Title: r3PG – an R package for simulating forest growth using the 3-PG process-based model

Running Head: The r3PG R package

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Abstract

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1. Process-based forest models (PBMs) are important tools for quantifying forest growth and vulnerability, particularly under climate change. The 3-PG model (Physiological Processes Predicting Growth) is one of the most widely used forest growth simulators for this purpose worldwide.

2. Here, we present r3PG, a new Fortran implementation of 3-PG, wrapped into an R package. r3PG can simulate monospecific as well as mixtures of evergreen and deciduous tree species in even-aged or uneven-aged stands.

3. The combination of Fortran functions with an R interface makes the model extremely fast. This facilitates the use of r3PG for extensive computer experiments and sensitivity analysis. We demonstrate this in a case study including i) single model runs; ii) a sensitivity analysis and a full Bayesian calibration of the model, and iii) spatial simulations of forest growth across Switzerland.

4. r3PG is faster and easier to use than previous implementations of 3-PG in visual basic. We believe that this will make 3-PG even more useful and popular for ecologists and climate change scientists.

Introduction

Forest growth models are widely used by practitioners and scientists to project forest productivity, management effects, and vulnerability, particularly under climate change. Currently, there are more than 50 different forest growth models in use, which operate at different temporal and spatial scales (Fontes et al., 2010; Pretzsch, Forrester, & Rötzer, 2015). One of the most popular models worldwide is the Physiological Processes Predicting Growth (3-PG) model (Landsberg & Waring, 1997). Its relatively simple structure, readily obtainable input data, and a relatively low number of parameters have facilitated the widespread use of 3-PG in many forest types as described in at least 90 international peer-reviewed articles in ISI-

listed journals published from 1997 to 2017 (Gupta and Sharma, 2019).

Despite its popularity, currently available 3-PG implementations had limitations that prevented a seamless integration of the model into the typically R-centered workflow of data-oriented ecologists. 3-PG was originally designed for monospecific, evenaged and evergreen forests and implemented in Visual Basic (Sands, 2010). This model implementation was recently extended to also describe deciduous, uneven-aged or mixed-species forests (Forrester & Tang, 2016) and to calculate wood $\delta^{13}\text{C}$ (Wei et al., 2014). These Visual Basic versions did not easily interface to R and were relatively slow, which made runtime-intensive calculations, such as calibrations or sensitivity analyses (e.g. Hartig et al., 2012) challenging. Several recent studies that calibrated 3-PG or made larger spatial simulations (e.g. Augustynczyk et al., 2017; Thomas et al., 2017; Trotsiuk et al., 2020) therefore used Fortran re-implementations of 3-PG. These, implementations however, were not designed for “end users” with appropriate help and instruction files, were not made available on the comprehensive R archive network (CRAN), and did not include the above-mentioned extensions of the model for deciduous, uneven-aged or mixed-species forests.

Here, we present r3PG, a newly developed R package, which provides a flexible and user-friendly R interface for Fortran re-implementations of 3-PG, including important extensions. With the package, users can conveniently start model simulations from R (R Core Team, 2018), and flexibly switch between various options and submodules. In the remainder of this article, we give a short description of the model and explain the structure of the r3PG package, followed by three case studies which demonstrate the basic functionality of the package, performs a sensitivity analysis and a Bayesian calibration of the model, and use the calibrated model to simulate forest growth across Switzerland.

