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Predictive and prescriptive analytics for ESG performance evaluation: A case of Fortune 500 companies

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ABSTRACT

Given the growing importance of organizations' environmental, social, and governance (ESG) performance, studies employing AI-based techniques to generate insights from ESG data for investors and managers are limited. To bridge this gap, this study proposes an AI-based multi-stage ESG performance prediction system consolidating clustering for identifying patterns within ESG data, association rule mining for uncovering meaningful relationships, deep learning for predictive accuracy, and prescriptive analytics for actionable insights. This study is grounded in the big data analytics capability view that has emerged from the dynamic capabilities theory. The model is validated using an ESG dataset of 470 Fortune listed 500 companies obtained from the Refinitiv database. The model offers practical guidance for decision-makers to maintain or enhance their ESG scores, crucial in a business landscape where ESG metrics significantly affect investor choices and public image.

1. Introduction

The last two decades have witnessed an increased attraction toward environmental and climate change trends and a general concern about the environmental impact of business operations, with public demand forcing corporate transparency (Azmi, Ng, Dewandaru, & Nagayev, 2019). Given this recent mindset change towards these environment-sensitive topics, investors are becoming more interested in different characteristics of companies instead of just their turnover. Investors are moving their investments towards companies operating transparently, using practices to preserve the environment, and promoting societal well-being. Accordingly, companies are faced with the necessity of abiding by these environmental activities and documenting their strategies to cope with this trend. In light of this pressure, sustainability is moving to the top of the corporate agenda (Klettner, Clarke, & Boersma, 2014).

Regulators, governments, non-governmental organizations (NGO), society, and researchers powered by social media increasingly encourage companies to pursue non-monetary goals relating to environmental, social, and governance (ESG) practices while putting a spotlight on sustainability (Ahlström & Monciardini, 2022). The Global Reporting Initiatives and the United Nations Sustainable Development Goals propose standardized metrics and frameworks for companies to disclose information on their sustainability practices. To evaluate the success of sustainability, ESG metrics of companies are derived from various sources (i.e. annual reports, websites, stock exchange filings, NGO websites, corporate social responsibility reports, new content from ESG-trained research analysts, etc.) on different aspects (i.e. air emission, waste management, resource use, workforce, human rights, employee diversity, shareholders, etc.).

ESG measurement uses a triple-bottom-line strategy covering three main metrics regarding companies' sustainability in three pillars – environmental, social, and governance. The environmental pillar covers the orientation and practices of companies toward environmental issues.

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This pillar measures the company's activities regarding energy consumption, energy efficiency, gas emissions, waste, water, and resource management. The social pillar regards the company's strategies related to human rights protection, workplace and product safety, labor standards, gender policies, and public health issues. The governance pillar views the factors linked to the good governance of companies, such as board independence, protection of shareholder rights, control and monitoring activities, anticompetitive procedures, plus compliance with laws and regulations.

ESG rating agencies analyze and measure the ESG performance of companies by using various criteria for all these aspects. With the increased attention to measuring the sustainability performances of companies, a necessity for developing a standardized ESG scoring system becomes apparent. Accordingly, all these aspects are consolidated into a combined ESG score rating (Thomson Reuters, 2017). In this scoring system, the environmental pillar constitutes three components labeled emission (E1), resource use (E2), and innovation (E3). The social pillar combines four components labeled human rights (S1), product responsibility (S2), workforce (S3), and community (S4). The governance pillar is formed by management (G1), shareholders (G2), and corporate social responsibility strategy (G3) components. This consolidated system makes quantitative measurement of a company's ESG performance much more straightforward.

Calculating the ESG score of a company is a step-by-step process starting with collection of data from various sources on each component. The company rating on all ten components is calculated numerically according to the transparency in reporting material and the company's relative performance on each component. Then, the weighted average of E1, E2, and E3 features is calculated to measure the company's environmental pillar performance. Similarly, while the weighted average of S1, S2, S3, and S4 is calculated for assessing the social pillar, the weighted average of G1, G2, and G3 is taken to evaluate the governance pillar. Finally, the weighted average of these obtained E, S, and G pillar scores is calculated to find the overall ESG score of the company.

Although this consolidated system for ESG score rating is widely accepted and practically used, researchers are still searching for alternative ratings (Hughes, Urban & Wójcik, 2021) due to various reasons. First of all, there still exists a significant divergence in ESG ratings between main rating agencies based on the scope, measurement, and weight, where measurement constitutes the most critical portion of divergence (Berg, Koelbel, & Rigobon, 2022). This is mainly because the data generation stage is still challenging. Data being collected manually is prone to error and is time-consuming; the degree of reporting standardization is low, while the authenticity and credibility of reports are questionable as the entire process lacks transparency (Wu, Chen, Fu, Jiang, & Huang, 2022). Moreover, since ESG information disclosure is voluntary and publicly listed companies may select from different regulatory fillings to disclose information, this affects investment decisions for potential clients who want to evaluate alternative companies' ESG performance (Consolandi, Eccles, & Gabbi, 2022; Schiehll & Kolahgar, 2021). Thus, in many cases, publicly available ESG information does not satisfy the investors' needs. This gap in required and available information is not only due to the different levels of compliance with disclosure requirements but also due to explanations of the material information issued by companies (Madison & Schiehll, 2021).

In ESG performance assessment, the rating systems must assign scores to the ESG components and weights for each component. As presented in existing studies, the differences between the ESG scores of different rating agencies can be due to the weight selection (Berg et al., 2022). Thus, the decision on the optimal weights in ESG score calculation is the other challenge in this system (Gholizadeh & Fazlollahtabar, 2021). Last but not least, the selection of these weights may require to be updated dynamically with changing conditions and external factors affecting sustainability operations (Chen & Mussalli, 2020).

This paper proposes a multi-stage system for companies' ESG performance prediction using advances in data analytics and deep learning technologies. Data analytics has become a leading method for companies to cope with various business problems and to make better decisions. In today's business environment, data analytics is one of the essential tools for a company to improve its performance. Data analytics is defined as analyzing data to detect patterns immediately, obtain valuable insights, and support decision-making (Choi & Park, 2022; Wu, Hitt, & Lou, 2020). Due to their superiority in analyzing complex data sets, being free of strict assumptions of basic statistical techniques, high prediction accuracies, time efficiency, and many other benefits, these technologies now command significant attention from researchers and decision-makers (Sariyer, Kahraman, Sözen, & Ataman, 2023).

While traditional businesses have focused on descriptive and predictive analytics, today's dynamically changing competitive business environment creates an increasing need for prescriptive and cognitive analytics (Mithas, Chen, Saldanha, & De Oliveira Silveira, 2022). Due to their superiority in analyzing and modeling complex data sets, data analytics and deep learning technologies are now crucial in descriptive, predictive, prescriptive, and cognitive analytics.

Despite the high interest in these promising technologies, their integration in the context of sustainability is in its early stages. Most existing studies evaluate companies' corporate social responsibility activities (Calic & Ghasemaghaei, 2021; Choi & Park, 2022; Chouaibi, Chouaibi, & Rossi, 2022; Vo, He, Liu, & Xu, 2019). Developing an intelligent ESG data reporting system based on these technologies is also studied in recent literature (Sethi, Rovenpor, & Demir, 2017; Wu et al., 2022). Implementing these techniques in ESG performance analysis and ESG score prediction is also examined in this context (D'Amato, D'Ecclesia & Levantesi, 2021; Lee et al., 2022). However, since these existing studies benefit from the descriptive and predictive powers of data analytics, machine learning, and deep learning technologies, a gap exists in the literature on using prescriptive and cognitive analytics in sustainability. Besides, most of these studies use only the prediction function of these technologies, although they have many other tools and functions.

Therefore, this study contributes to existing literature by proposing a novel ESG score prediction system. Firstly, the system is weight-free; hence, the calculation of the ESG score does not require any weighted averaging in this study. Secondly, the proposed method does not use the exact numerical measurements in the pre-defined ten ESG components (E1, E2, E3, S1, S2, S3, S4, G1, G2, G3). Thirdly, this system offers a holistic approach by combining the clustering, association rule mining, and prediction functions of data analytics technologies in a multi-stage process. Interpreting the predicted ESG scoring in a prescriptive way using a simulation is a further contribution of this research. The proposed model is validated on listed Fortune 500 companies.

The organization of the paper is as follows. The theoretical background of the proposed model is discussed in Section 2. The methodological framework is presented in Section 3. The data set used to validate the model is described in Section 4. Empirical findings and model performance are shown in Section 5. Discussions and implications are proposed in detail in Section 6. The concluding remarks, limitations, and future research directions are suggested in Section 7.

2. Theoretical background

2.1. Dynamic capabilities view and big data analytics capabilities (BDAC)

This study is grounded in the big data analytics capability view, which evolved from the dynamic capabilities theory.

Dynamic capabilities define an organization's ability to innovate, adapt to change, and improve positively for the benefit of its customers (Teece, Peteraf, & Leih, 2016). To properly deal with environmental uncertainties, dynamic capabilities make best use of the organization's internal and external resources (Teece, Pisano, & Shuen, 1997). Dynamic capabilities are the main processes for sensing, integrating, learning, and reconfiguring resources and capabilities (Birkinshaw, Zimmermann, & Raisch, 2016) and stress an organization's capacity to create, extend, or modify its resources purposefully. It has become imperative for companies to embrace sustainability in their strategies and operations, as a recent change in mindset towards environmentally sensitive issues has been promoted. A general concern about the environmental impact of business operations has also forced a public demand for corporate transparency. The global dispositions toward environmental and climate change trends and corporate transparency now place sustainability at the center of business operations. As the need for sustainability has become more prominent, companies have immediately started engaging in these activities to contribute to social welfare (Kolk, 2016). These changing topics have also caused new trends in performance evaluations of organizations (Büyüközkan & Karabulut, 2018) and, thus, investment decisions (Steinmeier & Stich, 2019). Traditionally, investors evaluate companies mainly based on their earnings. Still, there is a movement towards investing in companies adopting suitable environmental, social, and governance activities, being transparent in data sharing, and contributing to society. These differences have mainly been seen in the last two decades and have forced companies to adopt dynamic changes rapidly. In this environment, only companies that can create, extend, and modify their internal and external resources appropriately can embrace these new trends and dynamically change their processes. This highlights a dynamic capabilities theory in sustainability research and practices (Buzzao & Rizzi, 2021). There is now a considerable amount of literature grounding sustainability research in dynamic capability theory (Al-Shami & Rashid, 2022; Dias, Gouveia Rodrigues, & Ferreira, 2021; Rebs, Thiel, Brandenburg, & Seuring, 2019; Tiberius, Stiller, & Dabić, 2021).

