Diagnostics for multiple regression

February 5, 2015

1 Diagnostics in multiple linear model

1.1 Outline

- Diagnostics – again
- Different types of residuals
- Influence
- Outlier detection
- Residual plots:
  - partial regression (added variable) plot,
  - partial residual (residual plus component) plot.

1.2 Scottish hill races data

The dataset we will use is based on record times on Scottish hill races.

```
In [2]: make_table(Description)
        apply_theme('basic')
```

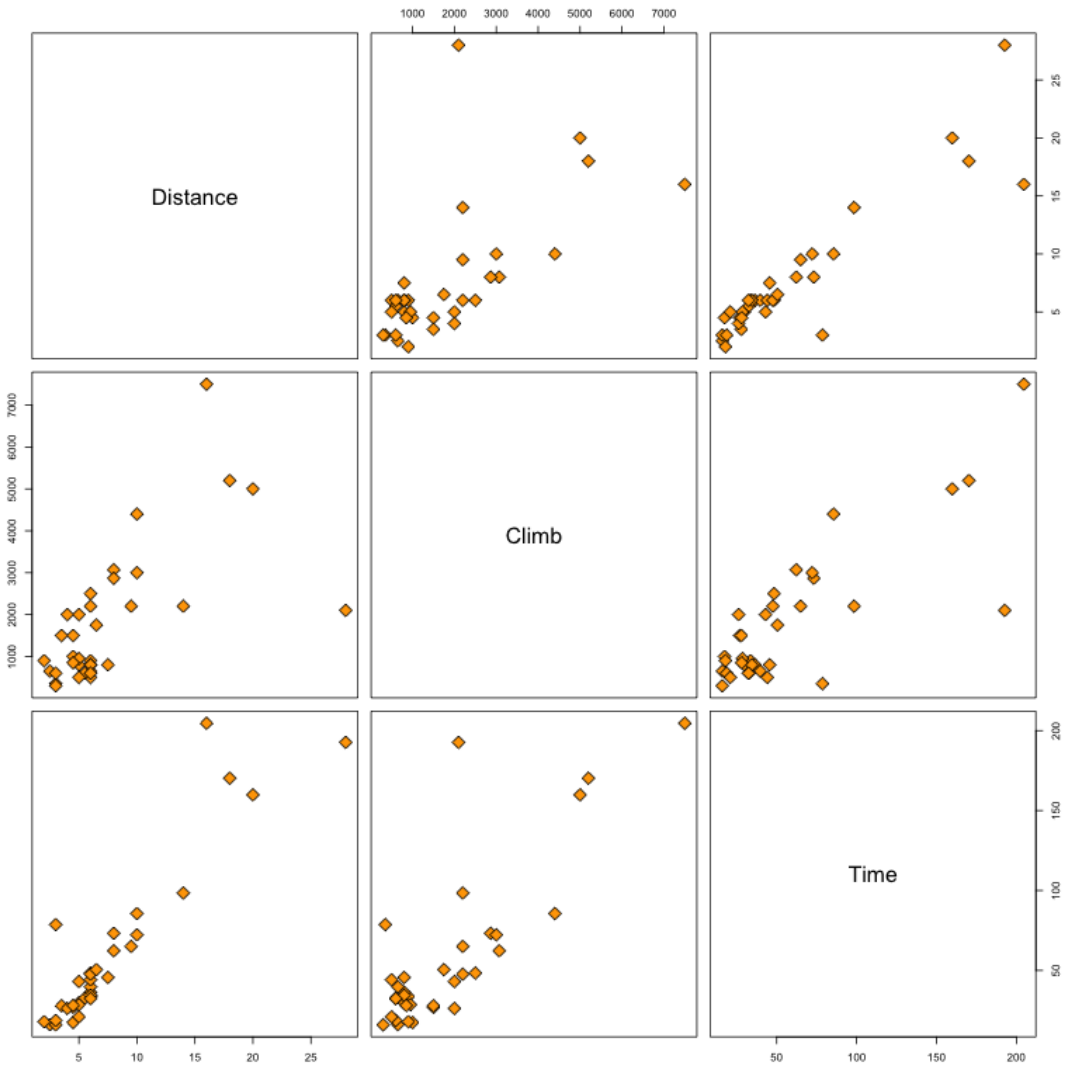
```
Out[2]: <ipy_table.IpyTable at 0x106cbca50>
```

```
In [3]: %%R
        url = 'http://www.statsci.org/data/general/hills.txt'
        races.table = read.table(url, header=TRUE, sep='\t')
        head(races.table)
```

```
         Race Distance Climb   Time
1 Greenmantle      2.5   650 16.083
2    Carnethy      6.0  2500 48.350
3 CraigDunain      6.0   900 33.650
4      BenRha      7.5   800 45.600
5   BenLomond      8.0  3070 62.267
6    Goatfell      8.0  2866 73.217
```

As we'd expect, the time increases both with `Distance` and `Climb`.

```
In [4]: %%R -w 800 -h 800
        plot(races.table[,2:4], pch=23, bg='orange', cex=2)
```



Let's look at our multiple regression model.

```
In [5]: %%R
        races.lm = lm(Time ~ Distance + Climb, data=races.table)
        summary(races.lm)
```

```
Call:
lm(formula = Time ~ Distance + Climb, data = races.table)

Residuals:
    Min      1Q  Median      3Q     Max
-16.215  -7.129  -1.186   2.371  65.121

Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) -8.992039   4.302734  -2.090   0.0447 *
```

```
Distance     6.217956   0.601148  10.343 9.86e-12 ***
Climb        0.011048   0.002051   5.387 6.45e-06 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 14.68 on 32 degrees of freedom
Multiple R-squared:  0.9191,Adjusted R-squared:  0.914
F-statistic: 181.7 on 2 and 32 DF,  p-value: < 2.2e-16
```

But is this a good model?

1.3 Diagnostics

What can go wrong?

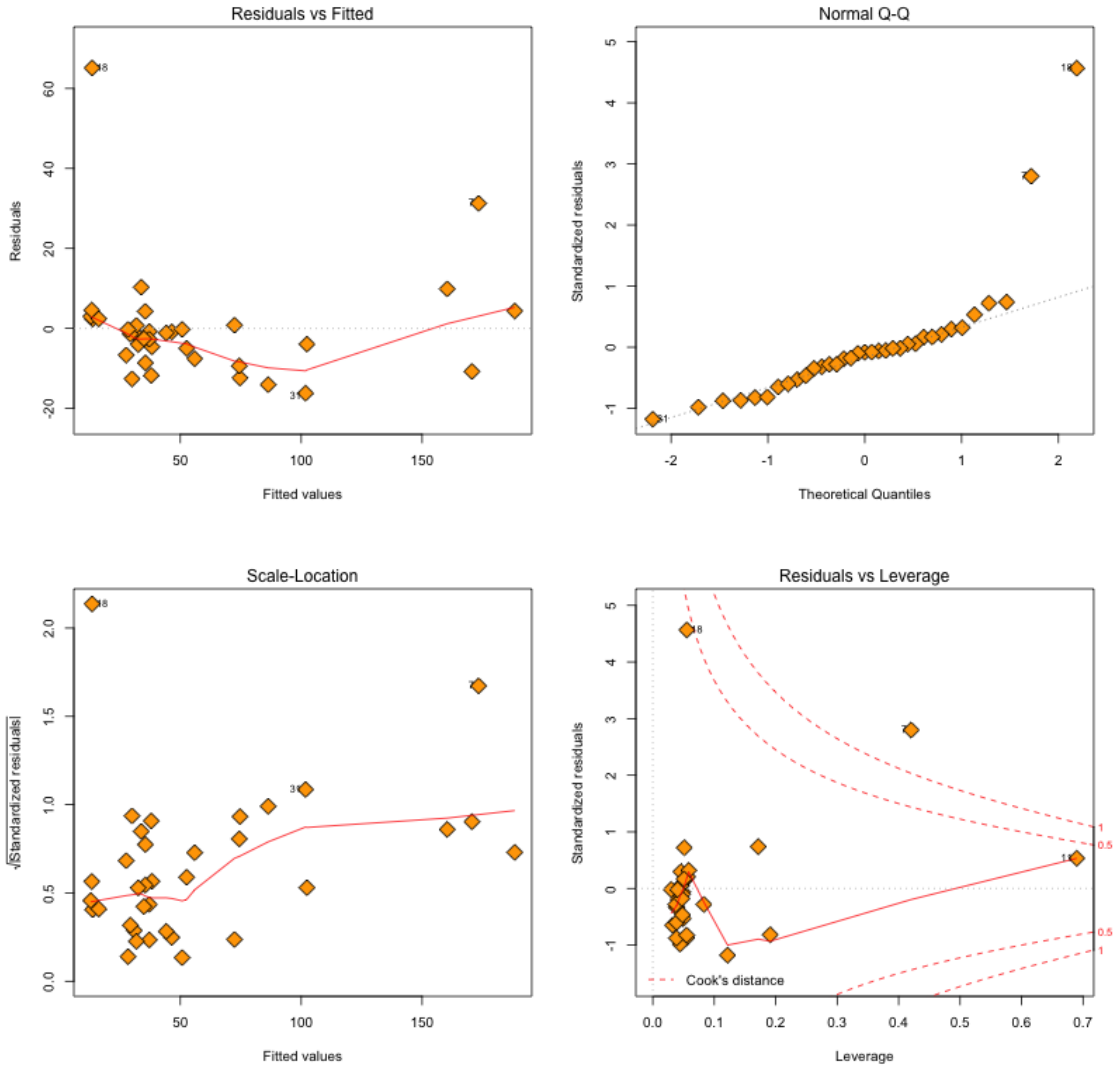
- Regression function can be wrong: maybe regression function should have some other form (see diagnostics for simple linear regression).
- Model for the errors may be incorrect:
  - may not be normally distributed.
  - may not be independent.
  - may not have the same variance.
- Detecting problems is more *art* then *science*, i.e. we cannot *test* for all possible problems in a regression model.
- Basic idea of diagnostic measures: if model is correct then residuals $e_i = Y_i - \widehat{Y}_i, 1 \leq i \leq n$ should look like a sample of (not quite independent) $N(0, \sigma^2)$ random variables.

1.4 Standard diagnostic plots

`R` produces a set of standard plots for `lm` that help us assess whether our assumptions are reasonable or not. We will go through each in some, but not too much, detail.

As we see below, there are some quantities which we need to define in order to read these plots. We will define these first.

```
In [6]: %%R -h 800 -w 800
        par(mfrow=c(2,2))
        plot(races.lm, pch=23 ,bg='orange',cex=2)
```



1.5 Problems with the errors

Possible problems & diagnostic checks

- Errors may not be normally distributed or may not have the same variance – qqnorm can help with this. This may not be too important in large samples.
- Variance may not be constant. Can also be addressed in a plot of $\boldsymbol{X}$ vs. $\boldsymbol{e}$: *fan shape* or other trend indicate non-constant variance.
- Influential observations. Which points "affect" the regression line the most?
- Outliers: points where the model really does not fit! Possibly mistakes in data transcription, lab errors, who knows? Should be recognized and (hopefully) explained.

