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Biogeosciences Discussions

Interactive comment on "Modeling the vertical soil organic matter profile using Bayesian parameter estimation" *by* M. C. Braakhekke et al.

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1 General comments

Braakhekke et al. present an application of a soil organic carbon (SOC) turnover and transport model (SOMPROF, previously introduced by the same authors) to two sites that differ greatly in terms of pedology and vegetation, and consequently, also in terms of the processes that govern the formation of the soil organic matter profile. They used various types of observations, among these a fallout radioisotope, to calibrate the model using Bayesian parameter estimation.

I read this manuscript with great interest. It is very well written, clear, balanced, and easy to follow. The authors did a great job in developing this model, which I think will be of great benefit and may help to improve current knowledge and understanding of SOC turnover and transport processes in the soil profile. This work nicely illustrates the difficulties that typically arise when applying such sophisticated, process-based models. Using Bayesian techniques, however, the authors also show how to deal with these difficulties.

My review is intended to complement the referee comments given on the previous version of the manuscript. I found that these comments have been addressed adequately. Therefore, I focused my review on statistical and technical aspects of the present manuscript, which have not been covered by the previous comments.

2 Specific comments

(2.1) The presentation of Bayes' theorem should be revised. I am aware of the referee comment on this topic given by Marcel van Oijen on the previous version of the manuscript and the changes made in response to this comment. I think, however, that these changes went in the wrong direction. The probability density of the observations given the parameters (which can be interpreted as the likelihood of the parameters) should be written as $P(\mathbf{O}|\theta)$. The order of the arguments is important in this context and cannot be switched, as it was done in the current version of the manuscript. I propose to write Bayes' theorem as $P(\theta|\mathbf{O}) = cP(\theta)P(\mathbf{O}|\theta)$, which is actually very close to the equation given in the previous version of the manuscript, except that L is replaced with P for the likelihood term.

(2.2) There is a misconception in the definition of the uncertainty model. This model accounts for the stochastic nature of the model residuals, not of the observations! This makes a fundamental difference and deserves special attention because any wrong assumption made here will propagate into the results and may distort them. A common assumption often made in inverse modelling – and a reasonable starting point – is that the model residuals are independent and identically distributed following a normal distribution. This assumption has been shown to hold approximately true for a wide range of environmental models (even so the independence assumption is sometimes violated). I strongly recommend to repeat the Bayesian analysis using a normal likelihood function. In addition, I recommend to check whether this assumption was actually justified. This can be tested a posteriori (see, for example, Scharnagl et al., 2011, Hydrology and Earth System Sciences, 15:3043-3059). I am quite sure that these a posteriori tests would indicate that the log-normal likelihood (based on misleading assumptions) used in the present study was actually inadequate and should be revised.

(2.3) There is another misconception in the use of σ, which was interpreted here as the standard deviation of the observations. This is only true if the model is correct and all forcing and additional input variables are perfectly known. This, of course, is never the case when dealing with real-world problems. In fact, σ represents the standard deviation of the residuals, which is always larger than that of the observations, sometimes even substantially larger. The reason for this is that inadequacies in the model structure and uncertainties in the input variables will generally lead to some systematic misfit that adds to the uncertainty stemming from observational errors. This has two important practical implications. First, the actual value of σ is typically unknown a priori. Using the standard deviation of the observations instead, as it was done in this study, results in a likelihood function that is overly sharply peaked. One of the consequences is that the information content of the measurements is overestimated, and hence, the uncertainty in the estimated parameters is underestimated. Another consequence is that jumps from one mode to another become more difficult. The authors encountered exactly this problem, even though they used an MCMC algorithm that was especially designed to facilitate such inter-modal jumps (Laloy and Vrugt, 2012). Second, since the standard deviation of the residuals is not known a priori, we have to take special measures to deal with this situation. One option is to treat σ as an additional unknown parameter that needs to be estimated simultaneously with the other parameters. Another option, which is frequently applied in Bayesian parameter estimation, is to integrate σ out of the likelihood function assuming a special type of prior distribution for σ. More detailed information on this last issue appears, for example, in Scharnagl et al. (2011, Hydrology and Earth System Sciences, 15:3043-3059) and the literature cited therein.

