Response to Editor:

We thank the editor for the detailed explanations and helpful suggestions, and we have thought carefully about the limitations of the algorithm from a theoretical perspective. Our reply is listed in the following sections. The comments from the editor are provided in blue text and our responses are organized in black text. The manuscript text after the proposed changes is shown in "*black italics*". The number of the line, equation and section refers to the revised version of the manuscript without track changes, shown in yellow highlight.

In most cases, I agree with the reviewer's comments and with the answer of the authors to those comments. There are, however, certain reviewer comments with which I fully agree and which are not yet properly addressed in the answers of the authors. Unfortunately, some of these are quite major comments and I hope that the authors can address them properly. I explain these concerns in more detail in the following.

Most importantly, it is not clear what the consequences of the reordering step in the secant method are on the acceptance probability of the sampler that forms the outer loop (in this case a ABC-SMC algorithm). Changing the acceptance probability of any sampler almost always has consequences on the convergence proofs for that algorithm, i.e. on its ability to sample the intended distribution, which in this case is the posterior. Note that this concern is still there if one uses BEAR together with other samplers such as MCMC methods or SMC algorithms, as mentioned by the authors in their replies. This means that there are doubts about which distribution the BEAR algorithm actually samples. This point was raised by Reviewer 3 in comment 1. The authors try to address this concern in Appendix B of their response, but they do not manage to show that BEAR samples the posterior distribution. Since the εX are sampled a new in each iteration of the outer loop (sampler), we have different chances to reach τs for each s and therefore different chances of accepting the proposed parameter sample (i.e. different acceptance probability). Also the ranks, kq, are re-initialized in each iteration. In the same answer, in Eq. 7, the authors claim that εX are a deterministic function of the parameters, but in the sentence below and in the scheme in Figure 1, they say that they are sampled from $f(\eta)$. According to Fig. 1, even η changes during the inference.

Thanks very much for the editor's comment here. We concur the BEAR method does not update the posterior distribution of input errors, "the εX are sampled a new in each iteration of the outer loop (sampler)", and the calculation of input errors are re-initialized in each iteration. Instead, our approach leads to an optimized estimate of εX dependent on the model parameters and constrained by the prior distribution of εX.

To explain: if the sample size is large (i.e. in the case of identifying the data-based input errors) and the error distribution is fixed, there is no significant difference among the error populations in subsequent samplings. Therefore, the error series εX is determined by the optimal error rank series as estimated via the secant method. When a model parameter is generated, the residual error only depends on the input error in this study. In other words, for a set of model parameters, the optimal input error series will lead to the minimized residual error. Therefore, we have revised the manuscript to state "εX are a deterministic function of the parameters" in Appendix B.

In cases where the error distribution is not fixed in the calibration (η changes during the inference), η (μ_X, σ_X in Appendix B) is regarded as a hyperparameter, calibrated along with the model parameters. Again in this case, the optimal input error will lead to the minimized residual error. Here, "εX are a deterministic function of the model parameters and input error parameter". To avoid confusion in the core idea of the rank estimation, "η changes during the inference" has been deleted in Figure 1 and the methodology is based on the assumption that the error distribution can be pre-estimated. But to explore the ability of the BEAR method in wider applications and fully discuss its limitations, the concept of changing η has been considered in a synthetic case and Appendix B.

To sum up, the reordering step is implemented when the model parameters and input error distribution have been updated and aims to find the optimal input error series corresponding to the minimized residual error (not the posterior distribution of the input errors, as the Editor and reviewers have noted). Thus, after the reordering step, the optimal input error εX is a deterministic function of the model parameter and input error parameter. It is re-calculated via the secant method for a new set of the model parameter and input error parameter and does not update its posterior distribution. We hope these revisions clarify the contribution of the work.

I see two possibilities: either the authors can provide a mathematical proof that their algorithm samples the posterior distribution, or they clearly state in the manuscript that the resulting distribution of the parameters has an interpretation that is not clear and possibly different from the actual posterior distribution. In that case, the approach cannot be considered a Bayesian approach (which doesn't mean that it cannot be useful).

Thanks very much for your suggestions. As we concur in the previous point, the BEAR method does not update the posterior distribution of the input errors, and due to this point, it would be inaccurate to refer to it as a formal Bayesian approach to identify the input errors. We have clarified this as follows:

"*The reordering step is implemented when the model parameter has been updated and aims to find the*

optimal input error series corresponding to the minimized residual error. After the reordering step, the optimal input error is a deterministic function of the model parameter. Thus, unlike formal Bayesian inference, the BEAR method does not update the posterior distribution of the input errors, but identifies the input error through the deterministic relationship between the input error and model parameter." (line 318-322)

In the second case, I suggest to provide a more thorough synthetic case study, where the model parameters κ, Smax, a and b are known and re-inferred by BEAR, which is not shown at the moment. One thing to investigate in such a case study is also the effect of the temporal resolution (see comments in the next paragraph).

The synthetic case we provided in the manuscript is just the case where the model parameters κ, Smax, a and b are known and re-inferred by BEAR. Rather than providing the posterior distribution of each model parameter in the manuscript, we have added results demonstrating the overall effect of the model parameters in Figure 2(5). The explanation is as follows: "*In the validation period, the simulated output corresponds to the true input and estimated model parameters, and its NSE compared to the true output can assess the accuracy of the model parameter estimation*." (line 229-231)

BEAR assumes a direct correspondence between the input and the output at each time-step. This necessitates that the number of input and output time-steps are the same and assumes that the model output at each time-step is only affected by exactly one input value: the one at the same time. However, memory effects introduced by water quality models can be substantial. For example, in the model used by the authors, the differential equation will lead to significant memory and input that happened multiple time-steps ago will affect the model output later on. This also depends on the temporal resolution of the model. The BEAR method will have significant problems with models that show a pronounced memory effect, especially when the temporal resolution of the data is high and one model output is affected by many model inputs.

We strongly agree with the editor and reviewers' opinion that the memory effect in the model response is very important in identifying the input error and we have carefully considered how to address this problem. In previous work, we have thoroughly investigated the memory effect in quantifying the input error in a hydrological model. We applied an autoregressive (AR) model to represent autocorrelation in the model residual error and remove this from the original model residual error. The results demonstrate that the ability of the BEAR-AR method in a hydrologic model is stable, it

outperforms the BEAR method (the details please see the paper (Wu et al., 2021)).

To investigate the usefulness of this approach here, we applied an autoregressive (AR) model with order 1 to represent autocorrelation in the model residual error and remove this from the original model residual error. The resultant error series is used to adjust the input error ranks. The results are denoted as "BEAR-AR" in the following Figure D 1 and demonstrate that the ability of the AR model is not stable. Compared with the results of the BEAR method (green bars), the BEAR-AR method (pink bars) in some cases improves the input error identification but in other cases, it worsens. We think this is a function of the degree of autocorrelation relative to the observational error magnitude, and the simple autoregressive function used here. While the approach does not properly solve the potential issue of autocorrelation, we believe the additional analysis demonstrates the potential avenues to address this and future work for BEAR.

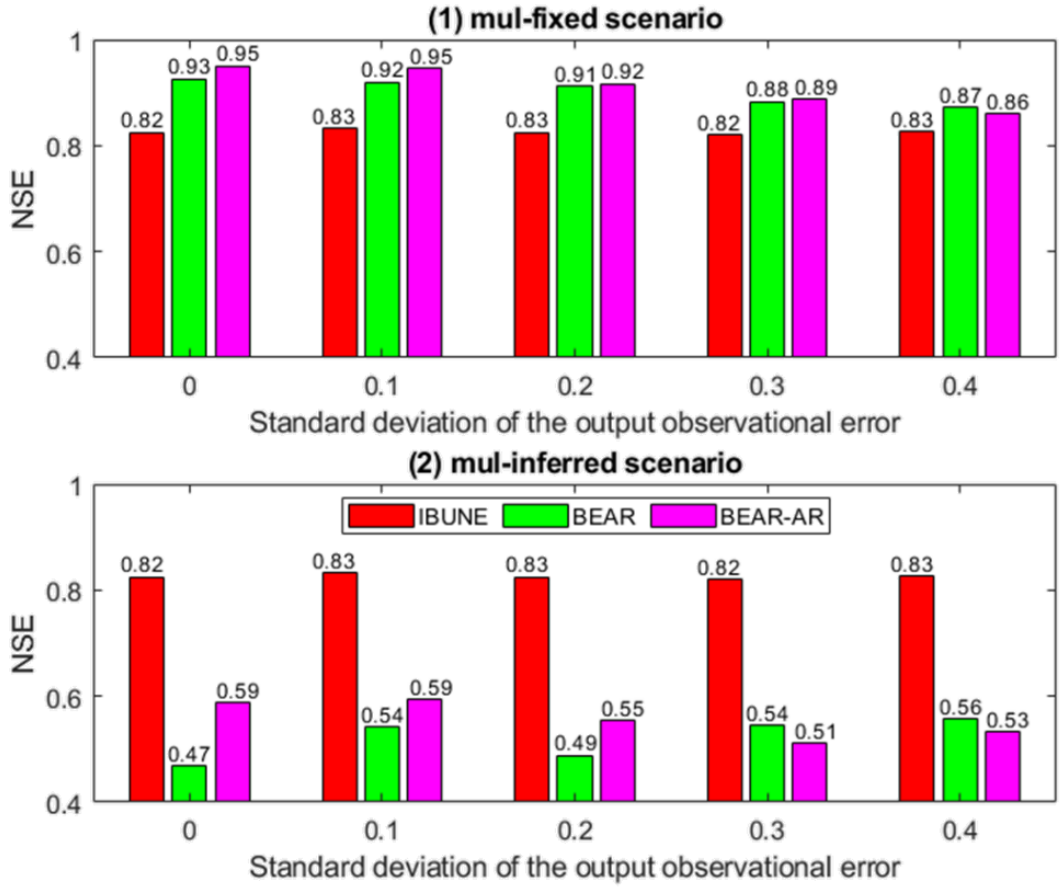


Figure D 1 Comparison of Nash-Sutcliffe efficiency (NSE) of the modified input v.s true input under the interference of the output observational errors with the increasing standard deviations in two calibration scenarios in synthetic case 2 (including *mul-fixed* and *mul-inferred*; notations are given in Table 2) via three calibration methods (including the IBUNE method and the BEAR method and the BEAR-AR method)

The possible reason and related discussion have been added in the manuscript as follows:

"If the response caused by an input is not instantaneous but exhibits persistence (i.e. occurs over several time steps), the autocorrelation in the output should be addressed to ensure the independence assumption of the rank updating is satisfied. Current ways to deal with this problem in hydrologic modelling can provide a reference to the potential modification of the BEAR method. Autocorrelation in the residual errors can be represented by an autoregressive moving average (ARMA) model (Kuczera, 1983) or autoregressive (AR) (Schaefli et al., 2007, Bates and Campbell, 2001). The correlated part of the error is removed from the residual error and the remaining part will be only impacted by the input error. Thus, the correspondence between the input error and the residual error part is ensured and the latter process will be the same as the application of the BEAR method in this study. Following this idea, the autoregressive (AR) model has been integrated with the BEAR method in the study of Wu et al. (2021) to deal with the autocorrelation of residual errors in a hydrologic model. The results prove this integration is effective to improve the input error estimation.

However, this treatment may not guarantee the improvement of the input error estimation in this study where the sediment concentrate is simulated at the daily time scale (Figure D 1). At this time scale, one input (streamflow) cannot impact the response (sediment concentration) for multiple time steps and the autocorrelation may not be well represented via a simple autocorrelation function. When the temporal resolution of the data is high (i.e. minute) and one model output is affected by many inputs, the memory effect may be addressed effectively via the AR model. Therefore, the specific representation of the autocorrelation in the residual error needs further discussion through comparisons in different time scales or with different characteristics in the memory effect." (line 356-372)

Reference:

WU, X., MARSHALL, L. & SHARMA, A. 2021. Quantifying input error in hydrologic modeling using the Bayesian Error Analysis with Reordering (BEAR) approach. Journal of Hydrology, 126202.

Response to Reviewer #1:

The study proposes and demonstrates an algorithm for quantifying input uncertainty called BEAR (Bayesian error analysis with reshuffling). It is claimed that the method is suitable to overcome restrictions of current state-of-the-art approaches like high dimensional computational problems or underestimation and misidentification of error sources. For this purpose, the algorithm employs the secant method to estimate a certain rank of error associated to input data from an underlying rank distribution of errors. After introducing the method, it is demonstrated on the task of total suspended solids modelling in, first, a synthetic case study and, second, a real test case. Thereby, both, the effectiveness and the limitations are shown and discussed. Finally, transferability of the method within the field of water quality modelling and potential routes of improvement are presented.

General comments:

The issue of uncertainty quantification in modelling is for sure one of high importance. By focusing on input uncertainty this study addresses a branch that is particularly challenging in this field. Contributions in this direction deserve attention and the topic of this manuscript is suitable for the journal. However, certain issues regarding content and presentation of the material require to be addressed:

We thank the reviewer for the overall positive assessment of the manuscript and helpful comments, which we believe have helped improve the quality of the manuscript. We have responded to each point in turn in the following sections. The comments from the reviewer are provided in blue text and our responses are organized point-by-point in black text. The manuscript text after the proposed changes is shown in "*black italics*". The number of the line, equation and section refers to the revised version of the manuscript without track changes, shown in yellow highlight.

