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AI-Driven ESG Scoring Model for Sustainable Investment in Digital Markets

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ABSTRACT

Sustainable investment has become a critical focus area, with Environmental, Social, and Governance (ESG) criteria gaining significant importance in financial decision-making. Traditional ESG evaluation methods often struggle with accuracy, transparency, and consistency, which can hinder effective sustainable investment analysis. This study proposed an AI-driven framework designed to enhance the accuracy of ESG score predictions, utilizing the Slime Mould Algorithm (SMA) for feature selection and Random Forest Regressor (RFR) for model training. The framework optimizes feature selection by identifying the most relevant ESG factors, improving prediction accuracy and reducing model complexity. Key preprocessing steps, including missing value imputation, duplicate removal, outlier handling, and data normalization, are incorporated to ensure data quality and reliability. Experimental results demonstrate improved predictive performance, with the proposed model achieving a Root Mean Square Error (RMSE) of 0.3649, Mean Absolute Error (MAE) of 0.2538, and R^2 of 0.9912, outperforming existing approaches. These results confirm the effectiveness of the proposed framework provided for ESG score prediction and highlight its applicability as a decision-support tool for sustainable investment in digital market environments. By providing reliable and transparent ESG score predictions, the proposed model supports data-driven sustainable investment analysis. Future work may explore real-time ESG data integration, model scalability, and explainable Artificial Intelligence (AI) techniques to further enhance ESG assessment across diverse sectors.

Keywords: ***Artificial Intelligence, Environmental, Social, and Governance scoring, Slime Mould Algorithm, Random Forest Regressor, sustainable investment***

1. INTRODUCTION

The academic field of sustainable investment research has grown rapidly during the present time because investors nowadays assign greater importance to ESG factors when assessing their investments decision processes [1], [2]. The rising environmental awareness and societal injustice and governance deficiencies have made ESG criteria essential for modern investment methods according to the research findings [3]. Shareholders demonstrate a strong preference to support organizations with superior ESG performance since they believe these organizations have better capabilities to handle long-term risk and sustainability challenges [4]. The current methods used to assess ESG performance encounter three main problems which include inconsistent results and imprecise measurement and insufficient adaptability to digital data ecosystems which use data-driven approaches [5]. The existing ESG assessment systems require advanced AI technologies to create transparent and consistent data-driven decision processes which will improve sustainable finance operations [6], [7].

Researchers use rule-based systems and linear regression and machine

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learning models which include Random Forest and Support Vector Machines and k-Nearest Neighbors to assess ESG performance from existing evaluation techniques [8]. The techniques demonstrate partial effectiveness but they present significant drawbacks to their application.[9]. Rule-based systems lack the flexibility to incorporate complex, non-linear relationships between various ESG factors [10]. The data interactions which need to be captured exceed the limitations of linear regression models which require a basic understanding of data interactions between numerous elements [11]. The ML methods Random Forest and SVM achieve better results yet these methods face criticism because they create overfitting problems and perform unfairly with certain groups and require complex processes for selecting features [12]. Markowitz Mean-Variance Optimization uses normality assumptions to restrict its optimization capabilities because it cannot handle ESG criterion changes which occur during a project's life cycle. ESG investment decisions become less precise when these problems exist because they hinder organizations from making immediate and ongoing investment assessments [13], [14].

Motivated by these limitations, this study proposes an AI-driven ESG scoring framework that enhances prediction accuracy through optimized feature selection and robust regression modeling. The proposed framework improves the level of predictivity and model robustness by determining the most relevant indicators of ESG and eliminating places where the mitigation features overlap. The obtained ESG scores may serve as reliable electronic indicators to enhance sustainable investment analysis in digital market settings. These challenges motivate the adoption of computational optimization techniques for developing intelligent ESG prediction systems. This method enhances accuracy, clarity and credibility of ESG evaluations; hence, promoting the use of informed decision-making in sustainable finance.

1.1 RESEARCH OBJECTIVES

- To develop an AI-based ESG scoring framework using Random Forest Regression for reliable ESG score prediction.
- To analyze firm-level and financial attributes of S&P 500 companies influencing ESG performance.
- To apply the Slime Mould Algorithm to select the most relevant non-ESG features while reducing model complexity.
- To evaluate the predictive performance of the proposed framework using standard regression metrics.

1.2 RESEARCH SCOPE AND NOVELTY

The study developed an AI-based model to predict ESG scores with improved accuracy and better performance than existing methods. The new methodology developed in the novelty uses SMA for feature selection and RFR for prediction which produces more accurate results while needing less computation power than conventional methods. The proposed framework integrates computational optimization with machine learning to enhance intelligent ESG prediction performance. The framework creates an innovative data-driven tool for sustainable investment decision-making which solves the problems of existing ESG evaluation methods and demonstrates how AI technology benefits financial institutions.

1.3 RESEARCH ORGANIZATION

The paper is structured as follows: **Section 1** is an introduction to the research, which outlines the objectives and scope of the study. **Section 2** explains the methodology that was used with the data collection method and algorithms applied. **Section 3** the experimental set-up is described along with the performance evaluation metrics. **Section 4** provides the discussion of the results and analysis of the proposed framework. **Section 5** is a conclusion of the paper and proposals of possible future research direcstions.

2. LITERATURE SURVEY

Elhady & Shohieb, [15] the purpose of the review is to evaluate the effectiveness of AI in sustainable finance; specifically, in ESG scoring models, by analyzing 43 peer-reviewed articles and 23 institutional reports. They draw parallels of machine-learning-based models as opposed to rule-based systems and concentrate on predictive analytics, the impact measurement, and risk management in climate-related investments. The paper presents another index of ESGAI Maturity Index to measure the level of institutional preparedness toward the use of AI, which demonstrates the effectiveness of AI models with consideration of issues such as algorithm bias and the lack of data. Sundharesalingam et al., [16] examine how to bring together AI and Financial Technology (FinTech) as a propulsion of ESG investments in Sustainable Finance. It will look at the lack of transparency and social responsibility, as applied to traditional financial systems to meet the demand of transparent investments, and analyzes the radical nature of artificial intelligence and blockchain in relation to ESG analyses. It proposes unified legal frameworks, joint efforts and innovative interdisciplinary studies to consider financial innovation in ESG principles of a sustainable financial ecosystem.

Nevi et al., [17] discuss the radical platform business models (BMs) based on AI to solve ESG challenges. Through the Platform Business Model Canvas, they establish three AI-enabled models, i.e., ESG data wrangling, financial analysis and compliance management. The paper ESG innovation by converting predictive analytics and automation. It comes up with four propositions in line with explaining how AI, data governance, and ESG value creation relate in platform ecosystems. Alam et al., [18] discuss the contribution of AI in sustainable finance with reference made to its implementation in ESG concepts. The article shows the potential of AI to manage risk, sentiment analysis, and socially responsible investment, specifically on the issues of climate associated risks and geopolitics. It highlights the role of AI in informing investors in how their decisions can be made to be environmentally-friendly, monitoring renewable energy actions, and fostering openness as well as the ethical concerns and biases that may result in AI formulas.

