Interactive comments on "Forward and inverse modeling of water flow in unsaturated soils with discontinuous hydraulic conductivities using physics-informed neural networks with domain decomposition" by Toshiyuki Bandai and Teamrat A. Ghezzehei

Reviewer comments are in black, while reply to comments in red.

Review of "Forward and inverse modeling of water flow in unsaturated soils with discontinuous hydraulic conductivities using physics-informed neural networks with domain decomposition" by Bandai and Ghezzehei.

In this manuscript the authors tested a physics-informed neural networks (PINNs) method to solve the Richardson-Richards equation for simulating unsaturated soil water dynamics. The authors also investigated the capability of the method for obtaining inverse solutions. As coupling data-driven and physics-based approaches have received much attention these days, the topic fits well with the scope of HESS. The authors have done a great job on demonstrating how PINNs performed when simulating unsaturated water flow in soils and showing applicability and limits of the method. Although the paper was well organized and written, I believe the paper has a room for some improvement. I have some comments that should be addressed prior to accepting this paper for publication. For my curiosity, I am wondering if this approach can be applied to simulate preferential type flow in soils. Is it going to be straightforward? Does it require some modifications in the model? If it can be applied to such phenomena, it would be a great breakthrough in the field of soil physics and hydrology.

Response: We sincerely thank the reviewer for spending efforts in reviewing our manuscript. Before we answer the questions below, we would like to clarify the application of PINNs to preferential flow here. Although it is highly important to simulate preferential flow, the current PINNs cannot be applied to general preferential flows. This is because reliable mathematical models for preferential flow have not been developed yet. The basis of PINNs is well-defined mathematical equations (e.g., differential equations) that describe the processes of interest. This is an identical requirement to other traditional numerical methods such as finite difference and finite element methods. Nevertheless, some aspects of preferential flow could be simulated using PINNs. For example, Cueto-Felgueroso and Juanes (2009) proposed to model finger flow in a homogeneous soil by adding a fourth-order term to the Richardson-Richards equation. The fourth term describes the formation of gravity fingers during water infiltration into soils. In principle, we can apply PINNs to solve the fourth-order Richardson-Richards equation, though it requires further computational cost due to the fourth-order term. Alternatively, it might be possible for us to use PINNs to study the gravity finger using laboratory infiltration experiments using imaging-based soil moisture data (e.g., Sadeghi et al. (2017)). Compared to traditional numerical methods, PINNs do not require initial and boundary conditions, which would be useful for the experimental laboratory setup too. In conclusion, PINNs are limited to processes that mathematical equations are available for. We require more experimental and theoretical work on formulating mathematical models for preferential flow in general (Nimmo, 2021).

General comments:

In Fig. 5, the evolution of PINNs solution is plotted. At the initialization, some of the solutions are beyond the limit of the water content as the water content values are greater than the saturated water content. Would it be possible to put some constraints to the solutions in PINNs? If so, would that improve training and overall performance? Any discussions on this matter will helpful for those who are interested in using this method. A similar question goes to the inverse solutions. I am wondering if any constraints can be applied to the target parameters that are inversely estimated. There is always a need to put some constrains to the parameters being estimated.

Response: We appreciate your keen comments on Figure 5. The oversaturation at the initialization is because we did not implement the conditional statement such as $\theta = \theta_s$ for $\psi \geq 0$. Thus, the neural networks gave unphysical volumetric water content over the saturated water content based on the Gardner model (Equation (5)).

We had some technical issues that prevented us from implementing the conditional statement. But, we have now implemented such conditional statements. An example of the results from this implementation is shown below in addressing your questions on saturated-unsaturated flow.

In terms of your question on the constraint on inverse modeling in general, yes, we can constrain the range of target variables in this framework. For example, if the range of a variable α is $0 < \alpha < 1$, then we can use the sigmoid function to represent α (note that the range of the sigmoid function is between 0 to 1). Alternatively, we might set bounds for each parameter by adding conditional statements. Nevertheless, as standard inverse modeling frameworks, imposing such bound constraints might make the minimization problem more difficult than that for unconstrained optimization.

In the demonstration of getting inverse solution with PINNs, the authors used a 2-layered soil system. Why? If the boundary fluxes are being estimated, wouldn't be better to start with a homogenous case? Was there a specific reason that the layered soil system was used in this demonstration?

Response: We appreciate your reasonable suggestion. The reason we used a two-layered soil for the inverse modeling is twofold: 1) we knew PINNs work well for a homogeneous soil from our previous study (Bandai and Ghezzehei, 2021); 2) soil moisture sensors are inserted into multiple layers in our target field data, which is often the case for most situations. We believe it is important to test this algorithm for two-layered soils because the physical property of the very surface soil is often different from the below ones due to crust, organic matter accumulation, and surface processes.

Specific comments:

L189: It sounds a bit strange to say that soil dynamics is "controlled by the volumetric water content at the bottom."

Response: Thank you for pointing out this. To avoid confusion, we will change the sentence:

"which corresponds to when soil moisture dynamics is controlled by the surface water flux q(0, t) (i.e., evaporation or infiltration) and the volumetric water content at the bottom θ(−Z, t)."

to

"which corresponds to when soil moisture dynamics is induced by the surface water flux q(0, t) (i.e., evaporation or infiltration) while the volumetric water content at the bottom θ(−Z, t) is kept to h(-Z, t)."

L193 (Eq.15): A little bit more explanations will be helpful to understand this transformation. I have no idea why the beta value gives better initial guess.

Response: We appreciate your comment. The initial guess for the homogeneous simulation is shown in Figure 5 (a). This distribution is determined by Equation 15 with the parameter β and the initial neural network parameters Θ. The initial neural network parameters are given by the Glorot initialization (Line 262). By tuning the parameter β, we can begin our simulation at a better initialization. The parameter β is also important for the question below (L311).

