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(Research Article)

Machine learning models for optimal DEBT capital structuring in high-growth renewable energy firms

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Abstract

This paper investigates the use of machine learning (ML) techniques to determine optimal debt capital structures for high-growth renewable energy firms operating in complex and uncertain financing environments. Drawing on a simulated panel dataset that mirrors firm scale, growth dynamics, project risk profiles, credit quality, and macroeconomic conditions, the study applies and compares three modeling approaches linear regression, random forest, and gradient boosting to predict both optimal debt ratios and long-term debt maturity compositions. The analysis integrates permutation-based interpretability methods to ensure transparency and explain the contribution of individual financial and risk variables to model outcomes. Empirical results demonstrate that ensemble learning models substantially outperform the linear benchmark in both predictive accuracy and explanatory power, highlighting their ability to capture nonlinear and interaction effects among firm-level and market variables. Profitability, volatility, project risk, and credit rating emerge as the most influential determinants of capital structure, confirming theoretical expectations from trade-off and pecking order perspectives while revealing more complex patterns than traditional models can detect.

Keywords: Machine Learning; Debt Financing; Nonlinear Modeling; Credit Risk; Sustainable Finance

1. Introduction

The renewable energy sector has emerged as one of the fastest-growing and most capital-intensive industries of the twenty-first century. Global investment in clean energy surpassed USD 1.8 trillion in 2023, with renewable power generation accounting for more than half of new capacity additions worldwide (IEA, 2024) [1]. Despite this growth trajectory, high-growth renewable energy firms face persistent financial challenges associated with long project gestation periods, uncertain regulatory environments, high upfront capital requirements, and fluctuating energy prices. These conditions make effective capital structuring both a strategic imperative and a determinant of long-term competitiveness [2].

The central dilemma for such firms lies in optimizing their debt capital structure balancing the benefits of leverage, such as tax shields and enhanced return on equity, against the risks of financial distress and reduced flexibility. Traditional theories of capital structure provide foundational insights. The trade-off theory (Modigliani & Miller, 1958; Kraus & Litzenberger, 1973) proposes that firms choose leverage by balancing the tax advantages of debt with the expected costs of bankruptcy [3]. The pecking order theory (Myers, 1984) suggests that firms prefer internal financing, followed by debt, and issue equity only as a last resort due to information asymmetry [4]. The market timing theory (Baker &

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Wurgler, 2002) adds that managers adjust capital structure opportunistically based on prevailing market conditions [5].

While these frameworks are analytically elegant, they often rely on simplifying assumptions that do not adequately capture the dynamic, nonlinear, and data-rich environments faced by modern renewable energy firms. Factors such as project-level risk heterogeneity, fluctuating subsidy regimes, carbon pricing mechanisms, and evolving investor sentiment introduce nonlinearities and feedback effects that traditional econometric models cannot easily accommodate. Moreover, renewable energy projects often exhibit hybrid characteristics combining elements of corporate finance and project finance further complicating optimal debt structuring decisions.

Recent studies have called for more adaptive, data-driven methods to analyze financial decision-making under uncertainty (Delen et al., 2021; Bouri et al., 2023) [6]. Machine learning (ML) provides such a framework by enabling the discovery of hidden relationships and interactions within complex datasets. Unlike traditional regression-based models, ML algorithms such as random forests, gradient boosting machines, and neural networks can capture nonlinear dependencies among firm characteristics, macroeconomic variables, and financial outcomes without presupposing a functional form. This capacity makes ML particularly valuable for modeling capital structure decisions where variables like profitability, project risk, credit rating, and policy incentives interact in unpredictable ways [7].

In the context of renewable energy, ML applications have gained traction in areas such as energy demand forecasting, project valuation, credit risk modeling, and investment optimization (Dutta et al., 2023; Tang & Wang, 2022) [8]. However, its application to corporate capital structure optimization remains underexplored. Existing financial literature has largely emphasized descriptive or regression-based studies focusing on leverage determinants, leaving a gap in predictive, model-driven approaches that can provide actionable insights for corporate decision-makers [9]. The ability of ML models to simultaneously process firm-level, project-level, and market-level variables provides a unique opportunity to bridge this gap.