With the advances in data and data analytics technologies, dynamic capabilities theory has led to big data analytics (BDA) capability theoretical framework, where data analytics is viewed as a valuable resource for companies in dealing with uncertainties (Sariyer, Mangla, Kazancoglu, Xu, & Tasar, 2022; Sariyer, Ataman, Mangla, Kazancoglu, & Dora, 2022; Gupta & George, 2016). The theoretical framework highlights that merely having access to big data technology is insufficient for organizations to benefit from it. Instead, combining technological, human, organizational, and strategic capabilities is essential to effectively leverage big data analytics (Huynh, Nippa, & Aichner, 2023; Mikalef, Framnes, Danielsen, Krogstie, & Olsen, 2017). BDAC is defined as an ability to provide awareness by using data management, technology, and labor capabilities to gain competitive strengths (Kiron, Prentice, & Ferguson, 2014). Companies implement BDA, large-scale analytics using different advanced analytical methods, functions, tools, and techniques to convert and create value from raw data sets, contributing to organisationally valued outcomes, including sustainable practices and innovation. Additionally, companies must constantly adapt their resources in response to evolving market dynamics (Gupta & George, 2016; Teece, 2014). Nonetheless, for effective adaptation, it is crucial for companies to understand the different resources necessary to develop a capability that not only integrates predictive and prescriptive analytics but leverages this combined analytics capability for generating value across various organizationally valued applications (Charles, Emrouznejad, Gherman, & Cochran, 2022).

Since extensive knowledge and advanced analytics are needed for various sustainability-related issues, companies are increasingly implementing characteristics and initiatives incorporating BDA. In addition, to appropriately adapt to the new environment-sensitive trends and the dynamically changing environment created by these innovations, companies are now required to have BDA capabilities. Accordingly, studies exploring the role of BDA and BDA capability in sustainability have gained prominence in recent literature. Existing research presents the theoretical underpinnings of using BDA and sustainability (Pandya & Kumar, 2022). Studies also demonstrate the BDA techniques that can be used to identify sustainability components in big data (Nguyen, Li, Spiegler, Ieromonachou, & Lin, 2018). A few researchers also focus on BDA capability, particularly for investigating ESG performance analysis (Zhu, Du, Shahzad, & Wattoo, 2022). Despite the existence of these studies, proposing an alternative ESG scoring model that can be used in real life to evaluate companies' sustainability performances remains a gap in the literature. Thus, by presenting a deep learning-based multi-stage ESG performance model, this study aims to highlight the significance of BDA capabilities in sustainability research and practices; this will also address this gap in existing literature. While current studies show the benefits of BDA's descriptive and predictive power in sustainability (Acar, Sarıyer, Jain, & Ramtiyal, 2023; Sariyer & Taşkın, 2022), this research additionally uses prescriptive techniques for presenting insights to companies using a simulation method. Although dynamic capability theory and the recent view of BDA capability have been well represented in the sustainability context, this study attempts to extend the use of these theories, particularly for the investigation of the sustainability performances of companies through their ESG scores.

3. Methodological framework

This study presents a deep learning-based multi-stage ESG score prediction (*DLB-MS-ESG*) system to evaluate a company's sustainability performance. The system uses a holistic approach and sequentially integrates clustering, association rule mining, and prediction functions of data analytics. It also benefits from the prescriptive power of data analytics by using the simulation method to create prescriptions for companies about their ESG scoring.

To form a homogenous grouping of companies based on their sustainability performances, the system's first stage takes advantage of the clustering function of data analytics and implements the kmeans++ algorithm. The second stage attempts to discover hidden associations between scores of the pillar components and obtained clusters of the companies on corresponding pillars; this uses the Apriori algorithm. Using the sector, obtained grouping for each pillar, and ranged scores (described in Section 4.1) of each of the ten components, the third stage aims to predict the overall ESG score of the company numerically by implementing deep neural networks (DNN). In the final stage, prescriptions are provided for the purposively selected companies using a simulation method, with rules obtained based on what-if scenarios.

3.1. Stage 1 clustering

Various sustainability performances exist among companies, even though they are all listed in sustainability indexes. There may also be a variety between the performance of the same firm on other pillars of sustainability. Clustering the companies according to their performance in each pillar can provide useful methods and practical advantages. With clustering, companies that are more similar in terms of their performances on each pillar, rather than those in different clusters, are grouped. Since the obtained homogenous groups represent the companies with similar performances on the sustainability pillars, these companies can be analyzed together in decision-making. Thus, instead of making separate analyses and decisions for each company, managers can use the obtained groups to improve time and cost efficiency (Sariyer, Mangla, et al., 2022). This also enables companies to create prescriptions by analyzing the groups that they can target according to their performance expectations. The clustering approach also reduces algorithmic complexity, as evaluating the homogenous groups obtained separately, instead of considering all companies separately, will reduce variation in the data set. The proposed ESG score prediction system implements clustering analysis in its early stages to benefit from these practical and methodological advantages of clustering analysis. Cluster analysis is performed separately for E, S, and G pillars to obtain a grouping of companies with similar performance in each sustainability pillar. Thus, in the proposed system, the output of the first stage is the company clusters obtained based on E, S, and G pillar scores. The system performs a k-means++ algorithm to obtain these clusters. The algorithmic details of this algorithm are summarized in Appendix A. The data processing steps are initialized using *Pandas* and *NumPy* libraries, and the clustering stage is performed using the *Scikit-learn* library of Python programming language.

3.2. Stage 2 finding frequent associations between component scores and obtained clusters

The second stage of the proposed system aims to generate hidden associations among the company's performance on each pillar component and obtained grouping regarding the pillar. The acquired associations may also prescribe the rules regarding pillars between component scores and targeted clusters. According to the associations obtained, the components with higher effects on the particular pillar can also be identified. The associations between the variables of the big data sets are generated in a rule structure presenting the antecedent and consequent of the rule by using association rule mining. As in the first stage of the model, association rule mining is performed separately for E, S, and G pillars. The association between the company scores on E1, E2, and E3 components and the company grouping based on the E pillar score is used for the rule generation regarding the environmental dimension. Thus, while the component scores (E1, E2, E3) represent the antecedent of the rules regarding the company's performance on the environmental dimension, the obtained clustering based on the E pillar score represents the rule's consequence. Similarly, to analyze the hidden rules regarding social and governance dimensions, associations between S1, S2, S3, and S4 components and the company grouping based on the S pillar score, and G1, G2, G3 components and the company grouping based on the G pillar score, are obtained.

However, quantitative measurement of the components creates complexity regarding the method's applicability, the interpretation of the obtained rules, and their use in decision-making. Therefore, component scores are converted into quartile-ranged scores to generate the rules at this stage. This model is worth highlighting where identifying the existing/targeted quartiles is sufficient for making decisions instead of exact measurements on component performances.

The Apriori algorithm is used to experiment with the association rule mining; algorithmic details are given in Appendix B. Python's PyPI library is used to implement the Apriori algorithm.

3.3. Stage 3 predicting the overall ESG score

The sustainability performances of companies are measured by their overall ESG score; this score is traditionally calculated as the weighted average of component and pillar scores. The proposed system quantitatively predicts the overall ESG score of a company, given the outputs obtained in the previous two stages. The grouping or cluster numbers of the companies based on E, S, and G pillar scores obtained as the output of the first stage are used as the first input variables of the ESG score prediction. The quartile ranged scores of each of the ten components, validated in the second stage with the obtained associations, are also used as input variables of the overall ESG score prediction. To obtain sector-based scoring, the sector in which the company operates is defined as the other input of the ESG score prediction. The system uses fourteen input variables to numerically predict the company's overall ESG score in this stage. A deep neural network algorithm is implemented for this stage of experimentation. The algorithmic details are shown in Appendix C. Deep neural networks are implemented with the *TensorFlow* library and related functions.

Although deep neural networks offer many advantages compared to other algorithms, the main challenge of this technique is the requirement of parameter tuning for many parameters. Learning rate refers to the rate at which the algorithm converges to the optimal solution, while the batch size defines the number of samples used in one epoch to train the network; these are essential hyperparameters affecting algorithm training. Parameter tuning requires a large amount of time to complete algorithm training. However, optimization algorithms such as Stochastic Gradient Descent optimizers can be used to deal with these challenges in parameter tuning.

3.4. Stage 4 simulation for prescriptive analytics

While predictive analytics addresses "What will happen?" and "Why will it happen?" in the future, prescriptive analytics addresses the "What should I do?" and "Why should I do it?" questions (Lepenioti, Bousdekis, Apostolou, & Mentzas, 2020). While prescriptive analytics is less mature than predictive and descriptive analytics (Charles et al., 2022), it has started to gain significant attention from researchers (Larson & Chang, 2016).