It should be noted that the method name has been changed from the "Bayesian error analysis with reshuffling" into "Bayesian error analysis with reordering". This is based on suggestions by one of the reviewers, as the word "shuffling" implies randomness in the reordering, while the reordering in our method is determined by the model residual error. The term "reordering" better reflects the deterministic nature of error quantified via this new method.

1) Maybe it is just the presentation, but it was not straightforward to see how the method exactly works. Aside of a more detailed explanation, providing more illustrations to support explanations about how the method exactly works might help, e.g. displaying the secant method itself, error distribution in rank space, etc.

Thanks for your suggestion. We have addressed this by modifying the methodology in the following points to make the algorithm clearer:

(1) Summarize the main steps in the BEAR method upfront:

"Thus, the procedure of input error quantification has been developed into the following key steps: 1) Sample the errors from the assumed error distribution to maintain the overall statistical characteristics of the input errors; 2) Update the input error ranks to minimize the model residual via the secant method (Eq. (5) and (6)); 3) Reorder these sampled errors according to the updated error ranks; 4) Repeat 2) and 3) for a few iterations until a defined target is achieved. This new algorithm is referred to as the Bayesian error analysis with reordering (BEAR)." (line 135-139)

(2) Integrate an example and its illustration in Appendix A to explain the specific steps involved. More explanation for the rank estimation via the secant method and the reordering steps has been added.

(3) Separate the description of the BEAR method from the ABC-SMC calibration scheme in Section 2.3 following suggestions from other reviewers. We changed this because the ABC-SMC calibration algorithm is not necessary in the BEAR method, and the core idea of the BEAR method (identifying the input errors by estimating their ranks) can be easily applied in any other calibration algorithm, for example, MCMC and SMC algorithms.

(4) Change the ABC-SMC calibration scheme to the SMC scheme because it is easy to derivate the BEAR method from a Bayesian perspective in Appendix B.

2) By design, the BEAR method seems to shuffle and pick errors (by their ranks) such that maximum fit to the data is achieved. Is this a proper addressment of the input errors in terms of quantification of input uncertainty? For instance, in L.232 it is discussed that "method R always has much higher correlations with the true error series" and in L.243 it outperforms the other methods with highest NSE values. Both seem to be effects from the BEAR method searching

for optimally fitting errors until exactly the error is found that minimizes the gap between model predictions and observations.

The reviewer raised an important question. The BEAR method works well under the circumstance where the input error is dominant in the total uncertainty, where minimizing the residual error has a similar effect as minimizing the input error. From this point of view, the sampling and reordering strategy in the BEAR method provides an effective way to identify the input error according to the residual error. This is what the Reviewer refers to as "searching for optimally fitting errors until exactly the error is found that minimizes the gap between model predictions and observations". Like current methods that BEAR seeks to demonstrate an improvement over, the input error compensates for other errors, a step that is constrained by accurate prior information of the input error distribution being available (Figure 3). However, the compensating effect in the BEAR method is more apparent because it is much more effective than other current methods in minimizing the gap. Thus, the accuracy of the input error model is particularly important in the BEAR method. The analysis and discussion in Section 4.2 have been modified to convey this as follows:

"The IBUNE method takes advantage of stochastic error samples to modify the input observations (Ajami et al., 2007). Figure C 2 demonstrates compared with O-fixed and O-inferred scenarios, S-fixed and S-inferred scenarios applies the simulated streamflow whose input error is more significant, and the resultant simulations (black line) via the IBUNE method are further away from the observed outputs (red dots). As per the finding in the previous study of Renard et al. (2010), if the σ of input errors is inferred with the model parameters, the IBUNE method will underestimate σ (in Fig. 2(1) and Fig. 4(1)). If σ is fixed via prior information, the input modification and model simulation cannot be improved, especially in the scenarios with large intrinsic σ of input errors, demonstrated in Fig. 2 and Fig. 3. From the above, the ability of the IBUNE method depends on the input data quality and the improvement of the input data and model simulation only happens when the standard deviation of the estimated input error is small. The availability of prior information is insignificant for the IBUNE method, especially when the intrinsic σ of the input error is large.

However, the findings in the BEAR method are quite different. Accurate prior information about the input error model is important in the BEAR method. Figure 3 demonstrates fixed scenarios

calibrated via the BEAR method always produce a higher NSE of the modified input than inferred scenarios. This is likely because the prior information can constrain the input error distribution and reduce the impacts of other sources of errors. The availability of prior information of the input error relies on studies about benchmarking the observational errors of water quality and hydrologic data, and the selection of a proper input error model is important. Comparing the results in Figure 2, when the input error model is an additive formulation, the BEAR method consistently brings the best performance regardless of the prior information of the error σ. When the input error model is a multiplicative formulation, the BEAR method cannot improve the input data if the prior information of the error σ is not accurate. This illustrates that the compensating effect between the input error and parameter error is weaker in the additive form of the input error. This is probably related to the specific model structure, as the exponent parameter b in BwMod has a stronger interaction with the multiplicative errors than the additive errors. Thus, more comprehensive comparisons should be taken to explore the capacity of different input error models in different model applications.

To sum up, the ability of the BEAR method depends on the accuracy of prior information of the input error parameter and the selection of the input error model. The IBUNE method can modify the input data when the standard deviation of the estimated input error is much smaller than the true value. It is most likely to make use of the stochastic errors to improve the original input data, but not effectively identify the input error." (line 324-349)

3) Expectations are raised that the method overcomes issues of state-of-the-art frameworks like BATEA and IBUNE. Yet, no direct comparison is shown which makes it hard to see the benefit of the method. Both these methods are frequently mentioned and a comparison is claimed. So far, there is a comparison of cases abbreviated by "T" (traditional), "D" (distribution) and "R" (BEAR method itself). "D" is referred to be "similar to the basic framework of the IBUNE method". However, this does not provide an actual comparison.

The reviewer is correct. We have changed the abbreviation to the full name of the methods as per the reviewer's suggestion, and added more explanations about this comparison, as follows:

"*The application of the BATEA framework is limited by high dimension computation (Renard et al., 2009). It probably becomes impractical in quantifying the data-varying errors (rather than the*

event-varying errors in the study of BATEA (Kavetski et al., 2006)), where the dimension easily exceeds 1000 (Haario et al., 2005). Therefore, the BATEA method is not considered in the comparison. In this study, three methods, including the "Traditional" method, "IBUNE" method and "BEAR" method, are compared to evaluate the ability of the BEAR method in estimating the model parameters and quantifying input errors. "Traditional" method regards the observed input as error-free without identifying input errors (i.e. Eq. (2)), while the other two methods employ a latent variable to counteract the impact of input error and build the modified input (i.e. Eq.(3)). In the "IBUNE" method, potential input errors are randomly sampled from the assumed error distribution and filtered by the maximization of the likelihood function (Ajami et al., 2007). Although the comprehensive IBUNE framework additionally deals with the model structural uncertainty via the Bayesian Model Averaging (BMA) method, this study only compares the capacity of its input error identification part. The "BEAR" method adds a reordering process into the "IBUNE" method to improve the accuracy of input error quantification." (line 162-173)

4) The method is supposed to reduce "the potential search space for input errors" (L.360). I wonder whether this is the objective quantification of input uncertainty? Isn't it rather a comprehensive assessment of the errors and noise associated to input error and not searching in a sub-space of already collected errors and then selecting the one that fits best during predictions?

We apologize for the lack of clarification. We have added more explanation in the revision. Here "reduce the potential search space for input errors" (L.360) is because "*In a continuous sequence of data, the potential error values have an infinite number of combinations, while the error rank has limited combinations, dependent on the data length. For example, in Table A1, the estimated error at the 1st time step could be any value. Even under a constrain of a range from the minimized to the maximized sampled errors (i.e. [-0.29,0.16] in the 1st iteration), its value estimation still has infinite possibilities due to its continuous nature. While the rank is discrete, having only 20 possibilities (i.e. the integrity in [1,20]). From this point of view, it is more efficient to estimate the error rank than estimate the error value, although the rank estimation will suffer from the sampling bias problem.*" (line 296-302)

To avoid the misunderstanding the current manuscript created, we have deleted "reduce the potential search space for input errors" (L.360), and changed this sentence as follows:

"*The estimation focuses on the error rank rather than the error value, which enhances the constraints of the input error model on the estimated errors and avoids the high dimensionality problem resulting from calibrating all the errors with the model parameter as a whole."*(line 378-380)

5) Generally, a thorough discussion on the used error distributions is missing, e.g. why is a bias of 0.2 in the error function assigned without further discussion (l.211)

Thanks for your comments. We have added clarification as follows:

"*If the input errors are estimated based on a rating curve, like the procedure in the following real case, the mean of the input error should be 0. But in order to test the ability of the BEAR method in wider applications, a systematic bias 0.2 has been considered in the synthetic case. An additive formulation (denoted as 'add' in Table 2) is suitable to illustrate the error generation in measurements, while the multiplicative formulation (denoted as 'mul' in Table 2) is specifically applied for errors induced from a log-log regression procedure, which is common for water quality proxy processes (Rode and Suhr, 2007)."* (line 207-213)

6) There is at least one article cited in the manuscript, that does not appear in the list of references (please see specific comments, l.190). Please assure correct referencing.

Thanks for your comments. We have corrected all the missing references.

Specific comments

1) L. 37-38: "…estimate the residuals between the measurements and proxy values…" -> yet, measurement error is not addressed

Thanks for your comments. we have clarified this as follows:

"*In this process, the measurement errors are ignored given the errors introduced from the surrogate process are commonly much more than the measurement errors (McMillan et al., 2012).*" (line 35-36)

2) L. 68: “variable” -> “scalar“– both, vectors and scalars represent variables

“variable” has been changed into “scalar”. (line 69)

3) Eq. 3: unnecessary, since given by equation (1)

Yes, Equation (3) has been deleted.

4) L. 84-91: repetitive, add details to the corresponding paragraph in the introduction

Thanks for your suggestion. We have moved these details into the introduction, as follows:

“The Bayesian total error analysis (BATEA) method provides a framework that has been widely used (Kavetski et al., 2006). Time-varying input errors are defined as multipliers on the input time series and inferred along with the model parameters in the Bayesian calibration scheme. It leads to a high-dimensionality problem, which cannot be avoided (Renard et al., 2009) and restricts the application of this approach to the assumption of event-based multipliers (the same multiplier applied to one storm event). In the Integrated Bayesian Uncertainty Estimator (IBUNE) (Ajami et al., 2007) approach, multipliers are not jointly inferred with the model parameters, but sampled from the assumed distribution and then filtered by the constraints of simulation fitting. This approach reduces the dimensionality significantly and can be applied in the assumption of the data-based multiplier (one multiplier for one input data) (Ajami et al., 2007). However, this approach is less effective because the probability of co-occurrence of all optimal error/parameter values is very low, and it results in an underestimation of the multiplier variance and misidentification of the uncertainty sources (Renard et al., 2009). From the above, a new strategy should be developed to avoid high dimensional computation and ensure the accuracy of error identification.”(line 43-54)

5) L. 92: “innovation” -> rather “introduction” or simple “The secant method” as chapter header – the innovation was made before

Thanks for your comment. The section titled *“innovation”* has been changed to *“introduction”*. (line 103)

6) L. 98-99: Rank definition and concept -> requires further explanation

We have added further explanations, as follows:

"Here, the rank is defined as the order of any individual value relative to the other sampled values, and determines the relative magnitude of each error in all data errors. For example, in the 1st iteration in Table A 1, the error at 15th time step, -0.29, is the smallest value among all the sampled errors, therefore, its rank is 1." (line 106-109)

7) L. 128ff: it sound like in ABC the requirements on the likelihood function are looser and therefore the method is easier to apply. However, requirements are also strict but ABC allows for Bayesian inference if the likelihood function is intractable. -> Please reformulate and clarify.

Thanks for your comments. Given the BEAR algorithm could be implemented via SMC, GLUE or SCE-UA, or any common model calibration approach, and this description about ABC confuses the main contribution of the paper (i.e. the core idea of BEAR method, which is to optimize input error ranks rather than input error magnitudes), we have recast the implementation of our optimization algorithm via SMC (the clarification is in Section 2.3).

8) L. 132ff: Notation "OF" not explained. Overall, the introduction of ABC and SMC is not clear. Further, the motivation why SMC is used here is not given.

Thanks for your comments. "OF" here means "objective function". But according to the above reply, we have recast the implementation via SMC, which target is the likelihood function rather than the objective function. Therefore, this sentence has been deleted.

9) L. 146: "…when 1000 proposed parameter sets…" -> is this suggested as a general approach or an arbitrary choice for this study. Please explain.

According to the reply for 7), we have recast the implementation via SMC. If the BEAR method is implemented using a likelihood-based calibration procedure, the proposed parameter is

compared to the previous entry in the chain and there is no need to set this stop criterion, just follow traditional convergence rules.

10) L.171ff: Please replace abbreviations T, D and R by their names. With all abbreviations that follow it is hard to keep track.

Thanks for your suggestion. We have changed the abbreviations into the full names in the below descriptions and related figures.

