A CRAN-based model development and reporting paradigm for NONMEM

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Objectives: Model development and reporting for NONMEM [1] can be organizationally daunting. Run management can be addressed by third-party tools [2-3] and reporting is greatly simplified by scripted approaches [4-5]. However, the ubiquity of R makes attractive a CRAN-based solution [6]. My objective was to create a paradigm that minimizes installation requirements, organizes metadata for model inputs and outputs, formalizes relationships among individual models, and maximizes availability of reporting features.

Methods: R Markdown [7] was chosen as the script format for its familiarity and support. An existing tab-delimited metadata format [8] was adopted to document NONMEM model inputs.   An R package [9] was developed to interconvert between NONMEM control streams and equivalent R objects, giving programmatic read/write access to model details.   Functions were included to modify models and extract model results.   By convention, models use problem statements consisting of the name of a reference model and a related feature difference; model parameters and tabled items are documented in the control stream.

Results: All additional software is acquired from CRAN in R by executing "install.packages('nonmemica')". NONMEM models are linked to each other through their problem statements; lineages may be succinctly summarized as run logs and parameter tables. A single function call merges tabular inputs, outputs, and metadata. Model files may be modified manually or programmatically. Output can be viewed at the console or rendered in any format supported by R Markdown, such as Word or PDF; reporting features for the latter include table of contents, list of tables, list of figures, linked table/figure captions, nested section headings, equations, and references.

Conclusions: A CRAN-based NONMEM model development and reporting paradigm was implemented that enabled flexible, interactive access to model details as well as a rich set of reporting features for a variety of formats.   The paradigm emphasizes scripted reporting by means of R Markdown and makes systematic use of metadata for model inputs and outputs. Using this paradigm, modelers may develop and report analyses efficiently and reproducibly using familiar technology.

References:
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