

A Neuro-Causal Fusion Architecture for Outlier-Robust ESG Forecasting and Policy Simulation

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Abstract—The global transition toward mandatory sustainability governance has exposed a critical “prediction-action” gap, where conventional black-box models fail to provide actionable strategic roadmaps. Current ESG forecasting is further compromised by the systemic risk of corporate greenwashing and the structural inability of standard machine learning to handle the heavy-tailed anomalies inherent in volatile financial datasets. To bridge this epistemological divide, the Neuro-Causal Fusion (NCF) framework is introduced as a dual-stream architecture designed for high-fidelity prediction and prescriptive policy simulation. The methodology synthesizes hierarchical Out-Of-Fold (OOF) tree meta-features with a bidirectional Long Short-Term Memory (BiLSTM) attention network, using an outlier-robust Huber Loss to ensure stable convergence amid market volatility. Furthermore, Fuzzy-set Qualitative Comparative Analysis (fsQCA) is integrated to derive specific “causal recipes” for ESG excellence across diverse firm lifecycles. Empirical results demonstrate superior predictive fidelity ($R^2 = 0.9603$), significantly outperforming traditional boosting and neural baselines. Beyond prediction, the Digital Twin simulation module identifies non-linear marginal returns for resource optimization, empowering C-suite executives to virtually stress-test sustainability policies before physical capital expenditure. This research ultimately provides an audit-ready strategic consultant for navigating the rigorous regulatory demands of the Paris Agreement and CSDDD. The framework’s reliability is further validated through comprehensive ablation studies and cross-seed stability tests, ensuring reproducible intelligence for institutional sustainability auditing.

Keywords—ESG risk prediction; neuro-causal fusion; digital twin; huber loss; fsQCA; sustainable finance

I. INTRODUCTION

Environmental, Social, and Governance (ESG) performance is no longer just a ‘nice to have’ ethical issue. It is one of the key parameters of corporate stability and competitiveness in the modern financial system [1]. In the world’s capital markets, attention is on sustainability rather than short-term profit maximization. This is confirmed by

recent empirical evidence from the banking sector. High-level sustainable ESG performance is a strategic asset. It is a buffer mechanism that transforms the market’s competitive forces into a stronger system of financial resilience [2,3]. This correlation is even more important during times of macroeconomic volatility. Systematic risk is also protected by mature sustainability practices [4, 5]. To protect capital against the risk of future climate and governance shocks, ESG must be predicted and managed properly for all global investors and regulators [6]. One of the emerging economic challenges is corporate greenwashing, which has accompanied high ESG ratings. A significant portion of sustainability reporting is self-reported and not audited by a standardized framework. This enables corporations to control narratives to overstate their sustainability attractiveness [7]. As analyses of corporate disclosures using natural language processing (NLP) show, there is a significant transparency gap.

In general, companies tend to focus on external factors and forget internal factors such as governance [8]. A study of LEED-certified buildings found that only 10% of the reports demonstrated transparency in governance [9]. This type of selective reporting covers up systemic risks under a sustainability facade [10]. An information veil is a major discrepancy in information between the corporate board and shareholders. Advanced AI-auditing systems need to be designed to assess the actual impact on operations to restore the integrity of the market [11]. The complexity of building these AI-powered systems stems from the complexity of corporate data. Financial and ESG indicators can be highly non-linear and vary widely across the world. These datasets commonly have extreme outliers and are heavy-tailed [12]. Markets have “Black Swan” moments, like geopolitical changes or taking an instant environmental “fine”. These anomalies give rise to abrupt changes in the structure of financial time series [6].

The majority of current machine learning models assume normal distributions and employ the Mean Squared Error (MSE) loss function. However, MSE is not well-suited to sustainability data that is heavy-tailed, since the squared residuals are more likely to be influenced by outliers. This

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results in gradient instability and biased convergence, which has a significant impact on the robustness of the prediction, making it challenging to capture the underlying pattern due to noisy data [13,14]. If the anomalies are heavy-tailed, the MSE harshly penalizes large deviations. This can make the gradient unstable and heavily overfit to local noise. Therefore, the traditional model fails to generalize in volatile markets. There is also an epistemological gap between prediction and strategic execution.

Descriptive “black-box” models abound in the current literature. However, corporate executives require more than just a forecast ESG value to make strategic managerial decisions based on enhanced disclosures of their social sustainability [15]. Many Explainable AI (XAI) techniques, such as SHAP and LIME, offer only retrospective insights. They describe what has happened but do not guide as to how to optimize future outcomes [16]. A forecasted ESG score isn’t enough for corporate executives. They need roadmaps that provide some direction for operational transitions. The need can be met with prescriptive analytics, specifically Digital Twin technology. In manufacturing, Digital Twins help optimize processes, moving from the “As-Is” to the “To-Be”. This technology significantly shortens process timelines and eliminates information gaps within the organization. The use of these simulation systems is a key enabler for improving the performance of the green supply chain and managing strategic risk [17,18]. To overcome these algorithmic and strategic difficulties, the NCF framework is presented. The NCF model can fill the gap between structural intelligence and temporal memory. It combines OOF tree meta-features with an elaborated BiLSTM-Attention temporal stream. The network is optimized using the Huber Loss function for robustness to outliers. The negative impact of heavy-tailed anomalies is suppressed with Huber Loss without any loss of predictive accuracy. The framework is also designed to account for the mapping of complex causal configurations for the use of fsQCA. Lastly, it uses a Digital Twin simulation environment to create a model that becomes an audit-ready strategic consultant. This enables companies’ boards to model the effects of policies and allocate resources as they go. The research makes many contributions, both multidimensional and at the forefront of computer finance and sustainable corporate governance. In particular, this paper brings the following:

- **The Neuro-Causal Fusion (NCF) Architecture:** We develop and validate a hybrid neural-boosting framework that successfully synthesizes the hierarchical rule-extraction capabilities of tree-based ensembles with the longitudinal sequence-modeling strengths of BiLSTM networks, achieving enhanced predictive accuracy in multidimensional ESG forecasting.
- **Outlier-Robust Optimization:** We introduce a robust mathematical approach in ESG modeling by replacing the conventional MSE loss with the Huber Loss function, empirically demonstrating its capacity to stabilize gradient convergence and maintain robust predictive performance amidst heavy-tailed financial data and market volatility.
- **Causal Configuration via fsQCA:** Moving beyond traditional linear feature attribution, we implement

fsQCA to extract complex “causal recipes,” providing corporate management with explicit, configurational pathways that support high ESG outcomes across varying stages of the Firm Life Cycle.

- **Digital Twin Policy Simulation:** We build a dynamic Digital Twin sensitivity analysis module that turns static AI predictions into quantified, forward-looking strategic roadmaps, so C-suite executives can virtually simulate the net impact of specific resource-optimization policies before physical capital expenditure.

II. LITERATURE REVIEW

History of the sustainability governance system changing from voluntary disclosure to mandatory disclosure. A key element of this development is the ratification of the EU’s Corporate Sustainability Due Diligence Directive (CSDDD), which introduces fault-based civil liability. It obligates large enterprises to implement climate transition plans that are firmly anchored in the 1.5 °C Paris Agreement target [19]. Theoretically, this regulatory wave is based on Stakeholder Theory, which asserts that companies must meet a wider range of environmental and social expectations to be legitimate. The ‘Management Score’ is included as a significant measure of the firm’s overall ESG effectiveness across the Firm Life Cycle, drawing concepts from the Firm Life Cycle theory. Corporate resources shift from SMEs to mature, and a good management is the only single way to maintain stewardship to satisfy the demands of stakeholders and to avoid greenwashing. However, the risks of “technological greenwashing” have emerged when financial institutions have been quick to leverage AI to automate compliance obligations, yet have not realized that, behind the black box, lie high-frequency metrics that mask underlying systemic risk. This requires a shift toward “Responsible AI” architectures that address Information Asymmetry by enforcing strict algorithmic auditing and human-in-the-loop review and control, thereby improving transparency and verifiability of corporate disclosures [10].