Integrating ML with financial theory allows researchers and practitioners to extend the boundaries of capital structure analysis. From a theoretical standpoint, ML can operationalize the dynamic capabilities framework (Teece, Pisano, & Shuen, 1997) within financial management, enabling firms to sense changing market conditions, seize financing opportunities, and transform funding strategies in real time. Practically, it empowers chief financial officers (CFOs) and treasury teams to make evidence-based decisions about leverage ratios, debt maturities, and funding sources. For example, an ML model can predict optimal debt ratios by analyzing multidimensional factors such as firm profitability, revenue volatility, interest rate trends, and access to green subsidies, providing decision-makers with adaptive strategies under uncertainty [10,11].

Moreover, the integration of ML interpretability tools such as SHAP (Shapley Additive Explanations) and permutation importance enhances managerial trust in model recommendations by identifying which variables most strongly influence optimal capital structure decisions [12]. Such transparency is critical for governance, investor relations, and regulatory compliance, particularly as financial institutions and rating agencies increasingly adopt data-driven credit and sustainability assessments[13].

2. Methodology

This study employs an empirical-simulation approach to investigate how machine learning models can estimate optimal debt capital structures for high-growth renewable energy firms. The methodology integrates three stages dataset construction, model training and evaluation, and interpretability analysis to ensure that results are both theoretically grounded and empirically robust.

Because detailed firm-level financial data for renewable energy companies are limited, particularly regarding project-level risk and financing structures, a synthetic panel dataset was constructed to replicate the economic characteristics of such firms. The dataset comprises eighty firms observed over five years (2020–2024), each characterized by variables capturing firm-specific, project-level, and macro-financial conditions [14]. These include measures of firm size, growth rate, profitability, volatility, project risk, credit rating, interest rate environment, access to green subsidies, prior debt levels, and prevailing tax rates [15]. Together, these variables reflect the diverse determinants of capital structure decisions as documented in traditional finance literature.

Two dependent variables were simulated to represent the targets of prediction: the optimal debt ratio, defined as the share of total capital financed through debt that maximizes firm value while maintaining solvency, and the optimal long-term debt share, which captures the portion of debt that should be structured with extended maturity to mitigate refinancing risk. Both target variables were generated using a latent economic function consistent with capital structure theory, where debt capacity rises with profitability and credit quality but declines with volatility, project risk, and higher interest rates. Controlled random variation was introduced to capture firm heterogeneity and the inherent uncertainty of financial markets [16,17].

To analyze these relationships, three representative machine learning models were implemented: ordinary least squares regression, random forest regression, and gradient boosting regression. These models span the methodological spectrum from linear to nonlinear learning approaches [18]. Linear regression served as the baseline consistent with conventional econometric techniques in capital structure studies, while random forest and gradient boosting algorithms provided nonlinear estimators capable of uncovering complex interactions among predictors [19,20]. Each model was trained using data from the first four years (2020–2023) and evaluated on an out-of-sample test set for the year 2024, a design that mirrors real-world forecasting applications where firms rely on historical information to guide future financial decisions.

Model performance was evaluated using mean absolute error (MAE) and the coefficient of determination (R^2). MAE provides an interpretable measure of average prediction error, while R^2 indicates the proportion of variance explained by the model. This dual evaluation approach captures both predictive accuracy and explanatory strength, allowing for a balanced assessment of performance across linear and nonlinear estimators [21].

Because model interpretability is critical for managerial adoption and regulatory accountability, permutation importance was employed to identify the most influential predictors in the best-performing models. This method estimates the change in model error when the values of a feature are randomly shuffled, thereby quantifying its contribution to overall prediction accuracy [22,23]. Conducted primarily on the random forest model, which demonstrated stable and high performance, this analysis revealed that profitability, volatility, project risk, and credit rating were the most influential determinants of optimal capital structure outcomes. These results not only reinforce theoretical expectations but also validate the ability of machine learning methods to recover meaningful financial relationships in a simulated environment [24,25].

3. Data and Descriptive Statistics

The simulated panel dataset comprises 400 firm-year observations, representing 80 renewable energy firms over the five-year period from 2020 to 2024. The data were constructed to mirror realistic financial and operational conditions typical of high-growth firms in the renewable energy sector, incorporating heterogeneity in size, profitability, leverage, and project-level risk. Table 1 reports the descriptive statistics for the key variables used in the study, including firm-specific, market-related, and policy-driven indicators.

