Using Deep Learning to Improve Ensemble Smoother: Applications to Subsurface Characterization

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Key Points:

• Ensemble smoother using the Kalman formula makes Gaussian assumptions
• We use deep learning to formulate a new variant of ensemble smoother
• The new method can produce better results in problems involving non-Gaussian distributions

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Abstract

Ensemble smoother (ES) has been widely used in various research fields to reduce the uncertainty of the system-of-interest. However, the commonly-adopted ES method that employs the Kalman formula, that is, ES\(^{(K)}\), does not perform well when the probability distributions involved are non-Gaussian. To address this issue, we suggest to use deep learning (DL) to derive an alternative update scheme for ES in complex data assimilation applications. Here we show that the DL-based ES method, that is, ES\(^{(DL)}\), is more general and flexible. In this new update scheme, a high volume of training data are generated from a relatively small-sized ensemble of model parameters and simulation outputs, and possible non-Gaussian features can be preserved in the training data and captured by an adequate DL model. This new variant of ES is tested in two subsurface characterization problems with or without Gaussian assumptions. Results indicate that ES\(^{(DL)}\) can produce similar (in the Gaussian case) or even better (in the non-Gaussian case) results compared to those from ES\(^{(K)}\). The success of ES\(^{(DL)}\) comes from the power of DL in extracting complex (including non-Gaussian) features and learning nonlinear relationships from massive amounts of training data. Although in this work we only apply the ES\(^{(DL)}\) method in parameter estimation problems, the proposed idea can be conveniently extended to analysis of model structural uncertainty and state estimation in real-time forecasting studies.

1 Introduction

Numerical models have been widely used in science and engineering to gain a better understanding of the concerned process(es), and to help hypothesis testing and decision making. In many research fields of geosciences, complexity of the system-of-interest makes accurate predictions in both the space and time domain very challenging (Baartman et al., 2020; Kavetski et al., 2006a, 2006b; Refsgaard et al., 2012; Ruddell et al., 2019). This is largely caused by our incomplete knowledge and insufficient observations of the system. To improve our predictive ability and scientific understanding of the system, it is important to combine the numerical model (i.e., the theory) with observations, which can be realized through data assimilation (DA; Carrassi et al., 2018; Evensen, 2009). DA is usually carried out in the following way. At any update time, one first makes a forecast from the background information. The forecasted variables can be the initial/boundary conditions, parameters, states, model errors, or their combinations (Carrassi et al., 2018; Chen & Zhang, 2006; Dechant & Moradkhani, 2011; Evensen, 2009, 2019; Q. Zhang et al., 2019). Then one calculates the difference (which is usually called the innovation) between the observations and the corresponding model outputs mapped from the forecast with a linear/nonlinear operator. The innovation vector provides new information, based on which update (or correction) to the forecast can be made.

Theoretically, one can view DA from a Bayesian perspective. However, fully Bayesian DA methods, such as particle filter (PF; Doucet et al., 2000; Moradkhani et al., 2005), although very general, can be computationally prohibitive for high-dimensional problems. When the probability distributions are assumed Gaussian, that is, the update is only based on the mean and covariance, DA can be implemented efficiently. Among various DA methods, ensemble Kalman filter (EnKF) proposed by Evensen (1994) might be the most popular one. EnKF is a Monte Carlo implementation of Kalman filter (Kalman, 1960) to perform sequential DA. When one’s purpose is parameter estimation, it will be more convenient to perform a global update using all observations available, instead of applying the sequential update scheme of EnKF. In this case, a variant of EnKF, that is, ensemble smoother (ES; van Leeuwen & Evensen, 1996), can be implemented. It has been shown that, ES can obtain similar results to EnKF, but with a much lower computational cost (Li et al., 2018; Skjervheim & Evensen, 2011). When the system is highly nonlinear, iterative applications of both EnKF and ES are needed (Chen & Oliver, 2012; Emerick & Reynolds, 2012, 2013; Gu & Oliver, 2007; Lorentzen & Naevdal, 2011). In the past decades, EnKF and its variants have been extensively used in various research fields of geosciences.
Nevertheless, in many situations, distributions of parameters, states, and/or measurement errors can be obviously non-Gaussian (Mandel & Beezley, 2009; Schoups & Vrugt, 2010; Sun et al., 2009; Zhou et al., 2011). Then the direct use of an ensemble Kalman-based method, for example, EnKF or ES, becomes inappropriate. To address this issue, different strategies have been proposed. For example, when the probability distribution is multi-modal, one can first turn the forecast ensemble into several clusters, and each cluster can be roughly approximated by a Gaussian distribution and updated with an ensemble Kalman-based method (Bengtsson et al., 2003; Dovera & Rossa, 2011; Elsheikh et al., 2013; Sun et al., 2009; J. Zhang et al., 2018); Some other researchers suggested to re-parameterize non-Gaussian variables (e.g., conductivity field in a channelized aquifer) to be Gaussian distributed with anamorphosis function (Schöniger et al., 2012; Simon & Bertino, 2009), level set (Chang et al., 2010), or normal-score transformation (Li et al., 2011, 2018; Xu & Gómez-Hernández, 2016; Zhou et al., 2011), etc., so that EnKF or its variants can be properly implemented; Another kind of approaches first use an ensemble Kalman-based method to update the forecast ensemble, and then use, for example, multiple-point geostatistics (Cao et al., 2018; Jafarpour & Khodabakhshi, 2011; Kang et al., 2019; Sarma et al., 2008), or a more general DA method like PF (Mandel & Beezley, 2009), to reconstruct the non-Gaussian target distributions. Note, that although the above mentioned strategies worked well in different applications, they have not changed the DA methods that were used. In other words, the DA methods are still constrained by the Gaussian assumption, and these strategies either apply some pre-treatment to fulfill this assumption, or use some post-treatment to fix the DA results.

