

Simulation Functions in the DAAG Package

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1 Calibration of Regression Diagnostics

Indications of departures from regression assumptions in diagnostic plots may reflect sampling variation. This is an especial issue for relatively small datasets. Diagnostic plots for a number of sets of simulated data may be an essential aid to judgement. In effect, the observed diagnostic plot is judged against a simulated sampling distribution for such plots.

1.1 A 'simple' straight line regression example

We use data that compares record times for Northern Island hill races between males and females. Data values are not log transformed, precisely because this will show up problems that will largely be avoided if a logarithmic transformation is applied to the data.

The data that are plotted in Figure ?? are, as they stand, problematic for least squares fitting. A least squares line has nevertheless been added to the plot:

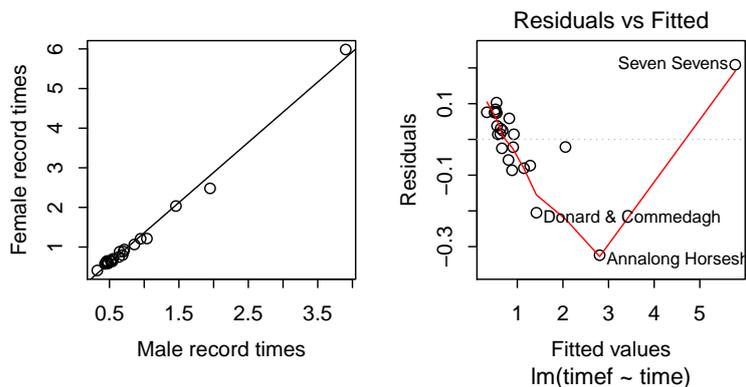


Figure 1: Record times for hill races are compared – females versus males. A least squares line is added. The diagnostic plot of residuals against fitted values (which=1), using the plot method for an lm object, is shown alongside. The “curve” is a crude attempt to identify any pattern in the residuals.

Code is:

```
library(DAAG)
plot(timef~time, data=nihills,
      xlab="Male record times",
      ylab="Female record times")
mftime.lm <- lm(timef ~ time, data=nihills)
abline(mftime.lm)
plot(mftime.lm, which=1)
```

1.2 The function `plotSimScat()`

The function `plotSimScat()` is designed for use with straight line regression. It plots either actual data values and simulated values against the x -variable, or residuals and simulated residuals.

Figure ?? shows four scatterplots that overlay residuals from the actual data with residuals that are simulated from the model. The coefficients used are those for the fitted least squares line, and the standard deviation is the estimate that is returned by R's `lm()` function.

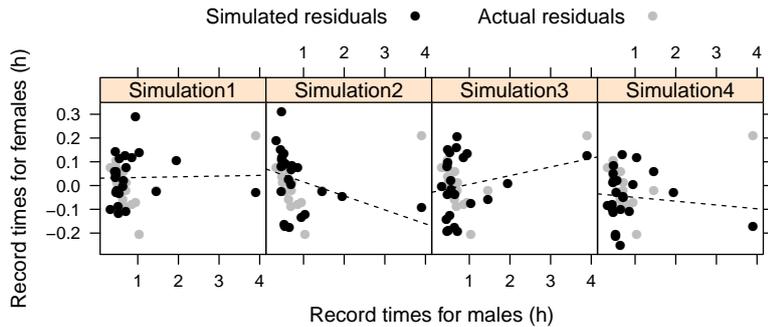


Figure 2: The plots are four simulations of points. The coefficients used, and the standard deviation, are from the fitted least squares line.

The largest simulated value lies consistently above the data value. Code is:

```
mftime.lm <- lm(timef ~ time, data = nihills)
gph <- plotSimScat(mftime.lm, layout = c(4, 1), show = "residuals")
gph <- update(gph, xlab = "Record times for males (h)",
             ylab = "Record times for females (h)")
print(gph)
```

2 Diagnostic Plots for Simulated Data – `plotSimDiags()`

The function `plotSimDiags()` can be used with any `lm` object, or object of a class that inherits from `lm`. For simplicity, the function is used here with a straight line regression object. Here are the diagnostic plots, for the object `mftime.lm` that was created earlier, from use of `plot.lm()`.

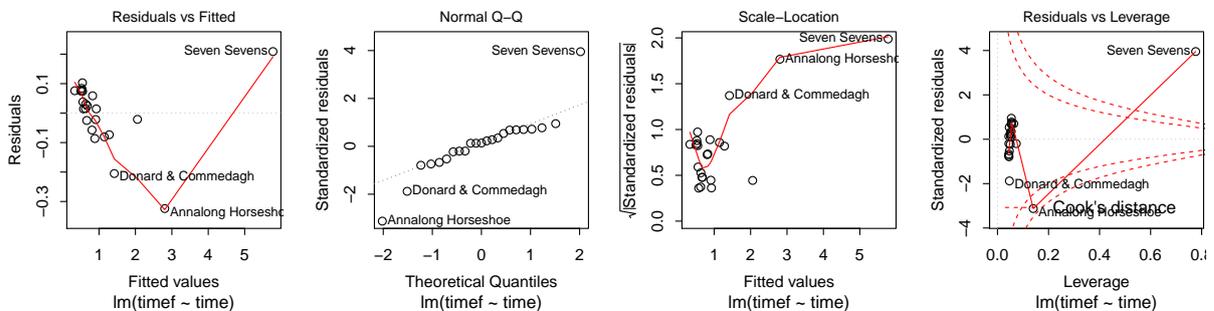


Figure 3: Diagnostic plots from the regression of `timef` on `time`.