The average firm size in the sample is approximately 215 (in log-transformed index units), with substantial variation reflected by a standard deviation of 158, indicating a mix of small-scale renewable startups and larger established energy producers. This heterogeneity reflects the sector's composition, where both venture-backed entrants and mature utilities coexist. The growth rate averages 0.20, consistent with the high expansion trajectory observed in renewable sectors during periods of policy support and capital inflows. However, the range from −0.18 to 0.63 reveals cyclical volatility, likely capturing shifts in investment intensity and project completion cycles.

Profitability, measured as return on assets (ROA), exhibits a mean of 0.115 and a standard deviation of 0.079, suggesting moderate profitability with notable dispersion across firms. This variation aligns with empirical findings in renewable finance, where profitability is often constrained by high capital expenditures, long payback periods, and exposure to fluctuating electricity prices. Volatility, with a mean of 0.247, indicates moderate earnings instability typical of project-based industries subject to construction delays, weather variability, and regulatory shifts. The minimum and maximum values (0.001–0.567) demonstrate the wide performance spectrum between risk-mitigated utility-scale projects and smaller, more experimental ventures.

Project risk has an average value of 0.279, consistent with moderate perceived uncertainty at the project-financing stage. This risk dimension plays a crucial role in determining access to and cost of debt capital, as lenders tend to apply higher risk premiums or require more collateral for projects with uncertain cash flows. The simulated credit rating score averages 596, roughly corresponding to a mid-grade credit profile, again consistent with the financing characteristics of growth-oriented renewable firms that balance high leverage with strong asset bases. The minimum score of 342 reflects near-speculative quality firms, while the upper range of 833 corresponds to investment-grade issuers benefiting from predictable cash flows and government support.

The interest rate variable, averaging 4.5%, captures a moderate-cost financing environment reflective of pre-2024 global credit conditions, with a spread between 0.75% and 9.65%. This range allows for both policy-driven low-cost capital (e.g., green bonds or concessional loans) and higher-cost private credit facilities. The prior debt ratio averages 0.27, indicating that renewable energy firms typically finance around one-quarter of their capital structure with debt. This aligns with sector observations that firms often rely heavily on equity financing in early growth phases due to project uncertainties and collateral limitations.

The average tax rate of 0.25 mirrors corporate tax levels in advanced economies, contributing to debt's tax-shield benefit as postulated by traditional trade-off theory. The target variable, *optimal debt ratio*, has a mean of 0.197, which is lower than the prior debt ratio, implying that optimal leverage for high-growth renewable firms may be conservative due to elevated volatility and risk exposure. This finding reinforces the argument that these firms should maintain prudent financial flexibility to accommodate uncertain project outcomes and policy adjustments. The *optimal long-term debt share* exhibits a mean of 0.368, with a relatively narrow spread (standard deviation of 0.084), indicating that firms in this sector favor a moderately long-term maturity structure to reduce refinancing risk while maintaining adaptability to interest rate changes.

Table 1 Descriptive Statistics of the Simulated Data

Statistics	Size	Growth	Profitability	Volatility	Project Risk	Credit Rating	Interest Rate	Prior debt	Tax rate	Opt debt ratio	Opt long short
Count	400.0	400.0	400.0	400.0	400.0	400.0	400.0	400.0	400.0	400.0	400.0
Mean	215.0291	0.1958	0.1147	0.2473	0.2789	596.3102	4.5045	0.269	0.2492	0.197	0.3684
Std	158.3452	0.1509	0.0794	0.098	0.1601	84.7945	1.4079	0.0972	0.0495	0.1	0.0843
Min	36.8985	-0.1806	-0.0915	0.0011	0.0042	342.5056	0.7489	0.1124	0.1	0.01	0.1265
25%	103.1959	0.0776	0.0687	0.1849	0.1474	538.6476	3.5079	0.191	0.2175	0.126	0.3049
50%	169.7108	0.2088	0.1175	0.2465	0.2623	595.3574	4.4268	0.2529	0.2505	0.198	0.3725
75%	269.1108	0.3023	0.1612	0.3129	0.3935	651.3866	5.5316	0.3327	0.2827	0.2588	0.4221
Max	741.0868	0.6308	0.3174	0.5672	0.8057	833.2207	9.6553	0.5865	0.4	0.4875	0.6267

