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Data-Driven Facies Prediction: A Comparative Study of Random Forest, XGBoost, SVM, CatBoost, and K-Means

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Data-Driven Facies Prediction: A Comparative Study of Random Forest, XGBoost, SVM, CatBoost, and K-Means

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ABSTRACT

Facies classification plays a critical role in characterizing subsurface heterogeneity and supporting effective reservoir development. Traditional methods, which often rely on core interpretation and manual log analysis, are limited by subjective interpretation and sparse data coverage. This study aims to improve facies prediction by comparing the performance of five machine learning models: Random Forest, XGBoost, Support Vector Machine, CatBoost, and K-Means clustering. The dataset is derived from sandstone formations in Labuan Island, Malaysia, and is enhanced using synthetic data generated through Latin Hypercube Sampling to address data scarcity. Feature selection is performed using three independent techniques to identify the most informative variables, and Principal Component Analysis is used to investigate feature relationships. Model evaluation is based on classification accuracy, precision-recall metrics, receiver operating characteristic curves, and confusion matrices. Among the models tested, CatBoost achieved the highest cross-validation accuracy at 95.4%, followed by XGBoost at 93.7%. Random Forest achieved a test accuracy of 89.5%, while Support Vector Machine performed less reliably with a test accuracy of 85.6%. The K-Means clustering approach yielded an overall accuracy of 49.7% in aligning predicted clusters with true facies labels. The results demonstrate the effectiveness of ensemble methods in facies classification and support the use of augmented data in enhancing model performance. This approach provides a practical framework for applying machine learning in geological settings, with potential benefits for reservoir modeling and development planning.

KEY WORDS

Facies classification; Machine learning; Geostatistics; Synthetic data augmentation; Ensemble models

1. INTRODUCTION

Facies classification is a fundamental step in geological interpretation, providing insight into depositional environments, stratigraphic architecture, and reservoir heterogeneity (Babai et al., 2025; Hall, 2016; Miall, 2022). It plays a key role in guiding exploration and development by helping identify lithological boundaries, predict reservoir properties, and support volumetric assessments. When integrated with seismic and petrophysical data, facies models improve the continuity and reliability of subsurface interpretations between wells (Luoni et al., 2004; Xu et al., 2017). This is especially important in sedimentary systems where facies transitions can be abrupt or spatially complex. Traditional methods, such as core and log-based interpretation, while valuable, are often limited in spatial coverage and resolution, particularly in data-scarce settings (Al-Ali et al., 2020; Renard et al., 2009). To improve model accuracy, facies classification is increasingly used to constrain 3D reservoir simulations and guide fluid flow modeling (Dzhalalov, 2025; Ezati et al., 2020; Saikia et al., 2019).

Machine learning (ML) techniques have become powerful tools in facies classification, offering improvements in speed, accuracy, and scalability compared to traditional manual methods(Bentéjac et al., 1911; Emmert-Streib et al., 2020; Probst et al., 2019; Risha & Liu, 2025). These algorithms can handle high-dimensional well log data and detect subtle lithological variations that may be overlooked by human interpreters (Maehara et al., 2021; Risha et al., 2025). Supervised models such as support vector machines, random forests, and neural networks have demonstrated high predictive accuracy in classifying complex lithofacies, particularly when trained on large, annotated datasets (Al-Ali et al., 2020; Asedegbega et al., 2021). In addition, unsupervised learning approaches such as clustering algorithms and self-organizing maps are useful in situations where labeled data is scarce, allowing for objective facies groupings based on data patterns alone. More recent studies have integrated multiple ML methods such as combining Principal Component Analysis with Gaussian Mixture Models and Hidden Markov Models to capture both vertical and lateral lithological trends across wells, enhancing the reliability of reservoir models (Chen & Zeng, 2018a; Fadokun et al., 2020a).

While machine learning methods have improved the efficiency and accuracy of facies classification, several limitations persist that affect their robustness and generalization. One major challenge is the quality and quantity of training data. Most algorithms require extensive labeled datasets, yet many subsurface datasets lack sufficient

core-calibrated facies labels, which increases the risk of overfitting or poor performance on new wells (Alaudah et al., 2019a; Bestagini et al., 2017a). Another key issue is the high dimensionality and redundancy in input features, particularly in seismic facies classification. Without careful feature selection, models can become unnecessarily complex and sensitive to noise, reducing interpretability and stability. In addition, the lack of standardized benchmarks and inconsistencies in how training and validation are performed make it difficult to compare model performance across studies. Finally, geological realism is not always guaranteed by data-driven models. Without incorporating domain knowledge, even highly accurate models may produce facies distributions that are inconsistent with stratigraphic context or depositional settings (Babikir et al., 2024a; Halotel et al., 2019a; Shashank & Mahapatra, 2018).

Integrating geological knowledge into machine learning models has proven to improve the accuracy and geological consistency of facies classification. Traditional models often rely only on well log measurements and treat each depth point independently, which can overlook stratigraphic context and depositional patterns. Several studies have demonstrated that incorporating features derived from geological rules, such as density-neutron separation, sequence stratigraphy, and grain or pore size estimates, leads to more reliable classifications. These additional features help the models recognize patterns that are meaningful in a geological sense, rather than just statistical associations (Halotel et al., 2019b; Przybysz-Jarnut et al., 2020). The inclusion of facies zonation maps and stratigraphic markers further enhances classification by guiding the model with prior geological knowledge. These approaches also support better handling of uncertainty, as they allow models to consider a broader set of plausible interpretations that remain consistent with geological understanding (Egorov et al., 2018; Tran et al., 2020). New architectures that combine machine learning with geological logic and structural constraints have also been shown to produce more coherent facies distributions across wells (Jaikla, 2019).

This study aims to evaluate the performance of multiple machine learning models for classifying sandstone facies using a combination of real and synthetically augmented data. The models tested include Random Forest, XGBoost, Support Vector Machine, CatBoost, and K-Means, covering both supervised and unsupervised learning approaches. The use of Latin Hypercube Sampling for synthetic data generation allows for a more robust evaluation by expanding the feature space beyond the limitations of a small field dataset. Feature selection is

addressed using three independent techniques, each highlighting different aspects of feature relevance, while dimensionality reduction is explored through Principal Component Analysis to better understand the underlying data structure. The models are compared using a range of metrics including classification accuracy, precision-recall scores, receiver operating characteristic curves, and confusion matrices. Previous studies have often focused on a single method or dataset, which limits their generalizability (Alaudah et al., 2019b; Bestagini et al., 2017b). By integrating multiple models and evaluation methods on a semi-synthetic dataset, this study offers a broader perspective on the strengths and limitations of each algorithm in the context of geologically realistic data (Babikir et al., 2024b; Fadokun et al., 2020b; Rahimi & Riahi, 2022).

