APPLICATION OF MACHINE LEARNING METHODS TO FORECAST PETROPHYSICAL PROPERTIES IN BASALTS OF THE SERRA GERAL GROUP: IMPLICATIONS FOR CARBON STORAGE

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November 25, 2024

ABSTRACT

This study applies machine learning techniques to forecast petrophysical properties (density, porosity, and permeability) in the basalts of the Serra Geral Group, located in the Paraná Basin, Brazil. These properties are crucial for the successful implementation of carbon capture and storage (CCS), an important technology to combat climate change. Employing machine learning models—XGBoost, Gradient Boosting, and Random Forest—the research aims to overcome the limitations of traditional empirical methods that often fail to capture the complex variabilities in basalt formations. The models were applied to 28 wells within the study area. The interpolation of the well data indicated that the northern region of the Serra Geral Group in the State of Santa Catarina exhibits optimal conditions for geological storage. From 600 to 900 m, the basalts present suitable intervals ranging from 7 to 22 m thick, with density lows of almost 2.1 g/cm³, high peaks of 17.8% apparent porosity, and permeability of 55 μD. The results demonstrated significant improvements in accuracy of property predictions compared to empirical methods from the literature, highlighting the potential of machine learning to enhance the feasibility and reliability of CCS in basaltic formations. This study contributes to the ongoing efforts to optimize CCS technology by providing a more accurate geological assessment of suitable storage sites.

Keywords: Carbon Capture and Storage · Machine Learning Models · Petrophysics · Basalts

1 Introduction

Carbon capture and storage (CCS) is an important technology to combat climate change, by capturing carbon dioxide at the source, storing it underground, and preventing large amounts of CO2 from reaching the atmosphere (IPCC et al., 2018). Among the existing alternatives for geological storage, basalts stand out due to their unique chemical and physical properties, presenting as an attractive option for carbon storage due to their abundance and capacity for carbon mineralization (Cartier, 2020; Snæbjörnsdóttir et al., 2020). These rocks are rich in calcium and magnesium, which react with carbon dioxide to create minerals that securely sequester CO2 (Oelkers, Gislason, & Matter, 2008; Snæbjörnsdóttir et al., 2020).

Notable CCS projects have demonstrated the feasibility and potential of basalt formations for CO2 storage. In Iceland, the CarbFix project has successfully injected and mineralized CO2 in basaltic rocks, transforming over 95% of the captured CO2 into stable minerals in less than two years (Matter et al., 2016; von Strandmann et al., 2019; Snæbjörnsdóttir et al., 2020). Similarly, the Wallula project in the Columbia River flood basalt (USA) has explored the

capacity of basalt formations in the State of Washington for long-term CO2 storage, showing promising results in both CO2 injection and storage efficiency, with approximately 60% of the CO2 sequestered via mineralization within two years (McGrail et al., 2017; White et al., 2020). These projects exemplify the successful application of CCS in basalt formations, providing valuable insights and data that can be applied to other regions worldwide.

The basalts of the Serra Geral Group in Brazil represent a significant and still unexplored potential for CO2 storage. This extensive basalt formation, part of the Paraná Basin, erupted in the Early Cretaceous (Piccirillo & Melfi, 1988; Renne et al., 1992) and offers a vast geological environment suitable for CCS. The region's geological characteristics, including its thickness, density, porosity, permeability, and mineral composition, make it a promising candidate for CO2 injection and mineralization (Nardy, Machado, & Oliveira, 2008; Rossetti et al., 2019). Due to its volume, it may be considered one of the largest magmatic provinces potentially favorable for carbon fixation on Earth. Laboratory experiments with basalts from this region revealed facilitated, rapid carbonate precipitation beginning 72 hours post-injection, achieving an estimated CO2 storage of approximately 75% based on the availability of calcium, with carbonate precipitation comprising aragonite (75.9%), dolomite (19.6%), and calcite (4.6%) (Ferreira et al., 2024). Exploring the CCS potential of the Serra Geral basalts could significantly contribute to Brazil's carbon reduction efforts and provide a model for similar formations globally.

Understanding the petrophysical properties such as density, porosity, and permeability is crucial for effective geological storage of CO2 in basalts (McGrail, Spane, Sullivan, Bacon, & Hund, 2011; Zakharova, Goldberg, Sullivan, Herron, & Grau, 2012). Traditional empirical methods for predicting these properties often lack accuracy (Navarro, Teramoto, Engelbrecht, & Kiang, 2020; Rossetti et al., 2019), as they eventually mix data of basalt formations from different parts of the world and may not accurately predict new samples that deviate from the assumed data distribution (Breiman, 2001b). The variability and complexity of basalt formations necessitate more robust predictive models. Addressing these limitations requires advanced techniques that can provide accurate predictions for new, unseen data, ensuring the reliability and safety of CO2 storage projects.

