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Bayesian calibration of simple forest models with multiplicative mathematical structure: A case study with two Light Use Efficiency models in an alpine forest

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ABSTRACT

Forest models are increasingly being used to study ecosystem functioning, through simulation of carbon fluxes and productivity in different biomes and plant functional types all over the world. Several forest models based on the concept of Light Use Efficiency (LUE) rely mostly on a simplified mathematical structure and empirical parameters, require little amount of data to be run, and their computations are usually fast. However, possible calibration issues must be investigated in order to ensure reliable results.

Here we addressed the important issue of delayed convergence when calibrating LUE models, characterized by a multiplicative structure, with a Bayesian approach. We tested two models (Prelued and the Horn and Schulz (2011a) model), applying three Markov Chain Monte Carlo-based algorithms with different number of iterations, and different sets of prior parameter distributions with increasing information content. The results showed that recently proposed algorithms for adaptive calibration did not confer a clear advantage over the Metropolis–Hastings Random Walk algorithm for the forest models used here, and that a high number of iterations is required to stabilize in the convergence region. This can be partly explained by the multiplicative mathematical structure of the models, with high correlations between parameters, and by the use of empirical parameters with neither ecological nor physiological meaning. The information content of the prior distributions of the parameters did not play a major role in reaching convergence with a lower number of iterations.

We conclude that there is a need for a more careful approach to calibration to solve potential problems when applying models characterized by a multiplicative mathematical structure. Moreover, the calibration proved time consuming and mathematically difficult, so advantages of using a computationally fast and user-friendly model were lost due to the calibration process needed to obtain reliable results.

1. Introduction

Gross Primary Production (GPP) is a key component of the terrestrial ecosystem carbon balance (Chapin III et al., 2006; Nagy et al., 2006), representing the amount of CO_2 assimilated by photosynthesis per unit of time (Waring et al., 1998). The Eddy-Covariance (EC) technique (Burba, 2013) is one of the most commonly used approaches to calculate GPP at the ecosystem level: this method computes the net CO_2 turbulent flux between a given ecosystem and the atmosphere (Net Ecosystem CO_2 Exchange, NEE), and subsequently derives Ecosystem Respiration (ER) and GPP through the application of partitioning methods (Lasslop et al., 2010; Reichstein et al., 2005; van Gorsel et al., 2009). However, there are several theoretical assumptions (Burba and Anderson, 2010) that can seriously limit its application in topographically complex environments, and its estimates are limited to the footprint of the EC tower. GPP is also increasingly being estimated using remote sensing applications (Still et al., 2004; Wisskirchen et al., 2013; Zhang and Kondragunta, 2006): as an example, the MODerate

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Imaging Spectroradiometer (MODIS) sensor was designed in part for that purpose (Running et al., 2000). These latter methods have the clear advantage of covering very wide areas; on the other hand, they need to be validated by ground measurements in order to ensure the reliability of the data (i.e. due to cloud cover, or to the spatial and temporal aggregation processes). For those reasons, despite extensive efforts and several techniques tested, GPP quantification remains challenging in most ecosystems. Therefore, extensive modelling techniques have been applied to assist GPP estimates.

Nowadays, GPP is one of the central outputs of many forest ecosystem models (De Weirdt et al., 2012; Mäkelä et al., 2000; Tjiputra et al., 2013), most of which are detailed, multi-variable models that need much environmental information and careful parameterization before they can be run (Landsberg and Waring 1997). The modelling approach developed by Farquhar et al. (1980) is one of the most commonly applied to estimate GPP in forest modelling, but it is not free of disadvantages (van Oijen et al., 2004; Yin et al., 2004): its parameters are difficult to infer and have no physical meaning at the canopy scale, being chloroplast parameters with validity up to the leaf level only. Therefore, a process of simplification started in the 90′s (White and Running 1994; Landsberg and Waring 1997) with the aim of developing models that could be of use in applied forest management.

A widely-used group of simple models for GPP is based on the concept of Light Use Efficiency (LUE), defined as the ratio of GPP to Absorbed Photosynthetically Active Radiation (APAR). These models assume that vegetation has a potential LUE (which can be described as the ability of plants to use light for photosynthesis in absence of limiting factors), decreased by modifying factors that account for suboptimal conditions for photosynthesis (Landsberg and Waring, 1997; McMurtrie et al., 1994). GPP is then calculated as the product of LUE, incoming radiation, and modifiers, creating a quasi- or totally multiplicative mathematical structure. There are several LUE-based models in the existing literature: for example C-Fix (Veroustraete et al., 1994), 3PG (Landsberg and Waring 1997), Prelued (Mäkelä et al., 2008), and the Horn and Schulz (2011a) model. These models are often considered simpler and more “user-friendly” than process-based models (Landsberg and Waring 1997): they rely on few equations of simplified physiological processes, few often empirical parameters, do not require high computational power or many data to be run, and the computations are usually fast. On the other hand, their simple structure is likely to cause high correlation between parameters, leading to difficulties in calibration and ultimately to unreliable results and predictions (Bagnara et al., 2015). This is particularly true for the Prelued model (Mäkelä et al., 2008): despite its successful application in several biomes and plant functional types (Bagnara et al., 2015; Mäkelä et al., 2008; Peltoniemi et al., 2012), Bagnara et al. (2015) highlighted some calibration issues (possibly due to its multiplicative structure) that are likely to impair the reliability of the results and predictions, even in the presence of a very good fit to the data.

