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A Novel Bayesian Framework for Inverse Problems in Precision Agriculture

Zeyuan Songa, and Zheyu Jianga*

a Oklahoma State University, School of Chemical Engineering, Stillwater, Oklahoma, USA
* Corresponding Author: zheyu.jiang@okstate.edu.

ABSTRACT

An essential problem in precision agriculture is to accurately model and predict root-zone (top 1 m of soil) soil moisture profile given soil properties and precipitation and evapotranspiration information. This is typically achieved by solving agro-hydrological models. Nowadays, most of these models are based on the standard Richards equation (RE), a highly nonlinear, degenerate elliptic-parabolic partial differential equation that describes irrigation, precipitation, evapotranspiration, runoff, and drainage through soils. Recently, the standard RE has been generalized to time-fractional RE with any fractional order between 0 and 2. Such generalization allows the characterization of anomalous soil exhibiting non-Boltzmann behavior due to the presence of preferential flow. In this work, we focus on inverse modeling of time-fractional RE; that is, how to accurately estimate the fractional order and soil property parameters of the fractional RE given soil moisture content measurements. Specifically, we introduce a novel Bayesian variational autoencoder (BVAE) framework that synergistically integrates our in-house developed fractional RE solver and adaptive Fourier decomposition (AFD) to accurately estimate the parameters of time-fractional RE. Our proposed AFD-enhanced BVAE framework consists of a probabilistic encoder, latent-to-kernel neural networks and convolutional neural networks. The BVAE framework is theoretically explainable and enhanced by the AFD theory, a novel signal processing technique that achieves superior computationally efficiency. Through illustrative examples, we demonstrate the efficiency and reliability of our AFD-enhanced BVAE framework.

Keywords: Artificial Intelligence, Machine Learning, Numerical Methods, Food & Agricultural Processes, Water

INTRODUCTION

Precision modeling and forecasting of soil moisture are essential for implementing smart irrigation systems and mitigating agricultural drought. Most agro-hydrological models are based on the standard Richards equation [1], a highly nonlinear, degenerate elliptic-parabolic partial differential equation (PDE) with first order time derivative. However, standard RE is limited by its incapability of characterizing preferential flow in anomalous soil exhibiting non-Boltzmann behavior, a common and realistic scenario. To overcome this limitation, time-fractional RE of the following form [2] is developed and employed to model water flow dynamics in real soil systems:

$$\partial_t^\alpha \theta + \nabla \cdot \mathbf{q} = S, \tag{1}$$

$$\mathbf{q} = -(C(\theta)\nabla\theta + K(\theta)\nabla z). \tag{2}$$

where θ denotes the soil moisture content (in, e.g., m^3/m^3), $\mathbf{q}$ represents the water flux (in, e.g., $m^3/m^2 \cdot s$), S denotes the sink term measuring water uptake rate by roots, $K(\theta)$ is unsaturated hydraulic water conductivity (in, e.g., m/s), $C(\theta)$ is soil moisture diffusivity (in, e.g., m^2/s), $t \in [0, T]$ denotes the time (in, e.g., s), z corresponds to the vertical depth (in, e.g., m), and α is a soil-dependent parameter indicating subdiffusion ($0 < \alpha < 1$) and superdiffusion ($1 < \alpha < 2$) [2]. For unsaturated flow, both C and K are highly nonlinear functions of soil moisture content and soil parameters, thereby posing significant computational challenges for solving the standard Richards equation itself [3]. Thus, most existing research focuses on developing accurate and efficient numerical solvers for the time-fractional RE given soil parameters [2], which is also known as solving the forward problem. Meanwhile, an equally important problem, which is to accurately estimate soil parameters given the soil moisture profile, is known as the inverse problem and is often less studied. This is primarily because inverse problems are generally ill-posed due to insufficient and/or inaccurate information (e.g., soil moisture solutions) and thus face significant computational challenges. Nevertheless, with recent advancements in soil sensing technologies and increasing adoption

