

COMODCoordenação de Modelagem Computacional

Relatório de Atividades

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1 Introdution

1.1 MCMC

In 2000, Computing in Science & Engineering, a joint publication of the IEEE Computer Society and the American Institute of Physics, placed the Metropolis Algorithm on the list of the 10 algorithms with the greatest impact on the development of science and engineering practice in the 20th century ("Top Ten Algorithms of the Century" (Madey et al., 2005)).

1.2 Random permeability fields

Due to incomplete knowledge about the rock properties that show variability at multiple length scales, input parameters such as the permeability field, $\kappa(\mathbf{x},\omega)$, are treated as random space functions with statistics inferred from geostatistical models (here $\mathbf{x}=(x_1,x_2,x_3)^{\mathsf{T}}\in\mathbb{R}^3$ and ω is a random element in the probability space). In line with Dagan (1989) and Gelhar (1993) the permeability field is modeled as a log-normally distributed random space function

$$\kappa(\mathbf{x}, \omega) = \beta \exp\left[\rho \mathbf{Y}(\mathbf{x}, \omega)\right],$$
(1)

where $\beta, \rho \in \mathbb{R}^+$ and $Y(\mathbf{x}, \omega) \sim \mathbb{N}(\mu_Y, \mathcal{C}_Y)$ is a Gaussian random field characterized by its mean $\mu_Y = \langle Y(\mathbf{x}) \rangle$ and two-point covariance function

$$C_{Y}(\mathbf{x}, \mathbf{y}) = Cov(Y(\mathbf{x}), Y(\mathbf{y})) = E[(Y(\mathbf{x}) - \langle Y(\mathbf{x}) \rangle)(Y(\mathbf{y}) - \langle Y(\mathbf{y}) \rangle)].$$
(2)

Moreover, in this work, Y is a second-order stationary process (Gelhar, 1993), that is:

$$\langle Y(\mathbf{x}) \rangle = \mu_{Y}, \text{ (constant)}$$

$$C_{Y}(\mathbf{x}, \mathbf{y}) = C_{Y}(\|\mathbf{x} - \mathbf{y}\|) = C_{Y}(d).$$
(3)

1.3 Karhunen-Loève expansion

The Gaussian field Y can be represented as a series expansion involving a complete set of deterministic functions with correspondent random coefficients using the Karhunen-Loève (KL) expansion proposed independently by Karhunen (1946) and Loève (1955). It is based on the eigen-decomposition of the covariance function. Depending on how fast the eigenvalues decay one may be able to retain only a small number of terms in a truncated expansion and, consequently, this procedure may reduce the search to a smaller parameter space. In uncertainty quantification methods for porous media flows, the KL expansion has been widely used to reduce the number of parameters used to represent the permeability field (Efendiev et al., 2005, 2006; Das et al., 2010; Mondal et al., 2010; Ginting et al., 2011, 2012). Another advantage of KL expansion lies on the fact that it provides orthogonal deterministic basis functions and uncorrelated random coefficients, allowing for the optimal encapsulation of the information

contained in the random process into a set of discrete uncorrelated random variables (Ghanem and Spanos, 1991). This remarkable feature can be used to simplify the Metropolis-Hastings MCMC Algorithm in the sense of the search may be performed in the space of discrete uncorrelated random variables (θ), no longer in the space of permeabilities which have a more complex statistical structure.

2 Introdution

Variational auto-encoder (VAE) model is a stochastic inference and learning algorithm based on variational Bayes (VB) inference proposed by Kingma and Welling (2014). This is a generative technique whose central idea is the development of representations in a low-dimensional latent space that can be mapped back into a realistic-looking image.

Higgins et al. (2016) introduced the β -VAE, a modification of the original VAE, that introduces an adjustable hyperparameter β to balance latent channel capacity and independence constraints with reconstruction accuracy. They demonstrate that with tuned values of β ($\beta > 1$) the β -VAE outperforms VAE ($\beta = 1$).

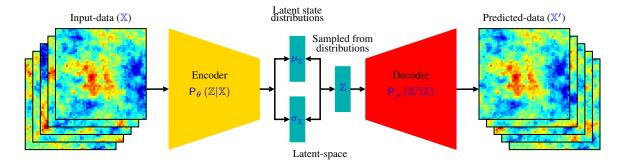
Makhzani et al. (2016); Louizos et al. (2017); Burda et al. (2016); Zheng et al. (2019); Vahdat and Kautz (2020)

3 ZHANG ET AL. (2022)

Variational auto-encoder (VAE) model is a generative network based on variational Bayes (VB) inference proposed by Kingma and Welling (2014).

Zhang et al. (2022) proposed a method to reconstruct porous media based on VAE and Fisher information with good quality and efficiency.

Consider the input data $\mathbb{X} = \left\{ \boldsymbol{x}^{(i)} \right\}_{i=1}^{\mathsf{N}}$ consisting of N independent and identically distributed (i.i.d.) samples of the continuous (or discrete) variable \boldsymbol{x} .



$$\mathbb{Z} = \mu_{\mathbb{Z}} + \sigma_{\mathbb{Z}} \cdot \varepsilon, \quad \text{where} \quad \varepsilon \sim \mathbb{N}(0, 1)$$
 (4)

3 Zhang et al. (2022)

The Kullback–Leibler divergence (also called relative entropy and I-divergence) is a measure of divergence between two distributions (Kullback and Leibler, 1951; Csiszar, 1975):

$$\mathcal{D}_{\mathsf{KL}}\left(f_{\mathbb{P}}||f_{\mathbb{Q}}\right) = \tag{5}$$

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