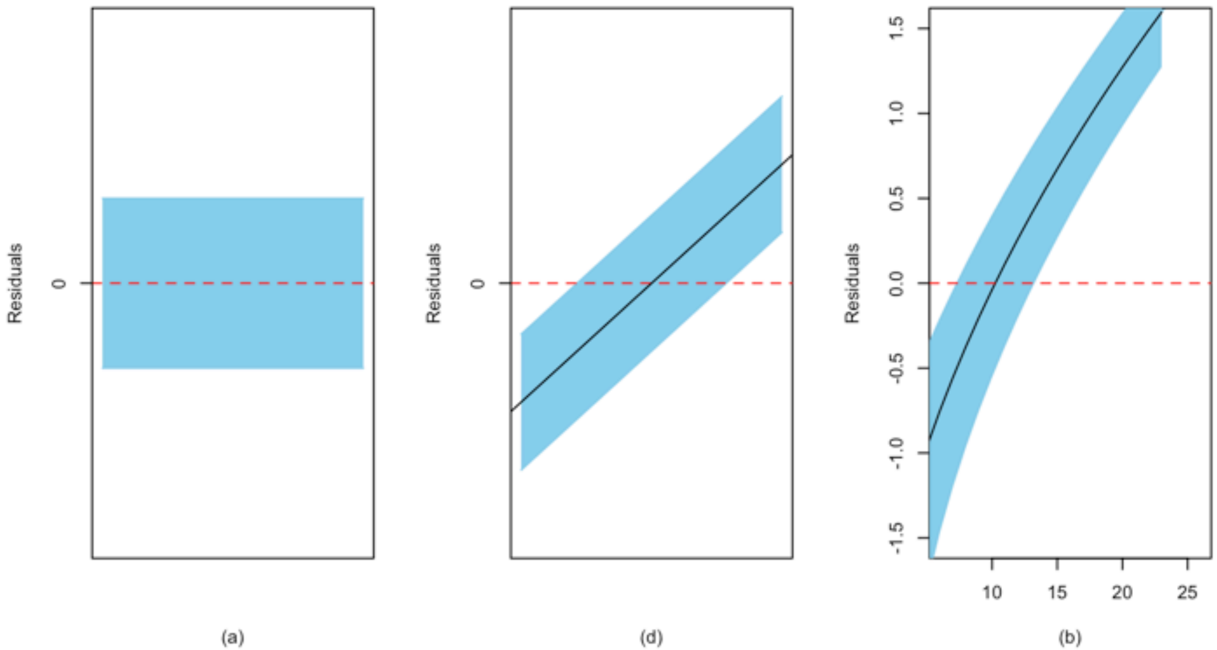
Test for non-constatnt variance

- If the data is separable in some way then a F test works
- Brown_Forsythe test (a t-test)
- Breusch-Pegan test (also known as Cook-Weisberg score test)
    - It is a chi-squared test

Added variable plot

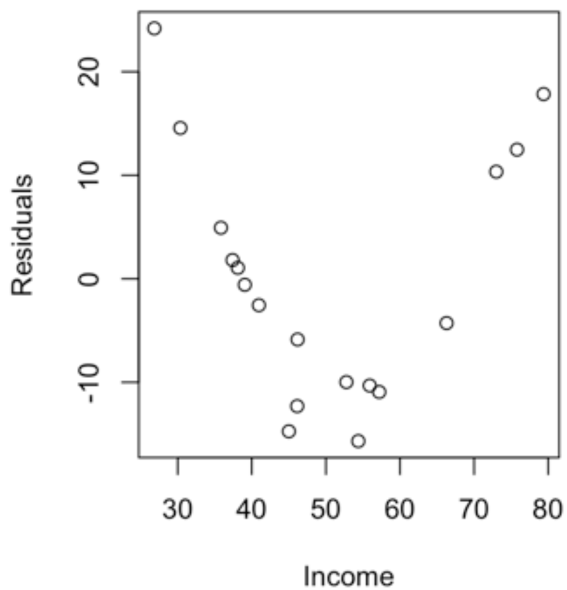
- Gives marginal relationship given the other predictors are in the model
- Can be used to investigate if a new variable is worthy to include in the model
- Provide clearer picture compared to residual vs predictor plot

