ENVIRONMENTAL DATA SCIENCE SESSION

ARTIFICIAL INTELLIGENCE-BASED FRAMEWORK FOR ANALYZING CRISES-CAUSED AIR POLLUTION

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Abstract:

Understanding the impact of air pollution processes during a crisis is crucial due to the significant risk to human health and to ensure global sustainability. Addressing this issue, this study introduces a novel artificial intelligence-based framework designed to analyze air pollution alterations caused by crises. The framework utilizes seven machine-learning regression models for making predictions: AdaBoost, CatBoost, ExtraTrees, Gradient Boosting, Histogram Gradient Boosting, LightGBM, and XGBoost regressor. Cross-validation is employed to ensure the robustness of the models and to prevent overfitting. The framework includes different metaheuristics algorithms, such as the Firefly Algorithm, Artificial Bee Colony, Harris Hawks Optimization, Sine Cosine Algorithm, Slime Mould Algorithm, and Quantum Superposition Algorithm. The top three performing ensemble models are optimized with the selected metaheuristic algorithm to find the optimal set of hyperparameters and to improve the results. After the optimization process, the best model is selected and evaluated on the dataset, then for explainability, SHAP and SAGE analysis are applied to provide deeper insight into the factors that influence the best model's predictions. These techniques ensure that the models are not only making precise predictions but also transparent and interpretable, which allows informed decision-making. Finally, the obtained results are visualized interactively for easier analysis of underlying patterns. This study lays the groundwork for a more effective crisis management system to mitigate the adverse of human health and environmental outcomes associated with air pollution caused by crises.

Keywords:

Artificial Intelligence, Machine Learning, Explainable Artificial Intelligence, Metaheuristics, Air Pollution.

INTRODUCTION

Air quality is a critical environmental factor that greatly impacts human health and global environmental sustainability. The quality of the air is directly linked to various health issues, including respiratory diseases, cardiovascular conditions, and overall well-being [1]. During crises, such as the COVID-19 pandemic and war, understanding and analyzing air quality becomes even more important due to the alterations of pollution levels. While extensive research has been conducted on air pollution and its impacts, there remains a need for innovative methodologies that can effectively characterize and predict air quality alterations during crises.

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Traditional monitoring and modeling approaches often fail to comprehensively capture air pollution patterns. This study introduces a novel artificial intelligence-based framework designed to characterize and predict air quality alterations during crises, the framework is named crAIRsis. The framework includes seven ensembles of advanced machine learning regression models and incorporates different metaheuristic optimization to precisely adjust the model parameters, enhancing the precision of the prediction. Additionally, the incorporation of explainable artificial intelligence (XAI) is crucial for supporting the output of a model [2]; the deployment of XAI techniques, such as SHapley Additive exPlanations (SHAP) and Shapley Additive Global importance (SAGE) analyses, allows users to understand better and to trust the result of the model, as well as helps in informed decision-making. This research presents significant advancement in environmental and crisis management.

The remainder of the paper is organized as follows: Section 2 describes the machine learning models incorporated into crAIRsis framework; Section 3 details the optimization and evaluation processes, as well as the application of XAI techniques; Section 4 outlines the workflow of the framework, and Section 6 concludes the work and gives potential directions for future work.

2. MACHINE LEARNING MODELS

This section briefly describes the regression ensemble machine learning algorithms employed in crAIRsis framework: AdaBoost, CatBoost, ExtraTrees, Gradient Boosting, Histogram Gradient Boosting, LightGBM, and XGBoost regressor, highlighting their strengths and uniqueness. In general, ensemble methods combine multiple machine learning models to create a single model, which results in improved quality of the prediction and robustness [3]. Additionally, ensemble methods effectively reduce overfitting, which is crucial for prediction reliability.