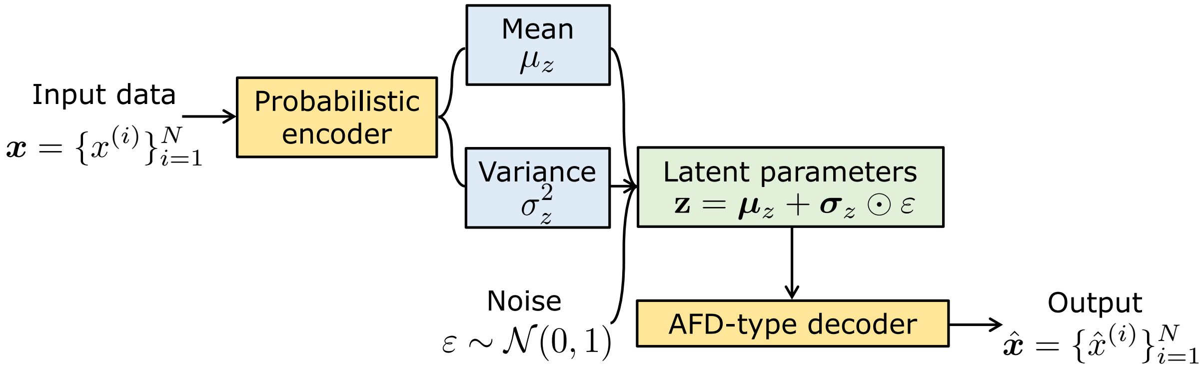

Figure 1. Our proposed AFD-enhanced BVAE architecture consists of two major components: an encoder that maps input $x = \{x^{(i)}\}_{i=1}^{N} \in D$ into a latent variable $z = \mu_z + \sigma_z \odot \varepsilon$ and a decoder that reconstruct $\hat{x} = \{\hat{x}^{(i)}\}_{i=1}^{N}$ from z.

of in situ soil moisture sensors, farmers now have real-time access to massive arrays of root-zone soil moisture data. This poses great need and opportunity to develop more accurate and computationally efficient algorithms for solving inverse problems of time-fractional RE, so that one can extrapolate soil parameters estimated from local in situ soil sensing measurements to model field-wide soil moisture profiles.

Existing approaches to solve inverse problem for standard and/or time-fractional RE can be categorized into deterministic or probabilistic methods. Deterministic methods, which solve the inverse problem as a nonlinear optimization problem [4-6], tend to be trapped in local optima and are sensitive to data noise. Meanwhile, probabilistic methods, such as Markov chain Monte Carlo (MCMC) [7] or variational autoencoder (VAE) [8], can explore the entire solution space. However, state-of-the-art probabilistic methods scale poorly as problem size (e.g., the number of parameters to be estimated) increases, leading to scalability issues [9].

To address these challenges, in this work, we propose a novel Bayesian variational autoencoder (VAE) framework that is built upon our in-house developed time-fractional RE solver [11] and the adaptive Fourier decomposition (AFD) techniques [12,13]. This integration enables precise parameter estimation for time-fractional RE. The AFD-enhanced BVAE framework consists of a probabilistic encoder, latent-to-kernel neural networks, and convolutional neural networks. The probabilistic encoder will map the input data (i.e., soil moisture measurements) to a latent space. To preserve useful mathematical properties and physical insights, we further restrict the latent space to its reproducing kernel Hilbert space (RKHS) via the use of latent-to-kernel neural networks. The AFD-based convolutional neural networks are then applied to the resulting RKHS as decoder for parameter estimation. These neural networks are trained end to end, in which the training data are soil moisture profiles produced by our time-fractional RE solver. Through a simple 3-D time-fractional RE example, we demonstrate the accuracy of our AFD-enhanced BVAE framework in solving inverse problems by comparing it with conventional BVAE approach whose decoder structure is not specially designed.

AN EXPLAINABLE BAYESIAN FRAMEWORK

Bayesian VAE framework

Here, we first provide a brief overview of the BVAE framework. The standard variational autoencoder (VAE) is a generative model that learns a structured latent space while reconstructing input data. As shown in Figure 1, VAE consists of two primary components, an encoder that maps input $x \in D$ into a set of latent variables z, and a decoder that reconstruct x from z.

VAE defines the marginal likelihood as the probability of the observation x under the generative model. Given latent variables z, the marginal likelihood is expressed as:

$$p(x) = \int p(x|z)p(z)\, dz, \tag{3}$$

where $p(z)$ is the prior distribution over latent variables (often a standard Gaussian). Since direct computation of the RHS of Equation (3) is intractable, VAE approximates the true posterior $p(z|x)$ using a variational distribution $q(z|x, \phi)$, and maximizes the Evidence Lower Bound (ELBO):

$$\mathcal{L}_{ELBO} = \sum_{x \in D} \mathcal{L}_{\Theta,\phi}(x), \tag{4}$$

$$\mathcal{L}_{\Theta,\phi}(x) = \mathbb{E}_{q(z|x,\phi)} \log p(x|z,\Theta) - D_{KL}[q(z|x,\phi) \| p(z)] \tag{5}$$

where the first term of Equation (5) ensures accurate reconstruction and the second term regularizes the latent space by minimizing the Kullback-Leibler (KL) divergence between the approximate posterior and the prior distribution.

