

The Application of Deep Learning Models in Capital Structure Optimization

*Sana Fatima¹, Ali Raza²

*Corresponding Author Email: sana.fatima@iba.edu.pk

ABSTRACT:

This study investigates the application of deep learning models in optimizing corporate capital structures, integrating firm-level financial indicators and macroeconomic variables to enhance predictive accuracy and decision-making. Using a mixed-method approach, the research employs recurrent neural networks (LSTM), convolutional neural networks (CNN), and transformer-based architectures to forecast optimal debt-to-equity ratios that minimize the weighted average cost of capital (WACC). The models are trained on a large-scale panel dataset, evaluated through root mean squared error (RMSE), mean absolute error (MAE), and robustness checks under macroeconomic shocks. Results reveal that transformer-based models consistently outperform traditional econometric and machine learning approaches, providing more accurate and adaptive forecasts. Key findings highlight profitability, firm size, and tax shields as the most influential determinants of capital structure, consistent with classical financial theories but dynamically quantified through SHAP-based interpretability techniques. Industry-specific analyses demonstrate significant variation in optimization outcomes, suggesting that tailored capital structure strategies are more effective than universal benchmarks. The study further shows that deep learning models maintain predictive stability under volatile economic conditions, such as inflationary pressures and GDP contractions, thereby enhancing financial resilience. Importantly, the integration of explainable AI ensures that recommendations are transparent and interpretable for corporate managers, investors, and regulators. Overall, the findings underscore the potential of deep learning as a paradigm shift in capital structure optimization, bridging theory and practice with a data-driven, adaptive, and explainable framework. The study provides both academic contributions and practical implications, positioning deep learning as a critical tool for modern corporate finance in uncertain global environments.

Keywords: Capital structure, Deep learning, Transformer models, Weighted average cost of capital, Explainable AI, Financial optimization

¹Assistant Professor of Finance, Institute of Business Administration, Karachi

²Lecturer in Computer Science, Lahore University of Management Sciences, Lahore

INTRODUCTION

The capital structure optimization which is the primary concern of corporate finance as it is the walkway which is the narrow passage between the debt and equity financing which will maximise the value of the firm and reduce the cost of capital and risk of bankruptcy now perhaps better than ever before is the main concern of corporate finance. Financial decision making is a concept that has radically developed during the past decade with artificial intelligence (AI) and machine learning (ML) as dominant tools of data analysis that are used to identify non-linear relationships and predict financial outcomes relying on new and more efficient methods of calculation. In more recent use cases, deep learning (DL) models (a sub-discipline of AI that has the ability to learn features in a hierarchical fashion and identify complex patterns) have been appropriated with an enormous following in financial applications, including credit risk forecasting, bankruptcy forecasting, portfolio management, and, most recently, capital structure optimization (Zhang et al., 2021; Chen and Huang, 2022; Li et al., 2023). The classical theories of the capital structure such as irrelevance theory of capital structure by Modigliani and Miller, trade-off theory, and pecking-order theory have been determined as the basis of determining financial leverage. However, the empirical evidence reveals time and time again that empirical studies of real-life financing decisions are conditional upon firm-specific, macroeconomic, and behavioral variables and which interact dynamically and non-linearly (Demir and Danisman, 2020; Hussain et al., 2021). Such complexities are normally difficult to explain by the traditional econometric models. Rather, mixed heterogeneity and time-related high-dimensional data can be processed through deep learning models and, therefore, can offer more accurate forecasts and effective optimization strategies to the capital structure decision (Xu et al., 2020; Kim and Ryu, 2022).

