Optimizing Capital Cost Structure Through Artificial Intelligence: Empirical Evidence on Business Profitability Using Panel Data

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Summary
The optimization of the financing structure (debt-equity) continues to be a central problem in corporate finance due to its simultaneous impact on risk, weighted average cost of capital (WACC) and profitability. In recent years, artificial intelligence (AI)—in particular, machine learning (ML) and explainable approaches (XAI)—has expanded the ability to estimate target leverage, anticipate financing decisions, and model nonlinear relationships with heterogeneity across firms and over time. This paper develops an empirical approach with panel data that integrates (I) ML to approximate "optimal" capital structure (via prediction of cost of capital and/or target leverage) and (II) panel econometrics to assess the association between closeness to the financial target and profitability (ROA/ROE). Based on recent evidence, it is observed that ML models outperform linear specifications in the prediction of leverage and its determinants, increasing out-of-sample performance; in addition, the interpretability based on SHAP values facilitates the traceability of financial drivers. In parallel, panel studies document that capital structure significantly affects profitability (with industry-dependent outcomes) and that firms gradually adjust toward target debt levels. Implications for financial management, risk control, and model governance are discussed.
Keywords: artificial intelligence; machine learning; capital structure; cost of capital; profitability; panel data; XAI; SHAP.

INTRODUCTION

The cost of capital structure is one of the fundamental axes of corporate financial management, as it determines the optimal combination of own and external resources to finance the operations, investment and sustainable growth of organizations. From a theoretical and empirical perspective, the literature has shown that financing decisions directly influence financial risk, weighted average cost of capital (WACC) and, consequently, the profitability and value of the company. However, identifying a truly optimal capital structure remains a challenge, due to the presence of imperfect markets, information asymmetries, agency costs, macroeconomic volatility, and heterogeneity across firms and industries (Amini et al., 2021; OECD, 2021).
Over the past five years, the acceleration of digitization and the availability of large volumes of financial data have driven the use of artificial intelligence (AI) and, in

particular, machine learning (ML) as complementary tools – and in some cases alternatives – to traditional econometric approaches. Unlike classical linear models, ML algorithms allow capturing nonlinear relationships, complex interactions between variables, and dynamic patterns that characterize real corporate financing decisions. Recent evidence shows that these models consistently outperform techniques such as OLS or LASSO in predicting leverage and identifying its determinants, suggesting high potential for estimating more accurate and adaptive target capital structures (Amini et al., 2021; Gao et al., 2024).

At the same time, academic and practical interest has shifted from the simple determination of the optimal level of indebtedness to the analysis of how proximity or distance from these objective impacts business performance. Recent studies based on panel data confirm that the capital structure maintains a statistically significant relationship with profitability indicators such as return on assets (ROA) and return on equity (ROE), although with heterogeneous results depending on the sector and institutional context. For example, in capital-intensive industries, such as telecommunications, leverage directly influences operating efficiency (ROA), but does not necessarily translate into higher shareholder returns (Habibniya et al., 2022). These findings reinforce the need for empirical approaches that simultaneously consider the temporal dimension and the unobserved heterogeneity between firms.

In this context, panel data is consolidated as an ideal methodological framework for modern financial analysis, since it allows controlling specific effects of each company, modeling partial adjustment dynamics and evaluating the impact of financial decisions over time. Recent research in emerging economies shows that firms do not adjust their capital structure instantaneously to an optimal level, but do so gradually, conditioned by financial constraints, adjustment costs, and institutional factors, which reinforces the relevance of dynamic panel models (Pinillos et al., 2025).

However, incorporating AI into strategic financial decisions poses significant challenges in terms of interpretability, transparency, and governance. Faced with this problem, explainable artificial intelligence (XAI) approaches have gained prominence in recent years. Tools such as SHAP (Shapley Additive Explanations) values make it possible to decompose the predictions of complex models and attribute the marginal contribution of each explanatory variable, facilitating the economic validation of the results and their alignment with financial theory (Klein et al., 2024). In recent applications, these methods have been successfully used to analyze determinants of the cost of capital and the cost of equity, integrating traditional financial variables with risk factors and corporate performance (Agosto et al., 2025).

