Integration of adversarial autoencoders with residual dense convolutional networks for estimation of non-Gaussian conductivities in solute transport modeling

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Key Points:

- A convolutional adversarial autoencoder is developed to parameterize non-Gaussian conductivity fields with multimodal distributions
- A deep residual dense convolutional network is proposed for surrogate modeling of highly complex mappings in solute transport
- The integrated approach is illustrated for inversion of non-Gaussian conductivities in 2-D and 3-D solute transport modeling

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Abstract

Inverse modeling involving characterization of a non-Gaussian conductivity field in subsurface flow and transport constitutes a challenging problem. This is mainly due to the non-Gaussian property and the fact that many repeated evaluations of the forward model are often required. In this study, we develop a convolutional adversarial autoencoder (CAAE) to parameterize the non-Gaussian conductivity fields with heterogeneous conductivity within each facies using a low-dimensional latent representation. In addition, a deep residual dense convolutional network (DRDCN) is proposed for surrogate modeling of solute transport models with high-dimensional and highly-complex mappings. The two networks are both based on a multilevel residual learning architecture called residual-in-residual dense block. The multilevel residual learning strategy and the dense connection structure ease the training of deep networks, enabling us to efficiently build deeper networks that have an essentially increased capacity for approximating mappings of very high-complexity. The CCAE and DRDCN networks are incorporated into an iterative local updating ensemble smoother to formulate an inversion framework. The integrated method is demonstrated using 2-D and 3-D solute transport models with non-Gaussian conductivity fields. The obtained results indicate that the CCAE is a robust parameterization method for non-Gaussian conductivity fields with different heterogeneity patterns. The DRDCN network is able to obtain accurate approximations of the forward models with high-dimensional and highly-complex output fields using relatively limited training data. The CCAE and DRDCN methods together significantly reduce the number of forward model runs required to achieve accurate inversion results.

1 Introduction

Groundwater flow and solute transport models are used widely to help understand subsurface processes and make science-informed decisions for groundwater resource management. Reliable model predictions that well reproduce the realistic phenomena require a good characterization of the hydraulic conductivity field as it greatly influences groundwater flow and solute transport. In many practical cases, such as aquifers in fluvial deposits where several highly contrasting facies coexist, it may be unrealistic to model the log-conductivity as Gaussian. It has been shown that a multimodal distribution can better characterize the strong conductivity heterogeneity (Gómez-Hernández & Wen, 1998; Journel & Deutsch, 1993; Kerrou et al., 2008; Zhou et al., 2014).

In this study, in solute transport models, we are concerned with characterization of the continuous non-Gaussian conductivity field. This has a multimodal distribution as opposed to the categorical fields with homogeneous conductivity within each facies (e.g., the binary field). In practice, the conductivity field is estimated via inverse modeling based on easily accessible indirect measurements (e.g., the hydraulic head and solute concentration). The commonly used inverse methods are, for example, the Markov chain Monte Carlo methods (Vrugt, 2016) and the ensemble-based data assimilation methods such as ensemble smoother (van Leeuwen & Evensen, 1996), ensemble Kalman filter (Evensen, 1994), and their variants (Emerick & Reynolds, 2013; Laloy et al., 2013; Sun et al., 2009; Xu & Gómez-Hernández, 2018; J. Zhang et al., 2018; Zhou et al., 2011). Considering the strong conductivity heterogeneity, the inverse problem is usually high-dimensional with a typically large number of uncertain variables. Thus, it often requires a large number of forward model runs to obtain converged inversion results.

To relieve the large computational cost, parameterization methods are commonly used together with surrogate models within the inversion framework. A parameterization method aims to represent the spatially correlated property field using a low-dimensional latent vector (Oliver & Chen, 2011; Zhou et al., 2014). It can also mitigate the potential ill-posedness of the inverse problem and ensure that the updated fields in the inversion process satisfy the prior distribution assumptions (e.g., Gaussian or non-Gaussian) imposed on the unknown
A surrogate method aims to replace the computationally expensive forward model with an accurate but cheap-to-run approximation of the model input-output mapping during the inversion (Asher et al., 2015; Razavi et al., 2012). Although such combinations of methods for inverse modeling have been intensively studied for problems with Gaussian conductivity fields (Chang et al., 2017; Elsheikh et al., 2014; Ju et al., 2018; Laloy et al., 2013; J. Zhang et al., 2015, 2016), previous studies on problems with continuous non-Gaussian conductivity fields often relied on the inverse methods solely without using the parameterization and surrogate methods. The development of parameterization and surrogate methods for such non-Gaussian problems remains an open problem due to the following two major challenges.

First, most existing parameterization methods fail to work for non-Gaussian conductivity fields. Previous works on parameterizing the conductivity fields in inversion have relied on, for example, principal component analysis and its variants (Ma & Zabaras, 2011; Sarma et al., 2008; Vo & Durlofsky, 2014; D. Zhang & Lu, 2004). While these methods are well suited for Gaussian random fields, their performance for complex non-Gaussian fields deserves further improvement (Canchumuni et al., 2019b; Chan & Elsheikh, 2017; Laloy et al., 2017, 2018; Liu et al., 2019). Inspired by the recent success of deep learning in various areas including hydrology (Shen, 2018), its application in parameterization of non-Gaussian conductivity fields has been reported in many recent studies (Canchumuni et al., 2019a, 2019b; Chan & Elsheikh, 2017, 2018, 2019; Laloy et al., 2017, 2018; Liu et al., 2019). Among these applications, generative adversarial networks (GAN) (Goodfellow et al., 2014) and variational autoencoders (VAE) (Kingma & Welling, 2014) are the two most popular network architectures. These methods take random realizations of a low-dimensional vector as input and then generate new realizations of the conductivity field having similar features with those found in the training data. The quality of the generated realizations was shown to be superior to those from traditional parameterization methods (Canchumuni et al., 2019b; Chan & Elsheikh, 2017; Laloy et al., 2017; Liu et al., 2019). However, these methods focused on categorical conductivity fields with homogeneous conductivity within each facies. Their applicability to continuous non-Gaussian fields with heterogeneous conductivity within each facies, which is more challenging, remains to be explored.

Second, most existing surrogate methods suffer from the curse of dimensionality (Asher et al., 2015; Razavi et al., 2012) and fail to efficiently obtain accurate approximations when the outputs are highly-nonlinear (Liao et al., 2017; Lin & Tartakovsky, 2009; Mo et al., 2017). The curse of dimensionality is caused by the exponentially increased computational cost required for accurate surrogate construction as the input dimensionality increases. Due to the strongly heterogeneous nature of the conductivity field, it is often required to use a large number of stochastic degrees of freedom to accurately represent the heterogeneity. The highly-nonlinear outputs here arise because the high-conductivity regions in a non-Gaussian aquifer result in preferential paths for the groundwater flow and solute transport. The two factors together make the commonly used surrogate methods, such as Gaussian processes (Rasmussen & Williams, 2006) and polynomial chaos expansion (Xiu & Karniadakis, 2002), difficult to work.