The 3-PG model

3-PG describes the development of a forest stand via five sub-modules: light, productivity, water, allocation and mortality. These sub-modules update the forest structure in monthly time steps (Fig. 1). The *light* sub-model calculates light absorption using species-specific light extinction coefficients and leaf area index. The horizontal canopy structure is quantified using the fractional ground cover of the canopy (Landsberg, & Sands, 2011). The 3-PG extension for species mixtures calculates the light absorption of each species or age class by considering the vertical and horizontal structure of the canopy, and can be used for deciduous as well as evergreen species (Forrester & Tang, 2016). In this case, the horizontal canopy structure depends on the leaf area of the given canopy layer, crown architecture and latitude (Forrester & Tang, 2016). The consideration of the canopy structure also allows the calculation of vertical gradients in radiation, vapor pressure deficit (VPD) and aerodynamic conductance. The *productivity* sub-model calculates gross primary productivity (GPP) based on a species-specific canopy quantum efficiency (α_c) that is reduced due to limitations imposed by temperature, frost, VPD, soil moisture, soil nutrient status, atmospheric CO₂ and stand age (Landsberg & Waring, 1997; Sands & Landsberg, 2002; Almeida, Landsberg, & Sands, 2004). Net primary productivity (NPP) is then calculated as a constant fraction of GPP (Waring, Landsberg, & Williams, 1998). In the *water* sub-model, the Penman–Monteith equation is used to calculate tree transpiration and soil evaporation and, together with canopy interception, predicts evapotranspiration. Here, the wood's $\delta^{13}\text{C}$ fraction can be calculated to facilitate comparison to field observations (Wei et al., 2014). The *allocation* sub-model distributes NPP to roots, stems and foliage depending on soil nutrient status, VPD and soil moisture. The *mortality* sub-model calculates density-dependent mortality based on the $-3/2$ self-thinning law by Yoda (1963) and density-independent mortality, e.g. caused by pests, diseases or drought (Sands, 2004; Gonzalez-Benecke, Jokela, Cropper, Bracho & Leduc, 2014). After each time step, the simulated biomass is converted into output variables such as mean tree diameter,

height, basal area, wood volume, size distributions etc., using allometric relationships. Thinning, defoliation and irrigation can also be performed at this step if desired. For a more detailed description, published parameter sets and information about measurements needed to calculate each parameter, see Forrester (2020).

Figure 1 The 3-PG model structure. Processes are calculated in monthly time-step, and are forced by standard climatic variables.

The r3PG package

We re-implemented all major published sub-modules and functions of 3-PG in Fortran 95 (Adams, Brainerd, Martin, Smith, & Wagener, 1997). This implementation is particularly relevant for parallel computing while performing large scale, spatial simulation (see case studies). Unlike previous implementations of 3-PG in Fortran (Minunno, Hartig, & Trotsiuk, 2019; Thomas et al., 2017), R (Griffith, Still, & Kim, 2018) or JavaScript (Merz & Hart, 2016), our code implements major available extensions. We confirmed that model results are numerically identical to their original Visual Basic implementations in the unit tests of the R package (Wickham, 2011). The package contains a vignette, as well as help files, which will

be the best starting point for an up-to-date overview about the available functions and their use in the future.

Case studies

Single model runs

To demonstrate the functionality of the r3PG R package, we first simulate the growth of a 40-year-old mixed *Fagus sylvatica* and *Pinus sylvestris* stand for a period of 15 years (Fig. 2). The initial conditions and parameters were based on Forrester et al. (2017) who used 3-PG to examine the growth of *P. sylvestris* and *F. sylvatica* mixtures along site and climatic gradients. The code for this and all further examples, together with additional comments for the user, is provided in the package vignette (accessible via <https://cran.r-project.org/web/packages/r3PG/vignettes/r3PG-ReferenceManual.html>).

Figure 2 15-yr projections of stand structure and above- and belowground dry biomass for a mixed *F. sylvatica* and *P. sylvestris* stand using the 3-PG model.

Sensitivity analysis and Bayesian calibration

As a second case study, we calibrate the model for the Solling flux site, which is dominated by *Picea abies*. We obtained data for this site via the PROFOUND database for evaluating vegetation models and simulating climate impacts on forests (Reyer et al., in press).

