Seeing Macro-dispersivity from Hydraulic ConductivityField with Convolutional Neural Network

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Motivation

For applying the advection-dispersion models under field conditions, hydro-geologists have proven that the magnitude of field-scale dispersivity (macro-dispersivity) can be several orders of magnitude higher than lab-scale value for the same material (Fiori et al., 2017). This increase mainly attributes to the spatial variability of aquifer structure which can be generally described by the spatial distribution of the hydraulic conductivity. Considering the heterogeneous distribution of hydraulic conductivity as a random field and relating flow and transport to its statistical moments has been one of the primary goals of the field of stochastic modelling (e.g. Dagan, 1989; Gelhar, 1993). A fundamental issue addressed by these works is how macro-dispersivity can be related to the statistical properties of the hydraulic conductivity field. However, the general applicability of the stochastic approach is sometimes questionable due to several foundational assumptions. And the first and second-order spatial statistics cannot provide sufficient information on estimating of macro-dispersivity. The conductivity fields with the same first two moments may produce very different solute spreading because of the spatial patterns that are not characterized by these statistics (e.g. Zinn and Harvey, 2003; Bianchi and Pedretti, 2018). The concepts of connectivity and geological entropy then emerge as other attempts to characterize the transport behavior from the heterogeneous conductivity fields (e.g. Rizzo and de Barros, 2017; Bianchi and Pedretti, 2017, 2018). In short, researchers have made great efforts to predict solute transport behavior only from a characteristic description of the conductivity field. Despite the helpfulness of these works in understanding the correlation between the heterogeneity of conductivity field and the transport behavior, a direct and efficient functional mapping between the conductivity field and the transport behavior for predictive purposes remains to be solved.

Methodology

a) Generating training datasets. Two-dimensional random fields of the hydraulic conductivity are generated. Direct simulations with the random walk particle tracking method (Salamon et al., 2006) are then used to compute the macro-dispersivities of the generated conductivity fields. The field dispersivity pairs consist of the training datasets for the deep neural network model.

b) Training the CNN. The training datasets from the previous step are then used to train our CNN that takes a heterogeneous conductivity field as input and gives macro-dispersivity as output.

c) Estimating macro-dispersivities. The trained CNN is then used to estimate macro-dispersivities of new conductivity fields that are not in the training datasets.

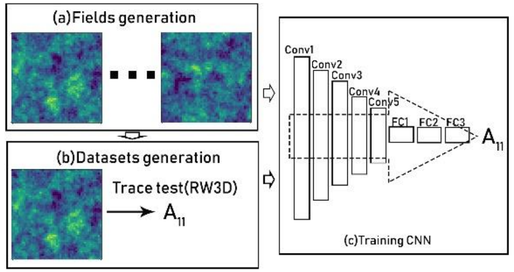

Figure 1: Sketch of the framework.

Table 1: 8 layers neural network architecture

Layer	Type	Maps and Neurons	Kernel Stride Padding
0	Input	1 field of 140 × 140 data points	-
1	Convolutional[a]	16 feature maps	7 2 1
2	Convolutional[a]	32 feature maps	7 1 2
3	Convolutional[a]	64 feature maps	7 1 2
4	Convolutional[a]	128 feature maps	7 1 2
5	Convolutional[a]	256 feature maps	5 1 2
6	Fully connected[b]	256 neurons	-
7	Fully connected[b]	256 neurons	-
8	Fully connected	256 neurons	-

[a] The convolutional layers are followed by a bacth normalization, a ReLU activation and a max pooling.
[b] The fully connected layers are followed by a ReLU activation.

Trace test set

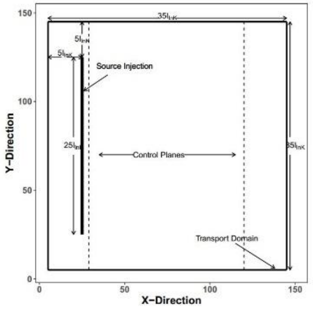

Figure 2: Sketch of domain of transport simulations showing the initial location of trace source, the control planes.

Physical Model Validation

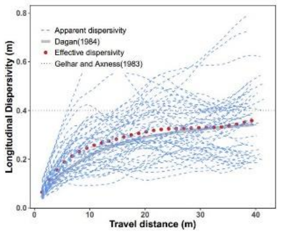

Figure 3: Comparison of effective and apparent macrodispersivities with the Dagan's (Dagan, 1984) and Gelhar's (Gelhar and Axness, 1983) analytical models ($\sigma_{\ln K}{}^2 = 0.1$).

Synthetic Experiments Setting

Synthetic experiments are conducted to demonstrate the capability of the neural network to estimate the macro-dispersivity by considering different variances of conductivity fields.

Table 2: Setup of experiments investigated in this work.