1.6 Residuals

1.6.1 Possible problems & diagnostic checks

- Errors may not be normally distributed or may not have the same variance – qqnorm can help with this. This may not be too important in large samples.
- Variance may not be constant. Can also be addressed in a plot of X vs. e: *fan shape* or other trend indicate non-constant variance. One of `R`'s plots is $\hat{Y}$ vs $e = Y - \hat{Y}$.
- Influential observations. Which points "affect" the regression line the most?
- Outliers: points where the model really does not fit! Possibly mistakes in data transcription, lab errors, who knows? Should be recognized and (hopefully) explained.

1.7 Types of residuals

- Ordinary residuals: $e_i = Y_i - \widehat{Y}_i$. These measure the deviation of predicted value from observed value, but their distribution depends on unknown scale, σ.
- Internally studentized residuals (`rstandard` in R):

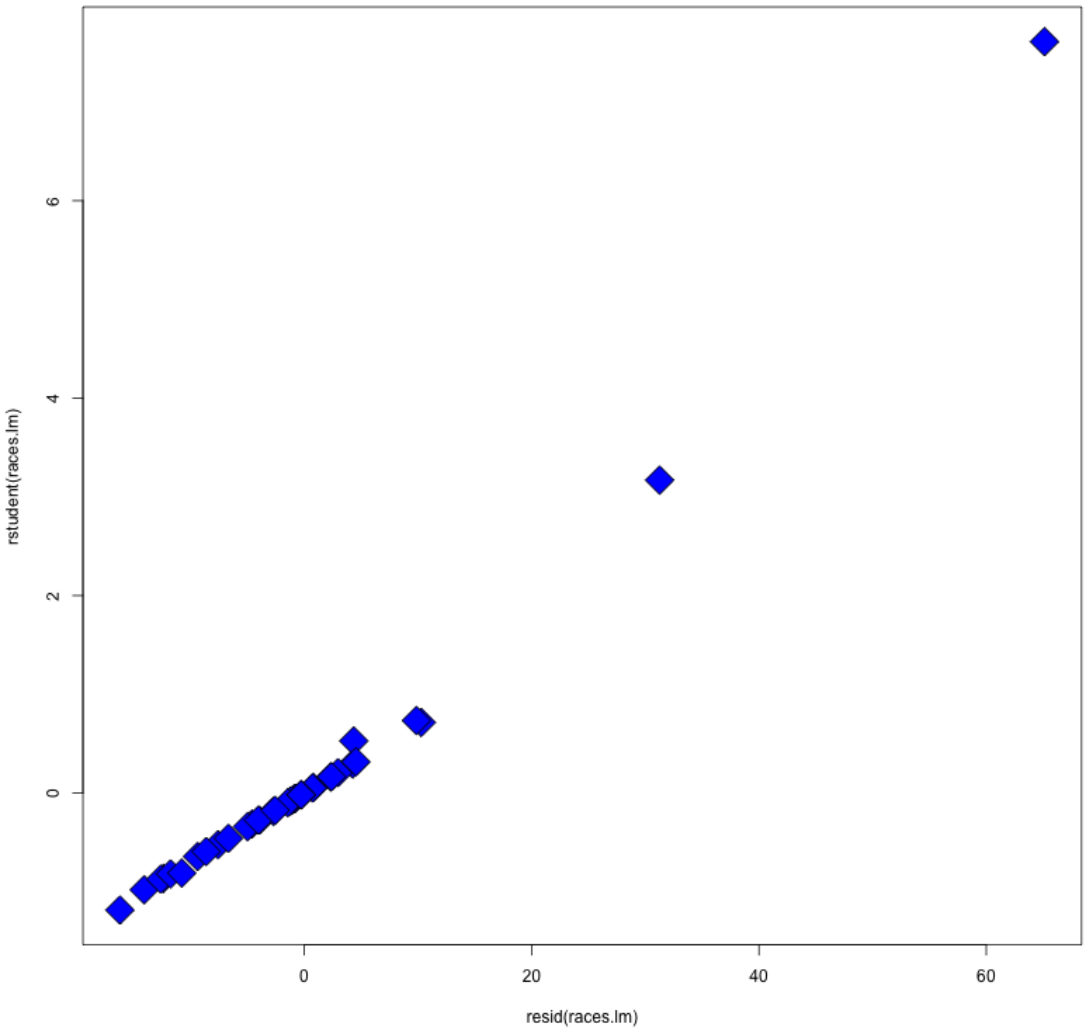
$$r_i = e_i / s(e_i) = e_i / \widehat{\sigma}\sqrt{1 - H_{ii}}$$

  ,
- Above, H is the "hat" matrix. These are almost t-distributed, except $\widehat{\sigma}$ depends on e_i.
- Externally studentized residuals (`rstudent` in R):

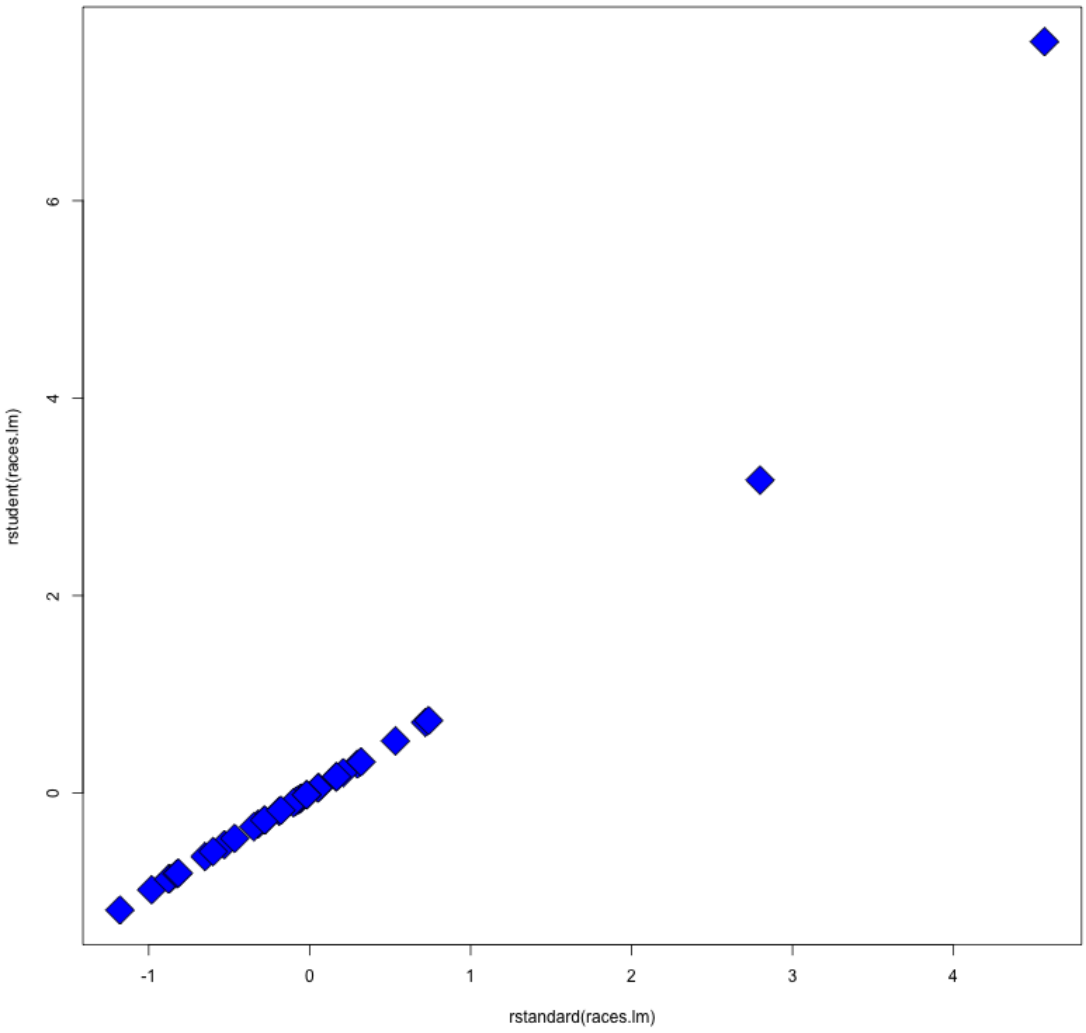
$$t_i = e_i / \widehat{\sigma_{(i)}}\sqrt{1 - H_{ii}} \sim t_{n-p-2}.$$

  These are exactly t distributed so we know their distribution and can use them for tests, if desired.
- Numerically, these residuals are highly correlated, as we would expect.

```
In [7]: %%R -h 800 -w 800
        plot(resid(races.lm), rstudent(races.lm), pch=23, bg='blue', cex=3)
```



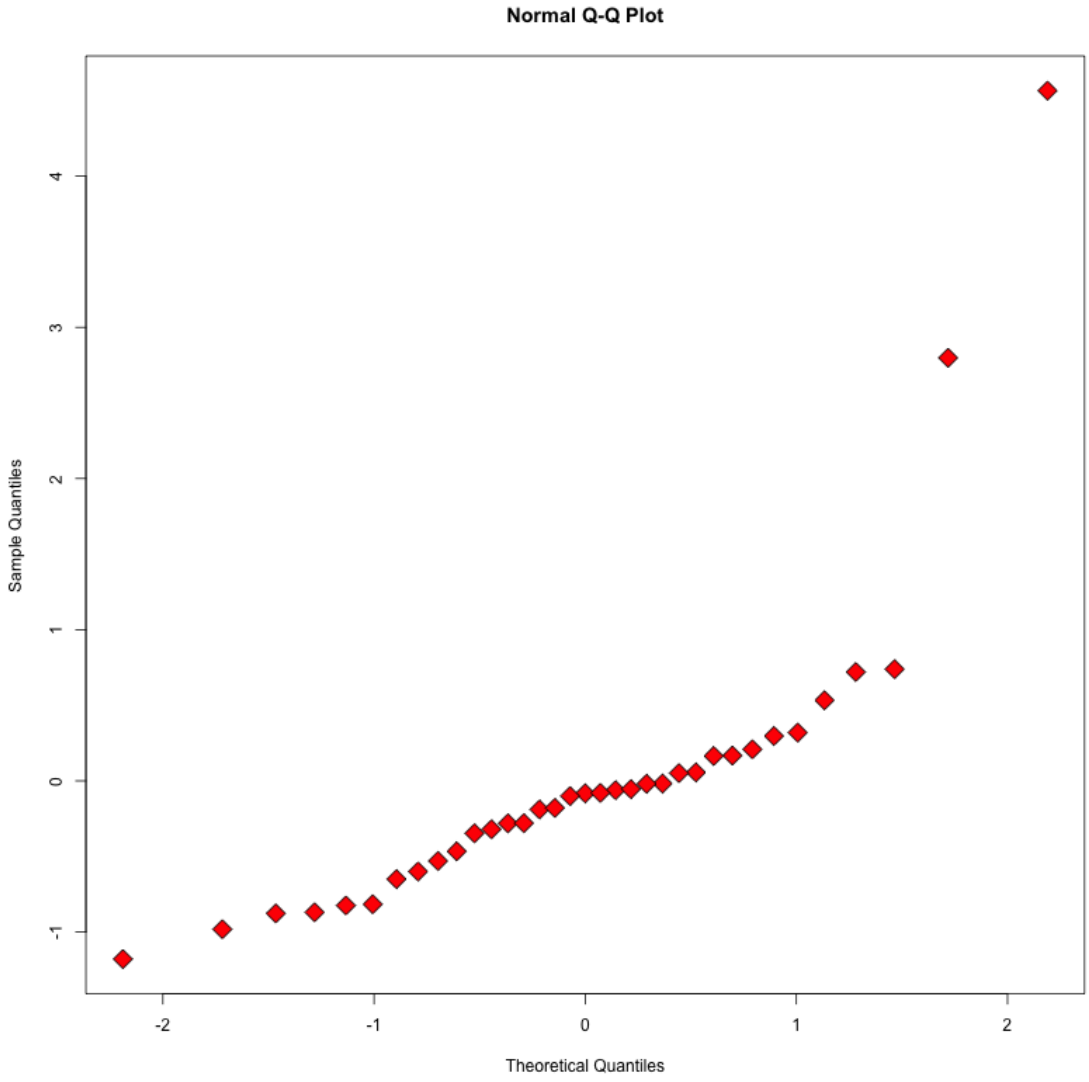
In [8]:
```
%%R -h 800 -w 800
plot(rstandard(races.lm), rstudent(races.lm), pch=23, bg='blue', cex=3)
```