(2.4) The description of the MCMC scheme given in Appendix A made me puzzled. I do not understand why the authors used the Metropolis-Hastings ratio (Eq. A1) instead of the Metropolis ratio. My questions are the following: First, if (some of) the parameters are transformed, the Markov chain samples the transformed parameter space, right? Consequently, the transformed parameters must be used in the Metropolis ratio. The notation of Eq. A1 suggests, however, that the untransformed parameters were used. Is that really true? And if so, why? Second, the Metropolis-Hastings ratio is used in case of an non-symmetric proposal distribution, that is, when jumps of the Markov chain in one direction and in the opposite direction do not have the same probability. This, however, is not true in the case of the MCMC algorithm used in this study. What is the reason for using the Metropolis-Hastings ratio then? And third, what is meant by "transformations affect the distribution sampled"? Why should the Hastings factor be used to compensate for that? And why is the Hastings factor the Jacobian of the transformation? Please provide some more explanation or some references here.

(2.5) The caption of Tab. 3 and the discussion of the numbers given therein is rather confusing to me. The authors argue that the mode with minimum misfit corresponds to the most reasonable model hypothesis (Sec. 4.2). However, the mode with minimum misfit has maximum posterior probability, not minimum as stated in the caption. On one hand, reporting the "minimum value of $\log\left(P(\theta)L(\theta|\mathbf{O})\right)$" would not make any

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sense. On the other hand, if in fact the (log of the) maximum posterior probability is given here, the interpretation of these numbers would be completely different. Please clarify this issue.

(2.6) In case of the Hainich site, effective decomposition rate coefficients determined under laboratory conditions were used for model calibration in addition to other observations. I wonder what the information content of these particular measurements is. Information on the effective decomposition rate coefficients is not readily available in most applications and it is interesting to know how much additional information it provides. Is it actually worth the effort of performing these measurements? Would the posterior distribution look substantially different if this information was missing? In general, the posterior uncertainty seems to be considerably smaller for Hainich compared to Loobos, where information on effective decomposition rate coefficients was not available. Does this explain these differences?

3 Technical comments and corrections

(3.1) p.11240 l.12: Remove the line break here. The abstract should be a single paragraph.
(3.2) p.11240 l.27: "a" should be removed here.
(3.3) p.11243 l.20: The reference of the SOMPROF model (Braakenhekke et al., 2011) should be inserted here, not in the following sentence.
(3.3) p.11243 l.23-26: This sentence is grammatically incorrect. The best thing might be to split it in two: "...years to centuries. The model includes...".
(3.4) p.11244 l.1-15: I suggest to change the order of these two paragraphs, such that the research questions appear at the end of the Introduction section.

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(3.5) p.11244 l.22: The word "explicitly" should be removed. It is not needed here.
(3.6) p.11246 l.16: "of" is missing: "...the total organic matter stock of the respective layers."
(3.6) p.11247 l.11: Insert "which" after the comma.
(3.6) p.11249 l.14-15: "pedologically very poor" is not a meaningful expression. Please rephrase.
(3.6) p.11249 l.21: Use "were" instead of "are".
(3.6) p.11251 l.14-15: This sentence is repetitive. The same information was given before (p.11250 l.28).
(3.6) p.11254 l.7: The expression "random guided walk" sounds a little bit strange to me. Usually, the term "random walk" is used in this context.
(3.6) p.11254 l.15: "MCMC" was not previously defined.
(3.6) p.11255 l.7: A constant is missing in this equation (see, for example, Mosegaard and Sambridge, 2002). Additionally, the symbol C_i was already used to denote the ith carbon pool.
(3.6) p.11260 l.9: "a decrease of the formation" instead of "a decrease formation".
(3.6) p.11260 l.13: "DOM" was not previously defined.
(3.6) p.11262 l.1-2: The expression "root input dominates the mineral soil as a mechanism for organic matter input" should be rephrased.
(3.6) p.11262 l.5: Add the word "to": "...compared to material...".
(3.6) p.11262 l.26: "Further comparison..." instead of "Comparison further...".
(3.6) p.11264 l.22: Insert the word "the" here: "...explained by the fact...".
(3.6) p.11270 l.16: The authors mention a factor of 0.1 here, whereas in Fig. 2 of the supplementary material they mention a factor of 5. Which one is correct?

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