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Machine Learning Interpretability Methods to Delineate the Aerosol Formation in the Arabian Sea Near Kerala Coast

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ABSTRACT

Atmospheric aerosols have a significant function in atmospheric systems and hence play a crucial role in climatic changes. Machine learning (ML) models are highly preferred for aerosol estimation because of their exceptional predictive capability. However, it is challenging to justify and understand the predictions made by these ML models. The purpose of this research is to show how model-agnostic interpretation methods - permutation feature importance (PFI) and SHapley Additive exPlanations (SHAP) can be used to enhance and clarify machine learning model prediction of aerosols in the Arabian Sea region near the Kerala coast. Initially, the performance of 3 ML models, Polynomial regression, Bayesian ridge regression and Support Vector Regression (SVR) models are analyzed for estimating the aerosol optical depth (AOD). The study employed Pearson correlation to investigate the relationships between AOD and the various input features and to find the best features for building the ML models. Mean Squared Error (MSE) and Coefficient of Determination (R2) are the performance metrics used to assess these models' performance. Results indicated that SVR model (with R2 = 0.7933 and MSE = 0.0063) provided better predictive performance. Then the predictions of the most accurate model are explained by PFI and SHAP. The ML interpretability analysis showed that the main factors strongly associated with aerosol formation are aerosol radiative forcing at the top of the atmosphere (ARF_TOA), radiative forcing at the surface of the atmosphere (ARF_SURF), sea salt and temperature profile at 250hPa.

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INTRODUCTION

Aerosols are tiny liquid or solid particles suspended in the atmosphere, which originate from natural sources like volcanic eruptions, dust storms, and sea spray, as well as man-made events like burning fossil fuels and industrial operations (Khan et al., 2023). Aerosols are microscopic particles that harm lung tissue and thus result in lung illnesses when inhaled (Yousefi et al., 2020). Situated along the southeast coast of the Arabian Sea, the coastal regions of Kerala, Karnataka, and Goa are significant biological and socio-economic environments that are intricately linked to the climate dynamics of the area. Because landmasses encircle the Arabian Sea on three sides, it is particularly susceptible to aerosol pollution from industrial emissions and dust-laden winds from arid regions. Numerous studies have demonstrated that the thermodynamic structure and cloud properties over this maritime region are greatly impacted by aerosol loading (Elshora, 2023; Yeom et al., 2022). Aerosol-induced perturbations can alter

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various climate parameters, and the resulting changes can have significant impacts on water availability, agricultural productivity, and ecological balance (de Leeuw et al., 2023). Kerala is an agrarian state, hence climatic elements like temperature, precipitation, and cloud formation have a significant impact on the state's water resources and agricultural production. Aerosol Optical Depth (AOD) measures the amount of sunlight blocked by atmospheric particles from reaching the earth (Wei et al., 2020). It measures the amount of light that is lost due to aerosol absorption and scattering. Since AOD has no units, it is a dimensionless quantity. An atmosphere with a higher concentration of aerosols and a higher AOD value is said to be hazier; an atmosphere with a lower AOD value is said to be clearer.

Aerosol pollution, which is defined as the presence of particles smaller than 10 micrometres (PM10), is a major health and environmental hazard, especially in coastal areas of the Arabian Sea that are close to the states of Kerala, Karnataka, and Goa. Recent research has made significant progress in understanding and characterizing aerosols in the marine regions. In order to anticipate PM10 concentrations, ML techniques are employed in several studies by combining meteorological and land-use parameters with satellite-based AOD data (Babu & Thomas, 2023; Karimian et al., 2023). Research on seasonal variability and cloud interactions in oceanic regions of Asia highlights the complex interactions between AOD and cloud and temperature parameters, providing insight into the regional climate dynamics influenced by aerosol-cloud-temperature interactions (Alam et al., 2014). Research works established correlation properties between meteorological indicators and AOD and studies revealed strong connections, especially with respect to atmospheric indices like relative humidity (Boiyo et al., 2018). Deep learning techniques are used for approximating the spatiotemporal characteristics of AOD, with enhanced precision, thus surpassing the drawbacks of traditional techniques and offering significant insights into AOD fluctuations at more precise temporal and spatial resolutions.

