Estimating soil hydraulic parameters for unsaturated flow using Physics-Informed Neural Networks

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Abstract. Water movement in soil is essential for weather monitoring, prediction of natural disasters, and agricultural water management. Richardson-Richards' equation (RRE) is the characteristic partial differential equation for studying soil water movement. RRE is a non-linear PDE involving water potential, hydraulic conductivity, and volumetric water content. This equation has underlying non-linear parametric relationships called water retention curves (WRCs) and hydraulic conductivity functions (HCFs). This two-level non-linearity makes the problem of unsaturated water flow of soils challenging to solve. Physics-Informed Neural Networks (PINNs) offer a powerful paradigm to combine physics in data-driven techniques. From noisy or sparse observations of one variable (water potential), we use PINNs to learn the complete system, estimate the parameters of the underlying model, and further facilitate the prediction of infiltration and discharge. We employ training on RRE, WRC, HCF, and measured values to resolve two-level non-linearity directly instead of explicitly deriving water potential or volumetric water content-based formulations. The parameters to be estimated are made trainable with initialized values. We take water potential data from simulations and use this data to solve the inverse problem with PINN and compare estimated parameters, volumetric water content, and hydraulic conductivity with actual values. We chose different types of parametric relationships and wetting conditions to show the approach's effectiveness.

Keywords: Physics-Informed Neural Networks · Richardson-Richards equation · Computational Hydrology

1 Introduction

Understanding the movement of water in near-surface levels of soil is of utmost importance for agricultural water management, prediction of floods, and microbial activities inside the soil. This understanding is heavily dependent on our capacity to model these hydrological processes. A partial differential equation called *Richardson-Richards equation* [28] (RRE) is at the heart of modeling water movement in soils. This non-linear partial differential equation (PDE)

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represents water movement in porous media. It involves the relationship between three quantities, namely pressure head or water potential (ψ), volumetric water content (θ), and hydraulic conductivity (K) [7]. To make the RRE solvable, two parameterized relations called water retention curve (WRC) and hydraulic conductivity function (HCF) are used. The parameters used in these relationships characterize the hydraulic properties of soil. This double non-linearity makes solving RRE difficult and is of utmost interest to mathematicians and physicists. A detailed review of the history and significance of RRE in computational sciences is provided in the review by [7]. They referred to the equation as arguably one of the most difficult equations to reliably and accurately solve in all hydro-sciences.

Machine learning and deep learning are used in many applications to model and simulate physical processes. A new and exciting paradigm for using deep learning for physics involves solving problems related to differential equations, providing a robust framework to integrate physical knowledge into data-driven deep learning systems. Physics-Informed Neural Networks (PINNs) were introduced in the seminal works of Raissi et al. [24, 25], showing the use of deep learning to solve forward and inverse problems involving differential equations.

Applying PINNs to solve problems involving RRE effectively has greatly interested the scientific community. Tartakovsky et al. [32] used PINNs and estimated saturated and unsaturated hydraulic conductivity and pressure from saturated hydraulic conductivity measurements. Bandai et al. [3] introduced a PINN-based framework for the inverse solution of the Richards equation to estimate both the water retention curve (WRC) and the hydraulic conductivity function (HCF). This involved training three neural networks, with one approximating the solution, the Richards PDE, regarding the water content and the remaining two describing, respectively, the WRC and HCF. Depina et al. [13] addressed the inverse problem by deriving individual formulations for potential-based and volumetric water content-based extensions of the classic mixed form of RRE, while Chen et al. [5] investigated the impacts of the loss weights and random state on the performance of the RRE-solving PINNs and possible solutions to mitigate such impacts.