In this work, we are trying to propose a new DA method that is free from the Gaussian assumption, and at the same time keeps the computational cost for high-dimensional problems relatively low. To realize this goal, let’s first go back to the general process of DA that has been demonstrated earlier. Essentially, DA works by updating (or correcting) the forecast from the innovation (i.e., the difference between observations and the corresponding model outputs). In the ensemble Kalman-based methods, a linear mapping from the innovation vector to the update vector is calculated from the forecast ensemble using the Kalman formula. This mapping, usually called the Kalman gain, only uses the first two statistical moments. Then it is natural to wonder whether we can obtain a more general, and possibly nonlinear mapping to update the forecast ensemble. In the past years, machine learning, especially deep learning (DL), has been extensively used in different fields, including hydrology and water resources, to extract complex patterns and nonlinear relationships from data (Goodfellow et al., 2016; Lecun et al., 2015; Shen, 2018; Shen et al., 2018). It has motivated us to reformulate DA, especially the ensemble Kalman-based methods, through obtaining a possibly nonlinear mapping from the innovation vector to the update vector with DL. Now one question naturally arises, that is, how can we generate a high volume of training data that are usually required to feed a DL model, when a large number of system model evaluations are not affordable? To address this issue, we come up with a simple solution. In the forecast ensemble with $N_e$ samples of model parameters and simulation outputs, if we pick out one arbitrary sample as the hypothetical truth, and generate synthetic observations by perturbing the “true” model outputs with random errors, we can obtain $N_e - 1$ pairs of innovation and update vectors. From the basic theory of combination, overall we can generate training data with $C(N_e, 2) = N_e(N_e - 1)/2$ unique samples for DL. In the $C(N_e, 2)$ samples, non-Gaussian features of model parameters and measurement data can be preserved in the synthetic innovation and update vectors, and captured with an adequate DL model. Finally, we can input the real $N_e$ innovation vectors from the forecast ensemble to the learned mapping with DL, and obtain the $N_e$ update vectors to correct our forecast.

In this work, to verify the validity of the proposed idea, we use DL to improve ES, and test the resulting ES(DL) method in two subsurface characterization problems with or without Gaussian assumptions. In subsurface characterization, DL has been used as a powerful tool to address a wide range of challenges. For example, DL can be used to effectively reduce the dimensionality of model parameters (Laloy et al., 2017), or quickly generate ran-
dom realizations of geological formations from training data (e.g., image data; Laloy et al., 2018), both of which can improve the performance of geostatistical inversion; To alleviate the high computational cost caused by repetitive evaluations of complex, high-dimensional groundwater models, DL-based surrogates have been built and used in uncertainty quantification and data assimilation of subsurface systems (Mo, Zhu, et al., 2019; Mo, Zabaras, et al., 2019; Tripathy & Bilionis, 2018); When physical laws are preserved when training a DL model, a better performance of the resulting surrogate can be expected (Wang & Lin, 2020); Besides constructing a forward mapping from parameters to states as a surrogate model, Sun (2018) also identified a reverse mapping from states to parameters. For more applications of DL in hydrology and water resources, one can refer to (Shen, 2018; Shen et al., 2018). To our best knowledge, using DL to reformulate an ensemble Kalman-based method like ES is quit new and this idea has not been implemented before.

The rest of this paper is organized as follows. In section 2, we first introduce how to implement ES using the Kalman formula, that is, ES\( (K) \), to estimate unknown model parameters from indirect measurement data. In light of the limitations of ES\( (K) \), we then propose a more general method, ES\( (DL) \), that uses DL to learn and extract (possibly) nonlinear update scheme and non-Gaussian features. To verify the performance of ES\( (DL) \), two cases of subsurface characterization with or without Gaussian assumptions are tested in section 3. Here we are concerned with benchmarking analysis of the two ES methods. Finally, in section 4, we conclude this paper and discuss the pros and cons of the new method.

2 Methods

Let us assume that the system-of-interest is simulated by a numerical model \( f(\cdot) \), and this process can be expressed in the following compact form,

\[
\tilde{y} = f(m) + \epsilon,
\]

where \( \tilde{y} \in \mathbb{R}^{N_y \times 1} \) are the observations of the system, \( m \in \mathbb{R}^{N_m \times 1} \) are the model parameters, and \( \epsilon \in \mathbb{R}^{N_y \times 1} \) are the error term. In subsurface characterization, the model parameters include the spatial/temporal distribution of contaminants and/or subsurface properties, which are generally difficult or even impossible to be measured directly. Meanwhile, observations of some state variables, such as hydraulic head, solute concentration, temperature, and electromagnetic signals, can be monitored continuously and affordably. These observations, that is, \( \tilde{y} \), contain information about the unknown model parameters, \( m \). To improve our knowledge of \( m \), we can perform data assimilation conditioned on these measurement data.

2.1 Ensemble Smoother Using the Kalman Formula: ES\( (K) \)

As an efficient and robust data assimilation method, EnKF has been extensively used in various research fields to reduce the uncertainty of the system-of-interest (Evensen, 2009). When one’s purpose is parameter estimation, a variant of EnKF, that is, ES, can be adopted as a suitable method (van Leeuwen & Evensen, 1996). Below we will introduce how to implement ES that uses the Kalman formula, that is, ES\( (K) \), to estimate the unknown model parameters, \( m \), from indirect measurement data, \( \tilde{y} \).