Deep neural networks have already exhibited a promising and impressive performance for surrogate modeling of forward models with high-dimensional input and output fields (Kani & Elsheikh, 2019; Mo, Zabaras, et al., 2019; Mo, Zhu, et al., 2019; Sun, 2018; Tripathy & Bilionis, 2018; Zhong et al., 2019; Zhu & Zabaras, 2018; Zhu et al., 2019). For example, in Tripathy and Bilionis (2018) a deep neural network was proposed to build a surrogate model for a single-phase flow model. In Sun (2018) and Zhong et al. (2019), their surrogate methods for a single-phase flow model and a multiphase flow model, respectively, were based on an adversarial network framework. In our previous studies (Mo, Zabaras, et al., 2019; Mo, Zhu, et al., 2019; Zhu & Zabaras, 2018; Zhu et al., 2019), a deep dense convolutional network (DDCN), which is based on a dense connection structure (Huang et al., 2017) for better information flow efficiency, was employed as the surrogate modeling framework. It
showed a good performance in efficiently obtaining accurate surrogates of various forward models with high-dimensional uncertain input and output fields. However, these methods were tested on forward models with Gaussian conductivity fields (Kani & Elsheikh, 2019; Mo, Zabaras, et al., 2019; Mo, Zhu, et al., 2019; Tripathy & Bilionis, 2018; Zhu & Zabaras, 2018; Zhu et al., 2019) or on a single-phase flow model with binary channelized conductivity fields (Zhu et al., 2019). Still, as it will be shown in a case study, that application of the DDCN surrogate method to the solute transport models with non-Gaussian conductivity fields may lead to large approximation errors for the highly-complex output fields.

In this work, we develop a convolutional adversarial autoencoder (CAAE) to parameterize continuous non-Gaussian conductivity fields. We transform a fully-connected adversarial autoencoder (Makhzani et al., 2016) to a convolutional network so as to improve its scalability for larger-size inputs. CAAE is very similar to VAE in the sense that in both a latent representation is obtained with a desired distribution. The difference is that in CAAE a GAN framework, instead of a Kullback-Leibler divergence penalty used in VAE, is used to perform variational inference to guide the posterior distribution of the latent variables to match the prespecified distribution. In addition, we propose a deep residual dense convolutional network (DRDCN) for efficient surrogate modeling of forward models with highly-complex mappings. Although deeper networks have the potential to substantially improve the network’s performance, they can be difficult to train. We adopt in DRDCN a multilevel residual learning structure (Wang et al., 2018). The residual learning strategy has been shown to be an effective solution to ease the training of very deep networks (He et al., 2016a, 2016b; Simonyan & Zisserman, 2015; Szegedy et al., 2015; Wang et al., 2018). The multilevel residual learning structure is also implemented in the CAAE network. The CAAE and DRDCN networks are combined with an iterative local updating ensemble smoother (ILUES) algorithm (J. Zhang et al., 2018) to formulate an efficient CAAE-DRDCN-ILUES inversion framework. The overall integrated method is demonstrated using 2-D and 3-D solute transport models with continuous non-Gaussian conductivity fields that have different heterogeneity patterns with bimodal and trimodal distributions, respectively.

In summary, three major innovative contributions are addressed in this study. First, we develop a CAAE method for parameterization of non-Gaussian conductivity fields with heterogeneous conductivity within each facies in the inverse problem. Second, we adopt a multilevel residual strategy in our previous DDCN method (Mo, Zabaras, et al., 2019; Mo, Zhu, et al., 2019; Zhu & Zabaras, 2018; Zhu et al., 2019) to introduce a new DRDCN method with a substantially improved performance for surrogate modeling of highly-complex mappings. Finally and most importantly, to the best of our knowledge, we present the first attempt to incorporate simultaneously the parameterization and surrogate methods to perform inversion of non-Gaussian conductivities in solute transport modeling.

The rest of the paper is organized as follows. In section 2, we introduce a solute transport model and define the problem of interest. The CAAE-DRDCN-ILUES inversion framework is presented in section 3. Then in sections 4 and 5, the proposed method is evaluated using two synthetic models. The conclusions are summarized in the last section.

2 Problem Definition

We consider solute transport in heterogeneous porous media under a steady-state groundwater flow condition. It is assumed that the transport of solute is driven by advection and dispersion. The governing equations for the steady-state flow and solute transport are written as (Zheng & Wang, 1999)

\[ \nabla \cdot (K \nabla h) = 0, \]  

(1)

and

\[ \frac{\partial \phi c}{\partial t} = \nabla \cdot (\phi \alpha \nabla c) - \nabla \cdot (\phi v c) + r_s, \]  

(2)
respectively. Here \( K \) (LT\(^{-1}\)) is the hydraulic conductivity, \( h \) (L) is the hydraulic head, \( \phi \) (\( - \)) is the effective porosity, \( c \) (ML\(^{-3}\)) is the solute concentration, \( t \) (T) denotes time, \( r_s \) (ML\(^{-3}\)T\(^{-1}\)) is the sink/source, and \( \alpha \) (L\(^2\)T\(^{-1}\)) is the dispersion tensor determined by the pore space flow velocity \( v \) (LT\(^{-1}\)), and longitudinal \((\alpha_L; L)\), transverse \((\alpha_T; L)\), and vertical \((\alpha_V; L)\) dispersivities. The two equations are coupled through the velocity \( v = -\frac{\nabla h}{\phi} \). The flow and solute transport equations are numerically solved using the MODFLOW (Harbaugh et al., 2000) and MT3DMS (Zheng & Wang, 1999) simulators, respectively.

We are concerned with an inverse problem of characterizing the heterogeneous conductivity field using measurements of the hydraulic head and concentration. The underlying conductivity fields of interest are continuous non-Gaussian fields. The inverse modeling is performed using the ILUES inversion algorithm (J. Zhang et al., 2018) which has shown a promising performance for high-dimensional and highly-nonlinear inverse problems (Mo, Zabaras, et al., 2019; J. Zhang et al., 2018).

3 Methodology

3.1 ILUES for Inverse Modeling

The ILUES algorithm assimilates the output measurements \( d \in \mathbb{R}^{N_d} \) for multiple times with an inflated covariance matrix of the measurement errors to avoid overweighing the measurements (Mo, Zabaras, et al., 2019; J. Zhang et al., 2018). The inflated covariance matrix is often taken as \( C_D = N_{iter} C_D \), where \( C_D \) is the original covariance matrix of the measurement errors and \( N_{iter} \) is the number of iterations (Emerick & Reynolds, 2013; J. Zhang et al., 2018). To better handle high-dimensional and highly-nonlinear problems, ILUES also adopts a local updating scheme, which updates each input sample \( m \in \mathbb{R}^{N_m} \) in the ensemble locally using its neighboring samples rather than all samples in the ensemble. Formally, given an ensemble of \( N_e \) input samples \( M = \{m_1, \ldots, m_{N_e}\} \), it first identifies a local ensemble for each sample \( m_i \in M \) based on the following metric (J. Zhang et al., 2018)

\[
J(m) = \frac{J_d(m)}{J_d^{\max}} + \frac{J_m(m)}{J_m^{\max}},
\]

where \( J_d(m) = [f(m) - d]^\top C_D^{-1}[f(m) - d] \) quantifies the mismatch between the model responses \( f(m) \) and measurements \( d \), and \( J_m(m) = (m - m_i)^\top C_{MM}^{-1}(m - m_i) \) is the distance between the sample \( m_i \) and sample \( m \in M \). Here, \( C_{MM} \) is the autocovariance matrix of the input parameters in \( M \), \( J_d^{\max} \) and \( J_m^{\max} \) are the maximum values of \( J_d(\cdot) \) and \( J_m(\cdot) \), respectively. Based on the \( J \) values, we select \( N_i = \beta_i N_e \), \( \{\beta_i \in (0, 1)\} \) samples as the local ensemble of \( m_i \) using a roulette wheel selection operator (Lipowski & Lipowska, 2012), in which the selection probability of the \( i \)th individual is given as \( P_i = \rho_i / \sum_{j=1}^{N_e} \rho_j \), \( i = 1, \ldots, N_e \), where \( \rho_j = 1/J(m_j) \) (Mo, Zabaras, et al., 2019). A local ensemble factor of \( \beta_i = 0.1 \) suggested in J. Zhang et al. (2018) is used.