We aim to complement and build upon this body of work in this study. We use PINNs to solve the inverse problem of one-dimensional RRE. Specifically, we use data on water potential (ψ) to estimate the remaining two variables, θ and K, thereby learning the complete system. This is done by inferring the parameters in WRC and HCF, which characterize the hydraulic properties of soil. We do this for different types of parametric relationships: Gardner [9] and van-Genuchten [10]. Depina et al. [13] use different formulations to solve the inverse problem using data from other variables. In contrast, our approach uses a single general mixed formulation that can handle water potential and volumetric water content measurements without rewriting the RRE. Additionally, Bandai et al. [3] use three separate neural networks to capture the RRE, WRCs, and HCFs, while our single neural network finds a representation by simultaneously resolving all of them by training on a multi-objective loss. This is illustrated in the Figure 1.

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2 Theoretical Background

This section offers an overview of the Richardson-Richards equation (RRE) with Physics-Informed Neural Networks (PINNs) [24, 25, 28], combining computational hydrology and machine learning. The RRE is fundamental for modeling water movement in unsaturated soils and is essential for understanding soil water dynamics. PINNs integrate deep learning to solve complex differential equations by enforcing physical laws. We provide a concise overview highlighting their combination and synergy to alleviate current challenges.

2.1 The Richardson-Richards Equation

Richardson-Richards equation [28] is used extensively for modeling water movement in unsaturated porous media. The equation applies when assuming isothermal water transport (heat exchange is negligible) and when soil hydraulic properties are homogeneous and isotropic, indicating uniform behavior across the soil. The general mixed formulation of the equation is given as

$$\frac{\partial \theta(\psi)}{\partial t} = \frac{\partial}{\partial z}\left[K(\theta)\left(\frac{\partial \psi}{\partial z} + 1\right)\right], \tag{1}$$

where $\theta[L^3L^{-3}]$ is the volumetric water content, $t[T]$ is the time, $z[L]$ is the depth, $K[LT^{-1}]$ is the hydraulic conductivity and $\psi[L]$ is the water potential (hydraulic pressure). The measurement units of all the quantities are given in square brackets.

Since the number of unknowns is greater than the number of equations in Equation 1, additional equations are required to solve the equation completely. These two additional equations are $K(\theta)$ and $\theta(\psi)$. The function $\theta(\psi)$ is called the water retention curve (WRC), and $K(\theta)$ is called the hydraulic conductivity function (HCF). These non-linear parametric relationships are used to solve the Equation 1. They are of different types. Some of the most used ones in the community are relations given by Gardner [9], given by Equation 2 and van-Genuchten [10], given by Equation 3

$$\begin{aligned} \theta &= \theta_r + (\theta_s - \theta_r)\, e^{\alpha\psi}, \\ K &= K_s e^{\alpha\psi}, \end{aligned} \tag{2}$$

$$\begin{aligned} \theta &= \theta_\mathrm{r} + \frac{\theta_\mathrm{s} - \theta_\mathrm{r}}{(1 + (-\alpha\psi)^n)^m}, \\ K &= K_\mathrm{s} S_\mathrm{e}^l \left(1 - \left(1 - S_\mathrm{e}^{1/m}\right)^m\right)^2. \end{aligned} \tag{3}$$

The parameters given in Equation 2 and Equation 3 characterize the hydraulic properties of soil. The parameter $\theta_r[L^3L^{-3}]$ is the residual water content, $\theta_s[L^3L^{-3}]$ is the saturated water content, $\alpha[L^{-1}]$ is the pore-size distribution

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parameter and $K_s[LT^{-1}]$ is the saturated hydraulic conductivity. There are additional quantities in van-Genuchten relationships. l is the tortuosity parameter, and n, m are shape parameters. The intermediate quantity S_e in Equation 3 is the effective saturation given by

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r}. \tag{4}$$

A more detailed review of the numerical solutions and the significance of RRE is provided in [7]. This study focuses on the three parameters common in both relationships: α, K_s, θ_s.