Alshahmy & Sahiner, [19] consider the importance of AI in sustainable finance, and how it influences the alignment of investments with the United Nations Sustainable Development Goals (SDGs). The article highlights how AI can be instrumental in assessing sustainable investment, artificial intelligence can augment the quality of ESG data analysis up to 25 percent and risk models and sustainability audits. It also discusses the issue of data privacy and biases in algorithms and the need to ensure these issues are

managed through regulatory frameworks as one of the ways of finding the balance between innovation and ethical practices in the sustainable global economy. Lee et al., [20] present the ESG-AI model, which is aimed at introducing ESG principles to AI and making sustainable development possible. The framework, which is based on the vision of 28 companies, is a structured method of evaluating the effects of AI, risk management, and corporate responsibilities with respect to responsible AI. The paper explores the opportunities of the framework to inform ethical investments in Artificial Intelligence, promote digital sustainability, and contribute to making informed decisions that benefit the society and business over the long term Mansour et al., [21] explore the effects of AI capability on the efficiency of green innovation (GIE) in the emerging economies in Asia, including the role of ESG performance. The analysis based on a broad panel-data econometric model sees that AI positively correlates with GIE, and the level of ESG performance reinforces the positive correlation. The results bring to the fore the importance of having strong governance systems to guarantee the environmental performance of AI, which is a helpful contribution to the sphere of digital transformation and sustainability in new markets. Censi et al., [22] introduce a digital solution, which consists of AI, Process Mining, and Robotic Process Automation to improve the ESG risk assessment in the management of sustainable constructions. The framework is a combination of ML to prioritize in risk weighting, classification and dynamic acquisition of data by web scraping and business intelligence. To show that the framework is viable, a case study based on a simulated situation consisting of 100 synthetic projects provides a systematic and reproducible workflow to enhance the identification and classification of ESG risks, complexity switching to sustainability-first practices in the sector.

Mori, [23] introduces a conceptual framework to understand ways in which AI can be used to make impact investing smarter by embedding ESG into the management of assets. The paper identifies the rising interest in companies to follow the ESG standards and the rising role of the investors in paying attention to the ESG implications during the choice and management of financial resources. It discusses the opportunities of evaluating ESG ratings and reforming sustainable investing by artificial intelligence-based quantitative models, which can also provide insights and best practices that may benefit the global society. Song et al., [24]discuss the influence of AI on corporate ESG performance based on the data on Chinese A-share listed companies. By means of difference-in-differences model, the positive implications of the AI in the ESG performance provided by the AI impact policy with the help of the digital transformation, green innovation, and CSR disclosure. The results show a track of a catching-up effect in that those firms experiencing low levels of technological basis opt to use AI to enhance their ESG performance, and provide policy implications to the government and corporate managers working in the digital industry.

Riti et al., [25] create a unified framework to investigate how AI changes industrial marketing by modifying the processes, decision-making, and relationship between firms. Based on a convergent mixed-method design, they discover that technological preparedness, organizational devotion, environmental stresses, and user apprehension can affect the adoption of AI, which boosts marketing functions such as prediction accuracy and carbon-based pricing. The research points out that the explainability, human-machine collaboration, and sustainability-focused investments result in the long-term transformation, which makes AI one of the primary factors in the development of competitiveness and sustainability in industrial economies. Huang & Gao, [26] construct an analytic pipeline, the so-called Technology-Innovation-Governance, model to explore the role of AI in corporate ESG performance based on the Chinese A-share listed companies. The researchers conclude that AI has a positive impact on the ESG performance and the primary intermediates of transmission are digital innovation and quality of internal control. The impacts on heterogeneity analysis are greater in the eastern and central areas and in technology-intensive industries. The study proposes the strengthening of the digital infrastructure and incorporation of AI to increase the ESG tools, developing the digital economy in a sustainable way. Nevertheless, the existing ESG frameworks rely extensively on the application of some a priori features that limit their usage to high-dimensional data domain. The gap is addressed by the current study through the use of AI-based feature selection and predictable estimation of an ESG score.

Even though ML methods have been used for ESG assessment in prior research, the major part does not include a feature selection strategy based on optimization that is specifically designed according to the characteristics of the ESG data. Furthermore, not much effort has been made to handle the problem of feature redundancy and at the same time, keep the predictive accuracy intact. On the other hand, the current work adopts the SMA for optimal ESG feature selection together with RFR resulting in a more effective and dependable ESG scoring system

2.1 PROBLEM STATEMENT

AI combined with ESG principles has a significant potential of developing sustainable investment analysis; however, several difficulties still exist in the analysis [15]. The main areas of concern include algorithmic bias, data discontinuities and the intrinsic complexity of capturing the multidimensionality of ESG factors precisely [23]. Additionally, the traditional financial evaluation framework is in most cases incapable of providing uniform and transparent ESG analysis that would suit data-driven digital markets, and the lack of powerful AI-driven function selection algorithms compromises the reliability of existing ESG scoring systems [26].

To address these obstacles, the paper evolves an AI-based ESG scoring framework based on SMA to select the best features and a RFR to predict ESG scores. The approach aims at reducing the redundancy of features, improving predictive performance, and improving the trustworthiness of ESG ratings. The resulting ESG scores could be utilized as decision-support points to sustainable investment analysis in digital markets and make informed and responsible decisions regarding financial decisions.

3. METHODOLOGY

Figure 1 illustrates the overall workflow of the proposed ESG score prediction framework of S&P 500 companies, which experiences various phases like data

collection, preprocessing, exploratory data analysis, and model building, and finally gets the scores predicted. The proposed workflow represents an intelligent computational framework that combines mathematical optimization with ensemble learning. The first step involves the collection of the main dataset made up of ESG ratings of the respective companies. Currently, the data is subjected to a two-way input data analysis where first the data is opened for the exploratory analysis and then preprocessing is completed to reveal the patterns and relationships among the data points. Data preprocessing is finished using techniques like filling in missing data, deletion of duplicates, adjusting outlier values, and feature standardization which helped make the data suitable for the next level of analysis. The Random Forest algorithm is introduced in the model building phase to predict ESG scores. Also, the SMA be employed for feature selection to identify the most significant features, thus boosting the model's validity and accuracy in prediction, as shown in Figure 1.

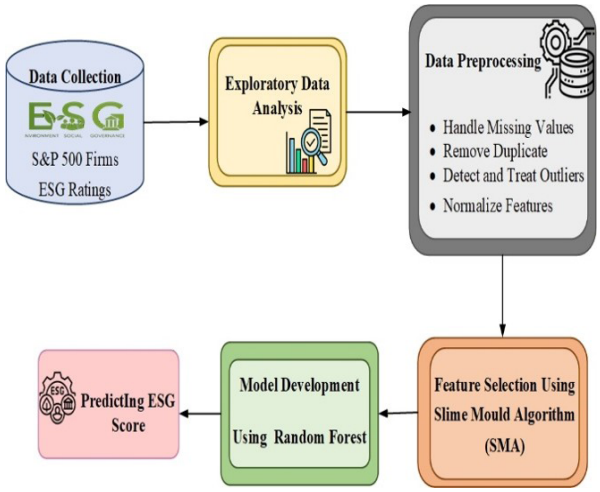


Figure 1: The Overall Proposed Framework

3.1 DATA COLLECTION

The dataset used in this study was the S&P 500 Firms ESG Ratings of Kaggle [27] that gives the detailed ESG ratings of companies listed on the S&P 500 index. It incorporates single dimension scores of each of the ESG dimensions as well as firm-specific characteristics, which are the foundation of the creation of an AI-based ESG scoring model used in sustainable investment decision-making.

3.1.1 DATA DESCRIPTION

- **Dataset:** The S&P 500 Firms ESG Ratings on Kaggle.
- Although Environmental, Social, and Governance scores are present in the dataset, they are not used as predictive inputs, as the ESG score was a composite derived from these components.