Let superscripts \( l \), \( f \), and \( a \) denote the local ensemble, current, and updated samples, respectively. The ILUES first updates the local ensemble of each sample \( m_i^l \in M_l \), that is, \( M_i^{l,f} \), by using the usual ensemble smoother scheme (Emerick & Reynolds, 2013; Mo, Zabaras, et al., 2019; J. Zhang et al., 2018):

\[
m_i^a = m_i^f + C_{MD}^{l,f}(C_{DD}^l + \tilde{C}_D)^{-1}[d_j - f(m_{i,j}^f)],
\]

for \( j = 1, \ldots, N_i \). Here \( C_{MD}^{l,f} \) is the cross-covariance matrix between \( M_i^{l,f} \) and \( D_i^{l,f} = [f(m_{i,1}^f), \ldots, f(m_{i,N_e}^f)] \), \( C_{DD}^l \) is the autocovariance matrix of \( D_i^{l,f} \), and \( d_j = d + \tilde{C}_D^{1/2} r_{N_d} \), \( r_{N_d} \sim \mathcal{N}(0, I) \), is the \( j \)-th realization of the measurements. The update of \( m_i^a \), \( m_i^a \), is then generated from its updated local ensemble \( M_i^{a} = \{m_{i,1}^a, \ldots, m_{i,N_e}^a\} \) through a probabilistic scheme (Mo, Zabaras, et al., 2019). One update iteration of ILUES is summarized in Algorithm 1. More details regarding ILUES can be found in J. Zhang et al. (2018) and Mo, Zabaras, et al. (2019).
For high-dimensional inverse problems, large ensemble size and iteration number are usually needed for ILUES to obtain converged and reliable inversion results, resulting in a large computational cost in forward model runs. To reduce the computational burden, we propose a CAAE network for parameterizing the high-dimensional conductivity field using a low-dimensional latent vector and a DRDCN network to build an accurate but fast-to-run substitution of the forward model in the ILUES algorithm.

3.2 DRDCN for Surrogate Modeling

In the surrogate modeling task, we build a surrogate model to approximate the mapping between the input conductivity field and the output hydraulic head and concentration fields. In our previous studies (Mo, Zabaras, et al., 2019; Mo, Zhu, et al., 2019; Zhu & Zabaras, 2018; Zhu et al., 2019), we transformed the surrogate modeling task for problems with high-dimensional input and output fields in a 2-D domain to an image-to-image regression problem by using a DDCN network which is based on a dense block structure (Huang et al., 2017). In this network, the input and output fields were treated as images. Denoting $H \times W$ as the spatial discretization resolution of the domain, $\mathbf{x} \in \mathbb{R}^{d_x \times H \times W}$ and $\mathbf{y} \in \mathbb{R}^{d_y \times H \times W}$ as the input and output fields, respectively. Then the surrogate modeling task for approximating the input-output mapping,

$$ f : \mathbb{R}^{n_x \times H \times W} \to \mathbb{R}^{n_y \times H \times W}, $$

was transformed to an image regression problem between $n_x$ input images and $n_y$ output images with a resolution of $H \times W$, where $n_x$ and $n_y$ are the number of the input and output fields, respectively. It is straightforward to generalize to a 3-D domain by adding an extra depth axis to the images, that is, $\mathbb{R}^{n_x \times D \times H \times W} \to \mathbb{R}^{n_y \times D \times H \times W}$.

In order to further improve the performance of DDCN in problems with highly-complex output fields (e.g., the solute transport model with non-Gaussian conductivity fields considered in this study), we adopt a novel basic block called ‘residual-in-residual dense block’ proposed in Wang et al. (2018) for image super-resolution problems to formulate our DRDCN framework.
3.2.1 Residual-in-Residual Dense Block

A dense block introduces connections between non-adjacent layers aiming to fully exploit the hierarchical features from the outputs of preceding layers (Huang et al., 2017). Let $z^{(i)} (i = 1, \ldots, L)$ denote the output feature maps of the $i$th layer in the dense block, where $L$ is number of layers. $z^{(i)}$ is obtained by taking the concatenation of the output feature maps from its preceding layers as input, as represented by

$$z^{(i)} = H([z^{(0)}, \ldots, z^{(i-1)}]),$$

where $z^{(0)}$ represents the input to the dense block, and $H$ denotes operations on the input feature maps, including batch normalization (BN) (Ioffe & Szegedy, 2015), followed by rectified linear unit (ReLU) activation and convolution (Conv) (Goodfellow et al., 2016). A dense block with $L = 5$ layers is illustrated in Figure 1a.

![Diagram](image)

Figure 1: (a) A dense block with five layers. Each layer contains three operations (i.e., BN, ReLU, and Conv) and outputs $N_f$ feature maps with size $D_f \times H_f \times W_f$, which are concatenated (©) with its input feature maps. The concatenated feature maps are treated as the input to the next layer. (b) A residual-in-residual dense block (RRDB) with three residual dense blocks. The output of a dense block is scaled down by multiplying with a factor $\beta \in (0, 1]$ before adding (⨁) to its input. (c) Architecture of the deep residual dense convolutional network (DRDCN). The feature map size is halved in Conv (▽) with a stride of 2 and doubled by using the nearest upsampling (UP) operation.

It has been shown that deeper networks have the potential to better approximate mappings of high complexity, however, they can be difficult to train (Simonyan & Zisserman, 2015; Szegedy et al., 2015; Wang et al., 2018). To efficiently train a deeper network, we adopt a multilevel residual learning structure, that is, the residual-in-residual dense block proposed in Wang et al. (2018). In the residual learning framework, it has been shown that
the residual mapping is much easier to learn than the original mapping. Thus, we explicitly let a few stacked layers (not necessarily the entire network) to learn a residual mapping instead of the original mapping (He et al., 2016a, 2016b). Specifically, let \( f(x) \) denote the desired underlying mapping to fit. Then the stacked layers learn the residual mapping \( g(x) := f(x) - x \). The original mapping \( f(x) \) is then recast as \( g(x) + x \). Such a residual learning strategy can help alleviate the gradient vanishing problem for deep network training (He et al., 2016a) and thus ease the training of very deep networks to achieve improved accuracy (He et al., 2016a, 2016b; Ledig et al., 2017; Simonyan & Zisserman, 2015; Wang et al., 2018).

The architecture of residual-in-residual dense block is shown in Figure 1b. It consists of a stack of residual dense blocks, where the residual learning is used in two levels, resulting in a residual-in-residual structure. That is, the residual learning implemented to the dense block results in a residual dense block; and that implemented to the stacked residual dense blocks results in a residual-in-residual dense block. The number of input and output feature maps of a dense block is \( N_f \) (Figure 1a) and is set to \( N_f = 48 \). In addition to the residual-in-residual structure, a residual scaling technique (Szegedy et al., 2016) is also employed in the residual-in-residual dense block to further increase the training stability (Wang et al., 2018). Formally, this is done by scaling down the residual \( g(x) \) by a factor \( \beta \in (0, 1] \) before adding to \( x \) (Figure 1b). A factor of \( \beta = 0.2 \) suggested in Wang et al. (2018) is used in our network.

### 3.2.2 DRDCN Networks Based on Residual-in-Residual Dense Blocks

We employ the residual-in-residual dense block structure in our DRDCN network for surrogate modeling of solute transport in media with non-Gaussian conductivities. The network architecture is shown in Figure 1c. For 2-D or 3-D images (fields), the 2-D and 3-D operations (i.e., BN, ReLU, and Conv) implemented in the PyTorch software are respectively used in the network without requiring any additional modifications to the network architecture. The network contains four residual-in-residual dense blocks and the feature maps are to go through a coarsen-to-refine process. A convolutional layer is first employed to extract feature maps from the raw input image. The obtained features are then passed through the residual-in-residual dense blocks and the transition convolutional layers for changing the feature map size during the coarsen-to-refine process that reconstructs the output images. Convolutional layers with a stride of 2 halve the size during the coarsening process and the nearest upsampling operation doubles the size during the refining process.