L311: If the logarithmic transformation of water potential is used, the approach is limited to "unsaturated" systems. But there are many cases you will have both positive and negative potential values. How do you deal with that?

Response: Thank you for your insightful comment. As you suggested, the output of the negative logarithmic transformation is always negative. However, the parameter β in Equation (15) makes the PINNs possible to have positive water potential (i.e., saturated flow). For example, if we use $\beta = 10$, the range of $\hat{\psi}$ would be $-\infty < \hat{\psi} < 10$.

Although we limited ourselves to unsaturated cases in this paper, we tested the applicability of PINNs to saturated-unsaturated cases by changing the surface flux of the homogeneous problem in the main text from 0.9 cm/h to 1.05 cm/h, where the saturated hydraulic conductivity is 1.0 cm/h. Figure 1 below shows that the volumetric water content reached the saturated volumetric water content at t = 3 h for half of the soil, while the water potential becomes positive, as shown in Figure 2. The slope of the water potential is close to 0.05 cm/cm, which is reasonable to satisfy the surface flux to be 1.05 times the saturated hydraulic conductivity.

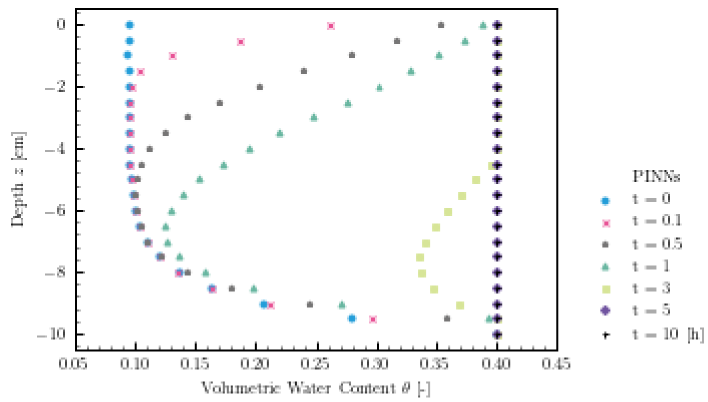

Figure 1. The PINNs solution for saturated-unsaturated flow into a homogeneous soil in terms of volumetric water content.

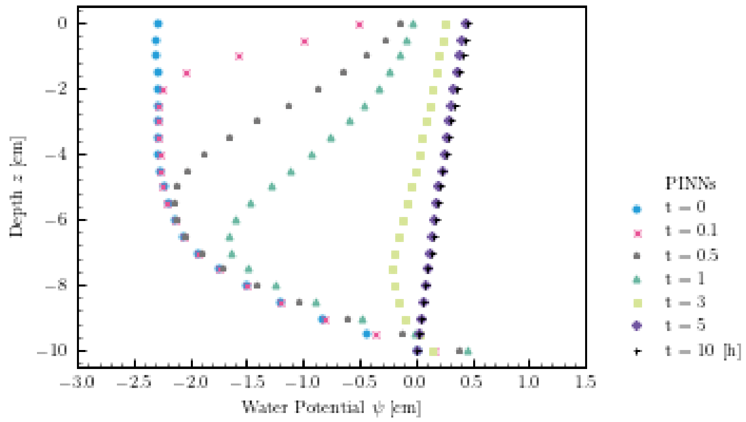

Figure 2. The PINNs solution for saturated-unsaturated flow into a homogeneous soil in terms of water potential.

We sincerely appreciate you gave us a chance to test PINNs against the saturated-unsaturated flow. However, we can foresee the potential difficulty of PINNs for saturated-unsaturated cases because the solution to the governing equation will not be smooth (i.e., not differentiable) at the saturated-unsaturated interface, and it is difficult to know the location of the interface a priori. Please note that traditional numerical methods have also issues for saturated-unsaturated interfaces (convergency of non-linear solver). The application of PINNs to saturated-unsaturated flow requires further verification and comparison with other numerical methods, and we would like to limit ourselves to unsaturated scenarios in this paper, as suggested in the title. We will add these comments in the discussion section of the revised manuscript as a future perspective.

Figure 3(b): There are some systematic differences between FDM and PINNs. Why? Are these because of the choice of spatial and temporal discretization in FDM?

Response: Thank you for pointing out the systematic difference. Yes, the difference comes from the discretization used in FDM. In FDM, the temporal derivative is approximated by a finite difference, and the FDM solution and the corresponding numerical error propagate with time marching. Major errors come from a steep wetting front, and thus we see a clear trend in FDM errors. On the other hand, PINNs do not use time marching for temporal discretization and minimize the residual of the partial differential equations in both time and space simultaneously. Therefore, we see PINNs errors distributing broadly in the spatial and temporal domains.

Figure 10: Looks like something is wrong with the texts at the top of the figures.

Response: We regret that we left the weird texts in the figure. We will fix this in the revised manuscript.

Figure 16: For all three cases, the PINN solutions show that the inversely estimated initial surface flux is much smaller than the true flux. Are there any specific reasons for this?

Response: We appreciate your close investigation. According to our empirical experiences, PINNs tend to learn the solution backward in time. Please see Figure 13, where PINNs learned the solution at t = 10 h first and other solutions backward in time. We believe the same thing happened to the inverse modeling case too. Please see Figure 15 (a), where the solutions at t = 0 and t = 1 are not satisfactory near the surface. The estimated water content at t = 0 and t = 1 would be closer to the solution at t = 3 because neural networks are continuous, and thus estimated water content is higher than the true water content. If the estimated water content is higher than the true one, then there is less water flux required, which is the result of the underestimation (in absolute value) of initial surface water flux.

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