Prescriptive analytics is the most advanced type of BDA and may create the most significant business intelligence and value (Oesterreich, Anton, Teuteberg, & Dwivedi, 2022). The main goal of prescriptive analytics is to provide or prescribe the best decisions based on the generated predictions to support decision-making. Prescriptive analytics take the outcome of a predictive algorithm as input and create prescriptions for businesses based on these predictions (Šikšnys, Pedersen, Liu, & Özsu, 2016). It helps companies achieve their targets by recommending all probable scenarios and tasks to optimize these targets, presenting a wide landscape for decision-makers (Charles et al., 2022).

To provide competitive advantages to businesses by enhanced decision-making in an optimized way, prescriptive analytics apply different methods classified as probabilistic, machine learning, optimization or mathematical programming, evolutionary computation, simulation, and logic-based models. While most existing studies employ optimization models for prescriptive analytics (Belhadi, Zkik, Cherrafi, & Sha'ri, 2019), simulation is also a popular topic for researchers (Rezaei, Raeesi Vanani, Jafari, & Kakavand, 2022).

Simulation is modeling a situation on a computer to investigate how a system works. Using simulation, consciously modifying the values of the input variables of a model, and generating estimations on the target variable, it is possible to analyze how the system reacts in response to these modifications. In prescriptive analytics, simulation can be applied to enhance effective decision-making by testing new ideas or investigating how a probable modification will affect the system (Lepenioti et al., 2020). Stochastic simulation, simulation over Random Forest, risk assessment, and creating what-if scenarios are the most widely used techniques in simulation.

In the final stage of this research, by creating what-if scenarios, simulation is used as a prescriptive analytics method. Some of the study data set companies are purposively selected in the simulation process in light of Stage 1 clustering results. Various simulation experiments are conducted to see how these selected companies' ESG scores will be affected by the ten pillars' modified (decreased/increased) scores. A deep learning-based ESG score prediction model presented in Stage 3 is used to assess the effect of modified scores of each pillar on the ESG score. Thus, prescriptions are provided for these companies on which pillar score should be achieved in which quartiles to maintain or improve the overall ESG scores (Fig. 1).

4. Empirical experiment

4.1. Dataset

Currently, there are various ESG rating and ESG score calculation services (Schäfer, 2016); many charge a subscription fee for data access, limiting its accessibility to the public. In 2018, as a London Stock Exchange Group subsidiary, the Refinitiv Company was founded (Refinitiv, , 2022). Refinitiv ESG scores are designed to transparently and objectively measure a company's relative ESG performance based on publicly available and auditable data. Refinitiv ESG is a primary ESG rating provider, offering one of the most comprehensive databases in the industry. For each company listed in sustainability indexes, Refinitiv assigns a score between 0 and 100 to each of the E, S, and G components.

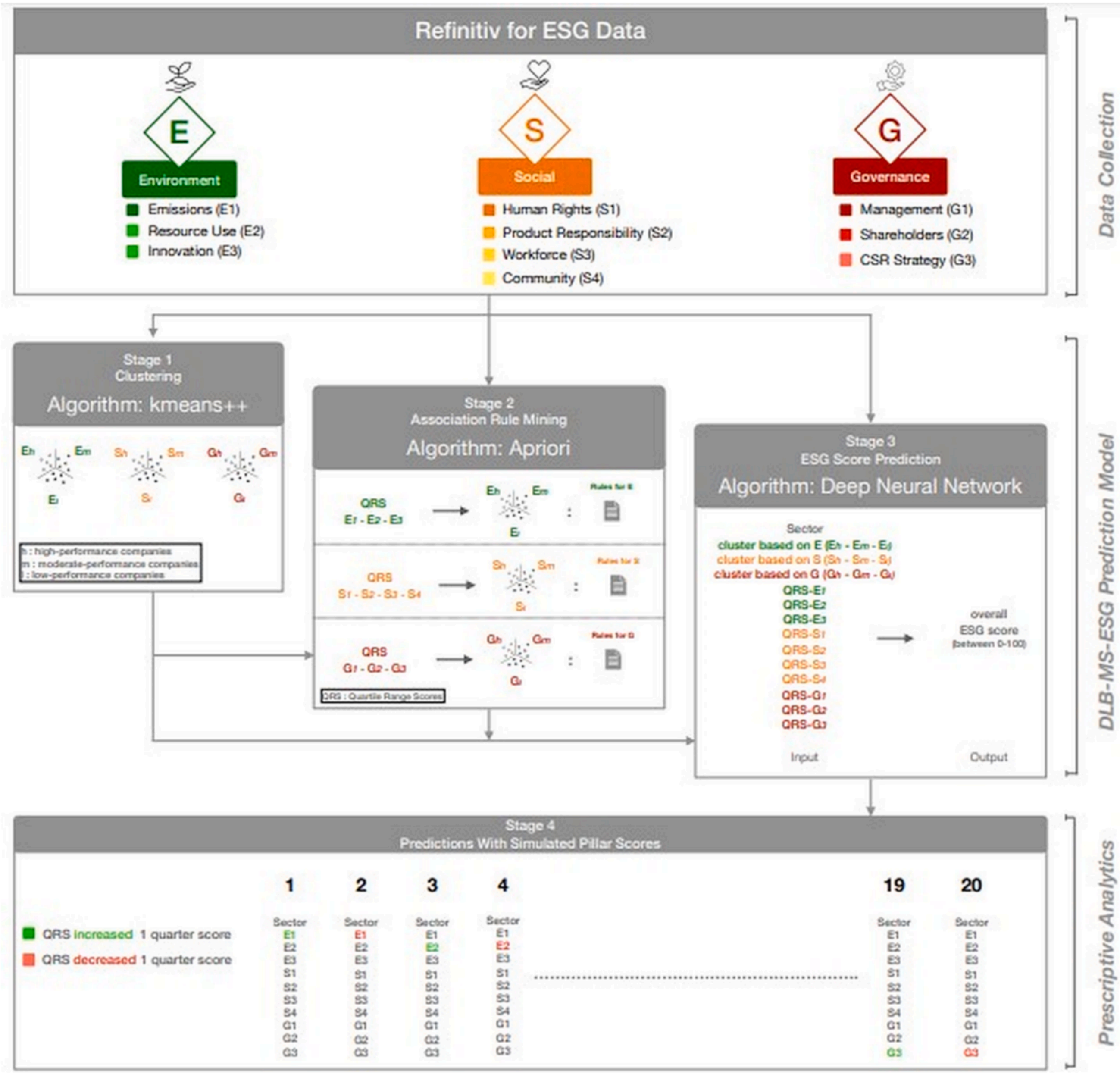

Fig. 1. Research flowchart.

Refinitiv then calculates each pillar score by taking the weighted averages of these components to evaluate the overall ESG score of the listed company (Thomson Reuters, 2017). With technological advances, BDA has become essential for researchers to analyze, model, and obtain prescriptive implications on large data sets such as Refinitiv. We, therefore, concentrate on BDA tools and techniques to analyze the study data set from this large database.

In this study, the company's scores on these ten components, three pillars, and overall ESG scores calculated for 2021 are downloaded from the Refinitiv database. Although these components are numerically measured, Refinitiv also uses a range scoring based on the quartiles. This range scoring is presented in Table 1.

The model is validated in a sample of companies from the Fortune 500 list. In this study, Fortune 500 companies are selected since these listed companies are widely explored in the context of sustainability (Bendell & Huvaj, 2020; Rosamartina, Giustina, & Angeloantonio, 2022). The most up-to-date list of Fortune 500 companies is downloaded. Four hundred and seventy listed companies have ESG scores data in the Refinitiv 2021 database.

Table 1
Range scoring based on quartiles used in the modelling.

Score range	Description	
0 to 25	The first quartile (Q1)	poor relative performance and insufficient degree of transparency in reporting data publicly.
>25 to 50	Second quartile (Q2)	satisfactory relative performance and a moderate degree of transparency in reporting data publicly.
>50 to 75	Third quartile (Q3)	good relative performance and above-average degree of transparency in reporting data publicly.
>75 to 100	Fourth quartile (Q4)	excellent relative performance and a high degree of transparency in reporting data publicly.

Source: Refinitiv, 2022.

Thus, the study data set includes data from 470 companies for components, pillars, and overall ESG scores. Since the proposed ESG scoring system also uses the sector as a parameter, the sector data in which the companies in the study data set operate are also downloaded.

4.2. Evaluation metrics

The obtained grouping of the companies based on E, S, and G pillar scores is evaluated by the significance of the differences in these scores and the sectoral distributions within the groups.

Generated association rules are evaluated based on support and confidence levels. The calculation details are given in Appendix B. The rules satisfying 0.8 confidence are listed to present only the rules with strong-level associations.

The performance of the overall ESG prediction is evaluated based on root mean square error (RMSE) and mean absolute performance error (MAPE) measures; these are calculated as follows:

$$RMSE = \sqrt{1 \Big/ n\sum_{i=1}^{n}(ESG_i - \widehat{ESG}_i)^2} \quad (1)$$

$$MAPE = 1 \Big/ n\sum_{i=1}^{n}\left|\frac{ESG_i - \widehat{ESG}_i}{ESG_i}\right| \quad (2)$$

In equations (1) and (2), ESG_i and $\widehat{ESG}_i$ respectively show the actual and predicted overall ESG score of the company I; n indicates the total number of companies in the study data set.

5. Empirical findings

5.1. Stage 1 clustering results

In the experimentation of clustering, for simplicity and better interpretation, the k value representing the number of clusters is taken as 3. Thus, 470 companies of the study data set are divided into three groups based on their E, S, and G pillar scores.

Table 2 represents the number of companies clustered in each group, the mean and standard deviation statistics of each group's E, S, and G pillar scores, and the significance of the differences between the obtained groups.

The results in Table 2 show that significant differences exist between the clusters for all pillar scores. With these findings, identified groups of companies are labeled as given in the last column of this table based on the average ESG scores.

To comparatively analyze the performance grouping of the study data set companies, another investigation is applied; these findings are presented in Fig. 2.