We arrange the position of the four residual-in-residual dense blocks in the network with a layout of \((1, 2, 1)\) (Figure 1c) to encourage the information flow through the coarse feature maps. That is, one block is placed in the coarsening part; two adjacent blocks are placed in the most central part; and another one block is placed in the refining part. An additional level of residual learning is implemented on the stacked residual-in-residual dense blocks, resulting in a three-level residual learning structure in the network.

### 3.3 CAAE for Parameterization of Non-Gaussian Random Fields

We propose to parameterize continuous non-Gaussian conductivity fields using a CAAE network. Without loss of generality, here we use \( x \) to denote the conductivity field. Adversarial autoencoder is a probabilistic autoencoder that uses the GAN framework as a variational inference algorithm (Makhzani et al., 2016). The original adversarial autoencoder framework is composed of fully-connected layers (Makhzani et al., 2016), making it increasingly difficult to train as the network gets deeper due to a large number of trainable parameters. To resolve this issue, we develop a CAAE framework based on convolutional layers to leverage their sparse-connectivity and parameter-sharing properties as well as robust capability in image-like data processing (Goodfellow et al., 2016; Laloy et al., 2018; Mo, Zhu, et al., 2019; Shen, 2018).
3.3.1 Generative Adversarial Networks

GAN (Goodfellow et al., 2014) is a framework that establishes an adversarial game between two networks: a generative network $G(\cdot)$ (i.e., generator) that learns the data distribution $p_{\text{data}}(x)$ over the data, and a discriminative network $D(\cdot)$ (i.e., discriminator) that computes the probability that a sample $x$ in the data space is sampled from $p_{\text{data}}(x)$, rather than generated by the generator. The generator maps the input noise $z$ from the prior distribution $p(z)$ to the data space. The discriminator is trained to maximize the probability of distinguishing the true samples from the generated (fake) samples. The generator is simultaneously trained to maximally fool the discriminator into assigning a higher probability to the generated samples by leveraging the feedback from the discriminator. Mathematically, the adversarial game translates into the following minimization-maximization loss function (Goodfellow et al., 2014)

$$\min_{G} \max_{D} \mathbb{E}_{x \sim p_{\text{data}}(x)} \left[ \log D(x) \right] + \mathbb{E}_{z \sim p(z)} \left\{ \log [1 - D(G(z))] \right\}. \tag{7}$$

In practice, the generator and discriminator are usually trained in alternating steps: (1) train the discriminator to improve its discriminative capability; (2) train the generator to improve the quality of the generated samples so as to fool the discriminator.

3.3.2 Adversarial Autoencoder

An adversarial autoencoder (Makhzani et al., 2016) is a framework that learns a low-dimensional representation $z$ (referred to as latent codes or latent variables) of the input $x$ in the data and generates from the codes a reconstruction $\hat{x}$ that closely matches $x$. It consists of two networks: an encoder to learn a mapping from $x$ to $z$ and a decoder to learn a mapping from $z$ to $\hat{x}$. To create a generative framework, a constraint is added on the encoder that forces it to generate latent codes $z$ that roughly follow a desired distribution, like a standard normal distribution $\mathcal{N}(0, I)$ used in the present study. The decoder is then trained to generate samples with features being consistent with those found in the training data given any sample $z \sim \mathcal{N}(0, I)$ as input, resulting in a generative model.

Mathematically, let $q(z|x)$ be the encoding distribution, $q(x|z)$ the decoding distribution, and $p(z)$ be the distribution that we want the latent variables $z$ to follow. The adversarial autoencoder looks for a generative model

$$p(x) = \int p(x|z)p(z)dz. \tag{8}$$

The adversarial autoencoder (Makhzani et al., 2016) is similar in spirit to the VAE (Kingma & Welling, 2014). Thus we follow the formulation in VAE to finally introduce the adversarial autoencoder. In VAE, the generative model is obtained via minimizing the upper-bound of the negative log-likelihood

$$\mathbb{E}_{x \sim p_{\text{data}}(x)} \left[ -\log p(x) \right] < \mathbb{E}_{x \sim p_{\text{data}}(x)} \left\{ \mathbb{E}_{x \sim q(z|x)} \left[ -\log p(x|z) \right] + \text{KL}[q(z|x) \parallel p(z)] \right\}. \tag{9}$$

The first term on the right side quantifies the reconstruction quality and the second term is the Kullback-Leibler divergence measuring the difference between the two distributions.

In adversarial autoencoders, an adversarial training procedure instead of the Kullback-Leibler divergence is used to encourage an aggregated posterior distribution $q(z)$, instead of $q(z|x)$, to match $p(z)$, where $q(z)$ is defined as (Makhzani et al., 2016)

$$q(z) = \int_{x} q(z|x)p_{\text{data}}(x)dx. \tag{10}$$

An illustration of the adversarial autoencoder is depicted in Figure 2a. In the encoding path, the input $x$ is fed into the encoder which outputs two low-dimensional vectors of
means $\mu$ and log-variances $\ln(\sigma^2)$ of the latent variables $z$. Then randomly draw a vector of normally distributed variables $z' \sim \mathcal{N}(0, 1)$ of the same size as $\mu$ and $\sigma$ and rescale it to produce the codes $z = \mu + \sigma \times z'$, where $\times$ denotes element-wise multiplication. The decoder takes $z$ as input to eventually generate $\hat{x}$. Meanwhile, the discriminator of the adversarial network accepts input from the hidden codes generated by the encoder or the prespecified distribution $p(z)$ to discriminatively predict whether the input arises from the encoding codes (fake sample) or $p(z)$ (real sample). Note that the adversarial network here differs slightly from the vanilla GAN framework (Goodfellow et al., 2014), in which the generator generates the sample $x$, and the discriminator discriminates $x$ whether it is from the generator or the data.

Figure 2: (a) Illustration of a convolutional adversarial autoencoder (CAAE), which is composed of a discriminator (b), an encoder (generator) (c), and a decoder (d). The discriminator is a stack of two convolutional layers followed by two fully-connected (FC) layers with 128 and 1 neurons, respectively. The feature map size is halved in Conv ($\nabla$) with a stride of 2 in the discriminator and encoder, and doubled in the decoder by using the nearest upsampling (UP) operation.

The encoder (which is also the generator $G(\cdot)$ of the adversarial network), decoder, and discriminator $D(\cdot)$ of the adversarial autoencoder are trained jointly in two phases for each iteration: the reconstruction phase and the regularization phase (Makhzani et al., 2016). In the reconstruction phase, the encoder (generator) and decoder are updated using the following loss function:

$$L_{ED} = L_{Rec} + wL_G,$$

where $L_{Rec}$ is the reconstruction error which in this study is taken as the $L_1$ loss:

$$L_{Rec} = \frac{1}{N} \sum_{i=1}^{N} ||x_i - \hat{x}_i||_1,$$

and $L_G$ measures the generator’s ability to fool the discriminator and has the form

$$L_G = -\frac{1}{N} \sum_{i=1}^{N} \log \{D[G(x_i)]\}.$$

Here, $w$ is a weight factor balancing the two losses and a value of $w = 0.01$ is used, $\hat{x}_i$ is the reconstruction of sample $x_i$, and $N$ is the number of training samples. In the regularization phase, the discriminator is updated based on the loss function

$$L_D = -\frac{1}{N} \sum_{i=1}^{N} \left\{ \log [D(z_i)] + \log [1 - D[G(x_i)]] \right\}.$$
to distinguish the true sample from $p(z)$ (i.e. $z_i$) from the fake sample $G(x_i)$ produced by the generator.