1.8 Standard diagnostic plots

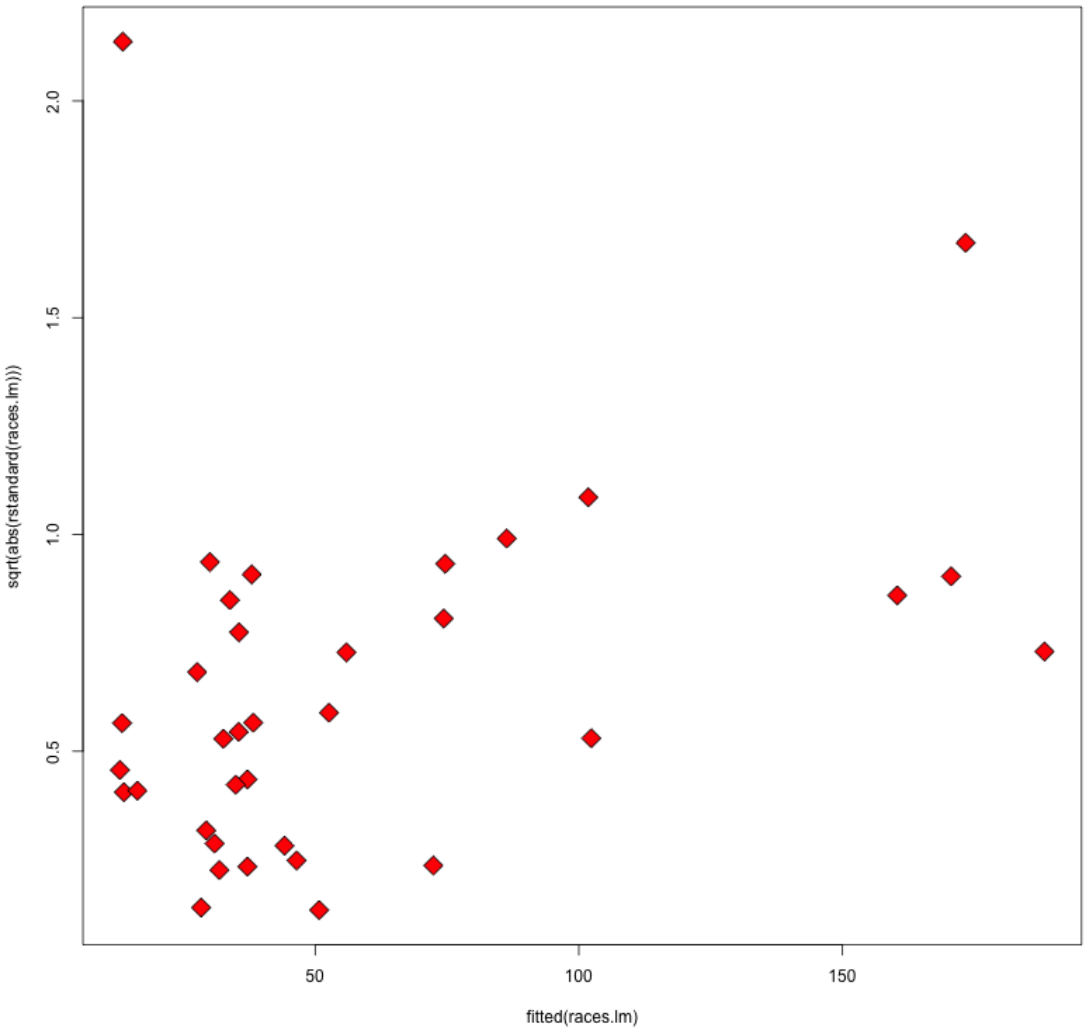
The first plot is the quantile plot for the residuals, that compares their distribution to that of a sample of independent normals.

```
In [9]: %%R -h 800 -w 800
        qqnorm(rstandard(races.lm), pch=23, bg='red', cex=2)
```

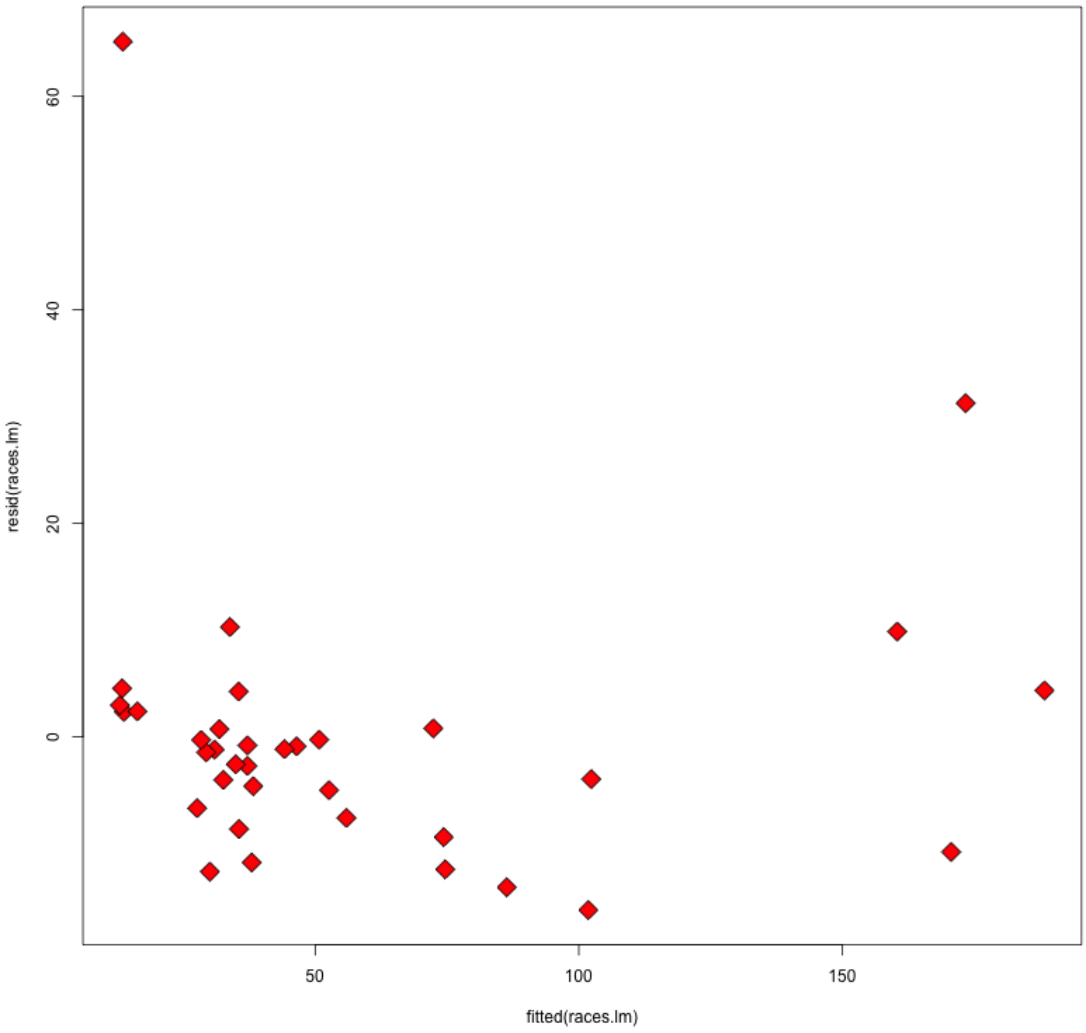


Two other plots try address the constant variance assumptions. If these plots have a particular shape (maybe the spread increases with $\hat{Y}$) then maybe the variance is not constant.

```
In [10]: %%R -h 800 -w 800
         plot(fitted(races.lm), sqrt(abs(rstandard(races.lm))), pch=23, bg='red', cex=2, text.cex=4)
```




```
In [11]: %%R -h 800 -w 800
         plot(fitted(races.lm), resid(races.lm), pch=23, bg='red', cex=2)
```



1.9 Influence of an observation

Other plots provide an assessment of the `influence` of each observation. Usually, this is done by dropping an entire case (y_i, x_i) from the dataset and refitting the model.