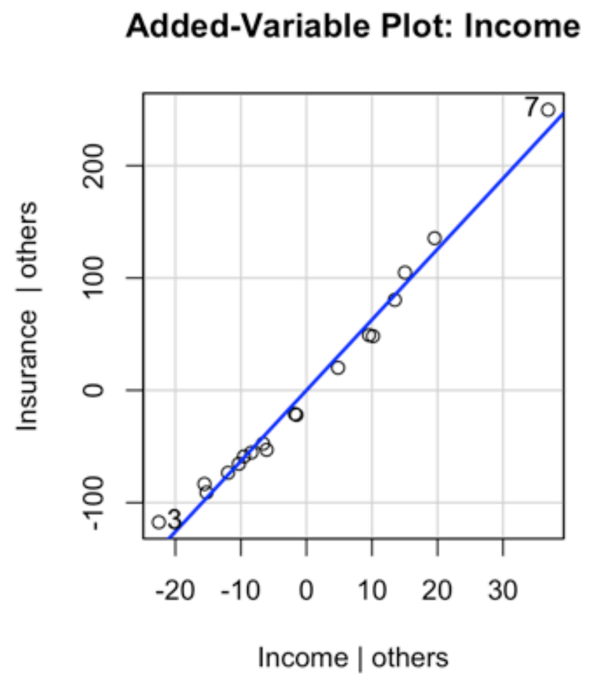
Simulated Scenarios



1. No additional information from the predictor
2. Helpful addition of the predictor
3. Inclusion of the predictor with some transformation.

AV plot example





Component plus residual (CR) plot

The **component plus residual (cr) plot** (a.k.a, **partial residual plot**) is a competitor to the added variable plot.

The **cr plot** shows $\hat{\beta}_i x_i + \hat{\epsilon}$ versus x_i.

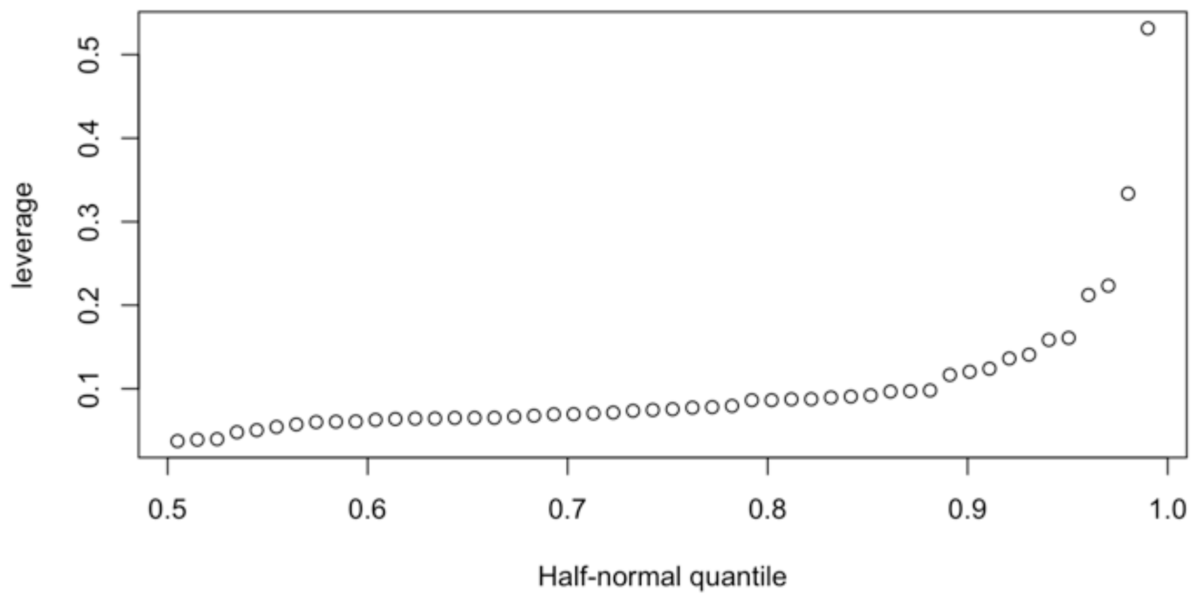
- **cr** plots are useful for checking nonlinear relationships in the variable being considered for inclusion in the model.
- They can also suggest potential transformation of the data so that the relationship is linear.
- If the scatter plot does not appear to be linear, then there is a nonlinear relationship between the regressor and the response (after accounting for the other regressors).
- The slope of the line fit to the cr plot is $\hat{\beta}_i$.