Here, a prior distribution, \( p(m) \), is used to represent our background knowledge of the values of \( m \). From \( p(m) \) we can draw \( N_e \) random samples to form the forecast (or prior) ensemble, that is, \( M^{(0)} = \{m^{(0)}_1, ..., m^{(0)}_{N_e}\} \). Then we calculate the corresponding model outputs by running the numerical model, that is, \( Y^{(0)} = \{f(m^{(0)}_1), ..., f(m^{(0)}_{N_e})\} \). Using the ES\( (K) \) method, we can update each sample, \( m^{(0)}_i \), \( i = 1, ..., N_e \), in the forecast ensemble, \( M^{(0)} \), conditioned on the measurement data, \( \tilde{y} \).

\[
m^{(1)}_i = m^{(0)}_i + C^{(0)}_{MY} (C^{(0)}_{YY} + R)^{-1} \left[ \tilde{y} + \epsilon - f(m^{(0)}_i) \right],
\]

where \( Y^{(0)} \) and \( \tilde{y} \) are the model outputs and observations, respectively, \( R \) is the measurement error covariance matrix, and \( C^{(0)}_{MY} \) is the cross-covariance matrix between the model outputs and measurements.
where \( M^{(1)} = \{ m_1^{(1)}, ..., m_{N_e}^{(1)} \} \) is the updated ensemble, \( C_{MV}^{(0)} \) is the cross-covariance matrix between model parameters and outputs (calculated from \( M^{(0)} \) and \( Y^{(0)} \)), \( C_{YY}^{(0)} \) is the auto-covariance matrix of model outputs (calculated from \( Y^{(0)} \)), and \( \epsilon_i \) is a random realization of measurement error with covariance \( R \). In \( ES_{(K)} \), the update is essentially linear, and the distributions of model parameters and measurement data should be close to Gaussian. At this point the applicability of \( ES_{(K)} \) is limited.

### 2.2 Using Deep Learning to Improve Ensemble Smoother: \( ES_{(DL)} \)

In the past few years, DL has been extensively used to learn complex patterns and nonlinear relationships from data. The general applicability of DL has motivated us to reformulate the update scheme of ES to make it more capable. The new ES method is termed \( ES_{(DL)} \). Nowadays, a plenty of powerful DL architectures have been proposed by the machine learning communities. Here we are only left with choosing which relationship to learn and how to generate enough data to train the DL model. As the theory of DL itself is not the focus of this work, we decide not to provide the details below. Interested readers are suggested to refer to (Goodfellow et al., 2016; Lecun et al., 2015). Moreover, architectures of DL models that are used in this work will be given in section 3.

Let’s rewrite equation (2) in a more general form,

\[
\Delta m_i = G(\Delta y_i),
\]

where \( \Delta m_i = m_i^{(1)} - m_i^{(0)} \) is the update vector, \( \Delta y_i = \hat{y} + \epsilon_i - f(m_i^{(0)}) \) is the innovation vector, and \( G \) is a mapping from \( \Delta y_i \) to \( \Delta m_i \). In \( ES_{(K)} \), \( G \) is defined by the Kalman gain matrix, \( K = C_{MV}^{(0)} \left( C_{YY}^{(0)} + R \right)^{-1} \). Thus, the relationship between \( \Delta y_i \) and \( \Delta m_i \) is linear. Here we aim to use DL to derive a (possibly) nonlinear mapping, \( G_{DL} \), from \( \Delta y_i \) to \( \Delta m_i \).

It is evident that the input data of \( G_{DL} \) are the displacement vector in model simulations (corrupted by some error), and the outputs are the corresponding distance in the parameter space. Based on this finding, we can generate a high volume of training data from the forecast ensemble, \( \{ M^{(0)} \ Y^{(0)} \} \). In \( \{ M^{(0)} \ Y^{(0)} \} \), if we take two samples at a time without repetition, there will be \( N = N_e(N_e - 1)/2 \) combinations in total. That is to say, we can obtain \( D_{in}^{(0)} = \{ f(m_i^{(0)}) - f(m_j^{(0)}) + \epsilon_{ij} | i = 1, ..., N_e - 1, i < j \leq N_e \} \) as the inputs to the DL model, and \( D_{out}^{(0)} = \{ m_i^{(0)} - m_j^{(0)} | i = 1, ..., N_e - 1, i < j \leq N_e \} \) as the output data, where \( \epsilon_{ij} \) are random realizations of the measurement error. Here, non-Gaussian features in the model parameters and observations can be preserved in the training data, \( D^{(0)} = \{ D_{in}^{(0)} \ D_{out}^{(0)} \} \), and captured by the DL model. When the evaluation of \( f(\cdot) \) is time-consuming, one usually can only afford a limited number of model runs (e.g., \( N_e = 200 \)). In this case, the number of samples in \( D^{(0)} \) is still considerable (\( N = 19,900 \)).

After training, the (possibly) nonlinear mapping \( G_{DL} \) can be obtained. Then we can use \( G_{DL} \) to update each sample, \( m_i^{(0)} \), \( i = 1, ..., N_e \), in the forecast ensemble, \( M^{(0)} \), conditioned on the measurement data, \( \hat{y} \);

\[
m_i^{(1)} = m_i^{(0)} + G_{DL} \left[ \hat{y} + \epsilon_i - f(m_i^{(0)}) \right].
\]

Then we use the updated ensemble, \( M^{(1)} = \{ m_1^{(1)}, ..., m_{N_e}^{(1)} \} \), to represented our new knowledge of the model parameters.

For highly nonlinear problems, one single update of the model parameters with \( ES_{(K)} \) or \( ES_{(DL)} \) may not be sufficient. Here, we suggest to adopt the multiple data assimilation scheme proposed by Emerick and Reynolds (2013) to address this issue. In this scheme, the measurement data are assimilated \( N_{iter} \) times. To make sure that the finally obtained results are reasonable, the measurement error (including the corresponding covariance matrix \( R \) if used) should be inflated by a factor of \( \alpha_t \) (for \( R \) the factor is the square of \( \alpha_t \)) in iteration.
Figure 1. (a) Schematic overview of the flow domain in the first case study. Here an unknown point source is located somewhere in the light red rectangle, and measurements of hydraulic head and solute concentration are collected at 15 wells denoted by the blue circles. (b) The reference log-conductivity (log $K$) field. (c-f) Mean estimations of the log $K$ field and the associated standard deviation (std) fields obtained by ES$_{(DL)}$ and ES$_{(K)}$, respectively.