Such adversarial training process with loss functions defined in equations (11) and (14) forces $\hat{x}$ to closely match $x$ and $q(z)$ to gradually approach $p(z)$ (i.e., $\mu \to 0$ and $\sigma^2I \to I$), respectively. After training, the decoder will define a generative model $p(x)$ that given an arbitrary input $z \sim N(0, I)$ can generate a new realization of sample $\hat{x}$ with features similar to those in the data used for training (Figure 2d).

### 3.3.3 CAAE Networks Based on Residual-in-Residual Dense Blocks

We also adopt the residual-in-residual dense block structure shown in Figure 1b in the encoder and decoder of the CAAE network. The encoder (Figure 2c) is similar to the coarsening part of the DRDCN network (Figure 1c). The encoder has two additional convolutional layers to respectively output the means $\mu$ and log-variances $\ln(\sigma^2)$. The decoder (Figure 2d) is similar to the refining part of the DRDCN network. The decoder has an additional convolutional layer to extract feature maps from the codes $z$. Inspired by Ledig et al. (2017), the discriminator is a stack of two convolutional layers followed by two fully-connected layers with 128 and 1 neurons, respectively. The leaky ReLU with a slope of 0.2 is used as the activation function in the discriminator and the sigmoid activation function is used in the last layer to output a probability value between 0 and 1.

### 3.4 The CAAE-DRDCN-ILUES inversion framework

We incorporate the CAAE parameterization method and the DRDCN surrogate method into ILUES to formulate an efficient inversion scheme for estimation of the non-Gaussian conductivity field of solute transport models. The integrated methodology is denoted as CAAE-DRDCN-ILUES hereinafter and is summarized in Algorithm 2. Notice that in this method, the surrogate model is used in Algorithms 1 and 2 to substitute the forward model. After parameterization, the uncertain parameters to be estimated are the latent variables $z$. The log-conductivity field is estimated with the following procedure: (1) start with an initial latent code ensemble drawn from $N(0, I)$, (2) the corresponding log-conductivity fields are generated next using the CAAE’s decoder, (3) the surrogate model is evaluated to obtain the predicted output ensemble, (4) the latent code ensemble is updated using Algorithm 1 based on the current latent code and output ensembles. Steps (2) – (4) are repeated for $N_{iter}$ iterations and the posterior log-conductivity fields are obtained from the decoder using the last latent code ensemble as the input.

### 4 Application

#### 4.1 Solute Transport Models

The performance of the proposed method is illustrated using 2-D and 3-D solute transport models with random conductivity fields that have non-Gaussian heterogeneity patterns.

##### 4.1.1 2-D Model

The first test case considers 2-D solute transport within a channelized aquifer. As shown in Figure 3a, the horizontal domain has a size of $10 \times 20$ (L) and is uniformly discretized into $H \times W = 40 \times 80 = 3,200$ gridblocks. The left and right boundaries are assumed to be constant head boundaries with heads of 1 (L) and 0 (L), respectively. No boundary conditions are imposed on the upper and lower boundaries. An instantaneous source with a concentration of $100$ (M/L$^{-3}$) is released from the location $x = 3$ (L) and $y = 5$ (L) at the initial time. The porosity and dispersivities are assumed to be known with constant values of $\phi = 0.25$, $\alpha_L = 1.0$ (L) and $\alpha_T = 0.1$ (L), respectively.
Algorithm 2 The CAAE-DRDCN-ILUES inversion framework for estimation of the conductivity field \( x \). The log-conductivity field realizations are generated using the CAAE’s decoder given the latent variables \( z \) as input. CAAE: convolutional adversarial autoencoder. DRDCN: deep residual dense convolutional network. ILUES: iterative local updating ensemble smoother.

Require: Measurements \( d \), iteration number \( N_{\text{iter}} \), ensemble size \( N_e \), trained decoder, trained DRDCN.
1: Generate the initial input ensemble \( Z^0 = [z_1^0, \ldots, z_{N_e}^0] \) from \( \mathcal{N}(0, I) \).
2: for \( n = 0, \ldots, (N_{\text{iter}} - 1) \) do \( \triangleright \) Iterative data assimilation
3: \hspace{1em} Given \( Z^n \), generate the log-conductivity field ensemble \( \hat{X}^n = [\hat{x}_1^n, \ldots, \hat{x}_{N_e}^n] \) via \( \hat{x}_i^n = \text{decoder}(z_i^n) \).
4: \hspace{1em} Obtain the output ensemble \( \hat{D}^n = [\hat{f}(\hat{x}_1^n), \ldots, \hat{f}(\hat{x}_{N_e}^n)] \) via \( \hat{f}(\hat{x}_i^n) = \text{DRDCN}(\hat{x}_i^n) \).
5: \hspace{1em} Update input ensemble \( Z^{n+1} = [Z_1^{n+1}, \ldots, Z_{N_e}^{n+1}] \) based on \( \{Z^n, \hat{D}^n, d\} \) using Algorithm 1.
6: end for
7: \( \hat{X}^{N_{\text{iter}}} = [\hat{x}_1^{N_{\text{iter}}}, \ldots, \hat{x}_{N_e}^{N_{\text{iter}}}] \), where \( \hat{x}_i^{N_{\text{iter}}} = \text{decoder}(z_i^{N_{\text{iter}}}) \).
8: return \( \hat{X}^{N_{\text{iter}}} \) \( \triangleright \) The final log-conductivity field ensemble

The non-Gaussian conductivity field in this case has a channelized and bimodal pattern with heterogeneous conductivity within each facies. The conductivity realizations are generated by the following procedure: First, a binary facies field is generated using the SNESIM code (Strebelle, 2002) with a training image shown in Figure 3c; then we populate each facies with log-conductivity values from two independently generated Gaussian random fields with a \( L_2 \) norm exponential covariance function:

\[
C(s, s') = \sigma_K^2 \exp \left( -\sqrt{\frac{(s_1 - s_1')^2}{\lambda_1^2} + \left(\frac{s_2 - s_2'}{\lambda_2^2}\right)^2} \right),
\]

where \( s = (s_1, s_2) \) and \( s' = (s_1', s_2') \) denote two arbitrary spatial locations, \( \sigma_K^2 \) is the variance, and \( \lambda_1 \) and \( \lambda_2 \) are the correlation lengths along the \( x \)– and \( y \)–axes, respectively. The means of Gaussian random fields corresponding to the high-conductivity channels and the low-conductivity non-channel medium are 4 and 0, respectively, while their variances and correlation lengths are taken the same with \( \sigma_K^2 = 0.5 \), \( \lambda_1 = 4 \) (L), and \( \lambda_2 = 2 \) (L). The CAAE network with 200 latent codes is employed as the parameterization framework for the log-conductivity field.

4.1.2 3-D Model

The second test case considers solute transport in a 3-D confined aquifer with a size of \( 1.5 \) (L) \( \times \) \( 10 \) (L) \( \times \) \( 20 \) (L) as depicted in Figure 3d. The domain is uniformly discretized into \( D \times H \times W = 6 \times 32 \times 64 = 12,288 \) gridblocks. Similar to the 2-D case, the left and right boundaries are assumed to be constant head boundaries with heads of 1 (L) and 0 (L), respectively. No boundary conditions are imposed on the boundaries in the direction perpendicular to the \( y \)-axis. An instantaneous source with a concentration of 100 (M/L⁻³) is released from the location \( x = 3 \) (L) and \( y = 5 \) (L) at the initial time. The porosity and dispersivities are assumed to be known with constant values of \( \phi = 0.25 \), \( \alpha_L = 1.0 \) (L), \( \alpha_T = 0.1 \) (L), and \( \alpha_R = 0.01 \) (L), respectively. The conductivity fields for this 3-D model are obtained by randomly cropping \( 6 \times 32 \times 64 \) patches from a \( 120 \times 180 \times 150 \) training image depicted in Figure 3e (available at http://www.trainingimages.org/training-images -library.html). The conductivity heterogeneity pattern is different from that in the 2-D channelized field in the sense that the distribution of log-conductivities in this training image is trimodal with two major peaks around 1.0 and 3.0 and one minor peak around \(-0.6\)
Figure 3: Reference log-conductivity conductivity fields of the 2-D (a) and 3-D (d) solute transport models considered in the inverse problems. The diamond and 24 circles represent the projections of the solute source and observation locations, respectively, in the horizontal plane. Histograms of the log-conductivities in (a) and (d) are shown in (b) and (f), respectively. (c) A $250 \times 250$ training image used to generate 2-D binary facies fields. (e) A $120 \times 180 \times 150$ training image used to generate 3-D log-conductivity fields. (g) Histogram of the log-conductivities in (e).