ML models are effective instruments for estimating AOD, as demonstrated by the reviewed literature. All of them are regarded as black-box models, nevertheless. This implies that the user will find it challenging to understand these models' internal logic (Ahmed et al., 2024). Interpretability and feature importance analysis are crucial elements of machine learning because they enable users to comprehend how a model makes decisions and determine which features have a major impact on predictions (Ullah et al., 2023). Consequently, interpretable ML contributes to the understanding of the model's behaviour and enhances user trust in its results. Finding the most useful features for the prediction process and comprehending their role in the model's overall performance are the objectives of feature importance analysis (Lundberg & Lee, 2017). Many strategies like SHapley additive explanations (SHAP), accumulated local effects (ALE), permutation feature importance (PFI), and local interpretable model-agnostic explanations (LIME) have been developed recently to overcome these limitations (Jabal et al., 2022).

The interpretability technique PFI is employed to assess the significance of individual features inside a prediction model. PFI is regarded as a model-agnostic technique, which means that any machine learning model can be used to interpret its predictions (Casalicchio et al., 2019). It offers a means of comprehending the characteristics that accelerate the model's results. The effect of permuting or rearranging a particular feature's values on the model's performance is measured by permutation feature significance (Musolf et al., 2022; Oh, 2022). It measures how much the model's performance drops when a feature's values are arbitrarily permuted, highlighting how significant that feature is (Gilpin et al., 2018). Developed around the idea of SHapley values from cooperative game theory, SHAP is a potent framework for analysing machine learning model predictions that permits an equitable distribution of contributions across characteristics according to their influence on the model's predictions (Chaibi et al., 2021). Based on the average contribution of each feature to all potential combinations, the approach assigns an importance value to each feature in the dataset, accounting for every possible combination of feature values (Feng et al., 2021).

In numerous domains, including science, engineering, aeronautics, agriculture, medicine, business, etc., the most important factors affecting a predictive model are now identified using both PFI and SHAP model-agnostic explanation methodologies. This study is carried out with the objective to investigate the intricate relationships that exist between atmospheric aerosols and temperature variations and radiative forcings, in the Arabian Sea region near the Kerala coast, using ML models with PFI and SHAP approaches. This study concentrates on the narrow coastal zone of Kerala, which serves as a transitional area. The aerosol mixture here is a unique combination of sea salt, biogenic emissions originating from the Western Ghats, and pollutants from urban areas. Forecasting AOD in this mixed geospatial setting is considerably more challenging compared to a uniform inland region. Therefore, this research is important as it examines the aerosol dynamics of the Southeast Arabian Sea (coastal corridor)—a region characterized by its distinct location between the Western Ghats and the open sea. This study aims to (1) examine the AOD prediction performances of SVR, Polynomial and Bayesian Ridge Regression Models (2) quantify the relevance of inputs, clarify their effects on each individual estimation, and emphasize their interaction in order to explain the predictions of the best machine learning model using PFI and SHAP approaches, and (3) determine which characteristics are most important in influencing the aerosol production in the study area.

MATERIALS AND METHODS

Study Area and Dataset

The study area of this work is the southeast Arabian Sea region (8-20 °N, 68-76 °E) on the Indian peninsula's southwest coast of the Indian states Kerala, Karnataka, and Goa. The data set contained daily data of 365 days of the year 2015 with 34 features pertaining to air temperature, radiative forcing at different altitudes, and atmospheric aerosols. The year 2015 is selected for the study because of two major climatological events that occurred in the study region: the strongest El Niño ever recorded and notable cyclone activity. In 2015, one of the strongest El Niño events in history occurred, and such strong El Niño occurrences generally lead to a weakening of the Indian Summer Monsoon and change the dust transport patterns from the Arabian Peninsula (Chatterjee et al., 2022). Additionally, the year 2015 was noteworthy because two Extremely Severe Cyclonic Storms namely Chapala and Megh, formed in the Arabian Sea within just eight days of each other, in late October to early November 2015 (Najah et al., 2025). The most potent El Niño intensified the transport of Arabian dust to the shores of Kerala, while the unusual cyclones Chapala and Megh increased the levels of sea salt aerosols, resulting in heightened and fluctuating AOD conditions that were perfect for evaluating advanced prediction models. All the data are obtained from MODIS, MERRA-2 and CALIPSO satellite reanalysis datasets. Measurements of aerosol components namely dust, black carbon, organic carbon, sea salt, and sulphate, as well as aerosol optical depth (AOD) and aerosol radiative forcing (ARF) parameters expressed in Watts per square meter (Wm^-2), namely ARF at the surface (ARF_SURF), ARF at the top of the atmosphere (ARF_TOA), and ARF in the atmosphere (ARF_ATM) and temperature values expressed in Kelvin (K), at various altitudes ranging from 1 meter to 1000 meters are included as features.

