Energy Proceedings
Vol 56, 2025
ISSN 2004-2965

Interpretable Characterization of Carbon Sequestration Reservoirs Using Kolmogorov-Arnold Networks

Jiayu Li [1,2], Xingwen Jiang B [3], Siwei Meng [4,5], Yuwei Li [6], Jizhou Tang B [1,2*]

1 School of Ocean and Earth Science, Tongji University, Shanghai 200092, China

2 State Key Laboratory of Marine Geology, Tongji University, Shanghai 201306, China

3 National Key Laboratory of Continental Shale Oil, Northeast Petroleum University, Daqing 163318, China

4 Research Institute of Petroleum Exploration and Development, PetroChina, Beijing 100083, China

5 National Key Laboratory of Continental Shale Oil, Daqing 163002, China

6 School of Environment, Liaoning University, Shenyang 110036, China
(*Corresponding Author: jeremytang @ tongji.edu.cn)

ABSTRACT

In recent years, AI technology has been used to evaluate carbon sequestration reservoirs and caprocks, but the black-box nature of neural networks raises credibility concerns. This study employs the Kolmogorov-Arnold Network (KAN) to interpretably characterize carbon sequestration caprocks, including lithology identification and porosity prediction. Inspired by the Kolmogorov-Arnold representation theorem, KANs feature learnable activation functions on edges and univariate spline functions, enhancing both accuracy and interpretability. Smaller KANs achieve accuracy comparable to larger MLPs in data fitting and solving partial differential equations. For lithology identification, well log datasets from the Daniudi and Hangjinqi Gas Fields were used, with a KAN achieving a test accuracy of 0.806, surpassing traditional MLPs. For porosity prediction, datasets from the Gulf of Mexico wells were used, with a KAN achieving an MSE of 0.055. Fine-tuning and retraining derived a physical formula representing porosity based on well log data, elucidating the relationship between porosity and various parameters. This study demonstrates that KANs provide accurate and interpretable predictions, offering promising prospects for carbon sequestration site selection and reservoir characterization, thereby enhancing model credibility and advancing AI applications in geological sciences.

Keywords: Kolmogorov-Arnold Networks, Carbon Storage, Lithology Identification, Porosity Prediction, Explainable AI

NONMENCLATURE

Abbreviations	
KAN	Kolmogorov-Arnold Network
MLPs	Multi-layer perceptrons
AI	Artificial intelligence
MSE	Mean squared error
Symbols	
Φ	A KAN layer
$\phi_{q,p}$	Learnable functions
$\phi_{i,j}$	Activation function
l	Layer
x_l	Input vector

1. INTRODUCTION

In recent years, the pressing issue of climate change has driven significant interest in carbon sequestration as a viable solution for reducing atmospheric CO2 levels [1][2]. Carbon sequestration involves capturing carbon dioxide from the atmosphere and storing it in geological formations, such as reservoirs and caprocks, to mitigate its impact on global warming [3]. Accurate characterization of these geological formations is critical for ensuring their suitability and effectiveness for long-term carbon storage. Advanced technologies, including artificial intelligence (AI), have been increasingly employed to evaluate the properties of carbon

This is a paper for International CCUS Conference 2024 (ICCUS 2024), June 20-22, 2024, Beijing, China.

sequestration reservoirs and caprocks, aiming to enhance the reliability and efficiency of these assessments [4][5].

Traditional AI methods, particularly neural network models, have been widely utilized for geological evaluations due to their powerful data processing capabilities.

For instance, Xu et al. (2018) used active learning to reduce labeling costs in lithology identification, achieving high accuracy with Uncertainty Entropy methods [6]. Zhao et al. (2018) proposed a CE-SGAN model to address data imbalance in lithology identification, achieving significant improvements in classification accuracy and data enhancement on small-sample logging datasets [7]. Baouche et al. (2018) used a two-step approach for permeability prediction, combining electrofacies classification with non-parametric regression techniques, showing robust results compared to traditional methods[8]. Wang et al. (2018) developed an integrated neural network combining 1D CNN and bidirectional GRU, which improved porosity prediction accuracy by reducing RMSE and MAE by 10.81% and 9.85%, respectively [9]. However, the black-box nature of these neural network models has raised concerns about the credibility and interpretability of the results. The lack of transparency in how these models arrive at their predictions makes it challenging for researchers and practitioners to fully trust and understand the AI-driven evaluations.