This study uses machine learning models to enhance the predictive accuracy of petrophysical properties of the Serra Geral basalts. By applying machine learning techniques, we aim to predict the density, porosity, and permeability of the basalts in the Paraná Basin, specifically in the State of Santa Catarina. Based on the predicted petrophysical properties, this approach will help identify the most suitable regions and sections for CO2 storage within the Serra Geral layer. Achieving this objective will advance the understanding of CCS in the Serra Geral basalts and provide a framework for applying machine learning methods to future geological storage projects elsewhere.

2 Material and Methods

2.1 Study area

Identifying regions and sections suitable for carbon capture and storage is crucial for mitigating climate change. This study focuses on the basalts of the Serra Geral Group, located in the western portion of the State of Santa Catarina (Figure 1). These basaltic rocks exhibit significant compositional variations (Nardy et al., 2008; Wildner et al., 2014) and are situated near stationary sources that could benefit from carbon storage (Ketzer, Machado, Rockett, & Iglesias, 2016). Additionally, the area has a good coverage of wells with petrophysical data (ANP-SGB, 2023), making it an ideal candidate for prospective research.

However, due to the intrinsic heterogeneity and variability of petrophysical properties of basalts, empirical equations used to predict the petrophysical properties of basalts have considerable limitations. They typically use a single property as input and can be less flexible than machine learning approaches. These equations may perform poorly with new, unseen data, especially if it deviates from the assumed data distribution and comes from different regions (Breiman, 2001b). In the following subsections, we describe the application of machine learning techniques to predict density, porosity, and permeability in the study area's basaltic rocks.

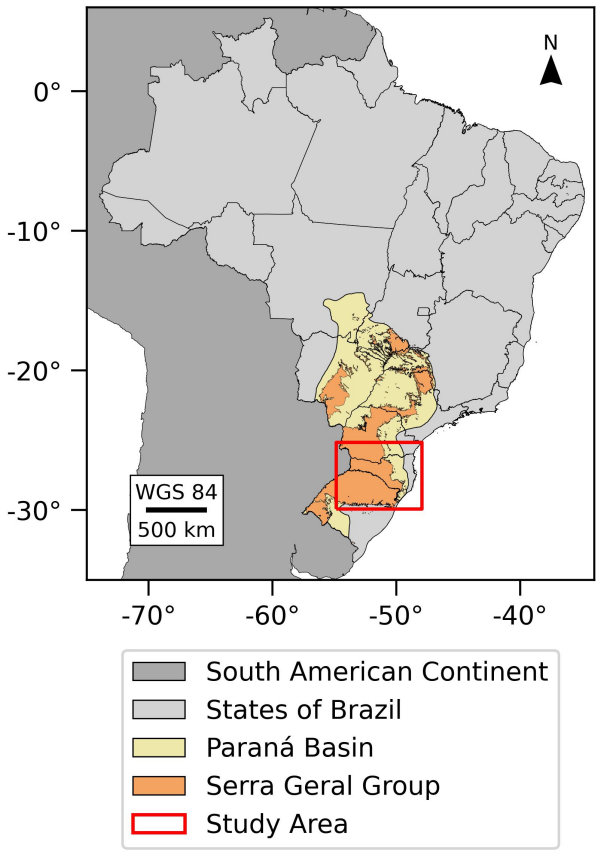

Figure 1: Location map of the study area. The focus is the basaltic rocks in the Serra Geral Group area at the Paraná Basin in the State of Santa Catarina.

2.2 Density model

Previous works applied p-wave velocity (Vp) to predict density, employing linear to second-degree equations (e.g. X. Chen et al. (2015); Rossetti et al. (2019); Vedanti, Malkoti, Pandey, and Shrivastava (2018)). In this work, we applied four variables as input to predict density: sonic velocity (DT or Vp), gamma ray (GR), spontaneous potential (SP), and induction log deep resistivity (ILD). The XGBoost model was used due to its robust performance in handling various data characteristics and complexities.

XGBoost, or Extreme Gradient Boosting, is an advanced implementation of gradient boosting algorithms designed for speed and performance. It constructs an ensemble of decision trees sequentially, where each subsequent tree is built to correct the errors of the previous trees. This is achieved through an additive model, where new trees are added to minimize a loss function. XGBoost incorporates regularization terms to prevent overfitting and uses decision tree pruning and parallel processing to enhance efficiency. This makes it particularly well-suited for handling large datasets with complex relationships and managing linear and nonlinear interactions among the input features (T. Chen & Guestrin, 2016).

To supply the model, we used freely available data from the REATE database (ANP-SGB, 2023). Data from 3 wells (14463 samples) containing the curves of DT, GR, SP, ILD, and density (RHOB) were used (Figure 2). Subsequently, the model was applied to 25 additional wells in the study area.