During pre-processing stage, the missing or invalid records are removed and the pre-processed dataset contained 363 records. Since the dataset contained 34 features, a feature selection method is applied for finding the most appropriate features that affect AOD. For feature selection, Pearson correlation method was followed to investigate the linear, and monotonic relationships between AOD and predictors like temperature at different altitudes, aerosol constituents like organic carbon, black carbon, dust, sea salt, and radiative forcings.

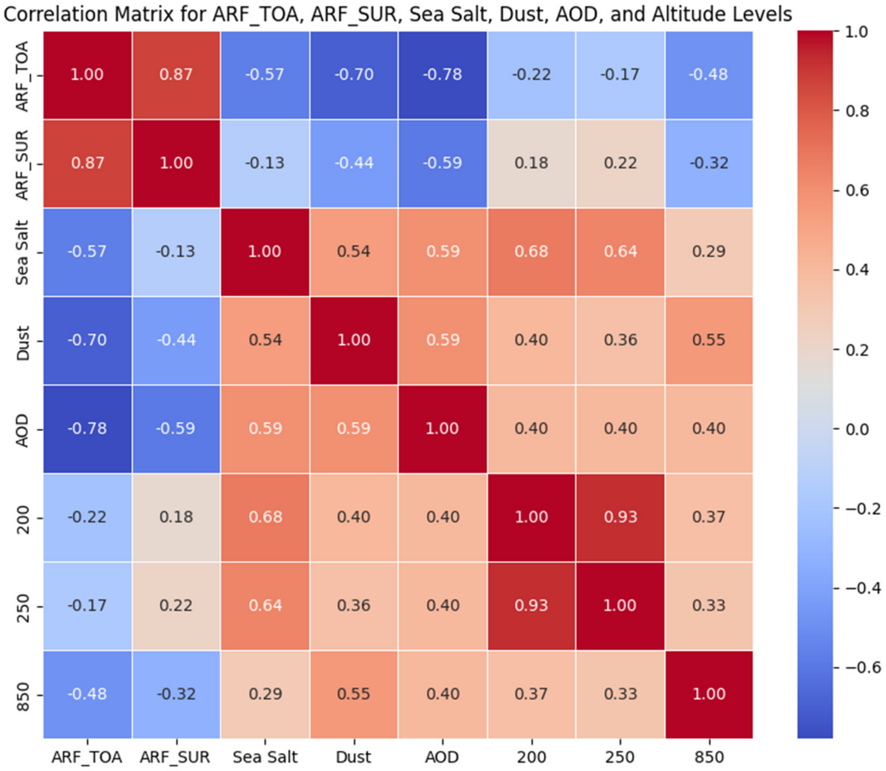

Fig. 1. PCC Heatmap of AOD with 7 Significant Features

The Pearson correlation coefficient (PCC) is used as an initial and computationally efficient filter to identify features that show at least a moderate linear relationship with AOD within a high-dimensional atmospheric dataset. This is a common pre-processing step in climatic ML studies aimed at reducing the dimensionality issue and removing irrelevant predictors prior to SVR training (Jebli et al., 2021a). Although PCC identifies linear relationships, SVR's kernel is specifically designed to capture non-linearities in the reduced feature space; this combined methodology is supported by post-hoc explainable AI techniques: PFI and SHAP, that validate significant non-linear effects among the selected features, such as humidity and wind speed (Z. Liu et al., 2024). This method improves transparency without the need for initial expensive non-linear selections, guarantees training stability in the face of multicollinearity in Kerala's coastal meteorological variables, and is consistent with classical atmospheric modeling.