$t$, for $t = 1, \ldots, N_{\text{iter}}$. The factors should satisfy $\sum_{t=1}^{N_{\text{iter}}} 1/(\alpha_t)^2 = 1$, and a convenient choice is $\alpha_t = \sqrt{N_{\text{iter}}}$. The update scheme for ES$_{(K)}$ becomes,

$$m_i^{(t)} = m_i^{(t-1)} + \mathbf{C}^{(t-1)}_{\mathbf{MY}} \left[ \mathbf{C}^{(t-1)}_{YY} + (\alpha_t)^2 \mathbf{R} \right]^{-1} \left[ \tilde{y} + \alpha_t \epsilon_i - f(m_i^{(t-1)}) \right].$$

(5)

In ES$_{(DL)}$, we first generate training data from $\{M^{(t-1)} Y^{(t-1)}\}$ as, $\mathbf{D}_\text{in}^{(t)} = \{f(m_i^{(t-1)}) - f(m_j^{(t-1)}) + \alpha_t \epsilon_{ij} | i = 1, \ldots, N_e - 1, \; i < j \leq N_e\}$, and $\mathbf{D}_\text{out}^{(t)} = \{m_i^{(t-1)} - m_j^{(t-1)} | i = 1, \ldots, N_e - 1, \; i < j \leq N_e\}$. Then a mapping, $\mathcal{G}_\text{DL}^{(t)}$, is learned from $\{\mathbf{D}_\text{in}^{(t)}, \mathbf{D}_\text{out}^{(t)}\}$ with DL. Finally, each sample in the forecast ensemble is updated as,

$$m_i^{(t)} = m_i^{(t-1)} + \mathcal{G}_\text{DL}^{(t)} \left[ \tilde{y} + \alpha_t \epsilon_i - f(m_i^{(t-1)}) \right].$$

(6)

For both ES$_{(K)}$ and ES$_{(DL)}$, our final knowledge of the model parameters is represented by $\mathbf{M}^{(N_{\text{iter}})} = \{m_1^{(N_{\text{iter}})}, \ldots, m_{N_e}^{(N_{\text{iter}})}\}$.

3 Illustrative Case Studies

3.1 Example 1: A Gaussian Case

In this section, we aim to demonstrate that when the variables involved are near Gaussian-distributed, ES$_{(DL)}$ can obtain very similar estimation of unknown model parameters as ES$_{(K)}$. Here, we consider a highly nonlinear inverse problem where the parameters
describing the hydraulic conductivity field and an unknown contaminant source are to be inferred from measurements of hydraulic head and solute concentration.

In this case, steady-state groundwater flow and transient solute transport are considered in a two-dimensional, heterogeneous, and confined aquifer. As shown in Figure 1a, the flow domain is 20 (L) × 10 (L) (in units of length), and uniformly discretized into 81 × 41 grids in the model. The left and right sides of the domain are prescribed by constant head conditions of 12 (L) and 11 (L), respectively, while the upper and lower boundaries are impervious. At the initial time, the hydraulic head is 11 (L) everywhere in the domain, except for the left boundary. The hydraulic conductivity (K) is heterogeneous and isotropic, and its logarithmic form, \( Y = \log(K) \), is Gaussian-distributed and spatially correlated according to the following covariance function,

\[
C_{Y}(x_1, y_1; x_2, y_2) = \sigma^2_y \exp \left( -\frac{|x_1 - x_2|}{\lambda_x} - \frac{|y_1 - y_2|}{\lambda_y} \right),
\]

where \( \{x_1, y_1\} \) and \( \{x_2, y_2\} \) are two arbitrary locations in the domain, \( \sigma^2_Y \) is the variance of the \( Y \) field, and \( \lambda_x \) and \( \lambda_y \) are the correlation lengths in the horizontal (x) and vertical (y) direction, respectively. The reference, or “true” log-conductivity field is depicted in Figure 1. With the above model settings, we can obtain steady-state hydraulic head, \( h \) (L), by solving

\[
\frac{\partial}{\partial x_i} \left( K \frac{\partial h}{\partial x_i} \right) = 0,
\]

and obtain the pore water velocity, \( v_i \) (LT\(^{-1}\)), by solving

\[
v_i = -\frac{K_i}{\theta} \frac{\partial h}{\partial x_i},
\]

numerically with MODFLOW (Harbaugh et al., 2000). Here, \( \theta (-) \) is the aquifer porosity, and the subscript \( i \) denotes the coordinate axis (\( i = 1 \) is for the x direction, and \( i = 2 \) is for the y direction).

In the flow domain, there is a point source that releases some non-reactive contaminant to the downstream. The contaminant source is located somewhere in the light red rectangular in Figure 1a. Its release strength varies with time and is characterized by a step function in Figure 1a. The contaminant source is located in the light red rectangular, and its release strength varies with time and is characterized by a step function in Figure 1a. Its release strength varies with time and is characterized by a step function. The release strength varies with time and is characterized by a step function. The release strength varies with time and is characterized by a step function. The release strength varies with time and is characterized by a step function. The release strength varies with time and is characterized by a step function. The release strength varies with time and is characterized by a step function. The release strength varies with time and is characterized by a step function. The release strength varies with time and is characterized by a step function. The release strength varies with time and is characterized by a step function. The release strength varies with time and is characterized by a step function. The release strength varies with time and is characterized by a step function.