To ensure the reliability of our model, several preprocessing and validation steps were implemented (Figure 3). Outliers were identified and treated to prevent skewed predictions. The dataset was split into training and testing sets, with 20% of the data reserved for testing to evaluate model performance (Geron, 2019). We applied scaling to stabilize variance and make the data more Gaussian-like. Model validation was conducted using K-fold cross-validation (k=5) to ensure the model generalizes well to unseen data (Anguita, Ghio, Ridella, & Sterpi, 2009; James, Witten, Hastie, Tibshirani, & Taylor, 2023). Hyperparameter tuning was performed using a randomized search over a parameter grid

(Bergstra & Bengio, 2012; Pedregosa et al., 2011), including 'n_estimators,' 'learning_rate,' 'max_depth,' 'subsample,' 'min_child_weight,' and 'gamma,' to optimize model performance.

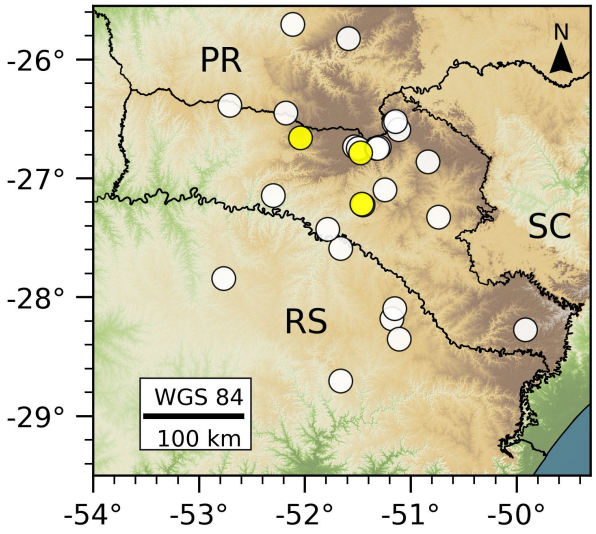

Figure 2: Location map of the 28 wells where the machine learning models were applied to predict the petrophysical properties of basalts and then used to create the interpolated maps. The wells in yellow were used to train-test the density models. The yellow wells are the only ones in the area with density curves.

2.3 Porosity model

Previous works used the relationship between Vp or density to predict porosity, employing linear to exponential equations (e.g. Al-Harthi, Al-Amri, and Shehata (1999); X. Chen et al. (2015); Navarro et al. (2020); Rossetti et al. (2019); Vedanti et al. (2018)). Based on tests with bagging and boosting models, we used the Gradient Boosting model to predict porosity using Vp and density as inputs.

Gradient boosting is an ensemble learning technique that builds a model sequentially. It trains a series of weak learners, such as decision trees, where each new tree corrects the errors of the previous ones. The process starts with an initial prediction, and subsequent models are fitted to the residuals of the previous predictions, gradually improving the overall model performance. This results in a robust predictive model that captures complex patterns in the data (Friedman, 2001; Geron, 2019; James et al., 2023).

The porosity model was supplied with data (175 samples) containing Vp, density, and porosity from Rossetti et al. (2019), Goulart (2019), and Famelli (2020). Subsequently, the model was applied to 28 wells in the study area. The preprocessing and validation steps were similar to those applied to the density model (Figure 3). Hyperparameter tuning was conducted using a randomized search over a defined parameter grid (Bergstra & Bengio, 2012; Pedregosa et al., 2011), including 'n_estimators,' 'learning_rate,' 'max_depth,' 'min_samples_split,' and 'min_samples_leaf.'

2.4 Permeability model

For permeability, previous empirical equations explored exponential relationships between porosity and permeability to predict data (e.g. Lamur et al. (2017); Mueller, Melnik, Spieler, Scheu, and Dingwell (2005); Navarro et al. (2020); Yokoyama and Takeuchi (2009)). Based on the tests, we used the Random Forest model to predict permeability, using Vp, density, and porosity, and a feature was created using Vp multiplied by density squared as inputs.

Random Forest is an ensemble learning method that constructs multiple decision trees during training and outputs the mean prediction of the individual trees. Each tree is built from a random subset of the training data using a bootstrap aggregating or bagging technique. Additionally, random forests select random subsets of features at each split in the decision tree. This randomization reduces the variance of the model, leading to better generalization of unseen data. Aggregating multiple trees helps mitigate overfitting and improves the model's robustness (Breiman, 2001a; Geron, 2019; James et al., 2023).

The permeability model was supplied with Vp, density, porosity, and permeability data (130 samples) from Rossetti et al. (2019) and Famelli (2020). Subsequently, the model was applied to 28 wells in the study area.

Further preprocessing and validation steps were applied, including cross-validation (k=3), which provided a balanced assessment of the model's generalizability and performance stability across different subsets of the data (Figure 3) (Geron, 2019; James et al., 2023). Hyperparameter tuning was performed using a grid search strategy over a defined parameter grid (Bergstra & Bengio, 2012; Pedregosa et al., 2011), including 'n_estimators,' 'max_features,' 'max_depth,' 'min_samples_split,' and 'min_samples_leaf.' This systematic search allowed us to identify the optimal combination of parameters, maximizing the model's predictive accuracy for permeability.