"In this study, three methods, including the "Traditional" method, "IBUNE" method and "BEAR" method, are compared to evaluate the ability of the BEAR method in estimating the model parameters and quantifying input errors. "Traditional" method regards the observed input as error-free without identifying input errors (i.e. Eq. (2)), while the other two methods employ a latent variable to counteract the impact of input error and build the modified input (i.e. Eq.(3)). In the "IBUNE" method, potential input errors are randomly sampled from the assumed error distribution and filtered by the maximization of the likelihood function (Ajami et al., 2007). Although the comprehensive IBUNE framework additionally deals with the model structural uncertainty via the Bayesian Model Averaging (BMA) method, this study only compares the capacity of its input error identification part. The "BEAR" method adds a reordering process into the "IBUNE" method to improve the accuracy of input error quantification.." (line 165-173)

11) LL. 190+196: "Sikorska et al, 2015" ! missing in references

Thanks, we have added all the missing references.

12) Eq. 9: define parameter "b"

The definition is shown in Table 1. A clarification has been added:

"*where the descriptions of a and b are shown in Table 1*" (line 196)

13) L. 215ff: incomplete sentence

This sentence has been completed as follows:

"The true output $\mathbf{Y}^*$ *is the simulated TSS concentration via BwMod corresponding to the true input* $\mathbf{X}^*$ *and model parameters set as the reference values in Table 1."*(line 203-204)

14) L. 229ff: "calibrated via method T,…" -> misleading explanation. Please provide a more specific explanation of the calibration process under error scenarios T, D and R

Please see the reply for 10)L. 171ff

15) L. 257: ":…the impacts of model structural error and output data error cannot be ignored." vs. L.264: ":…other sources of uncertainty can be ignored" -> sound like a contradiction, please elaborate

Thanks for your comments. We have modified the description as follows:

"*Case study 1 is an ideal situation that is used to test the effectiveness of the BEAR method in isolating the input error and the model parameter error. However, in real-life cases, other sources of errors (i.e. model structural error and output data error) will impact this effectiveness*." (line 253-255)

"*According to the results of Figure 3 and the assumption of the methodology derivation, the BEAR method works better when the input uncertainty is more significant, so another input data source with more significant data uncertainty, a streamflow simulation from a hydrological model, has been considered*." (line 271-274)

16) L. 282-283: "This illustrates that the impacts of other…" -> unclear phrase, please clarify and re-formulate

Thanks for pointing this out. This conclusion here is not clear and may lead to confusion. We have deleted this sentence and integrated the explanations into Section 4.2, as follows:

"The IBUNE method takes advantage of stochastic error samples to modify the input observations (Ajami et al., 2007). Figure C 2 demonstrates that compared with O-fixed and O-inferred scenarios, S-fixed and S-inferred scenarios uses simulated streamflow whose input error is more significant, and the resultant simulations (black line) via the IBUNE method are further away from the observed outputs (red dots). As per the findings in the previous study of Renard et al. (2010), if the σ of input errors is inferred with the model parameters, the IBUNE method will underestimate σ (in Fig. 2(1) and Fig. 4(1)). If σ is fixed as the prior information, the input modification and model simulation cannot be improved, especially in the scenarios with large intrinsic σ of input errors (in Fig. 2 and Fig. 3). From the above, the ability of the IBUNE method depends on the input data quality and the improvement of the input data and model simulation only happens when the standard deviation of the estimated input error is small. The availability of prior information is insignificant for the IBUNE method, especially when the intrinsic σ of the input error is large.

However, the findings in the BEAR method are quite different. Accurate prior information about the input error model is important in the BEAR method. Figure 3 demonstrates fixed scenarios calibrated via the BEAR method always produce a higher NSE of the modified input than inferred scenarios. This is likely because the prior information can constrain the input error distribution and reduce the impacts of other sources of errors. The availability of prior information of the input error relies on studies about benchmarking observational errors of the water quality and hydrologic data, and the selection of a proper input error model is important. Comparing the results in Figure 2, the BEAR method always brings the best performance regardless of the prior information of the error SD when the input error model is an additive formulation, while when the input error model is a multiplicative formulation, the BEAR method cannot improve the input data if the prior information of the error SD is not accurate. This illustrates that the compensating effect between the input error and parameter error is weaker in the additive form of the input error. This is probably related to the specific model structure, as the exponent parameter b in BwMod has a stronger interaction with the multiplied errors than the additive errors. Thus, more comprehensive comparisons should be undertaken to explore the capacity of different input error models in different model applications." (line 324-345)

17) L. 291: "…could be regarded as the reference value." -> Why? Please explain.

Thanks for pointing this out. The observed streamflow from the rating curve cannot be considered as the reference value, it is just closer to the reference value than the simulated streamflow via GR4J. The explanations have been corrected as follow:

"*According to the results of the traditional method in Fig. C2, the simulations from the "O" streamflow (in (a1)) catch the dynamics of observed TSS concentration better than the simulations from the "S" streamflow (in (a3)). Thus, compared with the simulated streamflow via GR4J ("S" streamflow), the observed streamflow from the rating curve ("O" streamflow) should be closer to the true input data."* (line 286-289)

18) L. 295-296: "…have an infinite number of combinations, while the error rank has limited combinations, dependent on data length." -> What is exactly meant here?

We have added the explanation as follows:

"In a continuous sequence of data, the potential error values have an infinite number of combinations, while the error rank has limited combinations, dependent on the data length. For example, in Table A.1, the estimated error at the 1st time step could be any value. Even under the constraint of input error ranging from the minimized to the maximized sampled errors (i.e. [-0.29,0.16] in the 1st iteration), error magnitude estimation still has infinite possibilities due to the continuous probability distribution the error represents. In contrast, the rank is discrete, having only 20 possibilities (i.e. an integer from [1,20]). From this point of view, it is more efficient to estimate the error rank than estimate the error value." (line 296-302)

19) L. 297ff. "Compared with the IBUNE framework…" -> there is no real comparison made, please see major comments

Please see the reply to the general comment 3).

20) L. 340: "for method R, an accurate input error model can constrain the adverse impacts…" -> wasn't this the problem to begin with? Please clarify this sentence.

This point has been clarified as follows:

"Accurate prior information about the input error model is important in the BEAR method. Figure 3 demonstrates fixed scenarios calibrated via the BEAR method always produce a higher NSE of the modified input than inferred scenarios. This is likely because the prior information can constrain the input error distribution and reduce the impacts of other sources of errors." (line 334-337)

Please also see the reply to the general comment 2).

21) L 354-355: "However, the ability of these approaches needs further discussion in systems with correlated responses." -> Please clarify – what is the exact problem and why do ARMA models fit here?

Thanks for your comments. According to our latest research, the AR model is a good tool to represent the autocorrelation of the model response in the input error identification, and we have clarified this as follows:

"If the response caused by an input is not instantaneous but exhibits persistence (i.e. occurs over several time steps), the autocorrelation in the output should be addressed to ensure the independence assumption of the rank updating is satisfied. Current ways to deal with this problem in hydrologic modelling can provide a reference in the potential modification of the BEAR method. The part of each residual error correlated with the previous residual errors can be represented by an autoregressive moving average (ARMA) model (Kuczera, 1983) or autoregressive (AR) model (Schaefli et al., 2007, Bates and Campbell, 2001). This correlated part is removed from the residual error and the remaining part will be only impacted by the input error. Thus, the correspondence between the input error and the residual error part is ensured and the latter process will be the same as the application of the BEAR method in this study. Following this idea, the autoregressive (AR) model has been integrated with the BEAR method in the study of Wu et al. (2021) to deal with the autocorrelation of residual errors in a hydrologic model. The results prove this integration is effective to improve the input error estimation.

However, this treatment can not guarantee the improvement of the input error estimation in this study where the sediment concentrate is simulated at the daily time scale (Figure D 1). At this time

scale, one input (streamflow) may not impact the response (sediment concentration) for multiple time steps and autocorrelation may not be well represented via a simple autocorrelation function. When the temporal resolution of the data is high (i.e. minute) and one model output is affected by many inputs, the memory effect may be addressed effectively via the AR model. Therefore, the specific representation of the autocorrelation in the residual error needs further discussion through the comparisons in different time scales or with different characteristics in the memory effect." (line 356-372)

22) L. 358: "developed" -> "proposed" – the methods are already known but used in a way to address input error here.

We have changed *"developed"* to *"proposed"*. (line 375)

23) L 362: "… addresses the high dimensionality problem…" -> not shown

Thanks for your comments. "Address" has been changed to "avoid" (line 379)

Figures

1) General: Legends in figures should be improved, e.g. in terms of colors or placing
2) General: Provide higher resolution and unify the legend (see especially Fig. 4 and 6)
3) Figure 3: please use colors that are better distinguishable (see cases "T" and "R")

Thanks for your suggestion. We have improved the quality of all the figures, including improving the resolutions and modifying the colors or placing of legends.

4) Figure 3(4): NSE = 1 is unrealistic. Please see major comments.

Thanks for your pointing this out. NSE is close to 1, not equal to 1. This occurs in the previous Figure 3 showing the results of the synthetic case where the modeling only suffers from input error and parameter error. The BEAR method is effective in isolating the input error and parameter error, which has been proved by the fact that NSE is much closer to 1. In the current manuscript,

we have implemented the BEAR method in the SMC calibration, and in new Figure 2, the NSE is still close to 1. However, when the BEAR method is applied in applications where other sources of errors will interfere, as Figure 3 shows, the fit to the output TSS observations reduces.

5) Figure 4 (c3,c4): model predictions are clearly shifted. Please elaborate on this offset.

The model applied is BwMod. When the input (streamflow) is large, the output (TSS concentration) will be reduced due to the wash-off effect. This is opposite to a hydrological model, where the large input (precipitation) will lead to a large output (discharge).

6) Figures 4 and 6: Maybe it is better to show these figures in the appendix and only present the most important subfigures in the main text

Thanks for your suggestion. We have moved these two figures into Appendix C.

Tables

1) Tables 1-1 and 1-2: The tables could be presented as additional files but are not helpful in the main article

Thanks for your comments. We have moved these two figures into Appendix A, integrating the descriptions and other figures to provide a more clear explanation about the BEAR method.

2) Table 3: the "fixed" scenarios in the real test case are not fixed but provide small hyperparameter ranges

Thank you for pointing this out. The small ranges have been changed into the fixed values in Table 2, and we have checked all the related results when the BEAR method is implemented in the SMC calibration scheme.

Technical corrections

1) L. 128: double ","

Thanks, this sentence has been deleted as the BEAR method has been recast in the SMC calibration scheme.

2) L. 142: “sth” -> make “s” italic

Thanks, this sentence has been deleted as the BEAR method has been recast in the SMC calibration scheme.

3) Eq. 8: unspecified symbol

We have removed this unspecified symbol. (line 192). Thanks.

4) L. 314: “q increasing until the objective: : :” -> incomplete sentence

Thanks, this sentence has been deleted as the BEAR method has been recast in the SMC calibration scheme.

Response to Reviewer #2:

This paper developed a new algorithm called BEAR for accurate quantification of input errors in water quality modeling. The precondition of the BEAR algorithm is that the input uncertainty should be dominant and that the prior information of the input error model can be estimated. Results of both synthetic data and observed data indicated the efficiency of the algorithm. Overall, the paper is well rewritten and the topic is suitable for the journal. However, the following issues should be further explained and clarified before its submission:

We thank the reviewer for the overall positive assessment of the manuscript and helpful comments. We have responded to each point in turn in the following sections. The comments from the reviewer are provided in blue text and our responses are organized point-by-point in black text. The manuscript text after the proposed changes is shown in "*black italics*". The number of the line, equation and section refers to the revised version of the manuscript without track changes, shown in yellow highlight.

It should be noted that the method name will change from the "Bayesian error analysis with reshuffling" into "Bayesian error analysis with reordering". This is based on suggestions by one of the reviewers, as the word "shuffling" implies randomness in the reordering, while the reordering in our method is determined by the model residual error. The term "reordering" better reflects the deterministic nature of error quantified via this new method. Besides, the abbreviations of methods (T, D, R) has been changed to the full names (Traditional, IBUNE, BEAR).

1) There have been many studies focusing on the uncertainty of input data errors for hydrologic modelling, and many methods including Bayesian algorithm can be used for handling the issue. However, the gap between previous studies and this study was not explained clearly in the Introduction. The motivation of this study should be clearly clarified.

Thanks for your suggestion. The research gap and motivation have been modified in the Introduction as follows:

"*Input uncertainty can lead to bias in parameter estimation in water quality modeling (Chaudhary and Hantush, 2017, Kleidorfer et al., 2009, Willems, 2008). Improved model calibration requires isolating the input uncertainty from the total uncertainty. However, the precise quantification of*

time-varying input errors is still challenging when other types of uncertainties are propagated through to the model results. In hydrological modeling, several approaches have been developed to characterize time-varying input errors, and these may hold promise for application in WQMs. The Bayesian total error analysis (BATEA) method provides a framework that has been widely used (Kavetski et al., 2006). Time-varying input errors are defined as multipliers on the input time series and inferred along with the model parameters in a Bayesian calibration scheme. This leads to a high-dimensionality problem, which cannot be avoided (Renard et al., 2009) and restricts the application of this approach to the assumption of event-based multipliers (the same multiplier applied to one storm event). In the Integrated Bayesian Uncertainty Estimator (IBUNE) (Ajami et al., 2007) approach, multipliers are not jointly inferred with the model parameters, but sampled from the assumed distribution and then filtered by the constraints of simulation fitting. This approach reduces the dimensionality significantly and can be applied in the assumption of data-based multipliers (one multiplier for one input data) (Ajami et al., 2007). However, this approach is less effective because the probability of co-occurrence of all optimal error/parameter values is very low, resulting in an underestimation of the multiplier variance and misidentification of the uncertainty sources (Renard et al., 2009). From the above, a new strategy should be developed to avoid high dimensional computation and ensure the accuracy of error identification." (line 39-54)

2) More detailed steps about how to use the BEAR algorithm should be explained. Besides, the advantages of the BEAR algorithm compared with conventional methods should be more clearly clarified for making clear understanding from readers.