Residuals versus fitted values: Figure ?? shows simulations for the first panel (Residuals vs Fitted) above. With just one explanatory variable, the difference between plotting against $\hat{\alpha} + \hat{\beta}x$ and plotting against x (as in Figure ?? using `plotSimScat()`) amounts only to a change of labeling on the x -axis. The plot against x -values in Figure ?? had the convenience that it allowed exactly the same x -axis labeling for each different simulation.

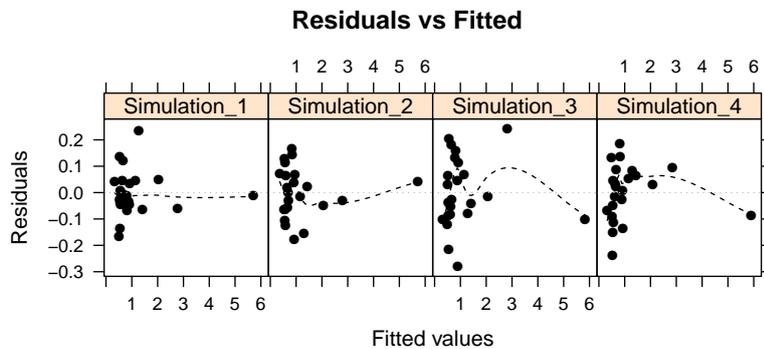


Figure 4: Residuals versus fitted values, for four sets of simulated data.

Code is:

```
plotSimDiags(obj=mftime.lm, which=1, layout=c(4,1))
```

The simulations indicate that, in these circumstances, there can be a pattern in the smooth curve that is added that is largely due to the one data value is widely separated from other data values.

A check for normality: Figure ?? (the second plot) identified two large negative residuals and one large positive residual.

Are the deviations from a line much what might be expected given statistical variation? Figure ?? shows normal probability plots for four sets of simulated data:

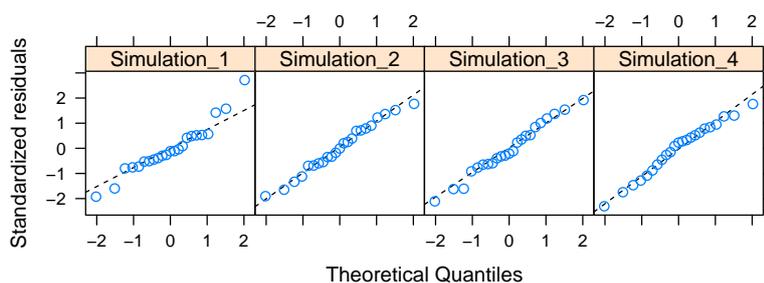


Figure 5: Normal probability plots for four sets of simulated data.

Code is as for Figure ??, but with the argument `which=2`.

Is the variance constant?: At the low end of the range in Figure ?? (the third plot), the variance hardly changes with increasing fitted

value. The sudden bend upwards in the smooth curve is due to the large absolute values of the residuals for the three largest fitted values.

Figure ?? shows the equivalent plots for four sets of simulated data. None of the plots show the same increase in scale with fitted value as in the third panel of Figure ??.

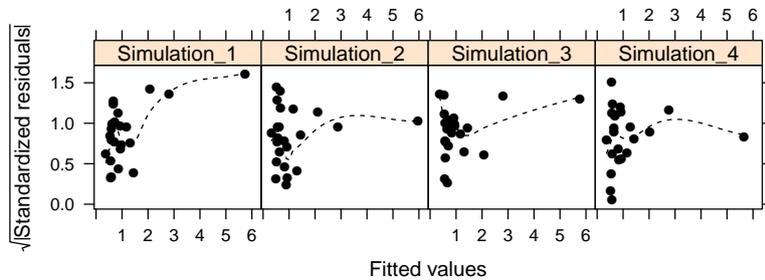


Figure 6: Scale-location plots for four sets of simulated data.

Code is as for Figure ??, but with the argument `which=3`.

Issues of leverage: Figure ?? (the third plot) warned that there are severe problems with leverage, as was already obvious from the scatterplot in Figure ?. Here, there is not much point in doing a simulation. We already know from the previous simulations that the large residual that is associated with the highest leverage point is unlikely to be due to statistical variation.