AdaBoost [4], short for Adaptive Boosting, is an ensemble technique that combines multiple weak learners to form a single strong model, the method assigns equal weights to the data points, and then iteratively adjusts the weights of instances based on their error, in every other iteration the instances with higher error have higher weights, which gives more importance and improves the prediction over time. This continuous refinement is particularly advantageous in the prediction of air pollution alterations, where predictions can be highly variable due to fluctuating environmental factors. CatBoost [5] is a relatively novel gradient boosting algorithm, the algorithm automatically handles categorical features, effectively reduces overfitting with a novel gradient-boosting scheme. The algorithm has two important innovations, the introduction of ordered boosting, and handling categorical features. Light Gradient Boosting Machine, in short LightGBM, is a high-performance gradient boosting method that uses tree-based learning algorithms [6]. This method is particularly efficient on large datasets because of the utilization of Gradient-based One-Side Sampling technique that is introduced by the authors of LightGBM. The second innovative techniuque in the paper is the Exclusive Feature Bundling, which allows handling large number of features. The algorithm is very efficient in terms of memory consumption and computational speed. Extreme Gradient Boosting (XGBoost) is well-known ensemble machine learning algorithm, with great performance on different problems, in terms of speed and quality of prediction. The algorithm supports several loss functions and enhancements to the basic gradient boosting algorithm, including regularization features to prevent overfitting. Additionally, the algorithm can manage missing data. XGBoost constructs trees in parallel, unlike other traditional Gradient Boosting Decision Tree (GBDT) methods [7] which builds trees sequentially. Gradient Boosting (GB) model is incorporated from the sklearn Python package [8], it is a powerful machine-learning technique that produces a prediction model in the form of an ensemble of weak prediction models. GB builds the model in forward stage-wise fashion and generalizes it by allowing optimization of an arbitrary differentiable loss function. Histogram-based Gradient Boosting is an advanced implementation of the gradient boosting method that uses histograms for decision tree learning, which speeds up the training process and reduces memory usage by discretizing the continuous feature values into bins and using these bins to construct the decision trees. This method is particularly useful for processing large and complex datasets.

The framework uses cross-validation to rigorously evaluate the performance of each model, and to ensure that each subset of the dataset is used both for training and validation [9]. This method helps in generalization to the dataset and minimizes the risk of overfitting. The cross-validation setup includes random shuffling of the data to prevent any biases that may influence the results due to the ordering of data points. Each of the seven ensemble models has unique strengths, making them suitable for inclusion in the crAIRsis framework. After the seven models are trained and evaluated on the dataset, the top three performing algorithms are selected for the given problem and further optimized to achieve better results and select the final best model based on the evaluation criteria.

3. MODEL OPTIMIZATION, EVALUATION, AND INTERPRETATION

The quality of machine learning models highly depends on the values of its hyperparameters. Hyperparameter tuning is an optimization process, and it belongs to NP-hard problems, where metaheuristics are shown to be successful [10], [11], [12], hence the crAIRsis framework, utilizes metaheuristic optimization algorithms for fine-tuning the best three models' hyperparameters and enhancing the quality of prediction. The following metaheuristic algorithms are implemented in crAIRsis framework to efficiently explore and exploit the search space and find near-optimal solutions: Firefly Algorithm (FFA) [13], Artificial Bee Colony (ABC) [14], Harris Hawks Optimization (HHO) [15], Sine Cosine Algorithm (SCA) [16], Slime Mould Algorithm (SMA) [17], and Quantum Search Algorithm (QSA) [18]. After optimizing the three best models and the set of optimal hyperparameters are identified by using the selected metaheuristic algorithms, the final best model is selected. For evaluating the performance of the models, different regression metrics are used, providing different insights, specifically: mean absolute error, mean squared error, mean absolute percentage error, R-squared, explained variance, and max error are used for evaluation purposes and the best model is selected based on the R-squared value.

In the domain of artificial intelligence, to create a trustworthy system and have human-understandable model, why specific decisions and actions made by the models are very important. Consequently, after selecting the best performing model, crAIRsis uses XAI techniques for interpretability, explainability, and transparency; specifically SAGE [19] and SHAP [20] XAI methods are used.

SAGE represents a global interpretability method that measures the importance of each feature in the dataset. The method extends the Shapley value concept from game theory to feature importance in machine learning. SHAP values explain the prediction of an instance by calculating the contribution of each feature to the prediction. By analyzing SHAP values across the entire dataset, we gain insights into the general behavior of the model, identifying patterns and trends in feature contributions. After obtaining all results, the dataset, the obtained results of the model and XAI are visualized in an interactive web application to make the AI system result analysis and interpretation more user-friendly.