2. METHODOLOGY

2.1 Data Collection and Description

This study focuses on Labuan Island, Malaysia, where data were collected using a combination of field sampling, laboratory analyses, and spectral gamma-ray measurements. These techniques provide a comprehensive understanding of the petrophysical and geological properties of the studied formations, allowing for high-resolution facies classification and predictive modeling (Freeman et al., 2019; Kuvichko et al., 2020).

A total of 41 rock samples were described, examined, and collected from different formations within the study area from 16 outcrops. Outcrops represented the exposed sandstone formation of Labuan including Crocker, Temburong, and Belait to ensure a representative dataset that captures lithological heterogeneity (Risha & Douraghi, 2021). The classification of samples and their facies was conducted using visual inspection, grain size, and sedimentary structures, which align with standard facies classification techniques (Crampin, 2008; Selley, 1968). Spectral gamma-ray was used to measure thorium (Th), and potassium (K) concentrations which are essential for facies differentiation based on mineralogical content as the Th/K ratio serves as an indicator of clay content and depositional conditions, with lower values signifying cleaner sandstone facies and higher values indicating more clay-rich or cemented formations (Freeman et al., 2019; Risha et al., 2023; Singh et al., 2022).

In the lab, grain size analysis was performed to determine the basic statistical distribution of particle sizes, including mean grain size, standard deviation, skewness, and kurtosis. Which are important in defining sorting, sizes range, and distribution which directly influence rock characteristics (Reinwarth et al., 2017). Mercury Injection Capillary Pressure (MICP) analysis was conducted on the collected samples to quantify porosity, permeability, microporosity, tortuosity, entry pressure in (MPa), and compressibility factor (CF) in (MPa·g/mm³) for this study. The MICP method is widely used to estimate pore throat distributions and capillary pressure curves, providing insights into fluid flow characteristics and reservoir connectivity (Mandal & Rezaee, 2019; Risha, 2025a). Entry pressure is important for predicting fluid displacement and permeability trends in reservoir rocks, while CF represents the mechanical response of the pore network under applied pressure, providing insights into rock deformation during fluid flow (Aji et al., 2021; Shikhov & Arns, 2013). Two other key indices were calculated to characterize pore structure and heterogeneity (Kuvichko et al., 2020):

1. Pore Connectivity Index (PCI) which quantifies the efficiency of the pore network and is calculated from:

$$PCI = \frac{Total\ Pore\ Volume\ (\frac{mm^3}{g})}{Modal\ Pore\ Diameter\ (nm)} \quad (1)$$

This provides an assessment of how well-connected the pore spaces are, which influences permeability and fluid flow efficiency (Wei et al., 2014).

2. Heterogeneity Index (HI) which reflects the variability and complexity of the pore structure:

$$HI = \frac{Span\ of\ Pore\ Size\ Distribution\ (nm)}{Modal\ Pore\ Diameter\ (nm)} \quad (2)$$

A higher HI value indicates greater variability in pore sizes, which may impact permeability and fluid retention properties (Yan et al., 2023).

These petrophysical parameters are good tools for facies classification based on the rock quality. The application of MICP techniques in evaluating permeability trends has been demonstrated to provide robust insights into pore structure and connectivity (Ciabarri et al., 2021; Kuvichko et al., 2020).

2.2 Data Preprocessing

Data preprocessing is a main step in machine learning-based techniques. Proper handling of numerical variables, synthetic data generation, and feature scaling significantly impact the performance of some classification models (Alshdaifat et al., 2021; Jadhav et al., 2022). This study follows a structured preprocessing workflow, addressing data uncertainty and resampling generation, which collectively enhance classification accuracy and generalizability (Araujo et al., 2022; Szeszko & Topczewska, 2016). Categorical variables, basically facies types that we want to predict, was encoded using the one-hot encoding technique which is widely used transformation that prevents numerical misinterpretation of non-ordinal categories like facies (Potdar et al., 2017). This encoding technique ensures that machine learning models do not assume inherent relationships between facies categories, which could otherwise lead to erroneous predictions (Johnson et al., 2023).

Two of the challenges in the data are the limited number of samples, which can lead to overfitting in machine learning models and the other was data representability where we can ask the question if this combination of values can represent the natural variation in the rock formation or even in the sample. To address this, data resampling by synthetic data augmentation was performed to generate multiple versions of the sample with independent variation between variables within a predefined range of uncertainty (Gameng et al., 2019; Kim & Byun, 2022). This technique was applied along with Latin Hypercube Sampling (LHS), a Monte Carlo-based sampling method that ensures a stratified representation of the dataset by dividing the range of each variable into equal probability intervals. Unlike random sampling, which can lead to overlapping or redundant data points, LHS ensures that each sample is representative of the full distribution of geological properties (Phromphan et al., 2024; Risha et al., 2025; Van Camp & Walraevens, 2009). The newly generated dataset expanded the original 41 samples into 4100 versions where each sample has new 100 versions, creating a more spread training dataset. The new versions were ensured to be version independency and equally spread in terms of variation. This approach improves model robustness, allowing for better generalization (Mishra et al., 2020; Mukherjee et al., 2023).

2.2 Feature Selection Techniques

Feature selection is aimed in this study to improve model performance by eliminating irrelevant or redundant variables in predicting the facies down to 10 features. This study utilized three feature selection techniques: Random Forest (RF) Feature Importance, Recursive Feature Elimination (RFE), and Least Absolute Shrinkage

and Selection Operator (Lasso) Regression. These techniques were chosen based on their ability to enhance model accuracy, reduce overfitting, and improve computational efficiency (Negi et al., 2023; Syed Mustapha, 2023).

Random Forest is a powerful ensemble learning method that operates by constructing multiple decision trees and aggregating their outputs (Risha, 2025b). One of its key advantages is its ability to compute feature importance scores based on the decrease in Gini impurity across the trees. In this study, an RF classifier was trained on the training dataset (80%), and the resulting feature importances were ranked to determine which geological attributes contributed most to facies classification (Gregorutti et al., 2017). The feature importance score of each predictor variable f_i was computed as:

$$I(f_i) = \frac{1}{N}\sum_{t=1}^{N}\left(\Delta Ginit(fi)\right) \quad (3)$$

where, $I(f_i)$ represents the importance score of feature f_i , N is the total number of decision trees in the Random Forest, and $\Delta Gini_t(f_i)$ denotes the decrease in Gini impurity due to the presence of f_i in tree t.

Recursive Feature Elimination (RFE) is a wrapper-based feature selection technique that iteratively removes the least important features while retraining a classifier. In this study, Logistic Regression with L1 penalty was used as the base model for RFE to select the most predictive subset of geological attributes (Ali et al., 2022; Priyatno & Widiyaningtyas, 2024).