Fig. 2 shows that among the 470 companies, only 146 are placed in the same performance groups based on all E, S, and G pillars. 96 of these companies are grouped in clusters of high-performance companies on all E, S, and G pillars. Similarly, using all E, S, and G pillars, 36 companies are grouped in moderate performance, and 14 are in the low-performance cluster. The performance grouping of the remaining 324 companies differs from one to all pillars.

Fig. 3 represents the performance grouping distribution for the sectors of the study data set that companies are operating.

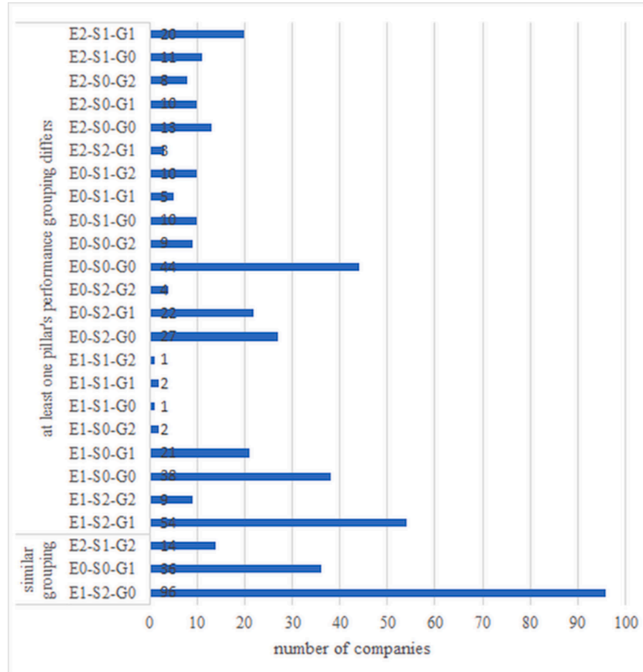

Fig. 2. Distribution of companies based on the obtained performance clusters.

Fig. 3 shows differences in the grouping distribution of the three pillars for different sectors. In the industrial, health care, utilities, and consumer defensive sectors, the percentage of the companies grouped in low performance is lower than the other sectors for each sustainability pillar. For information technology, while the companies clustered in the low-performance group are low for E and S pillars, the percentage is higher for G. The opposite finding is seen for the financial and materials sectors. In the healthcare and information technology sectors, the highest ratios observed for the companies clustered in high performance are worth noting for the S pillar. Similarly, for the G pillar, a relatively high percentage can be seen for the companies clustered in high performance in information technology.

5.2. Stage 2 Discovered top associations between component scores and obtained clusters

Various association rules are detected for the E, S, and G pillars. The notations E1 through E10 are used for the ten sustainability components, Q1 through Q4 for the quartile ranged scores, and C0, C1, and C2 for the regarding cluster. The generated rules are presented in Table 3.

Although various rules are generated, only 18, 25, and 15 top rules satisfy a confidence level higher than 0.8 for the E, S, and G pillars. As an instance, rule number 1 for the E pillar is read as if all of the three components of the E pillar of a company have a score between 0 and 25

Table 2
Summary results of obtained clusters.

Clustering based on	cluster id	number of companies	average ESG score	std. dev. of ESG score	p-value	cluster label
	E-0	167	48.731	8.741		Moderate-performance companies on the E pillar
	E-1	224	78.179	8.461		High-performance companies on the E pillar
	E-2	79	15.911	10.618		Low-performance companies on the E pillar
	S-0	181	61.022	6.998		Moderate-performance companies on the S pillar
	S-1	74	32.919	9.654		Low-performance companies on the S pillar
	S-2	215	83.367	6.616		High-performance companies on the S pillar
	G-0	240	80.175	7.948		High-performance companies on the G pillar
	G-1	173	55.133	7.783		Moderate-performance companies on the G pillar
	G-2	57	25.158	9.151		Low-performance companies on the G pillar

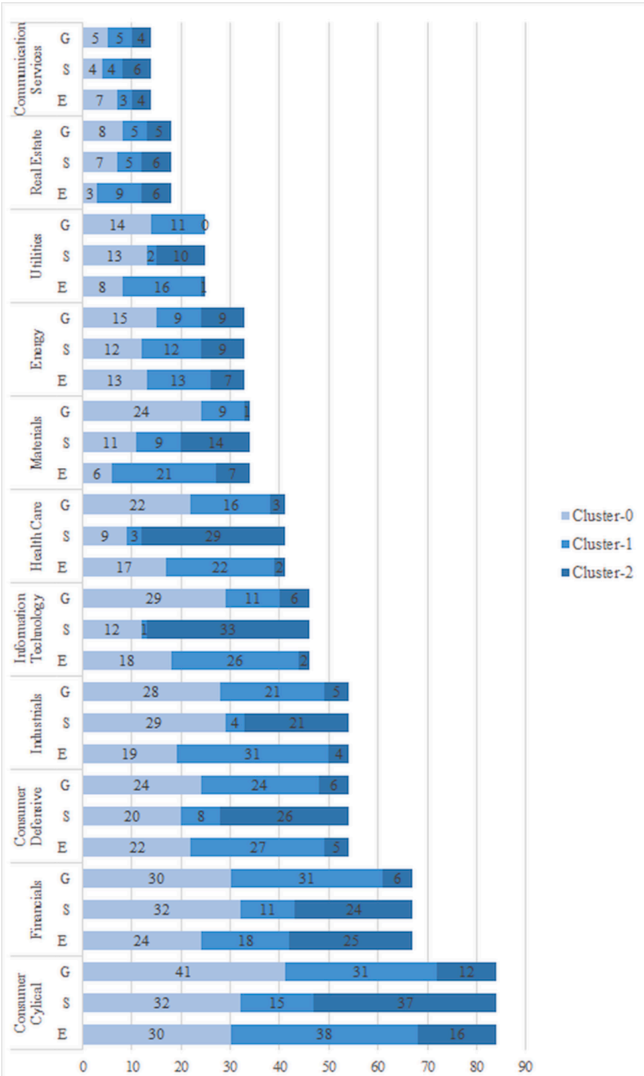

Fig. 3. Sector-based performance grouping analysis.

(namely Q1), then with a confidence of 1 (100 % probability), this company will be clustered in C2 – representing the low-performance companies according to the E pillar score. All other rules are interpreted similarly by following the rule's antecedents, consequences, and confidence.

Many findings are obtained based on the listed top rules representing the associations between the components' quartile-ranged scores and grouping based on pillar scores. If at least one component score of the E pillar is Q1, this company is most probably clustered in the low-performance group for the environmental dimension (rules # 1, 8, 9, 10, 16). All the other rules listed for the E pillar represent the high-performance group. These remaining rules show that if at least one component of the E pillar has a score in Q3 or Q4, this company is most probably grouped as high performance. Indeed, rules # 14, 17, and 18 show that a company can still be clustered in the high-performance group even if the E3 component has a Q2 score if at least one E1 and E2 component has a Q4 ranged score.

Based on the rules listed for the S pillar, it is observed that if, for the S3 component, a company has a ranged score of Q1, it is most probably grouped as a low-performance company (rule #23). Also, rule #17 indicates that even if a company has an S4 component score of Q4 if its S2 component score is Q2, it will be grouped as a moderate S-pillar performance. The remaining rules show that if at least two S components have a ranged score of Q3 and Q4, this company is grouped as high performance with high confidence.

In addition, reaching a Q4 ranged score for just the S1 component will be sufficient for a company to be grouped as high performance on the S pillar (rule #25).

Based on the rules listed for the G pillar, it is found that if the G1 component has a score ranging from Q1, this company is most probably labeled as a low-performance company on the G pillar (rule #12). If the G1 component has a ranged score of Q2, then this company will be clustered in the moderate performance grouping, even though it has a ranged score of Q3 or Q4 for its G2 and G3 components (rules # 1, 8, 9). A company is probably labeled with moderate G performance if only the G1 component score is Q2 (rule # 15). On the other hand, if at least two components of the G pillar have a ranged score of Q3 or Q4, the company is clustered in the high G performance group with high confidence. Besides, having a Q4 ranged score for just the G1 component will be sufficient for a company to be grouped as high performance on the G pillar (rule #11). On the other hand, even though the G2 or G3 components have a ranged score of Q2, this company is still most probably labeled as a high-performance group if its G1 ranged score is Q4 (rules # 13, 14).

The identified rules highlight the higher significance of E3, S1, and G1 components in evaluating sustainability performance based on the E, S, and G pillars, respectively.

5.3. *Stage 3 evaluation of DLB-MS-ESG prediction performance*

For two different structures of the implemented deep neural networks, the model's prediction performance is summarized in Table 4. Table 4 summarizes *DLB-MS-ESG* results of repeated (three) experimentation for two different layer structures of the DNN algorithm.

The layer structure starts with the number of input variables. Since all variables are required to be represented in binary form, fourteen model variables are converted into sixty binary variables. In the first network structure, sixty variables are put into the model's input layer. They are combined into fifty, forty, and fifteen variables in the hidden layers. Finally, one input is set through the output layer of the model to obtain the ESG score as the model output. The second DNN starts with sixty binary variables in the input layer. Forty and fifteen variables are processed in two hidden layers, and finally, one input is processed in the output layer for ESG prediction. The results show that root mean square error varies between 1.10 and 2.18 in this experimentation, meaning that the overall ESG score of the companies is predicted to be very close to their actual scores. The mean absolute percentage errors are similar: 1.4 % to 3 % errors are obtained. Thus, the ESG scores of the companies are predicted to be within 97 % to 98.6 % accuracy. The coefficient of determination values represent 98 % to 99 % of the variation in the model output, ESG score; this is explained by the fourteen input variables of the model.