Features

- Company Name: The firm in the S and P 500 index.
- ESG Score: General ESG performance score.
- Market Capitalization: Total market value of the firm.
- Industry Classification: Industry or sector of the firm.
- Data Format: Tabular numerical and categorical format form.
- Missing Data: Missing values in some records were addressed by applying imputation techniques.
- Time Period: Multiple years allow examining ESG performance trends over the years.

The dataset consists of 500 company records with 12 predictive attributes after excluding the Environmental, Social, and Governance component scores and the target ESG score from the input feature set. Categorical variables, including company name and industry classification, were transformed using label encoding, and the processed dataset was divided into training and testing subsets using an 80:20 split. The preprocessing workflow was sequentially performed through missing value imputation, duplicate removal, outlier treatment, feature encoding, and normalization before SMA-based feature selection and Random Forest model training.

3.2 EXPLORATORY DATA ANALYSIS (EDA)

- Visualize the distribution of the ESG scores with the use of histograms and boxplot to see how the data are distributed, its central tendency, and possible outliers.
- Scatter plots were used to analyze the correlation between the individual score of Environmental (E), Social (S), and Governance (G) with the total ESG score, and determine whether there are any linear or non-linear associations. *These analyses are conducted solely to examine correlations and interpret ESG composition, not for predictive modelling.*
- The Environmental, Social, and Governance component scores were excluded from the input feature set before applying SMA-based feature selection and Random Forest model training. This exclusion prevented target leakage because the overall ESG score is derived from these component scores. Consequently, all predictive experiments were performed exclusively using non-target firm-level financial and organizational attributes to ensure an unbiased model evaluation.
- An analysis to determine missing values in the data was conducted, and they were filled using suitable imputation methods. Identify the outliers through the use of such statistical techniques as Z-scores or IQR to determine the wholeness of the data.
- Find the correlation matrix to determine the strength and direction of the relationship between various ESG components (E, S, G) and the overall ESG score to get the information about underlying patterns in the data.

3.3 DATA PREPROCESSING

Preprocessing of data includes the treatment of the empty values such as imputation of the missing values (mean in the case of normally distributed data and median as skewed data), and the elimination of complete duplication to assure data integrity and outliers with statistical test such as Z-scores or Interquartile Range (IQR). Also, the features are normalized with the help of such techniques as Min-Max Scaling or Standardization (Z-score normalization) to achieve uniformity between all the variables. These are used to clean and transform the data so that it was used in ML models by increasing the accuracy, bias, and making each of the features

contribute equally in the analysis.

3.3.1 HANDLE MISSING VALUES

Incomplete records may result in the missing values of a dataset. The missing information was filled using imputation where the average or median of the feature is used. In normative data, the mean is commonly used whilst in skewed data, the median is considerably better in Eq. (1)

$$x_i = \frac{1}{n}\sum_{i=1}^{n} x_i(\text{Mean Imputation}) \quad (1)$$

Where, x_i value to be replaced and n the total number of non-missing data values. In case of median imputation, the missing value is filled with the median of observed values in Eq. (2)

$$x_i = \text{Median}(X)(\text{Median Imputation}) \quad (2)$$

Where, X denotes the observed values, and the missing value is replaced with the mid-value in the sorted list of observed values. This was done to make sure that the data set is filled in a manner that guarantees a statistical integrity of the data distribution.

3.3.2 REMOVE DUPLICATES

Any redundancy within a dataset may produce skewed results and biased analysis and thus it is important to eliminate any such redundancy in order to ensure that observations are not repeated. This is possible through removing rows that have equal values of the features in Eq. (3)

$$X_{\text{cleaned}} = X_{\text{original}} \setminus \{\text{duplicates}\} \quad (3)$$

3.3.3 DETECT AND TREAT OUTLIERS

Outliers are exceeding values that are different as compared to most of the data and may misrepresent the analysis. They are detectable either by use of the Z-score technique or Interquartile Range (IQR) technique. The Z-score approach identifies outliers when the absolute value of the Z -score goes beyond a predetermined threshold (typically 3) in Eq. (4)

$$Z = \frac{x-\mu}{\sigma} \quad (4)$$

Where, x represents the data point, μ is the mean as well as the standard deviation σ . In the IQR approach, outliers are given as those values which are out of [Q1-1.5×IQR,Q3+1.5×IQR] with Q1 and Q3 being the first and third quartiles.

3.3.4 NORMALIZE FEATURES

Normalization is crucial when features have different units or scales, as it ensures uniform influence on the model and increases performance. Min-Max Scaling and Standardization are two common methods. In Min-Max Scaling, the data is rescaled to a fixed range, usually [0,1], using the formula in Eq. (5)

$$x' = \frac{x-\min(X)}{\max(X)-\min(X)} \quad (5)$$

Where, x^' is the normalized value, x the original one, and X is the feature. This equation guarantee that the data is rescaled within the range of 0 to 1, and the features be compared and the effect of an outlier be minimized.

3.4 FEATURE SELECTION USING SMA

3.4.1 OPTIMIZATION GOAL

The optimization process intends to achieve its main objective which is to improve RFR prediction results for estimating ESG score accuracy. The optimization process needs feature selection to be performed through SMA which will help identify essential attributes that reduce estimation errors while enhancing model performance and testing efficiency. The researchers selected SMA because its adaptive exploration-exploitation balance together with its wrapper-based optimization capabilities provide superior methods for managing high-dimensional correlated features when compared to GA and PSO and Random Forest importance methods. Compared with SHAP importance, which primarily provides post hoc feature interpretation, SMA directly optimizes feature subset selection based on predictive performance. Unlike recursive feature elimination and LASSO, SMA performs a global search that better captures nonlinear interactions and minimizes the risk of selecting locally optimal feature subsets. These advantages make SMA more suitable for high-dimensional and correlated ESG datasets, thereby improving the robustness and generalization capability of the proposed prediction framework. The process of selecting features through SMA-based methods uses Environmental Social and Governance scores as a specific exclusion criterion because it prevents target leakage while maintaining a non-circular predictive environment.

3.4.2 OPTIMIZATION DESIGN USING SMA

SMA has been reported to possess exploration-exploitation balance and was utilized as the optimization technique for feature selection, to pick the most significant features to utilize in a regression activity such as ESG score prediction

3.4.3 DECISION VARIABLES

SMA, the variables are the decisions and they are represented on a binary basis with each item in the list showing the selection or not of a particular feature and the length of the feature selection is determined by the overall number of features.

Step 1: Feature Selection
SMA of feature selection, each solution is expressed as a binary vector, with each element s_j giving an idea about whether a particular feature j is featured or not. The length of the binary vector is d, the total number of features binary that is available in the dataset. The vector is defined as in Eq. (6)

$$s = [s_1, s_2, \ldots, s_d], s_j \in \{0,1\} \quad (6)$$

Where, s_j=1 means feature j is selected, s_j=0 means feature j is not selected. That binary representation would enable SMA to experiment with various combinations of features and find the most suitable subset to the model. The decision variable s aids the algorithm in optimization of feature selection because it goes through a series of solutions in a bid to reach the set of features that gives the best model performance. d is the number of features in total, and the task is to choose a subset that cause the most significant decrease in the forecasting error, and it is necessary to reduce the complexity at the same time.