On the other hand, the BVAE framework extends this by placing priors not only on the latent variables z but also on the model parameters θ, resulting in a Bayesian formulation:

$$p(\Theta|D) \propto p(D|\Theta)p(\Theta). \tag{6}$$

The likelihood function is then defined as:

$$p(x|z, D) = \int p(x|z,\Theta)p(\Theta|D)\, d\Theta \tag{7}$$

and the marginal likelihood as:

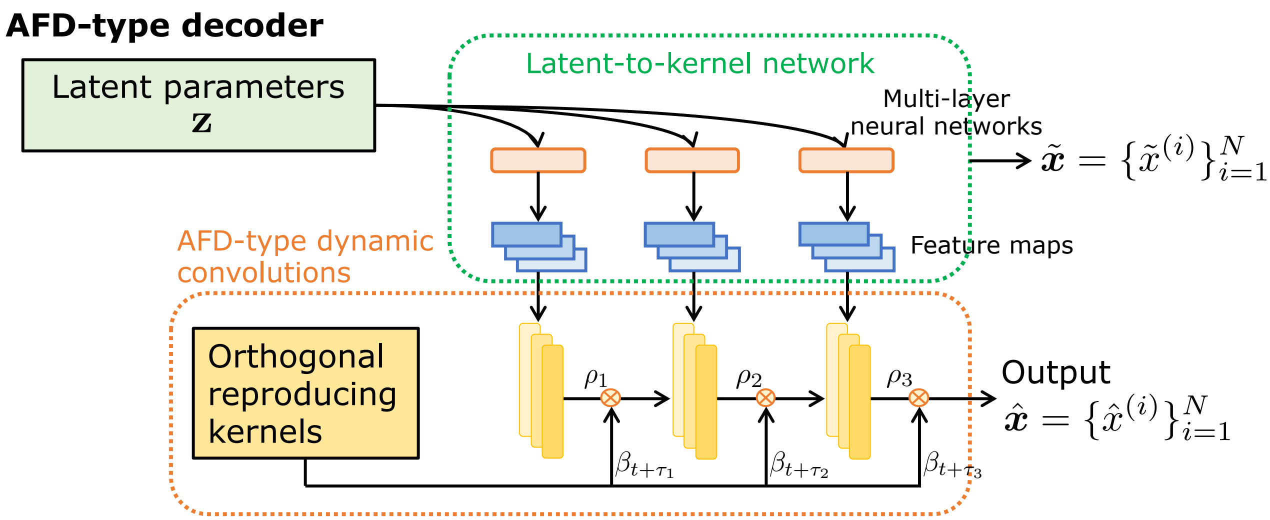

Figure 2. The decoder structure of our AFD-enhanced BVAE framework, which consists of two primary components: 1) latent-to-kernel neural networks which will map the latent variables z to $\tilde{x} = \{\tilde{x}^{(i)}\}_{i=1}^{N}$ lying on an RKHS, and 2) dynamic convolutional kernel network that will reconstruct $\hat{x} = \{\hat{x}^{(i)}\}_{i=1}^{N}$.

$$p(x|D) = \iint p(x|z, D)p(z)\, dz\, p(\Theta|D)\, d\Theta. \quad (8)$$

The BVAE enables more robust parameter estimation and improved uncertainty quantification. Instead of relying on a single point estimate for Θ, BVAE marginalizes over its posterior distribution, leading to better generalization and reliability in low-data regimes. By jointly inferring $p(z|x, D)$ and $p(\Theta|D)$, BVAE offers a fundamental way to incorporate uncertainty into both data representation and model parameters, making it particularly useful for applications requiring high-confidence decision-making.

