Interactive Discussion: Author Response to Referee #2

Spatio-temporal soil moisture retrieval at the catchment-scale using a dense network of cosmic-ray neutron sensors

Maik Heistermann et al.
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RC: ***Reviewer Comment***, AR: *Author Response*, ☐ Manuscript text

Dear Referee,

we would like to thank you very much for your positive comments and constructive suggestions to our manuscript. We very much appreciate the time and effort that you have invested in your report.

Please find below our detailed responses to all the issues you have raised in your report. Note that this response addresses both of your reports, part 1 and part 2, in one single document.

We are confident that the manuscript will improve as a consequence to addressing these issues. Yet, the final implementation of changes will also depend on another referee report that is still to be submitted in the interactive discussion.

Kind regards,
Maik Heistermann
(on behalf of the author team)

2.1. Sensitivity factor

RC: ***Sensitivity factor was assumed to be a constant for each sensor, which seems intuitively reasonable but needs scrutiny. Since these factors are essential to the uniform calibration, it at least requires some citations and/or explanation.***

AR: The detector-specific sensitivity or efficiency is a result of manufacturer-level variation of detector gas density, geometrical variation, and configuration parameters related to electricity. All of those were fixed once during manufacturing and cannot change over time. [Schrön et al., 2018] have shown that the resulting count rate efficiency is different from sensor to sensor, while significant variation in time is not evident. This is also known from experience with long running sensors of the COSMOS network in periods of more than a decade, where the duration of our 2-month campaign is negligible. On the basis of these explanations, we think that the application of constant, sensor-specific efficiency values is sufficient.

We will add a brief corresponding statement and citation in section 4.1.1 of the manuscript (Standardization of sensitivity).

2.2. Local uncertainty

RC: ***Please define/specify "local uncertainty". I think the "local" refers to the parameter space, not the spatial-temporal space. If I am correct, it creates some ambiguity in the text since the discussions are always related to space/time in this paper. (Line 271, 415, 665, etc.)***

AR: We apologize for the ambiguity, and we fully agree that the term "local uncertainty" requires a clear definition. In fact, we refer to "local uncertainty" as the uncertainty of our soil moisture estimate for a specific sensor footprint i, i.e. as the uncertainty of $\theta(N_i)$ and θ_i^{obs}, expressed as the width of the interval between two quantiles. It should also be clear that this uncertainty only refers to the point in time at which the manual soil moisture measurement campaign took place which was the basis of the N_0 calibration.

In the revised version of the manuscript, we will explain the term "local uncertainty" in section 5.2 where the actual results are discussed. In section 4.3, l. 271 of the original manuscript, we will avoid the use of the term instead of already defining it. That is because we think that the meaning of the term becomes more tangible for the reader in the context of the presentation of the actual results, hence we should not introduce it before.

2.3. Monte-Carlo simulation

RC: ***Please briefly explain the choice of "200 times" of the Monte-Carlo simulation on the sensitivity of N0. To my understanding, the number of simulations depends on the dimensions of the parameter space. Why are 200 times good enough to quantify the uncertainty of N_0 concerning these many parameters and disturbances.***

AR: The referee is correct that it would be good to have a formal justification of the number of runs that constitute our Monte-Carlo analysis. However, the parameters, their assumed probability distributions, and the corresponding stochastic disturbances are very different from each other. That makes it difficult to apply formal frameworks to assess the required numbers of runs. For example, some disturbances are rather a sub-sampling (e.g. the determination of the time interval over which the neutron count rates are averaged, or the selection of soil profiles that are included in the interpolation); for other input parameters, the definition of the underlying distribution and its parameters is necessarily arbitrary (e.g. the Kriging range, or the water equivalent from soil organic carbon and lattice water). Given these difficulties, we have addressed the issue rather pragmatically: we found that the results of the Monte-Carlo simulations with using 200 runs are robust, meaning that they do not vary substantially from simulation to simulation with regard to the output we were looking at (which is specifically the interquartile range, while the range between the 5th to the 95th percentile is purely for illustrative purposes). We also found that the results did not substantially change when we increased the number of runs per Monte-Carlo simulation.

We would like to emphasize that the Monte-Carlo-analysis is, in the context of this study, of rather qualitative relevance: its main purpose is to demonstrate that the disagreements that we observe in Fig. 4 can mostly be explained by the local uncertainties of $\theta(N_i)$ and θ_i^{obs}, while location 7 is clearly different.

In our view, arbitrary decisions in the design of the Monte-Carlo cannot be avoided at this point, and we have also been open with that in the conclusions. Yet, we fully understand and appreciate the referee's concern in this context. As a response, we suggest to very briefly mention, in section 4.3, the level of arbitrariness involved in this analysis, and the corresponding limitations in the interpretation of the results. Still, we could further increase the number of Monte Carlo runs if desired.

2.4. 2.4 Models

RC: ***Line 88 References for the concept of geophysical inversion are needed.***

AR: We suggest to cite [Zhdanov, 2015] in this context as a reference to the fundamental idea of geophysical inversion.