The Kolmogorov-Arnold Network (KAN) represents a significant advancement in addressing the interpretability issues associated with traditional neural networks. Inspired by the Kolmogorov-Arnold representation theorem, KANs are proposed as a powerful alternative to multi-layer perceptrons (MLPs) [10]. Unlike MLPs, which have fixed activation functions at nodes, KANs feature learnable activation functions on edges and replace linear weights with univariate spline functions. This simple change enhances both the accuracy and interpretability of the model. Smaller KANs achieve accuracy comparable to larger MLPs in data fitting and solving partial differential equations. Moreover, KANs offer intuitive visualization and easy interaction with users, proving useful in discovering mathematical and physical laws underlying the data [11][12].

This study employs the latest Kolmogorov-Arnold Network (KAN) to interpretably characterize carbon sequestration caprocks, focusing on lithology identification and porosity prediction. For lithology identification, well log datasets from the Daniudi and Hangjinqi Gas Fields were utilized, and a KAN with just 26 neurons (8-10-8) achieved a test accuracy of 0.806, significantly surpassing traditional MLP models. Different KAN architectures were analyzed to understand their performance variations. For porosity prediction, datasets from the Gulf of Mexico wells KC-151 and WR-313 were employed, with a KAN achieving an impressive test mean squared error (MSE) of 0.055. Additionally, the study involved fine-tuning and retraining the networks to derive a physical formula that represents porosity based on well log data. This formula elucidates the relationship between porosity and various well log parameters, enabling direct and interpretable evaluation of carbon sequestration reservoirs.

2. METHODOLOGY

2.1 Kolmogorov-Arnold Representation theorem

The Kolmogorov-Arnold representation theorem is the foundation of the Kolmogorov-Arnold network. It is a significant theorem in real analysis that describes how any continuous function can be represented as a combination of a finite number of continuous functions. The theorem has important theoretical implications for the representation and processing of multidimensional functions. Specifically, for any smooth function $f: [0,1]^n \to \mathbb{R}$, the theorem asserts that there exist continuous univariate functions $\phi_{q,p}: [0,1] \to \mathbb{R}$ and $\Phi_q: \mathbb{R} \to \mathbb{R}$ such that

$$f(x) = f(x_1, \dots, x_n) = \sum_{q=1}^{2n+1} \Phi_q \left(\sum_{p=1}^{n} \phi_{q,p}\left(x_p\right) \right)$$

where $x = (x_1, \dots, x_n)$. The history of this theorem dates back to 1957, when it was proposed by Andrey Kolmogorov and subsequently proven by Vladimir Arnold in 1963. The core idea of the theorem is to approximate any multidimensional continuous function by constructing an appropriate combination of one-dimensional continuous functions, thus simplifying complex high-dimensional problems into one-dimensional ones. This theoretical framework has broad applications in various fields, including machine learning, data mining, and signal processing. In machine learning, the Kolmogorov-Arnold representation theorem provides theoretical support for the design and optimization of neural networks. Multi-layer neural networks can approximate complex multidimensional inputs by combining one-dimensional activation functions. Specifically, the network structure can be designed with multiple parallel one-dimensional