4. DATASET AND FRAMEWORK WORKFLOW

The crAIRsis AI-based is a multiapproach framework. First, the data is collected from different reliable sources. Before modeling, data preprocessing is conducted to prepare the data for the framework. The selected datasets are input into the framework. The user selects the target or more targets and the metaheuristic algorithms for optimization. Initially, the framework automatically creates folders for saving all results, and then starts the training and optimization process. In this process, separate models are created for the period before the crisis, during the crises and after the crises, combined by each target and measurement site. Afterwards, the dataset split is carried out in 80:20 ratio, 80% for training and 20% for testing purposes. The preprocessed data for the given measurement site, period, and target is evaluated by the ensemble machine learning algorithms, using 5-fold cross-validation, then cross-validation prediction is carried out and the metrics are calculated and saved. Based on the evaluation metrics, the best three models are selected and optimized by one or more metaheuristic algorithms. In this process, the optimization history is saved, as well as the result of the three optimized methods. In the next step, the best model is selected, based on the R-squared value.

In the second stage, by using the best model, the crAIRsis framework works on the explainable part. The impact of each feature is analyzed by SAGE's marginal imputer and permutation estimator, and the calculated values of global impact, sensitivity, and their standard deviation, along with absolute and relative measures are saved. To understand the impact of individual features and their interaction on model prediction, the framework uses SHAP to compute the absolute, relative [21], and normalized impact and saves the results for further analysis. In this process, the main effect and the interaction values are also calculated and saved. For deeper understanding and interpretation, cluster analysis is performed using the SHAP values. Uniform Manifold Approximation and Projection (UMAP) [22] used for dimensionality reduction and clustering is performed by Hierarchical Density-Based Spatial Clustering of Applications with Noise (HDBSCAN) [23], which allows identifying groups of similar data points and outliers. The framework saves the dimensionality-reduced data, cluster probabilities, and detailed statistics. The crAIRsis flowchart is depicted in Figure 1 and an examples of the visualizations are presented in Figure 2-6.

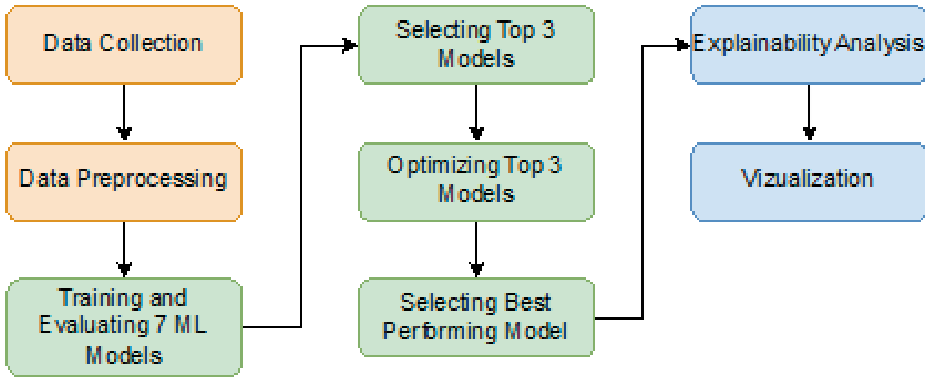

Figure 1. crAIRsis Framework Workflow.