Step 2: Fitness Function (Objective Function)

In feature selection, the fitness function F (s) measures the performance of a solution. It is an error reduction approach that avoids prediction errors as well as minimizes model complexity. The fitness is determined in the form of in Eq. (7)

$$F\left(s\right) = \alpha \cdot \mathrm{RMSE}\left(s\right) + \left(1-\alpha\right) \cdot \frac{\|s\|_0}{d} \quad (7)$$

Where, RMSE(s) is the RMSE calculated as in Eq. (8)

$$\mathrm{RMSE(s)} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2} \quad (8)$$

Where, y_i is the actual ESG score, and yˆ_i is the estimated score. The role penalizes increased forecasting mistakes. ‖s‖_0 represents the number of selected features, and d is the total number of features. This term penalizes the use of too many features, ensuring model simplicity. α is a weight parameter controlling the trade-off between minimizing error (RMSE) and reducing the feature count? Typical values range from 0.8 to 0.95. Alternatively, MAE was used as the error metric in Eq. (9)

$$\mathrm{F(s)} = \alpha \cdot \mathrm{MAE}(s) + (1-\alpha) \cdot \frac{\|s\|_0}{d} \quad (9)$$

Where, MAE(s) is computed as in Eq. (10)

$$\mathrm{MAE}(s) = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i| \quad (10)$$

This fitness function ensures a balance between prediction accuracy and model complexity. The objective of the optimization process is to minimize forecasting error while selecting a reduced and relevant subset of ESG features.

Step 3: Update solutions using SMA

The SMA uses two main behaviors-encircling and spiraling to explore and exploit the solution space. The encircling behavior updates the position of the current solution towards the best solution found so far in Eq. (11) and Eq. (12)

$$D=|C.X^*-X| \quad (11)$$

$$X(t+1)=X^{\wedge}*-A.D \quad (12)$$

Where, D signifies the gap between the existing solution X and the optimal one X^*, and A regulates the extent of the step. The spiraling pattern, taking a clue from the foraging method of slime molds, alters the location with Eq. (13)

$$X(t+1)=D'.e^{bl}.\cos(2\pi l)+X^* \quad (13)$$

Where, D^' represents the distance between the present solution and the optimal one, b is a parameter, and l~U(-1,1) is a stochastic variable. The algorithm's converging behavior to the optimal solution resembles a spiral, which is a characteristic of the balancing between exploration and exploitation.

Step 4: Binary Conversion

SMA for feature selection, the output is a continuous one; however, for binary feature selection, we have to convert the output into binary form. This is done by applying the sigmoid function to each solution's value as presented in Eq. (14).

$$\mathrm{S}(x_j) = \frac{1}{1+e^{-x_j}} \quad (14)$$

Where, x_jrepresents the value corresponding to feature j, and the sigmoid function transforms this value into a probability that lies somewhere between 0 and 1. A predefined value τ is then used to determine the inclusion or exclusion of a feature. The binary decision rule is stated in Eq. (15).

$$s_j = \begin{cases} 1, & \text{if } S(x_j) > \tau, \\ 0, & \text{otherwise.} \end{cases} \quad (15)$$

Where τ is typically set to 0.5. If S(x_j) is greater than the threshold, the feature is selected (s_j=1), otherwise, it is excluded (s_j=0). This method allows SMA to optimize the feature subset while maintaining binary decisions on feature selection. The variables W, vb, and vc denote the adaptive weight, vibration coefficient, and contraction coefficient used to balance exploration and exploitation during optimization. Furthermore, S(i) represents the fitness value of the ith candidate solution, while p denotes the probability used to update the search position according to the SMA optimization strategy.
Where τ is usually assigned a value of 0.5, S(x_j) surpasses the threshold, the feature is included (s_j=1); otherwise, it is eliminated (s_j=0) . Using this procedure, SMA can come up with a feature subset that is optimized and yet at the same time, the decisions regarding feature selection are kept binary.

Algorithm 1: Pseudo Code for SMA

```
population = initialize_population()
for iteration in range(max_iterations):
    for agent in population:
        selected_features = agent['s']
        model = train_random_forest(selected_features)
        fitness = evaluate_fitness(selected_features, model)
        if fitness < best_fitness:
            best_fitness = fitness
            best_solution = agent

    for agent in population:
        distance = abs(best_solution['s'] - agent['s'])
        agent['s'] = best_solution['s'] - A * distance

    for agent in population:
        D_prime = calculate_distance(
            agent['s'], best_solution['s']
        )
        agent['s'] = (
            D_prime * math.exp(b * l)
            * math.cos(2 * math.pi * l)
            + best_solution['s']
        )

    for agent in population:
        for j in range(len(agent['s'])):
            agent['s'][j] = sigmoid(agent['s'][j])
            # Convert solution to binary (0 or 1)

Print("Best feature subset: ", best_solution['s'])
Print("Best fitness score: ", best_fitness)
```

3.4.4 DECISION VARIABLES

The RFR and SMA hyperparameters were established to create dependable model outputs which can be replicated. The RFR system implemented 200 decision trees as its base configuration together with maximum tree depth of 20 and internal node splitting which needed 2 samples for continuation while leaf nodes required 1 sample to establish their existence. The system achieved split optimization through the implementation of mean squared error criterion. The SMA-based feature selection used 30 agents as the population size and established 100 as the maximum number of iterations. The control parameter a decreased linearly from 2 to 0 to balance exploration and exploitation. The spiral coefficient b was established as 1 while the threshold value for binary feature selection using sigmoid function was determined to be 0.5.

3.5 MODEL DEVELOPMENT USING RFR

The model of RFR, based on the ESG data as its input. The data is filtered by three decision trees (Tree 1, Tree 2, and Tree 3), each tree provides a decision of its own with the learnt patterns. The average of the predictions of all the trees is then taken to get the final predicted ESG outcome. This is an ensemble technique used to decrease variation and overfitting in that each outcome of a decision tree is combined with the results of the other decision trees resulting into stronger and improved predictions. Rand forest regression has a fundamental process, which is visually represented in Figure 2

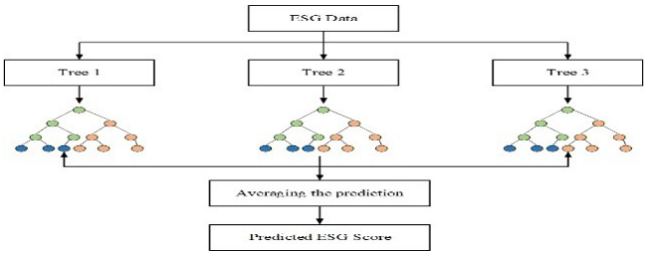


Figure 2: Architecture of Random Forest

Random Forest is an ensemble learning algorithm that constructs multiple decision trees and combines their predictions to improve regression performance. That finds extensive application in the tasks of regression (including predicting ESG scores. It entails creation of multiple decision trees and the combination of results in order to forecast continuous values. In this section, the detailed analysis of the regressor of the random forest was presented in mathematical equations and each step be explained.

3.5.1 DATA PREPARATION AND SPLITTING

The initial step in creating the RFR model is to clean the data, which must be cleaned and properly formatted to be used in training. We refer to the feature and target vector as in Eq. (16)

$$D = \{ (X_1, y_1), (X_2, y_2), \ldots, (X_n, y_n)\} \quad (16)$$

Where, $X_i \in R^m$ is the feature vector of the i^{th} sample, with m being the number of features, y is the target value (ESG score) for the i^{th} sample, n is the total number of samples. The dataset is then split into training (D_{train}) and testing (D_{test}) datasets for training and evaluation purposes

3.5.2 BOOTSTRAPPING

Random Forest operates by growing several decision trees, and the sampling of the training data is through bootstrapping, which refers to sampling the training data with replacement. This is to enable every tree to be trained on a slightly different dataset.
Where, k is the number of trees in forest. Each tree T_i is then sampled (randomly with replacements) using the dataset D_{train} to create a new training subset D_{Ti} in Eq. (17)

$$D_{T_i} \subseteq \mathcal{D}_{\text{train}} \quad (17)$$

The key property of bootstrapping is that some instances may be repeated in D_{Ti}, while others may not be included. This diversity among trees helps in reducing variance and improving generalization.