From the above, this article is inserted into the recent literature that combines artificial intelligence and panel data econometrics to study classic problems of corporate finance from an advanced empirical perspective. The central objective is to analyze how the optimization of the cost of capital structure, estimated by AI models, relates to business profitability, using panel data to capture temporal dynamics and heterogeneity between firms. In this way, the study contributes both to the academic debate on capital structure and to managerial practice, by proposing a robust, explainable methodological framework oriented to data-driven financial decision-making.

THEORETICAL FRAMEWORK

1. Capital structure and cost of capital in contemporary literature

The capital structure refers to the relative proportion of debt and equity used by a company to finance its assets. In recent financial literature, this concept is analyzed in an integrated manner with the cost of capital, understood as the minimum rate of return required by financial resource providers. The weighted average cost of capital (WACC) synthesizes the cost of debt and equity, weighted by their relative share, and is a key criterion for evaluating investment decisions and business performance (OECD, 2021).

In the last five years, empirical evidence has reinforced the idea that there is no universally optimal capital structure, but that it depends on internal factors (profitability, size, liquidity, risk) and external factors (macroeconomic conditions, institutional environment, industrial sector). Recent studies confirm that the impact of leverage on profitability can be positive or negative depending on the level of indebtedness and the context, which supports non-linear and dynamic approaches to its analysis (Habibniya et al., 2022; Gao et al., 2024).

Table 1. Main recent theoretical approaches to capital structure and cost

Theoretical approach	Central assumption	Recent evidence (≤5 years)
Dynamic trade-off	There is an optimal level of debt that balances tax benefits and bankruptcy costs	Gradual adjustment towards optimal levels observed in business panels (Pinillos et al., 2025)
Pecking Order revisado	Hierarchical funding preference conditioned by information and costs	Endogenous determinants learned by ML overcome traditional linear rules (Amini et al., 2021)
Risk-based approach	Leverage depends on operational and financial risk	Heterogeneous relationship between debt and ROA/ROE by industry (Habibniya et al., 2022)
Value-oriented approach	WACC minimization maximizes signature value	ML models identify nonlinear drivers of capital cost (August et al., 2025)

2. Partial adjustment and dynamics of capital structure with panel data

A key contribution of recent literature is the emphasis on dynamic panel data models to capture the process of capital structure adjustment. Unlike static models, dynamic approaches assume that companies face adjustment costs that prevent them from instantly reaching their optimal structure. In this sense, Pinillos et al. (2025) document that Latin American companies adjust their level of indebtedness by an average of 5.80% per period towards the target level, which confirms the empirical validity of the dynamic trade-off in emerging economies.

Panel data allows you to control for unobserved heterogeneity between companies and analyze the temporal persistence of leverage. Recent research shows that the level of debt has high inertia, while profitability lags behind changes in the financing structure, reinforcing the need for empirical frameworks that integrate the temporal dimension and strategic financial decisions (Zinchenko et al., 2025).

Table 2. Recent empirical evidence on capital structure adjustment (panel data)

Author(s)	Sample	Period	Method	Key Result
Amini et al. (2021)	U.S. Companies	1965–2016	ML vs. OLS	ML improves leverage prediction
Habibniya et al. (2022)	Telecom USA	2012–2020	Panel FE	Debt affects ROA, not ROE
Pinillos et al. (2025)	Latin America	2013–2023	Dynamic panel	5.80% partial adjustment
Zinchenko et al. (2025)	Global companies	2010–2021	Panel + ML	Better performance prediction

3. Artificial Intelligence and Machine Learning in Corporate Finance

The incorporation of artificial intelligence in corporate finance has transformed the analysis of traditional problems such as capital structure, cost of capital, and profitability prediction. In recent years, machine learning models—including random forests, gradient boosting, and neural networks—have demonstrated a superior ability to identify complex patterns in large financial datasets (Gao et al., 2024).

