Construction of elliptic stochastic partial differential equations solver in groundwater flow with convolutional neural networks

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Abstract. Elliptic stochastic partial differential equations (SPDEs) play an indispensable role in mathematics, engineering and other fields, and its solution methods emerge in endlessly with the progress of science and technology. In this paper, we make use of the convolutional neural networks (CNNs), which are widely used in machine learning, to construct a solver for SPDEs. The SPDEs with Neumann boundary conditions are considered, and two CNNs are employed. One is used to deal with the essential equation, and the other satisfies the boundary conditions. With the help of the length factor, the integrated neural network model can predict the solution of the equations accurately. We show an example of groundwater flow to evaluate the model proposed with Gaussian random field (GRF). The experimental results show that the proposed neural network solver can approximate the traditional numerical algorithm, and has high computational efficiency.

Keywords: stochastic partial differential equations, machine learning, convolutional neural networks, groundwater flow.

1. Introduction
The fact that the mathematical science community generally accepted is that the strict understanding of turbulence and other related problems in hydrodynamics is one of the most important problems in mathematics, and one of the challenging tasks of the future development of partial differential equations (PDEs) theory. SPDEs play an important role not only in mathematics but also in engineering field, especially in the field of groundwater flow research [1]. Randomness here usually refers to the existence of uncertainty coefficients in the equations.

There are many commonly used algorithms, and the suitable methods for different problems are also different, such as [2-4]. However, the traditional numerical algorithm has some disadvantages, such as high computational cost [5]. With the continuous progress of artificial intelligence (AI) technology, artificial neural networks (ANNs) are widely used in various fields, and various neural network algorithms are also increasing. CNNs are generally used in computer vision and other fields because of
their characteristics. The combination of neural networks and PDEs has also emerged in large numbers [6-10]. Among them, there are many algorithms using neural network to solve PDEs. Adel et al. summarized an algorithm using RBF neural network to solve fractional order PDEs, and theoretically proved the rationality of the method [11]. The approximate solutions of hyperbolic PDEs are obtained by using distributive cellular neural networks [12]. From a new point of view, [13] tried to conclude and derived a framework of the relationship between CNNs and PDEs. A framework of residual neural network solver for PDE is proposed, which provides detailed theoretical analysis for the model based on control theory [14].

At the same time, researchers in the field of groundwater have also made great progress in their respective research directions by using machine learning technology, such as prediction, optimization, image processing and so on [15-20]. More and more researchers are devoted to exploiting the neural network solvers to replace the traditional numerical solution simulators. In this way, it can not only approach the classical numerical method in accuracy, but also greatly reduce the waste of computing resources. The ANN was used to simulate the approximate relationship between transmissivity and water head in the basic groundwater flow equation [21]. Based on the physics-informed neural network (PINN) model, the one-dimensional advection equation was solved [22]. A neural network simulator for steady-state flow in complex set shape was proposed in [23], and the experimental results showed that the trained convolutional neural network can quickly predict the velocity field within a certain accuracy range. There are few studies on using CNN to solve groundwater flow problems, and generally only one neural network is used to add penalty term in the loss function or in a hard way to meet the boundary conditions, which cannot accurately solve the problems under Neumann boundary conditions.

This paper is devoted to the study of the solution of SPDEs under Newman boundary conditions in groundwater flow. Two CNNs are used to process the data from internal nodes and boundary nodes respectively, then integrate them with the help of length factor, and finally form a complete neural network solver. The experimental results show that the proposed method can approach the numerical solution of traditional numerical algorithm and has outstanding performance in calculation efficiency.

2. Methodology

2.1. Form of SPDEs

In this paper, we consider the following two-dimension SPDEs with the help of neural network solver:

\[
\begin{cases}
-\nabla \cdot (P(x, \rho) \nabla f(x, \rho)) = I(x, \rho), \text{ for } x \in \mathbb{R}^2 \\
P(x, \rho) \nabla f(x, \rho) \cdot n(x) = B(x, \rho), \text{ for } x \in \partial \mathbb{R}
\end{cases}
\]

The above equations can describe the diffusion phenomenon in different situations, and \( P(x, \rho) \) represents the diffusion coefficient. When considering the phenomenon of heat conduction, \( P(x, \rho) \) represents the conductivity and \( f(x, \rho) \) represents the temperature; When groundwater flow is considered, \( P(x, \rho) \) is permeability and \( f(x, \rho) \) is pressure.