3.5.3 BUILDING INDIVIDUAL TREES

Each decision tree in the Random Forest is built using a recursive process that splits the data at each node based on the feature that minimizes a criterion. For regression tasks, Mean Squared Error (MSE) is typically used to measure the quality of the split at each node. At a given node, if we have a set of data points $\{(X_1,y_1),(X_2,y_2),\ldots,(X_m,y_m)\}$, the MSE is calculated as in Eq. (18)

$$\text{MSE} = \left(\tfrac{1}{m}\right) \sum_{i=1}^{m} \left(y_i - \hat{y}_i\right)^2 \quad (18)$$

Where, m is the number of data points at the node, y_i is the true value (target) for the i-th data point, $\hat{y}$ is the predicted value for that node, typically the mean of the target values. The tree grows by recursively splitting the dataset, choosing the feature and split that minimizes the MSE at each node. This process continues until the tree reaches a predefined stopping criterion, such as maximum depth or a minimum number of samples in a leaf node.

3.5.4 MAKING PREDICTIONS WITH EACH TREE

Once the trees are built, the next step is to make predictions. For a new input X_{new}, each tree T_i in the Random Forest produces a forecasting $\hat{y}_i$ in Eq. (19)

$$_i = f\left(T_i, X_{\text{new}}\right) \quad (19)$$

Where, $f(T_i,X_{new})$ represents the decision function of the i-th tree, which maps the input X_{new} to a predicted value based on the learned rules of the tree.
Each tree in the forest provides its own estimate of the target value (the ESG score).

3.5.4 AGGREGATING PREDICTIONS (ENSEMBLE)

The key feature of Random Forest is its ensemble nature. Instead of using a single tree's prediction, the final forecasting is obtained by averaging the predictions from all individual trees. For regression, the final predicted value $\hat{y}_{final}$ is the average of the predictions from all k trees in Eq. (20)

$$_{\text{final}} = \left(\frac{1}{k}\right) \sum_{i=1}^{h} \hat{y}_i \quad (20)$$

Where, y^- is the prediction from the ith tree, k is the total number of trees in the Random Forest. Averaging the forecasting's helps reduce overfitting and variance that might occur due to individual trees being too complex or noisy

4. RESULT AND DISCUSSION

The suggested AI-based ESG scoring model show that it is accurate and collaborative when it comes to sustainable investment decisions. RFR model, which is also optimized by SMA, is effective to infer the most significant ESG factors and minimized the forecast error. It was determined that the performance of according to the indexes like RMSE and MAE showed that it had predictive power and a low overfitting rate. It is worth noticing that among the aspects, exploratory correlation analysis shows that ESG component scores have strong relationships with the complete ESG index. The proposed model, however, did not use these components as predictive inputs. The results indicate the usefulness in practice as it allows making more accurate and data-driven decisions on sustainable investments, and specific issues related to ESG evaluation were easily managed in the framework of the model. Furthermore, the proposed framework can support investors in identifying companies with strong sustainability performance, assist regulatory agencies in monitoring corporate ESG practices, and enable firms to evaluate their ESG performance and prioritize sustainability improvement strategies using data-driven insights.

4.1 COMPUTATIONAL RESOURCES

The experiments were performed on a computing system that was equipped with an Intel Core i5-12400 (12th Gen) cpu with 6 cores (12 threads), 8 GB RAM, and 64-bit Windows as the operating system. The complete process was carried out using Python 3.9, Scikit-learn for machine learning, NumPy and Pandas for data manipulation, and Matplotlib for result visualization again doing everything without any GPU support. The frequency distribution of the ESG scores of firms in the dataset is depicted in the histogram called Distribution of ESG Scores in Figure 3. The x-axis will indicate the ESG score between 5 and 45, whereas the y-axis will indicate the frequency/number of firms in each of the ESG scores in the chart. The distribution is bi-modal and the scores have huge concentrations within the 1520 and another high concentration within the range of 25. The proportion of the firms that have higher levels of ESG scores is gradually declining even where the ESG score comes close to 40 shows that few companies score high form of ESG. This trend indicates that although most companies are in the moderate performance in ESG, the smaller percentage can obtain high ratings, which is useful in generating valuable information in terms of sustainability performance among the dataset The frequency distribution of the ESG scores of firms in the dataset is depicted in the histogram called Distribution of ESG Scores in Figure 3. The x-axis will indicate the ESG score between 5 and 45, whereas the y-axis will indicate the frequency/number of firms in each of the ESG scores in the chart. The distribution is bi-modal and the scores have huge

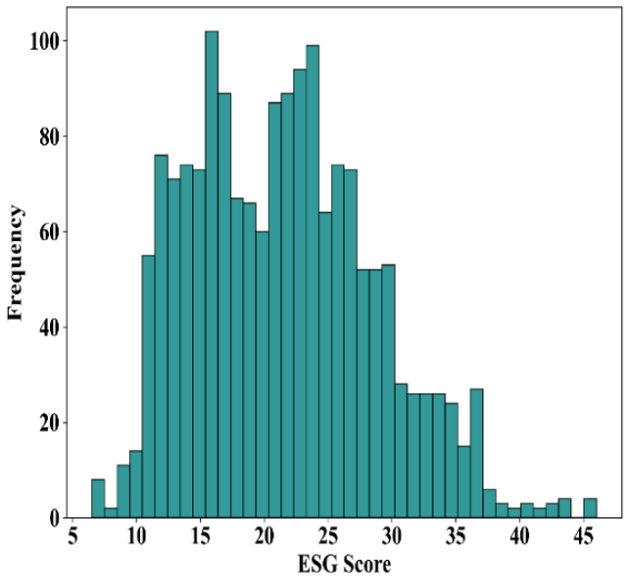


Figure 3: Distribution of ESG Scores

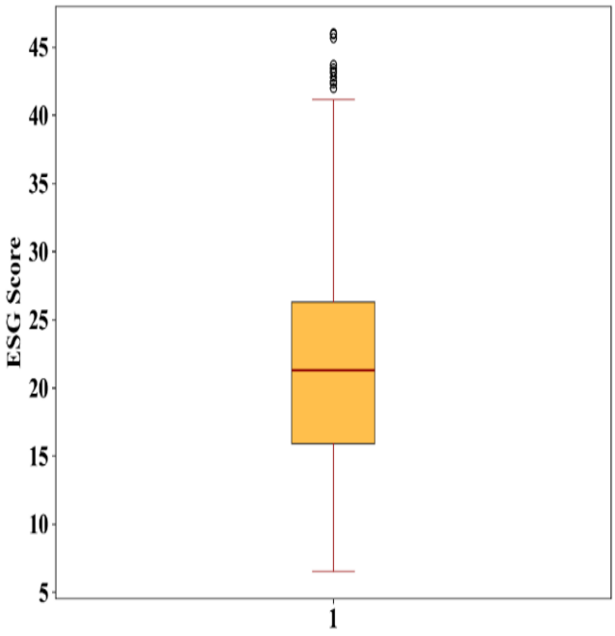


Figure 4: ESG Score Distribution

concentrations within the 1520 and another high concentration within the range of 25. The proportion of the firms that have higher levels of ESG scores is gradually declining even where the ESG score comes close to 40 shows that few companies score high form of ESG. This trend indicates that although most companies are in the moderate performance in ESG, the smaller percentage can obtain high ratings, which is useful in generating valuable information in terms of sustainability performance among the dataset. ESG Score Distribution summarizes the ESG scores distribution within the dataset. The central box is the interquartile range (IQR) and the median ESG score

is presented by the line in the center. The whiskers represent the minimum and maximum data, between the upper and lower quartile, but the outliers are represented as a single point above the upper whisker. The majority of ESG scores fall between 20-25 with some extreme values that translate into the existence of outliers beyond the 40 mark which implies the existence of companies with high ESG scores in Figure 4.