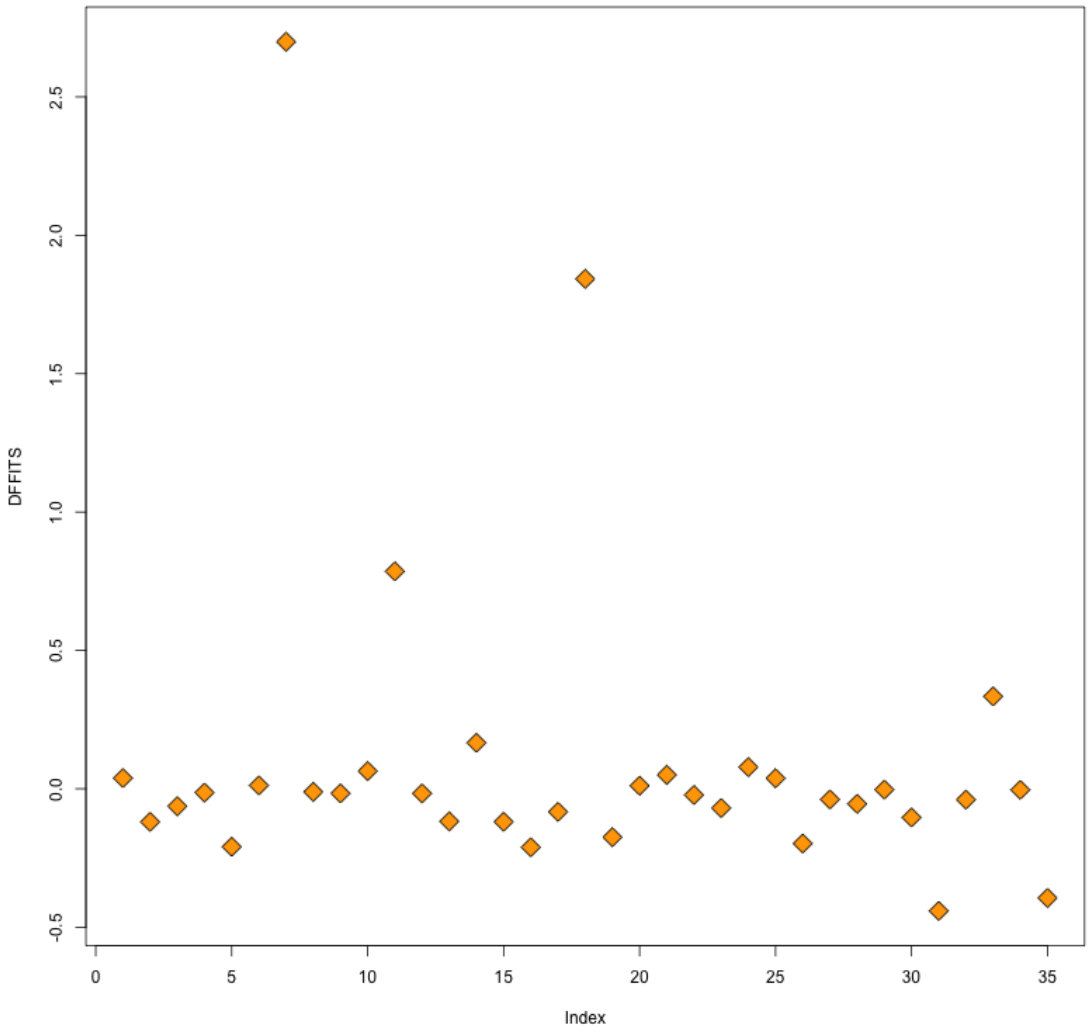
- In this setting, a $\cdot_{(i)}$ indicates i-th observation was not used in fitting the model.
- For example: $\widehat{Y}_{j(i)}$ is the regression function evaluated at the j-th observations predictors BUT the coefficients $(\widehat{\beta}_{0(i)}, \ldots, \widehat{\beta}_{p(i)})$ were fit after deleting i-th case from the data.
- Idea: if $\widehat{Y}_{j(i)}$ is very different than $\widehat{Y}_j$ (using all the data) then i is an influential point, at least for estimating the regression function at $(X_{1,j}, \ldots, X_{p,j})$.
- There are various standard measures of influence.

1.10 DFFITS

- $$DFFITS_i = \frac{\widehat{Y}_i - \widehat{Y}_{i(i)}}{\widehat{\sigma}_{(i)}\sqrt{H_{ii}}}$$

- This quantity measures how much the regression function changes at the i-th case / observation when the i-th case / observation is deleted.
- For small/medium datasets: value of 1 or greater is "suspicious". For large dataset: value of $2\sqrt{(p+1)/n}$.
- `R` has its own standard rules similar to the above for marking an observation as influential.

```
In [12]: %%R -h 800 -w 800
         plot(dffits(races.lm), pch=23, bg='orange', cex=2, ylab="DFFITS")
```



It seems that some observations had a high influence measured by $DFFITS$:

```
In [13]: %%R
         races.table[which(dffits(races.lm) > 0.5),]

         Race Distance Climb    Time
7  BensofJura       16  7500 204.617
11 LairigGhru       28  2100 192.667
18  KnockHill        3   350  78.650
```

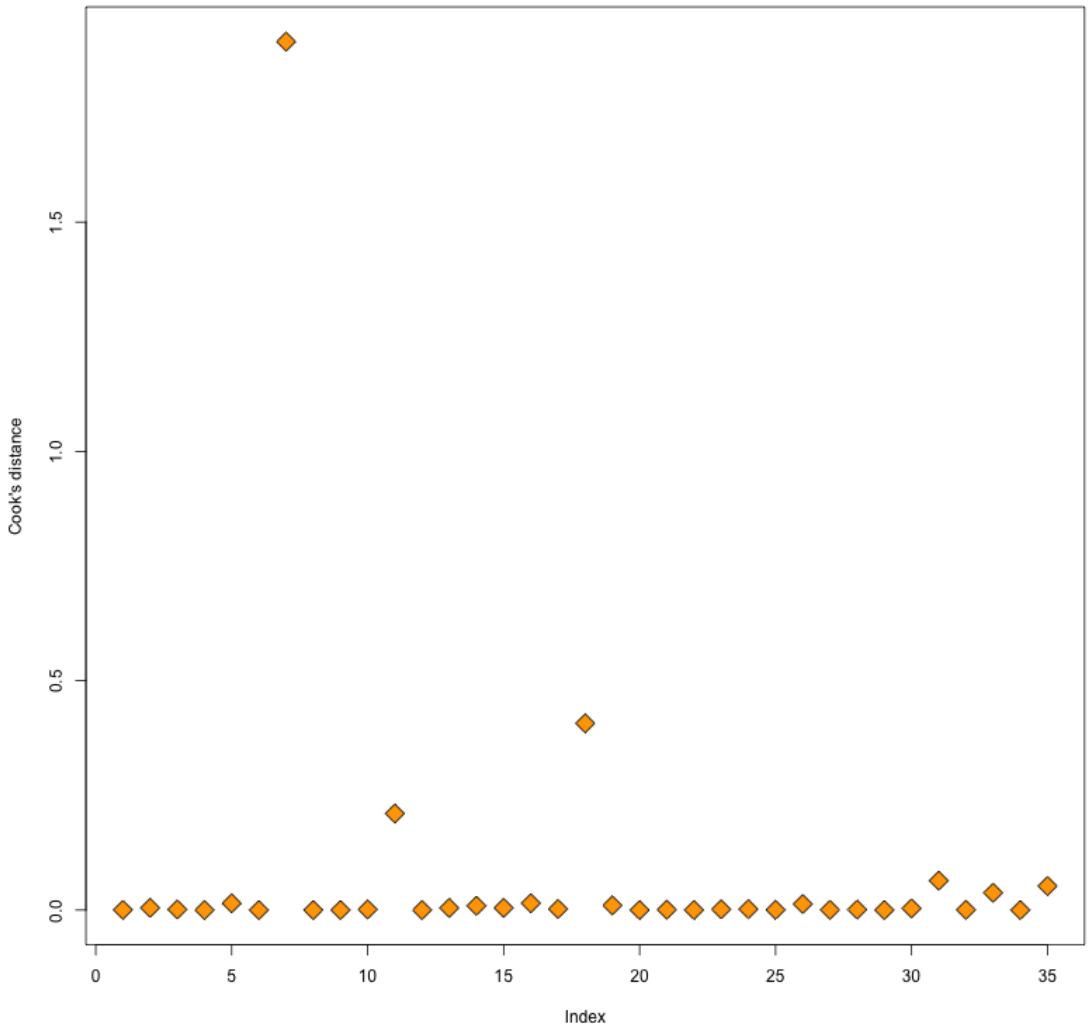
It is perhaps not surprising that the longest course and the course with the most elevation gain seemed to have a strong effect on the fitted values. What about `Knock Hill`? We'll come back to this later.

1.11 Cook's distance

Cook's distance measures how much the entire regression function changes when the i-th case is deleted.

- $$D_i = \frac{\sum_{j=1}^{n}(\widehat{Y}_j - \widehat{Y}_{j(i)})^2}{(p+1)\,\widehat{\sigma}^2}$$
- Should be comparable to $F_{p+1,n-p-1}$: if the "p-value" of D_i is 50 percent or more, then the i-th case is likely influential: investigate further.
- Again, `R` has its own rules similar to the above for marking an observation as influential.
- What to do after investigation? No easy answer.

```
In [14]: %%R -h 800 -w 800
         plot(cooks.distance(races.lm), pch=23, bg='orange', cex=2, ylab="Cook's distance")
```




```
In [15]: %%R
         races.table[which(cooks.distance(races.lm) > 0.1),]
```

```
         Race Distance Climb    Time
7  BensofJura       16  7500 204.617
11 LairigGhru       28  2100 192.667
18  KnockHill        3   350  78.650
```

Again, the same 3 races. This is not surprising as both $DFFITS$ and Cook's distance measure changes in fitted values. The difference is that one measures the influence on one fitted value, while the other measures the influence on the entire vector of fitted values.

1.12 DFBETAS

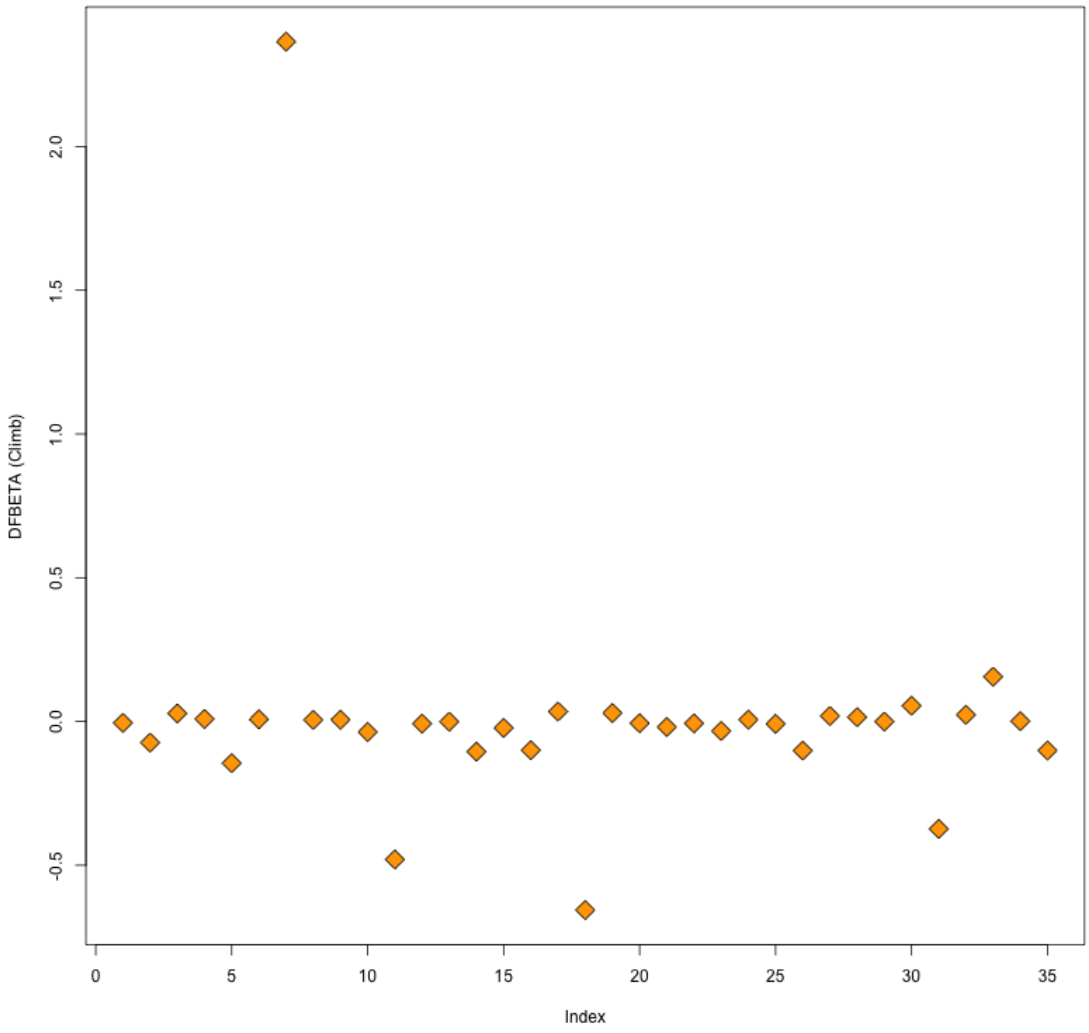
This quantity measures how much the coefficients change when the i-th case is deleted.