Although the regulatory mandate for this transparency, fundamental research in ESG forecasting has largely been confined to static machine learning approaches that do not account for the temporal nature of corporate actions. As a result, sectorial involvement data has been empirically shown to be more powerful than conventional financial data for predicting the ESG performance of mutual funds when used with non-linear ensembles such as Random Forests and Gradient Boosting [20]. Likewise, machine learning models such as Extreme Gradient Boosting (XGBoost) have demonstrated a strong ability to explain differences in ESG ratings for non-financial companies, relative to traditional statistical estimation models [21]. Moreover, the accuracy of the stacked ensemble models has been improved to evaluate the ESG risk of S&P 500 companies, and scientific evidence indicates that environmental and social factors are the most important in measuring total risk [13]. To improve predictive stability, recent literature has investigated the use of “Stacked Generalization,” which uses a meta-learner to combine multiple base learners via Bayesian Ridge Regression to reduce the variance commonly found in high-dimensional tabular data [14]. These architectures highlight the hierarchy of immediate structures, and sustainability is treated

as a point in time rather than a process. These models are static and do not reflect the longitudinal connections and historical context of ESG-related corporate action, and therefore lack dynamism in understanding long-term sustainability. To overcome this temporal gap, recent methodological developments have moved away from the traditional architectures to deep learning architectures that can learn sequential dependencies. A more complex approach has been used to forecast carbon emissions by combining structured financial indicators and semantic features extracted from corporate narratives using a hybrid framework that combines Long Short-Term Memory (LSTM) networks with Attention mechanisms [22]. In addition, the high-dimensional heterogeneity of corporate data has been addressed by designing advanced architectures, such as the Feature Balancing Transformer (FeBT), to ensure that low-dimensional signals are not overwhelmed by the dominant features in the data [23]. Some more complex relationships in the text have also been observed, for example, an inverted U-shaped relationship between ESG engagement and systematic risk under high economic policy uncertainty [4]. There is an important mathematical fact, though: an important data point in financial and ESG data is that “heavy tail” and “Black Swan” events, or extreme outliers, naturally exist. Standard deep learning models relying on Mean Squared Error (MSE) loss tend to over-penalize these anomalies, leading to destructive gradient explosions and destabilizing the model’s ability to generalize across volatile market conditions.

The pursuit of model transparency has subsequently led to the widespread adoption of Explainable AI (XAI), yet a profound epistemological gap remains between post-hoc explanation and strategic execution. XGBoost-SHAP-based models that can be interpreted have also been used to show that financial factors, including EBIT, tend to have a stronger effect on ESG ratings than non-financial measures [24]. At the same time, XAI-Ready Decision Support Systems are implemented to model carbon-emission pathways, enabling a shift from retrospective reporting to predictive governance [16]. Such improvements are commonly supported by Digital Twin technology to streamline the performance of the green supply chain and address information asymmetry in the manufacturing environment [25]. Effective implementation of these digital twins, however, strongly relies on firm readiness, which is a key driver of converting technological support into improved green supply chain operations at the corporate level [17]. However, the efficiency of this technological preparedness is frequently undermined by the institutional inertia of deeply rooted technologies and cross-scale competition in technology, which will slow the overall dynamics of green innovation even in favorable contexts [26]. Although some factors, such as green innovation, have been identified as positive catalysts, particularly when enhanced by the Paris Agreement, which is still considered in the literature, it is more descriptive in nature [27]. The majority of frameworks end with identifying the importance of features but do not offer an actionable roadmap or causal configurations to guide corporate strategy through the various phases of the Firm Life Cycle. Addressing these multifaceted constraints requires a shift to an integrated Neuro-Causal perspective. The proposed NCF architecture is specifically engineered to fuse the structural intelligence of tree-based ensembles with the temporal memory of BiLSTM-Attention streams. It is achieved by using the Huber Loss function,

an outlier-robust loss function, instead of the commonly used MSE loss function, resulting in more stable convergence in the framework and greater robustness to corporate data anomalies. The NCF framework not only predicts but also identifies specific recipes for causal excellence in ESG and simulates the future with precision using a Digital Twin. This method is not just about reporting risk; it provides a mathematically based, audit-ready strategic consultant that enables corporate boards to move beyond reactive compliance to proactive, data-driven sustainability optimization in line with current global regulations.

III. METHODOLOGY

The proposed Neuro Causal Fusion (NCF) framework follows an integrated multistage pipeline designed for high-fidelity ESG prediction and prescriptive analytics. As illustrated in Fig. 1, the workflow transitions from robust data engineering, incorporating sector median imputation and heavy-tailed anomaly control, to a dual-stream deep learning architecture. This architecture synthesizes temporal dependencies via a Bidirectional LSTM attention network with structural intelligence derived from out-of-fold tree meta features. Using an outlier-robust Huber Loss protocol, the framework produces a Digital Twin simulation environment for virtual stress testing and strategic assessment of sustainability policies.

A. Data Acquisition, Preprocessing, and Sample Characteristics

This paper is based on an in-depth, multi-sector global Environmental, Social, and Governance (ESG) data. The original raw matrix was a high-dimensional feature space comprising 509 sustainability and financial measures across 21,496 firm-years. Because global corporate reporting is inherently noisy and sparse, we implemented a rigorous mathematical preprocessing protocol to ensure maximum data integrity and structural independence. In the early days, strict longitudinal continuity was imposed to ensure that the evolutionary patterns of corporate behavior were captured as an evolving process rather than as a series of disjointed data points. Companies without 6 years of continuous reporting data were excluded. In parallel, the raw data matrix was sparsified to determine the sparsity thresholds. Observations and features that had more than 40% and 75% of their data missing were systematically excluded. Structural pruning is necessary to reduce the amount of synthetic noise added to the data, ensure the data remains real-valued, and then impute the data. The zero-variance constants were removed before handling the remaining missing values using a highly contextual imputation strategy. The use of global medians creates a distributional drift by obscuring important macroeconomic and industrial differences. We performed dynamic imputation of missing data points based on the intersection of the firm’s Global Industry Classification Standard (GICS) sector and the reporting year. To define the imputed value of a missing feature denoted by the value $\hat{x}_{i,j,t}$ of firm i in the sector S at year T , the imputed value of the feature is defined in Eq. 1:

$$\hat{x}_{i,j,t} = \text{median}(x_{k,j,t}) \quad \forall k \in S, T \quad (1)$$

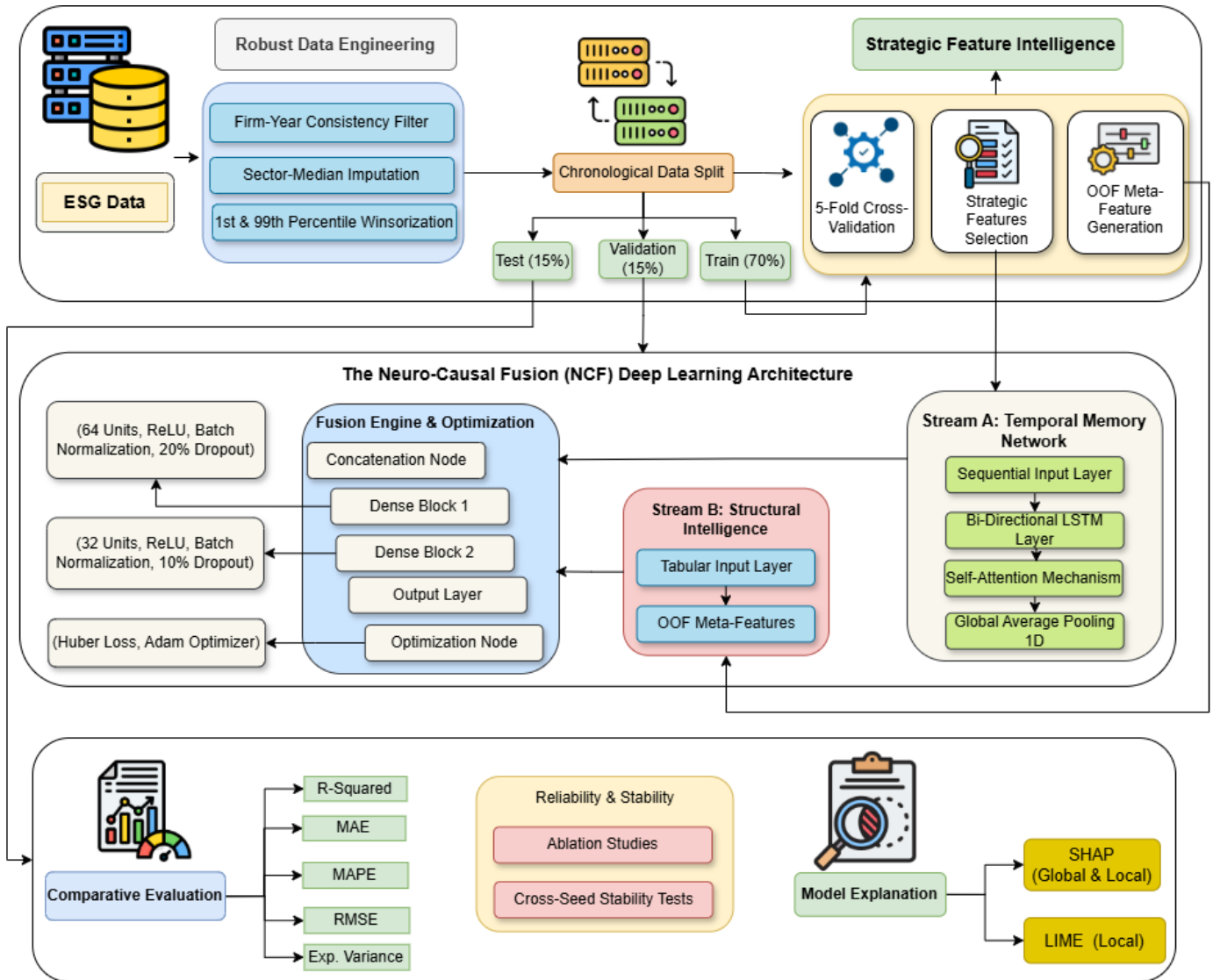


Fig. 1. The architecture of the proposed Neuro-Causal Fusion (NCF) framework.