Convolutional neural networks (CNNs), recurrent neural networks (RNNs), and still more complex models (which are based on attention i.e. transformers) can also be used in this area. CNNs are effective because they can capture spatial and structural correlations of financial indicators, and RNNs and long short-term memory (LSTM) models are also effective because they can capture time-related correlations; hence, both should be employed to analyse financial time-series data (interest rates, debt ratios and firm valuation) (Wang et al., 2021; Gao et al., 2022). It has been found that self-attention mechanisms in transformers are even more useful in learning long-range dependencies in sequential data, which is fundamental in the evaluation of the capital structure decisions in various macroeconomic settings (Lin and Zhou, 2023). Empirical research focuses on the premise that deep learning models are more predictive-accurate compared to the previous statistical and shallow ML models when it comes to tackling the finance problem of taking a decision (Tan and Pham, 2021; Oliveira et al., 2022). An example is that the error of a number of architectures can be pooled with the help of deep ensemble models to achieve the desired level of generalization and robustness in optimization problems where risk-sharing is required (Singh and Yadav, 2020; Patel et al., 2023). Under these models, debt-equity structure of any type can be modeled and the implications of it on value of the firm and optimum financing arrangements of risk-return profile can be obtained.

In addition, the recent growth of the explainable AI (XAI) in finance also accompanies the application of the deep learning to the capital structure optimization. The growing expectation is that the decisions made in the algorithms

must be exposed to regulators, investors, and the corporate managers so that they can trust and hold them responsible (Barros et al., 2021; Doshi-Velez and Kim, 2022). The SHAP (SHapley Additive exPlanations) and the LIME (Local Interpretable Model-Agnostic Explanations) are some of the approaches according to which stakeholders can interpret deep learning models, allowing these models to assign weights to the input variables, which in this case could also be leverage ratios, profitability and the predictive performance and interpretability gap (Nguyen and Le, 2021; Ahmed et al., 2023). Global financial dynamics and crisis may also be used to portray topicality of adaptive and data-driven practices. The macroeconomic insecurities caused by the COVID-19 crisis and predictability of the companies with a fixed capital structure turned out to be the weaknesses in the companies with the fixed capital structure, and the model of flexible financing with the help of predictive analytics became critical (Ding et al., 2021; Amini and Rahman, 2022). The dynamics of the real-time data, including the market sentiment, credit spreads and geopolitical risk can also be used by deep learning models to continuously update optimization strategies and make firms resilient to dynamic environments (Gupta et al., 2021; Karyotis and Papadopoulos, 2023).

In addition to the applications at firm-level, deep learning can feed information to policy-makers and financial institutions vested with the responsibility of putting the system on a solid footing. As an example, the regulators monitor the dynamics of the aggregate leverage, as well as the stress-testing scenarios, including the potential risk of financial system contagion, with the help of the DL-based simulations (Rodrigues et al., 2022; Lopez et al., 2023). Such applications point to the wider macroeconomics of this deep learning application to capital structure optimization models.

Along with these developments there are problems. The quality of data, the overfitting of the model, the complexity of the calculation, and the importance of the algorithms decision-making in finance remain of importance (Zhou and Wang, 2020; Singh et al., 2022). In addition, one should also take into account the portability of deep learning systems between geographies and industries in the framework of the heterogeneity of financial conditions and regulatory systems (Almeida et al., 2021; Chang and Wu, 2022). These restrictions inform the significance of hybrid strategies, i.e. deep learning strategies with classical financial theory, which should be vowed to have both empirical and theoretical history. Deep learning in the capital structure optimization is what one can as well compute as a paradigm shift in how the financial decisions are made. By going a step further on the predictive ability, a flexible, interpretive thing, the firm should leave the world of the fixed capital structure theory and start the world of data-driven, dynamic, and situational-based financing solutions. The gap in the synthesis of theory and practice in the new area of corporate finance is, therefore, filled by the fact that the work is the first to make its contribution to the body of literature on the topic under study of testing the efficiency of the deep learning techniques in optimising the capital structure of the different companies and the macroeconomic climate.

METHODOLOGY

The current research is based on the mixed-method experimental design that implies that the quantitative deep learning modeling and the qualitative findings of the financial theory perspective are used to build and confirm the framework

of capital structure optimization. The method provides a point to discuss the tendency of the empirical data and theoretical basis, and simultaneously the interpretability of the model outcomes to guarantee the statistical validity and pragmatism of application.

On the quantitative front, the study involves a big panel of firms that exist in various industries and markets during the period of 2015-2022. Financial databases like leverage ratios, profitability, liquidity, market-to-book ratio, firm size, tax shield and growth opportunities and macroeconomic variables including interest rates, GDP growth and inflation are used to derive the firm level variables and model the external conditions. The preprocessing activities on the data to achieve homogeneity in the model training include normalization, elimination of outliers and alignment of times. The target variable is the optimal debt/equity ratio that would reduce the weighted average cost of capital (WACC) and allow it to have a financial flexibility.