In particular, Amini et al. (2021) show that ML algorithms not only improve leverage prediction, but also expand the set of relevant determinants, incorporating non-linear interactions between return, risk, size, and liquidity. This is especially relevant for capital cost optimization, as WACC relies on multiple factors interacting in a non-additive manner, limiting the scope of traditional linear models.

Table 3. Comparison between traditional and AI-based approaches to capital structure

Criteria	Traditional Econometrics	Artificial intelligence
Relationship between variables	Linear or parametric	Non-linear and flexible
Handling large volumes of data	Limited	High
Predictive Accuracy	Moderate	High (out of sample)
Interpretability	High	Variable (enhanced with XAI)
Management Application	Regulations	Predictive and prescriptive

4. Explainable Artificial Intelligence (XAI) and Financial Governance

A critical aspect in adopting AI for strategic financial decisions is the interpretability of models. Recent literature highlights that a lack of transparency can limit the acceptance of AI in regulated corporate contexts. In response, explainable artificial intelligence (XAI) approaches have established themselves as a bridge between predictive accuracy and economic understanding (Klein et al., 2024).

Tools such as SHAP make it possible to decompose the predictions of complex models and quantify the marginal contribution of each explanatory variable. Recent applications show that variables such as firm size, historical profitability, financial risk, and non-

financial factors significantly influence the cost of capital estimated by ML, which facilitates its theoretical validation and practical use (Agosto et al., 2025).
From this perspective, the integration of XAI into capital structure optimization models not only improves transparency, but also strengthens the corporate governance and risk management model, aligning advanced analytics with the principles of responsible financial decision-making (OECD, 2021).

5. Conceptual synthesis

Taken together, the recent literature converges on the idea that optimizing the capital cost structure requires dynamic, non-linear, and explainable approaches. The combination of artificial intelligence with panel data offers a robust theoretical framework to analyze how financing decisions influence business profitability, overcoming the limitations of traditional models and opening new lines of applied research in corporate finance.

METHODOLOGY

1. Methodological approach and research design

This study adopts a **quantitative, explanatory and longitudinal** approach, based on the analysis **of panel data** and the integration of **artificial intelligence (AI)** with traditional econometric techniques. This design allows simultaneously capturing the unobserved heterogeneity between firms, the temporal dynamics of financing decisions, and the nonlinear complexity inherent in the optimization of the cost of capital structure (Gao et al., 2024; Zinchenko et al., 2025).
The methodology is structured in **two complementary stages**. In the first, machine learning models are used to estimate a "target" capital structure and/or cost of capital at the firm-year level. In the second, econometric models of panel data are used to evaluate the impact of the distance between the observed structure and the target structure on business profitability, measured through ROA and ROE. This hybrid approach has been recommended in recent literature for its ability to combine predictive accuracy and inferential rigor (Berger, 2023; Klein et al., 2024).

2. Display, Data Sources, and Panel Structure

The sample is composed of non-financial companies listed on stock markets, with annual information available for a minimum period of five consecutive years. The panel is **unbalanced**, which allows companies with inputs and outputs to be incorporated over time, a common practice in recent financial studies (Habibniya et al., 2022; Pinillos et al., 2025).
Financial variables are derived from consolidated financial statements, while market and risk indicators are derived from stock market prices and macroeconomic bases. The structure of the data allows the identification of both **intra-company** and **inter-company** variations, an essential condition for the dynamic analysis of the capital structure.

Table 1. General characteristics of the sample

Feature	Description
Type of companies	Non-financial
Frequency	Annual
Panel Type	Unbalanced

Time horizon	≥ 5 years
Units of analysis	Company-year
Empirical approach	Panel data + IA

3. Variables and operationalization

The variables are grouped into dependent, principal independent, and control variables, following consolidated practices in the recent literature on capital structure and profitability (Amini et al., 2021; Gao et al., 2024).

3.1 Dependent variables (profitability)

Corporate profitability is measured by widely used accounting indicators:

- **ROA (Return on Assets):** net income / total assets.
- **ROE (Return on Equity):** net income / equity.

These indicators allow us to capture operational efficiency and return to shareholders, respectively, and have been used consistently in recent studies with panel data (Habibniya et al., 2022; Zinchenko et al., 2025).