This Sector-Year anchoring ensures that the imputed values accurately reflect the regulatory environment and market conditions of that time frame. In addition to the loss of values, corporate financial data often has heavy-tailed distributions and extreme reporting distributions. Such extreme values severely penalize statistical loss functions and can lead to instability in numerical optimization. Bilateral Winsorization of all continuous non-protected variables at the 1st ($P_{0.01}$) and 99th ($P_{0.99}$) percentile was used to stabilize statistical variance. Transformation of an individual feature value $x_{i,j}$: mathematically, Eq. 2 expresses the transformation:

$$x'_{i,j} = \max(P_{0.01}(X_j), \min(x_{i,j}, P_{0.99}(X_j))) \quad (2)$$

Finally, a redundancy control system was introduced to prevent signal dilution. Using the Pearson correlation matrix, highly correlated features were identified. To compute the correlation coefficient with any two continuous features, X

and Y, the correlation coefficient between the two variables was computed as follows in Eq. 3:

$$\rho_{X,Y} = \frac{\text{cov}(X,Y)}{\sigma_X \sigma_Y} \quad (3)$$

Features exhibiting high collinearity ($|\rho_{X,Y}| > 0.98$) were systematically excised. This will guarantee structural independence of the other variables. Based on this thorough procedure, the data were reduced to a high-fidelity set of 17,611 firm-year observations and 397 structurally feasible features. To ensure the empirical representativeness of this streamlined sample, a descriptive analysis was conducted geographically, industrially, and temporally, as shown in Table I. The distributional properties give insights into salient structural heterogeneities. As shown in panel A, there is a sharp regional difference: mature Western markets (the US and Europe) have robust, positive mean ESG scores, whereas emerging Asian markets have negative mean ESG scores.

Regulatory shifts and the pressure of institutional investors in the West drive the development-sensitive industrialization of emerging market economies (EMEs). Moreover, there is no evidence of any industrial bias in panel B, with service sectors such as Banking (0.52) being represented well, relative to other sectors such as operationally intensive industries, Machinery (-0.12) and Chemicals (-0.08), and carbon-intensive industries, Engineering Components (-0.06). This disconnect is indicative of physical supply chains' systematic exposure to environmental penalties regardless of the management in place. Finally, the evolutionary process of Panel C has been steadily rising from a negative world average in 2010 to a very positive mean (0.38) in 2022, as the world moves towards compulsory institutional ESG reporting standards rather than voluntary corporate social responsibility reporting protocols. The fact that these spatial, sectoral, and temporal complexities overlap requires a complex, non-linear predictive structure developed in this paper, which, of course, cannot be provided by traditional linear regressions.

B. Target Formulation, Chronological Partitioning, and Feature Engineering

After data curation, the next stage of the methodological plan involves rigorous target formulation, elimination of predictive leakage, and feature engineering to fully exploit the mathematical space using deep learning. The main aim of the study is to predict the normalized global ESG index (INDEXESG1_N). Aggregated ratings in corporate sustainability ratings tend to suffer from target leakage, in which independent predictor variables inevitably contain a “leaky” component of the dependent variable. To prevent overly optimistic predictive accuracy, a strict protocol to eliminate leakage was in place. The feature space was systematically reduced only to include leakage predictors and granular sub-pillar scores that are precise and meaningful, such as `corpgov_tresgcoregrade`, `corpgov_env_pillarscoregrade`, `corpgov_socialpillarscoregrade`, and combined historical averages like `INDEXESG1_mean`. With these variables, the model would simply be predicting the ESG score based on the ESG score itself, thus missing the real drivers of operations. These variables are removed to ensure absolute transparency and force the model to adopt the basic corporate behavior that drives sustainability. The log transformation was applied to financial measures (total reported assets, net income, and total liabilities) to reduce their high positive skewness. The training history of a neural network can amplify very important governance and social cues by using unscaled financial magnitudes. All absolute financial characteristics were log-plus-one transformed; mathematically, this is expressed by Eq. 4:

$$x'_{i,j} = \ln(1 + \max(x_{i,j}, 0)) \quad (4)$$

Given that corporate ESG performance is very sensitive to macroeconomic cycles and shifts in global policy, the model can exhibit significant look-ahead bias when using standard randomized cross-validation, meaning it can predict past events based on future data. To maintain the causal ordering of the financial data, the original data was immediately processed using a strict chronological partitioning strategy after the first transformations were applied. The dataset was split into

Training (70%), Validation (15%), and Testing (15%) sets according to the year of reporting. To completely prevent information from crossing these temporal levels, all parameters for imputing missing values (median) and standard scaling were learned on the training manifold. These parameters were used for pre-computing the training set and were applied strictly to transform the validation and test sets. The scaling process is defined as follows in Eq. 5 with the mean and the standard deviation of the training set called μ_{train} and σ_{train} :

$$z_{i,j} = \frac{x_{i,j} - \mu_{\text{train},j}}{\sigma_{\text{train},j}} \quad (5)$$

Initial data pruning was applied to reduce the ‘technological greenwashing’ risks, namely the sparse features, which might result from selective disclosure by the corporations. This stringent filtering ensures that algorithmic production of pseudo-sustainability measures that could effectively mask real-world poor performance is not allowed. Even in this carefully cleaned-up feature space, the dimensionality was still fairly high. Directly feeding tabular data into sequential neural networks is likely to lead to the curse of dimensionality and overfitting. To tackle this, a robust feature selection algorithm was applied based on an Extra Trees Regressor ensemble (150 estimators). The algorithm selected the 20 most important and variable predictors from the large corporate dataset by minimizing Gini impurity via random decision splits. The correlation heatmap (Fig. 2) shows that the selected features are structurally independent and orthogonal, providing visual evidence that the selected inputs form a stable, non-redundant mathematical basis for the model.

To close the gap between structural decision-tree reasoning and deep sequential learning, an enhanced Out-Of-Fold (OOF) meta-learning strategy was developed. Instead of directly feeding the raw top 20 features into the neural network, LightGBM and Extra Trees regressors were fitted into a stringent 5-fold cross-validation framework on the training set. The tree-based models were trained on four data parts per fold and used to forecast the ESG results of the unknown fifth part. This particular OOF mechanism is tactically important; if the models merely predicted the training data used to train them, it would introduce a severe overfitting bias. The process produces mathematically clean and unbiased OOF meta-features by predicting on held-out folds only. After building these strong training meta-features, the base tree models were trained on the entire training set to produce the corresponding meta-features for application to the validation and test sets. This advanced stacking algorithm is far better than conventional architectures, as it effectively preprocesses tabular data by projecting complex, non-linear hierarchical decision boundaries into a dense, low-dimensional form. These tree-based OOF meta-features are an important complementary input channel, so that when temporal sequences are fed into the later deep learning architecture, they are already enriched with high-order structural intelligence.

C. The Proposed Neuro-Causal Fusion (NCF) Architecture

The core technical contribution of this study is the development of the Neuro-Causal Fusion (NCF) architecture. This dual-stream deep learning architecture can be used to

TABLE I. DESCRIPTIVE STATISTICS OF THE REFINED CORPORATE ESG SAMPLE

PANEL A: BY REGION					
Region	N	Mean ESG	Median ESG	CV (%)	Median Assets (M)
Asia	5135	-0.13	0.04	0.00	7959.23
Europe	3608	0.15	0.14	619.16	7581.52
Other	5911	0.04	0.12	2586.18	8006.47
US	2957	0.29	0.37	292.21	16008.00
PANEL B: BY INDUSTRY (TOP 10)					
Industry	N	Mean ESG	Median ESG	CV (%)	Median Assets (M)
Banks	780	0.52	0.72	177.85	208648.84
Chemicals	1086	-0.08	0.05	0.00	6593.62
Electronic Equipment	602	-0.06	0.14	0.00	4105.97
Food Products	571	0.06	0.20	1471.01	4928.75
Hotels & Leisure	557	-0.01	-0.01	0.00	4973.81
Machinery	677	-0.12	-0.05	0.00	6155.41
Metals & Mining	667	0.33	0.43	295.08	7716.14
Oil & Gas	668	0.22	0.32	409.45	21897.00
Real Estate	557	-0.03	0.03	0.00	13020.04
Semiconductors	513	0.03	0.15	3099.97	3657.21
PANEL C: TIME TRENDS					
Year	N	Mean ESG	Median ESG	CV (%)	Median Assets (M)
2010	935	-0.11	0.03	0.00	8430.64
2011	1010	-0.09	-0.03	0.00	8451.51
2012	1127	-0.13	0.04	0.00	8430.64
2013	1239	-0.16	-0.06	0.00	8430.64
2014	1357	-0.16	-0.13	0.00	8068.28
2015	1383	-0.13	0.03	0.00	7530.15
2016	1508	-0.06	0.03	0.00	7870.35
2017	1559	0.01	0.10	6731.47	8430.64
2018	1426	0.12	0.16	766.86	8430.64
2019	1299	0.21	0.26	416.55	8430.64
2020	1645	0.26	0.32	345.82	9577.64
2021	1539	0.31	0.38	277.94	10216.09
2022	1584	0.38	0.41	179.42	9677.62

concurrently learn temporal evolutionary dynamics and the decision boundaries of complex structures. There is a peculiar duality in corporate sustainability data: it is both longitudinal (e.g., gradual carbon reductions over time) and categorical (e.g., instant penalties for specific sector classifications). Regular monolithic machine learning algorithms cannot perform well in this area; gradient-boosted trees are more efficient at modeling tabular structural edges but lack time memory, whereas standard neural networks can model temporal chains but struggle to divide tabular hierarchies, absent rich feature crossing intrinsically. The suggested NCF concept addresses this gap through a complex integration paradigm.