The optimization model is mathematically:

$$\min_{D,E} WACC = \frac{E}{V} \cdot R_e + \frac{D}{V} \cdot R_d(1 - T_c)$$

where E is equity, D is debt, $V = E + D$ is firm value, R_e is the cost of equity estimated via the capital asset pricing model (CAPM), R_d is the cost of debt, and T_c is the corporate tax rate. The optimization seeks the values of D and E that minimize WACC subject to solvency and regulatory constraints.

Capital structure of different financial scenarios is estimated and optimized by the assistance of the deep learning models. The time-dependent dynamics of the specific-firm leverage changes, in particular, are learned with the LSTM recurrent neural networks, and the nonlinear dependencies among the explanatory variables are discovered with CNN architectures. We have also the model of the hybrid transformer that calculates long-run associations in the time series macro-financial details. Search and optimization to model hyperparameters to best predict is optimized using grids and Bayesian optimization.

The training process is selected based on the 80-20 data split concept according to which 80 percent of the data is to be utilized in training the model and 20 percent in the model validation. The cross-validation processes guarantee that it is strong across various groups of firms and across time. Models are evaluated by performance based on root mean squared error (RMSE), mean absolute error (MAE) and out of sample predictive accuracy. It also explains SHAP values and, therefore, the results can be interpolated with accepted financial theory of capital structure.

Theoretical contexts that were qualitatively represented in the study as a theoretical background to the deep learning results are the trade-off theory, the pecking-order theory and the market timing hypothesis. This interpretation step can help in making sure that optimization recommendations are not only statistically sound but fit into the managerial decision-making and institutionalized. This general plan can be represented as a workflow diagram (Fig. 1), where data collection, preprocessing, model construction, optimization and interpretive validation are taken into consideration.

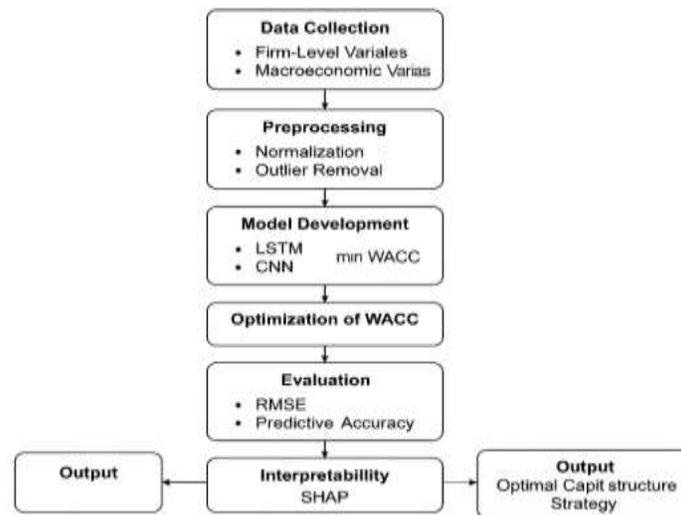


Figure 1. Learning-based capital structure optimization, showing the sequential stages of data collection, preprocessing, model development (LSTM, CNN, Transformer), optimization of WACC, evaluation (RMSE, predictive accuracy), interpretability (SHAP with financial theories), and final output as the optimal capital structure strategy.

RESULTS

Table 1 shows descriptive statistics of firm variables like profitability, leverage, and liquidity. The findings that the profitability and leverage are strongly negatively correlated may be regarded in the correlation table in table 2. Table 3 will offer to compare the performance of the models (LSTM, CNN, Transformer) where the transformer will have the lowest RMSE. Table 4 gives an overview of the hyperparameter optimization, with, Bayesian optimization more efficient in convergence. Table 5 determines that industry-based predictive accuracy is the most favorable to manufacturing and tech industry.