Thanks for your suggestion. The detailed steps of the BEAR method have been added in Appendix A and an illustration example has been moved from the methodology part to Appendix A to make the explanation clearer. In addition, the comparison with conventional methods has been clarified as follows:

"*The application of the BATEA framework is limited by high dimension computation (Renard et al., 2009). This becomes impractical in quantifying the data-varying errors (rather than the event-varying errors in the study of BATEA (Kavetski et al., 2006)), where the dimension easily exceeds 1000 (Haario et al., 2005). Therefore, the BATEA method is not considered in the comparison. In this study, three methods, including the "Traditional" method, "IBUNE" method and "BEAR" method, are compared to evaluate the ability of the BEAR method in estimating the model*

parameters and quantifying input errors. "Traditional" method regards the observed input as error-free without identifying input errors (i.e. Eq. (2)), while the other two methods employ a latent variable to counteract the impact of input error and build the modified input (i.e. Eq.(3)). In the "IBUNE" method, potential input errors are randomly sampled from the assumed error distribution and filtered by the maximization of the likelihood function (Ajami et al., 2007). Although the comprehensive IBUNE framework additionally deals with the model structural uncertainty via the Bayesian Model Averaging (BMA) method, this study only compares the capacity of its input error identification approach. The "BEAR" method adds a reordering process into the "IBUNE" method to improve the accuracy of input error quantification."(line 162-173)

3) Actually, the availability of prior knowledge of the input data error is important for modelling, but is also a difficult issue. It may be not enough only mentioning this issue in Conclusion. At least more discussions and the potential solutions should be provided.

The reviewer raised an important point. The discussion about this has been added in Section 4.2:

"*The availability of prior information of the input error relies on studies about benchmarking the observational errors of water quality and hydrologic data, and the selection of a proper input error model is important. Comparing the results in Figure 2, the BEAR method always brings the best performance regardless of the prior information of the error SD when the input error model is the additive formulation, while when the input error model is the multiplicative formulations, the BEAR method cannot improve the input data if the prior information of the error SD is not accurate. This illustrates that the compensating effect between the input error and parameter error is weaker in the additive form of the input error. This is probably related to the specific model structure, as the exponent parameter b in BwMod has a stronger interaction with multiplicative errors than additive errors. Thus, more comprehensive comparisons should be taken to explore the capacity of different input error models in different model applications."*(line 337-345)

4) The quality of some Figures in the manuscript should be improved to make all information clear.

Thanks for pointing this out. We have improved the quality of all the figures, including improving the resolutions and modifying the colors or placing of legends.

Response to Reviewer #3:

We have noted the reviewer's comprehensive remarks, and the following provides our response to each point. We appreciate the level of detail that the reviewer has gone into, and would like to thank the reviewer for the suggestions which have significantly improved how we convey the proposed approach. The comments from the reviewer are provided in blue text and our responses are organized point-by-point in black text. The manuscript text after the changes is shown in "*black italics*". The number of the line, equation and section refers to the revised version of the manuscript without track changes, shown in yellow highlight.

Complex patterns in input uncertainty such as spatial or temporal error correlations are an important topic in environmental science. In their present study, the authors seek to explore the ubiquitous issue of complex input uncertainty structures by proposing a novel method called Bayesian error analysis with reshuffling (BEAR). The proposed method is based on sampling an estimated input error and subsequently sorting the resulting realizations in an order which reduces residual mismatch to the observations. The authors then proceed to demonstrate the performance of their algorithm for a synthetic and a real case and compare its performance to a number of alternative setups.

I find the approach a very interesting and creative idea, and always appreciate it if someone takes the risks inherent to exploring a new methodological idea. Unfortunately, I have some reservations concerning its theoretical justifiability, which I hope the authors can address. Failing that, there might also be alternative ways to achieve similar effects which might stand on more robust theoretical foundations. Concerning these suggestions and the method itself, I have the following (major) comments:

Major comments:

1. Theoretical foundations: A key step of the approach is sorting input error realizations to reduce the residual mismatch between model predictions and system observations. I fear that this compromises the randomness of the error realizations, with potential consequences for the validity of the Bayesian inference that are difficult to predict. Rigorously deriving this algorithm from more basic theoretical foundations might better illustrate the consequences of the authors' assumptions

for Bayesian inference. If the authors do not have this expertise themselves (not to worry: few people in the environmental sciences do), I recommend seeking the help of the local statistics department – they are often keen to help. It seems an unfortunate truth of Bayesian statistics that interesting ideas for algorithms which sound nice on paper often tend to violate the Bayesian framework in unforeseen ways.

Thanks for your insightful comments. We have now added Appendix B that derives the BEAR algorithm, showing how we aim to optimise the input errors relative to the estimated model parameters. We believe the remarks of the reviewer here arise from the implementation of an Approximate Bayesian Computation (ABC) approach in model calibration, which is not a formal Bayesian method and confuses the main contribution of the paper (which is to optimize input error ranks rather than input error magnitudes). To address this, we have recast the implementation of our algorithm via the Sequential Monte Carlo (SMC) approach (see Section 2.3). The BEAR algorithm could be implemented via SMC, or GLUE, or SCE-UA, or any common model calibration approach, simply by optimising the latent-input errors on the error rank rather than error magnitude to realise the deterministic relationship between the residual error and the input error. It should be noted that we don't estimate the posterior distribution of the error ranks, we only optimise the error ranks by finding the deterministic relationship between the input error rank and model residual error (see Appendix B).

2. Improving future performance: While I am not intimately familiar with the alternative methods (BATEA, IBUNE) referenced by the authors, improving future model performance is a common motivation for learning complex uncertainty structures in hydrological models. The approach in this manuscript, however, requires a concurrent time series of observations. As a consequence, it does not really improve the error model itself and hence offers little value for improving future predictions. On the other hand, attempting to learn time-varying bias or correlation structures in the input errors – admittedly a sometimes computationally formidable task – can increase the likelihood of future predictions substantially. Such approaches would also be significantly easier to justify. I would recommend mentioning this limitation for the BEAR algorithm in the manuscript, or – better yet – either explore or propose ways on how this limitation could be circumvented.

The reviewer is correct in that the approach we propose does not 'improve' the error model but it improves the water quality model specification. It is assumed that the error model is known a priori and the overall objective is not to improve on this. We believe this is not an unreasonable assumption, as the model inputs are derived using a hydrologic model or rating curve whose error can be derived independently of the water quality model implementation, like the real case in this study. These independent observations provide insight into the distribution of input errors that can then be leveraged in the model calibration.This point has been clarified as follows:

"*The above approach does not improve the input error model itself but improves the WQM specification to have parameters closer to what would be achieved under no error conditions. Then the model can be more effectively used for scenario analysis (where we may know the hydrologic regime of a catchment in a hypothetical future), for forecasting under the assumption of perfect inputs (where the driving hydrologic forecast is independently obtained via a numerical weather prediction and a hydrologic model) or for regionalization of the WQM (where the model is transferred to a catchment without data). In all of these cases, an ideal model should have unbiased parameter estimates. This is our goal in identifying the optimal input errors, not to use the model for predictions with input data suffering the same errors."* (line 96-102)

In order to prove the BEAR method will provide better predictions under 'no input error' conditions, we added validation results in the synthetic case (Figure 2(5)), where the input is set as the true value (without error) and the model parameters are set as the calibrated values via different methods. Compared with the traditional and IBUNE methods, the BEAR method brings a simulation closer to the true output with similar reliability and smaller sharpness (Appendix C), which means a better quantification of the input errors will result in less biased model parameters and produce a better prediction.

3. The influence of other error types: It seems the authors focussed most of their attention on input uncertainty. While I agree that input uncertainty can play a very important role, the influence of observation errors and model structural uncertainty plays a substantial role as well. In this study, the authors assumed both the model and the output observations were error-free – and derived their algorithm accordingly –, but in practice these assumptions are virtually never met. I would encourage the authors to explore how (if at all) their algorithm can avoid surrogacy effects in the

presence of observation and model errors. (What I mean by "surrogacy effects" is that the algorithm's adjustments to the input error realizations also 'soak up' [and consequently mask] errors in the output observations and the model itself in a bid to reduce the output residuals. This is of course undesirable.) See also my penultimate minor comment below.

The reviewer has raised here a very important point, and we completely agree with the issue of compounding sources of error and potential 'surrogacy' effects.

We have aimed to address this by implementing a real data case which likely has issues of error surrogacy, to identify how our approach works in a 'real' setting. We believe this helps balance our discussion of the approach and its potential limitations.

To additionally ensure we do not oversell our method given other sources of error, we have added a synthetic example in Section 3.3 that examines how the BEAR method performs under increasing error on the model calibration data. We hope this will help properly identify the usefulness of our approach but its potential limitations depending on the settings in which BEAR might be implemented.

4. Deterministic functions as an alternative: If the authors find that their algorithm might be based on flawed assumptions (following a more detailed theoretical derivation or investigation of the distribution it effectively samples from), the authors might wish to explore possible alternatives. If reducing the output residuals through adjustments to the input data remains the goal, a safer route might be to couple a deterministic input pre-treatment routine with the WQM and add its parameterization to the WQM parameter vector. Functionally, this pre-treatment routine can simply be interpreted as part of the deterministic model. Choices for this pre-treatment routine could be, for example, a one-dimensional spline which re-scales input magnitudes non-linearly (see the attached Figure 1, for an example with three extra parameters). More complex function choices might allow the consideration of lag, temporal or spatial correlations, etc. This would have the additional advantage over the BEAR framework that this pretreatment routine could also improve future predictions, assuming that it compensated true bias and is not overfitted. This comment is not a request for change, but a hopefully constructive suggestion for alternatives so that the authors might salvage some of their work in case it would turn out theoretically indefensible.

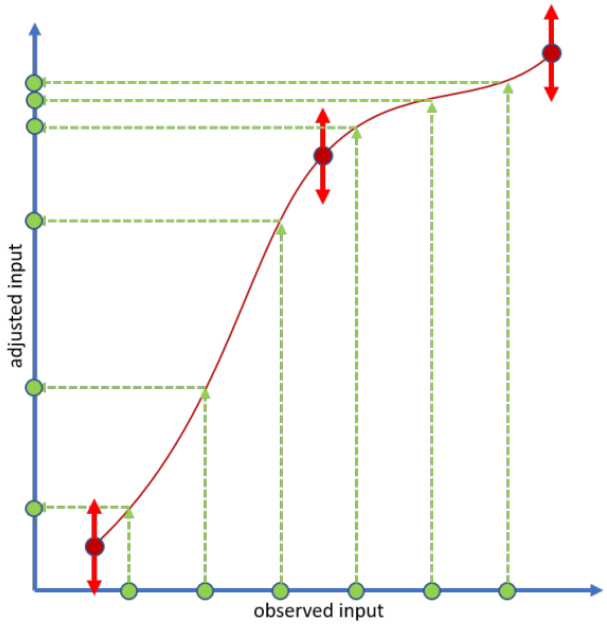


Fig. 1. Example of a non-linear re-scaling with a spline defined by three control points (red dots). You could use such a spline to scale the input values non-linearly.

We appreciate the thought that the reviewer has put into this comment, and we have considered this concept carefully, however, respectfully we do not see it as a viable pathway for the types of errors that we see in inputs to WQMs. The approach you suggested here is a non-linear bias correction to the input data which will correct systematic biases. However, the randomness of the observational error can't be explicitly identified and it does lead to biased model parameters in calibration. We present here a synthetic case to demonstrate such, where the model inputs are specified as $\boldsymbol{X}^o = \boldsymbol{X}^* + \boldsymbol{\varepsilon}_X, \boldsymbol{\varepsilon}_X \sim N(0, 0.2^2)$, the observed outputs are specified as $\boldsymbol{Y}^o = \boldsymbol{Y}^* = M(\boldsymbol{X}^*, \theta^*)$, and the likelihood function in the SMC approach is calculated in log-transformed space. The mean of Gaussian distribution of the input error is set as 0, where the observed inputs are not systematically biased from the synthetic true inputs (Figure R1). Implied in the approach suggested by the reviewer, the observed inputs do not need modification. However, in the comparison of different methods in Figure R1, if we do not deal with the stochastic errors in input data, like the traditional method (the same as the suggested approach by the reviewer), the model parameters will be biased from their reference values. In contrast, the BEAR method can effectively identify the stochastic errors, beyond the systematic unbias of input data, as the BEAR method can push each input error close to the true value by reordering its rank according to the

residual error, and alleviate the impacts of both stochastic and systematic errors in input data on the model parameters.