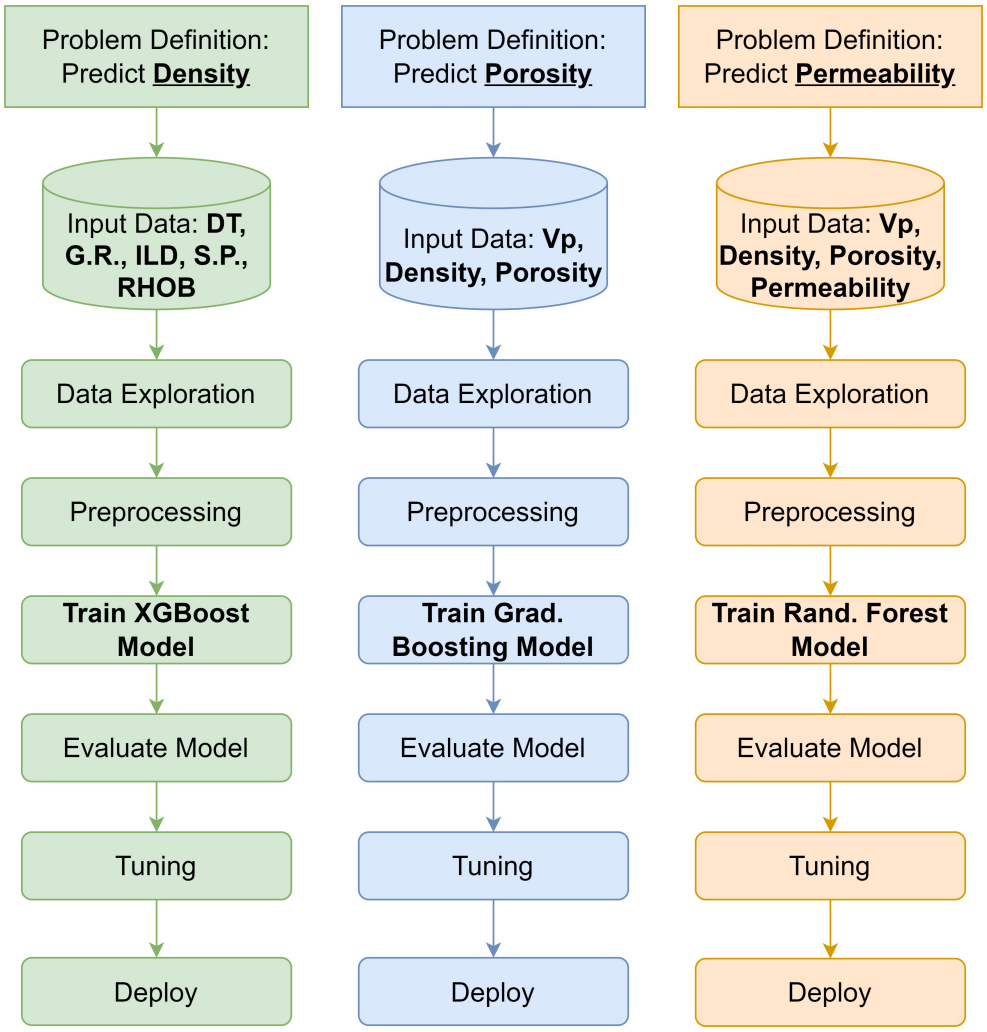

Figure 3: Flowchart used to predict density, porosity, and permeability of basalts in 28 wells of the Paraná Basin.

2.5 Models' performance evaluation

To evaluate the performance of the regression models, we used three metrics: R^2, Root Mean Squared Error (RMSE), and Mean Absolute Error (MAE). SHAP values (SHapley Additive exPlanations) were used to interpret the predictions made by the machine learning models. SHAP uses a game-theoretic approach to measure each input variable's contribution to the outcome (Lundberg & Lee, 2017). Additionally, residual plots were created to evaluate the quality of the model's outputs.

2.6 Models' application

To identify the most suitable sections in the basalts of the Serra Geral Group for carbon storage, the models were applied to the 28 wells in the study area. All well-logging curves were plotted together, focusing on areas with low density and high porosity and permeability. To delineate the most suitable areas, the average values of each petrophysical property were interpolated using regularized splines with tension in GRASS GIS (Cell size = 500 m, Tension = 20) (Team, 2023; Mitášová & Mitáš, 1993; Mitášová & Hofierka, 1993).

3 Results

3.1 Performance of the machine learning models

This study employs advanced machine learning models to analyze key geological parameters critical for carbon capture and storage in the Serra Geral Group basalts at the Paraná Basin. The models evaluated include XGBoost, Gradient Boosting, and Random Forest, each tested for their predictive accuracy and influence of input features.

Figure 4 presents the results of the XGBoost model applied to estimate the density. The bar graph illustrates the mean SHAP values, quantifying the impact of the features on the model's predictions. The P-Wave velocity (Vp) shows the highest mean SHAP value of 0.15, indicating its significant influence on the model's output. Vp had three times more impact on the model's output than the other inputs combined, suggesting that Vp is a critical predictor in the geological dataset.