PCC value is used to quantify the direction and strength of a linear relationship between two variables (Jebli et al., 2021b). PCC value falls between -1 and 1, where, perfect negative linear relationships are denoted by -1, perfect positive linear relationships by 1, and no linear relationships are denoted by 0. Those input features having a PCC value greater than 0.4 are considered as highly correlating variable to AOD. So, the features sea salt, dust, ARF_TOA, ARF_SURF, temperature in Kelvin at altitude levels 200, 250 and 850 are considered for building the models. Figure 1 illustrates the heatmap that describes the PCC between AOD and the input features. PCC showed a strong positive relationship between AOD and dust and sea salt, suggesting that elevated concentrations of these aerosol constituents are associated with elevated AOD values. Similarly, the selected temperature at 3 different altitudes indicated positive correlation with AOD. However, radiative forcing ARF_TOA and ARF_SURF showed a negative correlation with AOD.

Methodology

Three machine learning models namely Polynomial Regression, Bayesian Ridge Regression, and Support Vector Regression were evaluated for AOD estimation using Mean Squared

Error and R^2 as metrics. The most accurate model's predictions were then interpreted using Permutation Feature Importance and SHAP analysis to explain key contributing factors.

Polynomial Regression

Polynomial regression is a machine learning technique that uses a polynomial equation to describe non-linear correlations between predictor and result variables, and it is an extension of linear regression (Li & Yamamoto, 2016). The nth degree of the polynomial is used to model the relationship shared by the independent and dependent variables, x and y. Polynomial regression must be used when the given dataset's data points are ordered nonlinearly (Kim & Oh, 2021). When attempting to cover a non-linear model with a linear model, no data points will be covered. In order to make sure that all of the data points are covered, a polynomial model is employed. Here, a curve rather than a straight line will be appropriate for covering the majority of data points utilizing polynomial models (Matthew & Adeyinka, 2020).

Bayesian Ridge Regression

By incorporating Bayesian concepts, the ML technique called Bayesian Ridge Regression expands traditional linear regression (Y. Liu et al., 2020). Regression coefficients can be estimated while taking the model uncertainty factor into consideration. When there is little or poorly distributed data, this method is especially helpful. In contrast to conventional regression methods, this approach considers model coefficients as probabilistic variables that have predefined prior distributions (Imane et al., 2022). These distributions are then refined using Bayesian principles by incorporating observed data. The method integrates L2 regularization techniques, which add penalties for excessive coefficient values to combat overfitting, making it particularly useful when dealing with highly correlated predictor variables.

Support Vector Regression (SVR)

Support Vector Regression is a machine learning method that solves regression problems by utilizing support vector machines (Comito & Pizzuti, 2022; Zhang & O'Donnell, 2020). In situations when non-linear data patterns or complicated relationships cannot be adequately represented by linear regression, SVR is utilized. The aim of SVR model is to identify a function that maximizes the margin between the projected values and the actual data points and minimizes prediction error while predicting a continuous target variable (Quan et al., 2022). In order to handle variations from expected values, SVR includes determining the ideal hyperplane, which is specified by the weights and bias, as well as including the epsilon-insensitive loss function (Jaafari, 2024). SVR can handle non-linear interactions well because of the usage of kernel functions.

Permutation Feature Importance (PFI)

Machine learning algorithms are becoming increasingly powerful and accurate in their forecasting. But, as these models become more and more like "black boxes," it becomes harder and harder to figure out how they arrived at their predictions (Agarwal & Das, 2020). Thus, the model's interpretability and explainability become essential elements of the machine learning process. PFI is a widely used interpretable machine learning technique proposed by Leo Breiman for random forests and it is a widely used tool for illustrating how the features impact the overall prediction (Breiman, 2001). Fisher et al. made a substantial contribution to the comprehension and utilization of this technique by expanding its applicability to encompass all machine learning models, especially concerning feature evaluation and model interpretation (Fisher et al., 2019). PFI is a global model-agnostic explanation method that finds the most significant aspects underlying target variable prediction (Molnar et al., 2020). PFI helps to determine which features are most significant in the black-box model. In this study, the error term used in PFI is the mean squared error.