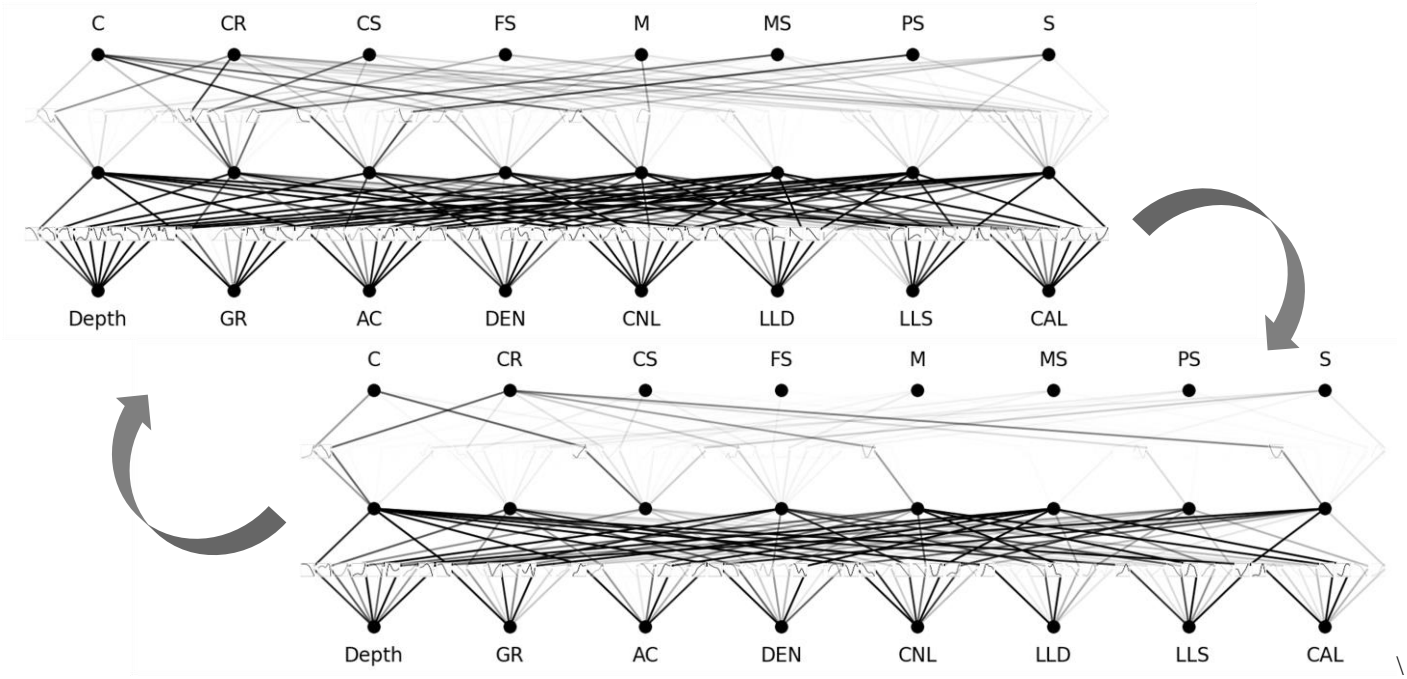


Fig. 1. KAN network structure [8,10,8]

function layers, which are combined and nonlinearly transformed through weighted sums to effectively represent and process high-dimensional inputs.

2.2 Kolmogorov-Arnold network

The Kolmogorov-Arnold Network (KAN) extends the original Kolmogorov-Arnold representation theorem by generalizing its two-layer structure to arbitrary widths and depths. In various tasks, KAN has demonstrated comparable or superior accuracy to traditional multilayer perceptrons (MLPs) while maintaining a smaller network size. The KAN network consists of multiple KAN layers, each utilizing a set of continuous functions to map inputs to outputs. Specifically, a KAN layer can be represented as

$$\Phi = \{\phi_{q,p}\}, \quad p = 1,2,\dots,n_{\text{in}}, \quad q = 1,2,\dots,n_{\text{out}}$$

where the functions $\phi_{q,p}$ have learnable parameters. A KAN network with L layers can be described by an integer array $[l_0, l_1, \dots, l_{L-1}]$. For two consecutive layers l and $l+1$, the i^{th} neuron in layer l is denoted as (l,i), and the j^{th} neuron in layer $l+1$ is denoted as $(l+1,j)$. The activation values of the neurons (l,i) and $(l+1,j)$ are denoted as $x_{l,i}$ and $x_{l+1,j}$, respectively. The activation function connecting neurons (l,i) and $(l+1,j)$ can be represented as

$$\phi_{i,j}, \quad l = 0,\dots,L-1, \quad i = 1,\dots,n_l, \quad j = 1,\dots,n_{l+1}$$