The core of the NCF architecture processes the top 20 strategically selected raw features across a three-dimensional temporal dimension. In contrast to conventional feed-forward networks, which assume that financial observations are independent and identically distributed, a sequence is fed into a Bidirectional Long Short-Term Memory (BiLSTM) layer with 32 hidden units. The two-way construct is remarkably rational in the case of corporate data; it considers the sustainability indicators of the past-to-future and future-to-past situations. This helps the network distinguish between a company that is continuously improving its governance and one that is temporarily faking its numbers before a downturn. To stabilize

recurrent learning and ensure that the network learns noise rather than the data, an L_2 regularization penalty (1×10^{-4}) is directly applied to the internal LSTM kernels. However, in financial and sustainability contexts, not all temporal signals are equally important. A major change in the board's diversity is predicted, rather than a sudden environmental controversy or a major shift in the environmental controversy. These important signals are diluted when all time steps are treated equally. A Self-Attention mechanism is deployed to counter this, right after the BiLSTM layer. The attention layer is a dynamic cognitive filter that computes alignment scores to ensure the most important latent events receive high scores, while irrelevant background volatility is suppressed. The attention-weighted output Z of a hidden state h_t is mathematically represented as in Eq. 6:

$$\alpha_t = \frac{\exp(e_t)}{\sum_{k=1}^T \exp(e_k)}, \quad (6)$$
$$Z = \sum_{t=1}^T \alpha_t h_t$$

where, α_t represents the attention weight assigned to each step, this weighted sequence is subsequently compressed via

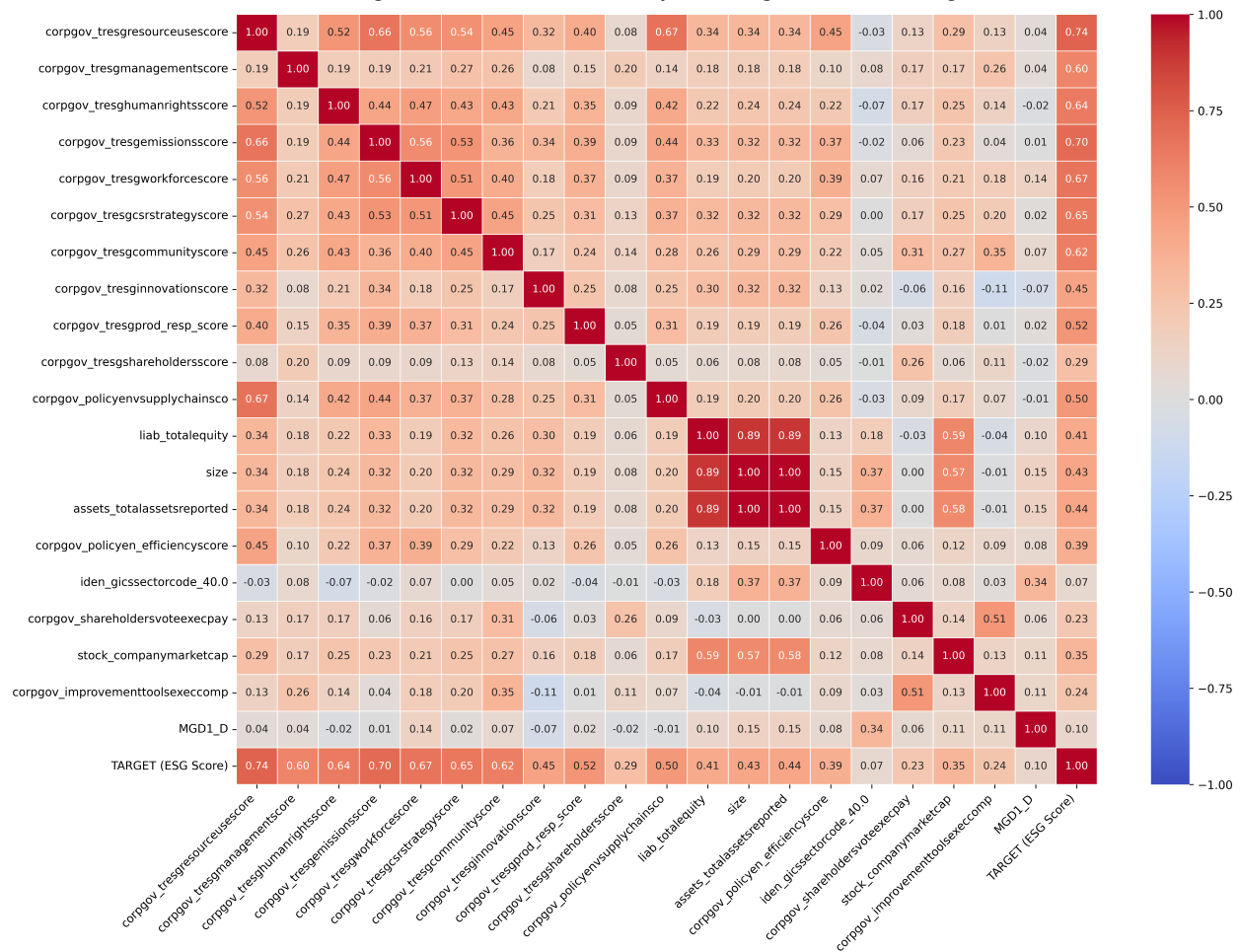


Fig. 2. Pearson correlation matrix validating the structural orthogonality of the top 20 features.

Global Average Pooling into a dense, high-order representation of the firm's temporal ESG trajectory. At the same time, the Out-Of-Fold meta-features produced by the LightGBM and Extra Trees ensembles are fed to the secondary input stream. These dense structural predictions are then fused with the attention vector that is temporally pooled at the fusion node. This particular operation mathematically constrains the neural network to condition its temporal predictions on the non-linear structural principles already identified by the tree algorithms. After concatenation, the resulting fused tensor is propagated through a Multi-Layer Perceptron (MLP) block with sequentially reducing dense layers (64 and 32 neurons) with Rectified Linear Unit (ReLU) activation functions. Financial datasets are highly vulnerable to internal covariate shift, with the distribution of network activations shifting radically during training due to macroeconomic volatility. In response, Batch Normalization is applied after every dense layer, ensuring stable, faster gradient flow. In addition, to avoid the network co-adapting to certain training samples (overfitting), stochastic Dropout layers (with drop rates of 0.2 and 0.1) are inserted strategically. These regularizations demand a framework to learn corporate behaviours in a strong and generalized way, instead of just memorizing local anomalies. The NCF framework has been thoughtfully optimized to address the

volatility of the global ESG assigning of scores. One of the commonly used loss functions in classical neural architectures is the Mean Squared Error (MSE). The financial figures of the companies are, however, fatally misaligned and include any extreme outliers: bad governance decision, a big unforeseen green tech initiative. The MSE smooths out these errors and causes a large gradient explosion and network destabilization. However, Mean Absolute Error (MAE) is robust to outliers, but hard to converge to the global minimum with a fixed gradient. This mathematical paradox is then removed by optimizing the architecture with Huber Loss to obtain the elegant piecewise solution. To a predicted ESG score $f(x_i)$, actual score y_i , and a tunable threshold parameter δ (set to 1.0), the Huber Loss L_δ is defined in Eq. 7:

$$L_\delta(y_i, f(x_i)) = \begin{cases} \frac{1}{2} (y_i - f(x_i))^2, & |y_i - f(x_i)| \leq \delta, \\ \delta |y_i - f(x_i)| - \frac{1}{2} \delta^2, & |y_i - f(x_i)| > \delta. \end{cases} \quad (7)$$

The dual-behavior loss function trades-off MSE when prediction errors are small, allowing for a smooth path toward reaching the target, while smoothly avoiding the catastrophic

behavior of large outliers by switching to linear MAE penalties on those errors. The Adam optimizer is used to train the network with an initial learning rate of 0.005. It has a ReduceLROnPlateau mechanism that reduces the learning rate by 50% when the validation loss has not improved for 5 consecutive epochs, helping the model navigate the complex loss landscape. Lastly, the EarlyStopping protocol automatically ends training when there is no progress after 15 epochs and restores the mathematically optimal weights. This strict optimization plan will give the best generalization to future unobserved corporate information.