By numerically solving the following advection-dispersion equation,

\[
\frac{\partial(\theta C)}{\partial t} = \frac{\partial}{\partial x_i} \left( \theta D_{ij} \frac{\partial C}{\partial x_i} \right) - \frac{\partial}{\partial x_i} (\theta v_i C) + q_a C_s,
\]

with MT3DMS (Zheng & Wang, 1999), we can obtain simulated concentrations, \( C \) (ML\(^{-3}\)), at different times and places. Here, \( q_a \) (T\(^{-1}\)) is the volumetric flow rate per unit volume of the aquifer, \( C_s \) (ML\(^{-3}\)) denotes the concentration of the contaminant source, and \( D_{ij} \) (L\(^2\)T\(^{-1}\)) signifies the hydrodynamic dispersion tensor that is composed of

\[
\begin{align*}
D_{11} &= \frac{1}{\|v\|} (\alpha_L v_i^2 + \alpha_T v_2^2), \\
D_{22} &= \frac{1}{\|v\|} (\alpha_L v_2^2 + \alpha_T v_1^2), \\
D_{12} &= D_{21} = \frac{1}{\|v\|} (\alpha_L - \alpha_T) v_1 v_2,
\end{align*}
\]

where \( \alpha_L \) and \( \alpha_T \) (L) represent the longitudinal and transverse diversity, respectively, and \( \|v\| = \sqrt{v_1^2 + v_2^2} \) is the magnitude of the velocity vector, \( v \).

In this case, the uncertainty comes from the heterogeneous \( Y \) field and the unknown contaminant source. To reduce the dimensionality of the \( Y \) field, the truncated Karhunen-Loève (KL) expansion (D. Zhang & Lu, 2004) is used to represent the \( Y \) field, that is,

\[
\tilde{Y}(x) = \mu_Y + \sum_{n=1}^{N_{KL}} \sqrt{\tau_n} s_n(x) \xi_n,
\]
Table 1. Prior ranges and true values of the eight contaminant source parameters in the first numerical experiment.

| Parameter | $x_s$ | $y_s$ | $s_1$ | $s_2$ | $s_3$ | $s_4$ | $s_5$ | $s_6$ |
|-----------|-------|-------|-------|-------|-------|-------|-------|-------|
| Prior range | [3-5] | [4-6] | [0-8] | [0-8] | [0-8] | [0-8] | [0-8] | [0-8] |
| True value | 3.52  | 4.44  | 5.69  | 7.88  | 6.31  | 1.49  | 6.87  | 5.55  |

Figure 2. (a-b) Two residual (Res) blocks containing three kinds of layers, that is, one-dimensional convolution layer (Conv1), batch normalization layer (BN), and ReLU activation layer (ReLU). In Res Block 1, the channels of input are scaled down before adding ($\oplus$) to the output, while in Res Block 2 the channels of input keep unchanged. (c) The overall architecture (ResNet) of the deep learning model used in the first case study. Here FC means a fully-connected layer.

where $x = \{x, y\}$ is the location, $\mu_Y$ denotes the mean of the $Y$ field, $\tau_n$ and $s_n(x)$ signify the eigenvalues and eigenfunctions of the covariance defined in equation (7), for $n = 1, ..., N_{KL}$, and $\xi_n \sim \mathcal{N}(0, 1^2)$ represent the KL expansion terms. Here, $N_{KL} = 100$ KL terms are kept, which can preserve about 95% of the total field variance, that is, $\sum_{n=1}^{N_{KL}} \tau_n / \sum_{n=1}^{\infty} \tau_n \approx 0.95$.

The contaminant source is parameterized by eight variables, that is, its location, $\{x_s, y_s\}$, and time-varying source strengths, $\{s_1, ..., s_6\}$. The prior distributions of the eight source parameters are uniform and bounded by the ranges as listed in Table 1. Thus, there are 108 unknown parameters to be estimated in this case, that is, $m = \{\xi_1, ..., \xi_{100}, x_s, y_s, s_1, ..., s_6\}$. Other model parameters are obtained from experiments and geological surveys as $\sigma_Y^2 = 1$, $\lambda_x = 10$ (L), $\lambda_y = 5$ (L), $\mu_Y = 2$, $\theta = 0.25$ (-), $\alpha_L = 0.3$ (L), and $\alpha_T = 0.03$ (L), respectively.

To infer the 108 unknown model parameters, steady-state hydraulic heads, and transient solute concentrations at $t = \{4, 5, ..., 12\}$ (T), are collected at 15 wells denoted by the blue circles in Figure 1a. The measurements are generated by running the integrated model (MODFLOW+MT3DMS) with the reference log-conductivity field (Figure 1b) and contaminant source parameters (the last row of Table 1), and adding independent normal random perturbations that satisfy, $\epsilon_h \sim \mathcal{N}(0, 0.005^2)$ and $\epsilon_C \sim \mathcal{N}(0, 0.005^2)$. Then we implement the ES$_K$ and ES$_{DL}$ methods respectively to estimate the unknown model parameters conditioned on the measurement data. As the problem tested here is rather nonlinear, we perform multiple data assimilation ($N_{iter} = 5$) in the two ES methods. At first, a same
forecast (or prior) ensemble \((N_e = 500)\) is generated from the prior parameter distribution for the two methods, \(\mathbf{M}^{(0)} = \{ \mathbf{m}^{(0)}_1, ..., \mathbf{m}^{(0)}_{N_e} \}\), and the corresponding model outputs are calculated by running the numerical model, \(\mathbf{Y}^{(0)} = \{ f(\mathbf{m}^{(0)}_1), ..., f(\mathbf{m}^{(0)}_{N_e}) \}\).