Additionally note that we do not propose a method for rescaling errors, we are simply re-ordering their positions in the data to better correspond to deviations from model fits.

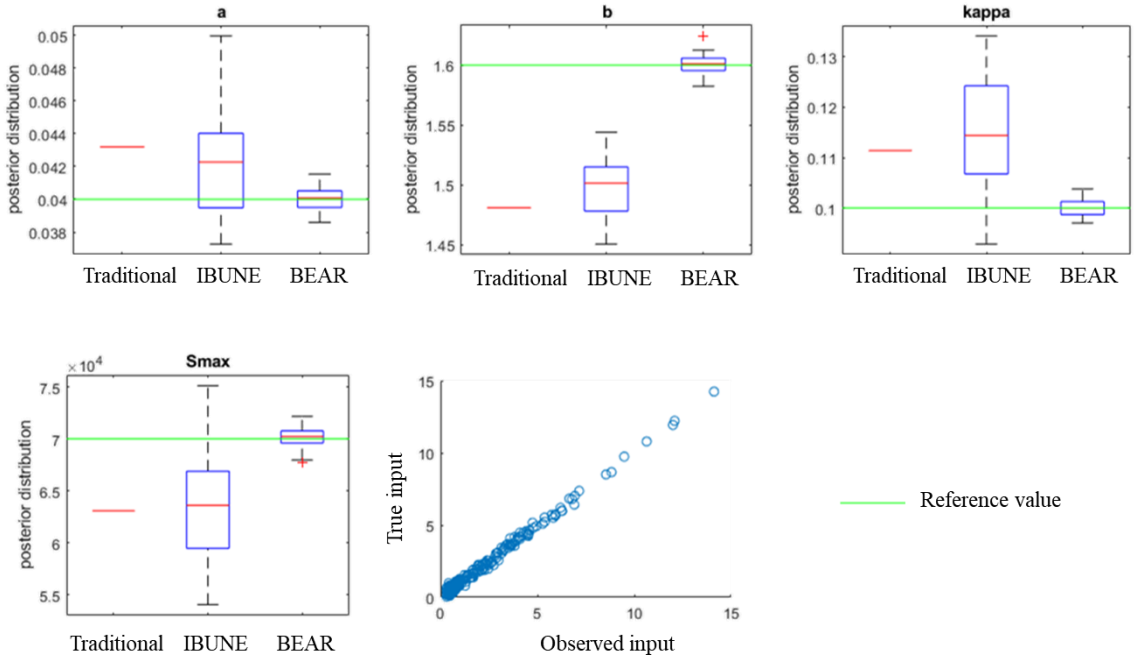


Figure R1 The posterior distributions of the model parameters estimated via the different methods and the scatter plot of the observed inputs vs true inputs in the synthetic case

5. BEAS instead of BEAR: This could be filed under nit-picking, but since the algorithm's name features so prominently, I chose to raise this to a major comment instead. The use of the word 'shuffling' implies randomness in the re-ordering. If I understood the authors' algorithm correctly, though, the re-ordering itself is entirely deterministic. As such, changing the name to something along the lines of "Bayesian error analysis with sorting" (BEAS) or "Bayesian error analysis with re-ordering" (if the authors like to retain their – admittedly very nice – acronym) might better reflect its deterministic nature.

We very much appreciate the valuable suggestion here, as the reviewer is completely correct. Yes, "reordering" better reflects the deterministic nature of error quantified via this new method.

Therefore, the method name will be changed into “Bayesian error analysis with reordering” to keep the BEAR acronym for short.

6. Why ABC: In the manuscript, the authors use an “Approximate Bayesian Computation via Sequential Monte Carlo” (ABC-SMC) approach. While I am not personally familiar with this approach, I struggle to see why it is necessary to resort to ABC, aside from any potential (forgive me) self-inflicted complications induced by the BEAR algorithm. The model and output variables seem pretty simple, so to my untrained eyes it is difficult to see why the formulation of an analytical likelihood should be impossible in this case. One could also cast the procedure the authors presented in Figure 1 with very few changes in terms of an MCMC routine, provided the re-ordering or error realizations ends up being statistically justifiable, of course. I would encourage the authors to provide a bit more detail on why ABC was necessary.

Thanks for the helpful suggestions here. The reviewer is completely correct that the ABC method is not necessary, and the core idea of the BEAR method (the reordering strategy according to the inferred ranks) can be easily applied in any other calibration algorithm, for example, MCMC or SMC algorithms. In order to clarify this point, we have recast the implementation of our algorithm via the Sequential Monte Carlo (SMC) approach (see Section 2.3), which is clearer to derive the BEAR algorithm from a Bayesian perspective under the assumption of optimised input errors (see Appendix B). This point has been clarified as follows:

“*The core strategy of the BEAR method is to identify the input errors by estimating their ranks, which can be easily integrated into formal Bayesian inference schemes (for example, Markov chain Monte Carlo (MCMC, (Marshall et al., 2004)) and Sequential Monte Carlo (SMC, (Jeremiah et al., 2011, Del Moral et al., 2006))) and other calibration schemes (for example, the generalized likelihood uncertainty estimation (GLUE, (Beven and Binley, 1992))). Based on a traditional calibration approach, the BEAR method works by replacing the observed input with the modified input that is obtained through the estimated input error rank via the secant method.*” (line 142-147)

7. Focus on a good fit: A key idea which seems to permeate the present manuscript is that it is desirable to obtain error realizations, if necessary by force (i.e., re-ordering), which match the observations as closely as possible. This is of course true, but not at all cost. Even assuming a severely mischaracterized prior input error distribution (e.g., a Gaussian with a standard deviation of 1E-10 and a mean of -1E8), one could theoretically obtain an error realization which causes the model to fit the observations perfectly if we only drew sufficiently (read: infinitely) many samples. The challenge, then, is not to find such a realization within our prior distribution (it will exist in any distribution with sufficiently broad support), but to find a distribution from which there is a high probability to obtain such a sample. Crucially, such a distribution should be independent from future observations, and I fear that this may not be the case for the approach proposed in this manuscript. In this approach, after re-ordering, the realizations are no longer i.i.d. samples from the input distribution (similarly to how one could interpret correlated Gaussian samples merely re-ordered independent Gaussian samples, but would nonetheless be wrong in claiming that an independent Gaussian distribution is identical to a correlated Gaussian distribution). If the authors decide to pursue my request for a derivation of a theoretical foundation for their approach (see comment 1), I recommend focussing on investigating from what effective distribution they are really sampling. Considering BEAR's ability to yield a reliably good fit with seemingly arbitrary prior input error realizations, I fear that the distribution you effectively sample from may be well approximated with (for example) a Gaussian with a mean inversely obtained from the observation residuals. If this turns out to be the case, the method would be more or less equivalent to just calculating the input error residuals through an inverse method of choice by minimizing the output residuals. This would not be very useful, and I would recommend exploring one of the approaches I suggested in comment 4 instead. See also my penultimate minor comment.

The reviewer has raised an interesting point here, that the reordered errors may include features (such as autocorrelation or dependency) that are not present in the original error sample. We have calculated the PACF of the reordered errors as a diagnostic for the case study on the potential interactions between observation error and other sources of error. The residuals show the reordering step does transform the autocorrelation of the residual error into input error. We have carefully considered the way to address this problem and applied an autoregressive (AR) model with order 1 to represent the autocorrelated part in the model residual error and remove this part from the original model residual error, the remaining part is used to adjust the input error ranks.

This approach was useful in a study of ours that considered the "memory effect" of hydrologic models and the persistence of input errors in the model outputs (Wu et al., 2021). The results are denoted as "BEAR-AR" in the following Figure D 1 and demonstrate that the ability of the AR model is not consistent in this study where the sediment concentrate is simulated at the daily time scale. Compared with the results of the BEAR method (green bars), the BEAR-AR method (pink bars) in some cases improves the input error identification but in other cases, it worsens.

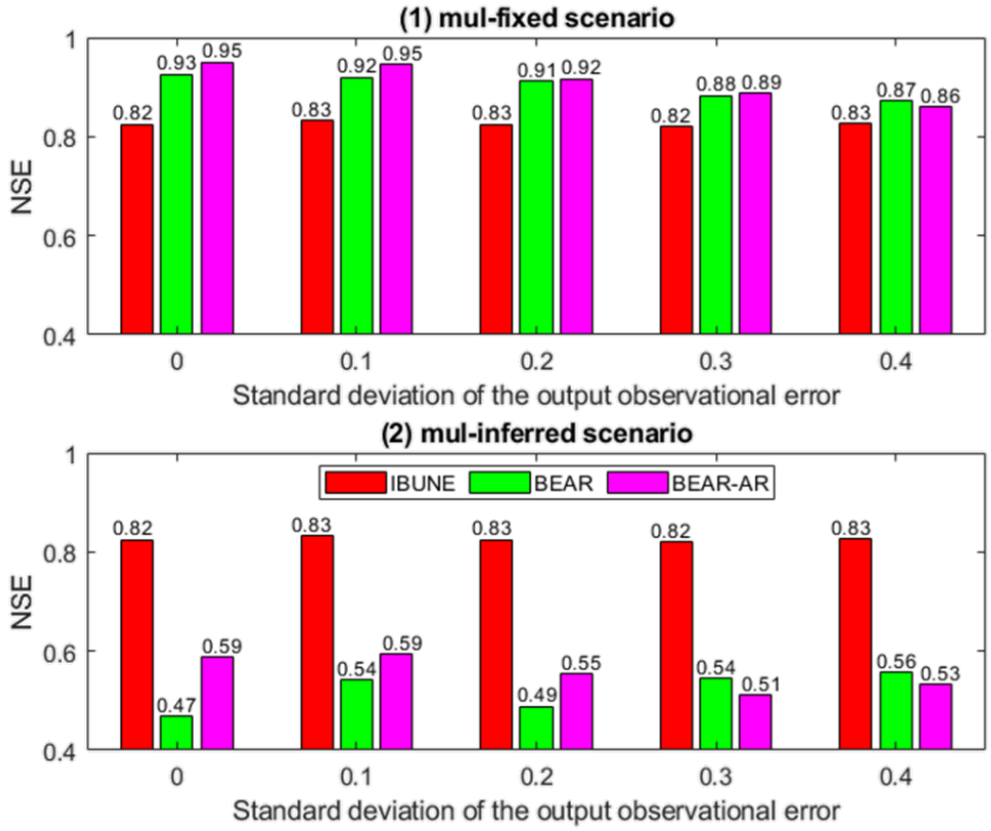


Figure D 1 Comparison of Nash-Sutcliffe efficiency (NSE) of the modified input v.s true input under the interference of the output observational errors with the increasing standard deviations in two calibration scenarios in synthetic case 2 (including *mul-fixed* and *mul-inferred*; notations are given in Table 2) via three calibration methods (including the IBUNE method and the BEAR method and the BEAR-AR method, the BEAR-AR method is the BEAR method after applying the autoregressive (AR) model to deal with the residual error)

In using the AR model for quantifying the input error in a hydrological model, the results demonstrate that the BEAR-AR method in a hydrologic model is stable, and outperforms the

BEAR method (the details please see the paper (Wu et al., 2021)). The possible reason for these differences and related discussion have been added in the manuscript as follows:

"If the response caused by an input is not instantaneous but exhibits persistence (i.e. occurs over several time steps), the autocorrelation in the output should be addressed to ensure the independence assumption of the rank updating is satisfied. Current ways to deal with this problem in hydrologic modelling can provide a reference to the potential modification of the BEAR method. Autocorrelation in the residual errors can be represented by an autoregressive moving average (ARMA) model (Kuczera, 1983) or autoregressive (AR) (Schaefli et al., 2007, Bates and Campbell, 2001). The correlated part of the error is removed from the residual error and the remaining part will be only impacted by the input error. Thus, the correspondence between the input error and the residual error part is ensured and the latter process will be the same as the application of the BEAR method in this study. Following this idea, the autoregressive (AR) model has been integrated with the BEAR method in the study of Wu et al. (2021) to deal with the autocorrelation of residual errors in a hydrologic model. The results prove this integration is effective to improve the input error estimation.

However, this treatment may not guarantee the improvement of the input error estimation in this study where the sediment concentrate is simulated at the daily time scale (Figure D 1). At this time scale, one input (streamflow) may not impact the response (sediment concentration) for multiple time steps and autocorrelation may not be well represented via a simple autocorrelation function. When the temporal resolution of the data is high (i.e. minute) and one model output is affected by many inputs, the memory effect may be addressed effectively via the AR model. Therefore, the specific representation of the autocorrelation in the residual error needs further discussion through comparisons in different time scales or with different characteristics in the memory effect." (line 356-372)

A point of clarification: in each subsequent iteration of the BEAR algorithm, a new population of input errors are sampled from their a priori distribution. This means that the distribution of errors at each iteration is the same prior to reordering, i.e. the population of errors do not converge to a distribution that has different statistical features (mean, standard deviation, skewness). However, we do recognize that the reordering process provides insight into how the input errors may be

ideally distributed across time that can inform how the surrogacy effect is manifested (see comment 3). For example, if the errors are highly autocorrelated, this could highlight potential model structural errors, resulting from that the WQM has not properly represented the storage characteristics of TSS in the catchment. We believe that including further diagnostics will help elucidate this effect.