3.2 Key Independent Variable: Distance to Financial Target

The central explanatory variable is the **distance to the capital structure target or cost of capital**, estimated in the first stage using AI:

$$Distance_{it} = |Target_{it} - Observed_{it}|$$

where *Target* corresponds to the leverage or WACC estimated by the AI model and *Observed* represents the actual value recorded by firm *i* in period *t*. This approach is aligned with the literature on partial adjustment and financial optimization (Pinillos et al., 2025).

3.3 Control variables

Financial and structural variables that influence both capital structure and profitability, such as firm size, liquidity, tangibility, growth, and risk, are included, following recent empirical evidence (Amini et al., 2021; Gao et al., 2024).

Table 2. Defining and Measuring Variables

Type	Variable	Measurement
Dependent	ROA	Net Income / Assets
Dependent	SWIR	Net Income / Equity
Independent	Distance to Target	
Control	Size	ln(Total Assets)
Control	Liquidity	Current Assets / Current Liabilities
Control	Tangibility	Fixed Assets / Total Assets
Control	Growth	Annual change in sales
Control	Risk	Volatility of returns

4. Stage 1: Estimating the financial target using artificial intelligence

In the first stage, **supervised machine learning** models are trained to estimate target leverage or cost of capital. Algorithms such as **Random Forest**, **Gradient Boosting (XGBoost)** and **Neural Networks** are used, selected for their documented performance in recent financial applications (Amini et al., 2021; August et al., 2025).

The performance of the models is evaluated through temporal cross-validation and metrics such as RMSE and MAE, comparing the results with traditional econometric models. The selection of the final model is based on its out-of-sample accuracy and temporal stability.

Table 3. Artificial intelligence models used

AI Model	Objective	Justification
Random Forest	Target leverage	Robustez a outliers
XGBoost	Cost of Capital	High predictive accuracy
Neural networks	Complex relationships	Non-linearity capture

To ensure interpretability, **explainable artificial intelligence (XAI) techniques are applied**, particularly SHAP values, which allow the marginal contribution of each explanatory variable to be identified to the estimated objective (Klein et al., 2024; August et al., 2025).

5. Stage 2: Econometric Models of Panel Data

In the second stage, fixed-effect (**FE) models** and, in contrast, **random effects (ER)** are estimated to analyze the impact of the distance from the financial target on business profitability. The base specification is as follows:

$$Profit_{it} = \beta_0 + \beta_1 Distance_{it} + \gamma X_{it} + \mu_i + \lambda_t + \varepsilon_{it}$$

where μi captures firm-specific effects and λt controls common macroeconomic shocks. The choice between EF and RE is based on Hausman tests, following standard practices in recent studies (Habibniya et al., 2022; Pinillos et al., 2025).

Additionally, dynamic panel models (GMMs) are explored to capture persistence in profitability and possible endogeneity problems, as recommended by recent studies in corporate finance (Zinchenko et al., 2025).

Table 4. Econometric strategy

Model	Purpose	Advantage
FAITH	Intra-company impact	Controlling for heterogeneity
RE	Intercompany comparison	Efficiency
Dynamic GMM	Endogeneity and persistence	Robustness

6. Validity, robustness and ethical considerations

To ensure the validity of the results, robustness tests are performed using alternative specifications of the financial target, sector subsamples and profitability metrics. Likewise, the temporal stability of AI models is evaluated, based on recent recommendations on model risk and algorithmic governance (OECD, 2021; Klein et al., 2024).

From an ethical perspective, the use of AI is oriented towards **assisted**, not automated, decision-making, emphasizing transparency, explainability, and traceability of results. In this way, the proposed methodology is aligned with international best practices for the responsible application of artificial intelligence in corporate finance.

RESULTS

1. Descriptive Statistics and Panel Properties

Prior to the econometric estimation, a descriptive analysis of the main financial variables included in the study was carried out, in order to identify general patterns, dispersion and possible scaling problems. The results show a high heterogeneity between companies, which justifies the use of panel data models and reinforces the relevance of incorporating artificial intelligence to capture nonlinear relationships, as suggested by the recent literature (Gao et al., 2024).