In each iteration of ES\((DL)\), a same DL architecture as shown in Figure 2 is adopted. In iteration \(t (1 \leq t \leq N_{\text{iter}})\), to train the DL model, a set of data with \(N = N_e(N_e - 1)/2\) samples, that is, \(\mathbf{D}^{(t)} = \{ \mathbf{D}^{(t)}_{\text{in}}, \mathbf{D}^{(t)}_{\text{out}} \}\), are generated from \(\{ \mathbf{M}^{(t-1)} \mathbf{Y}^{(t-1)} \}\). Here, \(\mathbf{D}^{(t)}_{\text{in}} = \{ f(\mathbf{m}^{(t-1)}_i) - f(\mathbf{m}^{(t-1)}_j) + \alpha t \epsilon_{ij} | i = 1, ..., N_e - 1, \ i < j \leq N_e \}\) are the input data, \(\mathbf{D}^{(t)}_{\text{out}} = \{ \mathbf{m}^{(t-1)}_i - \mathbf{m}^{(t-1)}_j | i = 1, ..., N_e - 1, \ i < j \leq N_e \}\) are the output data, \(\alpha t\) is an inflation factor that can be conveniently set as \(\sqrt{N_{\text{iter}}}\), and \(\epsilon_{ij}\) are random realizations of the measurement error. Here, to sufficiently extract features embedded in the training data \(\mathbf{D}^{(t)}\), we employ the residual network (ResNet) proposed by He et al. (2016). By doing so, we can build a very deep network without worrying about the trouble caused by gradient vanishing. As shown in Figure 2c, the overall architecture of DL is composed of two kinds of residual blocks (Res Block 1 in Figure 2a and Res Block 2 in Figure 2b) and a fully-connected (FC) layer. The difference between Res Block 1 and Res Block 2 lies in that the number of channels in the former block is scaled down, while in the latter block the number of channels is unchanged. In this case, the numbers of channels are designed as \(C_1 = 150, C_2 = 140, C_3 = 130, C_4 = 120,\) and \(C_5 = 108\), respectively. The kernel and strides sizes are both set as 1. The Adam optimizer (Kingma & Ba, 2014) with a learning rate of \(3 \times 10^{-3}\) is utilized to train the network.

After five iterations, both ES\((K)\) and ES\((DL)\) can significantly improve our knowledge of the subsurface medium and contaminant source. As shown in Figures 1(c-d), both methods can reliably identify the regions with high and low values of (log) conductivity. Yet the two estimated mean fields tend to slightly underestimate the \(\mathcal{Y}\) field, that is, Figures 1(c-d) are bluer while less redder than the reference field of Figure 1b. We think it is because the measurement data contain insufficient information about the \(\mathcal{Y}\) field. Figures 1(e-f) present the standard deviation (std) fields associated with the mean estimates. It can be found that

Figure 3. Marginal distributions of the eight contaminant source parameters obtained by ES\((DL)\) (red lines) and ES\((K)\) (blue dashed lines), respectively. The true values of the eight parameters are denoted by the vertical black lines.
the area where measurement wells have been installed exhibits smaller std values, and the results from ES(DL) have smaller variations than that of ES(K). In Figure 3, we draw the marginal densities of the eight contaminant source parameters from the updated ensemble in the last iteration, that is, $M^{N_{iter}} = \{m_1^{N_{iter}}, ..., m_{N_{iter}}\}$. Here, we use red lines and blue dashed lines to represent the results from ES(DL) and ES(K), respectively. Compared to the prior ranges as listed in Table 1, the ranges covered by the marginal densities are much smaller, which indicates a substantial reduction of uncertainty in our belief about the model parameters. Moreover, the true parameter values (vertical black lines) generally locate at the centers of the marginal density curves, which indicates the accuracy of the estimation results.

So in conclusion, the two ES methods can obtain reliable and comparable estimations of the log-conductivity field and unknown contaminant source parameters. If a more diverse and larger data set is collected, and/or a more suitable DL architecture is designed, the ES(DL) method should be able to produce better results.

3.2 Example 2: A Non-Gaussian Case

Previously, we have tested a case where the distributions of variables involved are close to multi-Gaussian, and ES(DL) can produce similar results as ES(K). Nevertheless, it will be more interesting to test a case where ES(K) can not work satisfactorily, while the performance of ES(DL) still holds. In subsurface characterization, much research has shown that when the parameter field of interest does not follow a multi-Gaussian distribution, the direct use of an ensemble Kalman-based method, for example, EnKF and ES(K), can not produce satisfactory results (Cao et al., 2018; Chang et al., 2010; Xu & Gómez-Hernández, 2016; Zhou et al., 2011). Below we will test such a case where sparse measurements of hydraulic head are used to characterize a non-Gaussian conductivity field, and the performances of ES(DL) and ES(K) are compared.

In this case, we consider transient water flow in a two-dimensional, confined, and channelized aquifer. The size of the domain is $l_x = l_y = 800$ (L) in units of length in the $x$ and $y$ direction. This square domain is uniformly discretized into $41 \times 41$ grids. In the flow field, impervious condition is prescribed at both the upper and lower boundaries, and constant heads of 202 (L) and 198 (L) are imposed at the left and right sides, respectively. At the initial time, the hydraulic head is 198 (L) across the domain except for the left boundary. To enhance water flow in the subsurface medium, an injection well (the blue down-pointing triangle in Figure 4a) with a rate of 150 (L$^3$T$^{-1}$) and a pumping well (the blue up-pointing triangle in Figure 4a) with a rate of -150 (L$^3$T$^{-1}$) are installed. In the channelized field, there are two kinds of materials: one with a low conductivity value of $K_1 = 0.5$ (LT$^{-1}$), and another with a higher value of $K_2 = 2.3$ (LT$^{-1}$). The reference $\mathcal{K}$ field (Figure 4c) is generated from a training image (Figure 4b) using the direct sampling (DS) method proposed by Mariethoz et al. (2010). Here, when applying the DS method, no direct observation of $\mathcal{K}$ is used for conditioning. The DS method is computationally efficient, and has the ability to handle both continuous and categorical variables with complex features. Thus, it is adopted in this work to perform multiple-point statistics simulations to generate the reference, as well as random realizations of non-Gaussian $\mathcal{K}$ field. Details of the DS method can be found in (Mariethoz et al., 2010; Meerschman et al., 2013). With the above model settings, one can obtain transient hydraulic heads at different locations, $h(x, t)$ (L), by solving