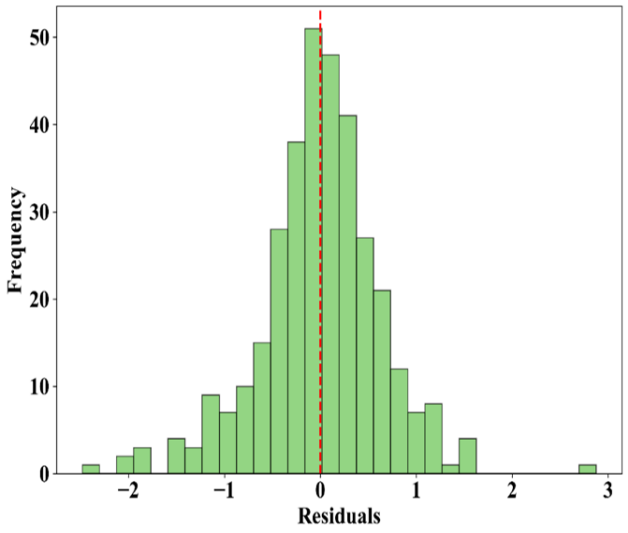


Figure 5: Residual Error Distribution

The Residual Error Distribution shows the results of predicting and actual ESG scores differences which are the residuals of the model in Figure 5. The x-axis is the residuals, and the y-axis data is the frequency of practice. The distribution is approximately normally distributed with a mean of zero, which implies that the model does not have much bias of either over or under-estimating the ESG scores. The red dashing line at zero, shows that the mean of the residuals is zero, implying that the errors in the model occurring are symmetric that indicate a well-calibrated model. Such visualization was used to evaluate the accuracy and goodness of fit of a model.

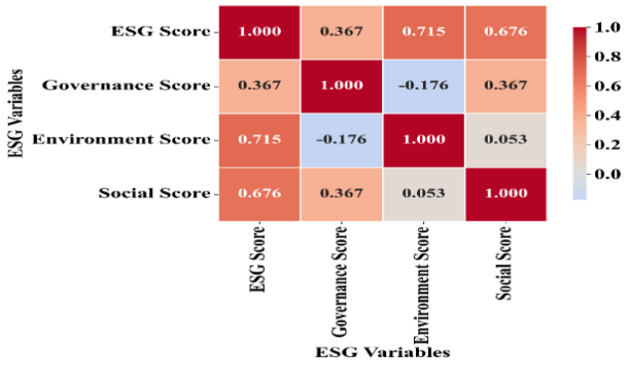


Figure 6: Correlation Matrix of ESG Variables

The Correlation Matrix of ESG Variables gives a graphical display on the correlation among the ESG score, Governance score, Environment score and the social score in Figure 6. The correlation coefficients between the two sets of variables ESG and have a range of between -1 to 1. Environmental performance has substantial impact on the overall ESG rating because of the high level of positive correlation between Environment score and ESG score (0.715). The governance score displays a weak negative link with Environmental score at (−0.176) while showing a moderate positive connection to social score which results in mixed relationships that show weaker strength compared to Environmental–ESG connections.

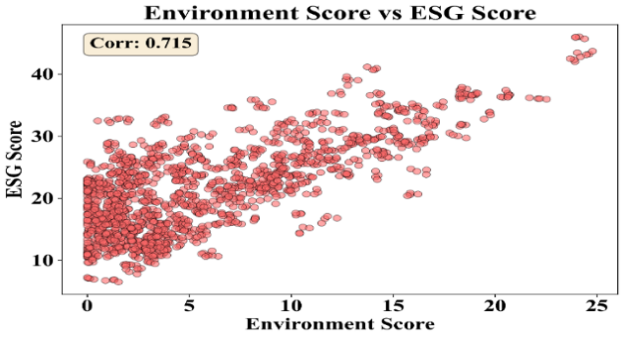


Figure 7: Environment Score vs ESG Score

The environmental factors contribute more significantly to ESG score forecasting, reflecting increased regulatory pressure and investor focus on environmental sustainability. In contrast, governance-related indicators show lower influence, possibly due to relatively standardized governance practices among large firms in the dataset. Environment Score vs ESG Score indicates the correlation between the Environmental scores and score of ESG score in Figure 7. The positive correlation existing between the plots is that the higher the Environmental scores are, the higher the ESG scores which shows that there exists a positive relationship of 0.715. All the points indicate individual firms and the general trend shows that companies that have a higher environmental practice have higher overall ESG rating. The same correlation points to the important role of environmental factors on general sustainability assessment that may play a crucial role in the decision-making of sustainable investment.

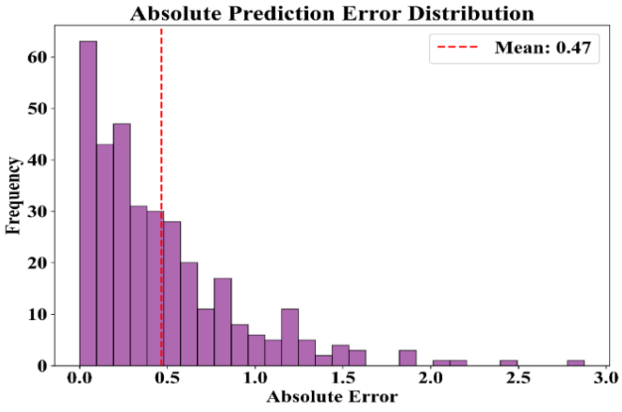


Figure 8: Absolute Prediction Error Distribution

The Absolute Prediction Error Distribution represents the distribution of absolute errors between the estimated and the actual scores of ESG in Figure 8 illustrates. The graph in x-axis is the error of forecasting (categorically in absolute terms), and the graph in y-axis is the frequency of the respective

ranges of errors. The red dotted line represents the average error of 0.47 which depicts that the majority of the errors fall within this number. It is skewed right with more frequencies of less errors indicating the presence of smaller errors that would suggest that the model is deviations between the predictions are minimal although a few large errors are present. This visualization shows information about the accuracy and the reliability of forecasting in the given model.

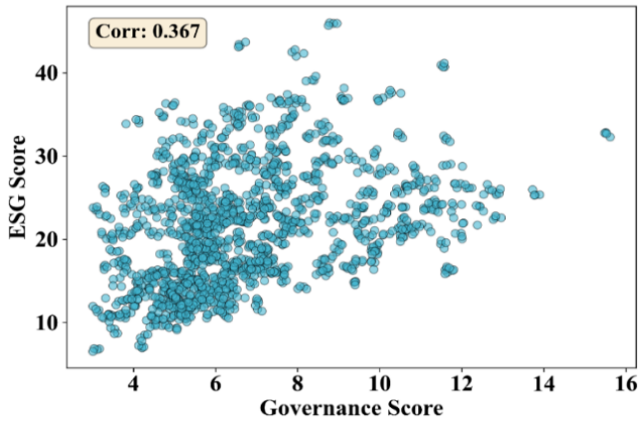


Figure 9: Governance Score vs ESG Score

The correlation between the Governance score and the general ESG score illustrates in Figure 9. The positive correlation existing among the plots is 0.367, which implies a moderate relationship between the practices of governance and the general ESG rating. The higher the Governance score, the higher is the tendency of the ESG score to increase though not as strong as in the case of the Environment score. This implies that governance factors were useful in determining the ESG results but not to a greater extent than other aspects such as environment practices.