A novel, explainable encoder structure in our AFD-enhanced BVAE framework

One common way to enhance the explainability of a neural network is to modify its structure based on the approximation theory (e.g., the universal approximation theorem [14]). In this work, we propose to achieve this by adopting AFD, a novel signal decomposition method that adopts adaptive orthogonal bases and thus leads to higher accuracy and significant computational speedup compared to conventional Fourier decomposition [12,13]. Specifically, as shown in Figure 2, we innovate the decoder structure by combining latent-to-kernel neural network with mathematically interpretable dynamic convolutional kernel network (CKN). In terms of latent-to-kernel network, our proposed structure consists of a multi-layer neural network that will first take the latent parameters z obtained from the encoder and generate $\tilde{x} = \{\tilde{x}^{(i)}\}_{i=1}^{N}$, which belongs to the Hilbert space H of the same manifold $\mathcal{M}$ that z belong to. Next, the latent-to-kernel network consists of feature maps $FM(\tilde{x})$ that project $\tilde{x}$ to its reproducing kernel Hilbert space (RKHS) [15]. This way, our latent-to-kernel network will try to learn the feature maps from $H(\mathcal{M})$ to its nearest RKHS, where the convolutional Kernel is unique and satisfies the reproducing property [16]. This naturally brings in dynamic CKN for local feature extraction, which is mathematically grounded in the RKHS framework. Furthermore, the dynamic CKN structure shown in Figure 2 mathematically resembles AFD in the sense that each dynamic convolutional layer performs cross-correlation between $FM(\tilde{x})$ and the orthogonal reproducing kernels β, i.e., $FM(\tilde{x}) \star \beta_i$. With this, the final output of the dynamic CKN, assuming that there are a total of N convolutional layers, is given by:

$$\hat{x} = \sum_{i=1}^{N} \rho_i (FM(\tilde{x}) \star \beta_i)\beta_{i+\tau_i}, \quad (9)$$

where $\rho_i \in (0,1)$ are scaling factors and τ_i can choose between 0 to $N - i$ for layer i. The choices of ρ_i and the orthogonal reproducing kernels must satisfy weak maximal selection principle and convergence theorem [10,12], respectively.

It can be shown that Equation (9) is equivalent to AFD operation [10,12,13]. Thus, with a specially designed structure, the AFD-type dynamic CKN will enjoy significant computational speedup and rigorous performance guarantees just like the AFD. The full AFD-enhanced BVAE model will be trained end to end by minimizing the following total loss function:

$$\mathcal{L} = \|x - \hat{x}\|^2_{H(\mathcal{M})} + \|\tilde{x} - FM(\tilde{x})\|^2_{H(\mathcal{M})} + wD_{KL}[q(z|x, \phi)\|p(z)], \quad (10)$$

where w is a regularization parameter.

Using AFD-enhanced BVAE framework to solve inverse problems

Here, we describe the procedure for applying our AFD-enhanced BVAE framework to solve the inverse problem. That is, we would like to reconstruct or estimate the soil-dependent parameters, including α and parameters of hydraulic conductivity function and water retention curve, from soil moisture content profiles through direct sensor measurements. Without loss of generality,

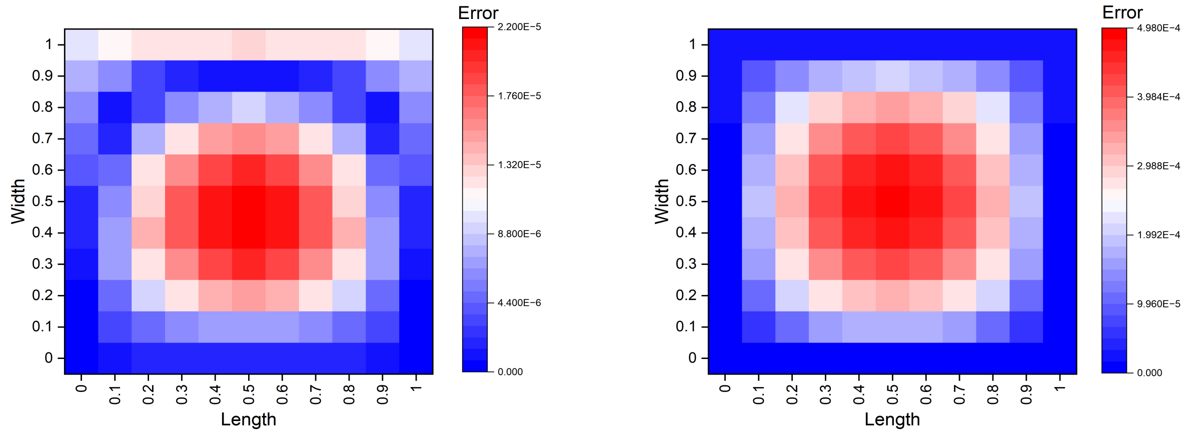

Figure 3. The error is obtained by substituting the parameters estimated by our proposed AFD-enhanced BVAE framework (Left) and conventional BVAE (Right) into the time-fractional RE solver [11] and taking the difference the numerical solution with the analytical solution of Equation (12). Ground truth value for the parameters are $\alpha = 0.5$ and $a = 0.001$. The parameters estimated by our proposed AFD-enhanced BVAE framework are $\alpha = 0.496 \pm 0.005$ and $a = 0.00102 \pm 7 \times 10^{-9}$, while those of conventional BVAE are $\alpha = 0.440 \pm 0.004$ and $a = 0.00094 \pm 3 \times 10^{-9}$.