Unusual observations

Leverage

- A **leverage** point is an observation that is unusual in the predictor space.
- h_{ii} is called the leverage value of the i th observation.
- h_{ii} is a measure of distance between the X values for the ith observation from the mean of the X values of all n observations.
- h_{ii} measures the role of the X values in determining how important y_i is in affecting $\hat{y}_i$
- A half-normal plot of the leverage values can be used to identify observations with unusually high leverage.
- A leverage value h_i is usually considered large if it is more than twice as large as the mean leverage value.

Example



Outlier

An outlier is a point that does not fit the current model.

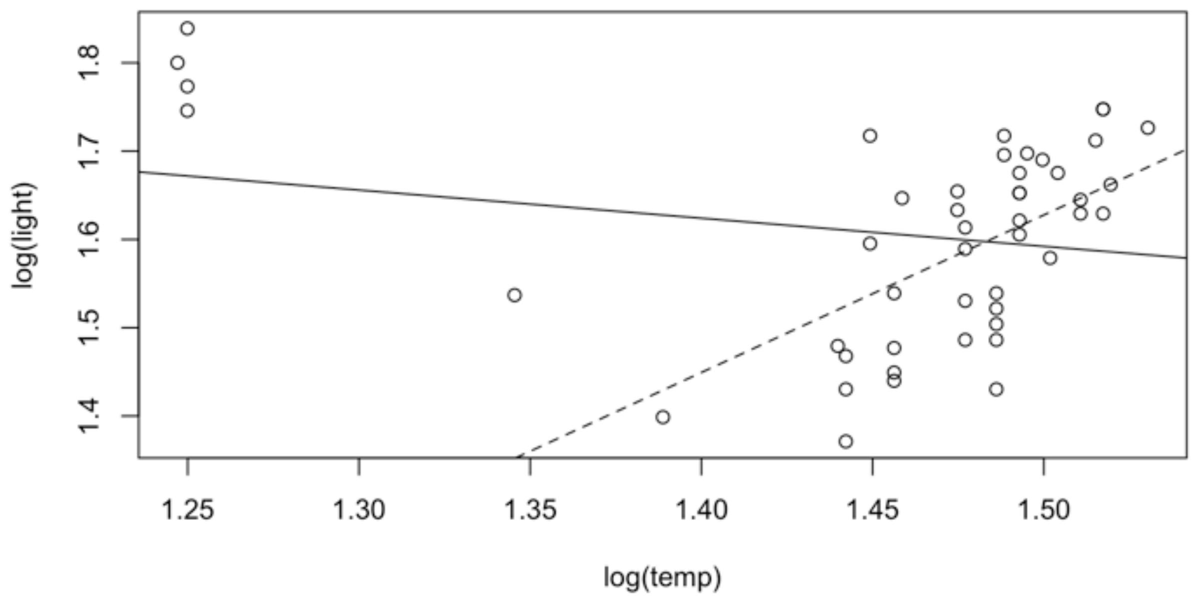
- An outlier is context specific! An outlier for one model may not be an outlier for a different model.

externally **studentized** residual

$$t_i = \frac{y_i - \hat{y}_{(i)}}{\hat{\sigma}_{(i)}\sqrt{1 + x_i^T \left(X_{(i)}^T X_{(i)}\right)^{-1} x_i}} \sim T_{n-p-1}.$$

