Mathematical modelling of the environment - are there enough data?

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Dynamic mathematical models are commonly applied to analyse ecological and biogeochemical data. They allow a.o. to estimate immeasurable quantities, such as reaction rates and fluxes, with the ultimate goal to acquire some predictive capabilities.

Whereas the most complex models are solved by numerical integration of differential equations to obtain rates, the data requirements for applying such models are large. In many real-life applications, essential observations are lacking to obtain a complete picture and the model needs to be simplified in order to still make some sense out of the data. The ultimate simplification is to express the natural system in terms of linear (mass balance) equations, without the need to specify rate equations or to find kinetic parameters.

Which modeling technique is chosen has great implications on the way the model is solved, and in order to deal efficiently with incomplete data sets, a flexible (mathematical) repertoire for model application is required. There are many good reasons to perform ecological modeling in a software package strong in statistics and graphical output (i.c. R), not in the least because of the extensive pre- and post-processing required by these models. Since the introduction of R-package **odesolve** (Setzer, 2001) that offered a numerical integration routine, R has been promoted as a platform to perform dynamic model simulations (Petzoldt, 2003).

To broaden the scope of models that R can deal with, several other packages were recently created, performing certain mathematical tasks or providing utilities to facilitate the modeling process or the confrontation of models with data.

An overview of several modeling types and how to solve them in R, will be given. Although the emphasis will be on environmental models, the techniques presented have a much wider scope.

References

Petzoldt, T. (2003). R as a simulation platform in ecological modelling. *R News*, 3(3):8–16.

Setzer, R. W. (2001). *The odesolve Package: Solvers for Ordinary Differential Equations*. R package version 0.1-1.

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