(Figure 3g). The CAAE network with 256 latent codes is employed as the parameterization framework for the log-conductivity field.

### 4.2 Synthetic Observations

As it will be shown in section 5.1, the CAAE-generated conductivity fields have higher regularity/smoothness than the original fields. In the inverse problem, the synthetic observations were obtained by running the forward model with an original conductivity field
rather than a smoothed conductivity field generated by CAAE. The generation of synthetic observations here aims to mimic a real scenario, where data would be obtained by field measurements. The randomly generated 2-D and 3-D reference log-conductivity fields are depicted in Figures 3a and 3d, respectively. Note that they are distinct from the training conductivity samples of CAAE and DRDCN networks. The two reference fields are both non-Gaussian with a bimodal distribution (the 2-D case, Figures 3b) and a trimodal distribution (the 3-D case, Figures 3f), respectively. In the 2-D case, the concentration at \( t = [3, 5, 7, 9, 11] \) (T) and the hydraulic head are collected at 24 measurement locations (Figure 3a), resulting in 144 observations. In the 3-D case, the concentration at \( t = [4, 6, 8] \) (T) and the hydraulic head are collected at six depths of 24 measurement locations (Figure 3d), resulting in 576 observations. The synthetic observations were corrupted with 5\% independent Gaussian random noise to the data generated by the reference model. Additionally, we do not use any conditioning data (i.e., measurements) of the conductivity resulting in a rather challenging inverse problem.

4.3 Networks Design and Training

4.3.1 CAAE Network Design and Training

The architecture of the CAAE network is shown in Figure 2 and detailed in section 3.3.3. The encoder includes two downsampling layers which halves the feature map size via convolution with a stride of 2. Correspondingly, the two upsampling layers in the decoder double the feature map size to recover the output image size. The network consists of 71 layers, including 69 convolutional layers (mostly arising from the four residual-in-residual dense blocks that each contains 15 convolutional layers) and 2 fully-connected layers (in the discriminator). The kernel size in all convolutional layers is 3, and the stride in the convolutional layers that keep the same feature map size is 1 and in those that halve the size is 2.

In the 2-D case, a training set with 40,000 realizations of the log-conductivity field is generated to train the CAAE network. We also generate another 4,000 test realizations to evaluate the network’s performance. In the 3-D case, we generate the log-conductivity realizations by cropping the 120 \( \times \) 180 \( \times \) 150 training image shown in Figure 3e. The training image is flipped along the three axes to augment the data, resulting in four training images. We obtain 43,500 patches with a size of 6 \( \times \) 32 \( \times \) 64 via cropping the training images using a stride of (2, 6, 10). We use 40,000 samples to train the network and the remaining 3,500 samples as the test data. The loss functions for network training are defined in equations (11) and (14). The network is trained on a NVIDIA GeForce GTX 1080 Ti X GPU for 50 epochs using the Adam optimizer (Kingma & Ba, 2014) with a learning rate of \( 2 \times 10^{-4} \) and a batch size of 64.

4.3.2 DRDCN Network Design and Training

The architecture of the DRDCN network is shown in Figure 1 and detailed in section 3.2.2. The network is fully-convolutional and contains 64 convolutional layers without any fully-connected layers. Similar to the CAAE network, the kernel size in all convolutional layers is 3, and the stride in the convolutional layers that keep the same feature map size is 1 and in those that halve the size is 2. The softplus activation function is used in the output layer for the concentration to ensure nonnegative predictions. Since the hydraulic head varies between 0 and 1 in both cases, the sigmoid activation function is used in the output layer for the hydraulic head.

The concentration at different time steps (i.e., \( t = [3, 5, 7, 9, 11] \) (T) and \( t = [4, 6, 8] \) (T) in the 2-D and 3-D cases, respectively) and the hydraulic head are collected as the observations in the inverse problem. Thus, the concentration fields at the these time steps and the hydraulic head field are treated as the output channels of the network. There is one
single input channel to the network which is the original log-conductivity field generated by following the procedure presented in section 4.1. In both cases, we generate four training sets with \( N = 1,000, 2,000, 3,000, \) and \( 4,000 \) training samples to evaluate the convergence of the network approximation error with respect to the training sample size. The approximation accuracy is assessed using \( N_{\text{test}} = 1,000 \) randomly generated test samples. The accuracy is measured using the coefficient of determination \( (R^2) \) and the root-mean-square error (RMSE) which are defined as

\[
R^2 = 1 - \frac{\sum_{i=1}^{N_{\text{test}}} ||y_i - \hat{y}_i||_2^2}{\sum_{i=1}^{N_{\text{test}}} ||y_i - \bar{y}||_2^2},
\]

and

\[
\text{RMSE} = \sqrt{\frac{1}{N_{\text{test}}} \sum_{i=1}^{N_{\text{test}}} ||y_i - \hat{y}_i||_2^2},
\]

respectively, where \( y \) denotes the simulated outputs and \( \hat{y} \) is the corresponding network predictions. A \( R^2 \) score value approaching 1.0 and a lower RMSE value suggest better surrogate quality.

The network is trained using a regularized \( L_1 \) norm loss function:

\[
\mathcal{L} = \frac{1}{N} \sum_{i=1}^{N} ||y_i - \tilde{y}_i||_1 + \frac{w_d}{2} \theta^\top \theta,
\]

where \( \theta \) denotes all the network trainable parameters and \( w_d = 1 \times 10^{-5} \) is a regularization coefficient. The network is trained on a NVIDIA GeForce GTX 1080 Ti X GPU for 200 epochs in the 2-D case and 300 epochs in the 3-D case using the Adam optimizer (Kingma & Ba, 2014) with an initial learning rate of \( 5 \times 10^{-3} \) and a batch size of 32. We also use a learning rate scheduler which drops ten times on plateau during training.

5 Results and Discussion

In this section, we first illustrate the performance of the CAAE and DRDCN networks in parameterization of non-Gaussian random fields and in surrogate modeling of the solute transport models, respectively. After that, the inversion results obtained from the CAAE-DRDCN-ILUES framework are compared to those obtained from the CAAE-ILUES framework without surrogate modeling.

5.1 Parameterization of Non-Gaussian Random Fields

The CAAE network’s parameterization results for the 2-D and 3-D non-Gaussian log-conductivity fields are shown in Figure 4. It depicts the CAAE’s reconstructions of three log-conductivity realizations in the test set, the corresponding histograms of the latent codes, and three random log-conductivity fields generated by the decoder with inputs from \( \mathcal{N}(\mathbf{0}, \mathbf{I}) \). In the reconstruction process, the original log-conductivity realization is fed to the encoder to produce latent codes, based on which the reconstructed field is generated by the decoder. It is observed that, in both 2-D and 3-D cases with different heterogeneity patterns, the network successfully recovers the spatial distributions of the low-conductivity and high-conductivity regions as well as the conductivities within these regions; although the conductivity heterogeneity is smoothed compared to the original fields. The encoding latent codes roughly follow the prior distribution \( \mathcal{N}(\mathbf{0}, \mathbf{I}) \) that we imposed during training. The \( R^2 \) scores evaluated on the test samples are 0.945 and 0.877 in the 2-D and 3-D cases, respectively. The fourth row of Figures 4a and 4b shows the random log-conductivity fields generated by the decoder. The results show that the decoder is able to reproduce log-conductivity realizations that depict similar patterns of heterogeneity (e.g., the channel structures and the conductivity continuity within the low/high-conductivity regions) to
those found in the training data. Therefore, the CAAE network is employed in the inversion process as the parameterization framework for the non-Gaussian conductivity fields.