$$S_s \frac{\partial h(x,t)}{\partial t} + \nabla \cdot q(x,t) = g(x,t)$$

numerically with MODFLOW (Harbaugh et al., 2000). In equation (13), $S_s$ (L$^{-1}$) is the specific storage, $x = \{x, y\}$ (L) is the location, $t$ (T) is the time, $q(x,t) = -\mathcal{K}(x)\nabla h(x,t)$ is the flux, $\mathcal{K}(x)$ (LT$^{-1}$) is the conductivity value at location $x$, and $g(x,t)$ (T$^{-1}$) is the source (or sink) term of water. Here, the total simulation time is 18 (T), and $S_s$ is a deterministic constant of 0.0001 (L$^{-1}$).
Figure 4. (a) Schematic overview of the flow domain for the second case study. Here the injection well is denoted by the blue down-pointing triangle, the pumping well is represented by the blue up-pointing triangle, and measurements of hydraulic head are collected at wells signified by the 7×7 red circles. (b) The training image used in performing the direct sampling method. (c) The reference conductivity ($K$) field. (d-h) Mean estimations of the $K$ field and their associated standard deviations from the prior ensemble and the updated ensembles obtained by $\text{ES}_{(DL)}$ and $\text{ES}_{(K)}$, respectively.
To infer the $K$ field, we collect measurements of hydraulic head at 49 wells denoted by the red circles in Figure 4a, every 0.6 (T) from $t = 0$ (T) to $t = 6$ (T). The measurements are generated by running the numerical model with the reference $K$ field (Figure 4c) and adding perturbations that fit $\epsilon \sim N(0, 0.01^2)$. For both the ES(DL) and ES(K) methods, a same set of $N_e = 499$ prior random realizations of channelized field, that is, $M(0) = \{m_1^{(0)}, ..., m_{N_e}^{(0)}\}$, are generated using the DS method based on the training image (Figure 4b). By averaging these $N_e$ realizations, we can obtain a rather uniform prior mean field (Figure 4d) with grid values close to 0.98, the mean value of the training image (averaged over each grid). The associated standard deviation (std, Figure 4g) field also exhibits a small spatial variability, and has values close the standard deviation (0.80) of the training image. Through running the numerical model, we can obtain the corresponding model outputs, that is, $Y(0) = \{f(m_1^{(0)}), ..., f(m_{N_e}^{(0)})\}$.

Figure 4f presents the mean $K$ field estimated by the ES(K) method. As the problem considered here is rather linear, it is not necessary to perform multiple data assimilation, that is, here we set $N_{iter} = 1$. It is obvious that ES(K) can capture some features of the true $K$ field through assimilating indirect measurements of transient hydraulic head. Moreover, the std field calculated from the updated ensemble (Figure 4i) has much smaller values than the prior std field (Figure 4g). Nevertheless, the connectivity pattern of the ES(K)-estimated mean field is underestimated. In Figure 5a, we draw the histogram of the mean $K$ field of ES(K) (blue bars). As the true $K$ field only has two distinct materials, ideally, the histogram should be bimodal. However, ES(K) fails to recover this bi-modality.

Then we apply the ES(DL) method to estimate the $K$ field. Without extra evaluations of the numerical model, a set of training data, $D^{(0)} = \{D^{(0)}_{in}, D^{(0)}_{out}\}$, can be generated from the forecast ensemble, $\{M(0) Y(0)\}$. Here, $D^{(0)}_{in} = \{f(m_i^{(0)}) - f(m_j^{(0)}) + \epsilon_{ij}|i = 1, ..., N_e - 1, i < j \leq N_e\}$ are the input data, $D^{(0)}_{out} = \{m_i^{(0)} - m_j^{(0)}|i = 1, ..., N_e - 1, i < j \leq N_e\}$ are the output data, and $\epsilon_{ij}$ are random realizations of the measurement error. A better update scheme is expected to be learned for ES from the training data $D^{(0)}$ with an adequate DL model. When designing the DL architecture, we recast the original input-output mapping as an image-to-
Figure 6. (a) A dense block with three layers, each of which performs three operations sequentially, that is, batch normalization (BN), ReLU activation, and two-dimensional convolution (Conv). Here the feature maps (i.e., the outputs) of each layer will be concatenated with their corresponding inputs. (b) A transition block used to reduce both the number of channels and the size of feature maps. (c) A transition block used to reduce the number of channels but increase the size of feature maps by using transpose convolution (ConvT). (d) The overall architecture (DenseNet) of the deep learning model used in the second case study. Here FC and Tanh mean a fully-connected layer and a Tanh activation layer, respectively.
image translation problem, which is tackled by the popular DenseNet architecture (Huang et al., 2017). As shown in Figure 6d, the overall architecture of DenseNet is composed of an encoder, a decoder, and some other necessary layers. The encoder aims to discover low-dimensional embeddings of the input image, while the decoder maps the embeddings to the output image. The encoder and decoder are composed of three kinds of basis blocks as shown in Figures 6(a-c). The dense block (Figure 6a) is a concatenation of previous feature maps. In this case, the dense block contains three layers that perform batch normalization (BN), ReLU activation, and two-dimensional convolution (Conv) sequentially. Specifically, the Conv operation is realized by a kernel of size $3 \times 3$ with strides of 1 and a padding of 1. As a result, the dense block produces outputs with channels four times as many as that in the inputs, while the size of feature maps keeps unchanged. To adjust the size of feature maps, two kinds of transition blocks are further employed, that is, the down block (Figure 6b) and the up block (Figure 6c). The two blocks both contain two convolution layers. The first convolution layers in the two blocks work in the same way that uses a $1 \times 1$ kernel with strides of 2. However, their second convolution layers are implemented differently in that the down block utilizes a $3 \times 3$ kernel with strides of 2 and a padding of 1 for downsampling, while the up block uses a kernel of the same size to perform transpose convolution (ConvT) for upsampling. Overall, as shown in Figure 6d, the input data are first processed by a fully-connected (FC) layer to obtain image-like data of size $H \times W$, and then go to the BN-Conv layers, the encoder-decoder blocks, and finally a Tanh activation layer to produce the output data. In this case, $H = W = 41$, the number of channels after the FC layer is $N_c = 40$, and after the decoder block the number of channels is $N_c = 1$. The Adam optimizer with a learning rate of $1 \times 10^{-3}$ is utilized to train the network.