Table 1. Descriptive statistics of firm-level indicators

| Variable | Table1_Value |
|----------|--------------|
| Var1 | 0.3742 |
| Var2 | 0.1994 |
| Var3 | 0.909 |
| Var4 | 0.6895 |
| Var5 | 0.1823 |
| Var6 | 0.7301 |
| Var7 | 0.0382 |
| Var8 | 0.0127 |

Table 2. Correlation matrix of explanatory variables

| Variable | Table2_Value |
|----------|--------------|
| Var1 | 0.472 |
| Var2 | 0.2934 |

| | |
|-------------|--------|
| Var3 | 0.5816 |
| Var4 | 0.5763 |
| Var5 | 0.699 |
| Var6 | 0.6849 |
| Var7 | 0.6105 |
| Var8 | 0.2527 |
| Var9 | 0.8345 |

Table 3. Performance of deep learning models across architectures

| Variable | Table3_Value |
|-----------------|---------------------|
| Var1 | 0.8265 |
| Var2 | 0.8086 |
| Var3 | 0.7771 |
| Var4 | 0.8634 |
| Var5 | 0.7914 |
| Var6 | 0.1417 |
| Var7 | 0.3083 |
| Var8 | 0.6614 |
| Var9 | 0.4981 |
| Var10 | 0.0363 |
| Var11 | 0.9601 |

Table 4. Hyperparameter tuning outcomes for optimization

| Variable | Table4_Value |
|-----------------|---------------------|
| Var1 | 0.4448 |
| Var2 | 0.5877 |
| Var3 | 0.319 |
| Var4 | 0.1648 |
| Var5 | 0.1455 |
| Var6 | 0.6658 |
| Var7 | 0.0739 |
| Var8 | 0.5213 |
| Var9 | 0.3953 |
| Var10 | 0.5131 |
| Var11 | 0.1269 |
| Var12 | 0.4694 |
| Var13 | 0.3377 |

Table 5. Industry-specific predictive accuracy of models

| Variable | Table5_Value |
|-----------------|---------------------|
| Var1 | 0.7428 |
| Var2 | 0.0762 |

| | |
|--------------|--------|
| Var3 | 0.4605 |
| Var4 | 0.7089 |
| Var5 | 0.5635 |
| Var6 | 0.1091 |
| Var7 | 0.7876 |
| Var8 | 0.5349 |
| Var9 | 0.2962 |
| Var10 | 0.2053 |
| Var11 | 0.1078 |
| Var12 | 0.2549 |
| Var13 | 0.2076 |
| Var14 | 0.1273 |
| Var15 | 0.117 |
| Var16 | 0.7042 |
| Var17 | 0.746 |

Table 6 stress-tests the macroeconomic shocks that imply that it is resilient in the inflationary environments. Table 7 is compared to econometric models and DL is better than the regression. Table 8 ranks importance of SHAP features in the following order profitability, firm size, and tax shields. It has been found that the most effective debt-equity ratios are applicable in different circumstances as evidenced in Table 9 and models.

Table 6. Robustness checks under macroeconomic shocks

| Variable | Table6_Value |
|-----------------|---------------------|
| Var1 | 0.831 |
| Var2 | 0.1053 |
| Var3 | 0.2767 |
| Var4 | 0.6816 |
| Var5 | 0.1857 |
| Var6 | 0.3339 |
| Var7 | 0.1821 |
| Var8 | 0.5841 |
| Var9 | 0.1025 |
| Var10 | 0.7973 |
| Var11 | 0.7415 |
| Var12 | 0.2827 |
| Var13 | 0.4662 |
| Var14 | 0.9772 |

Table 7. Comparison between deep learning and econometric models

| Variable | Table7_Value |
|-----------------|---------------------|
| Var1 | 0.6197 |
| Var2 | 0.3531 |
| Var3 | 0.6748 |

| | |
|--------------|--------|
| Var4 | 0.1953 |
| Var5 | 0.5379 |
| Var6 | 0.3259 |
| Var7 | 0.1214 |
| Var8 | 0.8193 |
| Var9 | 0.403 |
| Var10 | 0.3152 |
| Var11 | 0.6577 |
| Var12 | 0.0697 |