SHapley Additive exPlanations (SHAP)

A methodology for analyzing the machine learning model output is called SHapley Additive Explanations. In order to help users better understand model predictions, Scott Lundberg and Su-In Lee developed SHAP in 2017 (Lundberg & Lee, 2017). It is a model-agnostic tool that provides visually appealing explanations at both the local and global levels, making it a method for interpreting machine learning models (Ullah et al., 2023). The foundation of SHAP is the idea of SHapley values found in cooperative game theory. By giving each input feature an importance value, it may be utilized to explain the predictions of any ML model (Ahmed et al., 2024). To distribute the model's output's credit among its input features, we use the SHapley value. The contribution of each feature is indicated by its SHapley value, which indicates how the prediction would have changed if the feature hadn't been there. SHAP can assist in feature selection and model optimisation by highlighting the most important features (Babu & Thomas, 2025; Zheng et al., 2023).

Performance Metrics

The coefficient of determination (R^2) and mean squared error (MSE) are the performance measures chosen to assess the robustness of the developed ML models in predicting AOD. R^2 expresses relationship between actual and anticipated AOD values. MSE is the average of the squared differences between the actual and estimated values (Tatachar, 2021). When R^2 is close to 1 and MSE is close to 0, the ML model can attain excellent predictive performance.

RESULTS AND DISCUSSION

The dataset was randomly split into two subsamples, 20% for testing and 80% for training, in order to develop the ML models. The selection of hyperparameters in ML models as well as the training and testing data can have a significant impact on the models' performance.

In the initial run, the 3 models were fitted on the training data and then checked with the test data during testing phase. Then the predictive performance of three regression models was assessed. In terms of predictive capability, the polynomial regression model performed best at 78.4%, followed closely by SVR at 78.3%, whereas Bayesian ridge regression yielded 71.6%. Then hyperparameter tuning was done for the 3 models and again performance was analyzed. SVR's prediction increased to 79.3% after hyperparameter adjustment with Grid Search Cross-Validation. The optimal parameters of SVR model are listed in Table 1. On the other hand, Polynomial Regression model's predictive performance dropped to 76.3% following tuning process. The predictive capability of the Bayesian Ridge Regression reduced to 69.8% after hyperparameter tuning.

The performance measurements of 3 models in terms of the metrics MSE and R^2 are demonstrated in the Table 2. These results demonstrated that SVR attained the highest prediction performance, especially after hyperparameter modification. When using the ideal parameters, SVR produced R^2 score of 0.79 and MSE of 0.0063, which show excellent predictive performance and a good fit to the data. Polynomial Regression produced a somewhat less accurate fit, as

Table 1. Optimal Hyper Parameters of SVR model

Parameters	Value
C	0.10
Degree	3
Epsilon	0.01
Kernel	Poly

evidenced by its slightly higher MSE of 0.0066 and lower R^2 score of 0.78. Bayesian Ridge Regression performed inferior, with a higher MSE and a lower R^2, indicating less predictive performance. For AOD prediction, the SVR model's R^2 of 0.79 is reasonable and competitive, matching or surpassing standards in related atmospheric machine learning research (Song et al., 2023). The SVR model beats linear baselines like Polynomial Regression in spite of issues like data sparsity, multicollinearity from monsoon variability, and non-stationarity related to that year's delayed monsoon beginning and growing Arabian dust activity.

The prediction performance of the three ML models in predicting AOD values during testing phase is depicted in Figure 2, Figure 3 and Figure 4 respectively. In the test dataset, each point

Table 2. Performance Metrics of the three ML models

Model	MSE	R^2
Hyperparameter tuned SVR	0.0063	0.79
Polynomial regression	0.0066	0.78
Bayesian ridge regression	0.0086	0.71