- Bonferroni correction is needed

Example



Influential observations

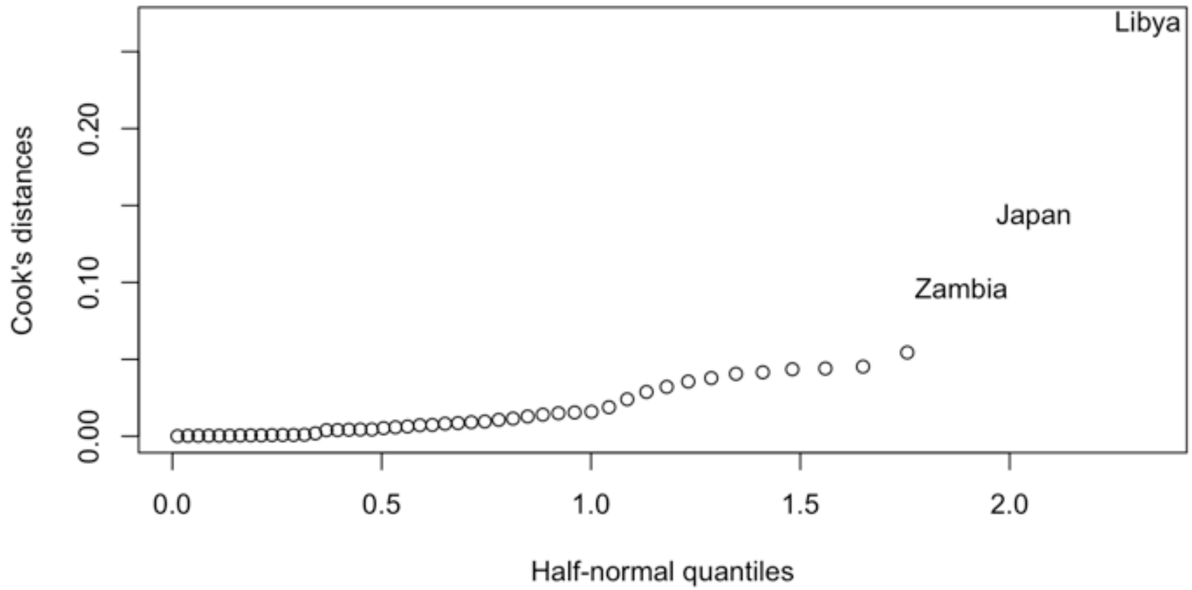
- An influential observation is one whose removal from the dataset would cause a large change in the fitted model.
- An influential observation is usually a leverage point, an outlier, or both.

The Cook's distance is a popular inferential tool because it reduces influence information to a single value for each observation.

The Cook's distance for the ith observation is

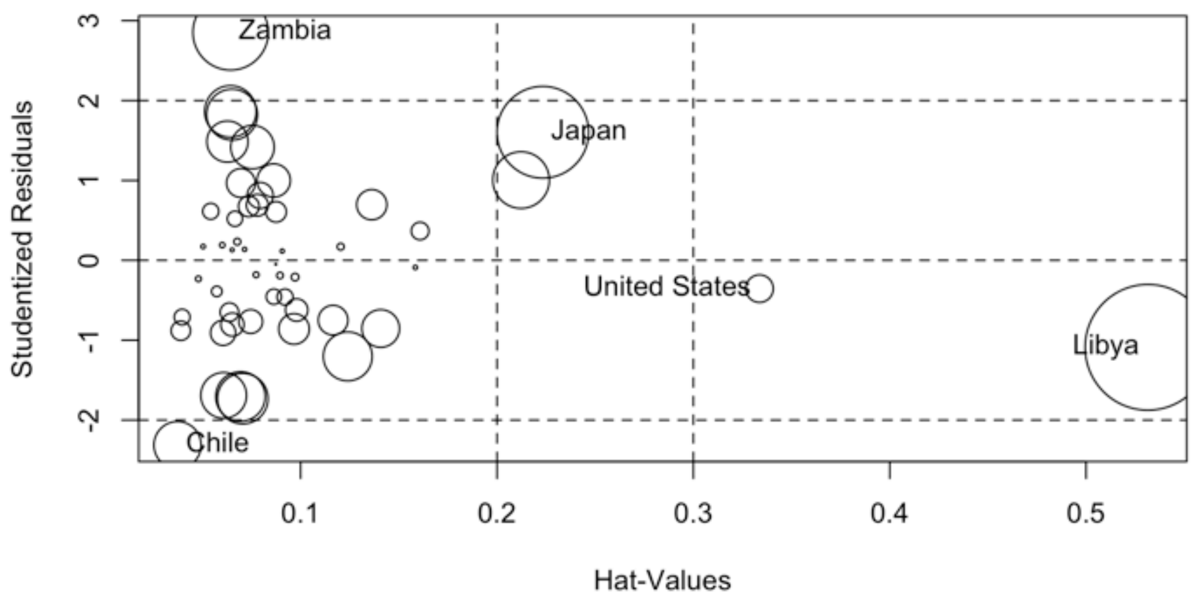
$$D_i = \frac{(\hat{y} - \hat{y}_{(i)})^T (\hat{y} - \hat{y}_{(i)})}{p\hat{\sigma}^2} = \frac{1}{p} r_i^2 \frac{h_i}{1 - h_i}$$