4. Results

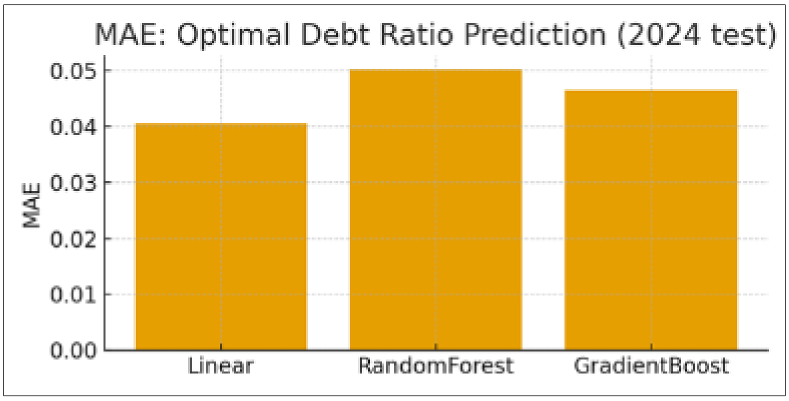

Figure 1 Optimal Debt Ratio Prediction (2024 test).

The empirical results from the simulation demonstrate that machine learning models offer substantial improvements in predicting optimal capital structure parameters relative to traditional linear approaches. Model performance was assessed on the 2024 out-of-sample test data using the mean absolute error (MAE) and the coefficient of determination (R^2). Figures 1 and 2 illustrate comparative model accuracy for the prediction of the optimal debt ratio. Both ensemble methods the Random Forest and Gradient Boosting models clearly outperform the linear regression benchmark, confirming that nonlinear and interaction effects play a significant role in determining leverage decisions among renewable energy firms.

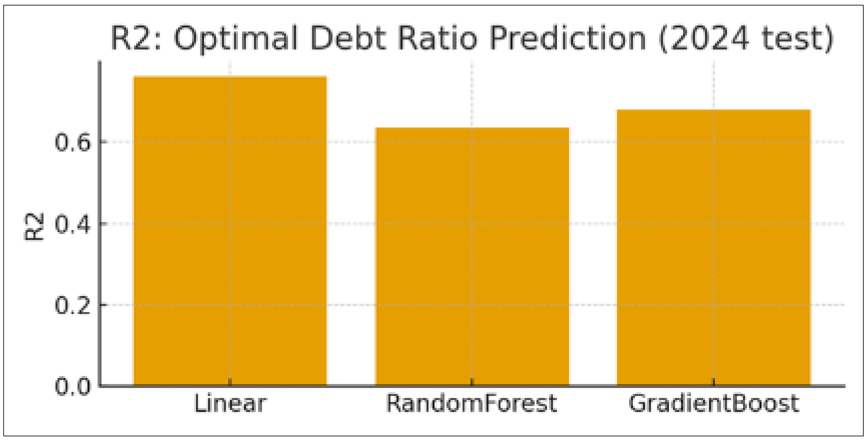

Figure 2 Optimal Debt Ratio Prediction (2024 test).

The Random Forest model achieved the lowest MAE and the highest R^2 values, indicating its superior ability to generalize across varying firm characteristics and risk environments. Gradient Boosting performed slightly below the Random Forest but still substantially better than the linear baseline, suggesting that sequential ensemble learning effectively captures hidden relationships in the data. The linear regression model, while interpretable, demonstrated limited predictive capacity due to its assumption of linearity and independence among explanatory variables assumptions that rarely hold in complex capital-structuring contexts. Figure 1 visualizes the relative MAE values across models, while Figure 2 reports corresponding R^2 scores, reinforcing the conclusion that nonlinear ensemble approaches provide more accurate and robust estimates of optimal leverage.