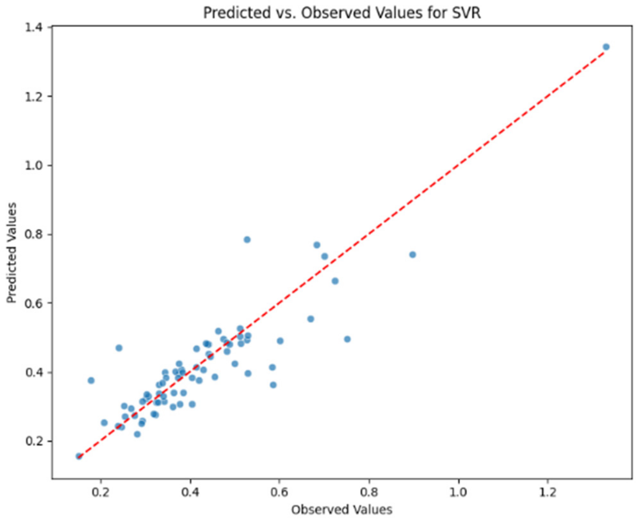

Fig. 2. Prediction Performance Plot of SVR Model

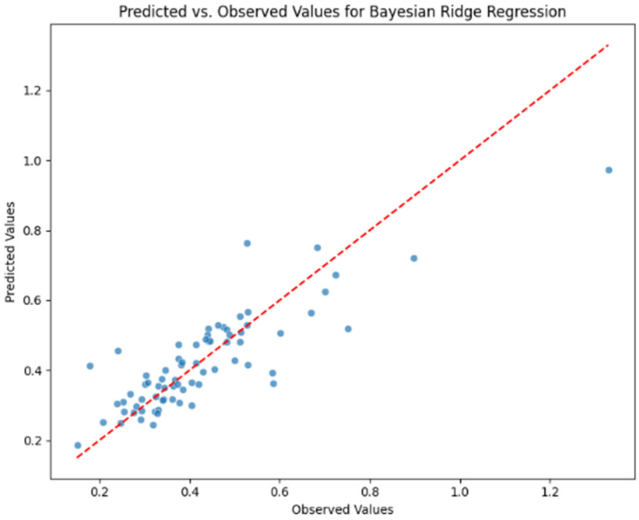

Fig. 3. Prediction Performance Plot of Bayesian Ridge Regression Model

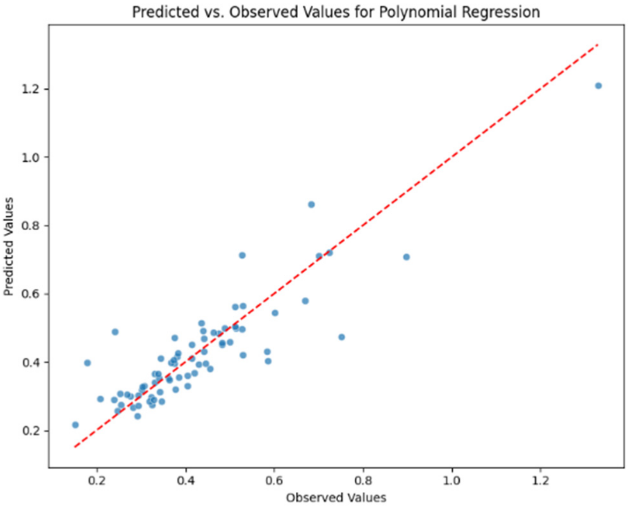

Fig. 4. Prediction Performance Plot of Polynomial Regression Model

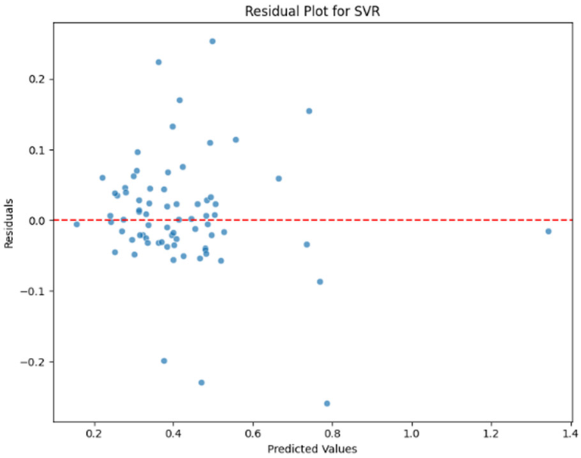

Fig. 5. Prediction Residuals of SVR Model

on the figure denotes a single observation. A diagonal line connecting every point signifies that the model's predictions and actual values are exactly in line with each other.

As shown in Figure 5, SVR model retains a reasonably low mean residual, providing predictions that are generally near to observed values. The SVR model, which strikes a balance between better prediction and dependability, is the best of the three for predicting AOD, given its lower MSE, consistent residual distribution, and higher R2 value. So, it can be concluded that SVR model exhibited better prediction performance in forecasting AOD values.

