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MACHINE LEARNING-AIDED THREE-DIMENSIONAL GEOLOGICAL MODELING WITH UNCERTAINTY QUANTIFICATION

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Three-dimensional (3D) geological modeling plays a crucial role in understanding and predicting subsurface features. This paper presents a machine learning-aided approach for 3D geological modelingto predict geological units at unsampled locations. Four popular machine learning algorithms, support vector machine (SVM),k-nearest neighbours (kNN), gradient boosting decision tree (GBDT) and random forest (RF), are compared for their performance using confusion matrix andF_1 score. The concept of information entropy is introduced to quantify uncertainty in the geological models. The proposed approach is applied to a site in Hong Kong. The distributions of underground geological layers are created from the developed model. Machine learning has shown promising applicability in 3Dgeological modeling.

Keywords: 3D geological modelling, Machine learning, Uncertainty.

1. Introduction

Three-dimensional (3D) modeling of subsurface stratigraphy has garnered escalating interest in site characterization due to its ability to illustrate 3D subsurface stratigraphic variances, significantly enhancing the design and analysis of geotechnical structures (Phoon et al., 2022; Shuku and Phoon, 2023).

In 3D geological modeling, various methods such as random field method have been employed. However, these methods often suffer from drawbacks like slow processing speeds and limited accuracy. Machine learning methods offer the potential for enhanced efficiency and increased accuracy (Lyu et al. 2024; Shi and Wang 2021). By leveraging machine learning approaches, these challenges could be effectively addressed (Hu et al. 2024).

Geological uncertainty can be substantial because of sparse site investigation data and the spatial diversity of geological strata (Shi and Wang, 2021; Yan et al., 2023; Zhao et al., 2024, 2025). While several softwares like Leapfrog and Rhino offer utility and ease of use, they frequently neglect to account for geological uncertainty. The implementation of 3D probabilistic geological modeling and uncertainty quantification becomes indispensable for engineering applications.

This study presents machine learning methods for 3Dprobabilistic geological modeling.The performance is evaluated using confusion matrix and F_1score, and information entropy is introduced to quantify the associated uncertainties. The method is verified using the Hong Kong International Airport (HKIA). The subsurface conditions of HKIA are identified. Machine learning methods show promising applicability in 3Dgeological modeling.

2. Method

2.1.*Machine learning method*

This study utilizes machine learning algorithms through Python code using scikit-learn. The rationale behind opting for machine learning over traditional spatial data analysis methods like kriging or random field simulation stems from machine learning's ability to offer more efficient estimations in scenarios involving non-Gaussian, non-stationary, and complex modeling (Hu et al. 2024).

Four machine learning algorithms including support vector machine (SVM), k-nearest neighbours (kNN),gradient boosting decision tree (GBDT) and random forest (RF) are considered. The hyperparameters are set by default in Python. The borehole data is randomly divided into 7:3 for training and testing sets.The inputs are 3D coordinates.

Among the four machine learning algorithms,the distance-basedweight is used in kNN, which issimilar to the commonly used inverse distance weighting approach for spatial interpolation. Additionally, a unified parameter, anisotropy ratio′ = x/x', where x = the horizontal coordinates and x' = the transformed horizontal coordinates, is introduced to eliminate the anisotropic effect between the horizontal and vertical scale (Xiao et al. 2022).

2.2.*Performance evaluation and uncertainty quantification*

The widely used confusion matrix and macro F_1 scoreused to evaluate model performance. The confusion matrix summarizes the model performance by comparing actual and predicted classes, detailing the performance for each class. The macro F_1 score amalgamates precision and recall, providing a holistic evaluation of the model performance.It is valuable for assessing models in the presence of imbalanced class distributions (Xiao et al., 2022).Since the borehole data was not evenly distributed, a 5-folder cross validation is used and macro F_1 score in each fold is calculated.

Information entropy is employed to measure geological uncertainty at each specific location (Yan et al., 2023). Entropy quantifies the degree of unpredictability regarding potential outcomes and is mathematically expressed as:

$$H(Y) = -\sum_{i=1}^{m} P(y_i) log\big(P(y_i)\big) \qquad (1)$$

where $P(y_i)$ = probability of possible geological condition; y_i = possible geological condition; n = number of possible geological conditions. A larger information entropy means a higher geological modelling uncertainty.