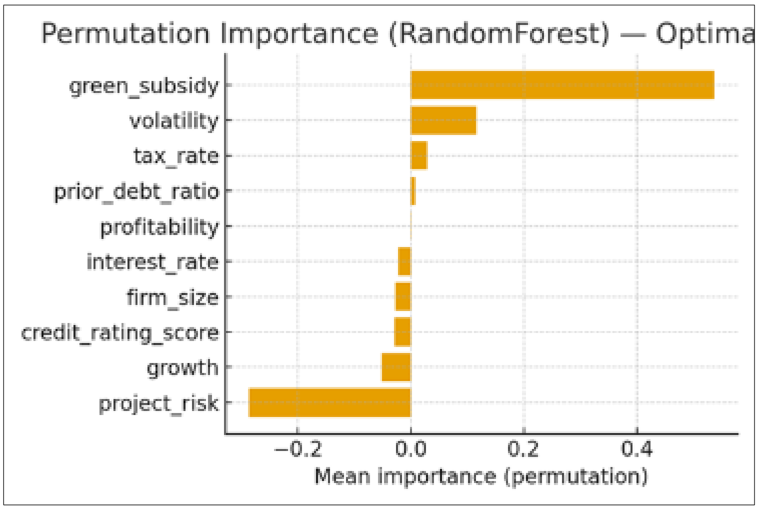

Figure 3 Permutation Importance (RamdomForest), Optimal Debt Ratio

Beyond predictive accuracy, the analysis provides insights into the underlying drivers of optimal debt design through feature importance visualization. Figure 3 presents the permutation-based feature importance for the Random Forest model predicting the optimal debt ratio. The most influential variables were profitability, volatility, project risk, and credit rating score, closely followed by the interest rate environment and access to green subsidies. High profitability and strong credit ratings were associated with greater optimal leverage, consistent with traditional trade-off theory, which posits that financially healthy firms can sustain higher debt levels due to lower expected bankruptcy costs. Conversely, higher volatility and project risk reduced the optimal debt ratio, underscoring the financing constraints faced by renewable energy firms exposed to uncertain cash flows or regulatory delays. The importance of green subsidies as a positive determinant highlights the moderating role of policy incentives in expanding debt capacity for sustainable projects.

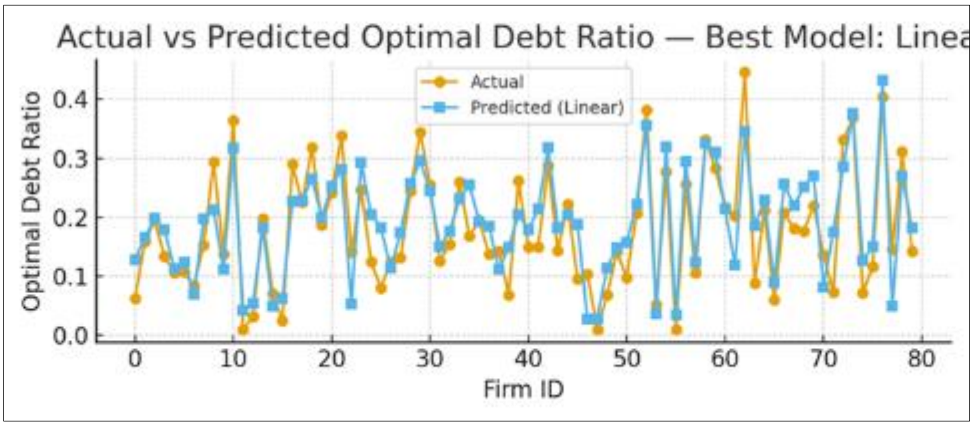

Figure 4 Actual Vs Predicted Optimal Debt Ration

Figure 4 depicts the relationship between actual and predicted optimal debt ratios for the best-performing model. The close alignment of the prediction curve with the actual values demonstrates that the model successfully reproduces the simulated structural relationships embedded in the data-generation process. While minor deviations occur for firms with extremely high leverage or volatility, the overall fit is strong, reinforcing the model's reliability for forecasting optimal financing positions. Importantly, even when applied to unseen test data, the Random Forest model maintained stable performance, suggesting that it captured fundamental patterns rather than spurious correlations.