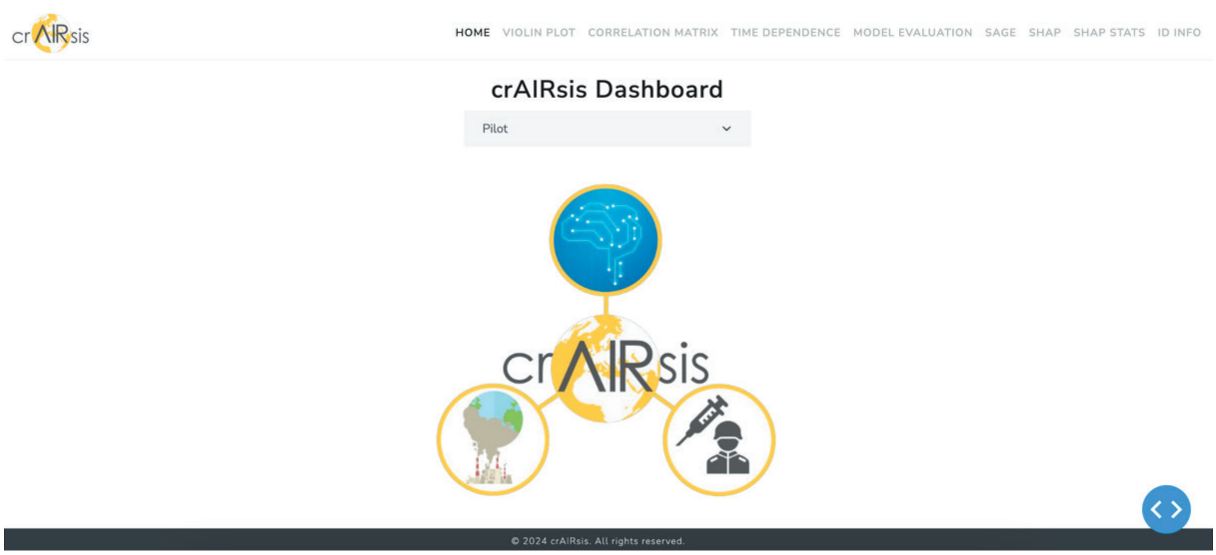

Figure 2. crAIRsis Dashboard visualization.

Figure 3. crAIRsis Dashboard visualization – Time series plots.

Figure 4. crAIRsis Dashboard visualization – Model Evaluation.

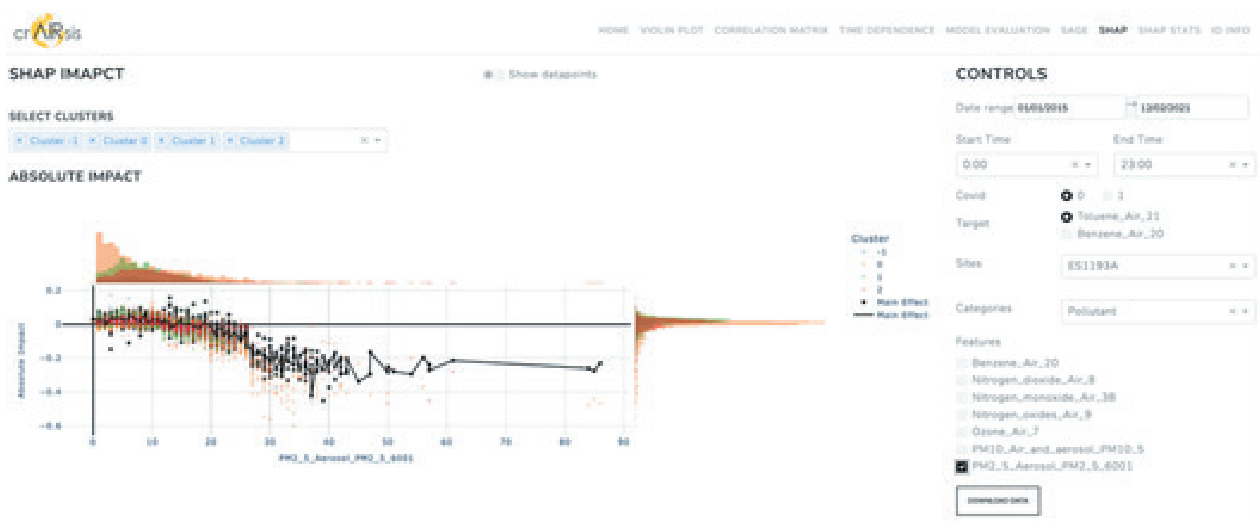

Figure 5. crAIRsis Dashboard visualization - SHAP.

Figure 6. crAIRsis Dashboard visualization - SAGE.

5. CONCLUSION

This study introduces a robust artificial intelligence-based framework, crAIRsis for analyzing and predicting alterations in air pollution during crises. By integrating advanced ensamble machine learning models for regression, cross-validation and optimization techniques, the framework has demonstrated a high degree of reliability. Additionaly, the explainable AI techniques providea deep insights into the driving factors behind the models' actions and decision. The deployment of crAIRsis offers significant potential in making informed decisions during environmental crises. The interactive visualizations allow easier interpretations and analysis for practicioners.

As future work, the framework presents opportunities for expansion, such as implementing methods for classification problems, development, and implementation of hybrid metaheuristics for more efficient hyperparameter optimization. Additionally, there is a potential for integrating Large Language Models (LLMs) and automatize the interpretation. The current framework lays a solid foundation for analysing air pollution alterations during crises, the continued incorporation of novel AI methodologies promises further improvement.

6. ACKNOWLEDGEMENTS

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