The calculation process from layer l to layer $l+1$ can be represented as

$$x_{l+1} = \Phi_l \circ x_l$$

where $x_l \in \mathbb{R}^{n_0}$ is an input vector, Φ_l is the function matrix corresponding to the l-th KAN layer. For a KAN with L layers, the network calculation process can be represented as

$$\text{KAN}(x) = (\Phi_{L-1} \circ \Phi_{L-2} \circ \cdots \circ \Phi_1 \circ \Phi_0)x$$

3. EXPERIMENTS

3.1 Lithology identification

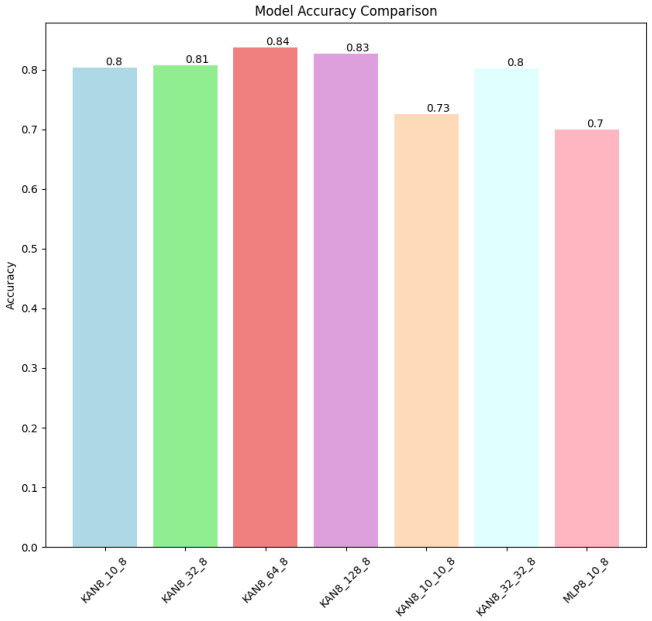


Fig. 2. Test accuracy after model training for lithology identification using KAN

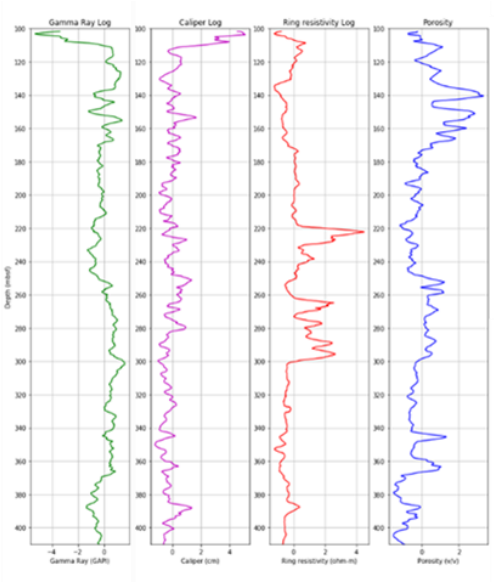
For lithology identification, well log datasets from the Daniudi and Hangjinqi Gas Fields were utilized. The logging parameters include gamma ray (GR), acoustic (AC), density (DEN), deep lateral (LLD), compensated neutron (CNL), shallow lateral (LLS), and caliper (CAL). The lithology types include pebble sandstone (PS), medium sandstone (MS), fine sandstone (FS), coarse sandstone (CS), siltstone (S), carbonate rock (CR), coal (C), and mudstone (M). The data were split into training and test datasets in an 8:2 ratio. Different KAN networks with varying numbers of neurons in the hidden layers were constructed, including [8,10,8], [8,32,8], [8,64,8], and [8,128,8], as well as networks with different numbers of layers such as [8,10,10,8] and [8,32,32,8], to explore the performance of KAN networks in lithology classification tasks. Additionally, an MLP network with [8,10,8] was constructed for comparison.