Experiment	Training set	Test set[a]
1	Var0.1	Var0.1
	Var0.2	Var0.2
	Var0.3	Var0.3
	Var0.5	Var0.5
2	Var0.2	Var0.1
	Var0.3	Var0.1 Var0.2
	Var0.5	Var0.1 Var0.2 Var0.3
3	Var0.1	Var0.2 Var0.3 Var0.5
	Var0.2	Var0.3 Var0.5
	Var0.3	Var0.5

[a] Each test set has 1000 samples which are not in the training set.

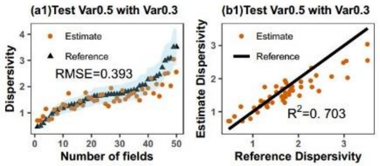

Figure 5: Estimating macro-dispersivities of felds with $\sigma_{lnK}{}^2$ =0.5 using neural network model trained by felds with $\sigma_{lnK}{}^2$ = 0.3.

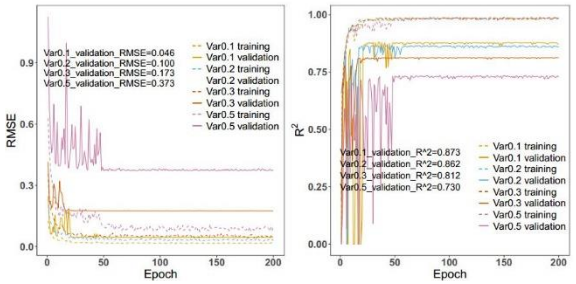

Figure 4: Training process of the neural network with the training sets of different variances.

Results and Discussion

Fig. 6 displays the comparison of R^2 from the above three experiments.

Generally, the CNN trained by conductivity fields with relatively large variances can achieve better performance on estimations of macro-dispersivities for conductivity fields with relatively small variances. The neural network trained by highly heterogeneous fields seems to have a high ability to extract features of heterogeneity. In Fig. 6(a4), the neural network trained by Var0.5 has much better performance than the neural network trained by Var0.1, although the neural network trained by Var0.5 has worse performance in its own test set.

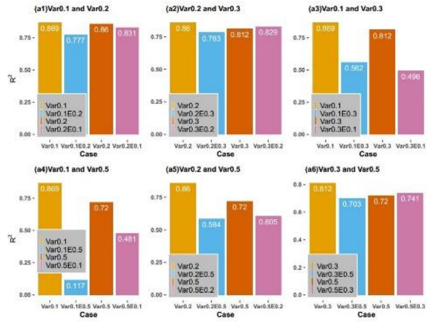

Figure 6: Comparison of R^2 for different cases; Var0.1 represents the results of using the CNN trained by the training set of Var0.1 to estimate conductivity fields in the test set of Var0.1; Var0.1E0.2 represents the results of using the CNN trained by the training set of Var0.1 to estimate conductivity fields in the test set of Var0.2; The other labels have similar meanings.

Sixteen typical fltered results from the frst convolutional layer are presented in Fig. 15(b) for estimating macro-dispersivityof the conductivity feld shown in Fig. 15(a). It can be seen that in Fig. 15(b) the CNN attempts to identify different features of the heterogeneous conductivity feld. Apparently, we can see that, feature 1, 3, 10, 13, 16 mainly capture the distributions of relatively high lnK values of the original lnK feld. While feature 2, 4, 7, 11, 12, 14 mainly capture the distributions of relatively low lnK values of the original lnK feld. Other features also reflect some other heterogeneous patterns that are not prominent.

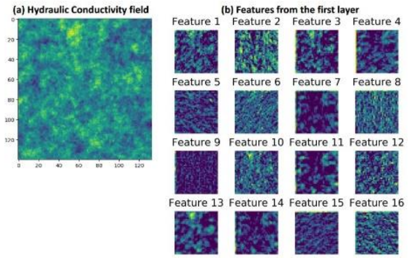

Figure 7: Illustration of features learned by the CNN, including (a) an input lnK feld and (b) corresponding features obtained from the frst convolutional layer.

Conclusions

The following conclusions can be drawn from these experiments:

1. The estimating performance of CNN generally drops with increasing variances of conductivity fields (increasing heterogeneity) for the given size of training datasets (4000 fields) and data points (140×140).
2. The CNN trained by conductivity fields with a specific variance has universality in estimating macro-dispersivity to a certain extent because a well trained CNN will have the capacity to extract different patterns of heterogeneity. Consequently, the trained CNN can extract some standard heterogeneous features of conductivity fields for estimating macro-dispersivities.
3. Furthermore, the universality of the trained CNN decreases with the increasing disparity between variances of conductivity fields in training set and test set. And the CNN trained by conductivity fields with relatively large variances can have stronger universality of estimating.
4. In general, the deep neural network is a very promising approach in building direct mapping between complicated subsurface structure and solute transport behavior.