Note that the approach does in fact rely on an appropriate prior distribution being identified describing the input error distribution. If this error distribution is mischaracterized and the statistical features are different from the real input, the resultant outputs will not converge to the calibration data, and will lead to larger residual errors. A new updating will be taken to find a more appropriate assumption of the input error to get a smaller residual error. In some cases, the parameter error compensates this mischaracterized error distribution of input error and leads to an overfitting problem. This impact depends on the selection of the input error model, but can not be avoided in all the methods unless a method can properly deal with all sources of errors together. More discussions have been added in Section 4.2.

Specific comments:

Line 22-25: You mention the importance of complex interactions of different error sources directly in the first paragraph but proceed to largely ignore their influence in the remaining manuscript. I think this part is important and should be discussed in greater detail in the remainder of the manuscript (particularly also the methods/theory section).

Thanks for your suggestion, we agree this was not being properly highlighted. We have added an explanation in the methodology that emphasizes this:

"It should be noted that the derivation of the BEAR method is based on the assumption that the model only suffers from input error and parameter error, but other sources of error (i.e. model structural error and output observational error) can also impair the estimation of the model parameters and are inevitable in the WQM. Considering this realistic situation, the ability of the BEAR method will be tested in a case study where the interference of other sources of error has been considered."(line 77-80)

Line 49-51: During this review, I have briefly glanced into the corresponding methods BATEA and IBUNE, and apparently there was quite a commentary battle between the authors over these methods (see doi:10.1029/2007WR006538 and https://doi.org/10.1029/2008WR007215), and Renard et al. 2009 noted that IBUNE may in fact not reduce dimensionality. The choice is of course ultimately up to the authors, but it might be useful to add a small comment noting that the claim of dimension reduction by IBUNE is also challenged.

Thanks for your comment. In the comments from Renard et al. 2009, there are two different interpretations of the IBUNE framework. Interpretation A is the same as method D (the IBUNE method in the current manuscript) and Renard et al. 2009 argue the randomness in this approach will lead to an underestimation of the input error variance. Interpretation B is the same as the BATEA approach, which can not reduce the computational dimension.

According to the IBUNE paper (Ajami et al., 2007), the authors state that IBUNE can circumvent the high dimensionality issues by randomly sampling the multiplier to each time step from an assumed normal distribution. Therefore, we consider Interpretation A as the 'true' version of IBUNE and provide discussion on this in the manuscript.

Line 69-75: I would be careful here. In reality, there are many different error sources, certainly not the least of which is model structural error. Calibrating (i.e., simply minimizing the residuals between simulated and observed output) in the presence of other error sources is prone to surrogacy effects, so you can never really be sure you recovered the 'true' parameters. Even making the (unrealistic) assumption that we could manage to completely remove all error sources in the model and its input, we could still only retrieve the 'true' model parameters if our inverse problem is unique. I would mention these restrictions here (only works if all error sources can be removed completely, unique inverse problem).

Thank you for pointing out the equifinality problem. We have modified the description here as follows:

"The proposed calibration (Eq. (3)) will turn into an ideal calibration where the optimal parameters $\boldsymbol{\theta}^p$ *will lead to the same simulation corresponding to the true values* $\boldsymbol{\theta}^*$ *and the model residual* $\boldsymbol{\varepsilon}^p$ *will decrease to zero. If the inverse problem (from the zero residual to find the optimal parameter) is not unique, the calibrated parameter* $\boldsymbol{\theta}^p$ *may not converge to the true parameter* $\boldsymbol{\theta}^*$*, but lead to the same simulation as the true parameter. In this study, these parameters are also denoted as* $\boldsymbol{\theta}^*$ *and called ideal model parameters."* (line 86-90)

Line 70-73: In Equation (2), the variables Y^o and Y^s are used without any introduction. I assume both variables stand for the observed and simulated output. Please introduce these variables.

Thanks for pointing this out. We have clarified this as follows:

"where $\boldsymbol{Y}^s$ *is the output simulated from the model M corresponding to the observed input* $\boldsymbol{X}^o$ *and model parameter* $\boldsymbol{\theta}^c$*, and the observed output* $\boldsymbol{Y}^o$ *is assumed without observational errors in the derivation, thus can be denoted as* $\boldsymbol{Y}^*$*."* (line 75-76)

Line 76-77: A critical thing here is that $\boldsymbol{\varepsilon}$ is previously introduced as an error, which implies that you consider it to be a random variable. However, subtracting a (say) Gaussian random variable from another Gaussian variable with the same properties does not reduce variance to zero but actually doubles it (if both random variables are independent). What you seem to have in mind

here only works if ε and ε^p have identical properties and are perfectly correlated (note that this implies a lot more than just sharing the same statistical moments!), or if you are talking about error realizations. You should clarify this. This relates to major comment 7. You can only create this perfect correlation if you can somehow extract the error realizations of ε (which only works under the assumption that you already have the input samples, that there are no other errors, and that the inverse problem is unique). Consequently, I fear that you may create/mimic this perfect correlation by implicitly solving an inverse problem, which would make the proposed method not very useful.

We agree with your argument that "Subtracting a (say) Gaussian random variable from another Gaussian variable with the same properties does not reduce variance to zero but actually doubles it (if both random variables are independent)". This is also the reason why the IBUNE method cannot provide accurate error identification by random sampling. The claim in this manuscript is "*If the equivalence between* ε_X *and* ε_X^p *can be ensured for each data point, the modified input* X^p *then becomes the same as the true value* X^**. The proposed calibration (Eq. (3)) will turn into an ideal calibration where the optimal parameters* θ^p *will lead to the same simulation corresponding to the true values* θ^* *and the model residual* ε^p *will decrease to zero*" (line 85-87). As the reviewer notes, we refer here to the error realizations, not the distribution of errors.

We also agree that the perfect identification of input error series and model parameters only happens when "there are no other errors, and that the inverse problem is unique". Considering the impacts of other error sources, we have added the clarification as follows: "*It should be noted that the derivation of the BEAR method is based on the assumption that the model only suffers from input error and parameter error, but other sources of error (i.e. model structural error and output observational error) can also impair the estimation of the model parameters and are inevitable in the WQM. Considering this realistic situation, the ability of the BEAR method will be tested in a case study where the interference of other sources of error has been considered."* (line 77-80). Considering the unique inverse problem, we have changed the description here to "*If the inverse problem (from the zero residual to find the optimal parameter) is not unique, the calibrated parameter* θ^p *may not converge to the true parameter* θ^**, but lead to the same simulation as the true parameter*." (line 87-89)

Line 79: In Equation (4), you also mark the parameters – on which this entire exercise should be conditional on – as changing due to your proposed approach. The equations you have shown so far imply that the procedure you describe here is applied after parameter calibration. During a first reading of this paper, it is not immediately clear why the calibrated parameter values should change with your proposed approach. On a second reading, it becomes evident that you do not really calibrate but sample the parameter posterior, but that this sampling process is inter-woven with your BEAR routine, hence the parameter values are also affected. I recommend commenting on this already here to save your readers some confusion. Maybe it would also help not to talk about calibration at all in this context.

Apologies for the lack of clarification here. The reordering step for the input errors is implemented after one set of the model parameters has been updated. Corresponding to this set of model parameters, the optimal ranks of input errors are inferred via the secant method (the detailed algorithm has been clarified in Appendix A). Although the sampled errors have been reordered, they still follow the assumed error distribution and the overall statistical characteristics remain unchanged. With the constraint of the input error distribution, in Equation (3), if the calibrated model parameters are far from the ideal model parameters, the reordered errors will not equal the true input errors and the residual error cannot be reduced effectively. If the model parameters are close to the true model parameters, the relative rank of the input errors can be identified precisely via the secant method, and the model residual error will approach zero. Minimizing the model residual error (or maximizing the likelihood function in Bayesian inference) here is the same as the goal of the model calibration. We have clarified the model calibration goal in the paper so that the intent is clear. The improved model calibration is the ultimate goal in properly identifying the input errors.

Line 81-83: I would be very careful with this statement. This only happens if the model parameters θp and the input error residuals $\boldsymbol{\varepsilon}_X^p$ cannot compensate each other, i.e. if there is only a single, unique combination of parameters and errors which yields zero residual. If you have a Pareto front along which different values of θp and input error residuals $\boldsymbol{\varepsilon}_X^p$ yield zero residual, you cannot be certain that you have correctly identified the 'true' parameter values and the 'true' input error, even in a scenario where no other errors/uncertainties exist. In addition to this, my reservations

concerning other error types raised in major comment 3 also apply. I would recommend changing this statement accordingly and exploring its consequences for your algorithm in greater detail.

We appreciate your comment. Yes, the input error and model parameter error might compensate each other, which leads to a Pareto front along which different values of θp and input error residuals yield zero residual. We have added the clarification as follows: "*Besides, if the identified input error and the model parameter can compensate each other, multiple combinations of model parameter and input error may yield zero residual and their estimates will be biased from the ideal values. A possible way to weaken this compensation effect will be explored in Sect. 4.2.*" (line 90-92).

In the manuscript, we compare two types of input error models: an additive formulation ($\boldsymbol{X}^o = \boldsymbol{X}^* + \boldsymbol{\varepsilon}, \boldsymbol{\varepsilon} \sim N(0.2, 0.5^2)$, *add* in Table 2) and a multiplicative formulation ($\boldsymbol{X}^o = \boldsymbol{X}^* \exp(\boldsymbol{\varepsilon}), \boldsymbol{\varepsilon} \sim N(0.2, 0.5^2)$, *mul* in Table 2). According to our synthetic cases, we find the multiplicative formulation is more likely to compensate the model parameter error, but the compensation effect will reduce with accurate prior information on the input error model. This is probably because the impacts of errors in the multiplicative formation are similar to the parameter *b* in Equation 8, or the nature of the multiplicative formulation is more likely to change with the model parameter than the additive formulation, due to having more flexibility. In sum, the compensation effect can be reduced through proper selection of the input error model as this affects the identification accuracy. But this problem is common in all the methods considering input error, and is not special to the BEAR method. More discussion has been added in Section 4.2.

Line 104-106: I would rephrase this a bit, because following the procedure you outlined in Figure 1 (a very nice schematic, by the way), it is not only two steps: you sample the error once, then iterate over a large number of re-ordering steps until you find an order which minimizes your output residuals. This could do with some clarification.

Thanks for your suggestion. We have rephrased the sentence as:

"*Thus, the procedure of input error quantification has been developed via the following key steps: 1) Sample the errors from the assumed error distribution to maintain the overall statistical characteristics of the input errors; 2) Update the input error ranks to minimize the model residual*

via the secant method (Eq. (5) and (6)); 3) Reorder these sampled errors according to the updated error ranks; 4) Repeat 2) and 3) for a few iterations until a defined target is achieved. This new algorithm is referred to as Bayesian error analysis with reordering (BEAR).” (line 135-139).

Line 115-116: If I understood your explanations here correctly, maybe an easier way of explaining what you are doing is that you sort your updated error ranks, then assign to each of them a new integer rank based on its position in the sorted list. This might be easier than trying to explain this procedure with scaling.

Thanks for your suggestion. We have modified this sentence as follows:

“*Sorting* $k_{i,q}$ *in all the ranks* $k_{i,q}(i=1,...,n)$ *can address this problem by effectively assigning to each of them a new integer rank based on its position in the sorted list*.” (line 125-126).

Line 125-131: As mentioned in major comment 6, please devote some space to explain why the models you use in the following necessitate the use of ABC. Even after going through the manuscript a few times, I struggle to see why standard Bayesian approaches would be impossible to use. At the risk of evoking the anger of our ABC-focussed colleagues: direct is usually better than approximate. It also does not become clear in the manuscript why an ensemble-based approach is used – couldn’t the same procedure be implemented in an MCMC-style acceptance/rejection algorithm? If there are some ABC reasons for requiring an ensemble, it you might also want to explain why and how it is used.

We apologize for the lack of clarification. The ABC is not necessary for the BEAR method to be implemented. We admit there is no difference in the calibration results between the standard Bayesian approaches and the ABC approach for this case study. We have clarified this as follows:

“*The core strategy of the BEAR method is to identify the input errors by estimating their ranks, which can be easily integrated into formal Bayesian inference schemes (for example, Markov chain Monte Carlo (MCMC, (Marshall et al., 2004)) and Sequential Monte Carlo (SMC, (Jeremiah et al., 2011, Del Moral et al., 2006))) and other calibration schemes (for example, the generalized likelihood uncertainty estimation (GLUE, (Beven and Binley, 1992))). Based on the traditional calibration approach, the BEAR method works by replacing the observed input with a*

modified input that is obtained through the estimated input error rank via the secant method." (line 142-147).

To avoid confusion, we have recast the implementation of our algorithm via the Sequential Monte Carlo (SMC) approach (Section 2.3) and redraw the flowchart (Figure 1). Besides, we have derived the foundation of the BEAR method in Appendix B.