Here, however, are plots for simulated data:

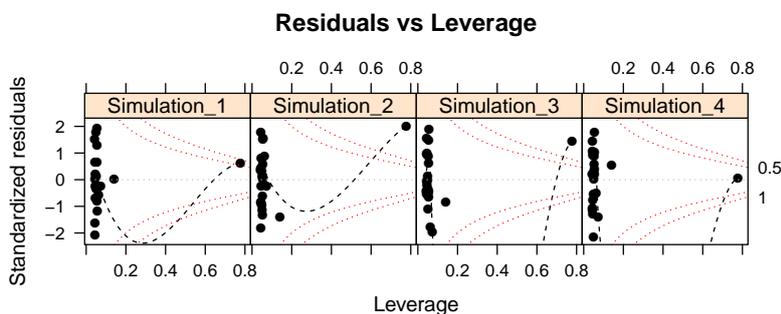


Figure 7: Scale-location plots for four sets of simulated data.

Code is as for Figure ??, but with the argument `which=5`.

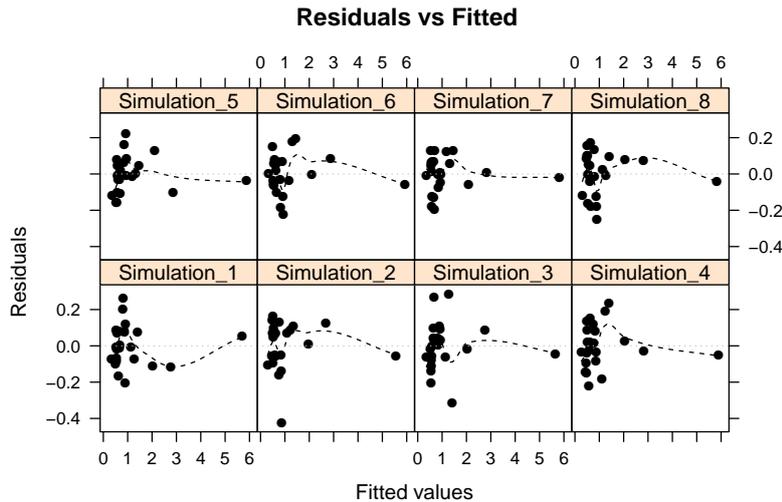
2.1 All 4 diagnostic plots in the same call

Do for example:

```
gphs1to6 <- plotSimDiags(obj = mftime.lm, which = 1:6,
  layout = c(4, 2))
```

Then do, for example:

```
update(gphs1to6[[1]], layout = c(4, 2))
```



This way of proceeding has the advantage that the same simulated data values are used for all diagnostics, without the need to set a prior random number seed.

Further checks: It bears emphasizing that, depending on the nature of the data, there may be further checks and tests that should be applied. Data that have been collected over a significant period of time is an important special case. Departures from a fitted line may well show a pattern with time. The functions `acf()` and `pacf()` should be used to check for autocorrelation in the residuals.

3 Simulation Checks on Stepwise and Related Methods

The function `bestsetNoise()` (*DAAG*) can be used to experiment with the behaviour of various variable selection techniques with data that is purely noise. ?, Section 6.5, pp. 197-198 gives examples from the use of this function. For example, try:

```
bestsetNoise(m = 100, n = 40, nvmax = 3)
bestsetNoise(m = 100, n = 40, method = "backward",
             nvmax = 3)
```

The analyses will typically yield a model that appears to have highly (but spuriously) statistically significant explanatory power, with one or more coefficients that appear (again spuriously) significant at a level of around $p=0.01$ or less.

The extent of selection effects – a detailed simulation: As above, datasets of random normal data were created, always with 100 observations and with the number of variables varying between 3 and 50. For three variables, there was no selection, while in other cases the

“best” three variables were selected, by exhaustive search. Figure ?? plots the p -values for the 3 variables that were selected against the total number of variables. The fitted line estimates the median p -value.

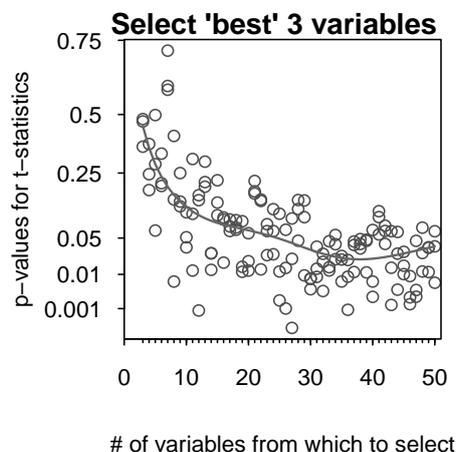


Figure 8: p -values, versus number of variables available for selection, when the “best” 3 variables were selected by exhaustive search. The fitted line estimates the median p -value. The function `bsnVaryNvar()` that is used for the calculations makes repeated calls to the function `bestsetNoise()`

```
## Code
library(DAAG)
library(quantreg)
library(splines)
set.seed(37) # Use to reproduce graph that is shown
bsnVaryNvar(m = 100, nvar = 3:50, nvmax = 3)
```

When all 3 variables are taken, the p -values are expected to average 0.5. Notice that, for selection of the best 3 variables out of 10, the median p -value has reduced to about 0.1.

Similar results will be obtained from use of forward or backward stepwise regression.

References

MAINDONALD, J. H. AND BRAUN, W.J. 2010. *Data Analysis and Graphics Using R – An Example-Based Approach*, 3rd edition, Cambridge University Press.

<http://www.maths.anu.edu.au/~johnm/r-book.html>