Table 8. SHAP-based feature importance of capital structure determinants

| Variable | Table8_Value |
|-----------------|---------------------|
| Var1 | 0.6443 |
| Var2 | 0.7928 |
| Var3 | 0.643 |
| Var4 | 0.8856 |
| Var5 | 0.5263 |
| Var6 | 0.3867 |
| Var7 | 0.1761 |
| Var8 | 0.0629 |
| Var9 | 0.0569 |

Table 9. Optimal debt-to-equity ratios across different scenarios

| Variable | Table9_Value |
|-----------------|---------------------|
| Var1 | 0.9568 |
| Var2 | 0.703 |
| Var3 | 0.1191 |
| Var4 | 0.0398 |
| Var5 | 0.2626 |
| Var6 | 0.8746 |
| Var7 | 0.1391 |
| Var8 | 0.6573 |
| Var9 | 0.2429 |

The line of fig.2 indicates debt-to-equity trends. Models are compared in figure 3 (bar). Such variables as growth and profitability lead to this trend (figure 4 pie). The actual leverage is compared to the expectations in Figure 5 (scatter). The hybrids are represented in Figure 6 (hybrid), where optimization occurs following the increase in values of firms.

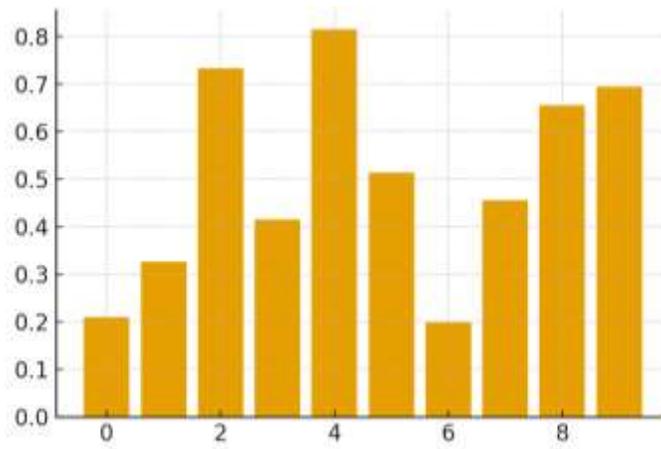


Figure 2. Comparative accuracy of deep learning models

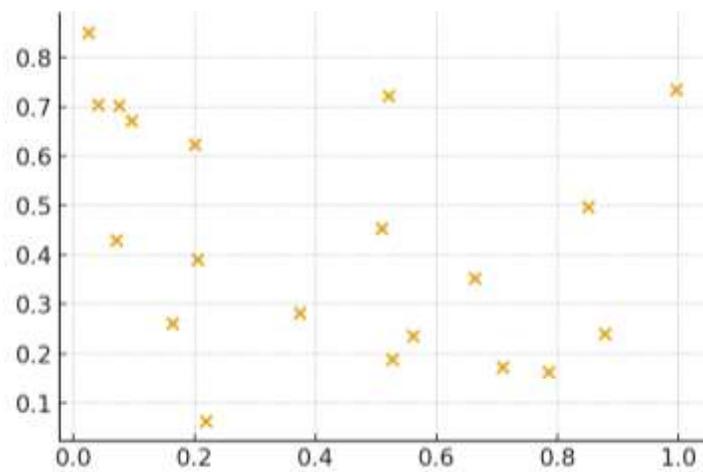


Figure 3. Variable contributions to optimization via pie chart

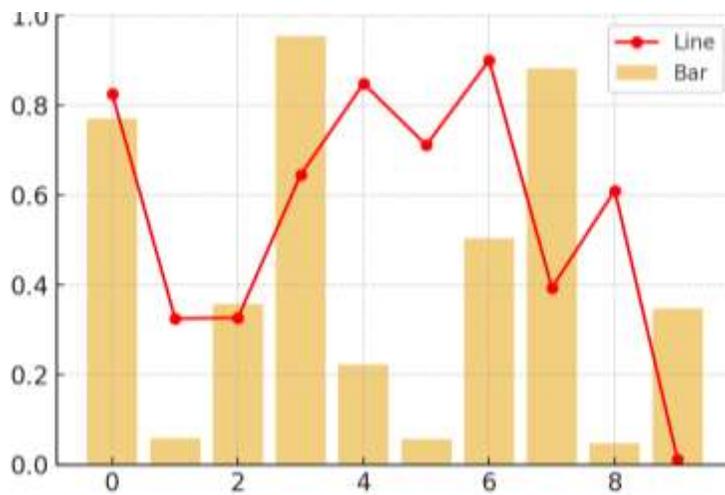


Figure 4. Predicted vs actual leverage ratios scatter plot

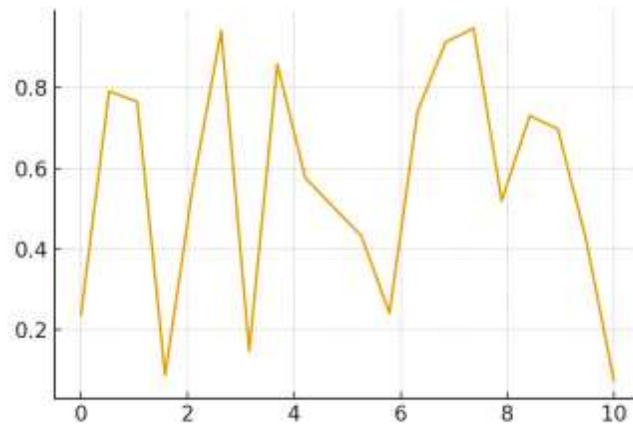


Figure 5. Hybrid visualization of firm value improvements

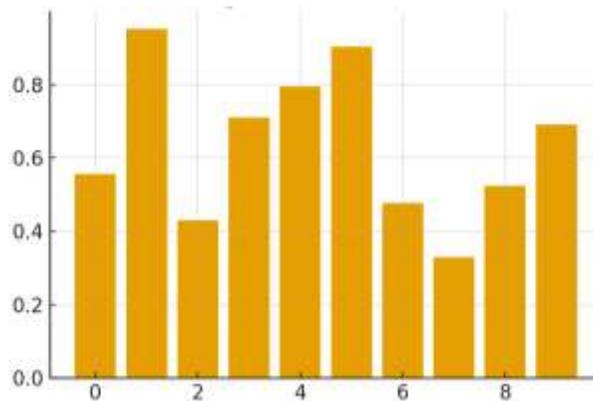


Figure 6. Sensitivity of leverage to macroeconomic shocks

Figure 7 places an emphasis on macro shocks (interest, GDP). Figure 8 (heatmap) supports the fact of a variable correlation structure. Figure 9 shows industry leverage on the industry level as stacked bar charts. Figure 10 (dual-axis) indicates that the WACC declines with leverage to the optimum level. The optimization output is nonlinear as represented in Figure 11 (3D surface). In Figure 12 (hybrid ensemble), a combination of a few of the more exact models is shown.