Line 132-136/Figure 1: This explanation of the method is very short, and essentially only explains that you approach the posterior distribution iteratively through a number of intermediate steps, but not how this is achieved exactly. Figure 1 provides more information and suggests some sort of acceptance/rejection scheme depending on whether your procedure can reduce the error residuals below a certain threshold, but the nature of the posterior distributions from which new parameter values are drawn remains undefined. You also seem to update an input error parameter ηx, which seemingly contradicts statements you made suggesting the input errors are sampled from a pre-estimated distribution (Line 10, Line 193-194). This step is also never mentioned in the text itself up to this point – you only mention that you estimate the input error distribution's hyperparameters much later. The text also frequently mentions 'populations', which evoke the idea of an ensemble-based method, but none of the steps mentioned in the text so far actually seem to require an ensemble. Please provide some more (written) detail about how your algorithm functions exactly.

Thanks for your comments.

1)To clarify the algorithm, we have recast the implementation via the Sequential Monte Carlo (SMC) approach (Section 2.3) and redraw the flowchart (Figure 1). Also, we have changed the description in the manuscript, as follows:

"The details of the SMC algorithm can be found in the study of Jeremiah et al. (2011). Figure 1 demonstrates the integration of the BEAR method into the SMC sampler. In the SMC scheme, s refers to the number of sequential updating populations of parameter vectors (particles). The maximum number of the population S is set as 200 in this study. In each sequential population, N particles of model parameters are calibrated. N is set as 100 in this study. For each particle of the model parameters, the corresponding input error ranks are updated over q iterations, where q increases until the acceptance probability is larger than a number randomly sampled from 0 to 1.

It should be noted that if the model parameters are far away from the true values, especially in the initial population, iterative updating of the error ranks will have little effect in reducing the model residual. Therefore, the maximum number of iterations should be set, referred to as Q. Q is set as 20 in this study. If q exceeds Q, the algorithm returns to the mutation step in Fig. 1." (line 151-160)

2) To avoid confusion, We have removed "update an input error parameter ηx" from the methodology part and Figure 1, but kept this consideration in the case study and added the clarification as follows:

"*Given the description in the introduction, the input error model can be pre-estimated independent of calibration by analysing the input data in some studies. While in other cases, the input error model cannot be estimated or the accuracy is in question. Therefore, two scenarios about the prior information of* σ *have been considered: one is fixed as the reference values (denoted as 'fixed' in Table 2), the other one is estimated as the hyperparameters with the model parameters (denoted as 'inferred' in Table 2)."* (line 214-218)

3) The term "population" is used as in the SMC algorithm, and it is like an ensemble-based method. We have clarified this by a better description of how the algorithm is implemented via SMC, as follows: *"A population means a group of parameter vectors (particles) that is updated in each iteration"* (line 153)

Line 145-148 and Line 159-162: This is just a comment towards the general "Why ABC?" discussion. It seems to me that a classic MCMC procedure would avoid the need for adjusting the acceptance threshold dynamically, as proposed parameters are always compared to the previous entry in the chain.

Yes, ABC is not necessary for the BEAR method and any MCMC procedure will avoid the need for adjusting the acceptance threshold. We have recast the implementation of our optimization algorithm via SMC. See the reply for Line 125-131.

Line 154-157: I confess that this explanation is quite impenetrable, and probably causes more confusion here than it does good. I recommend restructuring this explanation or removing it

altogether. A good alternative would be to visualize this with a small figure, possibly added to the supporting information if length limitations to not permit embedding it into the main text.

Thanks for your suggestion. We have integrated an example and its illustration in Appendix A to explain the specific steps involved, and a detailed explanation of this has been given in step (6).

Line 192: I do not see from Equation 8 or 9 or their surrounding text how the spatial scale factors into this model. Through the Sa variable? Please clarify this.

Thanks for your comments. "*The two formulations in Bwmod were developed in a small-scale experiment (Sartor and Boyd, 1972), while in applications at the catchment scale, the conceptualized parameters largely abandon their physical meanings and the formulations can be considered a "black-box" (Bonhomme and Petrucci, 2017).*" This study attempts to simulate the sediment dynamics in the catchment scale. Thus, we say "the spatial scale is set as the catchment in this study". This has been clarified as follows:

"*This study will test the BEAR algorithm in a case of simulating the daily sediment dynamics of one catchment, thus, the time scale is typically set as daily and the spatial scale is set as the catchment."* (line 183-184)

Line 200: In Equation 8, you do not introduce Smax and κ. Please introduce these variables as well.

Thanks for your comments. The introduction of Smax and κ is shown in Table 1. We have added clarification as follows:

"*where the descriptions of κ and Smax are shown in Table 1.*" (line 192)

Line 203: In Equation 9, you do not introduce a and Qt^b. Please introduce these variables as well.

Thanks for your comments. Qt^b should be $(Q_t)^b$, we have modified Equation (8) and the description as follows:

$$s(S_{a,t}) = a \cdot (Q_t)^b \cdot S_{a,t}$$

"*where the descriptions of a and b are shown in Table 1, and* Q_t *is the streamflow at the catchment outlet at time t.*" (line 196)

Line 205: In Equation 10, you do not introduce Qt. Please introduce this variable as well.

See the above reply.

Line 209-211: For this section, there are a few assumptions which could warrant greater discussion. If the errors are normally estimated in advance based on a rating curve, why is there a constant offset of 0.2? Couldn't this systematic bias be corrected through the rating curve itself? Alternatively, if the offset is necessary because your errors are asymmetrically fat-tailed, wouldn't a different distribution (such as a scaled beta or gamma distribution) be a better choice? It is commendable to make the synthetic test case more challenging by introducing bias as well, but how would this be recognized a priori in a real test case if it wasn't already considered in the rating curve? Some more information might clarify the authors' choice of distribution for the audience.

Thanks for your comments. Yes, we agree with your statement that if the errors are normally estimated in advance based on a rating curve, the mean of the normal distribution should be 0. By including the systematic bias of 0.2 in this synthetic study, we aimed to test the BEAR method in wider applications, even if these are not necessarily representative of true errors. Figure 2 indicates that in the synthetic case where the input errors have a systematic bias, the BEAR method can bring more accurate estimations of the input errors and the model parameters. Therefore, in situations where the input errors have no systematic bias, the BEAR method also works. According to your comments, we added the clarification as follows:

"*If the input errors are estimated based on a rating curve, like the procedure in the following real case, the mean of input error should be 0. But in order to test the ability of the BEAR method in wider applications, a systematic bias 0.2 has been considered in the synthetic case even though this is unlikely to manifest in real situations."* (line 207-210)

Line 224-226: This part here is a bit unclear. What I deduce from the context is that you looked at two scenarios – one, where you left the prior input error fixed, and one where you estimated the input error hyperparameters as well. I would not talk about 'conditions' in this context, but rather about 'scenarios'. If I understood your drift here correctly, I would also add a comment which puts more emphasis on the fact that you subvert one of the principal assumptions you made earlier in the second scenario (namely, that the input error distribution is a prior/pre-estimated).

Thanks for your comments. To clarify this, we have changed "conditions" to "scenarios" here and have modified the description as follows:

"*Given the description in the introduction, the input error can be pre-estimated independent of calibration by analysing the input data in some studies. While in other cases, the input error model cannot be estimated or its accuracy is in question. Therefore, two scenarios about the prior information of σ have been considered: one is fixed as the reference values (denoted as 'fixed' in Table 2), the other one is estimated as the hyperparameters with the model parameters (denoted as 'inferred' in Table 2).*" (line 214-220)

Line 232-234: I would recommend to critically re-examine this part in the light of major comment 7. The high correlation of scenario R with the realizations of the synthetic true error series – which are supposed to be realizations from an independent Gaussian distribution – might be reason for concern, as they suggest that you might be implicitly solving an inverse problem for the input error residuals. This would have little to do with a Bayesian framework.

Thanks for your comments. It should be noted that "correlation" here is not the correlation among the estimated input errors, but the correlation between the estimated input error and the true input error, which can be used to evaluate the ability of the method to identify the dynamics of the input error. Regarding the fact that reordering will break the iid assumption of the input errors, please see the reply of comment 7.

Figure 4: Unfortunately, this figure is really hard to read. If possible, I would recommend splitting this up into several figures and providing the figures for individual scenarios in the supporting

information. The choice of colors also makes it very difficult to see what's going on (especially the neon green and the soft peach color). I am not familiar with the HESS compiler, but I would also recommend either a significantly larger resolution and a different image format such as .tiff or .gif, as the current figure is in quite a low resolution and has serious compression artifacts. For graphs such as this one, vector-based formats such as .svg or .pdf (if saved straight from Python with pyplot.savefig) might also allow readers of the electronic version to zoom in arbitrarily close for details. This could be particularly valuable here, since most of the relevant details are quite small.

Thanks for your suggestion. We have improved the quality of the figures, including splitting this into several figures, improving the resolutions, using colours that are better distinguishable, and modifying the placing of legends. Please see Appendix C in the manuscript.

Line 296-297: I would remove this statement, as you have not experimentally backed this statement up and it is not immediately obvious. I see little reason why inverting the observation residuals to find optimal input error realizations would be a more difficult task than re-ordering a pre-existing set of realizations. Quite the opposite, in fact.

Thanks for your insightful comments. The approach suggested by the reviewer, "inverting the observation residuals to find optimal input error realizations", is BATEA, which calibrates all the input error series together with model parameters. This leads to a well established high dimension issue (Renard et al., 2009). The statement here "*It is far more efficient to estimate the error rank than estimate the error value*." is based on the explanation "*In a continuous sequence of data, the potential error values have an infinite number of combinations, while the error rank has limited combinations, dependent on the data length.*". To clarify this, we have added some explanations as follows:

"*For example, in Table A1, the estimated error at the 1st time step could be any value. Even under a constraint of the range from the minimized to the maximized sampled errors (i.e. [-0.29,0.16] in the 1st iteration), its value estimation still has infinite possibilities due to the continuous nature of the error. In contrast, the rank is discrete, having only 20 possibilities (i.e. the integrity in [1,20]). From this point of view, it is more efficient to estimate the error rank than estimate the error value.*" (line 298-302)

Considering the advantages of reordering a pre-existing set of realizations over directly optimizing the input error value, please see the explanation as follows:

"*Besides, to avoid the high-dimension calculation, modifying each input error according to the corresponding residual error only works in the rank domain. In the value domain, if there is no constraint on the estimated input errors, they will fully compensate for the residual error to maximize the likelihood function and subsequently be overfitted. There are two ways to impose restrictions. One is to regard errors and model parameters as a whole in calibration, like the BATEA framework (Kavetski et al., 2006), resulting in a high dimensional computation. The other is to sample error randomly from the assumed error model, like the IBUNE framework (Ajami et al., 2007), whose precision cannot be guaranteed due to the error randomness. However, in the BEAR method the inference focuses on the error rank where the value range of the sampled errors can be effectively limited by the assumed error model. Additionally, adjusting the order of the sampled errors according to the inferred error rank can reduce the randomness in the IBUNE framework (Ajami et al., 2007), which significantly improves the accuracy of the error estimation (as demonstrated by much higher NSEs than the IBUNE method in Fig. 2). The reordering step is implemented when the model parameter has been updated and aims to find the optimal input error series corresponding to the minimized residual error. After the reordering step, the optimal input error is a deterministic function of the model parameter. Thus, unlike formal Bayesian inference, the BEAR method does not update the posterior distribution of the input errors, but identifies the input error through the deterministic relationship between the input error and model parameter*" (line 309-322)

Line 301-307: This is a very important paragraph. As I suggested in comment 7, through re-ordering you are no longer sampling from the prior input error model, which makes the protection from perfect fits you mention here somewhat arbitrary. As an illustration, I would like you to consider the behaviour of this re-ordering for longer time series: For a single observation, re-ordering can yield no improvement, and the residual fit depends exclusively on the realization you drew. For a few observations, re-ordering will induce moderate improvements, and the residual fit depends somewhat on the realization you drew. However, in the limit of infinitely many observations (assuming the statistical moments of the prior input error distribution are correctly

characterized), re-ordering your error realizations should allow the residuals to be compensated completely at every single observation, irrespective of what specific realization you drew. This makes the protection against overfitting (and the expected residual error) dependent on the length of the observation time series and seems to converge towards deterministic (over) fitting. At the same time, the effective input error uncertainty decreases to zero. In a conventional Bayesian framework, even if the correlations in the input errors are perfectly identified, this would never happen.

The reviewer is correct that reordering will not be possible if a single observation is present, as the rationale behind reordering involves changing the position of the error but not the magnitude. As the number of samples increases, the fit will improve (assuming the error distribution has been identified properly a priori). However, an infinite number of observations will not lead to a good model fit if the prior distribution is seriously mischaracterized. For example, if the input error distribution underestimates the frequency of large streamflow errors (say with a mis-specified positive skewness) the model parameters will attempt to compensate for the reduction in overall TSS concentration and the model fit will be poorer than if a correct distribution of input errors was assumed, even with infinite observations. This highlights the need for the approach to properly identify the input error distribution ahead of time, and future work will demonstrate how model selection techniques could be used when there is limited information on input errors a priori. Please also see the reply for the comment 7.

Line 314: The dot after (Fig 1.) should probably be a comma

Thanks, this sentence has been deleted as the BEAR method has been recast in the SMC calibration scheme.