RFE follows an iterative approach by training the model on all features, rank features based on their contribution to classification performance, eliminate the least important feature and retrain the model, then finally repeat steps the last two steps until only a predefined number of features remain. Mathematically, feature ranking in RFE can be expressed as:

$$W_i = \sum_{j=1}^{N}\left|\beta_{i,j}\right| \quad (4)$$

where, W_i is the importance score of feature I, $\beta i,j$ represents the coefficient of feature i in model iteration j, and N is the number of iterations in RFE.

Lasso (Least Absolute Shrinkage and Selection Operator) Regression is a regularization-based feature selection method that applies an L1 penalty, forcing some feature coefficients to zero. In this study, Lasso Regression with

regularization parameter α = 0.01 was used to identify the most relevant geological attributes for facies classification (Tyagi et al., 2024). Lasso regression minimizes the following objective function:

$$\min_{\beta} \sum_{i=1}(y_i - X_i\beta)^2 + \alpha \sum_{j=1}^{p}|\beta_i| \quad (5)$$

where, y_i represents the target variable (facies classification), X_i represents the input features, β represents the regression coefficients, p is the number of features, α is the regularization parameter, controlling the strength of the penalty on feature coefficients, and $|\beta_j|$ enforces L1 regularization, shrinking some coefficients to zero, effectively selecting only the most relevant features.

2.4 Machine Learning Models for Facies Classification

Machine learning (ML) was used enabling data-driven identification of geological facies based on petrophysical, mineralogical, and geochemical properties. In this study, five ML algorithms were employed for facies prediction: Random Forest (RF), Extreme Gradient Boosting (XGBoost), Support Vector Machines (SVM), CatBoost, and K-Means clustering. Each algorithm was selected based on its ability to handle high-dimensional geological datasets and improve predictive accuracy.

For the supervised learning models, 20% of the data was kept as a holdout for model evaluation, and 80% of the data was trained using the same subset of features from the dataset. Training data included porosity (Por), permeability (Perm), Th/K ratio (Th_K_ratio), heterogeneity index (HI), Compressibility Factor (CF), clay grain size (Clay), sand/mud ratio (S_M_ratio), grain size standard deviation (STDV), skewness (skew), and kurtosis (kurt). For the unsupervised model, all variables were used with applying a 3D Principal Component Analysis (PCA) to reduce the features dimentionality. To ensure a fair comparison among the machine learning models, we aimed to maintain a similar level of hyperparameter complexity across all methods. While hyperparameter settings are not always directly comparable between different algorithms, we carefully selected values that balance model expressiveness and computational efficiency. This approach prevents any single model from gaining an advantage solely due to excessive hyperparameter tuning, ensuring that differences in performance are attributed to the models' inherent learning capabilities rather than parameter scaling (Table 1).

Table 1. Summary of machine learning models used for facies classification, including their learning type, ensemble status, key hyperparameters, and validation approach.

Model	Supervised/Unsupervised	Ensemble Method	Hyperparameters	Validation
RF	Supervised	Yes	Number of trees: 40, Max leaf nodes: 10	5-Fold
XGBoost	Supervised	Yes	Number of trees: 40, Max depth: 2, Learning rate: 0.1	5-Fold
SVM	Supervised	No	Regularization strength: 20, Gamma auto-tuned	5-Fold
CatBoost	Supervised	Yes	Iterations: 40, Tree depth: 3, Learning rate: 0.1	5-Fold
K-Means	Unsupervised	No	Number of classes: 6, 3D PCA applied	N/A

2.5 Model Evaluation Metrics

Multiple evaluation metrics were employed, including confusion matrices, receiver operating characteristic (ROC) accuracy comparison, and precision-recall (PR) curves to provide a strong comparison between the different model performances (Grau et al., 2015; Li & Guo, 2021). Accuracy is the most straightforward evaluation metric, measuring the proportion of correctly classified facies instances relative to the total number of samples and calculated from (6). PR curves evaluate model performance by plotting precision (the proportion of correctly predicted facies among all predicted facies) against recall (the proportion of correctly predicted facies among all actual facies) that are calculated from (7 and 8).

$$Accuracy = \frac{TP+TN}{TP+TN+FP+FN} \quad (6)$$

$$Precision = \frac{TP}{TP+FP} \quad (7)$$

$$Recall = \frac{TP}{TP+FN} \quad (8)$$

where: *TP* (True Positives): Correctly predicted facies classes, *TN* (True Negatives): Correctly rejected incorrect classes, *FP* (False Positives): Incorrectly predicted facies classes, and *FN* (False Negatives): Incorrectly rejected correct classes.

While accuracy provides an overall measure of model correctness, it can be misleading in cases of class imbalance, where some facies appear significantly more frequently than others (Eusebi, 2013). On the other hand, PR curves are particularly useful when dealing with imbalanced datasets, ensuring that models do not overpredict dominant facies while ignoring rarer ones (Jaskowiak & Costa, 2023).

3. RESULTS

3.1 Resampling Data Validation

To improve model generalization and enhance dataset robustness, LHS was applied to generate synthetic data based on the original facies' dataset. This approach ensured a controlled variability range for the features while maintaining geological consistency to prevent unrealistic deviations while expanding the dataset for machine learning training.

3.1.1 Distribution Comparison

A comparative Kernel Density Estimation (KDE) analysis was conducted to assess the similarity between the original and synthetic datasets (Figure 1). The KDE plots illustrate the probability density functions of key features, demonstrating the degree of alignment between synthetic and original data distributions. Tortuosity retained its primary distribution shape in synthetic samples. Porosity, microporosity, permeability, Th/K ratio, PCI, and entry pressure all showed a close match, indicating that the generated values fall within a realistic range of geological variability. HI and CF showed some divergence, suggesting a broader variability in synthetic data compared to the original dataset. Overall, the KDE comparison suggests that the synthetic dataset preserves the underlying statistical properties of the original data, with minor deviations expected due to the applied variability constraints.