The experimental results show that a Kolmogorov-Arnold Network (KAN) with just 26 neurons [8,10,8] achieved a test accuracy of 0.806, significantly surpassing traditional MLP models. While increasing the number of neurons in the hidden layers led to noticeable improvements in test accuracy, the improvement was not linear. The performance of [8,128,8] was weaker than that of [8,64,8]. Furthermore, the performance of multi-layer KAN networks did not improve with the addition of more layers, and in some cases, even showed a decline.

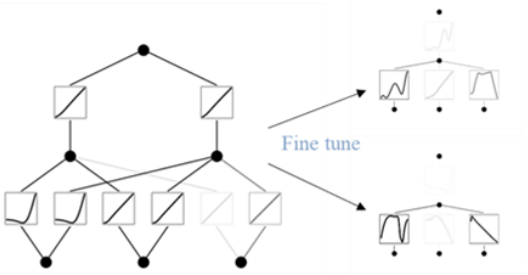
3.2 Porosity prediction

For porosity prediction, datasets from the Gulf of Mexico wells KC-151 were employed. A Kolmogorov-Arnold Network (KAN) with only 6 neurons achieved an impressive test mean squared error (MSE) of 0.055, demonstrating its efficiency in regression tasks. The study went beyond initial model training to include fine-tuning and retraining of the networks to derive a physical formula that represents porosity based on well log data. This formula clearly elucidates the relationship between porosity and various well log parameters, enabling direct and interpretable evaluation of carbon sequestration reservoirs from these measurements. This helps improve prediction accuracy and enhances the model's interpretability, allowing researchers to understand the specific impact of each logging parameter on porosity.

Additionally, by using the physical formula, well log data can be directly converted into porosity values, reducing reliance on complex numerical models and increasing the efficiency and reliability of the evaluation process. Moreover, this formula-based approach ensures greater transparency and verifiability of the results, facilitating broader acceptance and trust in practical applications.



(a) Well log data



(b) KAN network pruning

$$y = 0.08 \cdot \tan(0.06 \cdot (1 - 0.41 \cdot Caliper)^4 - 4.12 \cdot \sin(1.9 \cdot GR + 3.77) + 0.15 \cdot |3.0 \cdot Ring_{resistivity} - 8.58| + 0.57) + 0.42$$

(c) Interpretable porosity formula

Fig. 3. Porosity prediction using the KAN

4. DISCUSSION

This study demonstrates the performance advantages of the KAN model over the MLP model in the task of lithology identification. Under the same number of neurons, the accuracy of the KAN increased by nearly 10%, making KAN networks potentially more suitable for edge devices. However, increasing the number of layers in the KAN network did not lead to a significant improvement in test accuracy and even caused a decline. This might be a specific phenomenon occurring in deeper KAN networks, requiring further investigation to uncover the detailed characteristics of KAN networks. Additionally, for the porosity prediction task, this study provided interpretable physical formulas through network pruning and formalization, which significantly aids in understanding the physical implications behind the data. However, for larger-scale and more diverse input data, the physical interpretations derived from KAN networks may become more complex, making them difficult for researchers to comprehend. This complexity may necessitate the use of mathematical techniques to simplify the formulas.

5. CONCLUSIONS

This study demonstrates the use of Kolmogorov-Arnold Networks (KANs) for interpretable intelligent characterization of carbon sequestration reservoir properties. By leveraging the Kolmogorov-Arnold representation theorem, KANs offer a novel approach that enhances both the accuracy and interpretability of predictions. The research found that smaller KAN models can achieve prediction accuracy comparable to much larger Multilayer Perceptron (MLP) models while also providing physical explanations for their predictions. This not only makes KANs more efficient in terms of computational resources but also more suitable for deployment on edge devices where resources are limited. Moreover, the ability of KANs to offer interpretable results is a significant advancement, addressing one of the primary concerns associated with traditional neural networks—their "black-box" nature. By extracting physical meanings from data, KANs help elucidate the underlying mechanisms driving the predictions, thus enhancing the credibility and acceptance of AI models in critical applications like carbon sequestration. The promising results from this study suggest that KANs could play a crucial role in future carbon sequestration site selection and reservoir property characterization. Their ability to provide accurate and interpretable predictions can lead to better-informed decisions in the management and utilization of geological reservoirs for carbon storage. This advancement not only supports the fight against climate change by optimizing carbon sequestration efforts but also demonstrates the potential of AI technology in transforming geological sciences.