Summary:

In summary, I find the approach an interesting and ambitious idea, but have reservations concerning its theoretical validity, which I hope the authors can address in their revision. If my fears concerning it solving an implicit inverse problem for the input error residuals happen to be confirmed, the authors might consider the following alternative avenues:

a) The approach might be re-interpreted as a diagnostic tool for input error residuals; there is some value in identifying input error residuals and the correlations between them. In this case, however, it may be worthwhile to investigate whether the re-shuffling strategy is needed, or whether a more straightforward inverse method might be more efficient.

b) If predictive improvements are desired, following the suggestions in major comment 4 could be a viable and interesting alternative avenue.

I wish the authors the best of luck with the manuscript and hope that my comments are useful.

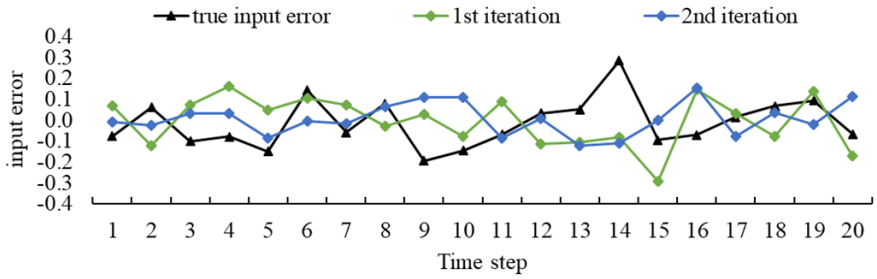
We thank the reviewer for their thought-provoking comments. We hope our responses above have helped clarify the concerns the reviewer has raised.

Appendix A: The illustration of the BEAR method

Table A 1 An example illustrating the BEAR method

1st iteration (the input errors are randomly sampled)																					
row	time step	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	sampled input error	0.07	-0.12	0.07	0.16	0.05	.0.07	0.07	-0.03	0.03	-0.08	0.09	-0.11	-0.11	-0.08	-0.29	0.14	0.03	-0.08	0.14	-0.17
2	input error rank	13	3	14	20	12	17	15	9	10	7	16	4	5	6	1	19	11	8	18	2
3	model residual error	-0.29	0.49	-0.58	-0.98	-0.78	0.29	-0.66	0.59	-1.31	-0.31	-0.87	0.76	0.46	0.54	0.25	-0.80	-0.07	0.56	-0.23	0.40
	MSE	0.40																			
2nd iteration (the input errors are randomly sampled)																					
4	sampled input error	-0.01	-0.02	0.03	0.03	-0.09	0.00	-0.02	0.06	0.11	0.11	-0.09	0.01	-0.12	-0.11	0.00	0.15	-0.08	0.04	-0.02	0.11
5	input error rank	9	6	14	13	3	10	8	16	17	18	4	12	1	2	11	20	5	15	7	19
6	model residual error	-0.13	0.23	-0.43	-0.41	-0.21	0.70	-0.23	0.09	-1.88	-1.52	0.20	0.17	0.53	0.60	-0.43	-0.72	0.36	0.12	0.47	-0.82
	MSE	0.47																			
3rd iteration (the error ranks are updated via the secant method)																					
7	calculated pre-rank	5.8	8.7	14.0	8.0	-0.3	22.0	4.3	17.3	-6.1	4.2	6.2	14.3	31.3	42.0	4.7	29.0	10.0	16.9	14.4	7.6
8	ranked rank (post rank)	6	10	12	9	2	17	4	16	1	3	7	14	19	20	5	18	11	15	13	8
3rd iteration (the input errors are reordered with the updated error ranks)																					
9	reordered input error	-0.02	0.00	0.01	-0.01	-0.11	0.11	-0.09	0.06	-0.12	-0.09	-0.02	0.03	0.11	0.15	-0.08	0.11	0.00	0.04	0.03	-0.02
10	model residual error	-0.23	0.20	-0.34	-0.24	-0.12	0.19	0.14	0.08	-0.40	-0.31	-0.22	0.03	-0.17	0.26	-0.09	-0.55	0.11	0.14	0.27	-0.23
11	MSE	0.06																			

(a) at the 1st and 2nd iteration where the input errors are randomly sampled



(b) at the 3rd iteration where the input errors are reordered according to the updated error ranks

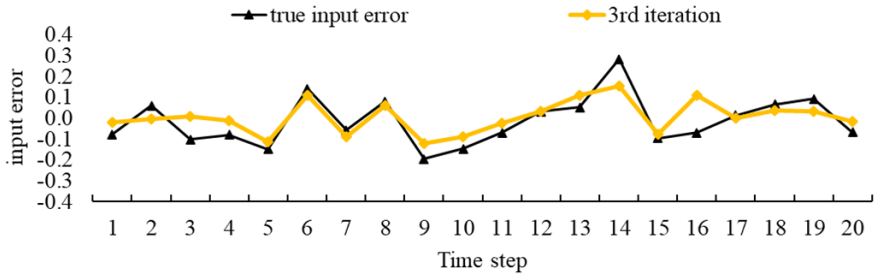


Figure A 1 Demonstration of the input error estimated in Table A.1

The BEAR method for identifying the input errors is implemented after generating the model parameters and contains two main parts: sampling the errors from an assumed error distribution and reordering them

with the inferred ranks via the secant method. An example is illustrated in Table A 1 and the explanation about the specific steps is presented in the following contents.

(1) In the 1st iteration (q=1), the errors are randomly sampled from the assumed error distribution (row 1), and then are sorted to get their ranks (row 2). This error series is employed to modify the input data, which corresponds to a new model simulation and model residual (row 3).

(2) Repeat step (1) in the 2nd iteration (q=2) as two sets of samples are prerequisites for the updating via the secant method. The results are shown in row 4, 5 and 6. Figure A 1(a) demonstrates that the ranges of the error distribution are the same between the true input errors (black line) and the sampled errors (blue and green lines) as they come from the same error distribution under the condition that prior knowledge of the input error distribution is correct. However, the values at each time step cannot match due to the randomness of the sampling.

(3) At the 1st time step in the 3rd iteration (i=1, q=3 in Eq. (4)), the pre-rank $K_{1,3}$ is calculated via the secant method (illustrated as the following Eq. (4)). The details are demonstrated in solid boxes in Table A.1.

$$K_{1,3} = k_{1,2} - \varepsilon_{1,2}^{p} \frac{k_{1,2} - k_{1,1}}{\varepsilon_{1,2}^{p} - \varepsilon_{1,1}^{p}} = 9\text{-}(\text{-}0.13)\frac{9-13}{-0.13-(-0.29)} = 5.8$$

(4) Repeat step (3) for all the time steps. The calculated pre-ranks are shown in row 7.

(5) Sort all the pre-ranks to get the integral error rank (row 8).

(6) According to the updated error ranks (row 8), the sampled errors in the 2nd iteration (row 4) are reordered. The example for the 1st time step is demonstrated in dotted boxes in Table A.1. The error rank at the 1st time step is updated as 6, and the rank 6 corresponds to the error value -0.02 in the 2nd iteration. Therefore, -0.02 is the input error at the 1st time step in the 3rd iteration. Following this example, the sampled errors at all the time steps are reordered. The results are shown in row 9. Figure A 1 (b) demonstrates that after reordering the errors with the inferred ranks, the estimated errors are much closer to the true input error, and the mean square error (MSE) of the model residual reduces in Table A 1.

(7) The reordered input error will lead to a new input data, a new model simulation and a new model residual. The residual result and its MSE statistic are shown in row 10 and 11 respectively.

(8) Check the convergence: If the objective function or likelihood function meets the convergence criterion, stop and the input error estimation is accepted. Otherwise, q=q+1, repeat step (3)~(8) until q is larger than the maximum numbers of iteration Q.

Appendix B: Theoretical foundation of the BEAR method

(1) Basic notation

In general, a model *M*() simulates the output $\boldsymbol{Y}^{s}$ given the observed input $\boldsymbol{X}^{o}$, model parameters $\boldsymbol{\theta}$, as follows:

$$\boldsymbol{Y}^{s} = M(\boldsymbol{X}^{o}, \boldsymbol{\theta}) \tag{1}$$

Here and in the following, ^{s} represents the simulated value, ^{o} represents the observed value, and * represents the true value.

(2) Input errors

The input errors $\boldsymbol{\varepsilon}_X$ are assumed to be represented by input multipliers, which are sampled from an uncorrelated lognormal distribution, and the observed input $\boldsymbol{X}^{o}$ can then be related to the true input $\boldsymbol{X}^{*}$ by the following equation:

$$\boldsymbol{X}^{o} = \boldsymbol{X}^{*} \exp(\boldsymbol{\varepsilon}_X), \boldsymbol{\varepsilon}_X \sim N(\mu_X, \sigma_X^2) \tag{2}$$

where $\boldsymbol{\varepsilon}_X$ are assumed to follow a Gaussian distribution with mean μ_X and variance σ_X^2.

(3) Output observational errors and model structural errors

In the derivation, these two parts are assumed to be error-free, therefore,

$$\boldsymbol{Y}^{o} = \boldsymbol{Y}^{*} \tag{3}$$

$$M() = M^{*}() \tag{4}$$

(4) Remnant errors

Based on the previous assumptions, the observed output equals the true output, and the difference between the simulated output and the observed output, $\boldsymbol{\varepsilon}$, will be equal to the difference between the simulated output and the true output, as follows:

$$\boldsymbol{Y}^{s} = \boldsymbol{Y}^{o} + \boldsymbol{\varepsilon} = \boldsymbol{Y}^{*} + \boldsymbol{\varepsilon}, \boldsymbol{\varepsilon} \sim (0, \sigma^2) \tag{5}$$

where the remnant errors $\boldsymbol{\varepsilon}$ are assumed to follow a Gaussian distribution with mean 0 and variance σ^2.

(5) Bayesian inference

According to the study of Renard et al. (2010), the posterior distribution of all inferred quantities is given by Bayes' theorem, as follows:

$$p(\boldsymbol{\theta}, \boldsymbol{\varepsilon}_X, \mu_X, \sigma_X, \sigma \mid \boldsymbol{Y}^o, \boldsymbol{X}^o) \propto$$
$$p(\boldsymbol{Y}^o \mid \boldsymbol{\theta}, \boldsymbol{\varepsilon}_X, \boldsymbol{X}^o)\, p(\boldsymbol{\varepsilon}_X \mid \mu_X, \sigma_X)\, p(\boldsymbol{\theta}, \mu_X, \sigma_X, \sigma) \tag{6}$$

The full posterior distribution comprises the following three parts: the likelihood of the observed output $p(\boldsymbol{Y}^o \mid \boldsymbol{\theta}, \boldsymbol{\varepsilon}_X, \boldsymbol{X}^o)$, the hierarchical parts of the input multiplier $p(\boldsymbol{\varepsilon}_X \mid \mu_X, \sigma_X)$ and the prior distribution of deterministic parameters and hyperparameters $p(\boldsymbol{\theta}, \mu_X, \sigma_X, \sigma)$.

Renard et al. (2009) argue that in the IBUNE method, $\boldsymbol{\varepsilon}_X$ are randomly sampled in each evaluation of the likelihood function and their different values at different evaluations will lead to the nondeterministic nature of the likelihood function (Equation (6)). In Bayesian inference, the likelihood function should return a fixed value for a given set of arguments. However, the randomness of the likelihood function in the IBUNE method breaks this theoretical foundation. Conversely, in the BEAR method, the secant method is applied to find a deterministic relationship between the rank of each input error and its corresponding model residual error. The residual errors depend on the model parameters $\boldsymbol{\theta}$. The magnitude of the whole input errors (i.e. their cumulative distribution function (CDF)) is related to the hyperparameters of the multipliers μ_X, σ_X. Given the value of each input error is determined by the CDF of the whole input errors and its relative rank among them, $\boldsymbol{\varepsilon}_X$ depends on μ_X, σ_X and $\boldsymbol{\theta}$, as follows:

$$\boldsymbol{\varepsilon}_X = f(\boldsymbol{\theta}, \mu_X, \sigma_X) \tag{7}$$

Considering $\boldsymbol{\varepsilon}_X$ are sampled from $N(\mu_X, \sigma_X^2)$, $p(\boldsymbol{\varepsilon}_X \mid \mu_X, \sigma_X)$ is fixed when μ_X, σ_X are determined and do not need to be considered in Equation (6). Therefore, the posterior distribution of all inferred parameters (Equation (6)) in the BEAR method will turn into:

$$p(\boldsymbol{\theta}, \boldsymbol{\varepsilon}_X, \mu_X, \sigma_X, \sigma \mid \boldsymbol{Y}^o, \boldsymbol{X}^o) \propto$$
$$p(\boldsymbol{Y}^o \mid \boldsymbol{\theta}, \mu_X, \sigma_X, \boldsymbol{X}^o)\, p(\boldsymbol{\theta}, \mu_X, \sigma_X, \sigma) \tag{8}$$

The above derivation states if the relationship between the input errors and model parameters (Equation (7)) can be determined, the problem of parameter estimation and input error identification (Equation (6)) can then be interpreted as the updating $\boldsymbol{\theta}, \mu_X, \sigma_X$ (Equation (8)) in the Bayesian inference. There are two ways to realize this determined relationship: one is to estimate the parameters and input errors together, as the BATEA approach, which will suffer from the high-dimensionality problem (Renard et al., 2010); the other one is to explore the relationship between each input error rank and model parameters via the secant method first, and then transform the error rank into the error value according to the estimated error parameters μ_X, σ_X, as the BEAR approach in this study.

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