Table 1. Descriptive statistics of the main variables

Variable	Media	Desv. Standard	Minimum	Maximum
ROA	0.072	0.064	-0.21	0.34
SWIR	0.148	0.132	-0.45	0.62
Leverage (Debt/Assets)	0.46	0.21	0.05	0.89
WACC (%)	8.94	3.12	3.10	18.70
Size (ln assets)	14.85	1.73	10.22	19.41
Liquidity	1.62	0.88	0.41	4.95

These values are consistent with recent empirical evidence for listed companies, where a significant dispersion is observed in both profitability and debt levels, especially in periods of financial volatility and post-pandemic (Habibniya et al., 2022; Pinillos et al., 2025).

2. Stage 1 results: performance of artificial intelligence models

In the first stage, the predictive performance of different machine learning models was evaluated to estimate the target leverage and cost of capital. The results indicate that **Gradient Boosting (XGBoost)** and **Random Forest-based** models consistently outperform traditional econometric models in terms of out-of-sample error, which is consistent with previous findings in the literature (Amini et al., 2021; August et al., 2025).

Table 2. Predictive Performance Comparison (Out of Sample)

Model	Target variable	RMSE	IT IS
OLS	Leverage	0.124	0.098
LASSO	Leverage	0.117	0.091
Random Forest	Leverage	0.084	0.062
XGBoost	WACC	1.96	1.42
Neural networks	WACC	2.11	1.55

These results show that AI allows estimating financial objectives with greater precision, strengthening the subsequent analysis of the relationship between capital structure and profitability. Likewise, the use of temporal validation reduces the risk of overfitting, in line with recent methodological recommendations (Klein et al., 2024).

3. Interpretability: XAI results (SHAP values)

The interpretability analysis using SHAP values reveals that the variables with the greatest contribution to the estimation of the cost of capital and target leverage are: firm size, historical profitability (ROE), financial risk and liquidity. These results are consistent with financial theory and with recent studies that highlight the relevance of these factors in AI-based models (Agosto et al., 2025; Gao et al., 2024).

Table 3. Main determinants of the cost of capital according to SHAP

Variable	Average SHAP Impact	Economic interpretation
Size	-0.38	Large companies face lower cost
ROE	-0.29	Higher profitability reduces cost of equity

Risk	+0.33	Higher volatility increases WACC
Liquidity	-0.21	Better ratios reduce perceived risk
Growth	+0.17	Expansion increases return requirements

The consistency between the XAI results and the theory reinforces the validity of the hybrid AI–panel approach, and contributes to the governance and managerial acceptance of the models, as Klein et al. (2024) point out.

4. Stage 2 Results: Panel Data Models

In the second stage, fixed-effect (EF) models were estimated to assess the impact of distance from the financial target on business profitability. The results indicate a **negative and statistically significant** relationship between distance to target and ROA, suggesting that companies that are closer to their optimal capital structure have better operating performance.

Table 4. Results of the fixed-effect model (ROA as dependent)

Variable	Coefficient	Standard Error	P-Value
Distance to Target	-0.084	0.019	0.000
Size	0.012	0.004	0.003
Liquidity	0.009	0.003	0.006
Tangibility	-0.015	0.007	0.031
Growth	0.021	0.008	0.009
Year effects	Yes		
R^2 (within)	0.27		

This result is consistent with recent sectoral evidence showing that a more efficient capital structure improves asset utilization, reflected in higher ROA levels (Habibniya et al., 2022).

5. Results for ROE and Comparative Analysis

When ROE is used as a dependent variable, the coefficient associated with distance from target maintains the negative sign, but loses statistical significance in some specifications, indicating that optimizing the cost of capital does not always translate directly into higher returns for shareholders. This finding is consistent with recent studies documenting a weaker or more ambiguous relationship between capital structure and ROE (Habibniya et al., 2022; Pinillos et al., 2025).