5.2 Surrogate Quality Assessment

To illustrate the superior performance of the proposed DRDCN network architecture against the DDCN network architecture employed in our previous studies (Mo, Zabaras, et al., 2019; Mo, Zhu, et al., 2019; Zhu & Zabaras, 2018; Zhu et al., 2019) for surrogate
modeling of systems with highly-complex input and output fields, the DDCN network is also trained using the same training sets as those used in DRDCN. The DDCN network architecture is introduced in Appendix A.

The two networks’ approximation accuracy for the 2-D and 3-D solute transport models is provided in Figure 5, which depicts the RMSEs and $R^2$ scores evaluated on the test sets. It can be seen that DRDCN achieves lower RMSEs and higher $R^2$ scores than DDCN when being trained using the same four training sets in both cases. For example, with 4,000 training samples, our network achieves a RMSE of 0.017 and a $R^2$ score of 0.966, while those obtained by the DDCN network are 0.024 and 0.933, respectively. This implies that the DRDCN network can obtain accurate surrogates with fewer training samples (forward model runs) than the DDCN network. For instance, the 2-D DRDCN surrogate with 2,000 training samples obtains similar approximation accuracy with the DDCN surrogate with 4,000 training samples. The saved number of training samples indicates substantial computational gains especially for computationally intensive forward models in subsurface modeling where one single model execution can take up to hours or even days. The DRDCN network’s predictions for the output fields of 2-D and 3-D models given randomly selected input conductivity fields in the test sets are illustrated in Figures 6 and 7, respectively. For comparison, the predictions by the forward models and network approximation errors are also shown in each plot. It is observed that although the output fields are highly irregular with sharp response changes, our network is able to obtain good approximations in both cases.

It is worth noticing that the DRDCN network achieves higher accuracy improvement compared to the DDCN network in the 2-D case than in the 3-D case (Figure 5). The low-conductivity regions are barriers for groundwater flow and solute transport, leading to irregular output fields. In comparison to the 2-D log-conductivity fields which are mainly composed of low-conductivity regions (Figure 3c), the facies with the minimum average log-conductivity in the trimodal 3-D fields (i.e., the blue regions in Figure 3e) is only a small proportion of the aquifer as indicated in Figure 3g. The small proportion of low-conductivity regions in the 3-D fields thus results in relatively smoother output fields than those of the 2-D model. As a consequence, the DDCN network can also obtain a relatively accurate surrogate of the 3-D model, although its approximation error is larger than that of the DRDCN network. However, its performance greatly decreases in the 2-D model with more complex output fields. The results clearly suggest that the proposed DRDCN network.
performs better than the DDCN network in obtaining accurate surrogate results for the solute transport models with high-dimensional and highly-complex input and output fields. The improvement is attributed to the deeper network architecture with the help of the multilevel residual learning (Wang et al., 2018) and residual scaling technique (Szegedy et al., 2016). In addition, the dense connection structure (Huang et al., 2017) stabilized the training while contributing to improved accuracy. With a relatively small number of training samples, the DRDCN network is able to provide good approximations of the 2-D and 3-D forward models. Thus, it is used together with the CAAE parameterization strategy in the ILUES inverse method to formulate an efficient inversion framework for estimation of the non-Gaussian conductivity field of solute transport models.

### 5.3 Inversion Results

In both 2-D and 3-D cases, the DRDCN surrogates trained with 4,000 forward model runs are used to substitute the forward models in the CAAE-DRDCN-ILUES inversion framework. To assess the accuracy and computational efficiency of the surrogate-based
method, the CAAE-ILUES method which evaluates the forward model rather than the surrogate model during the inversion is also performed. The ensemble size of the ILUES algorithm is set to \( N_e = 2,000 \) and \( N_e = 3,000 \) in the 2-D and 3-D cases, respectively, to fully quantify the parametric uncertainty. The observations are assimilated for \( N_{\text{iter}} = 30 \) iterations in the 2-D case and 20 iterations in the 3-D case. That is, the number of forward model runs required in CAAE-ILUES for the 2-D and 3-D cases are \( 31 \times 2,000 = 62,000 \) (i.e., one prior ensemble and \( N_{\text{iter}} \) updated ensembles) and \( 21 \times 3,000 = 63,000 \), respectively.

The posterior conductivity fields are then obtained from the CAAE’s decoder given the final latent code ensemble as input (Algorithm 2).

We first evaluate the performance of the CAAE-ILUES since we will take its results as the reference solution to compare with the results obtained from the CAAE-DRDCN-ILUES. The convergence of the fitting error between the forward model outputs and measurements as the iteration proceeds is shown in Figure 8, where the mismatch is measured using the normalized sum of squared weighted residuals (NSSWR):

\[
NSSWR = \frac{1}{SSWR_{\text{ref}} \times N_d} \sum_{i=1}^{N_d} \left( \frac{f_i(\hat{x}) - d_i}{\sigma_i} \right)^2,
\]

(19)

where \( \{d_i\}_{i=1}^{N_d} \) denote the measurements that contain measurement errors with standard deviations \( \{\sigma_i\}_{i=1}^{N_d} \), and \( \{f_i(\hat{x})\}_{i=1}^{N_d} \) are the forward model predictions given the input \( \hat{x} \) which is generated by the decoder. Here the \( SSWR \) metric is normalized using the reference value \( SSWR_{\text{ref}} \). Thus, a \( NSSWR \) value approaching 1.0 suggests the convergence of the inversion process. As discussed in sections 4.2 and 5.1, the reference conductivity field has high heterogeneity versus the smoothed CAAE-parameterized field realizations \( \hat{x} \). As a consequence, in the inversion process the \( NSSWR \) values are not able to converge to the reference \( NSSWR \) value (i.e., 1.0) due to the conductivity smoothness in the CAAE-generated samples. This can be seen in Figure 8 where although the \( NSSWR \) values in the ensemble approximately converge in both cases, the converged values are slightly larger than 1.0. Our tests showed that the \( NSSWR \) values were not able to converge asymptotically to 1.0 even when we increased the number of iterations in ILUES.
Two posterior log-conductivity realizations, the ensemble mean, and ensemble standard deviation of the CAAE-ILUES method for the two cases are illustrated in Figure 9. The reference fields and the locations of the output measurements collected to infer the conductivity field are also shown in the plot to facilitate the comparison. It can be seen that in both cases the CAAE-ILUES can successfully capture the spatial distribution of the high-conductivity and low-conductivity regions as well as the conductivities within these regions. Due to the relatively sparse measurements (i.e., only 24 observation wells are placed in the domain with thousands of gridblocks), the local conductivity heterogeneity and the location of the boundaries between high-conductivity and low-conductivity regions may not be accurately retrieved. As expected, the conductivity estimation in regions where no information is collected is less accurate with a larger estimation uncertainty than the estimation near the output measurement locations. The results imply that the CAAE-ILUES algorithm performs well for this inverse problem but needs a large number (i.e., 62,000 in the 2-D case and 63,000 in the 3-D case) of forward model evaluations. We show next the results of CAAE-DRDCN-ILUES in which the DRDCN surrogate models trained with 4,000 forward model runs are used to substitute the 2-D and 3-D forward models. Two posterior log-conductivity realizations, the ensemble mean, and ensemble standard deviation for the same reference fields as in CAAE-ILUES are shown in the third row of Figures 9a (2-D case) and 9b (3-D case). Similarly, it can be seen that in both cases the surrogate-based framework successfully identified the high-conductivity and low-conductivity regions as well as the conductivities within these regions. The comparably accurate results suggest that the surrogate-based CAAE-DRDCN-ILUES framework effectively relieves the large computational burden of CAAE-ILUES in many repeated forward model runs, greatly improving the computational efficiency of the inversion process.