5.3.1. *Robustness check*

Two different analyses are presented to test the robustness of the *DLB-MS-ESG* prediction model. Firstly, the impact of defined parameters in the two previous stages of the model is explored. The *DLB-MS-ESG* uses fourteen input variables: sector, obtained grouping on E, S, and G pillar scores, and quartile ranged scores of ten components. The model results for the sequential layer structures are presented in Table 4. For further analysis, two benchmark models are defined here. The first one, labeled as benchmark model-1, uses four parameters as sector and grouping companies based on E, S, and G pillar scores. Thus, this model presents the effect of clustering results on the overall ESG score prediction. The second benchmark, model-2, has eleven input variables: sector and quartile-ranged scores of the ten components. Therefore, the impact of quartile-ranged scores on the overall ESG score prediction is explored. The results are summarized in Table 5.

Similar DNN structures are used in the experimentation for robustness checks. However, since the number of input variables differs in

Table 3
Discovered top rules.

pillar	Rule number	Rule's antecedent	Rule's consequent	Performance group	support	confidence
E	1	if E1:Q1 & E2:Q1 & E3:Q1	then C2	low	0.057	1
	2	if E1:Q4 & E3:Q4	then C1	high	0.106	1
	3	if E2:Q4 & E3:Q4	then C1	high	0.149	1
	4	if E1:Q3 & E2:Q4 & E3:Q4	then C1	high	0.053	1
	5	if E1:Q4 & E2:Q4 & E3:Q3	then C1	high	0.064	1
	6	if E1:Q4 & E2:Q4 & E3:Q4	then C1	high	0.089	1
	7	if E2:Q4 & E3:Q3	then C1	high	0.078	0.974
	8	if E2:Q1 & E3:Q1	then C2	low	0.074	0.972
	9	if E1:Q1 & E2:Q1	then C2	low	0.068	0.969
	10	if E1:Q1 & E3:Q1	then C2	low	0.083	0.951
	11	if E1:Q4 & E3:Q3	then C1	high	0.079	0.948
	12	if E1:Q3 & E3:Q4	then C1	high	0.072	0.944
	13	if E3:Q4	then C1	high	0.196	0.939
	14	if E1:Q4 & E2:Q4 & E3:Q2	then C1	high	0.087	0.891
	15	if E1:Q4 & E2:Q4	then C1	high	0.287	0.859
	16	if E1:Q1	then C2	low	0.098	0.836
	17	if E1:Q4 & E3:Q2	then C1	high	0.098	0.821
	18	if E2:Q4 & E3:Q2	then C1	high	0.098	0.807
S	1	if S1:Q3 & S2:Q4 & S3:Q4	then C2	high	0.070	1
	2	if S1:Q4 & S2:Q4 & S3:Q4	then C2	high	0.129	1
	3	if S1:Q3 & S2:Q4 & S3:Q4 & S4:Q4	then C2	high	0.064	1
	4	if S1:Q4 & S2:Q3 & S3:Q4 & S4:Q4	then C2	high	0.053	1
	5	if S1:Q4 & S2:Q4 & S3:Q4 & S4:Q4	then C2	high	0.114	1
	6	if S1:Q4 & S3:Q4 & S4:Q4	then C2	high	0.198	0.989
	7	if S2:Q4 & S3:Q4 & S4:Q4	then C2	high	0.136	0.985
	8	if S1:Q4 & S2:Q3 & S4:Q4	then C2	high	0.078	0.974
	9	if S1:Q3 & S2:Q4 & S4:Q4	then C2	high	0.075	0.972
	10	if S1:Q4 & S2:Q3 & S4:Q4	then C2	high	0.057	0.964
	11	if S1:Q4 & S3:Q4	then C2	high	0.217	0.962
	12	if S1:Q4 & S4:Q4	then C2	high	0.248	0.951
	13	if S1:Q4 & S2:Q4	then C2	high	0.159	0.949
	14	if S2:Q4 & S3:Q4 & S4:Q4	then C2	high	0.194	0.938
	15	if S2:Q4 & S3:Q4	then C2	high	0.215	0.935
	16	if S1:Q3 & S2:Q4	then C2	high	0.081	0.927
	17	if S3:Q2 & S4:Q4	then C0	moderate	0.054	0.926
	18	if S1:Q4 & S3:Q3 & S4:Q4	then C2	high	0.051	0.923
	19	if S1:Q3 & S3:Q4 & S4:Q4	then C2	high	0.115	0.871
	20	if S2:Q4 & S4:Q4	then C2	high	0.229	0.857
	21	if S1:Q4 & S2:Q3	then C2	high	0.087	0.854
	22	if S2:Q3 & S3:Q4 & S4:Q4	then C2	high	0.087	0.854
	23	if S3:Q1	then C1	low	0.051	0.828
	24	if S3:Q4 & S4:Q4	then C2	high	0.339	0.815
	25	if S1:Q4	then C2	high	0.281	0.815
G	1	if G1:Q2 & G2:Q4	then C1	moderate	0.057	1
	2	if G1:Q3 & G2:Q2	then C1	moderate	0.053	1
	3	if G1:Q4 & G2:Q4	then C0	high	0.183	1
	4	if G1:Q4 & G3:Q4	then C0	high	0.209	1
	5	if G1:Q4 & G2:Q3 & G3:Q4	then C0	high	0.075	1
	6	if G1:Q4 & G2:Q4 & G3:Q4	then C0	high	0.106	1
	7	if G1:Q4 & G2:Q3	then C0	high	0.123	0.983
	8	if G1:Q2 & G2:Q3	then C1	moderate	0.057	0.964
	9	if G1:Q2 & G3:Q4	then C1	moderate	0.1	0.959
	10	if G1:Q4 & G3:Q3	then C0	high	0.1	0.959
	11	if G1:Q4	then C0	high	0.398	0.935
	12	if G1:Q1	then C2	low	0.089	0.933
	13	if G1:Q4 & G3:Q2	then C0	high	0.055	0.866
	14	if G1:Q4 & G2:Q2	then C0	high	0.072	0.850
	15	if G1:Q2	then C1	moderate	0.159	0.833

Table 4
Summary performance of *DLB-MS-ESG*.

sequential layers	experimentation trial	RMSE	MAPE	R^2
–50-40–15-1	1	1.17	0.015	0.99
	2	1.10	0.014	0.99
	3	1.44	0.017	0.99
–40-15–1	1	1.64	0.021	0.99
	2	2.18	0.030	0.98
	3	2.13	0.028	0.98

these benchmark models, the number of variables processed in the input layer differs. Thus, the sequential layer values are different in this analysis. Table 5 shows the findings. Firstly, similar to the original model findings summarized in Table 4, the models have higher performances when the number of hidden layers increases. The benchmark model-1, which considers only the clustering results and ignores the component scores, has the lowest performance among the three models. Although this model has the weakest statistics, its performance is still acceptable since only using the obtained performance groups achieves 91.5 % to 92.5 % accuracy. The results of benchmark model-2 are more similar to the proposed *DLB-MS-ESG* model. It has a varying performance between 96.8 % to 98.4 %. With this analysis, while the model robustness is tested, the impact of each identified input variable is also

Table 5
Robustness check with two benchmark models.

model	input variables	sequential layers	experimentation trial	RMSE	MAPE	R^2
Benchmark model-1	Sector, grouping on the E score grouping on the S scoregrouping on the G score	–15-10–5-1	1	4.99	0.077	0.91
			2	4.88	0.075	0.92
			3	5.20	0.081	0.90
		–10-5–1	1	5.15	0.081	0.91
			2	5.03	0.078	0.91
			3	5.32	0.085	0.90
Benchmark model-2	Sector,quartile ranged scores of E1, E2, E3, S1, S2, S3, S4, G1, G2, G3	–50-40–15-1	1	1.36	0.018	0.99
			2	1.32	0.016	0.99
			3	1.67	0.020	0.99
		–40-15–1	1	2.18	0.028	0.98
			2	2.28	0.032	0.98
			3	2.27	0.030	0.98

validated.

Different DNN hyperparameter combinations are also tried to test the model's robustness. The results are shown in Table 6. The first column of Table 6 represents different DNN structures with differing sequential layers. Differing batch sizes are taken as 1, 10, and 20. The number of other units in the DNN is 10 and 100. DNNs are tested with 0.01 and 0.001 learning rates. The data set is split into three train, validation, and test data sets with a ratio of [8:1:1]. Thus, the algorithm is trained in randomly chosen data from 376 companies. Then, the model is validated in the remaining randomly chosen 47 companies' data and tested in the remaining 47 companies' data. For both the validation and test data sets, the prediction performances based on MAPE, RMSE, and R^2 statistics are respectively presented in the last columns of Table 6. The performance statistics in Table 6 show that the prediction model achieved varying accuracies between 88.3 % to 94.1 % in the validation sets and 89.1 % to 95.5 % in the test data sets. These statistics are relatively lower than those in Table 4, showing the model's prediction performance tested with the 100 % train principle. However, the performance achieved according to train, validation, and test principles is still acceptable, showing the model's robustness.

5.4. Stage 4 simulation results for prescriptive analytics

In this stage, to propose prescriptions for sustaining or improving the ESG performance, we simulate scenarios by changing the ESG component scores of companies, generating predictions on overall ESG scores given these changes, and comparing these predicted scores with the real ones. We aim to create what-if scenarios based on the increased or decreased QRS of each of the ten ESG components. However, since the change in QRS level may also change the grouping of the companies, to see the effect of changing QRS levels of components, we decide to consider benchmark model-2 using the sector and QRS of ten components as model parameters. The results in Table 6 show that this benchmark model's performance is very close to the proposed DLB-MS-ESG prediction model, considering that this benchmark model does not make a significant difference in the obtained results and prescriptions.

We choose 146 companies grouped in similar performance clusters on each pillar. We first consider 96 companies clustered in high-performance groups on all E, S, and G pillars and run the simulations using these companies' data. We then run the simulations for the remaining 50 companies with moderate or low performance on each pillar. Thus, we propose prescriptions comparatively and appropriately based on their current performances.