D. Experimental Setup and Implementation Details

All empirical experiments were conducted in a high-performance computing environment, where strict reproducibility and high computational efficiency were guaranteed. Main deep learning pipelines were constructed with the TensorFlow/Keras framework, while Out-Of-Fold (OOF) meta-learning ensembles were implemented with the LightGBM and Scikit-Learn libraries. Commonly used mathematical metrics were used to measure the predictive performance of the proposed architecture. The network configurations and dynamics of the proposed NCF framework were empirically adjusted to achieve robust convergence and prevent overfitting to the unseen chronological test set. Table II summarizes the detailed information on the hardware environment, software platforms, and specific network hyperparameters.

TABLE II. EXPERIMENTAL SETUP AND MODEL CONFIGURATION

Category	Parameter / Component	Value / Specification
Hardware & Environment	Hardware Accelerator	NVIDIA Tesla T4 GPU
	Programming Language	Python 3.12
	Deep Learning Framework	TensorFlow 2.x / Keras
	Tree-Boosting Framework	LightGBM, Scikit-Learn
Network Hyperparameters	Optimizer Algorithm	Adam
	Initial Learning Rate	0.005
	Mini-Batch Size	32
	Maximum Epochs	150
	Loss Function	Huber Loss ($\delta = 1.0$)
Regularization & Stability	Dropout Rate (Dense Layer 1)	0.2
	Dropout Rate (Dense Layer 2)	0.1
	Weight Decay (L2 Penalty)	1×10^{-4}
	Batch Normalization	Enabled
Training Control	Early Stopping	Patience = 15 epochs (restore best weights)
	Learning Rate Scheduler	ReduceLROnPlateau (factor = 0.5, patience = 5)

IV. RESULT ANALYSIS

A. Experimental Results and Discussion

Table III presents the empirical results for the proposed Neuro-Causal Fusion (NCF) framework, contrasted with the

TABLE III. PERFORMANCE BENCHMARKING OF NCF VS. BASELINE MODELS

Model	R^2	RMSE	MAE	MedAE	Exp. Variance	MAPE (%)
LightGBM	0.9510	0.1684	0.1259	0.1022	0.9510	75.75
Gradient Boosting (GBR)	0.9450	0.1783	0.1344	0.0997	0.9460	71.93
Linear Regression	0.9368	0.1912	0.1477	0.1208	0.9428	72.72
Ridge Regression	0.9368	0.1912	0.1477	0.1209	0.9428	72.72
XGBoost	0.9329	0.1970	0.1491	0.1154	0.9329	69.03
Random Forest	0.9289	0.2029	0.1548	0.1233	0.9290	84.49
K-Nearest Neighbors	0.8579	0.2867	0.2244	0.1853	0.8579	91.34
AdaBoost	0.8318	0.3119	0.2497	0.2053	0.8330	88.87
Decision Tree	0.8090	0.3324	0.2499	0.1918	0.8090	146.22
Fixed-Effects	0.9501	0.1698	0.1292	0.1026	0.9536	71.95%
NCF (Proposed)	0.9603	0.1514	0.1096	0.0815	0.9593	64.99

various predictive structures. The NCF model had a better R-Squared (R^2) of 0.9603, which effectively explained the greater variance of global ESG performance (more than 96%). An important result is that the Tree-based ensembles LightGBM ($R^2 = 0.9510$) and Gradient Boosting ($R^2 = 0.9450$) perform well. This means that the interactions between ESG datasets are high-dimensional and non-linear, making them challenging to model with linear models. However, the NCF framework offers a synergistic benefit of combining the BiLSTM layers with Tree-based meta-features. Although the tree-based elements are very effective at capturing structural complexity, the BiLSTM layers are particularly designed to capture longitudinal dependence and temporal trends. This is a “Neuro-Causal” version of the integration that allows the NCF to complement the static structural analysis with the time-series dynamism needed to forecast and create a comprehensive representation of sustainability trajectories. Moreover, to explicitly validate this temporal ability against the gold standard in financial econometrics, the NCF was benchmarked against a classical Fixed-Effects model. The results indicated that the Fixed-Effects baseline model overall had a high R^2 and RMSE. Still, the proposed NCF model consistently achieved higher results, demonstrating that our hybrid approach was more suitable for complex panel data than the Fixed-Effects baseline approach.

In addition, the elegant error profile of the NCF yields the lowest RMSE (0.1514) and MAE (0.1096), further establishing its accuracy. The most significant results are Median Absolute Error, where NCF achieves the lowest performance with 0.0815. In the corporate governance domain, there are many examples of “extraordinary events” or “outside the range” in the datasets, and the lower MedAE indicates that the NCF is less sensitive to such events than other models, such as XGBoost or Random Forest. Moreover, the MAPE of 64.99% is a strategic innovation to reduce the global ESG noise, which is a well-recognized problem. The model also has a high Explained Variance (0.9593) which corroborates that the model is not contaminated with noise but picking up the underlying ESG drivers. The NCF is a stable, reliable forecasting platform, with a backbone of ensemble learning, giving stakeholders the ability to make accurate forecasts and validate their strategies over the long term.

The ablation study (Table IV) confirms the functional requirement and synergistic role of the architectural modules in the Neuro-Causal Fusion (NCF) model. Experimental results show that the full NCF model ($R^2 = 0.9603$) is a

more appropriate compromise between the predictability and structural stability than the shortened models. The inclusion of the Attention mechanism reduced R^2 to 0.9510, demonstrating that it is a cognitive filter that helps focus on salient governance signals. Without this layer, the higher the MedAE (0.0960), the lower the differentiation capacity between the important ESG drivers and environmental noises. Equally, the lack of Tree-based Meta-features greatly reduced the explained variance ($R^2 = 0.9450$), suggesting that structural complexities and non-linear interactions cannot be overlooked when basing neural predictions on a causal environment. The addition of BiLSTM layers resulted in the largest increase in MAPE (87.10%), indicating that BiLSTM is an essential temporal stabilizer. This growth underscores the critical role of temporal memory in navigating the longitudinal variability of global ESG indicators. Finally, the hybrid architecture can be justified by the fact that the high performance across all measures results from the hybrid structure, in which the elements mutually correct one another to achieve a consistent global optimum. Generally, the ablation results confirm the complementary contribution of both the tree-based meta-features and the BiLSTM–Attention components, with the complete architecture obtaining the highest R^2 , RMSE, and MAE of the tested variants.

TABLE IV. PERFORMANCE DEGRADATION ANALYSIS THROUGH COMPONENT ABLATION OF THE NCF FRAMEWORK

Model Variant	R^2	RMSE	MAE	MedAE	Exp. Variance	MAPE (%)
w/o Attention	0.9510	0.1683	0.1266	0.0960	0.9513	77.63
w/o Meta-features	0.9450	0.1783	0.1362	0.1063	0.9479	64.08
w/o BiLSTM (Dense)	0.9497	0.1705	0.1307	0.1000	0.9517	87.10
Simple BiLSTM (No Attn/Meta)	0.9355	0.1931	0.1474	0.1141	0.9400	56.56
Full Proposed Model	0.9603	0.1514	0.1096	0.0815	0.9593	64.99

To structurally validate the framework’s resilience against market volatility and heavy-tailed anomalies, a hyperparameter sensitivity analysis was conducted on the Huber loss threshold (δ). As depicted in Fig. 3, the dual-stream architecture was systematically re-evaluated across a spectrum of threshold constraints ($\delta \in \{0.5, 1.0, 1.5, 2.0\}$). The empirical results show that the model performs best when the parameter δ is set to the optimal value of 1.0, with $R^2 = 0.9604$ and RMSE = 0.1513, and that the loss of predictive fidelity across parameter variations is entirely negligible. In particular, the range of variance (R^2) is kept within a small margin (0.9587 to 0.9604), so that the variance is kept within 0.2%. To further evaluate the loss-function choice, a matched four-seed comparison was carried out, with the same NCF architecture and data splits. Huber trained model had a mean test R^2 of 0.9596 and a mean MAE of 0.1114, while MSE had a mean test R^2 of 0.9550 and a mean MAE of 0.1196 across these runs. The results confirm the use of Huber loss in the proposed fusion architecture.