In the next stage, the interpretability of the machine learning algorithms is explained using two interpretation methods - PFI and SHAP. PFI and SHAP methods are utilized to assess the impact of predictor variables on the predictions made by the most accurate model SVR only. The contribution of each feature to the SVR model's predictions was revealed via SHAP values, which gave a thorough grasp of how specific variables affected the SVR prediction performance. PFI was utilized to determine the significance of features by analyzing how feature permutation affected the SVR model's performance. Both PFI and SHAP illustrated the quantitative nonlinear interactions between AOD and the various predictor variables.

Feature Importance Analysis using PFI

In this section, the significance of each feature for AOD estimation is evaluated using PFI, in order to determine which features worked best. PFI scores of the 7 investigated predictors are shown in Figure 6. The top most features that affect AOD are radiative forcing at the top of the atmosphere (ARF_TOA), temperature at 250hPa altitude, dust, radiative forcing at the surface (ARF_SURF) and sea salt. These two radiative forcings are widely used in aerosol profile modelling conventionally. The PFI scores of the remaining features are negligible.

Feature Importance Analysis using SHAP

PFI technique finds the most significant features and provides global explanations. SHAP approach, on the other hand, can offer both local and global explanations. SHAP assesses the importance of features, clarifies their influence on model predictions, and explains individual observation results. SHAP values decompose model predictions into additive contributions from each feature, including AOD. Unlike PFI, SHAP provides instance-level explanations, revealing how AOD estimates are influenced by the specific input features.

The explanation produced by the SHAP approach for a randomly selected AOD value 0.40 from the test dataset is displayed in Figure 7. The negative SHAP values are shown on the left side of this figure and the positive SHAP values are shown on the right side. Local interpretations are averaged using absolute SHAP values for each feature to obtain a global interpretation of the SVR model for AOD predictions. The mean model prediction throughout the test data set is represented by the base value of 0.432. Red predictions are those that move the estimation beyond the base value, and blue predictions move it below. Table 3 displays the feature values for these observations together with the feature contribution to the 0.40 AOD output value for the SVR model. It is observed from Table 3 that the highest contribution is made by the feature ARF_TOA. Moreover, the features sea salt, 200hPa and 850hPa pushed the prediction

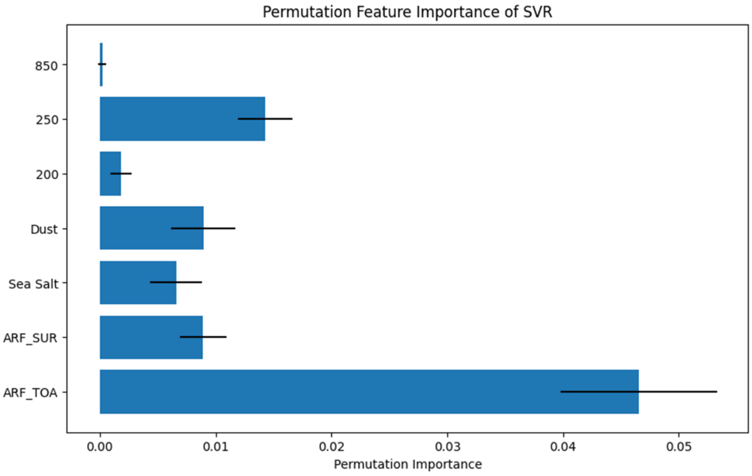

Fig. 6. PFI Scores of the Seven Features based on SVR model

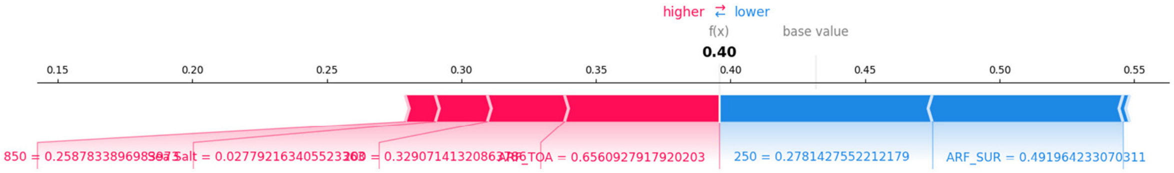

Fig. 7. Explanation of the SVR Model's Output Value of 0.40 using SHAP

Table 3. Feature Contribution for the SVR Model's Output Value of 0.40 using SHAP