2.2 Physics-Informed Neural Networks

Physics-Informed Neural Networks (PINNs) provide a framework to include rules of physics as differential equations in neural networks. PINNs leverage the fact that deep neural networks are universal functional approximations. Backpropagation enables the calculation of derivatives of any order between the input and output of deep neural networks. Raissi et al. [25] showed that loss function can be constructed using combinations of higher order derivatives, enabling the neural network to learn from physics. To illustrate the concept, consider a general differential equation of the form

$$\boldsymbol{u}_t + \mathcal{D}[\boldsymbol{u}] = 0, t \in [0, T], \boldsymbol{x} \in \Omega, \tag{5}$$

where $\boldsymbol{u(x,t)}$ is the solution of the differential equation in the domain $[\Omega X T]$. A neural network, represented by $\boldsymbol{u_w}$, with trainable parameters (weights and biases) $\boldsymbol{w}$ approximates the latent, hidden solution $\boldsymbol{u}$. The loss function to penalize the behaviour of $\boldsymbol{u_w}$ according to Equation 5 is given as

$$\mathcal{L}(w) = \frac{1}{N} \sum_{i=1}^{N} \left| \frac{\partial \boldsymbol{u_w}}{\partial t}(t^i, \boldsymbol{x}^i) + \mathcal{D}[\boldsymbol{u_w}](t^i, \boldsymbol{x}^i) \right|^2, \tag{6}$$

where N is the total number of sampled points in the domain $[\Omega X T]$. When trained with this loss function, the neural network is penalized on all these points such that the parameters θ are optimized to learn the behavior according to Equation 5. This framework of informing physics through loss function can be used for various applications where there is a need to enforce physics-based constraints. It can solve PDEs by adding additional loss functions for boundary and initial conditions. It can solve inverse problems using data samples and the physics constraint where parameters are trainable. This flexibility has made PINNs useful in various scientific and engineering disciplines [6, 22, 26, 30]. We recommend referring to Raissi et al. [25] and Karniadakis et al. [15] for a detailed overview of PINNs.

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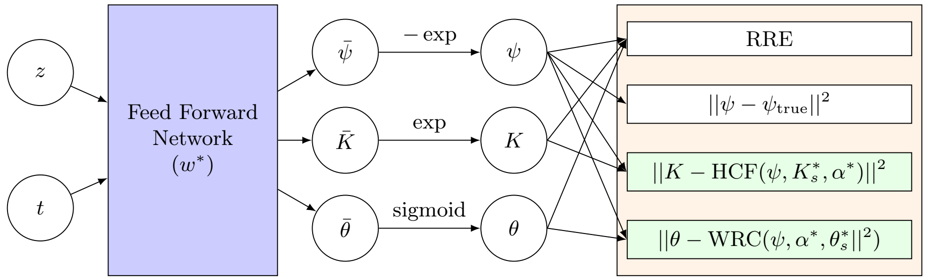

Fig. 1: Our proposed Physics-Informed Neural Network is designed to solve the Richardson-Richards equation, utilizing depth (z) and time (t) as input and giving ψ,K,θ as output. Specifically, the model can be trained using the observations of ψ, with the self-referential terms (highlighted in green). All learnable parameters are denoted by *. Please note that we additionally integrate knowledge about each output's value range to enforce reasonable results.

2.3 Inverse Problem of RRE

An inverse problem focuses on determining the unknown parameters and variables that govern a system based on already-known observations. This process entails using available data to work backward to identify the underlying factors or conditions that could have resulted in the observed outcomes. The system to solve Richard-Richardson-Equation consists of the three variables ψ, θ, and K. As described before, we solely observe ψ and have to uncover the remaining variables. However, knowing that θ and K can be described by hydraulic quantities of soil (either based on Gardner [9] or Genuchten [10]), we can introduce learnable parameters α^*, K_s^*, and θ_s^* to learn them on-the-fly. Given this setup, we could estimate the hydraulic behavior and type of soil given only the water potential ψ observations.