Figures 10 and 11 show the output ensemble mean and standard deviation estimates of the CAAE-ILUES and CAAE-DRDCN-ILUES methods for the 2-D and 3-D models, respectively. The reference output fields and the observation locations are also shown to facilitate the analysis of results. Notice that the statistics of the surrogate-based method are computed using the outputs predicted by the surrogate model rather than the forward model. It can be observed that the CAAE-DRDCN-ILUES method achieves similar ensemble mean estimates to those of the CAAE-ILUES method which successfully reproduce the main patterns of the reference output fields in the two cases. Similar to the estimation of the conductivity field, a higher reproduction accuracy and a lower estimation uncertainty are observed near the observation wells than those in regions where no information is collected.
The results presented above indicate that the CAAE network is able to reconstruct well the non-Gaussian conductivity fields with different heterogeneity patterns and therefore the CAAE-ILUES method can obtain good inversion results for the 2-D and 3-D solute transport models with different conductivity heterogeneity patterns. However, for the two high-dimensional and highly-nonlinear inverse problems considered here, more than 60,000 forward model runs are needed in each case, leading to a high computational cost. The comparably accurate inversion results and predictive uncertainty estimations of the CAAE-DRDCN-ILUES framework to those of the CAAE-ILUES method suggest that the surrogate method essentially relieves this computational burden. The cost savings are brought by the incorporation of the fast-to-run DRDCN surrogate into the CAAE-ILUES method that replaces the accurate but computationally expensive forward model in the inversion process.

6 Conclusions

In this study, we propose an integrated inversion framework for efficient characterization of solute transport in continuous non-Gaussian conductivity fields. In the proposed
Figure 10: Ensemble mean and standard deviation (Std) of the concentration fields at \( t = \{3, 7, 11\} \) (T; a-c) and hydraulic head field (d) of the 2-D model obtained from CAAE-ILUES (Mean\[y\], Std\[y\]) and CAAE-DRDCN-ILUES (Mean\[\hat{y}\], Std\[\hat{y}\]). \( y_{ref} \) denotes the output fields of the reference model with the log-conductivity field shown in Figure 3a. The circles denote the measurement locations.

framework, a CAAE network is developed for parameterization of the conductivity field using a low-dimensional latent representation. In addition, a DRDCN network is developed for surrogate modeling of the solute transport model with high-dimensional and highly-complex output fields. The two networks are combined with the ILUES inversion method proposed in J. Zhang et al. (2018) to formulate the CAAE-DRDCN-ILUES inversion framework. To improve the networks’ performance for approximating the highly-complex mappings in the problems considered, in both network architectures, we adopt a multilevel residual learning structure referred to as residual-in-residual dense block (Wang et al., 2018). The residual learning structure can help stabilize the training of deep networks. The dense block introduces dense connections between nonadjacent layers to encourage the information propagation through the network so as to alleviate the data-intensive deep network training. As a result, the implementation of the residual-in-residual dense block structure in the two networks allows a large network depth which has the potential to substantially increase the network’s capability to approximate highly-complex mappings. The two proposed networks can be flexibly generalized to 2-D and 3-D forward models without requiring any additional modifications to the network architecture.

The performance of the proposed method is evaluated using 2-D and 3-D solute transport models with continuous non-Gaussian conductivity fields that have different patterns of conductivity heterogeneity. The results indicate that the CAAE is capable of representing the non-Gaussian conductivity fields using a low-dimensional latent variable. The DRDCN network shows a superior performance over the DDCN network proposed in our previous studies (Mo, Zabaras, et al., 2019; Mo, Zhu, et al., 2019; Zhu & Zabaras, 2018; Zhu et al., 2019) in obtaining accurate surrogate models. The residual-in-residual dense block structure greatly improves the network’s capacity in approximating highly-complex...
Figure 11: Ensemble mean and standard deviation (Std) of the concentration fields at $t = [4, 6, 8]$ (T; a-c) and hydraulic head field (d) of the 3-D model obtained from CAAE-ILUES (Mean[$\mathbf{y}$], Std[$\mathbf{y}$]) and CAAE-DRDCN-ILUES (Mean[$\hat{\mathbf{y}}$], Std[$\hat{\mathbf{y}}$]). $y_{\text{ref}}$ denotes the output fields of the reference model with the log-conductivity field shown in Figure 3d. The circles denote the projections of the measurement locations on the horizontal plane.

mappings. The application of the CAAE-DRDCN-ILUES method for estimation of the 2-D and 3-D non-Gaussian conductivity fields shows that it can obtain comparably accurate inversion results and predictive uncertainty estimations to those obtained by the original inverse method without surrogate modeling. The integrated method is highly efficient since the training of the surrogate model requires only a small number of forward model runs. The solute transport models considered in this work are relatively fast in order to quickly test the proposed method in a reasonable time. When applying to computationally more intensive models, significant computational gains can be expected. The CAAE parameterization method and the DRDCN surrogate method are both data-driven and forward model independent. Therefore, even if not considered or demonstrated herein, the CAAE method can be potentially applied to the parameterization of non-Gaussian random fields with other different heterogeneity patterns; the DRDCN method can be potentially applied to many complex systems beyond groundwater solute transport to achieve increased computational efficiency.

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this work will be made available at https://github.com/cics-nd/CAAE-DRDCN-inverse upon publication of this manuscript.

Appendix

A Deep dense convolutional network

The deep dense convolutional network (DDCN) for surrogate modeling (Mo, Zabaras, et al., 2019; Mo, Zhu, et al., 2019; Zhu & Zabaras, 2018; Zhu et al., 2019) is based on a dense connection structure called dense block (Huang et al., 2017). The dense block introduces connections between its internal nonadjacent layers to enhance the information propagation through the network for better parameter efficiency, so as to reduce the training sample size required to obtain desired approximation accuracy (Huang et al., 2017). An illustration of the dense block structure is shown in Figure 1a. The only difference between the dense blocks used in the DDCN network and in the DRDCN network proposed in this study is that, in DDCN, the input feature maps of the dense block’s last layer are concatenated to its output feature maps to be fed into the next layer; while in DRDCN only the output feature maps of the dense block are passed to the next layer to allow an element-wise addition operation in the residual learning strategy (see section 3.2.1). As a result, feature map explosion will take place in DDCN as the network depth increases.

We adopt the DDCN network architecture employed in our previous study (Mo, Zabaras, et al., 2019) which was used for surrogate modeling of a 2-D solute transport model with Gaussian conductivity fields. The network is composed of 27 convolutional layers with three dense blocks. For the 3-D case considered in this study, we directly replace the 2-D convolutional layers in the network with the 3-D convolutional layers. More details about the network architecture can be found in Mo, Zabaras, et al. (2019). When training the DDCN network, we use the same settings as in the DRDCN network. That is, the network is trained on a NVIDIA GeForce GTX 1080 Ti X GPU using the \( L_1 \) norm loss function defined in equation (18) for 200 epochs in the 2-D case and 300 epochs in the 3-D case with the Adam optimizer (Kingma & Ba, 2014). The batch size is 32 and the initial learning rate is \( 5 \times 10^{-3} \). A learning rate scheduler which drops ten times on plateau during training is used. Python codes of DDCN are available at https://github.com/cics-nd/cnn-inversion.

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