To our knowledge, calibration issues are not usually properly addressed in studies that apply LUE models: those studies evaluate the models’ performance based only on their ability in reproducing the data, while little attention is given to the calibration process that generated those results. Therefore, there is no guarantee that calibration issues are specific to Prelued and not a general limitation to the application of LUE models. To answer this crucial point, we selected the model developed by Horn and Schulz (2011b) (as described in Horn and Schulz (2011a)) as a second LUE-based model to compare with Prelued in terms of convergence efficiency. This is a LUE model with the same time scale as Prelued’s, same number of parameters to avoid issues related to different dimensionality of parameter space, and comparable prior information about parameter values. The main difference between these two models is in their mathematical structure: overall, the structure of this latter model is slightly less multiplicative than Prelued, which should facilitate its calibration.

The Bayesian approach to calibration has become more and more popular in the last few years to obtain insights on both model predictions and uncertainties. This approach has been widely used in the past in different fields, and recently it has been applied to different kinds of ecosystem models, focusing on both croplands (Zhu et al., 2014) and forests (van Oijen et al., 2005; Svensson et al., 2008; Chevallier et al., 2006; van Oijen et al., 2011; van Oijen et al., 2013). Even so, the application of the Bayesian method to LUE-based models is not as common as its application to process-based models, with very few studies heading in this direction (Still et al., 2004; Xenakis et al., 2008; Bagnara et al., 2015). The main characteristic of a Bayesian calibration is that it quantifies model inputs and outputs in the form of probability distributions, and applies the rules of probability theory to update the distributions when new data are obtained (Sivia, 1996; van Oijen et al., 2005). In recent years, the increase in affordable computational power has allowed the Markov Chain Monte Carlo (MCMC) technique to become a popular choice for sampling the joint posterior probability distribution for the parameters of models. MCMC has a number of advantages for our purposes over other approaches that have been used for Bayesian Calibration, such as the adjoint method (Zhu et al., 2014) or the Kalman filter (Gao et al., 2011). These latter methods are special cases of Bayesian calibration (Wikle and Berliner, 2007), where a prior probability distribution for parameters is specified and updated using Bayes Theorem. However, they require assumptions of linearity and Gaussian distributions that are restrictive and inappropriate in the case of the highly nonlinear models that we study here. In contrast, the MCMC method allows for any type of prior and posterior distribution, including asymmetric and multimodal ones. Moreover, the sample from the posterior distribution generated by MCMC represents the full posterior probability distribution (in contrast to the adjoint method which only provides an estimate of the mode) and uncertainties can only be assessed fully with such global methods. The efficiency of the MCMC technique is highly dependent on the model structure (Browne et al., 2009; Gilks and Roberts, 1996): the high correlations between parameters induced by a multiplicative model structure generally make the convergence of the MCMC more difficult, impairing the reliability of the results of the calibration. Another important factor for the success of the MCMC is the *a-priori* information on the model parameters: poorly defined parameters, empirical parameters, or the lack of information in the existing literature force the modeller to assign non-informative prior distributions, which makes the calibration more difficult and time-consuming (Hartig et al., 2012). Different methods have been implemented to avoid or reduce such problems: the use of very long chains (Geyer, 1992; Gilks et al., 1996), model re-parameterization to avoid strong correlations (Buzzi-Ferraris and Manenti, 2010; Gilks et al., 1996), and the use of more efficient algorithms (Gilks et al., 1996; ter Braak, 2006). In this context the term “efficiency” can be ambiguous: for example, ter Braak (2006) calculates efficiency considering the mean square errors of different algorithms, but it can also be considered as the proper sampling from a posterior distribution (thus related to the acceptance rate). In this particular study, we considered efficiency as the capability of the algorithm to identify the convergence region minimizing the number of model evaluations, i.e. maximizing the speed of convergence.

This work aims at 1) identifying and solving possible and previously undetected calibration issues related to the multiplicative mathematical structure typical of LUE-based models; 2) assessing the importance of prior information on parameter values, and 3) determining if those issues are limited to a single model or affect the entire class of LUE models. We applied a Bayesian calibration with different algorithms, number of iterations, and different sets of prior distributions both to Prelued and to the Horn and Schulz (2011a) model employed as case studies, calibrating them over one year of daily GPP data from an EC tower in the Italian Alps.