We first performed a Morris screening (Morris, 1991) to determine which of the 52 model parameters are most influential for the model fit at this particular location (for details, see r3PG vignette). We calculated scaled Morris indices, meaning that sensitivities were scaled to the uncertainty of each parameter. As target variable for the screening, we used the fit to the observed data, expressed by the log-likelihood with normal (Gaussian) error assumptions for all six observed variables (basal area, DBH, height, stem biomass, root biomass, foliage biomass). The results from the Morris sensitivity analysis (Fig. 3) were comparable to previous studies (Esprey, Sands, & Smith, 2004; Xenakis, Ray, & Mencuccini, 2008; Forrester & Tang, 2016; Augustynczyk et al., 2017), highlighting that the parameters related to biomass partitioning, stand properties, and canopy properties are particularly important/sensitive for model performance.

Figure 3 Results from the Morris sensitivity analysis. The 52 parameters and 6 error parameters are listed on the x-axis. A high μ^* indicates a factor with an important overall influence on model output; a high σ indicates heterogeneity of the sensitivity across the parameter space,

which could indicate nonlinearities or interactions with other parameters. Higher μ^* also tends to produce larger σ , so σ should be interpreted relative to μ^* .

We selected the 20 most sensitive parameters based on Morris screening for calibration. We used the Differential Evolution Markov Chain Monte-Carlo algorithm (DEzs MCMC, Braak & Vrugt, 2008), implemented in the BayesianTools R package (Hartig, Minunno, & Paul, 2019) to estimate the joint posterior distribution for the model parameters, using the log-likelihood described earlier, and the same (uniform) priors that were used as uncertainty in the Morris screening. We ran three independent DEzs MCMC runs, each with three internal chains, for 5×10^6 iterations, which took 35 hours on our cluster. Convergence of the MCMCs was assessed via visual inspection of the trace plots and Gelman-Rubin diagnostic (Gelman & Rubin, 1992; McElreath, 2020), with convergence being accepted when the multivariate potential scale reduction factor was ≤ 1.1 . To evaluate the model performance, we calculated posterior predictive distributions by running the model with 500 random samples from the parameters' posterior distribution (Fig. 4).

Figure 4 Simulations of stand structural properties and above- and belowground dry biomass using default (orange) and calibrated (green) parameters for *P. abies*. The posterior predictive uncertainty (shaded green) was calculated by drawing 500 parameter combinations from the posterior distribution. The black dots represent the measured observational data.

Spatial simulations

As a third case study, we simulated *P. abies* stand biomass in monocultures with associated uncertainties for the forested area of Switzerland on a 1×1 km grid. The stands were initialized as 2-year-old plantations with an initial density of 2,500 trees ha⁻¹ and simulated until the age of 30 years under the average climate observed during the 1961–1990 period. The mean simulated stem biomass at age 30 was 115 Mg dry mass ha⁻¹, with the most productive areas located in the lowlands of Switzerland (Fig. 4a).

Figure 4 (a) Posterior mean predictions of stem biomass stocks for 30-year-old stands planted in 1960. (b) 95% posterior predictive credible interval for the biomass predictions.

Conclusions

The r3PG R package provides a faster and more convenient integration of several major 3-PG variants. It facilitates model-data integration with heterogeneous observational data, complex computer experiments, and access to advanced statistical tools in the R environment. With the faster model, sensitivity analysis and Bayesian calibration with r3PG can narrow down model uncertainties and allow faster and easier model parametrization for new tree species. With our new R package, all these tasks can also be performed for mixed and uneven-aged stands, which was previously hard or not possible. Finally, the ability to run 3-PG directly from within R, fosters transparent reporting of the computational protocol and reproducibility of simulation results.

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Author’s contributions

V.T., F.H., and D.F. conceived the study. V.T. implemented the model and the R package, and performed the analysis, with contribution from D.F. and F.H. All authors jointly wrote the manuscript.

Availability

The r3PG R package source code is publicly available via *The Comprehensive R Archive Network* (CRAN) <https://cran.r-project.org/web/packages/r3PG/index.html> or via <https://github.com/trotsiuk/r3PG>. The forest growth data for the Solling site can be obtained from the PROFOUND database (Reyer et al., in press). The climatic data for simulations on the Swiss scale were provided by the Landscape Dynamics group (WSL, Switzerland). Data required to reproduce the analysis are provided in the r3PG R package.

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