In Figure 4b, the high value of the Pearson correlation coefficient (R^2) of 0.94, along with low values of RMSE (0.05) and MAE (0.03), indicates that the model achieves an excellent level of accuracy in predicting the density of the basalts. The residuals plot in Figure 4c helps assess the prediction variance, showing a cloud of points centered around the zero line (dashed orange). This distribution suggests that the residuals are relatively small and randomly dispersed, implying that the model's predictions are consistent across different data points without systematic errors.

The application of the equations proposed by X. Chen et al. (2015), Rossetti et al. (2019), and Vedanti et al. (2018) to the test set yielded lower results than those achieved by the XGBoost model. The R^2 values from the empirical equations ranged from -0.63 to 0.65. Meanwhile, the RMSE and MAE varied from 0.11 to 0.25 and from 0.09 to 0.21, respectively.

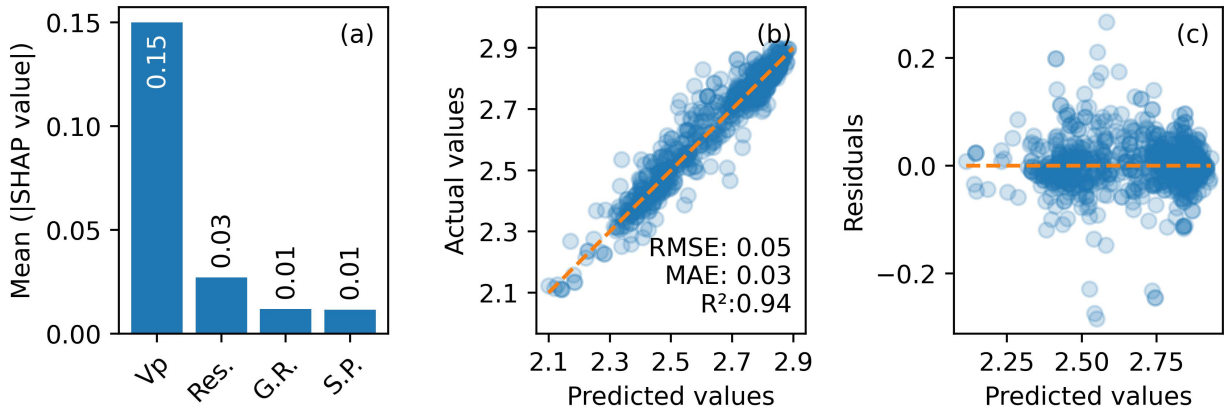

Figure 4: Performance of the XGBoost model used to predict the density of the basalts from Serra Geral Group. (a) Illustrates the mean SHAP values of input variables. (b) Illustrates the correlation between the predicted and actual values. (c) Residuals plot to assess the variance in predictions.

Figure 5 details the performance outcomes of the Gradient Boosting model applied to predict porosity. As in the previous model, the Vp represents the highest impact (SHAP value of 0.25), while the density has a lower impact with a SHAP value of 0.08 (Figure 5a). Although slightly lower than the XGBoost model, the Gradient Boosting model maintains a consistent accuracy, as reflected in the regression metrics (Figure 5b). In Figure 5c, the even distribution of residuals around zero suggests that the model's errors are random rather than systematic, validating the model's generalization ability across various data points.

The application of the equations proposed by Al-Harthi et al. (1999), X. Chen et al. (2015), Navarro et al. (2020), Rossetti et al. (2019), and Vedanti et al. (2018) to the test set yielded lower results than those achieved by the Gradient Boosting model. The R^2 values from the empirical equations ranged from -47.11 to 0.57. Meanwhile, the RMSE and MAE varied from 4.51 to 47.61 and from 3.86 to 46.31, respectively.

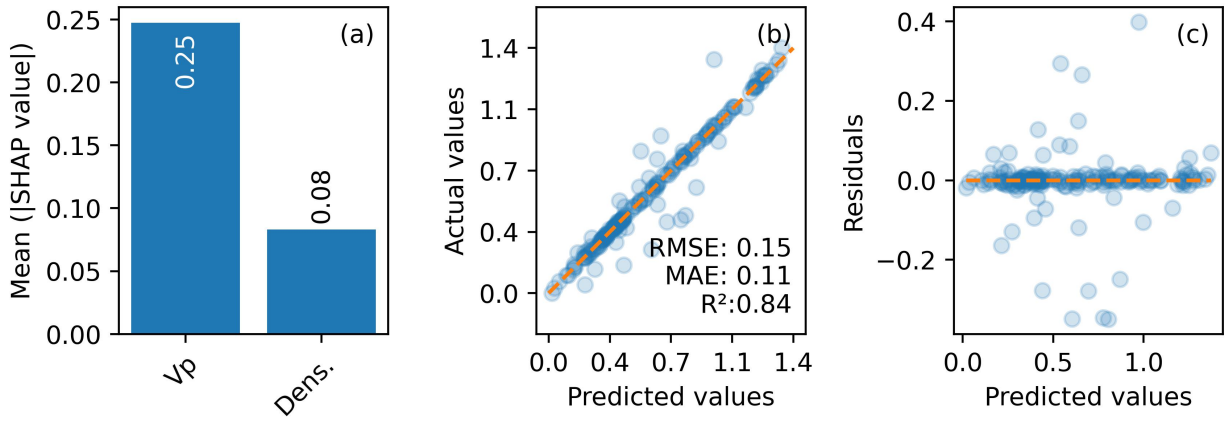

Figure 5: Performance of the Gradient Boosting model used to predict the porosity of the basalts from Serra Geral Group. (a) Mean SHAP values of input variables. (b) Predicted versus actual values graph. (c) Residuals plot to assess the variance in predictions.