Example



Libya
Japan
Zambia
Cook's distances
0.00
0.10
0.20
0.0
0.5
1.0
1.5
2.0
Half-normal quantiles

Influence plot




```
##                  StudRes        Hat      CookD
## Chile         -2.3134295 0.03729796 0.03781324
## Japan          1.6032158 0.22330989 0.14281625
## United States -0.3546151 0.33368800 0.01284481
## Zambia         2.8535583 0.06433163 0.09663275
```

Correct or Delete the Observation(s)

- If they're data entry errors, correct the problem. If they can't be fixed, remove them (they're wrong, so they don't tell us anything useful).
- Remove them if they're not part of the population of interest (you are studying dogs, but this observation is a cat).
- Remove them because they break the model.
- This is a bad idea.
- Make sure to indicate that you removed them from the data set and explain why.
- *THIS IS A BAD IDEA.*

Fit a Different Model

- An outlier/influential point for one model may not be for another.
- Examine the physical context—why did it happen?
- An outlier/influential point may be interesting in itself.
    - An outlier in a statistical analysis of credit card transactions may indicate fraud!
- This may suggest a better model.
- Use robust regression, which is not as affected by outliers/influential observations.
- Never automatically remove outliers/influential points!
- They provide important information that may otherwise be missed.
- Fit the model with and without the influential observation(s).
- Do your results substantively change?

Checking Error

Summary of methods for checking error assumptions

- Mean-zero error assumption:
  - Plot of residuals versus fitted values
- Constant error variance assumption:
  - Plot of residuals versus fitted values
  - Plot of $\sqrt{(|\hat{\epsilon}|)}$ versus fitted values.
- Normal error assumption:
  - q-q of residuals
  - Shapiro-wilk test
- Autocorrelated errors:
  - Plot of residuals versus time
  - Plot of successive pairs of residuals
  - Durbin-Watson test

Weighted Least Squares

Model

The generalized multiple regression model:

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

where,

- $\beta_0, \beta_1, \ldots, \beta_{p-1}$ are parameters
- $X_{i1}, \ldots X_{i,p-1}$ are known constants
- ϵ_i are independent $N(0, \sigma_i^2)$

Variance-covariance matrix

$$Var(\epsilon) = \begin{bmatrix} \sigma_1^2 & 0 & \dots & 0 \\ 0 & \sigma_2^2 & \dots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \dots & \sigma_n^2 \end{bmatrix}$$

- OLS assumes equal variance: $\sigma_1^2 = \cdots = \sigma_n^2 = \sigma^2$
- Using OLS we would get unbiased estimation of the parameters
- The OLS estimates no longer have minimum variance
- We must account for unequal variance in the estimation process
- Consider three cases:
  - Error variances are known (unrealistic)
  - Error variances are known up to proportionality constant
  - Error variances are known (realistic)

Error variances are known

Likelihood

$$L(\beta) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma_i^2}} \exp\left[-\frac{1}{2\sigma_i^2}(Y_i - \beta_0 - \beta_1 X_{i1} - \cdots - \beta_{p-1} X_{i,p-1})^2\right]$$

Define

$$w_i = \frac{1}{\sigma_i^2}$$

$$L(\beta) = \left[\prod_{i=1}^{n} \frac{\sqrt{w_i}}{\sqrt{2\pi}}\right] \exp\left[-\frac{1}{2}\sum_{i=1}^{n} w_i(Y_i - \beta_0 - \beta_1 X_{i1} - \cdots - \beta_{p-1} X_{i,p-1})^2\right]$$

Minimize

In matrix notation

$$W = \begin{bmatrix} w_1 & 0 & \dots & 0 \\ 0 & w_2 & \dots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \dots & w_n \end{bmatrix}$$

