Dose-response modelling using R

Christian Ritz

Faculty of Life Sciences, University of Copenhagen, Denmark

Rennes, July 8 2009
Package overview: \texttt{drc}

Principal idea: \textbf{use of self starter functions}

Model fitting function: \texttt{drm()}

- \textit{Feel} and interface much like \texttt{lm()} and \texttt{glm()}
- Response: continuous, count, or quantal
- One or more curves separately/simultaneously
- Parameter constraints possible

Methods: \texttt{anova, plot, predict, summary ...}
Applications

Some examples:

- **Hearing and speech science**
  - Estimation of psychometric functions

- **Screening of drugs**
  - Analysis of high-throughput dose-response data

- **Toxicity tests**
  - Estimation of effect concentrations
    (e.g. EC/ED/LC/LD50)

- **Weed science**
  - Modelling seed germination, yield loss
Elaborate infrastructure

Off-the-shelf model functions:

- **Symmetric**: log-logistic, log-normal (*Hill*)
- **Asymmetric**: Richards, Weibull models (2 types) (*also Gompertz*)
- **Other**: binary mixtures, fractional polynomials, hormesis models (*e.g. Brain-Cousens*)

Full flexibility in model specification:

- Special cases obtained by fixing parameter values
- **Examples**: asymptotic regression, exponential decay, logit, Michaelis-Menten, probit
Special functions

**After-fitting:** Accessing parameters of interest:

- \( \text{ED}() \), \( \text{SI}() \) – estimated effect concentrations
- \( \text{MAX}() \) – maximum hormesis effects
- \( \text{yieldLoss}() \)

Other useful functions:

- \( \text{compParm}() \) – comparison of parameters
- \( \text{maED}() \) – model-averaging
- \( \text{rdrm}() \) – simulation of dose-response models
Visualization – traditional graphics
Future developments

This is a **dynamic** package community

Ongoing work:

- Bootstrap and other types of confidence intervals
- Extending mixed model capabilities
- Handling other types of response
- Robustifying starting value procedures
- Variance modelling
- Visualization using **lattice**