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Discussions

Interactive comment on "Inverse modelling of in situ soil water dynamics: accounting for heteroscedastic, autocorrelated, and non-Gaussian distributed residuals" *by* B. Scharnagl et al.

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We thank Anonymous Referee #1 for the insightful comments. We have addressed each of them separately below. The numbering of our replies follows those of the original comments. Changes we made to the discussion paper in response to the comments are indicated by italic font.

1. We are particularly grateful for this comment because it points at an important

feature of the modified AR(1) scheme that we missed to mention in the discussion paper. We agree with the referee in that the decorrelated residuals obtained by Eq. (20) are indeed dependent on all residuals. We also agree on that this essentially makes Likelihood 3 an unnormalised likelihood function. This, however, has no practical implications for the present application since in MCMC simulation the likelihood must only be specified up to a normalizing constant. However, it is important to be stated explicitly. We consider Eq. (14) still appropriate to standardise the decorrelated residuals obtained with Eq. (20). Our reasoning is that the third term in Eq. (20) without the autocorrelation coefficient ϕ can be considered as a constant. As such, the variance of the decorrelated residuals is independent of this constant term. *In the revised discussion paper, we added two short paragraphs at the end of the description of Likelihood 3 that discusses these two important theoretical aspects of Likelihood 3 accordingly.*

2. The reviewer is right to point out that if the expected value of the standardised residuals is zero, so is the expected value of the decorrelated residual. However, the expected value of the decorrelated residual can also become zero if $\phi \rightarrow 1$ as we pointed out in the manuscript (p. 2167, l. 16-18). According to Eq. (13), the expectation of the decorrelated residuals will be zero if the expectation of the standardised residual is zero. However, the expectation of the decorrelated residual becomes also zero if ϕ is close to unity. In general, the expectation of η will always be smaller than the expectation of ε, because ϕ ranges from zero to unity as it becomes evident from the second row of Eq. (13). In the initial phase of exploration of the parameter space by the various Markov chains, the expectation of the residuals will deviate substantially from zero. Also, even in the vicinity of the optimum, the expectation of the residuals will only be close to zero, but never exactly zero. This leads us to the conclusion that the classical AR(1) introduces bias and makes the approach potentially unreliable. This effect diminishes in the vicinity of the optimum, but we argued that this effect may distort the inference

HESSD
12, C1526–C1529, 2015

scheme, leading to essentially meaningless results as obtained with Likelihood 2. *We added two additional sentences to the revised discussion paper, which clarify this issue.*

3. This is indeed what we did in a preliminary study. The problem in this approach is that it is not clear a priori which value to use as an upper bound for the autocorrelation coefficient ϕ. As shown in the present study, a value of 0.957 (Table 1) was found to be optimal if Likelihood 3 was used. We found that if the upper bound is chosen too large, the bias problem remains, while when chosen to small, not all of the autocorrelation was removed, resulting in lower values of the maximum posterior density. In the end, the choice of an upper limit is subjective, which is something we wanted to avoid if possible.

4. Good idea. *In the revised discussion paper, we add two sentences that will highlight the difference between Likelihood 2 and 3 on the one hand and the likelihood model proposed in Schoups and Vrugt (2010).*

5. We disagree. As both the prior and the posterior are formulated and interpreted/evaluated in terms of the transformed parameters, the inclusion of the Jacobian is not necessary in this analysis. If one is interested in probability statements regarding the untransformed parameters, one could simply backtransform the posterior sample accordingly.

6. In our preliminary tests using upper bounds of ϕ smaller than one, the problems with convergence and acceptance rates was reduced indeed. But it did not vanish. Please see our reasons against constraining the value of ϕ in our reply to comment 3 as well.

7. *We will comment on that in the revised discussion paper.* See also our reply to comment 13 by Thomas Wöhling (Referee #2).

HESSD

12, C1526–C1529, 2015

8. We did not try to relax the prior. The reason for this is similar to that given in our reply to comment 3. In our view, a relaxation would be a subjective modification of the prior information provided by the pedotransfer function (ROSETTA). The questions that arise next would be: How strong should we relax? Which degree of relaxation is “appropriate”? Is there a probabilistic justification for this relaxation? All these questions are important since the degree of relaxation would certainly have an influence on the parameter estimates. In the end, we personally prefer to stay as objective as we can and therefore took the prior as provided by ROSETTA.

9. *In the revised discussion paper, we included the parameters of the likelihood model in the scatter plot matrix of Figure 7, as suggested by the referee.*

10. Our notation here is indeed inconsistent and confusing. *We changed Eqs.(15) and (16) accordingly*.

11. No. We have independent measurements from a nearby location, which differ however substantially in the amount of the coarse fraction (>2 mm) in the upper soil. Also, there is plenty of evidence in the literature that shows that the soil hydraulic properties derived in the laboratory are not necessarily useful in describing in situ soil water dynamics. A brief discussion of this topic is provided in Scharnagl et al. (2011).

Interactive comment on Hydrol. Earth Syst. Sci. Discuss., 12, 2155, 2015.