Normal Equation

$$(X^T WX)\hat{\beta}_w = X^T WY$$

Estimators

$$\hat{\beta}_w = (X^T WX)^{-1} X^T WY$$

Variance of the estimators

$$Var(\hat{\beta}_w = (X^T WX)^{-1}$$

Properties of the estimators

- Unbiased
- Consistent
- Minimum variance among unbiased linear estimators
- When weights are known Var($\hat{\beta}_w$) is generally less than Var($\hat{\beta}$)

Error variances unknown

- We need to estimate the error variances.
- Residuals from an OLS gives valuable information about the error variances
- Two methods:
    - Estimation of variance function
    - Use of replicates or near replicates

Estimation of variance

- Squared residual $\hat{\epsilon}^2$ is an estimator of σ_i^2
- Absolute residual $|\hat{\epsilon}|$ is an estimator for σ_i
- Idea
  - We can estimate the variance function describing the relation of σ_i^2 to relevant predictor variables by first fitting the regression model using unweighted least squares and then regressing $\hat{\epsilon}^2$ or $|\hat{\epsilon}|$ against the appropriate predictor variables.
- $|\hat{\epsilon}|$ is preferred if outliers exist.

General guidelines

1. A residual plot against X_l exhibits a megaphone shape. $\Rightarrow$ Regress the absolute residuals against X_l

2. A residual plot against $\hat{Y}$ exhibits a megaphone shape. $\Rightarrow$ Regress the absolute residuals against $\hat{Y}$

3. A plot of the squared residuals against X_l exhibits an upward tendency. $\Rightarrow$ Regress the squared residuals against X_l

4. A plot of the squared residuals against X_l suggests that the variance increases rapidly with increases in X_l up to a point and then increases more slowly. $\Rightarrow$ Regress the absolute residuals against X_l and X_l^2.

What next?

After the variance function or the standard deviation function is estimated, the fitted values from this function are used to obtain the estimated weights:

$$w_i = \frac{1}{\hat{s}_i^2} \qquad \text{where } \hat{s}_i \text{ is fitted value from standard deviation function}$$

$$w_i = \frac{1}{\hat{v}_i} \qquad \text{where } \hat{v}_i \text{ is fitted value from variance function}$$

The parameters are then estiamted as

$$\hat{\beta}_w = (X^T W X)^{-1} X^T W Y$$

Use of Replicates or Near Replicates

- In designed experiments σ_i^2 is estimated suing replicate observations at each combination of levels of the predictor variables.

- In observation studies, near replicates many be used.

- For example, if the residual plot against X_l shows a megaphone appearance, cases with X_1 values can be grouped together and the variance of the residuals in each group calculated.

    - The reciprocal of these variances are the weights.