we denote those parameters and the corresponding soil moisture content as γ and θ, respectively. To train the model, various sets of soil parameters γ will be sent to our in-house developed fractional RE solver to generate a set of soil moisture profile solutions. These solutions and their associated soil parameters γ will then be sent to the encoder to extract latent parameters z, which are then used by the decoder to reconstruct soil parameters $\hat{\gamma}$. During the training process, the total loss function of Equation (10) will be minimized such that the output of the decoder, $\hat{\gamma}$, shall match with the given γ as closely as possible.

Once training is complete, our AFD-enhanced BVAE model will only take the actual soil moisture measurements or solution profiles θ as input and produce the soil-specific parameter estimates $\hat{\gamma}$ as output, which can be used by the fractional RE solver for extrapolation and field-wide soil moisture modeling.

AN ILLUSTRATIVE EXAMPLE

Here, we present a proof-of-concept example to demonstrate the accuracy enhancement of our proposed AFD-enhanced BVAE framework by considering a simple 3-D time-fractional RE where $K = \theta$ and $C = a(\theta + 1)$. The width, length as well as depth are 1. The boundary conditions are zero at all boundaries and the initial condition is given by:

$$\theta(x, y, z, 0) = (x - x^2)(y - y^2)(z - z^2). \qquad (11)$$

For $a = 0.1$ and $\alpha = 0.5$, the problem has an analytical solution and is given by:

$$\theta(x, y, z, t) = t(x - x^2)(y - y^2)(z - z^2). \qquad (12)$$

Assuming that we do not know the values of γ (i.e., α and a), we generate a total of 10,000 sets of (θ, γ) solutions using our in-house developed fractional RE solver. Both AFD-enhanced BVAE and conventional BVAE models contains three hidden layers and 256 neurons per layer. The Adam optimizer and ReLU activation function are used for training. Figure 3 shows the error of soil moisture profiles between analytical solution and the numerical solution obtained from substituting the estimated soil parameters into our fractional RE solver, where the solution across two dimensions (width and length) are drawn better visualization. For the third dimension (depth), the error employs a similar behavior due to symmetry of this problem. Our AFD-enhanced BVAE model not only produces more accurate parameter estimates, but also enhances the accuracy of our fractional RE solver by at least an order of magnitude compared to conventional BVAE model. This illustrates the synergistic improvement in model accuracy when combining advanced numerical solver (for solving the forward problem) with our AFD-enhanced BVAE model (for solving the inverse problem). Furthermore, the data-driven nature of our proposed framework makes it particularly suitable for integrating in situ soil moisture sensing technologies to equip farmers with accurate tools that will bring "eyes inside the soil".

For comparison, we also implement a simple Kalman filter (KF) algorithm as a benchmark method to solve the same inverse problem. The results of KF are $\alpha = 0.517$ and $a = 0.00114$, which are further away from the ground truth solutions compared to our AFD-enhanced BVAE model.

Lastly, we point out that, unlike MCMC approach, our AFD-enhanced BVAE algorithm does not experience a significant increase in computational time as the number of unknown parameters to be estimated grows. This suggests that the BVAE-type approaches are quite scalable with respect to the dimensionality of the parameter space [17].

CONCLUSIONS

In this work, we propose a novel AFD-enhanced BVAE framework to accurately solve the inverse problem of time-fractional Richards equation. Our proposed framework synergistically integrates BVAE, neural network, dynamic convolutions, and AFD theory to offer computational speedup and great mathematical explainability. Furthermore, by designing a tailored decoder structure that resembles AFD operation, our new framework significantly improves soil parameter estimation accuracy. In addition, by using this framework in conjunction with our accurate time-fractional RE solver [11], we can achieve synergistic advancement in root-zone soil moisture modeling. Moreover, we remark that our proposed AFD-enhanced BVAE model is a generalized framework that can be leveraged in solving various inverse problems in large-scale and/or complex partial differential equation systems (e.g., convection-diffusion equation, Schrödinger equation, etc.), as well as in other fields such as image processing, data analytics, and so on. We will explore these aspects in our future works.

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