We construct our Physics-Informed Neural Network as a standard feed-forward network. The water potential values ψ are recorded at a specific time (t) and depth (z); hence, we utilize them as input for training the PINN. Our model predicts the estimated water potential ψ, hydraulic conductivity K, and the volumetric water content θ. This model is trained on RRE, as given in Equation 1, along with samples of ψ. This model is also trained on the WRCs and HCFs to enforce the representation of the complete system. These loss terms are self-referential, i.e., one output of the neural network is used to compare to another. For example, As shown in Figure 1 (highlighted in green), in the third loss term, the output of the neural network K is compared to HCF, a function of ψ, also an output of the neural network. The same applies to the fourth loss term where θ and WRC are compared. Due to this, we found the model is prone to exploding gradients.

We leverage existent physical knowledge of the ψ, K, and θ to alleviate this effect during the model's training. We follow current best practices [3, 19]

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and restrict the possible value ranges for the model's output neurons through specific last-layer activation functions. We enforce ψ as always negative using a negative exponential function attached to the output neuron [3]. For K, we use an exponential function to ensure non-negative values. Lastly, knowing that θ can only be in $[0, 1]$, we utilize a *sigmoid* function to constrain the value range. Therefore, the initial model outputs, denoted as $\bar{\psi}$, $\bar{K}$, and $\bar{\theta}$, represent intermediate representations of the actual desired parameters. As shown by Bandai et al. [3], these stabilize the training significantly and enable the model to learn the complete system. As both *exponential* and *sigmoid* functions are computationally stable using backward passes, the gradients used for the optimization terms do not explode. The full self-regularization and knowledge integration approach is visualized in Figure 1.

Overall, the model minimizes its parameters w^* and the hydraulic soil parameters α^*, K_s^*, and θ_s^* by solving the following optimization problem:

$$\min_{w^*,\alpha^*,\theta_s^*,K_s^*} \|\mathrm{RRE}(\psi, \theta, K))\|^2 + \|\psi - \psi_{true}\|^2 + \\ \|K - \mathrm{HCF}(\psi, K_s^*, \alpha^*))\|^2 + \|\theta - \mathrm{WRC}(\psi, \alpha^*, \theta_s^*))\|^2 . \tag{7}$$

The model has to find a viable solution from the solution space defined by the following summarized objectives to predict the required parameters effectively:

1. The main target is solving the mixed formulation of the RRE based on Equation 1, such that valid solutions arise.
2. Further, minimizing the squared error between the predicted ψ and the measured values ψ_{true} for a specific time (t) and depth (z) value adds to the total loss term.
3. The parametric relationships, WRC and HCF, based on either Gardner [9] or van-Genuchten [10], are used as loss terms. During the learning, the values of α^*,θ_s^*, and K_s^* have to be updated to fit a suitable solution space. The initial values for these parameters are discussed in the experimental section.
4. Lastly, we avoid loss term weighting as in [20, 33, 35] to not interfere with output transforms used for value range restrictions.

3 Experiments

We first introduce our general experimental setup to validate our proposed model architecture and self-regularization approach to ensure comparable results. In our main experiments[1], we apply our approach to different types of parametric relationships for soil hydraulic properties.

3.1 Experimental Setup

To test the effectiveness of our proposed approach, we build our experiments on simulations of the Richard-Richardson-Equation [28]. We fix hydraulic quantities

[1] The code is available at `https://github.com/cvjena/InverseRRE`.

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of soil parameters (α, θ_s, K_s) and simulate RRE for certain depths until a certain time. We follow Ireson [12] to ensure correct simulations by setting an appropriate boundary and initial conditions. Accordingly, this is done for Gardner [9] and van-Genuchten [10]. The training data consists of 5000 samples of ψ from the simulations,

We evaluate the capabilities of our model, thus our approach, based on the following criteria:

1. The complete map of the water potential ψ is correctly estimated.
2. The learnable parameters describing the soil hydraulic properties (α^*, θ_s^*, K_s^*) converge towards the selected true parameters (α, θ_s, K_s).
3. The PINN output values of θ and K in the domain are close to that of the numerical simulations.
4. We investigate the qualitative results by comparing the predicted values and simulation over depth (z) and time (t).