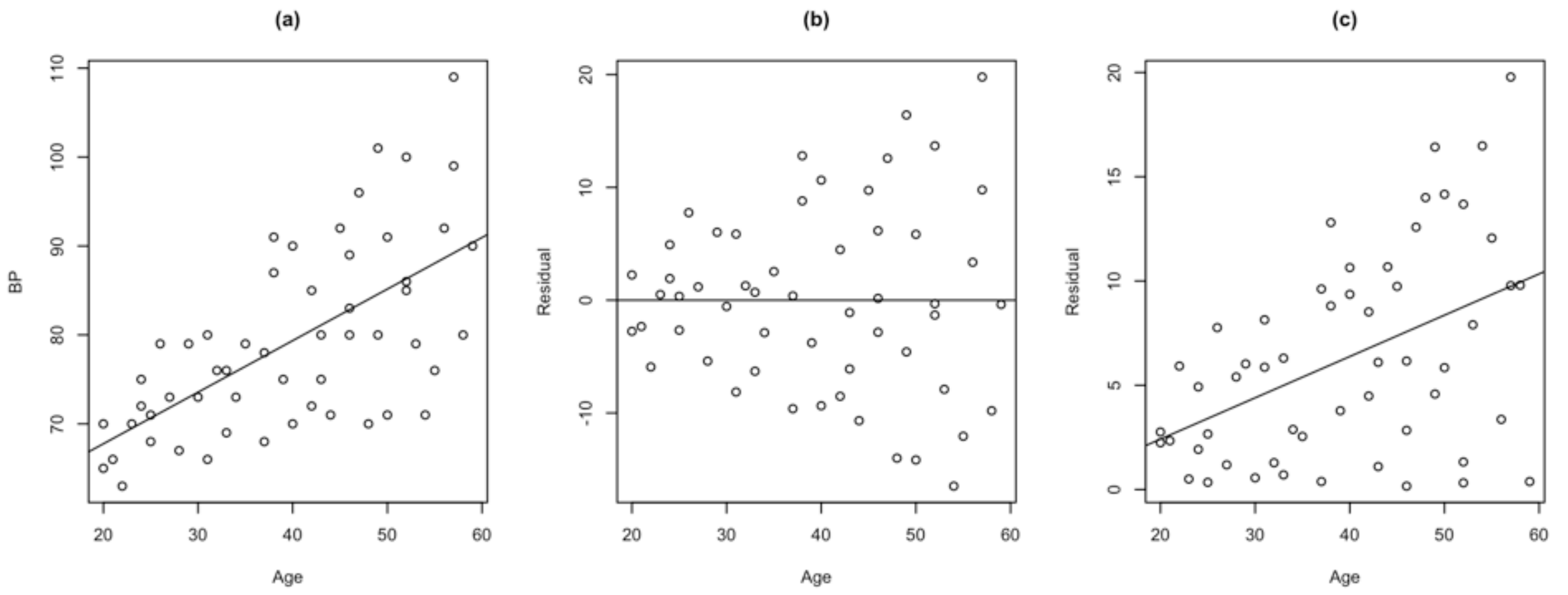
Example (Strong Interaction ALR4 page 157)

- Response : scattering cross-section (y), Predictor: square of total energy in the center of mass frame of reference (s)
- Designed experiment
- A very large number of particles was counted at each setting of s
- The variance of y is thus known almost exactly

Example (Strong Interaction ALR4 page 157)

```
##
## Call:
## lm(formula = y ~ x, data = alr4::physics, weights = 1/SD^2)
##
## Weighted Residuals:
##     Min      1Q  Median      3Q     Max
## -2.3230 -0.8842  0.0000  1.3900  2.3353
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)  148.473      8.079   18.38 7.91e-08 ***
## x            530.835     47.550   11.16 3.71e-06 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.657 on 8 degrees of freedom
## Multiple R-squared:  0.9397, Adjusted R-squared:  0.9321
## F-statistic: 124.6 on 1 and 8 DF,  p-value: 3.71e-06
```

Example (Blood pressure)



1. $\Rightarrow$ linear relationship (unweighted)
2. $\Rightarrow$ confirms the nonconstant error variance
3. $\Rightarrow$ a linear relation between Age and standard error is reasonable

Example (Blood pressure)

- Regress absolute residuals against `Age`

```
##               Estimate Std. Error t value  Pr(>|t|)
## (Intercept) -1.54948    2.18692 -0.7085 0.4817858
## blood$Age    0.19817    0.05309  3.7328 0.0004705
##
## n = 54, p = 2, Residual SE = 4.46057, R-Squared = 0.21
```

- Variance function

$$\hat{s} = -1.5494776 + 0.1981723Age$$

- Weights

```
w = 1/lmod_abs_res$fitted.values^2
head(w)
```

```
##          1          2          3          4          5          6
## 0.06920928 0.14655708 0.12661657 0.09725115 0.08625993 0.11048521
```

```
head(blood$Age)
```

```
## [1] 27 21 22 24 25 23
```

Example (Blood pressure)

- OLS

```
##              Estimate Std. Error t value  Pr(>|t|)
## (Intercept) 56.156929   3.993674 14.0615 < 2.2e-16
## Age          0.580031   0.096951  5.9827  2.05e-07
##
## n = 54, p = 2, Residual SE = 8.14575, R-Squared = 0.41
```

- WLS

```
wls_mod = lm(BP ~ Age, weights = w, data = blood)
sumary(wls_mod)
```

```
##              Estimate Std. Error t value  Pr(>|t|)
## (Intercept) 55.565766   2.520918  22.042 < 2.2e-16
## Age          0.596342   0.079238   7.526 7.187e-10
##
## n = 54, p = 2, Residual SE = 1.21302, R-Squared = 0.52
```