- $$DFBETAS_{j(i)} = \frac{\widehat{\beta}_j - \widehat{\beta}_{j(i)}}{\sqrt{\widehat{\sigma}^2_{(i)}(X^TX)^{-1}_{jj}}}.$$

- For small/medium datasets: absolute value of 1 or greater is "suspicious". For large dataset: absolute value of $2/\sqrt{n}$.

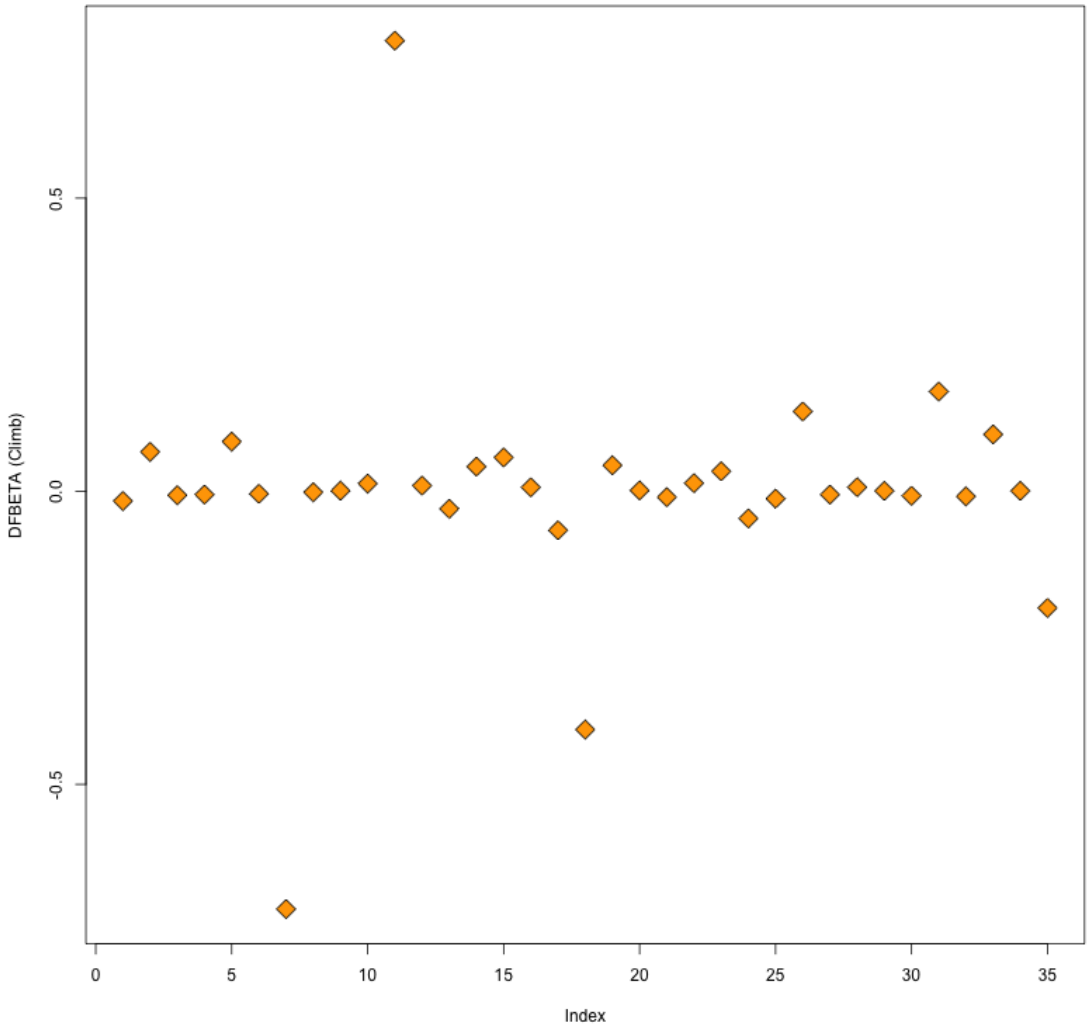
```
In [16]: %%R -h 800 -w 800
         plot(dfbetas(races.lm)[,'Climb'], pch=23, bg='orange', cex=2, ylab="DFBETA (Climb)")
         races.table[which(abs(dfbetas(races.lm)[,'Climb']) > 1),]
```

```
        Race Distance Climb    Time
7 BensofJura       16  7500 204.617
```



```
In [17]: %%R -h 800 -w 800
         plot(dfbetas(races.lm)[,'Distance'], pch=23, bg='orange', cex=2, ylab="DFBETA (Climb)")
         races.table[which(abs(dfbetas(races.lm)[,'Distance']) > 0.5),]

         Race Distance Climb    Time
7  BensofJura       16  7500 204.617
11 LairigGhru       28  2100 192.667
```



1.13 Outliers

The essential definition of an *outlier* is an observation pair $(Y, X_1, \ldots, X_p)$ that does not follow the model, while most other observations seem to follow the model.

- Outlier in *predictors*: the X values of the observation may lie outside the "cloud" of other X values. This means you may be extrapolating your model inappropriately. The values H_{ii} can be used to measure how "outlying" the X values are.
- Outlier in *response*: the Y value of the observation may lie very far from the fitted model. If the studentized residuals are large: observation may be an outlier.
- The races at `Bens of Jura` and `Lairig Ghru` seem to be outliers in *predictors* as they were the highest and longest races, respectively.
- How can we tell if the `Knock Hill` result is an outlier? It seems to have taken much longer than it should have so maybe it is an outlier in the *response*.

1.14 Outlying X values

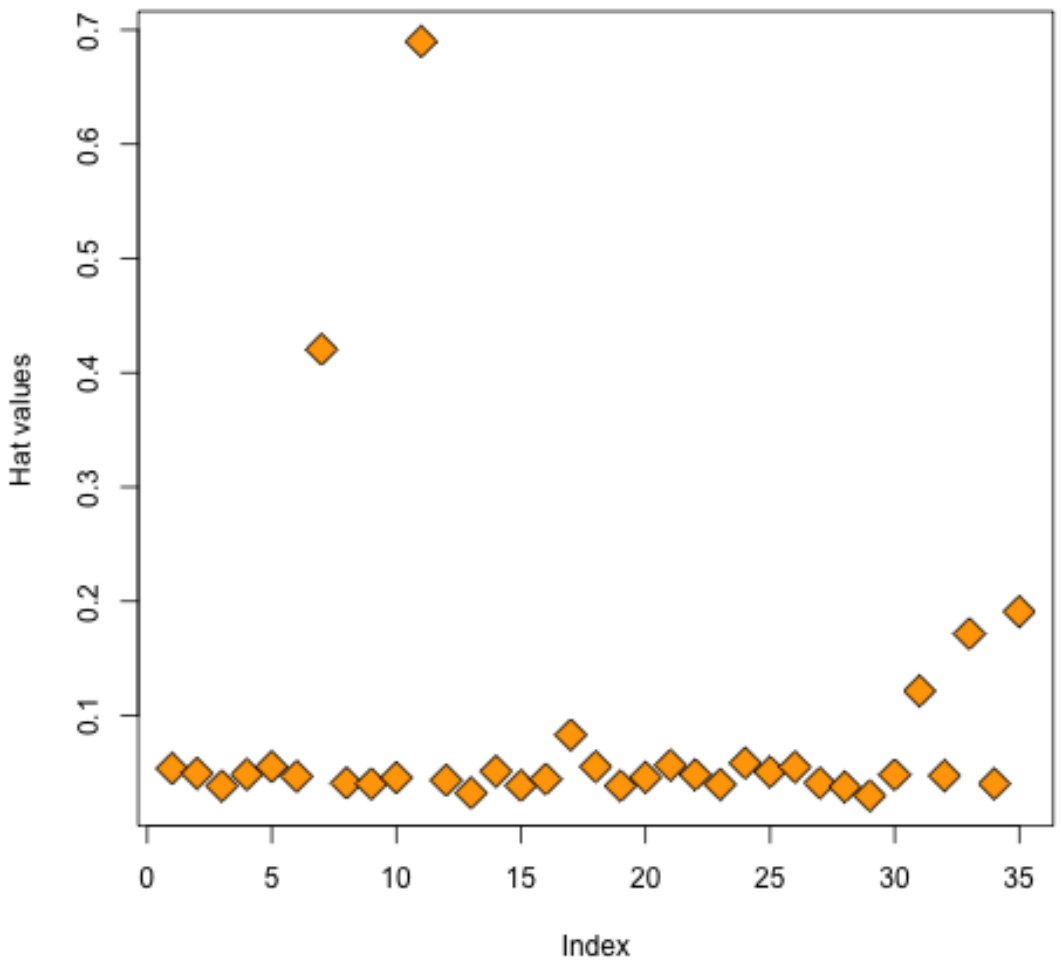
One way to detect outliers in the *predictors*, besides just looking at the actual values themselves, is through their leverage values, defined by

$$\text{leverage}_i = H_{ii} = (X(X^T X)^{-1} X^T)_{ii}.$$

Not surprisingly, our longest and highest courses show up again. This at least reassures us that the leverage is capturing some of this "outlying in X space".

```
In [18]: %%R
         plot(hatvalues(races.lm), pch=23, bg='orange', cex=2, ylab='Hat values')
         races.table[which(hatvalues(races.lm) > 0.3),]

         Race Distance Climb    Time
7  BensofJura       16  7500 204.617
11 LairigGhru       28  2100 192.667
```



1.15 Outliers in the response

We will consider a crude outlier test that tries to find residuals that are "larger" than they should be.