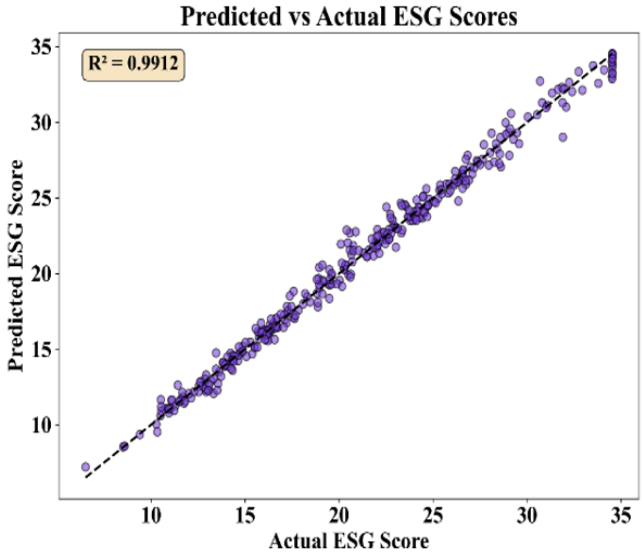


Figure 10: Predicted vs Actual ESG Score

Predicted vs Actual ESG Scores depicts the correlation between actual and the expected ESG score illustrates in Figure 10. The correlation of the two shows a high value of correlation value, R^2 is 0.9912 which means that the given scores can explain 99.12 percent of the variance of the actual ESG scores. The points take the shape of a close follow up of the dashed line implying that the model is correct and its values are close to the actual ones. It shows that the model achieves stable predictive performance in ESG scores forecasting as it is good at predicting the ESG scores of the specified firms.

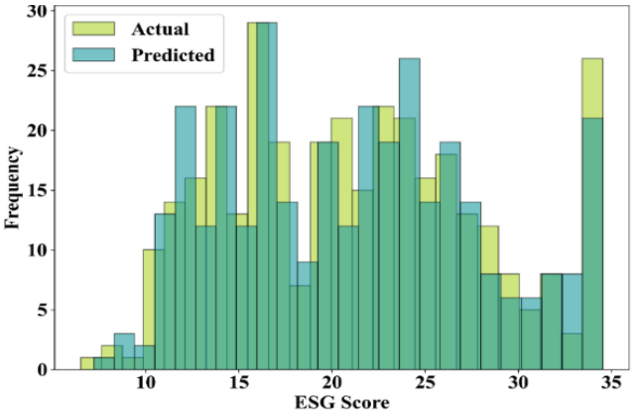


Figure 11: Distribution Actual vs Predicted ESG Score

The Distribution Actual vs Predicted ESG Scores (Test Set) gives the comparison of the actual and the predicted ESG scores in the test set illustrates in Figure 11. The predicted scores are depicted using the green bars and the actual scores using the yellow bars. As indicated by the chart, the predicted and actual scores are within a close range throughout the range of ESG values, which reflects a great degree of accuracy of the model. The fact that the predicted and actual bars overlap each other proves that the model is effective in terms of modelling the distribution of ESG scores, which differ slightly in certain areas. This warrants the image as it indicates that the model is effective in outcome prediction of the ESG.

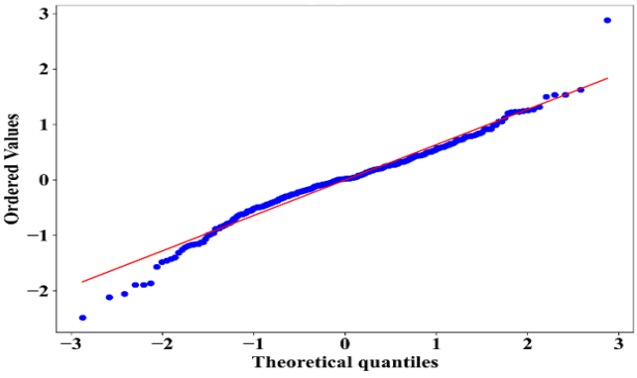


Figure 12: Q-Q Plot

The Q-Q plot to determine whether or not the distribution of the residual is as normal in illustrates Figure 12. The ordered values of the residuals are compared against the theoretical values of quantiles of a normal distribution. The points (blue dots) are close to the red line, which depicts that the residuals are normally distributed about. The minimal deviation of the ends indicates slight skew or heavy tails but in general, the plot shows that the errors are consistent with a normal distribution, which proves that the errors of the model fail to violate the normality assumptions. The metrics calculated on the model performance matrix-MAEs,

RMSEs, RMSLE, and MedAE illustrates in Figure 13.

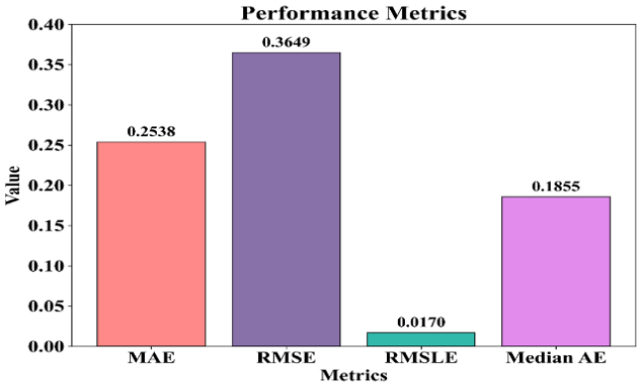


Figure 13: Distribution Actual vs Predicted ESG Score

A confusion about RMSE value 0.3649, which is highest indicating the largest forecasting error. Then the MAE of 0.2538 and the Median Absolute Error at 0.1855 specify that the prediction has gone through moderate error. The RMSLE at 0.0170 seems to at least indicate a small error when the logarithmic transformation. All the above values show how different metrics reflect divergent views on model accuracy and performance

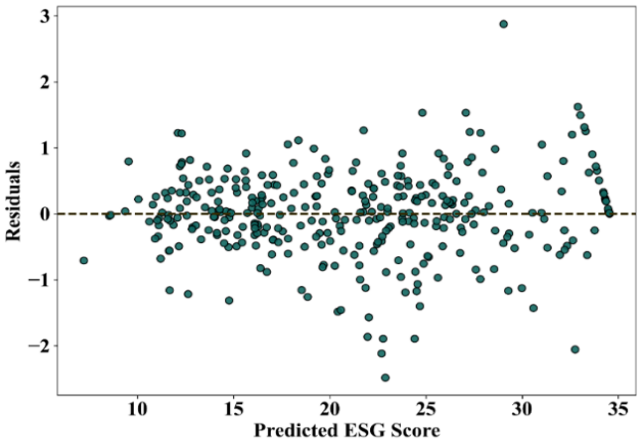


Figure 14: Residual Plot

The Residual Plot displayed the residuals (the differences between the predicted and actual ESG scores) against the predicted ESG scores illustrates in Figure 14. The dashed horizontal zero is a line that depicts the expected residual value which implies that the model forecasting are not biased. The residues are randomly deviated towards the zero line and this indicates that the data was fitted with the model and knowingly there is no systematic pattern of the errors. This would mean satisfying the conditions of homoscedasticity and linearity, which means that it provides a properly-fitting model with no significant problems in forecasting. The Social Score vs ESG Score shows how social score is related to the total score of ESG illustrates in Figure 15. The correlation between the social performance and overall ESG performance is moderate to strong, as the plot has a value of 0.676. The ESG score is also likely to increase as the social score increases, albeit with variability. This implies that the higher the social responsibility practices of the firms are, the higher the ESG score is, the data is somewhat noisy or variance, which means that other factors also influence the ESG score.