We use the same network architecture and learning hyper-parameters in all experiments shown. As we do not weigh the individual loss terms, we can refrain from additional hyper-parameter searches and focus solely on the general capabilities of our method. All models optimize the same optimization term in Equation 7.

Our feed-forward PINN is constructed and trained with the DeepXDE library [18]. We utilize eight hidden layers, each having 50 neurons followed by $SiLU$ activations, as prescribed in [2], Therefore, we require fewer parameters and only a single network compared to Bandai et al. [3] to solve the Richards-Richardson-Equation. All models are trained with Adam as optimizer [16] over 40000 epochs with a constant learning rate of $1e^{-4}$. All experiments are repeated for ten independent runs, and single training takes around one hour on an Nvidia GeForce GTX 1080 Ti.

3.2 Gardner Simulation

First, we solve the inverse problem of RRE with parametric relationships given by Gardner as given in the Equation 2. For this purpose, we use the simulation code

Table 1: The table compares original parameters and estimated parameters by PINN for RRE using Gardner's parametric relationships [9]. Additionally, we display the mean prediction errors between predicted variables by PINN with original simulated values. The given values are over ten independent trials.

Parameter	Original	Prediction
α	1.00	1.01 ± 0.07
θ_s	0.40	0.42 ± 0.15
K_s	1.00	1.02 ± 0.18

(a) Hydraulic Soil Parameters

RRE Parameter	Prediction Error
ψ	0.0361 ± 0.0075
K	0.0367 ± 0.0138
θ	0.0287 ± 0.0258

(b) Simulation Data

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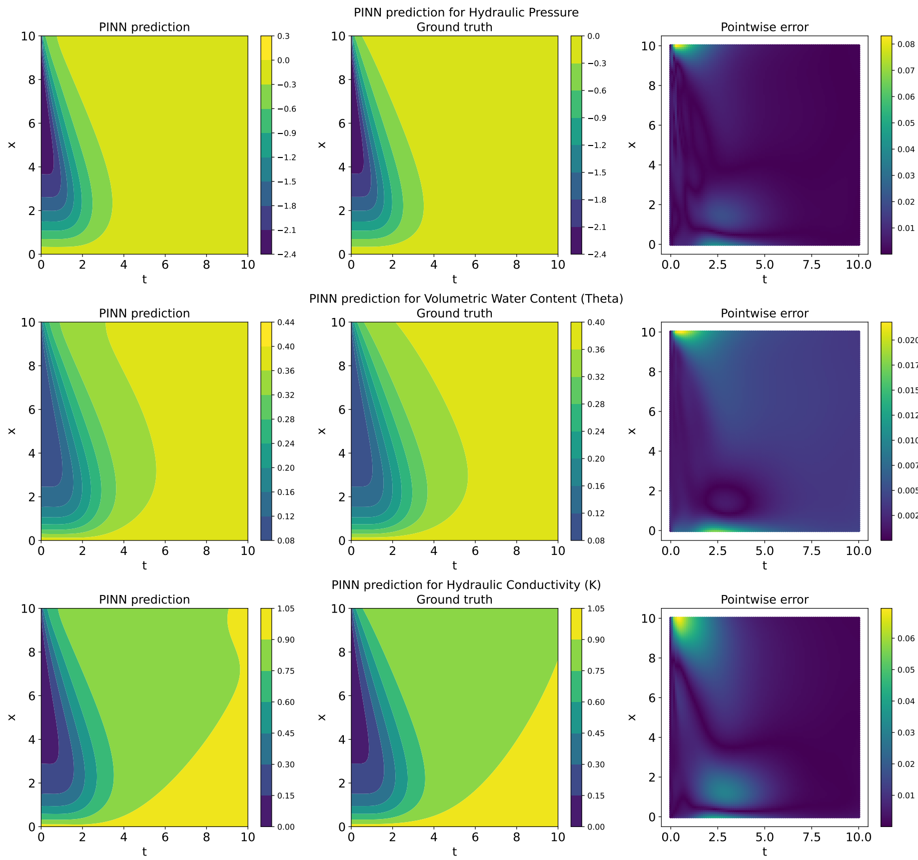

Fig. 2: Prediction of ψ, θ, and K using PINN for the inverse problem of RRE using Gardner relationships. The first column shows the PINN predictions, and the second column shows ground truth data from simulations [3]. The predictions are close to the ground truth, and the corresponding pointwise errors are shown in the third column.