3. Studied site

The HKIA is used as the case study (Fig. 1) (approximately 20km^2). A total of1908 boreholesare used, with ten geological types. Since some geological types have much fewer records than other dominant types, they are combined into five main geological types, namely fill, marine deposits (with estuarine, beach and debris flow deposits), alluvium (with colluvium), grade V-IV rocks, and grade III-I rocks.

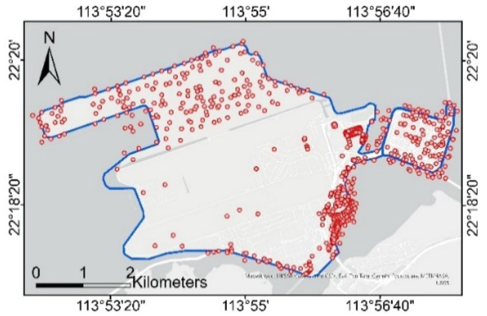

Fig. 1. Studied area and locations of boreholes (Red circles represent boreholes).

4. Results and discussions

The HKIA area is partitioned into voxels of 10m×10m×1m. The optimal anisotropy ratio is identified as about 40through a parameter analysis. This is attributed to the vertical variability surpassing the horizontal variability, a phenomenon also validated by Phoon and Kulhawy (1999).The performances of the four algorithms, expressed by confusion matrix andmacro F_1score, are shown in Figs. 2 and 3. The macro F_1scores of SVM, kNN, GBDT, and RF are 0.898, 0.904, 0.876, and 0.920, respectively.The RF and kNN perform relatively better while SVM and GBDT result in relatively poor performance. Thesemethodstend to misclassify grade III-I rocks as grade V-IV rocks, likely due to their similar characteristics and limited data on grade III-I rocks.

Typical geological layers and entropies from kNN are shown in Fig. 4. Table 1 shows that all the algorithms give comparable predictions on the thickness of marine deposits and grade V-IV rocks. RF gives a thicker alluvium layer than the other three algorithms. The depth order of the geological types is: fill, marine deposit, alluvium, grade V-IV rocks, and grade III-I rocks. This distribution aligns with the geological sedimentation patterns, indicating that the upper layers exhibit more severe weathering. Through summation of thickness of fill,marine deposits, and alluvium, kNN shows comparable results to the one given by the quaternary base from Geotechnical Engineering Office (GEO) while GBDT and RF present higher numbers. Hence, kNNismost reliable in this case considering both accuracy and HKIA geological conditions. This may be because kNN can consider spatial correlations through distance-basedweight.Compared to the edge areas with denser borehole coverage, the central region's data sparsity may result in less reliable interpolation and increased variability in the modeled outputs, therefore, should be interpreted with caution due to the inherent limitations of the available data.