2.2. Model framework

Due to the complexity of boundary conditions, two CNNs are used to construct the solution of the equations. One is used to deal with internal nodes, and the other is used to deal with boundary points. The whole model framework is shown in Figure 1, the algorithm flow is shown in Figure 1(a), and the structure of two neural networks is shown in Figure 1(b). The mean square error (MSE) loss function is used to train the neural network.

\[
L_1 = \sum_{n_1} (f_1(x, \rho) - Y_1)^2
\]

\[
L_2 = \sum_{n_2} (f_2(x, \rho) - Y_2)^2
\]
\[ L = L_1 + L_2 \] (4)

Where \( f_1(x, \rho) \) and \( f_2(x, \rho) \) are the outputs of neural networks dealing with internal nodes and boundary nodes respectively. \( Y_i \) and \( Y_B \) represent the output results of MODFLOW at internal nodes and boundary points respectively, \( N_i \) and \( N_B \) are the respective numbers of internal points and boundary points. Finally, the integrated network model is equivalent to a nonlinear mapping, i.e. \( f = F(x, \rho) \).

Figure 1. Model framework. (a) the algorithm flow (b) neural network structure

2.3. The solution of equations

The solution of the equations is integrated by the length factor \( l(x) \). Finally, the solution \( f(x, \rho) \) of the equations can be expressed as:

\[ f(x, \rho) = l(x)f_1(x, \rho) + f_2(x, \rho) \] (5)

When dealing with internal nodes, \( l(x) = 1 \); when dealing with boundary nodes, \( l(x) = 0 \). The application of \( l(x) \) makes the two neural networks in a parallel relationship, which can be trained without interference. Facing different problems, \( l(x) \) can be shown in detail.

3. Experiments

3.1. Case description

In this paper, the following groundwater flow equations are considered:

\[
\begin{align*}
-\nabla \cdot (P(x, \rho)\nabla f(x, \rho)) &= 0, \text{ for } x \in X = [0,1]^2 \\
\nabla f(x, \rho) \cdot n(x) &= 0, \text{ for } x \in \partial X
\end{align*}
\] (6)

Where \( P(x, \rho) \) is hydraulic conductivity, \( f(x, \rho) \) is hydraulic head. \( n(x) \) is the unit normal vector. In this case, \( l(x) \) can be written in detail according to the boundary range, and the solution of the Equation (6) is
\[ f(x, \rho) = x_1 (1 - x_1) x_2 (1 - x_2) f_1(x, \rho) + f_2(x, \rho) \]  

(7)

3.2. Evaluation criterion

In this paper, two metrics \( L_2 \) and \( R^2 \) are selected to compare the results of neural network solver and finite volume method (FVM) method:

\[
L_2 \left( f_{\text{fipy}}, f_{\text{NN}} \right) = \left\| f_{\text{fipy}} - f_{\text{NN}} \right\|_2
\]  

(8)

\[
R^2 \left( f_{\text{fipy}}, f_{\text{NN}} \right) = 1 - \frac{\sum_{m=1}^{M} \left( f_{\text{NN},m} - f_{\text{fipy},m} \right)^2}{\sum_{m=1}^{M} \left( f_{\text{fipy},m} - \bar{f}_{\text{fipy},m} \right)^2}
\]  

(9)

\( f_{\text{fipy}} \) and \( f_{\text{NN}} \) represent the output of a FVM solver named \( f\text{ipy} \) executed by TensorFlow and the model proposed in this paper respectively, and \( M \) is the total number of grids, \( \bar{f}_{\text{fipy},m} = \sum_{m=1}^{M} f_{\text{fipy},m} \).

3.3. Results and analysis

When the input is GRF data set, our neural network solver can well predict the output value within a certain accuracy. \( L_2 \) is stable within 0.1, with an average of 0.074; The maximum of \( R^2 \) is 0.9, and the average is 0.951. It reveals that our model can get the solution from SPDEs close to the traditional numerical solution to a certain extent. The training process of the network is presented in Figure 2. Some of the results can be found in Figure 3.

In addition, we have obvious advantages in computing time and efficiency. The trained neural network can give the verification results in 0.01s. With 2000 samples of verification set, the solution time of \( f\text{ipy} \) is 92.54s, and the model we proposed costs 17.16s. In this way, the waste of computing resources can be greatly reduced.

![Figure 2. The training process of the model.](image.png)
Figure 3. Part of the experimental results. The left side is the input random field graph, the middle is the prediction result of \textit{fipy}, and the right side is the prediction result of neural network.

4. Conclusions
In this paper, a neural network solver for SPDEs under Neumann boundary in groundwater flow is proposed. We use two CNNs to process the data from internal nodes and boundary nodes respectively, and then integrate them with the help of length factor to form a complete neural network solution model. The experimental results show that the proposed surrogate method can approximate the results of traditional numerical methods, and has outstanding performance in computational efficiency. In the future, we will consider the following three aspects:

• With the deepening of deep learning, more advanced neural network model can be used;
• Considering the improvement of loss function, we hope to train neural network in unsupervised learning way;
• The model proposed in this paper can be further used as an alternative to the simulator in parameter estimation and other tasks.

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