Reviewer 1:
General comments

The preprint deals with the analysis of the performance of different machine learning methods in inverse modelling of groundwater system. It compares the TNNA method described in previous papers by the authors' collective (J. Chen et al., 2021) with other machine learning methods and shows significantly better performance of the TNNA method compared to several other methods.

The scientific contribution of the preprint is fair, but not very good. The paper does not introduce a new method, but presents on two selected academic problems the good performance of a previously described method. It uses appropriate procedures and criteria for comparison and the results are presented in a very clear, lucid and convincing manner.

The study is well constructed and executed; its scientific quality is very good but I have one reservation about the chosen methodology that I will describe in the following paragraph.

Specific comments

My only comment on the methodology used in the preprint, which I consider to be significant, is the failure to include measurement error in the test problems used. The optimization problems are well chosen, but the measurements used to calibrate the parameters (inverse modeling) were not burdened with any random error emulating measurement error.

This may have a significant impact on the applicability of the method. In inverse modelling, in practice, we face two types of problems - the lack of ability to fit the measured data and the so-called overfitting of the data consisting in their too accurate replication by the model (by including the measurement error in the model parameters, i.e. damaging them in terms of the ability of further prediction). If the aim of the study was to show possible applicability of TNNA to solution of inverse models of groundwater problems, this feature of the study does not allow to fulfil the intended objective.

Technical corrections

The language of the preprint is clear, I did not notice any specific errors or typos.

Response:

We sincerely appreciate the reviewer's constructive comments and the time invested in reviewing our manuscript. Your insights are invaluable in helping us improve the quality of our works.

Regarding the reviewer's concern about the absence of measurement errors in the test problems, we apologize for the lack of clarity in the original manuscript. In fact, we incorporated measurement errors in both test cases by adding Gaussian noise to the normalized numerical simulation results, with a standard deviation of 0.01. This was explicitly stated in Section 3.2, Case 2, where we noted:

"The standard deviation of Gaussian noise for the normalized observations is set to 0.01." However, we recognize that the description in Case 1 was insufficiently detailed. To address this, we will revise the manuscript to explicitly clarify that both test cases included Gaussian noise with a standard deviation of 0.01 for the normalized observations.

Additionally, we agree with the reviewer's perspective on the impact of observational noise on inversion results, particularly in real-world scenarios. Nevertheless, these challenges often arise due to insufficiently defined inversion constraints. Because model parameters are strictly updated based on loss functions in available inversion algorithms. As a result, even minor noise perturbations can cause significant errors when constraints are ill-posed and rely on sparse, noisy data. Therefore, in practical applications, both providing effective inversion algorithms and establishing robust inversion constraints using sufficient data or regularized information are important. In this study, we primarily focus on the impact of differences in parameter optimization mechanisms between the machine learning-based TNNA inversion algorithm and traditional metaheuristic algorithms on inversion accuracy and algorithm efficiency. Accordingly, sufficiently well-defined constraints are included in both test cases to avoid inversion errors caused by external factor, which could mislead the performance assessment. When encountering significant observational noise in real-world scenarios, an effective approach is to improve the regularization terms, such as obtaining more measured parameter values, establishing prior information with lower uncertainty, or using other data sources as additional constraints.

We will supplement the manuscript with additional details on the potential challenges of applying the TNNA method to real-world scenarios, including considerations for observational noise and appropriate constraints construction.

Thank you once again for your valuable feedback and thoughtful suggestions.