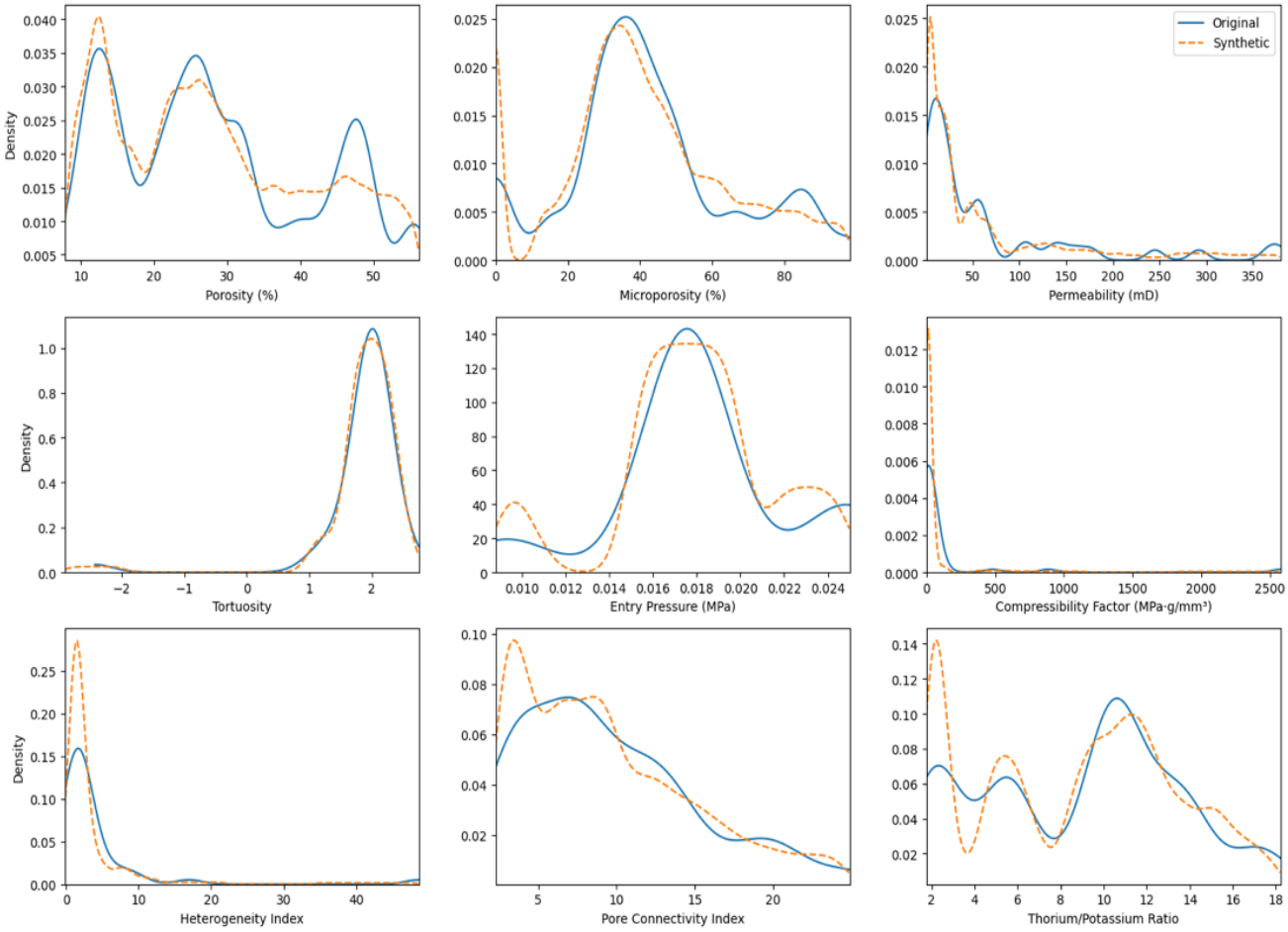

Figure 1 . Kernel Density Estimation (KDE) plots comparing the probability distributions of key features in the original (solid line) and synthetic (dashed line) datasets. The close alignment in most features suggests successful preservation of geological variability.

To quantify the statistical similarity, the mean values of each feature in the original and synthetic datasets were compared. Table 2 presents the absolute and percentage mean differences between the two datasets.

Table 2. Comparison of mean values between original and synthetic datasets for key geological features. The percentage difference indicates the deviation between the two datasets, with lower values suggesting closer alignment.

Feature	Variable Name	Original Mean	Synthetic Mean	Difference (%)
Porosity (%)	**Por**	28.505	28.157	1.22%
Microporosity (%)	**micro_por**	41.976	41.039	2.22%
Permeability (mD)	**Perm**	68.627	66.050	3.76%
Tortuosity	**Tortuosity**	1.859	1.851	0.47%
Entry Pressure (MPa)	**Entry_Press**	0.018	0.018	1.68%
Compressibility Factor (MPa·g/mm³)	**CF**	112.693	103.266	8.36%
Heterogeneity Index	**HI**	3.888	3.710	4.58%
Pore Connectivity Index	**PCI**	9.506	9.379	1.39%
Th/K Ratio	**Th_K_ratio**	8.908	8.822	0.97%
Clay Fraction (%)	**Clay**	2.833	2.858	0.87%
Sand Fraction (%)	**Sand**	81.124	81.371	0.28%
Silt Fraction (%)	**Silt**	15.652	15.771	0.82%
Sand/Mud Ratio	**S_M_ratio**	7.241	7.288	0.77%
Grain Size Mean	**mean**	3.275	3.249	0.08%
Grain Size Standard Deviation	**STDV**	1.507	1.495	0.78%
Grain Size Skewness	**skew**	0.998	0.995	0.31%
Grain Size Kurtosis	**kurt**	1.859	1.860	0.04%

The mean difference percentages remain below 5% for most features, confirming that the synthetic dataset retains the statistical characteristics of the original dataset. The largest deviation is observed in CF (8.36%), which may be attributed to its higher inherent variability.

3.2 Feature Selection Results

Feature selection was performed to identify the most relevant attributes for facies classification. The results from three different approaches, Random Forest, Recursive Feature Elimination (RFE), and Lasso (L1) regression which showed variations in feature importance rankings (Figure 2).

Random Forest provided a ranked list of features based on their relative contribution to classification accuracy, offering a more interpretable importance measure. The final selection included **nine** features based on their ranking in Random Forest, as it provided a more intuitive and continuous importance scale.