- Since `rstudent` are t distributed, we could just compare them to the T distribution and reject if their absolute value is too large.
- Doing this for every observation results in n different hypothesis tests.
- This causes a problem: if n is large, if we "threshold" at $t_{1-\alpha/2,n-p-2}$ we will get many outliers by chance even if model is correct.
- In fact, we expect to see $n \cdot \alpha$ "outliers" by this test. Every large data set would have outliers in it, even if model was entirely correct!

Let's sample some data from our model to convince ourselves that this is a real problem.

```
In [19]: %%R
         X = rnorm(100)
         Y = 2 * X + 0.5 + rnorm(100)
         cutoff = qt(0.95, 97)
         sum(abs(rstudent(lm(Y~X))) > cutoff)
```

```
[1] 10
```

```
In [20]: %%R
         X = rnorm(100)
         Y = 2 * X + 0.5 + rnorm(100)
         cutoff = qt(0.95, 97)
         sum(abs(rstudent(lm(Y~X))) > cutoff)
```

```
[1] 9
```

1.15.1 Multiple comparisons

- This problem we identified is known as *multiple comparisons* or *simultaneous inference.* We are performing n hypothesis tests, but would still like to control the probability of making *any* false positive errors.
- One solution: Bonferroni correction, threshold at $t_{1-\alpha/(2*n),n-p-2}$.

1.15.2 Bonferroni correction

- Dividing α by n, the number of tests, is known as a *Bonferroni* correction.
- If we are doing many t (or other) tests, say $m \gg 1$ we can control overall false positive rate at α by testing each one at level α/m.
- **Proof:** when the model is correct, with studentized residuals T_i:

$$\begin{aligned} P\left(\text{at least one false positive}\right) &= P\left(\cup_{i=1}^{m} |T_i| \geq t_{1-\alpha/(2*m),n-p-2}\right) \\ &\leq \sum_{i=1}^{m} P\left(|T_i| \geq t_{1-\alpha/(2*m),n-p-2}\right) \\ &= \sum_{i=1}^{m} \frac{\alpha}{m} = \alpha. \end{aligned}$$

Let's apply this to our data. It turns out that `KnockHill` is a known error.

```
In [21]: %%R
         n = nrow(races.table)
         cutoff = qt(1 - 0.05 / (2*n), (n -4))
         races.table[which(abs(rstudent(races.lm)) > cutoff),]
```

```
        Race Distance Climb  Time
18 KnockHill        3   350 78.65
```

The package `car` has a built in function to do this test.

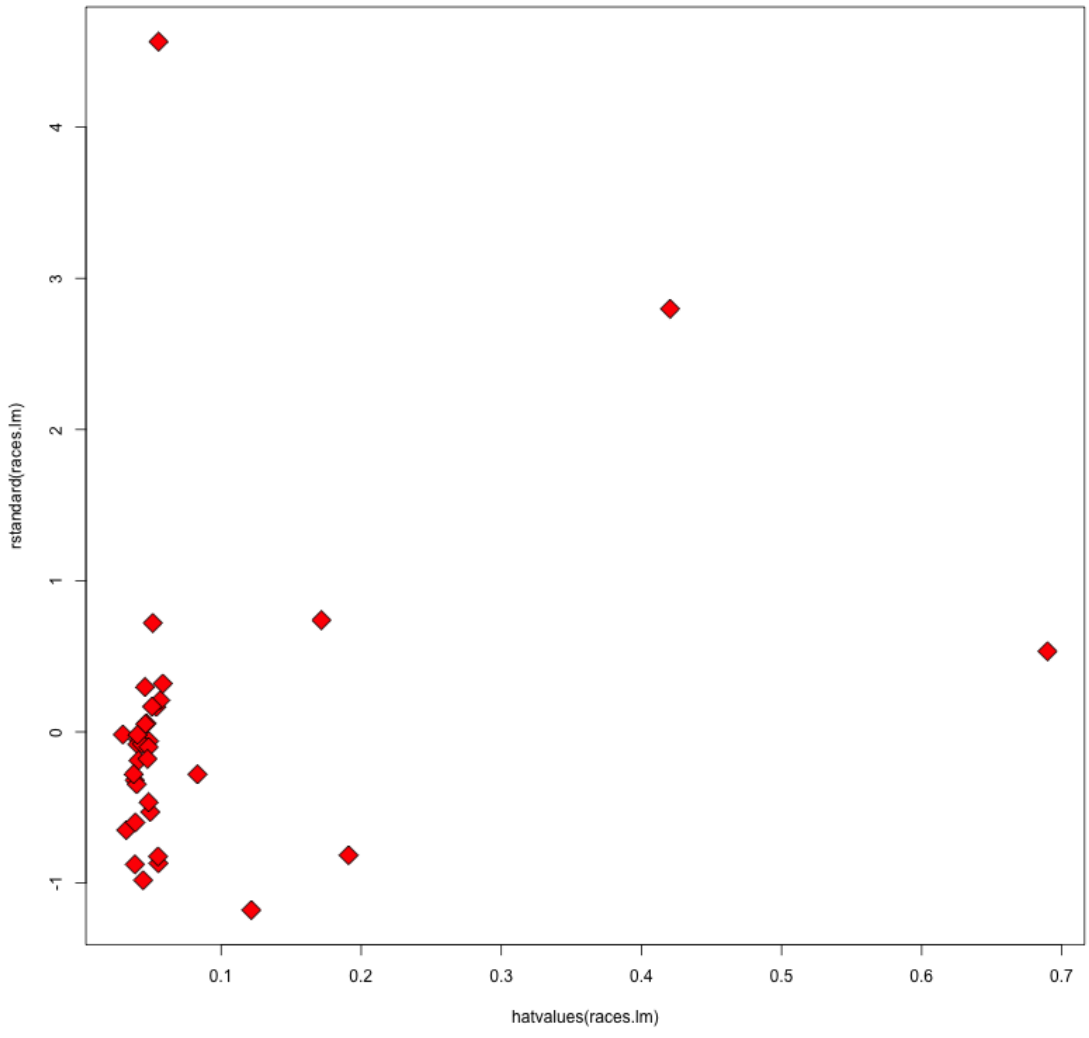
```
In [22]: %%R
         library(car)
         outlierTest(races.lm)
```

```
   rstudent unadjusted p-value Bonferonni p
18 7.610845         1.3973e-08   4.8905e-07
```

1.15.3 Final plot

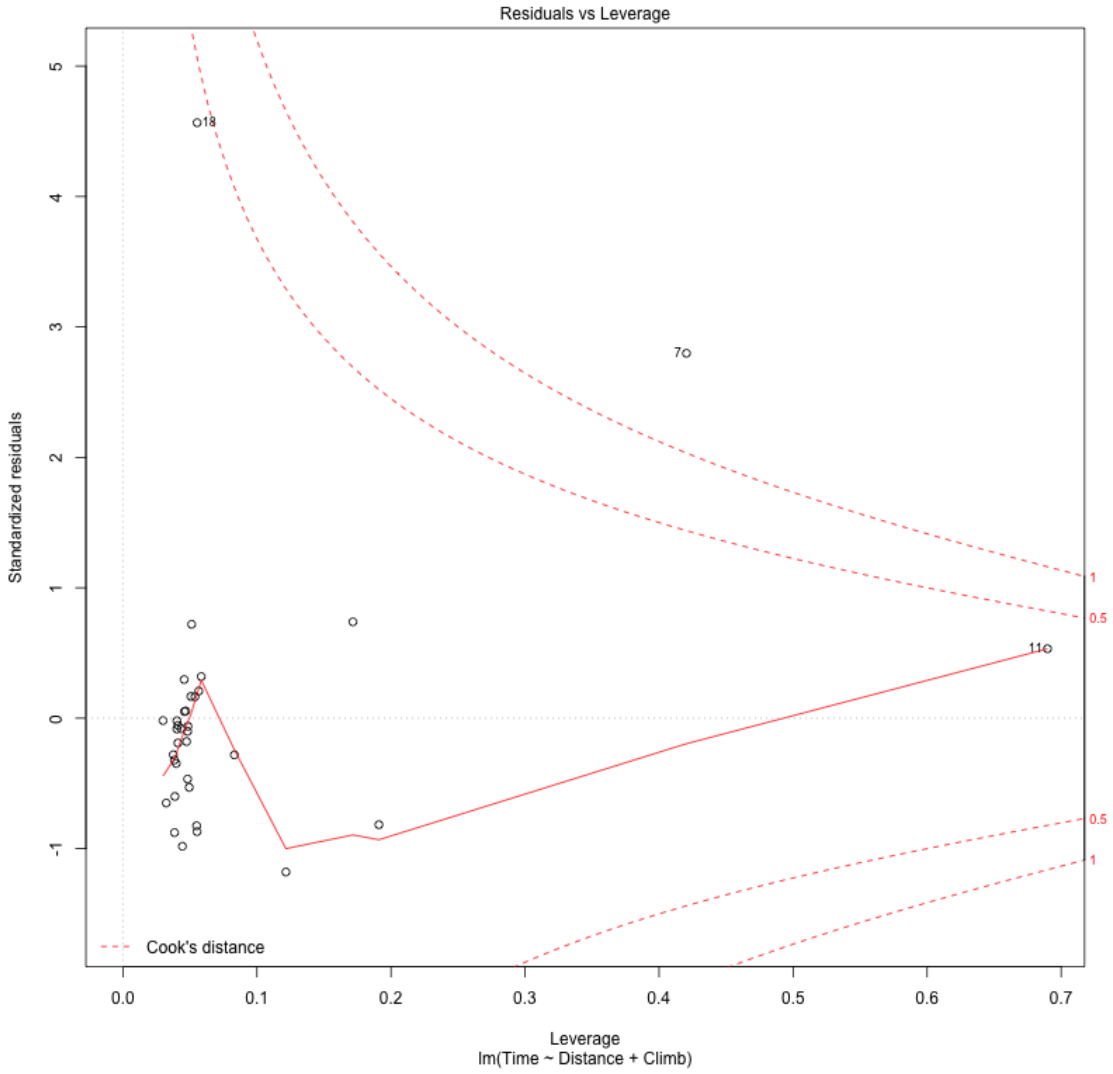
The last plot that R produces is a plot of residuals against leverage. Points that have high leverage and large residuals are particularly influential.

```
In [23]: %%R -h 800 -w 800
         plot(hatvalues(races.lm), rstandard(races.lm), pch=23, bg='red', cex=2)
```



R will put the IDs of cases that seem to be influential in these (and other plots). Not surprisingly, we see our usual three suspects.

```
In [24]: %%R -h 800 -w 800
         plot(races.lm, which=5)
```