RC: ***Line 329 There are three parameters for a variogram model, nugget, sill, and range. The paper only emphasized the range but did not mention the other two. Please specify the parameter selections.***

AR: We apologize for the incomplete documentation. We did not specify nugget and sill, as these do not affect the result of the predicted variable, but only the Kriging variance. Since we do not use the latter, nugget and sill can be chosen arbitrarily (in our case: nugget=0, sill=1). Nugget and sill become important when a theoretical variogram model is fitted to an empirical semi-variogram, as the choice of nugget and sill might affect the range, when the three parameters are fitted together. In our case, we did not fit a variogram model. Instead, the choice of the range of 300 m was rather a preference to express the scale at which we are interested in representing soil moisture heterogeneity.

Altogether, we will clarify these aspects in the revised version of the manuscript, and also state the values of nugget and sill used for our calculations.

RC: ***Line 297 The Kriging ranges for soil moisture and bulk density are quite different. Please justify this selection.***

AR: We agree that this should be explained better. The sampling intervals for the Kriging ranges in the Monte Carlo analysis (section 4.3) were based on the Kriging range values used for the interpolation of the soil variables as outlined in section 4.1.4, which were 50 m for all soil variables except soil moisture (150 m). These values were not obtained from fitting a variogram model, but rather heuristically: we chose a higher range value for soil moisture because the resulting estimates of θ^{obs} were more consistent with $\theta(N)$, although a systematic optimisation was not carried out. We addressed the apparent arbitrariness of this procedure by defining a sufficiently large interval around these range values from which we would sample in the Monte-Carlo analysis. We will point out, in the revised manuscript, that the selection of the Kriging range values could, in future studies, be subject to further systematic optimisation.

2.5. Footprint, model parameters, and scaling

RC: ***One of the unique features of CRNS is its large footprint, which could directly influence data visualization, model selection, and interpolation. The grid size for the interpolation process is 10 m * 10 m (Line 311), which is much smaller than the footprint. This implies that the modeling is not just an interpolation but also involves a downscaling process for the CRNS measurements. It is of great interest in terms of the CRNS studies. However, it also requires more clarification and cautiousness. For example, is it reasonable to use observed soil moisture, $\theta(N_{obs})$, to do Ordinary Kriging with a resolution much smaller than its footprint? Does it implicitly assume that observed soil moisture values are also representative at a smaller scale?***

AR: We thank the referee for this comment. Obviously, he or she is entirely right to demand that cautiousness. We hoped to express that caution with our statement from ll. 311-314 of the original manuscript:

> [ll. 311-314] The grid resolution is arbitrarily selected, and does not necessarily reflect the resolution at which the grid effectively conveys information of spatial heterogeneity; in other words, the product should not be interpreted at the scale of 10 m. Still, we require this comparatively fine horizontal resolution since some of the following steps require to re-aggregate (i.e. to average) the spatial soil moisture estimates inside a CRNS footprint.

Accordingly, we do not actually aim to represent soil moisture variation between 10 m grid tiles, but we require that resolution in order to reasonably apply the forward operator in order to obtain neutron intensity from a spatial soil moisture grid. In addition, one could see this sub-footprint resolution as a tool to represent gradients in the footprint, rather than values of the single cells. In the revised manuscript, we will attempt to clarify this more.

Furthermore, we emphasize in ll. 328-332 that Kriging is used as a "model" to represent our notion how soil moisture varies at a specific scale:

> [ll. 328-332] In this study, let us assume that the spatial distribution of soil moisture in the study area is smooth and continuous, and that this spatial pattern could be represented by a model m that corresponds to Ordinary Kriging with an exponential variogram model and a range parameter of, say, 300 m, using the CRNS sensor locations as points of support. We hope it is clear to the reader that the choice of such a model is arbitrary and subjective, although it should be based on our "expert" notion of how soil moisture varies at a specific scale.

Again, we will attempt, in the revised version, to emphasize that the use of Kriging with a grid resolution of 10 m does not mean that we should interpret variability at that scale.

Finally, the referee wonders whether we "implicitly assume that [$\theta(N)$ is] representative at a smaller scale". Our answer would be no, although it is true that the unconstrained model, technically, reproduces $\theta(N_i)$ at the sensor location i. However, that is rather a side effect and not a necessary requirement. The key property of our model m is that it represents soil moisture variation at a scale that is given by our (arbitrary) choice of the variogram (exponential with a range of 300 m). Please note that other models might well be able to represent soil moisture heterogeneity at an even finer effective resolution. Such a model could be a statistical relationship between surface properties (soil, terrain, vegetation) and soil moisture, or a physically-based model (see ll. 319-324). The effective resolution would be subject to their validity at a finer scale as well as the accuracy of their input data (please also refer to our response to next comment).