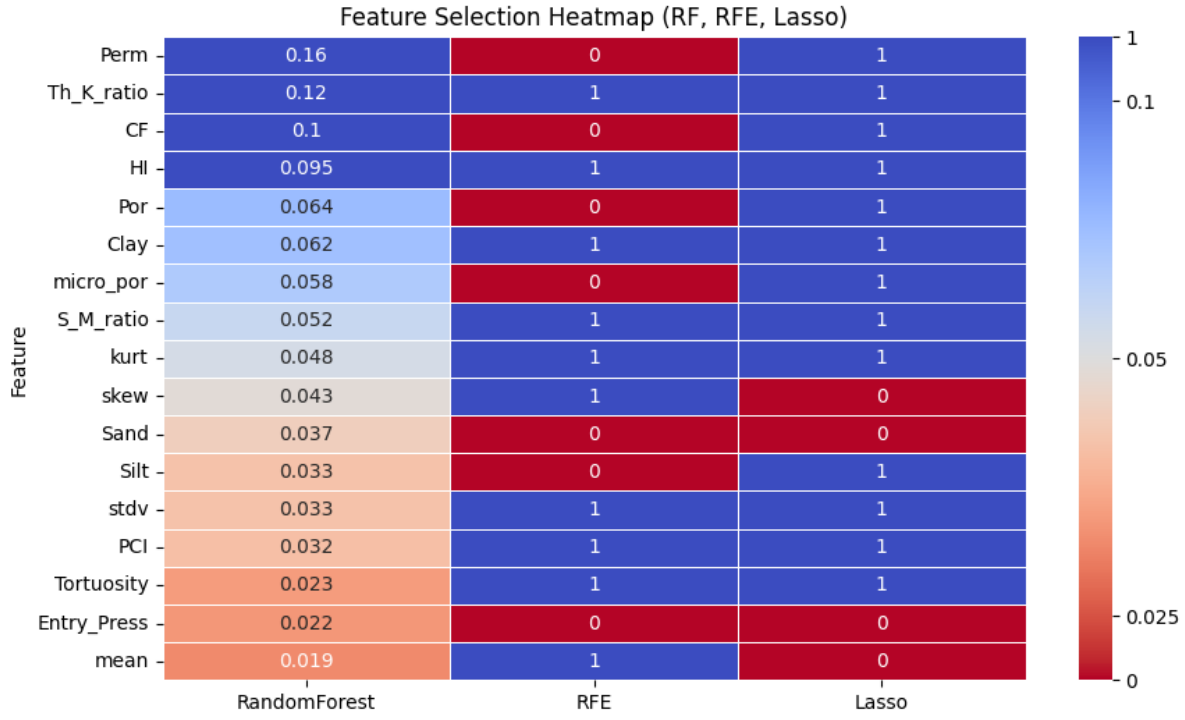

Figure 2. A heatmap summarizing the feature importance across all three methods, highlighting the agreement and differences in feature selection. The selected features were used for subsequent model training and evaluation.

3.3 Model Performance Evaluation

The classification performance of the supervised models Random Forest, XGBoost, SVM, and CatBoost was assessed using cross-validation accuracy, test set accuracy, and confusion matrices. Table 3 summarizes the cross-validation accuracy (mean ± standard deviation) and the test accuracy on the 20% holdout dataset. Among the models, CatBoost achieved the highest cross-validation accuracy (95.4% ± 0.93%), followed closely by XGBoost (93.7% ± 0.91%). SVM had the lowest test accuracy at 85.6%, while Random Forest performed moderately well with a test accuracy of 89.5%.

Table 3. Classification Accuracy and Cross-Validation Results.

Model	Cross-Validation Accuracy (%)	Test Accuracy (%) (Holdout 20%)
RF	89.3 ± 0.77	89.5
XGBoost	93.7 ± 0.91	93.9
SVM	82.7 ± 1.41	85.6
CatBoost	95.4 ± 0.93	93.8

The confusion matrices further illustrate how each model classified facies types, showing the patterns of correct classifications and misclassification (Figure 3). These matrices help identify facies that were consistently well-predicted and those that were more frequently confused with others. The Jointed Sandstone facies showed the highest misclassification rates across all models, particularly in Random Forest (67.3%), XGBoost (75.2%), SVM (77.2%), and CatBoost (71.3%). The primary misclassification trend for it was towards Massive Sandstone, indicating that the models struggled to distinguish between these two facies. On the other hand, Massive Sandstone was the most consistently well-classified facies across all models with high accuracy in Random Forest (99.3%), XGBoost (100%), SVM (98.6%), and CatBoost (99.7%) being rarely confused with other facies. However, despite its high classification accuracy, Massive Sandstone was also the most common target for other facies when misclassified, particularly for Interbedded Sandstone and Jointed Sandstone, which were frequently predicted as Massive Sandstone across different models. Other facies showed varied performance depending on the model. The Cross-Bedded and the Massive Cemented Sandstone had high classification accuracy in most models but showed a notably lower accuracy in SVM with (64.0%) and (57.7%) respectively, where it was misclassified primarily as Massive Sandstone (18.4%) and (20.5%) and as Interbedded Sandstone (16.0%) and (21.8%) respectively. Interbedded Sandstone also had higher misclassification rate in Random Forest (20.2%) misclassified as Massive Sandstone.