Features	Value	Contribution
ARF_TOA	0.656	+0.06
ARF_SURF	0.492	-0.07
250hPa	0.278	-0.08
Sea salt	0.028	+0.02
200hPa	0.329	+0.03
850hPa	0.259	+0.01
Dust	0.095	-0.001

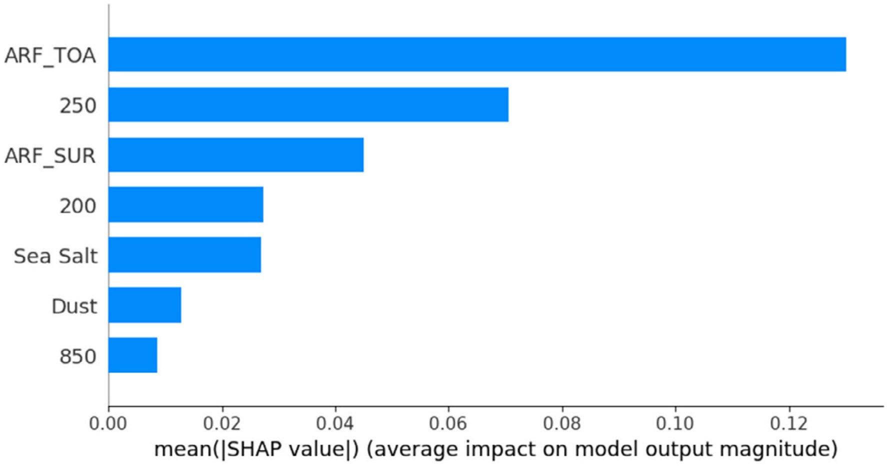

Fig. 8. SHAP Feature Importance Plot

to the right with values +0.02, +0.03 and +0.01respectively. On the other side, ARF_SURF and 250hPa pushed the prediction to the left by −0.07 and −0.08 respectively. The estimated AOD output value is $0.432 + 0.06 + 0.03 + 0.02 + 0.01 - 0.08 - 0.07 - 0.001 \approx 0.40$

The SHAP feature importance plot, shown in Figure 8, illustrates how each feature affects AOD estimation globally. SHAP method indicated that ARF_TOA, 250hPa temperature and ARF_SURF are the most significant features, while temperature at altitude 850hPa is the least effective feature. Sea salt and temperature at altitude 200hPa demonstrated similar moderate contribution in prediction of AOD, while dust showed lesser contribution in the prediction.

CONCLUSION

This research demonstrates how machine learning models, coupled with interpretability techniques like SHAP and Permutation Feature Importance (PFI), advance the precision and understanding of AOD predictions in Kerala's Arabian Sea region. The goal of this research is to leverage machine learning approaches for achieving superior accuracy and detailed characterization of atmospheric aerosols based on aerosol composition data, temperature distributions, and radiative forcing observations. Three ML models are employed for predicting AOD values in the Arabian sea region of Kerala. The results revealed that SVR model illustrated the best performance across the metrics MSE and R2, when compared to polynomial regression and Bayesian ridge regression models. Two model-agnostic interpretation techniques – PFI and SHAP are then used to explain the predictions of the SVR model. The analysis results of PFI and SHAP demonstrated the value of applying interpretation techniques to improve and clarify ML models' prediction capabilities. Both the PFI and SHAP methods demonstrated that ARF_TOA is the most important feature, followed by features namely temperature at altitude 250hPa, ARF_SURF and sea salt. By using these interpretation methods, it is possible to clarify the learned associations between predictors and aerosol formation, providing a data-driven perspective on potential drivers of regional aerosol variability in the study area. Overall, by bridging data-driven predictions and climate mechanisms, the study highlights the value of interpretable ML in reducing uncertainties in aerosol-climate models, guiding targeted monitoring of critical variables like ARF_TOA, and informing policies to mitigate aerosol-induced regional climate changes.

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CONFLICT OF INTEREST

The authors declare that there is not any conflict of interests regarding the publication of this manuscript. In addition, the ethical issues, including plagiarism, informed consent, misconduct, data fabrication and/ or falsification, double publication and/or submission, and redundancy have been completely observed by the authors.

LIFE SCIENCE REPORTING

No life science threat was practiced in this research.

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