Optimizing deep learning weights is stochastic, and careful analysis of predictive stability is required to ensure that performance numbers are not merely a result of good initial conditions. A robustness test was conducted using four random seeds (42, 1024, 123, and 2026) for the NCF framework. This choice criterion provides for a broad range of numerical initialization clusters and helps establish the claim of initialization invariance. The empirical results presented in Table V show a high stability, as the model has a stable mean R^2 of 0.9596. The

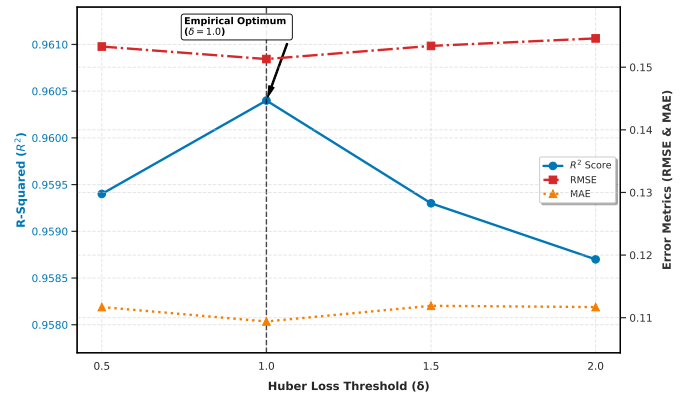


Fig. 3. Framework stability against market volatility via Huber loss.

low variance suggests that the NCF architecture can converge to a global optimum and successfully infer underlying drivers of ESG performance with high reproducibility. In addition, the NCF framework’s structural integrity is supported by the relative similarity of the error measures, with an average of RMSE (0.1529) and MAE (0.1114). From a scientific point of view, the consistency enables hybridizing BiLSTM layers with Tree-based meta-features to effectively flatten the loss landscape and prevent the optimization process from being driven by specific starting points. Further, the MAPE consistency (66.60%) supports the framework’s ability to eliminate systemic governance noise, which is a key property of its neuro-causal logic. The NCF model is a reliable tool for long-term sustainability predictions and strategic evaluation for institutional stakeholders and policy regulators.

TABLE V. PREDICTIVE STABILITY AND ROBUSTNESS ANALYSIS ACROSS DIVERSE NUMERICAL SEED CLUSTERS

Evaluation Metric	Seed 42	Seed 123	Seed 1024	Seed 2026	Overall (Mean)
R^2 Score	0.9593	0.9590	0.9596	0.9603	0.9596
RMSE	0.1534	0.1540	0.1529	0.1514	0.1529
MAE	0.1125	0.1114	0.1119	0.1096	0.1114
MAPE (%)	67.53	66.49	67.39	64.99	66.60

Note: Seed 2026 was designated as the primary seed before evaluation, while the remaining seeds were used to assess predictive stability.

As a further robustness check, all ESG-related score variables were excluded from the model. The resulting $R^2 = 0.8288$ indicates reduced predictive performance, highlighting the predictive relevance of ESG-related information.

B. Model Interpretability and Strategic Sustainability Drivers

The SHAP (Shapley Additive exPlanations) framework is used to understand the inner workings of the Neuro-Causal Fusion (NCF) architecture, not only as a validation tool but also as a guiding path for corporate sustainability. The hybrid design stacks BiLSTM layers to capture longitudinal volatility and Tree-based Meta-features to capture non-linear relationships, thereby guaranteeing predictive accuracy. Interpretability is explained via the SHAP Decision Plot (Fig. 4). This multi-instance decision plot shows the overall effect that features have had on various companies, unlike regular feature importance plots. The graph shows how the model’s prediction of

the company's ESG compliance moves in steps toward greater or lesser compliance, starting from the expected baseline (the central dashed line) as each corporate indicator is added or subtracted. The resulting "density cloud" of trajectories clearly shows a divergence. Of particular note, the highest-ranking features are `corpgov_tresmanagementscore`, `corpgov_tresinnovationscore`, and `corpgov_tresgmissionsscore`, which show up as the biggest and most important changes in the predictive route. This wide range of trajectories at these highest nodes suggests that strategic management and proactive green R&D are the key drivers that differentiate ESG leaders from laggards. These technical visualizations make the NCF framework into a "living advisor" for corporate leadership. Identification of decision routes enables stakeholders to focus on the pressure points and design interventions to target the pressure. The decision cloud was a very strong image to demonstrate the transformation of compliance to proactive sustainability and to directly link complex algorithmic calculations to managerial solutions within the model.

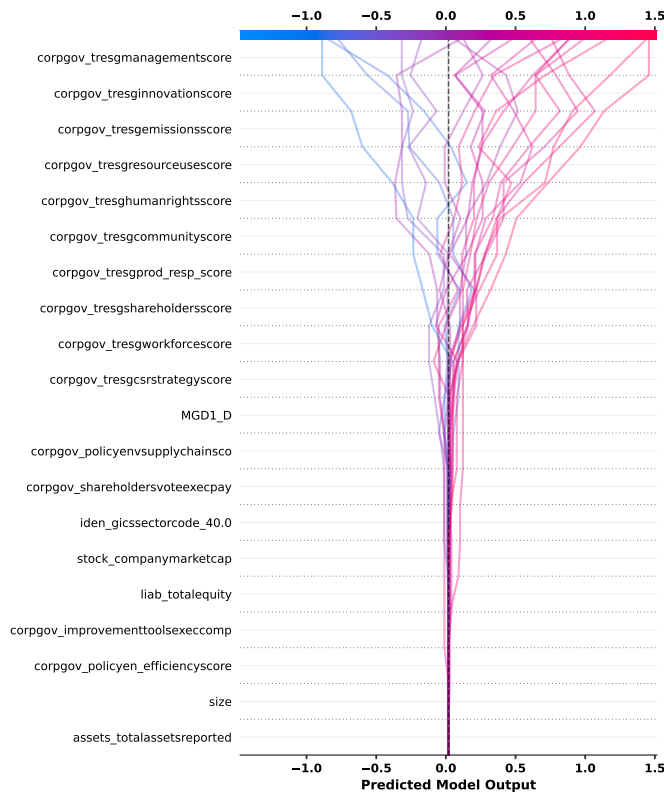


Fig. 4. Global feature hierarchy for ESG performance prediction via SHAP.

To instill granular transparency and build institutional trust, a local interpretability analysis has been conducted based on a SHAP Waterfall Plot of one representative entity (Firm ID: 0). This approach helps to decompose a single prediction additively, and the mathematical path through which the expected value ($E[f(X)] = -0.072$) transforms to the ultimate predicted ESG score ($f(x) = 0.081$). The NCF framework provides a visual representation of the positive/negative value added by certain features, thereby offering a forensic breakdown of why a particular firm was assigned its sustainability rating. Based on the analysis shown in Fig. 5,

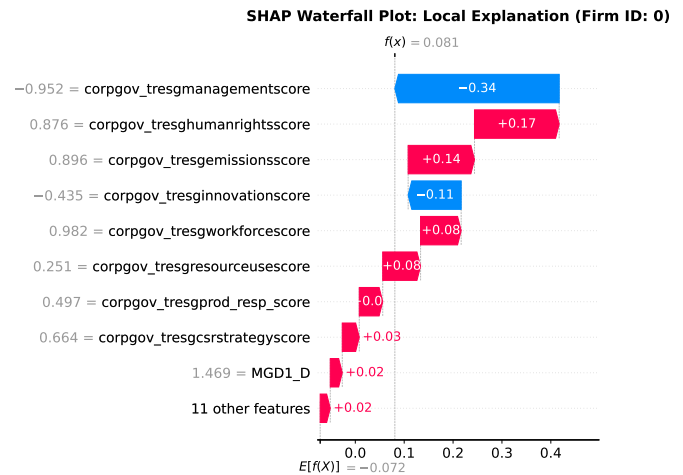


Fig. 5. Forensic ESG diagnosis via SHAP waterfall decomposition.

Management Quality (`corpgov_tresmanagementscore`) stands out as the most important detractor for Firm ID: 0, with a large negative pressure of -0.34. Given the low value of management input in the firm (-0.952), the model correctly identifies structural governance weaknesses and a lack of leadership oversight as the main inhibitors of sustainability. On the other hand, the firm's active Human Rights Compliance (`corpgov_tresgmissionsscore`, +0.17) and Emissions Control (`corpgov_tresgmissionsscore`, +0.14) performance serve as control mechanisms. These environmental and social pillars are effective in neutralizing the governance deficit, and the resulting prediction can move into the positive territory. Strategically, such a local diagnostic capacity will transform the NCF model into an active strategic advisor, rather than a Sustainability Consultant. Rather than providing an opaque aggregate metric, the framework offers an actionable roadmap: for Firm ID: 0 to achieve a superior ESG rating, leadership must prioritize governance reforms and innovation policies to mitigate the existing management-linked risks. This level of granular justification enables stakeholders such as corporate boards and institutional investors to pinpoint specific levers of change, enabling them to conduct targeted interventions that streamline corporate sustainability trajectories on a scientific basis.