1.16 Influence measures

As mentioned above, R has its own rules for flagging points as being influential. To see a summary of these, one can use the `influence.measures` function.

```
In [25]: %%R
         influence.measures(races.lm)

Influence measures of
 lm(formula = Time ~ Distance + Climb, data = races.table) :
```

```
     dfb.1_  dfb.Dstn  dfb.Clmb    dffit  cov.r   cook.d    hat inf
1   0.03781 -0.016614 -0.004744  0.03862 1.1595 5.13e-04 0.0538
2  -0.05958  0.067215 -0.073396 -0.11956 1.1269 4.88e-03 0.0495
3  -0.04858 -0.006707  0.028033 -0.06310 1.1329 1.37e-03 0.0384
4  -0.00766 -0.005675  0.008764 -0.01367 1.1556 6.43e-05 0.0485
5  -0.05046  0.084709 -0.145005 -0.20947 1.0837 1.47e-02 0.0553
6   0.00348 -0.004316  0.007576  0.01221 1.1536 5.13e-05 0.0468
7  -0.89065 -0.712774  2.364618  2.69909 0.8178 1.89e+00 0.4204   *
8  -0.00844 -0.001648  0.005562 -0.01115 1.1467 4.28e-05 0.0410
9  -0.01437  0.000913  0.006161 -0.01663 1.1453 9.52e-05 0.0403
10  0.04703  0.013057 -0.036519  0.06399 1.1431 1.41e-03 0.0457
11 -0.30118  0.768716 -0.479849  0.78569 3.4525 2.11e-01 0.6898   *
12 -0.01149  0.009656 -0.007488 -0.01672 1.1492 9.61e-05 0.0435
13 -0.03173 -0.029911 -0.000707 -0.11770 1.0922 4.70e-03 0.0323
14  0.11803  0.042034 -0.104884  0.16610 1.1039 9.34e-03 0.0513
15 -0.10038  0.057701 -0.022317 -0.11920 1.1062 4.83e-03 0.0388
16 -0.01852  0.006789 -0.099862 -0.21135 1.0501 1.49e-02 0.0444
17  0.01196 -0.066505  0.034455 -0.08337 1.1908 2.39e-03 0.0831
18  1.75827 -0.406545 -0.655934  1.84237 0.0493 4.07e-01 0.0554   *
19 -0.15889  0.044311  0.029414 -0.17484 1.0635 1.03e-02 0.0385
20  0.00866  0.001424 -0.005946  0.01102 1.1526 4.18e-05 0.0459
21  0.04777 -0.010019 -0.019199  0.05032 1.1611 8.70e-04 0.0566
22 -0.01889  0.013856 -0.006465 -0.02234 1.1546 1.72e-04 0.0483
23 -0.04131  0.034097 -0.033022 -0.06961 1.1326 1.66e-03 0.0398
24  0.07483 -0.046385  0.006428  0.07839 1.1571 2.11e-03 0.0584
25  0.03691 -0.012633 -0.008257  0.03808 1.1557 4.99e-04 0.0507
26 -0.13772  0.136124 -0.101306 -0.19782 1.0914 1.32e-02 0.0550
27 -0.02920 -0.005702  0.019239 -0.03857 1.1431 5.11e-04 0.0410
28 -0.04764  0.006936  0.014990 -0.05446 1.1345 1.02e-03 0.0376
29 -0.00214  0.000647 -0.000328 -0.00309 1.1338 3.29e-06 0.0299
30 -0.08532 -0.007705  0.054838 -0.10362 1.1323 3.67e-03 0.0482
31  0.02099  0.170124 -0.373634 -0.44138 1.0960 6.41e-02 0.1216
32 -0.02858 -0.008694  0.023275 -0.03931 1.1513 5.31e-04 0.0475
33 -0.15823  0.097014  0.155702  0.33384 1.2609 3.77e-02 0.1716
34 -0.00356  0.000704  0.001054 -0.00392 1.1461 5.29e-06 0.0403
35  0.20872 -0.199048 -0.100907 -0.39445 1.2764 5.24e-02 0.1910
```

While not specified in the documentation, the meaning of the asterisks can be found by reading the code. The function `is.influential` makes the decisions to flag cases as influential or not.

- We see that the `DFBETAS` are thresholded at 1.
- We see that `DFFITS` is thresholded at `3 * sqrt((p+1)/(n-p-1))`.
- Etc.

```
In [26]: %%R
         influence.measures
```

```
function (model)
{
    is.influential <- function(infmat, n) {
        k <- ncol(infmat) - 4
```

```
        if (n <= k)
            stop("too few cases, n < k")
        absmat <- abs(infmat)
        result <- cbind(absmat[, 1L:k] > 1, absmat[, k + 1] >
            3 * sqrt(k/(n - k)), abs(1 - infmat[, k + 2]) > (3 *
            k)/(n - k), pf(infmat[, k + 3], k, n - k) > 0.5,
            infmat[, k + 4] > (3 * k)/n)
        dimnames(result) <- dimnames(infmat)
        result
    }
    infl <- influence(model)
    p <- model$rank
    e <- weighted.residuals(model)
    s <- sqrt(sum(e^2, na.rm = TRUE)/df.residual(model))
    mqr <- qr.lm(model)
    xxi <- chol2inv(mqr$qr, mqr$rank)
    si <- infl$sigma
    h <- infl$hat
    dfbetas <- infl$coefficients/outer(infl$sigma, sqrt(diag(xxi)))
    vn <- variable.names(model)
    vn[vn == "(Intercept)"] <- "1_"
    colnames(dfbetas) <- paste("dfb", abbreviate(vn), sep = ".")
    dffits <- e * sqrt(h)/(si * (1 - h))
    if (any(ii <- is.infinite(dffits)))
        dffits[ii] <- NaN
    cov.ratio <- (si/s)^(2 * p)/(1 - h)
    cooks.d <- if (inherits(model, "glm"))
        (infl$pear.res/(1 - h))^2 * h/(summary(model)$dispersion *
            p)
    else ((e/(s * (1 - h)))^2 * h)/p
    infmat <- cbind(dfbetas, dffit = dffits, cov.r = cov.ratio,
        cook.d = cooks.d, hat = h)
    infmat[is.infinite(infmat)] <- NaN
    is.inf <- is.influential(infmat, sum(h > 0))
    ans <- list(infmat = infmat, is.inf = is.inf, call = model$call)
    class(ans) <- "infl"
    ans
}
<bytecode: 0x1139d01b8>
<environment: namespace:stats>
```

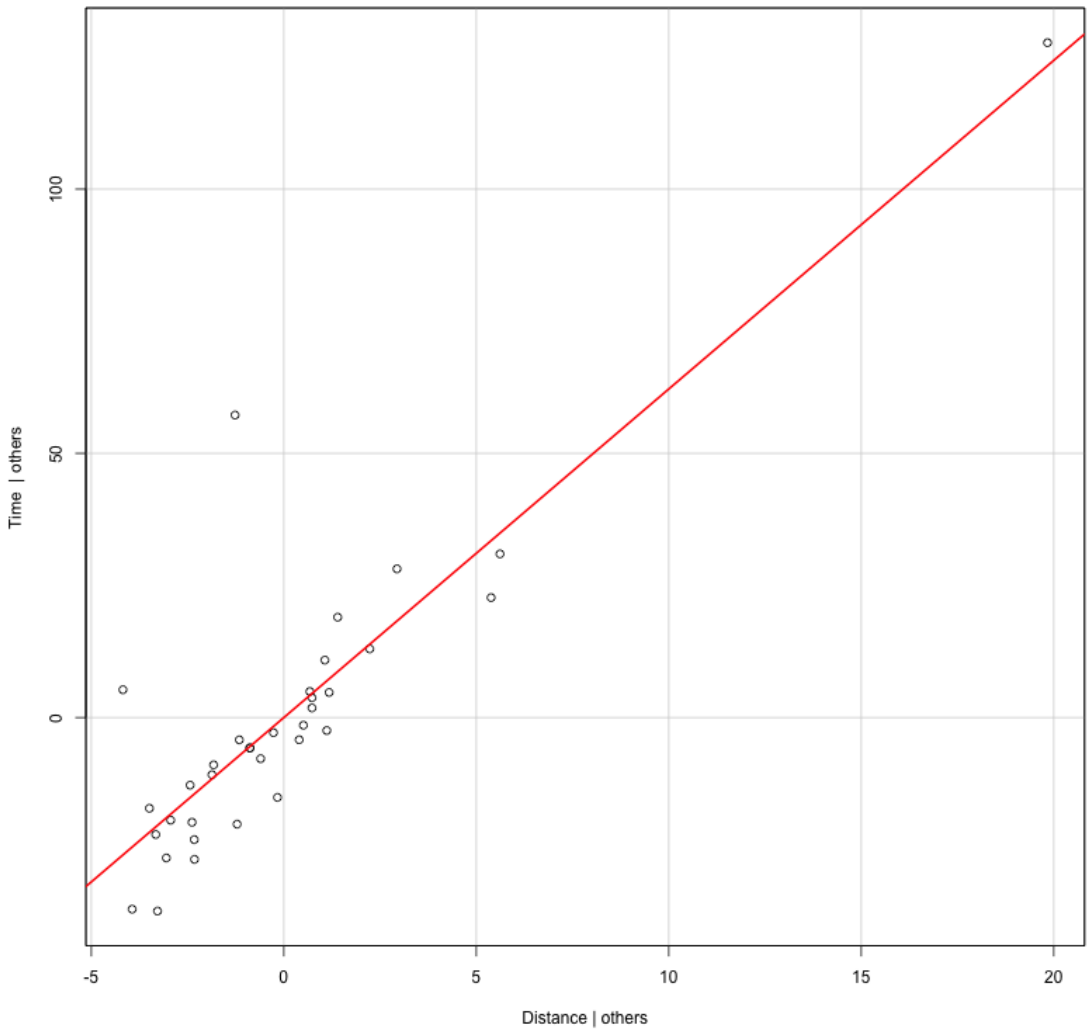
1.17 Problems in the regression function

- True regression function may have higher-order non-linear terms, polynomial or otherwise.
- We may be missing terms involving more than one $\boldsymbol{X}_{(\cdot)}$, i.e. $\boldsymbol{X}_i \cdot \boldsymbol{X}_j$ (called an *interaction*).
- Some simple plots: *added-variable* and *component plus residual* plots can help to find nonlinear functions of *one variable*.
- I find these plots of somewhat limited use in practice, but we will go over them as possibly useful diagnostic tools.