> [ll. 319-324] What we refer to as the "unconstrained" approach could imply any kind of (geostatistical) model or assumption m that represents the spatial distribution of soil moisture, θ, on the basis of any parameter set $\mathbf{p}$. For example, $m(\mathbf{p})$ could be the nearest neighbour algorithm. In that case, $\mathbf{p}$ would be the soil moisture values at a set of sampling points. As another example, $m(\mathbf{p})$ could be a statistical relationship between landscape attributes and soil moisture, hence $\mathbf{p}$ would comprise the parameters of that statistical model. Or, $m(\mathbf{p})$ could be a physical model of water movement in soils, with $\mathbf{p}$ being the entirety of (potentially spatially distributed) model parameters.

RC: ***The design of the forward operator and the optimization argument is innovative since it provides a way of downscaling CRNS measurement to almost any arbitrary scale/resolution, which may be only limited by computational capacity.***

The design of the dense network made the footprints of CRNS largely overlapped, which provides extra information about soil moisture spatial patterns. This may also make it logically possible and reasonable to do the downscaling and to improve the interpolation. Can the overlaps be used for results validation?

AR: We agree, in general, with the referee's view that the use of the forward operator allows for a certain level of downscaling (see our response to comment 2.5), and it certainly is one of the specific aims of this study to demonstrate that potential. However, we do not think that the achievable resolution is purely a matter of computational resources. In our view, it is rather a matter of how well our model m is able to represent patterns at high resolution. Example: We could enhance, in our setup, the spatial resolution of our target grid from 10 m to let's say 10 cm. That would involve a substantial increase in computational costs for the interpolation and the application of the forward operator, yet the effective/meaningful resolution of the results will not be higher than before.

Somewhat related to that point is the aspect of overlap: in general, we would expect that a large overlap from multiple sensors would help to better constrain the inverse problem, yet it does not, in our view, provide "extra information" for an independent validation. Even with a strong overlap, we still need a model of spatial soil moisture variation to make the problem solvable. The advantage of the overlap is particularly that the parameters of that model will probably be constrained better because changes of soil moisture in the region of overlap will affect multiple footprints and hence multiple values of N^{sim}.

While this discussion is certainly interesting, we would prefer not to extend it further in the context of this manuscript. We see the present study as a proof-of-concept, and both practical and theoretical aspects should be explored in future studies, as also outlined in ll. 722-730 of the original manuscript.

2.6. Technical Comments

RC: ***Line 26 "small spatial measurement support" and Line 330 "points of support". Support is an important concept in defining spatial scales of soil sampling and measurements. I recommend adding a definition and citations here. This would also help to present the results on soil moisture spatial patterns in the following sections.***

AR: In the revised version of the manuscript, we will refer, in section 1.1., to [Blöschl and Grayson, 2000] as the key reference with regard to the concept of spatial support in the observation and interpolation of spatial variables. We will also better explain, around l. 330 of the original manuscript, the meaning of "points of support", as this term does not refer to the concept of "measurement support" in the sense of [Blöschl and Grayson, 2000], but to the "nodes" of the interpolation, i.e. the locations at which an observation is assumed to be available. Alternatively, we could replace "points of support" by "node".

RC: ***Line 259 "assuming a spatially uniform value of N_0..." Modification required. Since N_0 mainly depends on the sensor itself after correcting all factors (air pressure, vegetation, lattice water, etc.), it is not a spatial variable.***

AR: We agree that this is misleading. We dropped "spatially" so statement becomes "[...] assuming a uniform value of N_0 [...]".

RC: ***Line 262 Eq. 1 - recommendation: replace comma with semicolon, i.e. $\theta(N_i; N_0)$. To my understanding, N_i is a variable, and N_0 is a parameter in Eq. 1.***

AR: We thank the referee for the suggestion, but we would prefer to keep the notation as it is: while in the context of Eq. 2, N_0 is the parameter (which is optimized), the constrained interpolation treats all N_i as parameters.

RC: ***Line 350 delete extra "suitable"***

AR: Thanks, will be deleted.

RC: ***Line 622 reliably -> reliability***

AR: Will be corrected.

References

[Blöschl and Grayson, 2000] Blöschl, G. and Grayson, R. (2000). Spatial observations and interpolation. In Blöschl, G. and Grayson, R., editors, *Spatial Patterns in Catchment Hydrology - Observations and Modelling*, chapter 2, pages 17–50. Cambridge University Press, Cambridge.

[Schrön et al., 2018] Schrön, M., Zacharias, S., Womack, G., Köhli, M., Desilets, D., Oswald, S. E., Bumberger, J., Mollenhauer, H., Kögler, S., Remmler, P., Kasner, M., Denk, A., and Dietrich, P. (2018). Intercomparison of cosmic-ray neutron sensors and water balance monitoring in an urban environment. *Geoscientific Instrumentation, Methods and Data Systems*, 7(1):83–99.

[Zhdanov, 2015] Zhdanov, M. S. (2015). Chapter 1 - forward and inverse problems in science and engineering. In Zhdanov, M. S., editor, *Inverse Theory and Applications in Geophysics (Second Edition)*, pages 3–31. Elsevier, Oxford, second edition edition.