To support the local forensic results and to guarantee the stability of the NCF framework, Local Interpretable Model-agnostic Explanations (LIME) were used as the secondary validation layer of Firm ID: 0. Although SHAP applies the additive feature attribution, LIME offers a different interpretative view by fitting the complex, non-linear NCF model with a locally linear surrogate. This ensures the predictions the model makes are neither high-dimensional object dependent nor verifiable and testable logic. The LIME surrogate aims to minimize a locally defined loss function that defines a feature neighborhood, and assigns weights to instances that are perturbed around the target instance via a proximity kernel. This mathematical method has proven to be useful in locally linearizing the behavior of the model, allowing careful inspection of the decision boundary. The LIME analysis closely aligns with the SHAP waterfall results, as shown in Fig. 6. Management Quality (`corpgov_tresmanagementscore`)

≤ -0.69) is the strongest predictor of the firm's performance decline, with the largest negative feature weight.

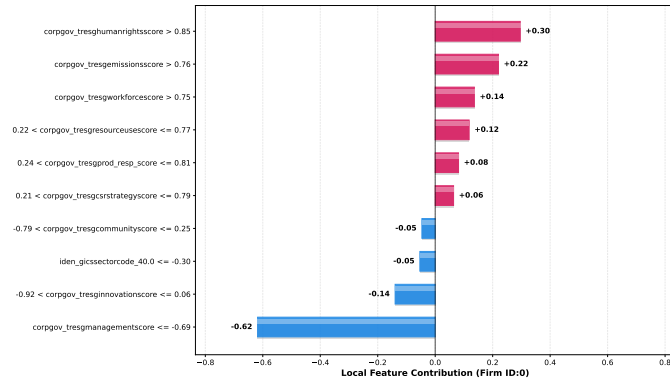


Fig. 6. Local feature contributions via LIME explanation.

On the other hand, the very high positive values of Human Rights Compliance (> 0.85) and Emissions Control (> 0.76) demonstrate the ability of operational excellence in certain social and environmental areas to protect a company against a serious governance risk. This local linear approximation shows that this model's sensitivity to the lack of governance is not due to stochastic variance but is a manifestation of a constant underlying causal structure that can be described in terms of the fusion architecture. The high level of convergence between SHAP and LIME for the same entity can be considered a vital cross-methodological validation, a characteristic of a rigorous Explainable AI (XAI) study. LIME converts the framework's output into a practical diagnostic report by providing specific operational thresholds and using if-then logic (e.g., keeping human rights scores above 0.85). This parallel interpretability shows that the NCF framework is a credible and transparent decision-support system, delivering the same diagnostic signals across mathematically divergent interpretive frames and thus meeting the high-transparency and accountability standards of institutional sustainability auditing.

C. Lifecycle-Driven Heterogeneity Analysis and Strategic Prescriptions

Corporate environmental, social and governance performance determinants are not singular but strongly influenced by the institutional context and stages of development of the firm. To examine this heterogeneity, this paper adopts a partitioning strategy based on quantiles and measures institutional maturity by means of total assets. The sample consists of three segments that are determined by the 33rd percentile and 66th percentile points: Small (SME), Medium-sized, and Large (Mature). Theoretically, the classification is based on the Firm Life Cycle, which theorizes the evolution of an organization's resources, regulatory activity, and strategic orientation as it evolves. To capture the overall evolution of corporate sustainability, the average effect of the feature scores over the maturity stages was estimated based on the NCF framework and KernelSHAP. The integrated attribution analysis (Table VI) proves the systematic and structural specification of sustainability priorities that adjust to the institutional expansion. The Management Score is the highest-ranked determinant across the maturity range and is

particularly strong in the Large (Mature) stage, with the highest predictive value of 0.2924. This pattern suggests that once companies are established, their ESG performance is highly responsive to governance scores, which reflect how well they manage ethics and transparency, as demanded by institutional investors worldwide. Strategic pivot in Medium-sized firms is at the intermediate stage of scaling, the Innovation Score is the highest, and the Rank is 3 (0.1581). This implies that, for mid-tier entities, technological change and green R&D score are the main distinguishing factors in market positioning. Small (SME) companies rely on the Resource Use Score (0.1262), indicating that the slimmer size of smaller companies may mean that efficiency measures such as waste management and energy optimization are the most direct approach to improving their overall sustainability scores. These stage-specific sensitivities are quantified, turning the NCF framework from prediction to a solid diagnostic roadmap. This enables stakeholders to stop using one-size-fits-all strategies and instead apply interventions that target the individual features for which the firm has the largest marginal gains, given its unique position in the corporate lifecycle.

TABLE VI. COMPREHENSIVE MATURITY-BASED ESG DRIVERS AND IMPACT MATRIX

Hierarchical Feature Ranking by Maturity Stage					
Firm Maturity Stage	Rank 1	Rank 2	Rank 3	Rank 4	Rank 5
Small (SME)	Management	Human Rights	Resource Use	Emissions	Innovation
Medium-sized	Management	Human Rights	Innovation	Emissions	Resource Use
Large (Mature)	Management	Human Rights	Resource Use	Innovation	Emissions

Quantitative Impact (Mean Absolute SHAP Values)			
Feature Name	Small (SME)	Medium-sized	Large (Mature)
Management	0.2423	0.2136	0.2924
Human rights	0.1464	0.1619	0.1845
Resource use	0.1262	0.1342	0.1730
Innovation	0.1046	0.1581	0.1501
Emissions	0.1128	0.1362	0.1244

In addition to institutional maturity, the macroeconomic and regulatory environment of individual jurisdictions plays a key role in moderating the effectiveness of sustainability drivers. To investigate this geographical heterogeneity, a cross-country comparative analysis was conducted on five large economies of the world, which have various institutional structures: the United States, the United Kingdom, Japan, Taiwan, and South Korea, these countries were chosen because they have a large market capitalization and a unique approach to ESG reporting between the market-oriented models of the West and the stakeholder-based and government-influenced models of East Asia. Comparative attribution analysis, as shown in Fig. 7, indicates that although the Management Score continues to be the predictor of foundation across the globe, its strength of influence across borders is extremely different. The empirical findings strongly indicate that the Management Score is disproportionately sensitive in the Taiwanese jurisdiction, with a Mean Absolute SHAP value of 0.37, compared to 0.25 in the United States and 0.22 in Japan. Financially speaking, this means that in young high-tech societies such as Taiwan,

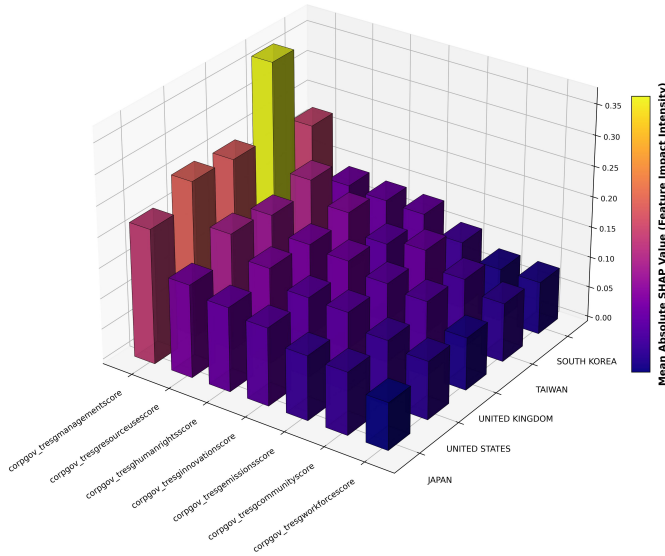


Fig. 7. Cross-country comparison of top ESG predictors.

corporate transparency and ethical leadership are the primary risk-reduction factors for external investors.

On the other hand, the United States and the United Kingdom show greater sensitivity to Resource Use Scores of 0.19 and 0.18, respectively. This indicates that operating efficiency and carbon footprint optimization are more established in the valuation of a company's ESG position in more developed capital markets. Moreover, the Score of Innovation appears to be a key distinguishing factor in the United Kingdom (0.15) and South Korea (0.14). In these innovation-based economies, the model finds that Green R&D is a strategic necessity, with technological advancement a more effective predictor of sustainability superiority than in more resource-intensive economies. These results can offer a critical "geographically-conscious" solution to the global investment strategies. To the portfolio managers, this analysis shows that using a global ESG weightage based on standardization is statistically inefficient. Rather, the NCF framework provides a localized diagnostic roadmap: investors in the Taiwanese market are advised to concentrate on governance-based forensic audits, whereas those in the US or UK markets are advised to focus on operational resource efficiency. The framework's quantification of these regional pressure points enables shifting generic global reporting to precision-based, regionally specific sustainability auditing.