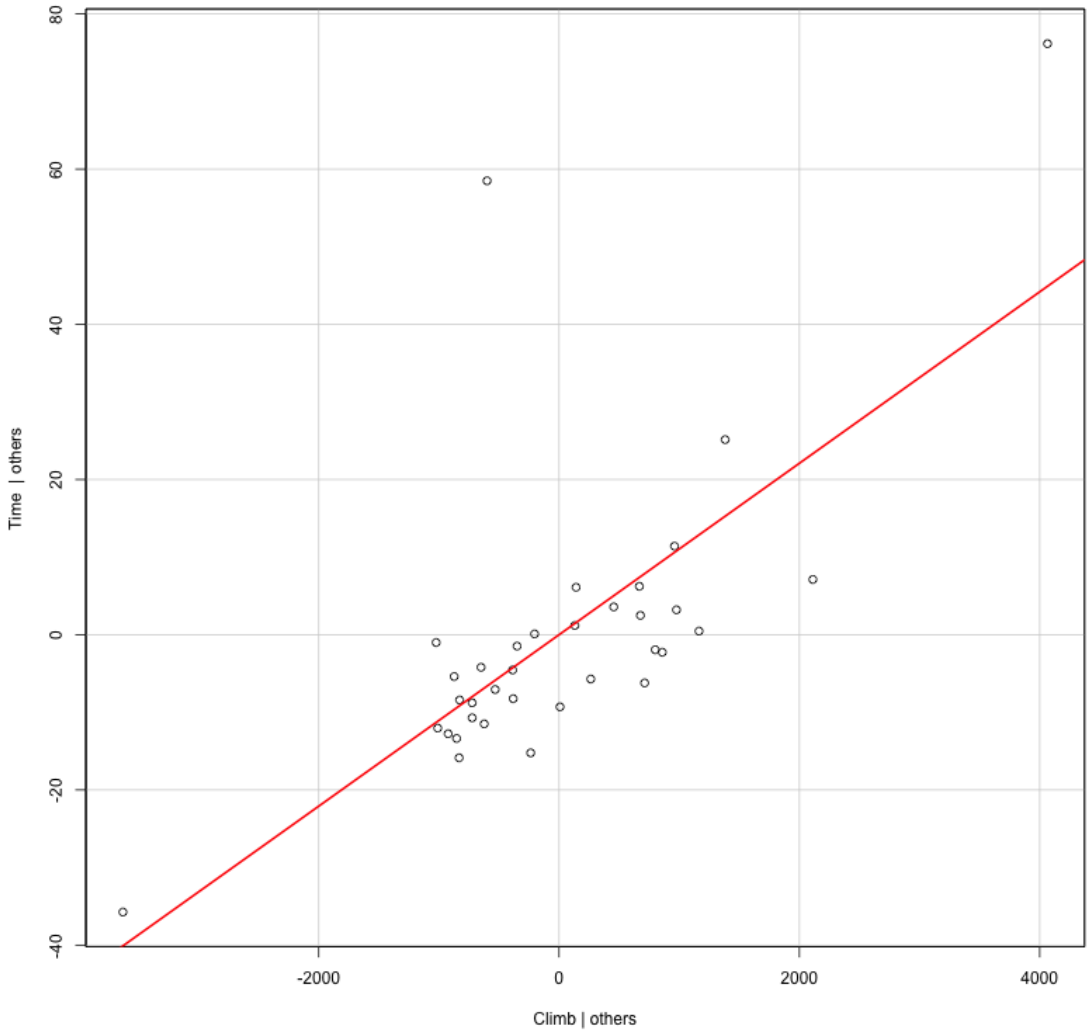
1.17.1 Added variable plots

- The plots can be helpful for finding influential points, outliers. The functions can be found in the `car` package.
- Procedure:
  - Let $\tilde{e}_{X_j,i}, 1 \leq i \leq n$ be the residuals after regressing X_j onto all columns of X except X_j;
  - Let $e_{X_j,i}$ be the residuals after regressing Y onto all columns of X except X_j;
  - Plot $\tilde{e}_{X_j}$ against e_{X_j}.
  - If the (partial regression) relationship is linear this plot should look linear.

```
In [27]: %%R -h 800 -w 800
         av.plots(races.lm, 'Distance')
```



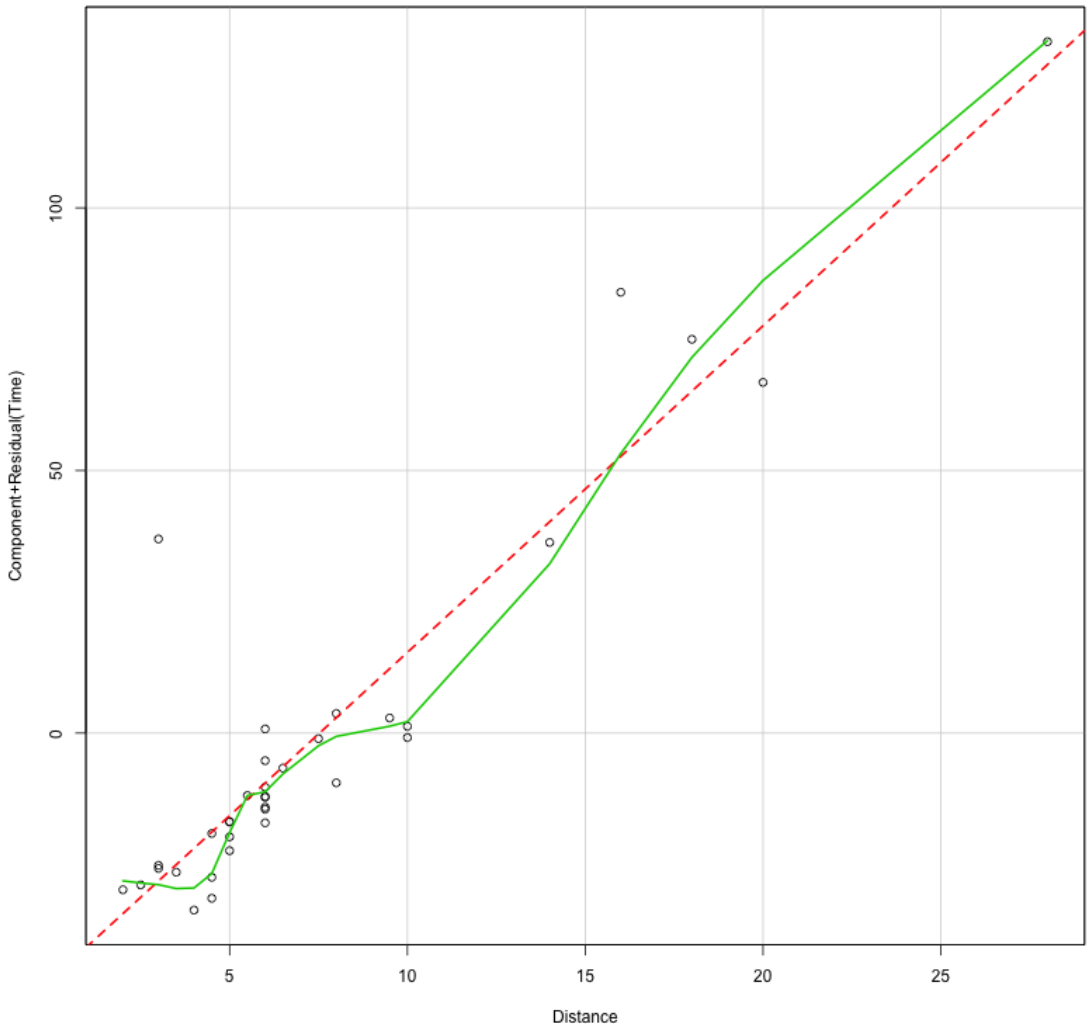
```
In [28]: %%R -h 800 -w 800
         av.plots(races.lm, 'Climb')
```



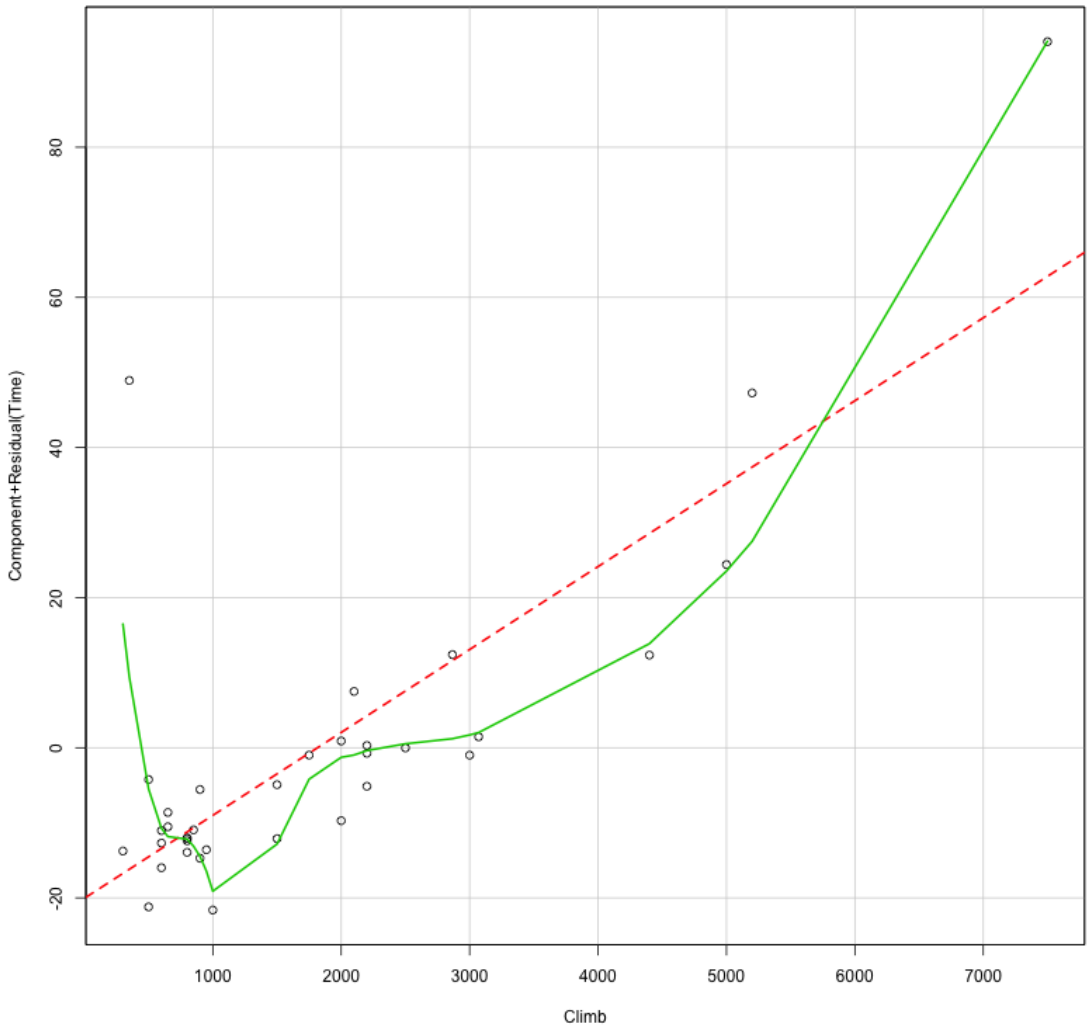
1.17.2 Component + residual plots

- Similar to added variable, but may be more helpful in identifying nonlinear relationships.
- Procedure: plot $X_{ij}, 1 \leq i \leq n$ vs. $e_i + \widehat{\beta}_j \cdot X_{ij}, 1 \leq i \leq n$.
- The green line is a non-parametric smooth of the scatter plot that may suggest relationships other than linear.

```
In [29]: %%R -h 800 -w 800
         cr.plots(races.lm, 'Distance')
```




```
In [30]: %%R -h 800 -w 800
         cr.plots(races.lm, 'Climb')
```


Component+Residual(Time)
80
60
40
20
0
-20
1000
2000
3000
4000
5000
6000
7000
Climb