Interactive comment on “Bayesian inverse modelling of in situ soil water dynamics: using prior information about the soil hydraulic properties” by B. Scharnagl et al.

Anonymous Referee #1

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1 General comments

(1) Does the paper address relevant scientific questions within the scope of HESS?

Yes. Hydrogeological inverse modeling of in-situ soil water content measurements and the use of more sophisticated statistical algorithms are important topics for this community.

Does the paper present novel concepts, ideas, tools, or data?

In my opinion, the novelty of this paper lies in applying a new MCMC algorithm to in-situ soil water content measurements, assimilating soil texture data and investigating the impact of correlation among parameters. The synthetic study shows excellent results that the posterior distribution captures the true values. However, the authors have overstated the novelty of using the prior and investigating the impact of prior, since they have been explored, for example, by Hou and Rubin [2005] (Hou, Z., and Y. Rubin (2005), On minimum relative entropy concepts and prior compatibility issues in vadose zone inverse and forward modeling, Water Resour. Res., 41, W12425, doi:10.1029/2005WR004082).

(3) Are substantial conclusions reached?

Although the paper presents interesting results, various aspects of the theoretical results are weak.

First, the definition of “prior” in this paper is confusing. In general, the term prior refers to any information before any data at the site. However, the authors use soil texture data at the site for their prior. In the sequential Bayesian sense, it could make sense since the distribution from the soil texture data become prior to the soil moisture measurements. Nonetheless, the authors need to state it more clearly. In addition, it might not be fair to compare to the uniform prior after assimilating the soil texture data. It might be straightforward to say that this paper is investigating the impact of soil texture data in hydrogeological data assimilation.

Second, the authors argue that the in-situ soil water content data alone does not give reliable estimates so that they need informative prior. At the same time, they say that different (biased) prior did not have any effect on the results so that their method is robust. At the first glance, these two sentences make this method more attractive, but
theoretically these two sentences are contradictory, since the different prior should give different results if the prior is informative and influential. The second sentence implies that the soil water content data is much more influential than the prior. In statistics, many people even seek noninformative prior in order to avoid bias from prior. Such contradictory situations often arise when the sampling method is ineffective and does not explore the true region. In this paper, the results, however, show that it is not the case, since the posterior distribution captures the true values. There could be some other reasons that the soil texture data is helpful for inverting the in-situ soil moisture measurements. More explanation and investigation are necessary.

(4) Are the scientific methods and assumptions valid and clearly outlined?

Although authors stated assumptions clearly, none of them have reasonable justification. It is always necessary to have physically possible assumptions or assumptions based on observations rather than just for convenience or computational reasons. Specific comments below elaborate further on these points. The way to determine the correlation among parameters in the prior distribution was questionable. The steps outlined in the paper transfer the covariance of soil texture data ($\Sigma_f$) to the correlation among hydraulic parameters through ROSETTA. This is equivalent to how measurement errors and/or variability in the soil texture data are translated into the uncertainty and correlation in hydraulic parameters. It does not account the correlation created by the pedotransfer function (PTF) through ROSETTA. For even a single soil texture, PTF can create correlation; for example, the clay content affects both saturated conductivity and residual water content. In addition, the sum of the percentages of sand, silt and clay should be always one, so that there should be only two random variables.

(5) Are the results sufficient to support the interpretations and conclusions?

It would be better to have additional results related to the issues described in (3).

(6) Is the description of experiments and calculations sufficiently complete and precise to allow their reproduction by fellow scientists (traceability of results)?

Yes.

(7) Do the authors give proper credit to related work and clearly indicate their own new/original contribution?

Yes.

(8) Does the title clearly reflect the contents of the paper?

It would be better to say “investigating the impact of prior” rather than “using prior”.

(9) Does the abstract provide a concise and complete summary?

Generally yes. However, after mentioning informative prior, stating “a biased prior did not distort the results” makes this paper less credible (the same reason as (3)).

(10) Is the overall presentation well structured and clear?

Yes.
Is the language fluent and precise?

Many definitions and phrases are informal and vague (e.g., "let data speak" and "this posterior distribution summarizes what we know about the parameters"). It would be better to have more precise definitions and terms that can be found in statistics textbooks.

Are mathematical formulae, symbols, abbreviations, and units correctly defined and used?

Specific comments below indicate some mistakes in the inverse modeling and MCMC formulation.

Should any parts of the paper (text, formulae, figures, tables) be clarified, reduced, combined, or eliminated?

Some specific points are shown below. More clarification and explanation are necessary for the issues described in (3) and (4).

Are the number and quality of references appropriate?

Yes.

Specific Comments

P2023, L29: "let the observational data speak" is informal.

P2024, L12: Symbols (e.g., L, Ks) are used before defining them.

P2025, L14: It seems that the soil texture (sand, silt and clay contents) was actually measured at the site. What is the uncertainty range of these measurements and variability within the model domain?

P2027, L12: It is necessary to have a physical reason to justify homogeneity rather than just for convenience. Otherwise, the whole inversion becomes meaningless.

P2030, L5: Although it is clearly defined, using $\hat{y}$ for measured observations still seems inappropriate, because hat is always used for estimates in statistics.

P2030, L12: "To formulate .... the model residuals" is not a precise statement but very vague. For example, "statistically meaningful inference" does not have any significant meaning. In addition, the statistical distribution should be based on observations or physical processes. This author’s statement seems to suggest that one can create a distribution just to make inference possible.

P2030, L16: It is important to state what $\epsilon$ physically means (measurement errors?) and why one can justify that they are independent and identically distributed.

P2030, L19, Equation (8): $\hat{y}$ should be replaced by $\hat{y}_i$. Equation (7) is a simple subtraction of vectors such that $\epsilon_i = y_i - \hat{y}_i(x_1, x_2)$. $\epsilon$ should be a function of $x_1$ and $x_2$, $\epsilon(x_1, x_2)$. The likelihood formation is wrong. It should be:

$$p(\hat{y} \mid x_1, x_2) \propto \exp[-\frac{1}{2\sigma^2} \sum_{i=1}^{N} \epsilon_i(x_1, x_2)^2]$$

P2030, L22, Equation (9): The equation assumes independence between $x_1$ and $x_2$ in prior. It needs to be justified.

P2031, L1: "This posterior distribution summarizes what we know about the parameters" is informal. It needs a more precise statement in statistics.

P2031, L10: "we can do better than this" is very informal. In addition, more system-
atic approaches to formulate prior has been already applied for estimating hydraulic parameters in the unsaturated zone (Hou and Rubin, 2005).

P2031, L18: The authors need to justify why they chose -250 and -50 cm for the bounds.

P2031, L19: We cannot omit the uniform prior from the posterior distribution, because the prior still affects the posterior such that the posterior probability density outside of the bounds is zero.

P2031, L25: Uniform distributions also require explicit prior knowledge for the upper and lower bounds.

P2032, L13: There are many other MCMC schemes (e.g., Gibbs sampling) which are widely used.

P2032, L16: The next position of the chain should also depend on the data, in addition to the current position, as is shown in Equation (11).

P2034, L26: "A normal distribution is computationally easy to implement...". Again, the authors need to justify use of a particular distribution based on physical processes or observations; otherwise the inverted results are meaningless.

P2035, L2: The authors need to state why they chose multivariate normal prior distribution.

P2035, L23: "0.25% was shown to work well in practice" needs a reference. In addition, the authors need to state what $\Sigma_f$ means physically (e.g., measurement errors and/or variability)