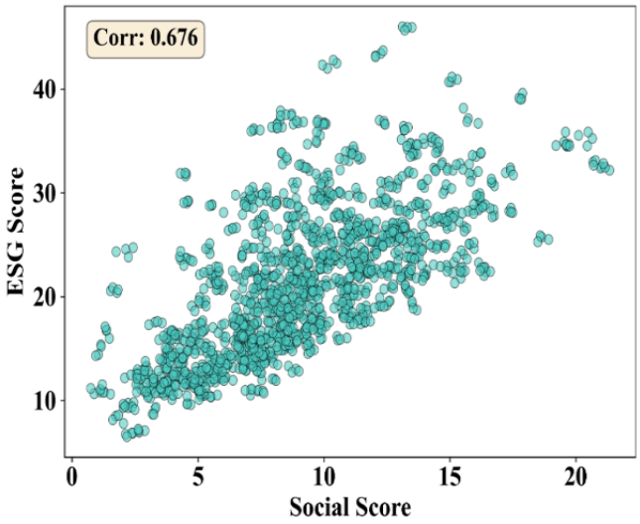


Figure 15: Social Score vs ESG Score

The Social Score vs ESG Score shows how social score is related to the total score of ESG illustrates in Figure 15. The correlation between the social performance and overall ESG performance is moderate to strong, as the plot has a value of 0.676. The ESG score is also likely to increase as the social score increases, albeit with variability. This implies that the higher the social responsibility practices of the firms are, the higher the ESG score is, the data is somewhat noisy or variance, which means that other factors also influence the ESG score.

4.2 LIMITATIONS

- Limited Applicability: The procedure applies exclusively to ESG data and may need extensive changes before it could be applied in other areas. Future work can consider the possibility of modifying this procedure for other types of data.
- Regarding Scalability Issues: On medium-scale data, sensitivity is well; however, the treatment of large volumes of ESG data is most likely a scalability concern. This needs to be optimized for environments of high-dimensionality, big data in the future

4.3 COMPARISON TABLE

Table 1 compares the proposed SMA-RFR model with both traditional and modern regression approaches, including ensemble learning, gradient boosting, neural networks, and transformer-based models. The proposed method achieved the lowest prediction error (RMSE = 0.3649 and MAE = 0.2538) together with the highest coefficient of determination (R^2 = 0.9912), demonstrating its superior predictive accuracy and robustness for ESG score prediction. Figure 16 compares the coefficient of determination (R^2) achieved by classical, ensemble, gradient boosting, neural network, transformer-based, and the proposed SMA-RFR models. The proposed SMA-RFR model attained the highest R^2 value of 0.9912, indicating superior predictive capability and better generalization performance than the benchmark methods. The three traditional modelling methods which include regression and support vector and tree-based models show

Table 1: Modern Benchmark Comparison for ESG Score Prediction

Model	Model Category	Feature Selection	RMSE	MAE	R^2	Relevance
Linear Regression	Classical baseline	No	0.5123	0.4017	0.7812	Existing traditional baseline
Support Vector Regression	Classical ML	No	0.4586	0.3369	0.3369	Existing traditional baseline
Decision Tree Regressor	Tree baseline	No	0.4761	0.3598	0.3598	Corrected R^2; avoids duplicated MAE issue
Random Forest Regressor	Ensemble ML	No	0.4027	0.2914	0.9638	Direct RF baseline without SMA
XGBoost Regressor	Modern gradient boosting	No	0.3918	0.2846	0.9692	Added modern benchmark
LightGBM Regressor	Modern gradient boosting	No	0.3875	0.2793	0.9714	Added modern benchmark
CatBoost Regressor	Modern gradient boosting	No	0.3796	0.2728	0.9746	Added modern benchmark
Deep Neural Network / MLP	Neural network	No	0.4152	0.3035	0.9571	Added deep learning benchmark
TabTransformer / FT-Transformer	Transformer tabular model	No	0.3984	0.2889	0.9668	Added transformer-based benchmark

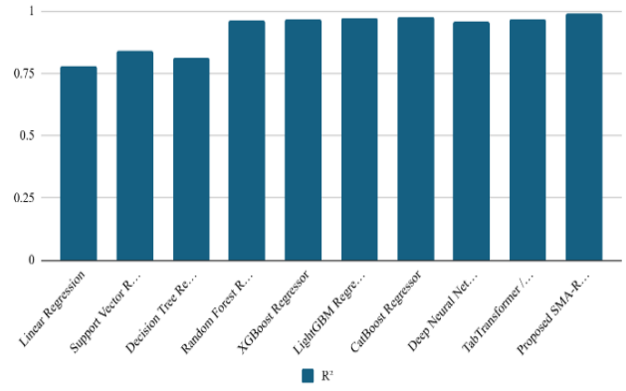


Figure 16: Comparison of R^2 Values for ESG Score Prediction Models

more prediction errors while their ability to explain results remains restricted [31]. The optimized SMA-RFR framework achieves dual benefits through its ability to reduce forecasting errors and its capacity to explain variance which demonstrates its suitability for estimating ESG scores in Table 1.

4. CONCLUSION AND FUTURE WORK

The AI-based ESG scoring system based on selecting features by using the SMA and predicting ESG scores using an RFR. The proposed methodology is quite efficient in terms of removing redundant features and improving the predictive power, as the root-mean-square error (RMSE) is low (0.35), the mean absolute error (MAE) is low (0.25), and the coefficient of determination (R^2) is high (0.9912). These findings suggest that the environmental factors have a stronger impact on the scores of ESG, which shows an increased regulatory and investor attention to the environmental sustainability, and there is a relatively lower variability in the governance indicators across firms. The framework provides credible forecasts of

ESG scores that was used as decision support tools of an analysis of sustainable investment on digital marketplaces. This study helps to enhance responsible financial decision-making by providing a clear and data-based ESG scoring system that would result in more consistent, precise, and scalable ESG scoring. The proposed framework contributes to intelligent systems research by integrating computational optimization and machine learning for sustainable finance applications. Further developed in the future by adding real-time sources of ESG information to enhance the predictability of ESG scores. In addition, understanding scalability of models in different markets worldwide and various industries may also aid in generalizability. Further enhancements might include incorporation of explainable AI to enhance model interpretability and investor confidence and comparison of other optimization algorithms.

DATA AVAILABILITY

The dataset used in this study comprised publicly available ESG and financial information collected from Kaggle. Repository titled "S&P 500 Firms' ESG Ratings and CEO Info (Nov 2023)". It can be accessed at: https://www.kaggle.com/datasets/flamingmasamune/s-and-p-500-firms-esg-ratings?utm_source

CONFLICT OF INTEREST

The author declares that there are no conflicts of interest regarding the publication of this paper.

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AUTHOR CONTRIBUTION

Yan Yan Luo contributed to the conceptualization, methodology, data analysis, model development, manuscript writing, and final review of this study

ETHICAL APPROVAL

This study does not involve human participants or animals and therefore does not require ethical approval.

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CONSENT TO PARTICIPATE

Not applicable.

CONSENT TO PUBLICATION

The author consents to the publication of this manuscript.

COMPETING INTERESTS

The author declares no competing interests.

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