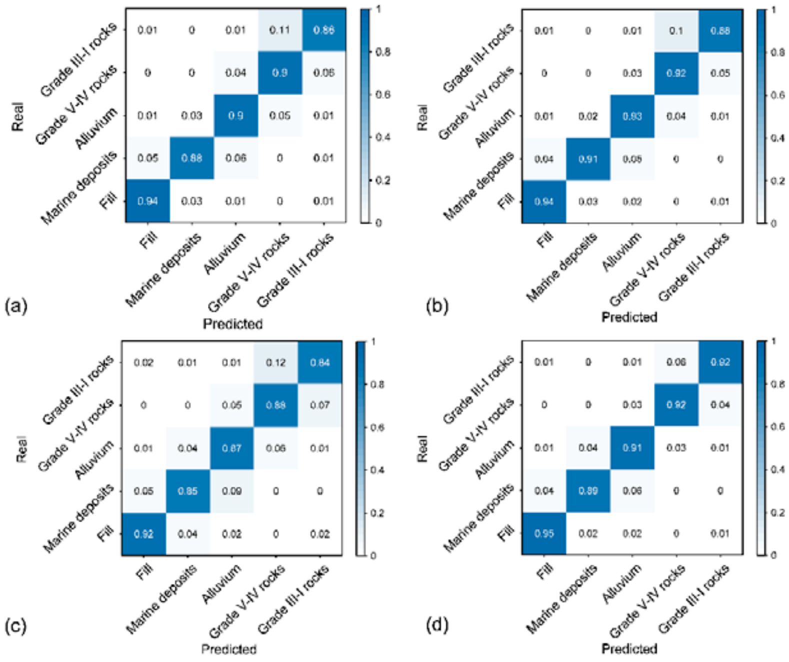

Fig. 2.Confusion matrix of (a) SVM (b) kNN(c) GBDT (d) RF.

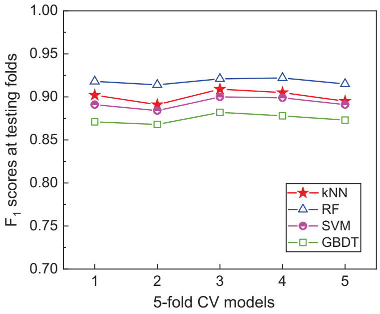

Fig. 3. Macro F_1scores at testing set under 5-fold cross validation.

The entropy values for the model are all less than 2, with most areas below 0.5 (Fig. 4 (b)), indicating a low level of uncertainty in the geological model, suggesting that the predictions are robust. Additionally, a higher degree of uncertainty is observed at the stratigraphic boundaries within the geological model, which is also observed by Shi and Wang (2021).

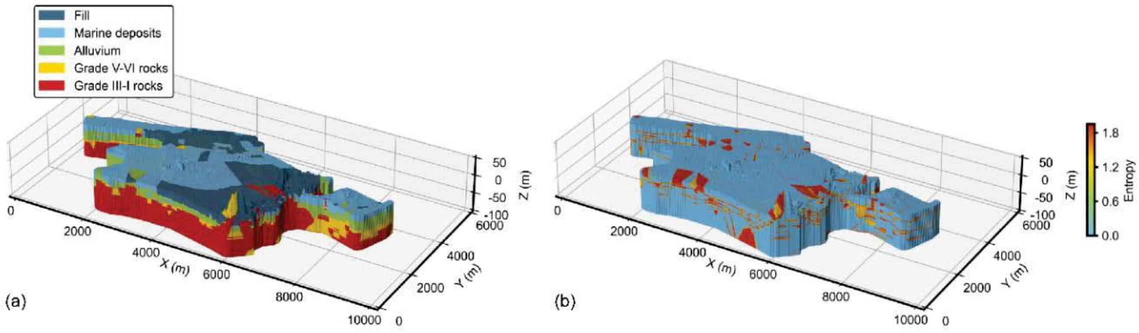

Fig. 4. (a) 3D geological model of HKIA and (b) the entropy using kNN.

Table 1. Statistics on geological layers of HKIA.

Algorithm	Mean thickness of geological layer (m)			
	Fill	Marine deposit	Alluvium	Grade V-IV rocks
SVM	5.8	12.7	22.5	15.1
kNN	5.3	12.1	24.4	13.5
GBDT	4.1	11.3	23.2	14.6
RF	6.2	12.9	29.4	16.6

5. Conclusions

This paper presents a machine learning-aided approach for 3D geological modeling. The proposed approach is applied to HKIA site.Main conclusions can be drawn as:

1) Four machine learning algorithms, SVM,kNN, GBDT and RF, are compared for their performance using confusion matrix and F_1 score. The RF and kNN perform relatively better. Thesemethodstend to misclassify grade III-I rocks as grade V-IV rocks, likely due to their similar characteristics and limited data on grade III-I rocks.
2) The algorithms give comparable predictions on the thickness of marine deposits and grade V-IV rocks. RF gives a thicker alluvium layer than the other three algorithms. The depth order of the geological types is: fill, marine deposit, alluvium, grade V-IV rocks, and grade III-I rocks. This distribution aligns with the geological sedimentation patterns, indicating that the upper layers exhibit more severe weathering.

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