The R package `nlstools`: a toolbox for nonlinear regression

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There is an increasing interest in the use of nonlinear regression models in a broad diversity of scientific fields (incl. chemistry, agricultural science, pharmacology, and microbiology). Various **R** functions are already dedicated to the fit of nonlinear models (Ritz & Streibig, 2008). The basic routine that provides nonlinear least squares estimates is the function `nls` from the `stat` package. The relative complexity of use of nonlinear optimization algorithms may prevent non-statisticians of using these models.

Unlike in linear regression, the fit of nonlinear models requires a great deal of attention regarding the definition of the starting values from which the algorithm will start its least-squares minimization procedure. Important issues associated with nonlinear regression relate, for example, to the assessment of the validity of the error model, the estimation of the parameters' confidence regions and confidence intervals, the identification of influencing observations (Bates & Watts, 1988; Huet et al., 2004). The available nonlinear regression modules lack some of these diagnostic functionalities, and there is a need to provide users with an extended toolbox of functions.

We developed the package `nlstools` which helps users to fit nonlinear regression models and provides a unified framework to test the error model assumptions and assess the quality of fit of the model. `nlstools` is designed to work directly with `nls` objects. This package includes a set of functions and graphical tools that will assist the user in creating `nls` objects and carrying out various diagnostics tests. These functions are organized as follows:

- Preparation of the fit of nonlinear regression models with `nls`: `preview`

- Summary of fit: `plotfit`, `overview`

- Validity of the error model assumptions: `nlsResiduals`

- Parameter's estimates confidence regions: `nlsConfRegions`, `nlsContourRSS`

- Confidence intervals and influencing observations using resampling techniques: `nlsBoot`, `nlsJack`

- Various examples of nonlinear regression models and illustrative datasets

Overall, the **R** package `nlstools` constitutes a useful add-on toolbox for nonlinear regression diagnostics. It is available on CRAN. Future developments are currently under way.

References

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