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Table 2: The table compares original parameters and estimated parameters by PINN for RRE using van-Genuchten's parametric relationships [31]. Additionally, we display the mean prediction errors between predicted variables by PINN with original simulated values. The given values are over ten independent trials.

Parameter	Original	Prediction
α	0.79	0.78 ± 0.06
θ_s	0.25	0.28 ± 0.08
K_s	1.08	1.07 ± 0.13

(a) Soil hydraulic parameters

RRE variable	Prediction error
ψ	0.0198 ± 0.0093
K	0.0238 ± 0.0146
θ	0.0104 ± 0.0139

(b) Simulation Data

by Bandai et al. [3], which is based on analytical solutions given by Srivastava et al. [31]. We simulate for depth $z = 10cm$ and time $t = 10h$, and the parameters are chosen to be $\alpha = 1.0$, $\theta_s = 0.4$, $K_s = 1.0$. The initial condition $\psi(0, t)$ is taken as parabolic. The simulation results of all variables are shown in Figure 2 (middle column). The details about architecture and training are described in subsection 2.3.

We train the PINN using the Adam optimizer for 40000 epochs with a learning rate $1e^{-4}$. In the first row of Figure 2, we show the predicted values of ψ as the first step to ensure PINN has learned from the data correctly. The θ and K predictions are shown in the second and third rows of the Figure 2. These figures show that the predicted values of PINN are accurate with reference solutions from simulations. Further, the estimated parameters are also close to the original values from the simulation, as shown in the table 1. This shows the effectiveness of PINN in solving the inverse problem of RRE with Gardner's parametric relationships.

3.3 van-Genuchten relationships

For the next experiment, we used van-Genuchten parametric relationships given by Equation 3, which are known to be more representative of real-world soils. We use the work by Ireson [12] to generate simulated data. We chose the soil type of Hygiene sandstone whose parameters are $\alpha = 0.79$, $\theta_s = 0.25$, $\theta_r = 0153$, $K_s = 1.08$. The simulation's starting condition is $\psi(0, z) = -z$. The generated data for ψ is shown in the Figure 3 (first row, middle figure). One thousand observations of ψ across the domain are randomly selected for training, and the basic training procedure remains the same as before; we use sampled points of ψ across the domain for training, and the PINN is trained with three types of loss functions. The second and third terms of loss function are now formulated based on van-Genuchten parametric relationships. We set the value of 0.1 as the starting value of trainable parameters. The PINN is trained and predicted volumetric water content, θ and hydraulic conductivity, K values are shown in the second and third rows of the Figure 3 and the estimated parameters in the table 2. We see that the predictions are accurate with the ground truth, showing the