For these two groups of companies, we use their actual data sets as a base. Keeping all other component scores as they are for each simulation, we increase and then decrease QRS by one quartile for each component score, respectively. By comparing the overall ESG score with the predicted score of these scenarios, we observe the impact of each

Table 6
Robustness check with multiple hyperparameter testing.

	Batch size	#of units	Learning rate	Validation set			Test set		
				MAPE	RMSE	R^2	MAPE	RMSE	R^2
60—50 – 40—15 – 1	1	100	0.001	0.082	4.581	0.915	0.065	4.417	0.941
60—50 – 40—15 – 1	10	100	0.001	0.070	4.291	0.925	0.060	4.587	0.936
60—50 – 40—15 – 1	20	100	0.001	0.070	4.221	0.928	0.051	3.975	0.952
60—50 – 40—15 – 1	1	10	0.001	0.076	4.389	0.922	0.060	4.056	0.950
60—50 – 40—15 – 1	10	10	0.001	0.086	4.226	0.928	0.056	3.746	0.957
60—50 – 40—15 – 1	20	10	0.001	0.115	5.739	0.867	0.077	4.809	0.930
60—40 – 15 – 1	1	100	0.001	0.072	3.825	0.941	0.066	4.541	0.937
60—40 – 15 – 1	10	100	0.001	0.060	3.652	0.946	0.059	3.789	0.956
60—40 – 15 – 1	20	100	0.001	0.059	3.666	0.945	0.046	3.396	0.965
60—40 – 15 – 1	1	10	0.001	0.071	4.117	0.931	0.051	4.019	0.951
60—40 – 15 – 1	10	10	0.001	0.105	5.033	0.898	0.070	4.661	0.934
60—40 – 15 – 1	20	10	0.001	0.117	6.906	0.780	0.109	6.055	0.795
60—50 – 40—15 – 1	1	100	0.01	0.091	4.868	0.904	0.064	4.482	0.939
60—50 – 40—15 – 1	10	100	0.01	0.079	4.723	0.910	0.074	5.226	0.917
60—50 – 40—15 – 1	20	100	0.01	0.075	4.184	0.929	0.059	4.285	0.944
60—50 – 40—15 – 1	1	10	0.01	0.080	4.569	0.915	0.057	4.243	0.945
60—50 – 40—15 – 1	10	10	0.01	0.080	4.470	0.919	0.052	4.359	0.942
60—50 – 40—15 – 1	20	10	0.01	0.076	3.937	0.937	0.045	3.130	0.970
60—40 – 15 – 1	1	100	0.01	0.078	4.479	0.919	0.056	4.107	0.949
60—40 – 15 – 1	10	100	0.01	0.086	5.431	0.881	0.069	4.801	0.930
60—40 – 15 – 1	20	100	0.01	0.086	4.929	0.902	0.065	4.486	0.939
60—40 – 15 – 1	1	10	0.01	0.083	4.655	0.912	0.057	3.690	0.959
60—40 – 15 – 1	10	10	0.01	0.073	4.041	0.934	0.047	3.492	0.963
60—40 – 15 – 1	20	10	0.01	0.078	4.022	0.935	0.049	3.281	0.967

ESG component on ESG performance and propose prescriptions for high-performing and moderate/low-performing companies comparatively. Figs. 4 and 5 represent the simulation method.

As seen in Figs. 4 and 5, by increasing and decreasing QRS scores by one quarter for each of the ten component scores for the two company groups, we create and simulate a total of 40 scenarios. If a company's actual QRS score on any pillar is Q4, the simulated score is also Q4 in the increase scenarios since this is the highest possible quarter score. Similarly, if a company's QRS score is Q1, there is no change in the simulated score for the decrease scenarios. We summarize the results of these simulations in Table 7.

In Table 7, the "avg. change" column represents the average change of the companies' actual and simulated ESG scores. Thus, for instance, when the E1 component score of the companies increases by one quarter, while on average, a 6.53 grade increase is observed for the 96 high-performance companies, a 3.44-grade increase is obtained for the 50 moderate or low-performance companies. The "max change" column shows the observed highest changes in the simulation, where this change can be decreased or increased. For instance, when the component score E1 is increased by one quarter, the most significant change is observed as a 17.48-grade increase in the ESG score in a company from the 96 companies. On the other hand, when E1 is decreased by one quarter for the high-performance companies, the highest change observed is a 13.43-grade decrease. Finally, the "n (inc./ dec.)" column represents the number of companies for which increases/decreases are seen between the actual and simulated ESG scores. Thus, when the E1 component score is increased by one quarter, the predicted ESG scores of 89 of the 96 companies are higher than the actual scores. The predicted ESG scores of 80 companies are lower than the actual scores when they decrease by one quarter.

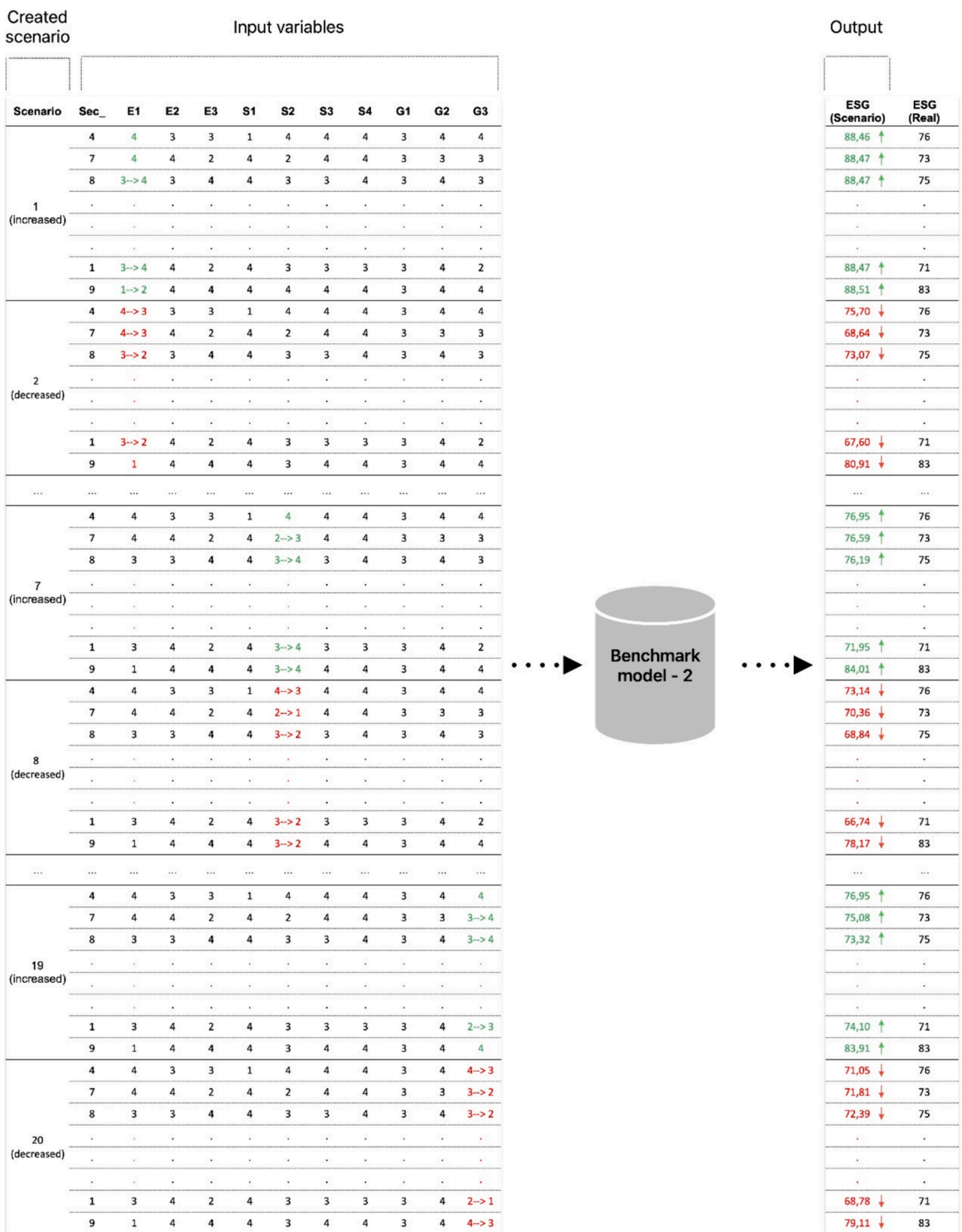

Fig. 4. Simulation method for 96 companies having high performances on each E, S, and G pillar.