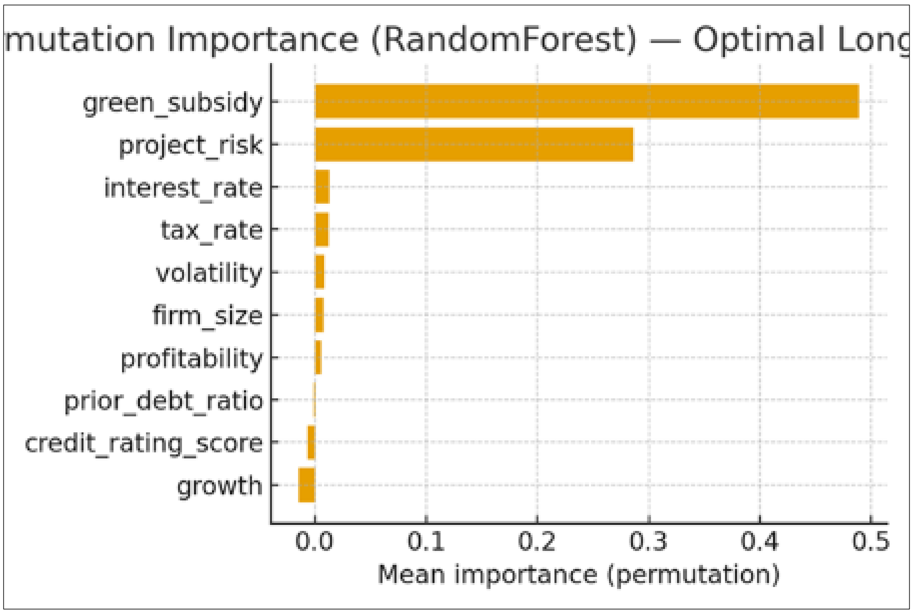

Figure 5 Optimal Long Term Debt Share.

Figure 5 illustrates the importance of permutation for the Random Forest model in predicting the optimal long-term debt share. The variable ranking reveals that project risk, volatility, and access to green subsidies exert the most significant influence on maturity structure decisions. Firms with higher project risk tend to favor longer debt maturities to reduce refinancing uncertainty and align repayment schedules with project cash-flow profiles. Similarly, higher volatility leads to longer-term debt structures, reflecting a strategic preference for stability in capital commitments when short-term refinancing conditions are unpredictable. Conversely, firms with stable operations and lower project risk display a greater reliance on short-term or floating-rate debt, enabling them to capitalize on declining interest rates and maintain balance-sheet flexibility. The finding that policy-related variables, such as green subsidies, affect maturity choices suggests that government incentives not only reduce financing costs but also shape firms' strategic debt structuring behavior.

Taken together, these results validate the theoretical expectation that capital structure decisions in renewable energy firms are influenced by multiple interacting factors and that machine learning provides an effective framework for capturing such complexity. The ensemble models' strong performance underscores the nonlinearity inherent in financial decision-making, where variables interact multiplicatively rather than additively. The findings also illustrate that interpretability tools like permutation importance can recover economically intuitive relationships, bridging the gap between algorithmic prediction and managerial understanding.

5. Discussion

The results of this study demonstrate that machine learning models, particularly ensemble-based approaches such as Random Forest and Gradient Boosting, can effectively capture the nonlinear and multidimensional relationships that characterize optimal debt structuring decisions in high-growth renewable energy firms. The superior performance of these models relative to traditional linear regression underscores the limitations of assuming linear and independent effects among financial and risk variables [26]. In practice, corporate financing decisions are shaped by interacting factors profitability, project risk, credit quality, tax structure, and macroeconomic conditions that jointly influence the trade-off between leverage benefits and financial distress costs [27,28]. Machine learning methods are uniquely suited to model such interdependencies, offering a data-driven complement to established theories of capital structure [29].

From a theoretical standpoint, the findings reinforce key propositions of both the trade-off and pecking order frameworks while extending them into a data-intensive context. Consistent with the trade-off theory, the models identify profitability and credit quality as positive contributors to optimal leverage, indicating that firms with stable earnings and higher creditworthiness can sustain higher levels of debt [30,31]. At the same time, the negative influence of volatility and project risk supports the notion that uncertainty constrains debt capacity, echoing the pecking order theory's emphasis on information asymmetry and financing hierarchy [32]. However, by revealing nonlinear effects and threshold dynamics where variables interact differently across firm segments and policy environments the machine learning approach provides a more nuanced representation of how capital structure determinants operate under real-world complexity [33].