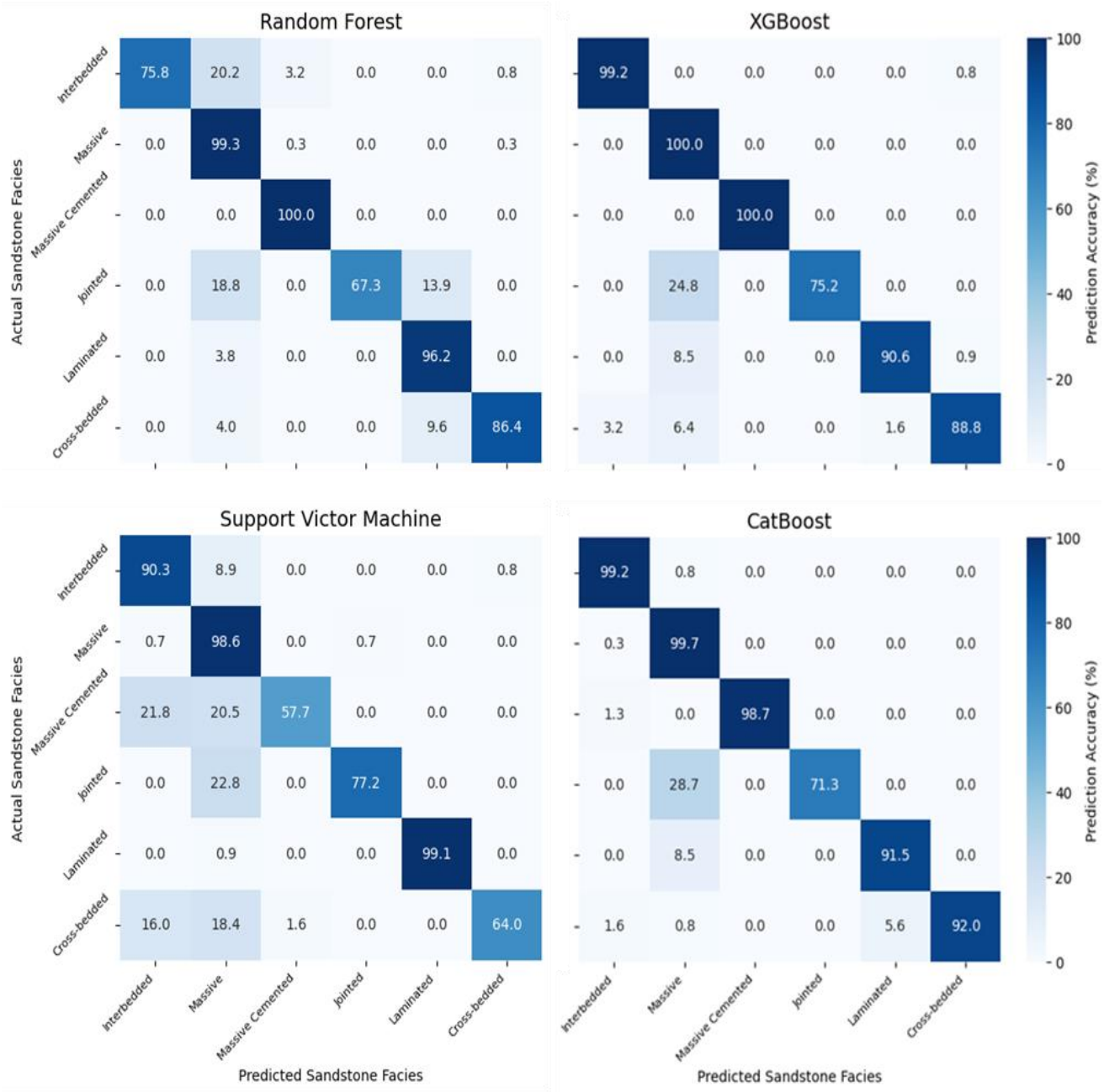

Figure 3. Confusion matrices for the supervised classification models, Random Forest, XGBoost, SVM, and CatBoost. Each matrix represents the percentage of correctly classified sandstone facies along the diagonal and misclassification distributions in off-diagonal elements. Darker shades indicate higher classification accuracy percentages, while lighter shades reveal misclassification trends of different facies categories.

3.4 PCA and K-Means Clustering

To evaluate the separability of facies within the dataset, Principal Component Analysis (PCA) was applied to reduce dimensionality while retaining the primary geological variations (Figure 4). The first principal component (PCA1) was largely influenced by porosity (-0.36), permeability (-0.33), and Th/K ratio (-0.36) in the negative direction, while clay content (0.41), standard deviation of grain size (0.38), and microporosity (0.32) contributed positively. PCA2 showed strong contributions from skewness (0.53), kurtosis (0.52), and mean grain size (0.39), whereas PCA3 was primarily driven by tortuosity (0.64) and CF (-0.52).

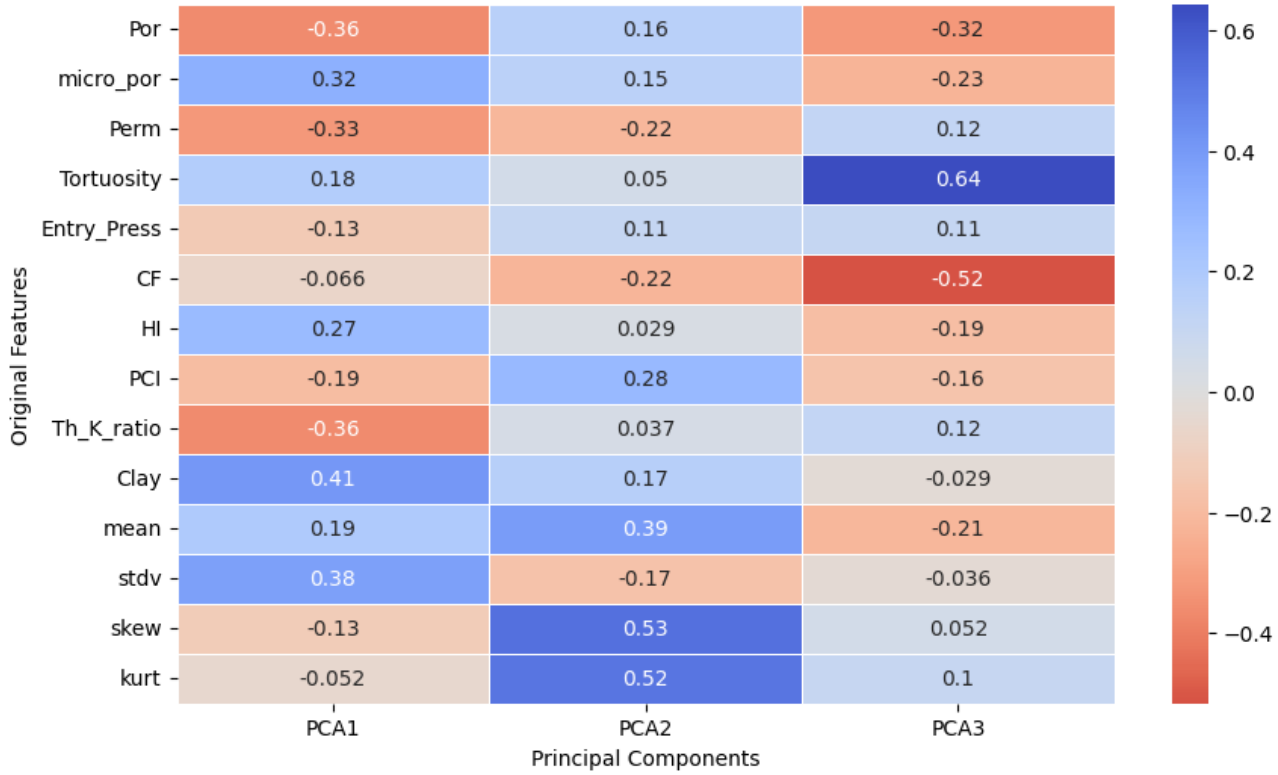

Figure 4. Feature Contributions to Principal Component Analysis (PCA). This heatmap visualizes the influence of each original feature on the first three principal components (PCA1, PCA2, and PCA3).

Following PCA transformation, K-Means clustering was performed to classify facies based on their feature distributions. The actual facies distribution and K-Means clustering results are visualized in Figure 5. The overall clustering accuracy was 49.66%, indicating moderate alignment between the K-Means classifications and the true facies labels. While some facies clusters were well-separated, others showed significant overlap. Clusters

corresponding to Cross-bedded and Interbedded Sandstone showed the best match of clusters and. However, Laminated and Jointed Sandstone displayed substantial overlap with the Massive Sandstone.