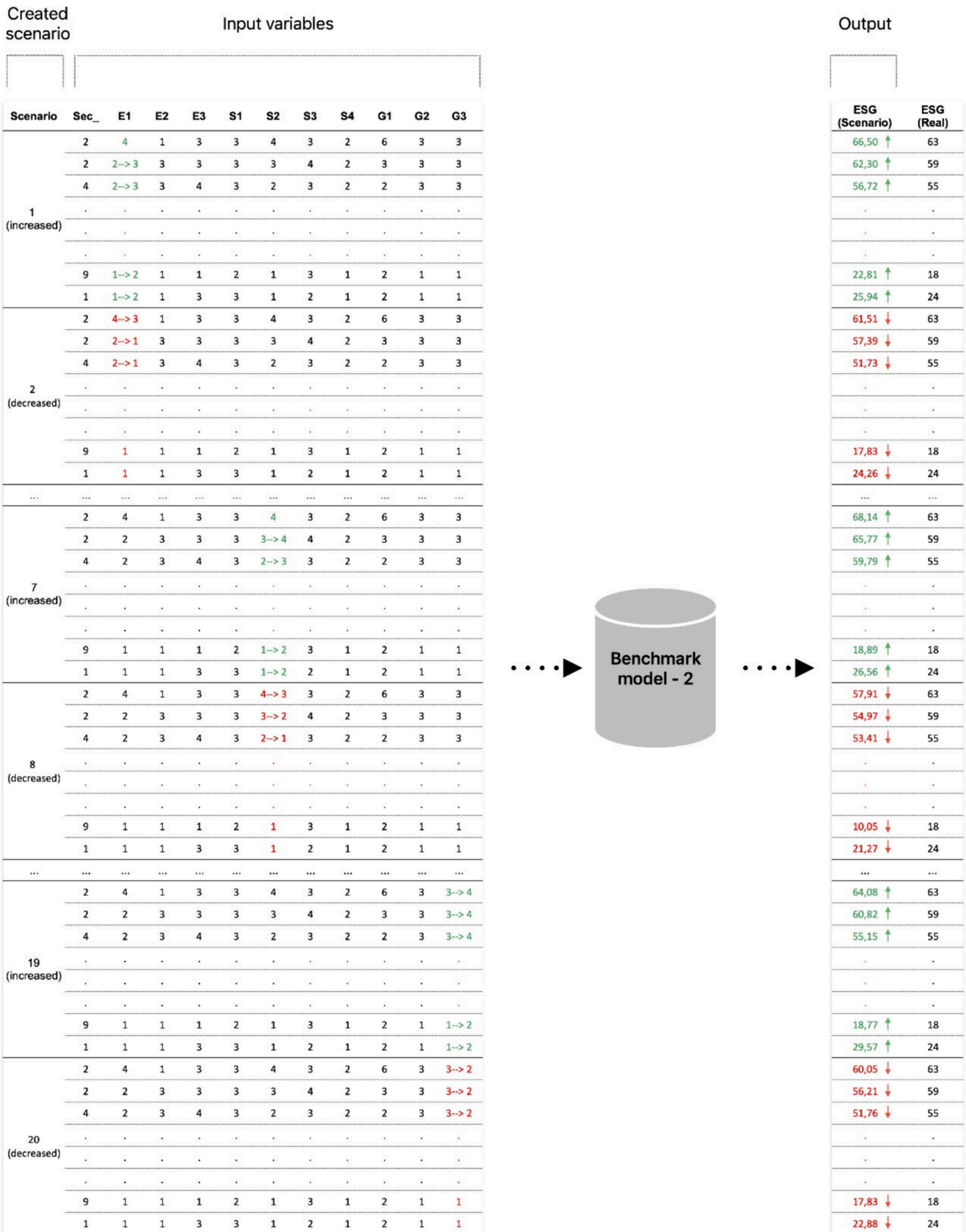

Fig. 5. Simulation method for 96 companies having moderate or low performances on each E, S, and G pillar.

Table 7
Summary results of the simulations.

Simulation id	scenario	Changed pillar scores	High-performance companies on each E, S, and G pillars (n = 96)			Moderate or low-performance companies on each E, S, and G pillars (n = 50)		
			Avg. change	max. change	n (inc. /dec.)	avg. change	max. change	n (inc. /dec.)
1	QRS increased 1 level	E1	6.53	17.48	89 (inc.)	3.44	10.07	44 (inc.)
2		E2	0.14	7.32	52 (inc.)	2.62	6.96	46 (inc.)
3		E3	0.65	6.98	58 (inc.)	2.34	5.86	42 (inc.)
4		S1	0.37	6.21	60 (inc.)	2.23	7.75	38 (inc.)
5		S2	0.72	7.63	63 (inc.)	2.77	9.03	42 (inc.)
6		S3	0.36	9.63	56 (inc.)	3.18	8.08	42 (inc.)
7		S4	0.06	6.72	52 (inc.)	1.62	8.13	41 (inc.)
8		G1	1.12	8.17	59 (inc.)	5.73	11.52	48 (inc.)
9		G2	0.33	6.91	57 (inc.)	2.00	7.43	41 (inc.)
10		G3	0.03	6.27	52 (inc.)	1.71	7.79	36 (inc.)
11	QRS decreased 1 level	E1	−3.24	−13.43	80 (dec.)	−0.98	−8.51	31 (dec.)
12		E2	−2.31	−7.51	79 (dec.)	−1.61	−7.04	32 (dec.)
13		E3	−2.07	−7.29	76 (dec.)	−0.37	−6.76	26 (dec.)
14		S1	−3.51	−11.76	86 (dec.)	−0.56	−4.69	27 (dec.)
15		S2	−3.22	−9.70	84 (dec.)	−1.74	−10.61	30 (dec.)
16		S3	−4.00	−11.13	87 (dec.)	−2.36	−8.24	33 (dec.)
17		S4	−3.96	−10.76	91 (dec.)	−1.95	−10.09	35 (dec.)
18		G1	−5.31	−11.17	92 (dec.)	−3.11	−9.49	38 (dec.)
19		G2	−1.96	−8.89	71 (dec.)	−0.59	−5.55	26 (dec.)
20		G3	−2.09	−9.16	73 (dec.)	−0.40	−6.50	23 (dec.)

Table 7 provides many prescriptions for the companies. For the companies having high sustainability performances on each E, S, and G pillar, increasing their performance on the emission (E1) component may cause the most considerable improvement in the overall ESG score; this is followed by the management (G1) component. A one-quarter increase in all other eight component scores will not cause a significant improvement on the ESG score. On the other hand, these high-performance companies are more sensitive to decreases in component scores. If component scores decrease by one quarter, the overall ESG scores in most companies will decrease, on average, between 2 and 5 grades. The highest decrease can be seen due to the reduction in the G1 component.

The low or moderate-degree performance companies on each pillar may be more sensitive to increases in their component scores. A one-quarter rise in any of the pillars may cause an average 2 to 6-grade increase for most companies. Components G1, E1, and S3 (workforce) may lead to the highest increases. These companies may be more sensitive to a one-quarter decrease in the components of G1, S3, and S2 (product responsibility) than the other seven components.

6. Discussion

With increased awareness of sustainability, companies' performance is now being evaluated, plus how and to what extent they are being environmentally friendly and benefiting society. As a result, while companies start to put sustainability at the top of their agendas and make their decisions accordingly, researchers, practitioners, and governmental institutions have begun to identify key metrics and evaluate the sustainability performance of organizations. Additionally, investors start to assess companies based on the performance of their environmentally sustainable activities instead of focusing only on their financial profitability and making their investment decisions within this framework. Various studies discuss the key themes in sustainability performance evaluation and reporting (Lee, Raschke & Krishen, 2022; Staniškis & Arbačiauskas, 2009). Since evaluating sustainability performance is highly subjective, analytical techniques and conceptual models are increasingly being used to overcome these complexities (Büyüközkan & Karabulut, 2018). Existing research aims to evaluate sustainability performance by constructing a composite index (Cottafava, Ascione, Corazza, & Dhir, 2022) or applying various analytical tools and techniques (Jain et al., 2022; Zhou et al., 2021).

The advances in data analytics technologies are receiving the attention of researchers; consequently, these technologies have started to be implemented in the context of sustainability performance evaluation. Many different techniques offered by data analytics technologies are used in this field; machine and deep learning techniques are the most significant among them (D'Amato et al., 2021; Lee et al., 2022; Vo et al., 2019).

Although models developed with these technologies are increasingly taking their place in current literature, most studies focus on a single function of these technologies. Therefore, to benefit more from these technologies, research needs to be improved by holistically combining different functions and techniques. With this aim, this study proposes a deep learning-based multi-stage model for predicting the sustainability performance of companies. The clustering function of these technologies is implemented in the initial stage of the model to create a homogenous grouping of companies to gauge their performances in the environmental, social, and governance pillars of sustainability. The second stage leverages the association rule mining function of these technologies. It generates hidden associations between the critical components of the three sustainability pillars and the companies' performance groups for these pillars. Using the obtained information from the previous stages, the last stage of the model aims to predict the overall sustainability performance of the companies in terms of their overall ESG scores. Besides attempting to fill the gap identified in existing literature, the proposed model contributes to the body of research by presenting an alternative means to perform ESG score and sustainability performance evaluation. In this regard, this study has many implications for both theory and practice.

6.1. Theoretical implications

Although various existing studies adopt dynamic capability (Al-Shami & Rashid, 2022; Buzzao & Rizzi, 2021; Dias, Gouveia Rodrigues & Ferreira, 2021; Rebs et al., 2019; Tiberius, Stiller & Dabić, 2021) and BDAC (Pandya & Kumar, 2022; Zhu et al., 2022) theories in the sustainability performance evaluation context, this study attempts to contribute to these theories from different aspects. Firstly, the findings reveal variability in companies' sustainability performances, both across different organizations and within their individual performances across the three sustainability pillars. The performance of companies on each pillar varies, depending on the industry sector. For instance, companies in the industrial, healthcare, utilities, and consumer defensive sectors are often categorized as having high or moderate performance levels on

E, S and G pillars. These findings emphasize the components that are particularly significant to a company's performance on each pillar. In a rapidly evolving business environment, models that examine these changes and identify the most critical features and parameters for performance evaluation could provide valuable insights for investors making investment decisions. Despite managers having proprietary information about their practices, this comparative analysis is equally beneficial for them, as it influences the attractiveness of their company stocks to investors. The rapidly shifting sustainability landscape continually reshapes decision-making processes for both investors and managers. The dynamic nature of company data sets warrants that decision-making processes quickly adapt to changes. Decision-makers, including investors and managers, face increased time pressures due to the swift and dynamic evolution of data, highlighting the growing necessity for BDAC, which becomes an essential framework for establishing a decision-making mechanism that fosters sustainability.

Thus, although dynamic capability theory and the recent view of BDAC have been well presented in recent literature, this study attempts to extend their usage in sustainability performance evaluation. By proposing a multi-stage model implementing various functions and tools of BDA and validating this model in Fortune 500 companies, this study aims to contribute to the context of these theories.