D. Causal Configuration Analysis via fsQCA

Although the above feature analysis (SHAP and LIME) effectively determines the relative importance of sustainability drivers, the practical relevance of corporate ESG excellence lies in the overall integration of multiple operational pillars. To fill this gap, a fuzzy set Qualitative Comparative Analysis was conducted. The set-theoretic approach is more than just linear attribution; it seeks to uncover "causal recipes", specific feature-wise combinations linked to good ESG rating. The continuous feature variables were calibrated to fuzzy sets (0-1) before generating these configurations using a strict quantile-based anchoring method (5th, 50th, and 95th percentiles). The

TABLE VII. SET-THEORETIC CAUSAL RECIPES AND CONFIGURATIONAL PATHWAYS FOR ESG EXCELLENCE

Recipe (Raw Feature Combination)	Consistency	Raw Coverage
Management * Humanrights	0.9438	0.4733
Innovation * Resourceuse	0.9379	0.4845
Management * Innovation	0.9375	0.4475
Humanrights * Emissions	0.9004	0.3357
Management * Emissions	0.8704	0.3947
Innovation * Emissions	0.8624	0.3549

performance of each ensuing causal recipe is gauged on two main set-theoretic measures: Consistency, the trustworthiness of the pathway, and the empirical footprint or popularity of the pathway among high-performing firms. As Table VII of the empirical findings indicates, there are multiple and strong configurational pathways to ESG excellence (all consistency scores > 0.85). Most significantly, the recipes show strategic dynamics of corporate sustainability. Last, all combinations without a high-emissions component also demonstrate an Environmental Veto model, such as Management * Emissions (0.8704). This confirms that excellent governance at the board level will not compensate for a poor carbon footprint and sets clear boundaries for sustainability ratings, aligning with existing regulatory requirements such as the Corporate Sustainability Reporting Directive (CSRD) and the Paris Agreement. These recipes would determine the NCF model as the analytical model of the roadmap that the corporate board is following. This fsQCA analysis provides a proven pathway to implementing the comprehensive sustainability changes needed by policymakers, portfolio managers, and corporate leaders. It shows that real sustainability can only be realized through coordinated changes rather than isolated, piecemeal ones.

E. Strategic Scenario Forecasting via Digital Twin Simulation

Although traditional predictive modeling provides a static analysis of corporate sustainability, institutional stakeholders need forward-looking, dynamic tools to develop policies and allocate capital. To meet this requirement, the last step in this paper operationalizes the NCF model architecture into a Digital Twin, a virtual simulation environment in which counterfactual sustainability scenarios can be systematically tested without financial risk in reality. A multi-firm sensitivity analysis was performed across the test set's 1,642 different company identifiers to evaluate the NCF-based Digital Twin scenario-forecasting capability. The scenario variable was chosen in a subsequent feature importance analysis, based on the analysis presented in the previous feature. Its value was systematically varied from -30% to +30%, with the rest of the inputs to the model fixed, and the prediction results were compared with the baseline predictions, which were made with the values of the other model inputs fixed. The predicted mean baseline was 0.36088 as reported in Table VIII. This relative increase of 10%, 20%, and 30% resulted in mean changes predicted to be 0.04547, 0.07542, and 0.09612, respectively, while a decrease resulted in a negative change. The 95% firm-level bootstrap confidence intervals did not include zero in any of the evaluated company identifiers, suggesting uniform model responses for each company identifier evaluated. These

results are complementary to the preliminary single-firm study and show the Digital Twin's ability to calculate scenario-specific prediction variations across a larger pool of firms. These results are model-based and *ceteris paribus* projections and not observed intervention effects; however they would serve as a quantitative basis for comparison of resource-use scenarios, resource allocation for sustainability planning, policy-oriented decision-making.

TABLE VIII. MULTI-FIRM DIGITAL TWIN SENSITIVITY ANALYSIS
UNDER RESOURCE-USE SCENARIOS

Score Shift	Mean Predicted ESG	Mean Impact	95% CI Lower	95% CI Upper
-30%	0.20851	-0.15236	-0.15583	-0.14898
-20%	0.26013	-0.10075	-0.10294	-0.09842
-10%	0.31101	-0.04987	-0.05113	-0.04864
0%	0.36088	0.00000	0.00000	0.00000
+10%	0.40635	0.04547	0.04416	0.04685
+20%	0.43630	0.07542	0.07328	0.07758
+30%	0.45699	0.09612	0.09328	0.09897

V. LIMITATIONS AND FUTURE WORK

The NCF framework outlined here shows promise in predictive fidelity and prescriptive strategy, but it needs its present conditions bounded. The biggest drawback is that the underlying data source itself is a “Garbage In, Garbage Out” (GIGO) source. The architecture is mathematically sound in handling heavy-tailed anomalies using the Huber Loss, but its predictive power depends primarily on structured corporate self-disclosures. Therefore, the outstandingly high R^2 of 0.9603 demonstrates the model's accuracy in predicting the reported ESG scores. Still, it does not rule out the possibility that the model is subject to the general risk of greenwashing. A framework that is “selectively transparent” in corporate reporting can lead to sub-optimal performance for environmental impact if it is set up to focus on consistency. For architecture to really break out of this restriction, it needs to become multimodal. The next step is to incorporate external, objective verification data to provide ground truth for comparison with the corporate narrative. For example, using independent NGO audits or high-resolution satellite imagery to monitor physical environmental footprints could provide an incorruptible audit layer. Moreover, further studies are needed to assess the framework's generalizability across various geographical jurisdictions, including comparisons with other jurisdictions with strict frameworks, such as the CSDDD in the EU. Lastly, the Digital Twin simulation module could be further enhanced with multi-agent reinforcement learning to create a more dynamic simulation environment. This would allow a corporate board to anticipate policy results in an interactive strategic political environment in which multiple stakeholders play a significant role. The following procedures are a logical step toward making the NCF a fully independent, multimodal ESG audit system.

VI. CONCLUSIONS

Governance of sustainability is moving from voluntary, discretionary reporting to obligatory, legally binding disclosure. The shift has created an unprecedented need for high-fidelity analytical frameworks. The present study aims to

bridgeto bridge the “prediction-action” gap in current sustainable finance by proposing a new framework called Neuro-Causal Fusion (NCF). Our study provides a solution to a key challenge in the industry: maintaining predictive power in the presence of heavy-tailed financial anomalies and industry-wide systemic risks arising from corporate greenwashing. The design of a hybrid architecture that seamlessly combines the hierarchical rule-extraction ability of tree-based ensembles with the longitudinal memory of BiLSTM-Attention streams in the model improves predictive accuracy, achieving a state-of-the-art R^2 value of 0.9603. This work's most noteworthy aspect is the mathematical optimization of neural learning with volatile data. The NCF framework is converging more robustly and is more generally applicable by using an outlier-robust Huber Loss function to replace the typical Mean Squared Error loss function, which is sensitive to “Black Swan” price swings. This algorithmic innovation makes this model a robust financial auditing tool that can uncover concealed structures in company reporting. This increases transparency and clarity and can, at least in theory, provide a more “audit-ready” real-world impact evaluation for institutional investors and global regulators, thereby reducing the information asymmetry common in the ESG space. The NCF paradigm shift is not only the most important value that goes beyond predictions, but it's also prescriptive sustainability management. The problems associated with retrospective feature importance are overcome in this study through Fuzzy-set Qualitative Comparative Analysis. Instead, it creates complex “causal recipes” that involve environmental, social, and governance factors necessary for achieving peak performance. The configurations provide clear, actionable next steps for corporate leadership across strategic areas, establish a living, methodological standard, and serve as a tool to change companies.

Besides, the framework can be integrated into a dynamic simulation environment for a Digital Twin and be used to simulate the effect of corporate policies under stress scenarios. This is the contribution of C-suite executives and corporate boards to shifting from a compliance mindset to a more proactive approach to optimizing resources. It helps decision-makers experience virtually the impact of sustainability measures and the potential of future resource reallocations before committing significant capital or resources to the organization. This forward-looking simulation capability is used by strategic consultants and as a key tool to bridgeto bridge business strategies with the stringent demands of the Paris Agreement and current regulatory environments. Lastly, the NCF is a holistic, multidimensional approach to overcoming the shortcomings of current ESG frameworks. It combines singular structural intelligence, temporal memory related to causes and prescriptions. The research provides a ‘scientific and auditable decision support system’ for global corporations and institutional investors to make more accurate decisions in today's complex sustainability governance landscape. Robust neural architectures and causal simulation will remain essential to achieving truly data-driven ESG excellence and financial sustainability in an increasingly volatile financial world, driven by climate change.

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DECLARATION OF COMPETING INTERESTS

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 AND CODE AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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DECLARATION OF GENERATIVE AI AND AI-ASSISTED TECHNOLOGIES IN THE WRITING PROCESS

During the preparation of this work the author(s) used [Grammarly] in order to [proofread]. After using this tool/service, the author(s) reviewed and edited the content as needed and take(s) full responsibility for the content of the publication.

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