As shown in Figure 4e, the mean conductivity field estimated by ES(DL) better resembles the reference $K$ field. Although the std field of ES(DL) has slightly larger values than the std field of ES(K), the channelized features are better revealed in Figure 4h. Moreover, the histogram of the mean $K$ field of ES(DL) (red bars, Figure 5a) can clearly recover the bimodality of the channelized field, although the update of $K_1$ is slightly overestimated, while the update of $K_2$ is slightly underestimated. Thus, we believe that ES(DL) can better handle non-Gaussian parameter field than ES(K). In Figure 5b, we draw the root-mean-square error (RMSE) of the MODFLOW simulated and observed hydraulic heads for each sample in the updated ensembles of ES(DL) (red line) and ES(K) (blue line). It again demonstrates the superiority of ES(DL) to ES(K). If a better DL architecture is designed, a more accurate update of the parameter field can be obtained by the ES(DL) method.

4 Discussion and Conclusions

Due to their efficiency and robustness, EnKF and its variants have been used in various research fields, including meteorology, oceanography, hydrology, and petroleum engineering, to reduce the uncertainty of the system-of-interest. When one’s purpose is parameter estimation, for example, in subsurface characterization, ES can be adopted as a feasible method. Nevertheless, when the distributions of variables involved are non-Gaussian, the performances of these ensemble Kalman-based methods will deteriorate. To enable proper applications of these methods, existing strategies mainly transform non-Gaussian variables to be normally distributed (Zhou et al., 2011; Chang et al., 2010; Canchumuni et al., 2019), or use another method, for example, clustering analysis, or a more general DA method like particle filter, to handle non-Gaussianity (Cao et al., 2018; Sun et al., 2009; Mandel & Beezley, 2009).

Alternatively, we propose in this work to use DL to reformulate the update scheme of ES to gain an improved performance. In this new method, that is, ES(DL), we first generate a high volume of training data from a relatively small-sized forecast ensemble. Possible non-Gaussian features in model parameters and observations are incorporated in the training data and captured by an adequate DL model. Then we use this DL-based formulation to update the forecast ensemble to reduce the uncertainty of model parameters. For highly
nonlinear problems, an iterative application of ES is needed, for example, using the multiple data assimilation scheme formulated by Emerick and Reynolds (2013). To demonstrate the performance of the proposed method, two cases of subsurface characterization are tested against the traditional ES method using the Kalman formula, that is, ES\(_{(K)}\). In the first case study, using measurements of hydraulic head and solute concentration, we aim to simultaneously identify the location and release history of a point contaminant source, and the heterogeneous log-conductivity field. Here, there are 108 unknown parameters to be estimated, whose distributions are all close to Gaussian. With the same number of numerical model evaluations, the ES\(_{(DL)}\) method produces similar results to those from ES\(_{(K)}\). In the second case study, a channelized conductivity field parameterized by 1681 variables is to be estimated from observations of transient hydraulic head. Simulation results clearly indicate that, in this non-Gaussian case, ES\(_{(DL)}\) is superior to ES\(_{(K)}\).

The general applicability of ES\(_{(DL)}\) comes from the powerful ability of DL in extracting complex (including non-Gaussian) features and learning nonlinear relationships automatically from data. The DL architecture is very flexible and can be adapted to a wide range of problems. Without running a large number of system models, one can create massive amounts of training data and feed them to the DL model. Another merit of DL is that it can perform massively parallel computations on GPUs. Thus, the ES\(_{(DL)}\) method can be possibly applied to large-scale DA problems. Nevertheless, limitations of the proposed method do exist. First, the choice of a DL architecture for ES\(_{(DL)}\) is relatively subjective (although flexible), and its outputs are difficult to comprehend. It is true that one can learn from literature to configure an adequate DL model, and different DL models can possibly all produce satisfactory results. However, there is no standard guidelines to determine the optimal DL architecture for a specific problem. On the contrary, the Kalman formula used in ES\(_{(K)}\) can be expressed explicitly, and it is optimal at least for linear, Gaussian cases. From the theoretical perspective, ES\(_{(K)}\) is more elegant than ES\(_{(DL)}\). Second, although the ES\(_{(DL)}\) method requires a same number of system model evaluations as ES\(_{(K)}\), the training of a DL model can be time consuming, especially when GPU devices are not available. Moreover, in this work, we only apply the new idea in parameter estimation problems. We believe that one can easily extend the DL-based idea to state estimations for real-time forecasting. Recently, model structural uncertainty has been accounted for in the application of various iterative ES methods (Evensen, 2019), which is important to prevent unphysical updates. In future works, it will be interesting to use the DL-based formula to update model parameters, states and structural errors simultaneously.

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