6.2. Managerial implications

The proposed model has direct managerial implications. While the whole model can be used to predict companies' ESG scores, each step can also be used separately. A decision-maker, manager or investor, can evaluate a company's performance on each sustainability pillar by comparing its scores with the average scores of each performance grouping for the benchmarked companies. By comparing the company performance on each pillar with high-performance companies, managers can set exact targets for the company, particularly on the pillars with relatively lower performances. Companies may also benefit from the second stage of the model by generating hidden associations between the component scores and the company's performance. The generated rules may also highlight the critical components of the sustainability pillars. These associations and identified components of higher importance may also be used in decision-making processes.

Investors may also use the proposed system. Regulators, governments, non-governmental organizations, and researchers can benefit from this study while evaluating the ESG performances of companies and suggesting efficient investment decisions. Overall, ESG performance measurement depends on different pillars and components in traditional models for calculating an ESG score. All of these pillars and components must have exact numerical measurements to make easier the comparisons and evaluations of the sustainability performance of firms. The proposed ESG score prediction system provides ease for practical usage since it does not require exact scoring for component scores or any weighting between them while evaluating the finalized ESG score. Besides, it presents an alternative way of assessing firms' performances on different pillars of sustainability and the relations between component scores and firms' groupings according to pillar scores.

This system's novel aspect is that it does not require any weighting on component and pillar scores in ESG evaluation. This model can be used practically to estimate the future ESG performance of a company given its current year performance grouping on each E, S, and G pillar score and the quartile ranged score of each of the ten components. In addition, a company can then concentrate on a specific component and introduce appropriate activities regarding this component during the year. The rating agencies periodically update the component, pillar, and overall ESG scores at the end of the year. But the situation may arise when a decision-maker is aware that the company increases its performance on this component, this will increase the exact scoring presented by rating agencies. In that case, the decision-maker may use the proposed model to estimate this firm's future ESG score by increasing the current quartile score of that particular component at least by one. Thus, without waiting for the updated scoring of the rating agencies, the decision-maker can obtain accurate predictions on the overall ESG scoring of the companies.

While this model can be used efficiently to generate predictions on the overall future ESG scores of the study data set of companies, it can also be used to evaluate the performance of an outside company. Assume that a company not currently listed in sustainability indexes is a candidate to be listed soon. The decision-maker may implement this model based on its possible grouping (low, moderate, high-performance) on each E, S, and G pillar score and the estimated quartile scores of each component to assess the possible ESG scoring of the company. These properties of the proposed system can prove to be very effective in managers' and investors' decision-making processes.

7. Conclusion

This study introduces a predictive tool for evaluating companies' ESG performance by leveraging advanced data analytics, deep learning technologies, and prescriptive methodologies to form a holistic perspective. The model's significant advantage lies in its utilization of quartile range scores for the ten components, rather than precise scores that range from 0 to 100, when determining the overall ESG score. Consequently, this approach eliminates the necessity to assess and assign weights to the components and pillars, as it does not rely on weighted averaging for its calculations.

The proposed system follows a multi-stage form where companies are initially grouped as high, moderate, and low performance based on their scores on each E, S, and G pillar of sustainability. Then, the hidden associations between quartile ranged scores of each component and obtained performance grouping of the regarding pillar are generated. Sector, obtained grouping on each pillar, and the quartile ranged score of each of the ten components are finally used as model input variables in the overall ESG score prediction. This model is tested in Fortune 500 companies, with around 99 % accuracy achieved in the experiment. Various experiments are also presented to demonstrate the robustness of the model.

The primary limitation of this study stems from the substantial volume of data required when working within the BDA framework. Our model validation involved 470 companies from the Fortune 500 list, alongside their sustainability scores from the Refinitiv database. Although the application of BDA techniques in real-world contexts requires large datasets, smaller datasets and analyses offer benefits, including simplified data collection and suitability for experimental analysis, particularly in domain-specific exploratory studies. Despite Refinitiv covering the sustainability performance of over 7,000 companies worldwide, our research focused on a subset of Fortune 500 companies to highlight the practical implications of Environmental, Social, and Governance (ESG) factors in fostering sustainable business practices within the Fortune 500 index. Looking forward, this model could be expanded to include other indices, such as the Fortune 1000, S&P, and Dow Jones, or applied to the entirety of companies listed in the Refinitiv database, for broader validation.

This study selects and implements a unique technique for each model step. As a future research direction, the multi-model approach can be used. Thus, different methods can be adopted for each stage of the model, and their performances can be compared. The proposed method can also be compared with other ESG rating systems such as Bloomberg, Sustainalytics, etc. A proposed prescriptive model can also be comparatively analyzed with updated data from the selected companies in future research. While this study focuses on sustainability and ESG scores, the proposed model can be extended to various contexts (such as renewable energy projects, carbon offsetting schemes, and urban development city planning projects) with a triple-bottom-line structure data set.

CRediT authorship contribution statement

Gorkem Sariyer: Writing – original draft, Supervision, Project administration, Methodology, Investigation, Conceptualization. **Sachin Kumar Mangla:** Writing – original draft, Validation, Supervision, Methodology, Investigation. **Soumyadeb Chowdhury:** Writing – original draft, Visualization, Software, Investigation, Formal analysis. **Mert Erkan Sozen:** Software, Investigation, Formal analysis, Data curation. **Yigit Kazancoglu:** Writing – original draft, Validation, Supervision, Resources, Project administration, Conceptualization.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

Appendix A. k-means++ clustering algorithm

Consider a collection of observations $(x_1, x_2, \cdots, x_n)$ where each node is a d-dimensional real vector. This algorithm aims to divide these n observations into k sets or clusters $(k \le n), S = \{S_1, S_2, \cdots, S_k\}$ to minimize the within-cluster sum of squared distances:

$$\underbrace{argmin}_{S} \sum_{i=1}^{k} \sum_{x \in S_i} \|x - \mu_i\|^2$$

by following the below step-by-step process:

Step 1. Select an initial center from $X(x_1, x_2, \cdots, x_n)$ uniformly randomly among all data points.

Step 2. Compute D(x) for any node x (the distance between x and the center selected in step 1.

Step 3. Choose another data node randomly as a new center, employing a weighted probability distribution, whereas x is chosen with probability proportional to $D(x)^2$.

Step 4. Repeat steps 2 and 3 until k centers have been chosen and finalize the initialization.

Step 5. Since the initial centers are appropriately chosen, move through, minimizing the within-cluster sum of squared distances given by equation (4).

Appendix B. Apriori algorithm

Let 'T' be a set of n transactions represented by $\{T_1, T_2, \ldots, T_n\}$ and 'I' be a set of items defined by $\{i_1, i_2, \ldots, i_n\}$ where $Ti \subseteq I$. In $X, Y \subseteq I$ and $X \cap Y = \emptyset$, X= >Y represents an association rule as X is the antecedent and Y is the rule's consequent. Antecedents or consequents are the items of the data set.

Support and confidence are used as performance metrics. For $X \subseteq I$, support(X) measures how frequently X is observed in the data set. Similarly, support of the rule is represented as support(X= >Y) = support($X \cup Y$) and indicates how frequently both X and Y are observed together in the data set. Confidence is the measure of reliability of a rule and is computed as (X= >Y) = support($X \cup Y$) / support(X).

The Apriori algorithm extracts association rules from the frequent item set combinations and filters through the given support and confidence threshold values. Let 'I' represent the item set with length n. I is frequent if every subset with length n-1 is also frequent.

Appendix C. Deep neural networks

A deep neural network is a tuple N = (L, T, Φ), where $L = \{L_k \mid k \in \{1..K\}\}$ is a set of layers, $T \subseteq L \times L$ is a set of connections between layers and $\Phi = \{\varphi k \mid k \in \{2, \ldots, K\}\}$ is a set of functions, one for each non-input layer. In a deep neural network, L_1 is the input layer, and L_K is the output layer. Other layers, excluding input and output layers, are the hidden layers. Each layer L_k contains s_k nodes. The l^{th} node of layer k is represented by $n_{k,l}$. Each node $n_{k,l}$ for $1 < k < K$ and $1 \le l \le s_k$ is connected with two variables $u_{k,l}$ and $v_{k,l}$ to record its values before and after an activation function, respectively. The ReLU function according to which the activation value of each node of hidden layers is defined as:

$$v_{k,l} = ReLU(u_{k,l}) = \begin{cases} u_{k,l} if u_{k,l} \ge 0 \\ 0 otherwise \end{cases}$$

Each input node $n_{1,l}$ for $1 \le l \le s_1$ is related to a variable $v_{1,l,}$ and each output node $n_{K,l}$ for $1 \le l \le s_K$ is associated with an irregular $u_{K,l}$ because no activation function is applied on them. We let $D_{L_k} = R^{s_k}$ be the vector space associated with layer L_k, one dimension for each variable $v_{k,l}$. Notably, every point $x \in D_{L_1}$ is an input.

Except for inputs, every node is connected to nodes in the previous layer by pre-trained parameters such that for all k and l with $2 \le k \le K$ and $1 \le l \le s_k$, we have:

$$u_{k,l} = b_{k,l} + \sum_{1 \le h \le s_{k-1}} w_{k-1,h,l} v_{k-1,l}$$

where $_{wk-1,h,l}$ is the weight for the connection between $n_{k-1,h}$ (i.e., the h-th node of layer $k-1$) and $n_{k,l}$ (i.e., the l-th node of layer k), and $b_{k,l}$ is the so-called bias for node $n_{k,l}$. We note that this definition can express both fully-connected functions and convolutional functions.

Finally, for any input, the deep neural network assigns a label, that is, the index of the node of the output layer with the largest value:$label = argmax_{1 \le l \le s_k} u_{K,l}$

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