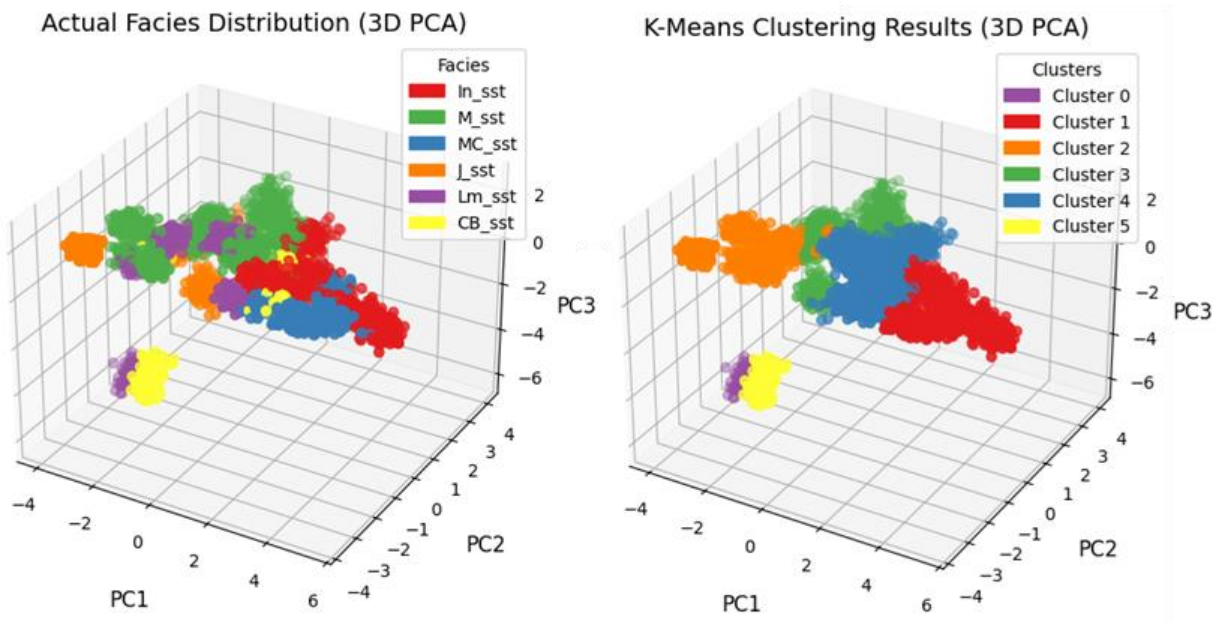

Figure 5. Comparison of Actual Facies Distribution and K-Means Clustering in 3D PCA Space. The clustering performance highlights areas of correct classification as well as facies misclassification, with certain facies being grouped together while others overlap.

3.5 Precision-Recall and ROC Evaluation

The classification performance of the models was further evaluated using the Precision-Recall (PR) and Receiver Operating Characteristic (ROC) curves. These metrics highlight the trade-offs between precision, recall, and false positive rates across different classification thresholds. The PR analysis shows distinct differences in model classification performance. The CatBoost model achieved the highest precision-recall score of 0.993, indicating its strong ability to maintain both high precision and recall. XGBoost followed with a score of 0.990, showing a similarly strong classification balance. The Random Forest model performed slightly lower at 0.958, while the Support Vector Machine demonstrated moderate effectiveness with a score of 0.859.

In contrast, the K-Means clustering approach resulted in a significantly lower score of 0.202, indicating poor precision and recall (Figure 6). The ROC curve further confirms these patterns. The CatBoost model showed the highest AUC value of 0.95, closely followed by XGBoost at 0.94. Random Forest also performed well, achieving

0.90, while the Support Vector Machine had a lower value of 0.85. The K-Means clustering model exhibited the lowest area under the curve at 0.50 (Figure 7).

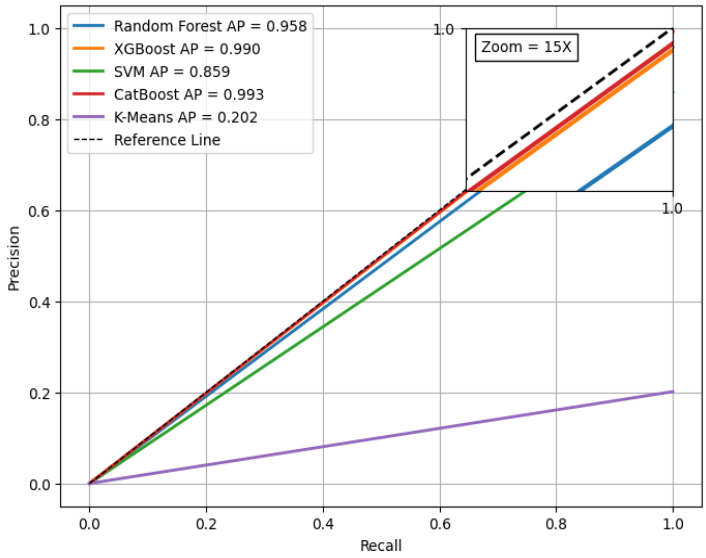

Figure 6. Precision-Recall curves for all models, between precision and recall across different classification thresholds. A zoomed-in section highlights differences in high-recall regions.

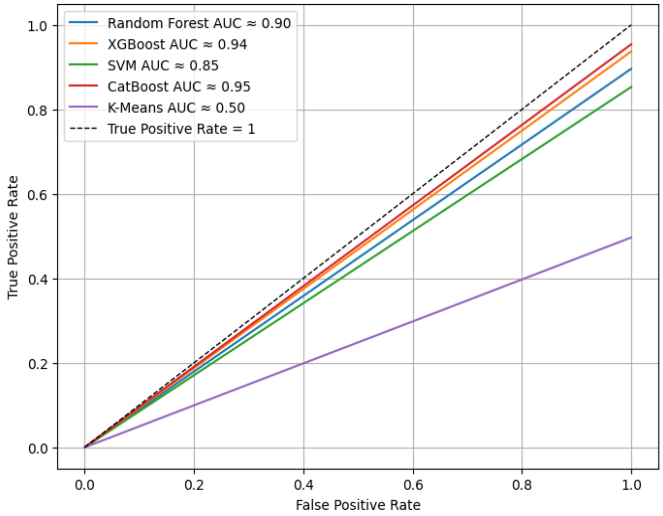

Figure 7. Receiver Operating Characteristic curves comparing model classification performance based on the true positive rate and false positive rate.

4. DISCUSSION

4.1 Interpretation of Model Performance

The classification results showed that CatBoost and XGBoost had the highest accuracy among the tested models. CatBoost achieved the best performance, correctly classifying most facies with minimal misclassification. XGBoost followed closely, showing similar trends in accuracy and precision. The strong results from these models can be attributed to their ability to handle feature interactions and optimize decision boundaries effectively. However, both of them showed misclassification Jointed as Massive Sandstone. Random Forest performed well but was slightly less accurate than the gradient boosting models. It showed good classification ability but had some difficulty in distinguishing between certain facies, particularly misclassifying Jointed and Interbedded with Massive Sandstone. This suggests that while Random Forest is effective, it does not refine decision boundaries as well as boosting methods. SVM had the lowest accuracy among the supervised models. The model particularly struggled with Cross-Bedded, Massive Cemented and a little less Jointed Sandstone being misclassified mainly as Massive Sandstone. The lower performance may be due to the difficulty of defining clear decision boundaries in a dataset with overlapping petrophysical properties. The reliance on support vectors may not have been as effective for this classification task compared to the tree-based methods.

K-Means clustering performed the worst, with an accuracy of 49.66%, which highlights some challenges when using an unsupervised approach for facies classification. The results suggest that while some facies formed distinct clusters, others showed significant overlap, making separation difficult. In particular, facies with similar characteristics were often grouped together like Interbedded and Massive Cemented Sandstone as both might have very low permeability, HI, and CF with high clay content, leading to misclassification. A similar misclassification occurred between Massive, Jointed, and Laminated Sandstone which has also been repeated in the other supervised models separately. This reinforces the advantage of supervised learning methods, which can better account for complex feature relationships.