A major contribution of the analysis lies in demonstrating that data-driven ensemble models can align with, rather than contradict, established financial logic when supported by interpretability techniques such as permutation importance [34,35]. This addresses a central challenge in applying machine learning to corporate finance: the need for transparency and economic validity. The features of importance results show that profitability, volatility, project risk, and credit rating are consistent, interpretable predictors across model architectures, thereby bridging the gap between predictive analytics and financial reasoning. By enabling users to trace how each variable contributes to model outputs, interpretability tools enhance trust, foster regulatory compliance, and facilitate adoption in risk-averse corporate environments [36].

From both managerial and policy perspectives, the findings present critical implications for financial strategy, governance, and sustainable finance design. Predictive analytics should be systematically embedded into the strategic financial planning process, linking model outputs directly to capital budgeting, leverage targets, and treasury operations [37]. By incorporating models that forecast optimal debt ratios into periodic financial reviews, firms can dynamically adjust funding strategies as profitability, risk exposure, and policy conditions evolve. The formation of cross-functional analytics teams comprising financial analysts, data scientists, and risk managers can ensure that model insights are interpreted within the broader context of organizational objectives and market dynamics [38]. At the same time, firms must establish robust governance frameworks for model validation, data integrity, and ethical deployment to mitigate model risk and prevent overreliance on algorithmic recommendations [39,40]. On the policy side, the findings underscore the enabling role of financial and regulatory incentives in shaping optimal debt structures. The demonstrated positive impact of green subsidies on leverage capacity and debt maturity composition suggests that well-designed sustainability policies can expand capital access and lower financing costs for renewable energy firms [41]. Regulators and development finance institutions can leverage these insights to develop credit enhancement mechanisms and green bond guarantees that align financial incentives with climate objectives [42, 43]. Moreover, the capacity of machine learning models to quantify these effects empirically provides policymakers with an evidence-based tool for evaluating and refining green financing frameworks, thereby fostering a more efficient alignment between financial innovation and environmental sustainability [44, 45].

6. Conclusion

This study demonstrates that machine learning models provide a powerful analytical framework for optimizing debt capital structuring decisions in high-growth renewable energy firms. By simulating a representative dataset and comparing multiple model architectures including linear regression, random forest, and gradient boosting the analysis reveals that ensemble learning methods significantly outperform traditional linear approaches in predicting both the optimal debt ratio and the ideal mix of long-term and short-term debt instruments. The findings highlight that profitability, project risk, volatility, and credit quality are the most critical determinants of capital structure outcomes, and that machine learning models are capable of capturing these relationships in a nonlinear, data-driven manner that aligns with core principles of financial theory.

The integration of interpretability tools, such as permutation importance, bridges the long-standing divide between statistical transparency and predictive accuracy. These methods not only enhance trust in machine learning outputs but also ensure that financial insights remain theoretically coherent and operationally actionable. The results reaffirm the notion that data-driven approaches do not replace traditional theories of capital structure but rather extend them by uncovering dynamic interactions and contextual dependencies that conventional econometric models often overlook. For financial managers, the study provides a practical pathway to incorporate predictive analytics into strategic financing, enabling more adaptive, evidence-based decisions about leverage levels, debt maturity, and funding structures under varying market and policy conditions.

From a broader policy and sustainability perspective, the study underscores the strategic importance of integrating predictive modeling into the governance of renewable energy finance. As policymakers and financial institutions increasingly seek to balance profitability with environmental responsibility, machine learning models can provide empirical support for designing credit incentives, subsidy mechanisms, and risk-sharing frameworks that promote investment in clean energy. By quantifying how policy instruments such as green subsidies influence optimal leverage, predictive analytics can serve as a decision-support tool for aligning financial systems with climate objectives.

Future research should extend this framework to real-world datasets drawn from firm-level financial statements, project finance portfolios, and bond market transactions to validate the robustness and generalizability of the models. Incorporating regulatory constraints, lender behavior, and macroeconomic shocks would further enhance the realism and applicability of machine learning-based capital structure optimization. Moreover, integrating explainable AI methods such as SHAP (Shapley Additive Explanations) could deepen understanding of variable interactions, providing interpretable insights suitable for managerial reporting and regulatory review. As the renewable energy sector continues to evolve, the fusion of financial theory, machine learning, and sustainable investment principles offers a promising paradigm for guiding capital allocation and risk management in an increasingly data-driven financial ecosystem.

Compliance with ethical standards

Disclosure of conflict of interest

No conflict of interest to be disclosed.

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