DECLARATION OF INTEREST STATEMENT

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper. All authors read and approved the final manuscript.

REFERENCE

[1] *Walther, G., Post, E., Convey, P., Menzel, A., Parmesan, C., Beebee, T., Fromentin, J., Hoegh-Guldberg, O., & Bairlein, F. (2002). Ecological responses to recent climate change. NATURE, 416(6879), 389–395.* https://doi.org/10.1038/416389a

[2] Zachos, J., Pagani, M., Sloan, L., Thomas, E., & Billups, K. (2001). Trends, rhythms, and aberrations in global climate 65 Ma to present. *SCIENCE*, *292*(5517), 686–693. https://doi.org/10.1126/science.1059412

[3] Lal, R. (2004). Soil carbon sequestration impacts on global climate change and food security. *SCIENCE*, *304*(5677), 1623–1627. https://doi.org/10.1126/science.1097396

[4] Ahmadi, M. A., Kashiwao, T., Rozyn, J., & Bahadori, A. (2016). Accurate prediction of properties of carbon dioxide for carbon capture and sequestration operations. *PETROLEUM SCIENCE AND TECHNOLOGY*, *34*(1), 97–103. https://doi.org/10.1080/10916466.2015.1107847

[5] Yan, H., Zhang, J., Zhou, N., & Li, M. (2020). Application of hybrid artificial intelligence model to predict coal strength alteration during CO2 geological sequestration in coal seams. *SCIENCE OF THE TOTAL ENVIRONMENT*, *711*. https://doi.org/10.1016/j.scitotenv.2019.135029

[6] Xu, T., Chang, J., Feng, D., Lv, W., Kang, Y., Liu, H., Li, J., & Li, Z. (2021). Evaluation of active learning algorithms for formation lithology identification. *JOURNAL OF PETROLEUM SCIENCE AND ENGINEERING*, *206*. https://doi.org/10.1016/j.petrol.2021.108999

[7] Zhao, F., Yang, Y., Kang, J., & Li, X. (2023). CE-SGAN: Classification enhancement semi-supervised generative adversarial network for lithology identification. *GEOENERGY SCIENCE AND ENGINEERING*, *223*. https://doi.org/10.1016/j.geoen.2023.211562

[8] Rafik, B., & Kamel, B. (2017). Prediction of permeability and porosity from well log data using the nonparametric regression with multivariate analysis and

neural network, Hassi R'Mel Field, Algeria. Egyptian Journal of Petroleum, 26(3), 763–778. https://doi.org/10.1016/j.ejpe.2016.10.013
[9] Wang, J., & Cao, J. (2022). Deep Learning Reservoir Porosity Prediction Using Integrated Neural Network. Arabian Journal for Science and Engineering, 47(9), 11313–11327. https://doi.org/10.1007/s13369-021-06080-x
[10] Liu, Z., Wang, Y., Vaidya, S., Ruehle, F., Halverson, J., Soljačić, M., Hou, T. Y., & Tegmark, M. (2024). *KAN: Kolmogorov-Arnold Networks* (arXiv:2404.19756). arXiv. http://arxiv.org/abs/2404.19756
[11] Li, Z. (2024). *Kolmogorov-Arnold Networks are Radial Basis Function Networks* (arXiv:2405.06721). arXiv. http://arxiv.org/abs/2405.06721
[12] Peng, Y., He, M., Hu, F., Mao, Z., Huang, X., & Ding, J. (2024). *Predictive Modeling of Flexible EHD Pumps using Kolmogorov-Arnold Networks* (arXiv:2405.07488). arXiv. http://arxiv.org/abs/2405.07488