4.2 Misclassification Trends and Facies Separability

The most consistent issue was the misclassification of Jointed Sandstone as Massive Sandstone. This trend appeared in every supervised model, with the highest confusion rates observed in Random Forest (67.3%), XGBoost (75.2%), SVM (77.2%), and CatBoost (71.3%). The similarity in petrophysical properties between Jointed Sandstone and Massive Sandstone likely contributed to the observed misclassification trends, as these models struggled to establish distinct decision boundaries between them. This challenge might be coming from joints is a large-scale structural, primarily defined by its macroscopic characteristics, which may not be adequately captured through finer petrophysical parameters from MICP. These differences are significantly influenced by the scale of the structural or the feature which is important in distinguishing different facies (Day-Lewis et al., 2005). These structural differences may not be sufficiently represented in the feature space used for classification, leading to systematic misclassification.

Massive Sandstone stood out as both the most accurately classified facies and the most frequent misclassification target. It consistently achieved high classification accuracy across all models. However, it also absorbed misclassified samples from other facies, particularly Jointed Sandstone and Interbedded Sandstone.

4.3 PCA Contributions, and K-Means Performance

The PCA results provided an understanding of the dominant geological properties influencing facies classification. PCA1 was primarily associated with variations in sandstone composition, with porosity, permeability, and Th/K ratio that might be indicating cleaner, well-sorted sandstones, while clay content, grain size variability, and microporosity, reflected the tight, heterogeneous nature of facies. PCA2 seemed to capture the depositional environmental effects, as indicated by high contributions from skewness, kurtosis, and mean grain size. PCA3 leaned towards the flow pathway complexity and diagenetic influence, with tortuosity and compressibility factor showing the highest loadings.

The supervised learning models retained high classification performance, indicating that the selected features effectively captured key geological distinctions. However, K-Means clustering struggled to distinguish facies that shared similar overlapped petrophysical attributes. The cluster overlap highlights the limitations of unsupervised

learning for facies classification, particularly in cases where petrophysical similarities between facies that are closely distributed from close depositional environments.

4.4 Learning Approach Comparison

The comparison between supervised and unsupervised learning approaches in facies classification showed big differences in the prediction performances. The supervised models, particularly ensemble methods like CatBoost and XGBoost achieved the highest classification accuracies, benefiting from their boosting mechanisms, which iteratively adjust for misclassifications, enhancing predictive performance which generally outperform traditional classifiers due to their ability to handle high-dimensional and complex data structures (Liu et al., 2023).

In contrast, SVM as a non-ensemble method showed the lowest accuracy among supervised models, indicating its limitations in distinguishing facies with overlapping properties. The challenges associated with SVM appears particularly when dealing with nonlinearly separable facies distributions (Mohamed et al., 2019). This suggests that kernel-based approaches may not always be suitable for facies prediction when petrophysical features overlap significantly.

K-Means clustering, representing the unsupervised approach, which was considerably lower in accuracy than the supervised methods. The low performance is attributed to its reliance on geometric distance measures, which fail to capture the subtle variations in petrophysical properties that define facies boundaries (Ippolito et al., 2021). The inability of K-Means to distinguish facies has also been noted in digital rock physics studies, where it struggled to cluster formations with similar depositional histories (Temizel et al., 2022).

4.5 Implications and Limitations of Machine Learning for Facies Classification

The study confirms the effectiveness of machine learning in facies classification of sandstone formations. Supervised learning models like XGBoost and CatBoost achieved high classification accuracy, demonstrating their potential to enhance traditional geological methods by reducing subjectivity and standardizing facies identification. Ensemble techniques, such as decision trees and gradient boosting, have been widely recognized for improving classification accuracy by capturing complex decision boundaries, making them valuable for geological applications (Mandal & Rezaee, 2019).

Using a relatively small dataset with overlapped sandstone features could be a limiting factor in this study. Even with applying uncertainty techniques to get a better representation of the natural distribution of features, using synthetic data augmentation can still be considered a limitation. Despite the role of data synthesis in improving data availability, it may introduce biases when applied to capturing geological variability. Previous research has highlighted that machine learning models trained on limited data may struggle with overfitting or reduced performance in different geological settings (Alaudah et al., 2019c).

Future research should incorporate additional geological features, such as mineralogical composition or depth, to improve model performance. Alternative clustering techniques, like self-organizing maps or Gaussian mixture models, could enhance the accuracy of unsupervised learning approaches. Deep learning methods, including convolutional and recurrent neural networks, have also been suggested as promising tools for improving facies classification (Chen & Zeng, 2018b). Further studies should evaluate these models on more diverse sandstone formations to ensure their broader applicability and reliability in different geological contexts.

5. CONCLUSION

This study demonstrates the effectiveness of machine learning models in classifying facies of complex sandstone samples. The results indicate that ensemble-based supervised learning models, particularly CatBoost and XGBoost, achieved the highest classification accuracy, outperforming Random Forest and the non-ensemble SVM model and the unsupervised learning K-Means method. These models effectively distinguished most facies, with CatBoost achieving a cross-validation accuracy of 95.4% and XGBoost reaching 93.7%. However, some facies, including Jointed Sandstone, faced difficulties with all models due to the overlapping petrophysical characteristics, often being misclassified as Massive Sandstone.

Dimensionality reduction through PCA provided insights into the dominant geological factors influencing facies classification with PCA1 mainly associated with sandstone quality features and PCA2 and PCA3 associated depositional environmental and diagenetic influence respectively. Despite its role in visualizing facies separability, PCA did not improve classification accuracy for the unsupervised K-Means clustering approach. The

K-Means model struggled to form distinct clusters, achieving only 49.66% accuracy, reinforcing the limitations of unsupervised learning in geological classification when features are strongly overlapped.

Despite the promising results and the integration of uncertainty analysis, this study has certain limitations. The reliance on synthetic data augmentation, coupled with a relatively small dataset, may introduce biases that affect the model's generalizability. Future research should aim to enhance uncertainty assessment, incorporate a broader range of geological parameters, and explore deep learning techniques to further improve classification accuracy.

Overall, this study highlights the potential of machine learning in facies classification, demonstrating its capability to enhance geological interpretation. By incorporating advanced computational techniques, geoscientists can achieve more accurate and objective facies predictions, improving decision-making in many geoscience applications.

Author Contributions

"The author, M.R., was responsible for conceptualization, methodology, software development, visualization, validation, formal analysis, investigation, writing original draft preparation, MR and PL did the review and editing, and supervision. The authors have read and approved the final manuscript."

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Competing Interests

"The authors declare no relevant financial or non-financial competing interests that could have influenced the research findings."

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