Figure 6 details the performance of the Random Forest model applied to predict permeability in basalts. Unlike previous models, all four input features significantly influence the model's output. The interaction term between Vp and density has the lowest impact (0.03), indicating that while the individual features are influential, their interaction provides additional but lesser predictive power.

The scatter plot (Figure 6b) indicates a moderate correlation between predicted and actual values, as reflected in its metrics, making this a model with weaker predictive power when compared to previous models. The residuals plot (Figure 6c) shows a concentration of residuals around zero, albeit with a wider spread than observed in the earlier figures. These results are due to the intrinsic difficulty in modeling permeability in basalts and the quality and quantity of samples available in the literature that were used to train the model. An improvement in these points can possibly help in modeling the complexity of this problem and result in greater predictive power.

The application of the equations proposed by Lamur et al. (2017), Mueller et al. (2005), Navarro et al. (2020) and Yokoyama and Takeuchi (2009) to the test set yielded significantly poorer results than those achieved by the Random Forest model. The R^2 values from the empirical equations ranged from -1.54×10^6 to -8.28×10^2. Meanwhile, the RMSE and MAE were both 0 in all cases.

The results of the three machine learning models show that the P-wave velocity (Vp) is the most impactful input feature, especially for the density and porosity models. The permeability model got moderate results due to the complex nature of the problem. The porosity model got fewer input features but still performed well. The density model performed the best among the models due to its direct correlation with Vp and a large amount of data for data training.

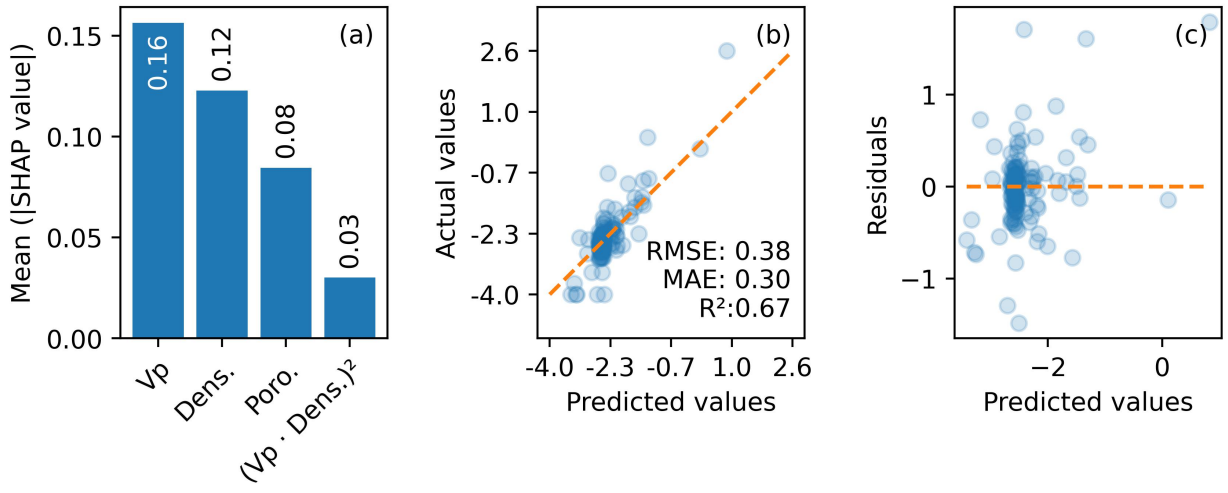

Figure 6: Performance of the Random Forest model used to predict the permeability of the basalts from Serra Geral Group. (a) Mean SHAP values of input variables. (b) Predicted versus actual values graph. (c) Residuals plot to assess the variance in predictions.

3.2 Interpolated maps

The machine learning models were applied to 28 exploratory wells available in the area. Figure 7 presents the interpolated maps of the density, porosity, and permeability of the basalts from the Serra Geral Group in Santa Catarina's State, Brazil.

In Figure 7a, the density map demonstrates notable density gradients, particularly in the southern part of the area, indicating possible subsurface heterogeneities—the areas with high density in the southern part correlate to areas with low porosity and permeability. Maps in Figure 7b and 7c indicate areas of higher porosity and permeability in the northern part, suggesting more permeable zones with higher carbon storage capacity.