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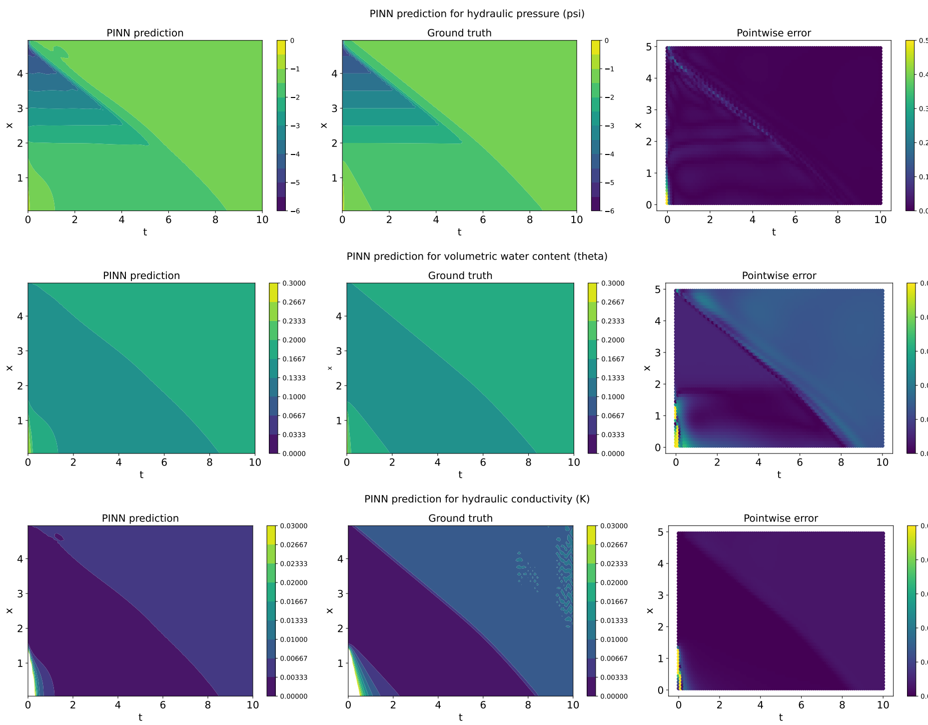

Fig. 3: Prediction of ψ, θ, and K using PINN for the inverse problem of RRE using van-Genuchten relationships. The first column shows the PINN predictions, and the second column shows ground truth data from simulations [12]. The predictions are close to the ground truth, and the corresponding pointwise errors are shown in the third column.

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effectiveness of PINN in solving the inverse problem of RRE with van-Genuchten parametric relationships.

4 Discussion and Conclusion

In this paper, we presented an interesting application of Physics-Informed neural networks to solve the inverse problem of the Richardson-Richards equation. We showed how it's useful for estimating the parameters (α, K_s, θ_s) and variables (Volumetric water content θ and hydraulic conductivity K) of the complete system from observations of a single variable (hydraulic potential ψ) across space-time domain. This is achieved by a multi-objective loss containing physics-based (RRE, parametric relationships) and data-based (ψ values) objectives highlighting the powerful characteristic of PINNs to combine physical knowledge into deep learning systems. We further used simple transformations for outputs to restrict their ranges, which helped in stable training and robust estimation of parameters. We show that PINNS accurately solve the inverse problem for different parametric relationships, namely, Gardner and van-Genuchten relationships.

This inverse problem setting could be useful for knowing the hydraulic properties of some unknown soil. This can also be used to regularly monitor hydraulic variables, which may provide significant information on agriculture water management, flooding, etc. This work focuses on simulation data with single-layered soil. The estimations depend on the starting values of the parameters, and often, if the starting values are too far off, the estimations are erroneous and this needs to be further investigated. The effects of various architectures and training procedures on performance also need further investigation.

Future research directions include assessing the behavior of PINNs when using experimental data with a lot of sparsity and noise, using multi-layered soils, and implementing complex wetting cycles. In this study, we are confined to using ψ data and predicting K and θ. This same approach is applicable if we exchange variables, i.e., use data samples of θ or K and predict the remaining variables. The data sampling strategy is also an interesting question because we observe, for example, in Figure 2 that most variables vary a lot in the first few time steps. Using adaptive sampling strategies [8, 34], which include more points of interest, might improve the training of PINNs.

Another interesting research direction is looking for efficient ways to improve multi-objective optimization for inverse settings because classical weighting techniques [20, 33, 35] might suffer due to the presence of trainable parameters and self-referential loss terms. New algorithms like DeepONets [17], which learn the operator of PDE rather than the singular solution, are also an interesting direction. Combining the proposed PINN approach with Remote sensing techniques [14, 21, 23, 27, 29] for automated estimation and monitoring of hydraulic properties of soil could have substantial real-life applications. The rapid progress in modern-day deep learning [1, 4, 11] ensures a unique and exciting future for studying PDEs using deep learning.

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