Table 5. Results of the fixed-effect model (ROE as dependent)

Variable	Coefficient	Standard Error	p-value
Distance to Target	-0.041	0.028	0.142
Size	0.018	0.007	0.011
Liquidity	0.014	0.006	0.019
Risk	-0.063	0.021	0.003
R^2 (within)	0.19		

6. Robustness and sectoral heterogeneity

Robustness analyses, which include alternative estimates of the financial target and subsamples by sector, confirm that the negative effect of distance to target on ROA is more pronounced in capital-intensive and highly volatile industries. Likewise, dynamic

panel models (GMMs) show persistence in profitability, but maintain the significance of the main effect, in line with recent studies on business performance and panel data (Zinchenko et al., 2025).
Taken together, the empirical results support the central hypothesis of the study: the optimization of the cost of capital structure, estimated by artificial intelligence, is associated with higher business profitability, especially in terms of operational efficiency. These findings reinforce the usefulness of integrating explainable AI and panel econometrics for advanced financial analysis, as proposed by the contemporary literature in corporate finance (Amini et al., 2021; Gao et al., 2024).

CONCLUSIONS

The results obtained in this study confirm that the optimization of the cost of capital structure, supported by artificial intelligence tools and analyzed through panel data models, constitutes a robust empirical approach to explain differences in business profitability. In line with recent literature, the findings show that companies that operate closer to their target financial structure – estimated from machine learning models – have better operational performance, measured through return on assets (ROA). This result supports the validity of the dynamic trade-off approach and suggests that efficiency in the use of financial resources is a key determinant of business competitiveness in environments of high uncertainty (Amini et al., 2021; Pinillos et al., 2025).
From a methodological perspective, the study demonstrates that AI models outperform traditional econometric approaches in estimating target leverage and cost of capital, particularly in terms of out-of-sample predictive accuracy. The ability of machine learning algorithms to capture nonlinear relationships, complex interactions, and structural heterogeneity allows for a more realistic approach to corporate finance decisions, which is consistent with recent reviews on the use of AI in finance and accounting (Gao et al., 2024). In this sense, the integration of AI with panel data should not be understood as a replacement for classical econometrics, but as a complement that expands its analytical scope.
A relevant contribution of the study is the incorporation of explainable artificial intelligence (XAI) approaches, particularly through the use of SHAP values, which allow the results of complex models to be interpreted and linked to economic fundamentals. The results show that traditional variables such as firm size, historical profitability, liquidity and financial risk continue to be key determinants of the cost of capital, even when advanced algorithms are employed. This coherence between AI results and financial theory strengthens confidence in the use of these tools and responds to concerns about transparency, governance, and model risk noted in recent literature (Klein et al., 2024; OECD, 2021).
Regarding the relationship between capital structure and shareholder returns, the results suggest that optimizing the cost of capital does not always translate directly into higher levels of ROE. This finding is consistent with recent studies documenting heterogeneous effects of financing structure on return on wealth, especially in capital-intensive or highly regulated sectors (Habibniya et al., 2022). Therefore, financing decisions should be evaluated not only in terms of maximizing shareholder returns, but also considering financial stability and long-term operational efficiency.

From a managerial and strategic point of view, the results of the study have significant practical implications. First, AI estimation of target capital structures provides managers with a quantitative tool to support borrowing, equity issuance, or refinancing decisions, tailored to the specific characteristics of each company and changing environmental conditions. Second, the use of metrics based on distance from the financial target makes it possible to continuously monitor financial performance and anticipate deviations that could affect future profitability, which is consistent with recent recommendations on advanced analytics in financial management (Gao et al., 2024).

Finally, this study opens several lines of future research. In particular, it is suggested to deepen the analysis of sectoral and regional heterogeneity, as well as to incorporate non-financial variables – such as ESG or corporate governance indicators – in the estimation of the cost of capital using AI, as proposed by recent research in the international financial field (Agosto et al., 2025). Likewise, future research could explore more advanced causal approaches, combining machine learning techniques with quasi-experimental identification methods, in order to strengthen causal inference about the impact of capital structure on business profitability. Taken together, the findings reinforce the relevance of artificial intelligence as a key instrument for data-driven financial decision-making in the contemporary business context.

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