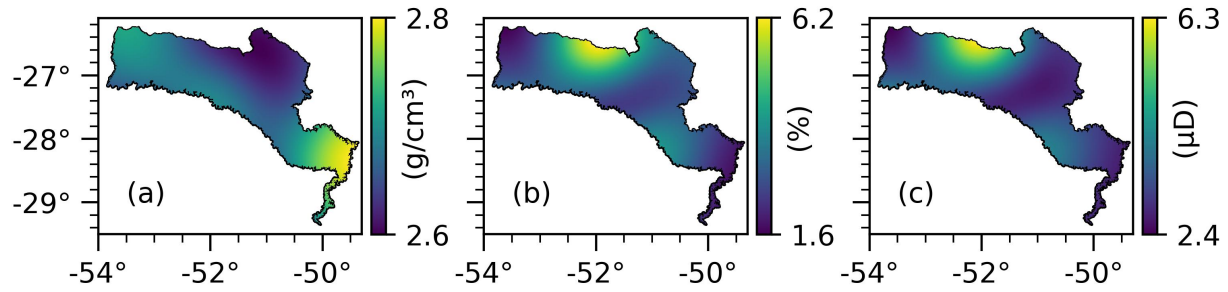

Figure 7: Interpolated maps of petrophysical properties of basalts generated from the application of machine learning models in 28 exploratory wells. (a) Density map. (b) Porosity map. (c) Permeability map. All three maps were interpolated using regularized splines with tension (Cell size = 500 m, T = 20).

3.3 Logging curves sections

The basaltic rocks from the Serra Geral Group present variations in their properties and internal fractures, generating sections more suitable for geological storage than others. Figure 8 presents the well logging curves from the exploratory well located in the high porosity and permeability part of the maps presented previously. The well log identified as 1-RCH-1-SC contains a basalt section from the Serra Geral group with 978 m thickness, and with average values of

2.69 g/cm³ for density, 7.23% for porosity, and 6.51 μD for permeability. The section from 600 to 900 m deep was plotted below.

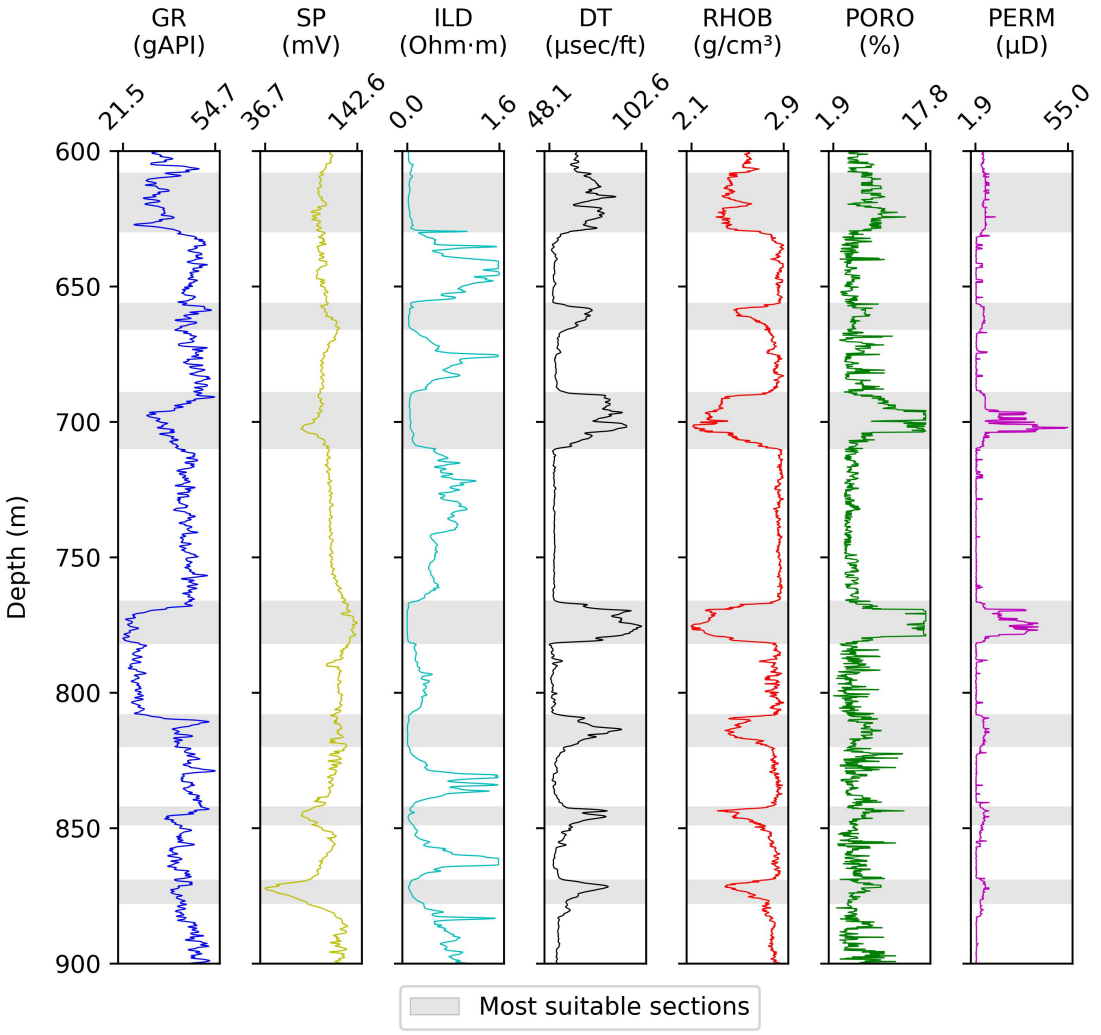

Figure 8: Borehole curves of 1-RCH-1-SC located in a region with high porosity and permeability basalts. Curve names: GR – Gamma Ray, SP - Spontaneous Potential, ILD – Induction Log Deep resistivity, DT – Sonic Velocity, RHOB – Bulk Density, PORO – Porosity and PERM – Permeability. The most suitable sections for geological storage are highlighted in grey.

The highlighted sections in grey represent intervals deemed most suitable for carbon capture and storage based on integrating these log data. From 600 to 900 meters, the most suitable intervals vary from 7 to 22 m thick, with density lows of almost 2.1 g/cm³, high peaks of 17.8% apparent porosity, and 55 μD permeability. These intervals exhibit a combination of favorable porosity, permeability, and other geophysical properties, suggesting they are optimal targets for further investigation and potential implementation of carbon storage solutions.

4 Discussion

By applying more robust solutions (more input features, advanced algorithms, train-test split, and cross-validation) and training the models only with data from basaltic rocks from Serra Geral Group, the models presented more satisfactory results to this dataset than other solutions available in the literature that use more classical statistical solutions and data from different places in the world.

The northern region of Santa Catarina's State has the best petrophysical properties for geological storage in basalts; however, due to the low population density in the area (most of the population of the state is concentrated in the coastal region), the area may not have enough stationary sources to make a project of this magnitude economically feasible (Ketzer et al., 2016). A deeper analysis considering other aspects of the business model is required, such as distance to stationary sources, geochemical factors, and other geological factors.

The logging curves display a cyclic pattern that correlates with different flow characteristics. Specifically, they show low density, high porosity, and high permeability in the top and bottom flows, which can be considered potential reservoirs. In contrast, the interiors of massive flows exhibit high density and low porosity-permeability, making them potential caprocks. Similar patterns are observed in the Columbia River flood basalts (Zakharova et al., 2012). The top and bottom flows are typically associated with vesicular and fractured basalts, whereas the interior flows are characterized by massive, less fractured basalts (Guidicini & de Oliveira Campos, 1968).

5 Conclusions

The success of carbon sequestration in basalts depends heavily on accessing a region with favorable physical properties for mineralization to occur. Predicting basaltic rocks' density, porosity, and permeability is complex, considering their nonlinear relationship and access to data from a specific region.

The three models built with different machine learning algorithms achieved very satisfactory results based on the evaluation of their capabilities of capturing the dataset's complexities and variabilities, surpassing previous solutions available in the literature. The versatility of the models allows them to be applied in other wells to generate maps of the most favorable regions and to determine the most suitable sections for carbon capture and storage.

The northern region of Santa Catarina's State presented the best-predicted properties, with low density and high porosity-permeability. In contrast, the southeast region presented the worst conditions near more stationary sources. Using the well curves, we identified layers that could serve as seal and reservoir layers. These layers exhibited densities of up to 2.1 g/cm³, porosities of up to 17.8%, and permeabilities of up to 55 μD.

The maps and borehole profiles presented can help subsequent investigations with savings in time and human and financial resources. Notwithstanding, the developed models can be applied to other regions of the Serra Geral Group at the Paraná Basin for applications in hydrology, carbon storage, and resource exploration.

6 Acknowledgments

The authors are grateful for the financial support from the Human Resources Program of the National Agency of Petroleum, Natural Gas, and Biofuels (PRH-ANP), supported with resources coming from the investment of qualified oil companies in the R&D Clause of ANP Resolution No. 918/2023 (PRH 33.1 - Regarding the announcement No. 1/2018/PRH-ANP; FINEP/FUSP/USP Agreement Ref. 0443/19). C. Riccomini is funded by the Research Productivity Grant #307471/2022-5 of CNPq-Brazil.

7 Code availability

The code for the machine learning models, along with the data used for training, testing, and map interpolation, is available on GitHub and Zenodo. This repository, titled "Application of machine learning methods to forecast petrophysical properties in basalts of the Serra Geral Group: Implications for carbon storage", is licensed under the MIT License and was developed by João Paulo Alves. For inquiries, please contact João Paulo Alves at joao.guilherme.alves@usp.br. The repository was first made available in 2024 and requires a platform to run a Jupyter Notebook, as the code is written in Python. The GitHub repository is avaliable at `https://github.com/jp-alves/ml_basalts_ccs`, and the Zenodo repository can be accessed at `https://doi.org/10.5281/zenodo.13821458`.

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