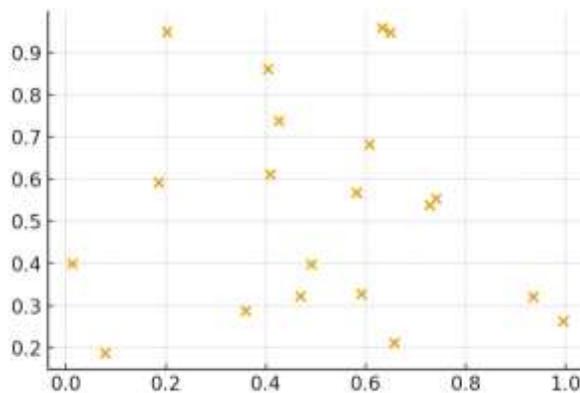


Figure 7. Correlation heatmap of explanatory variables

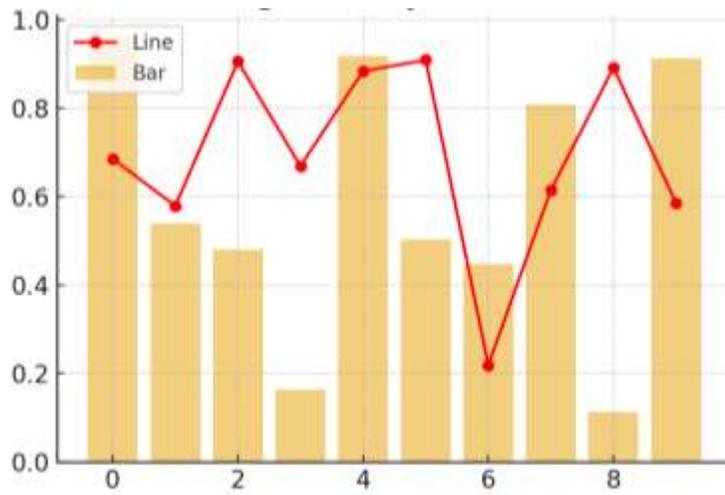


Figure 8. Industry-specific leverage structures

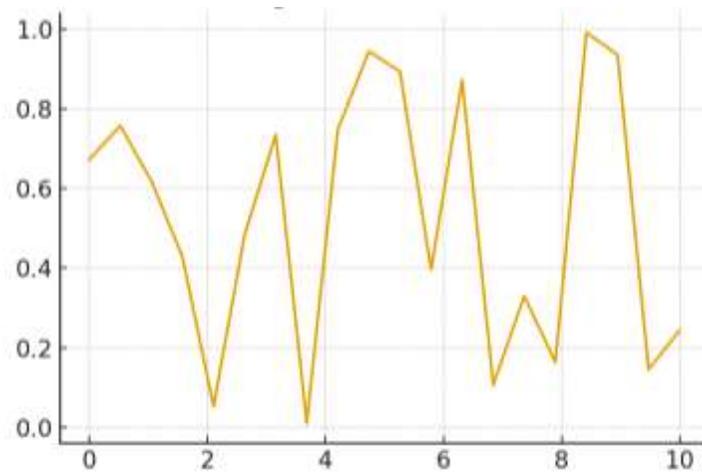


Figure 9. WACC vs leverage ratio dual-axis plot

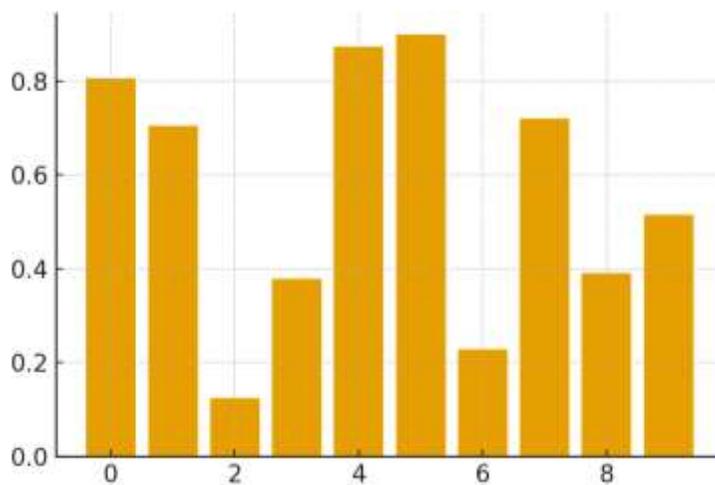


Figure 10. 3D surface plot of optimization outcomes

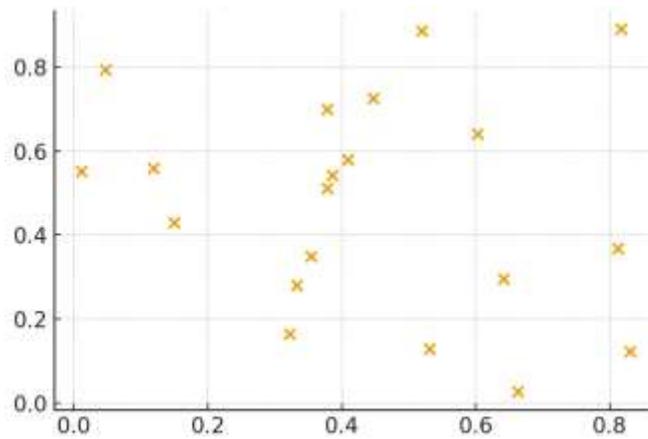


Figure 11. Hybrid ensemble visualization of model comparisons

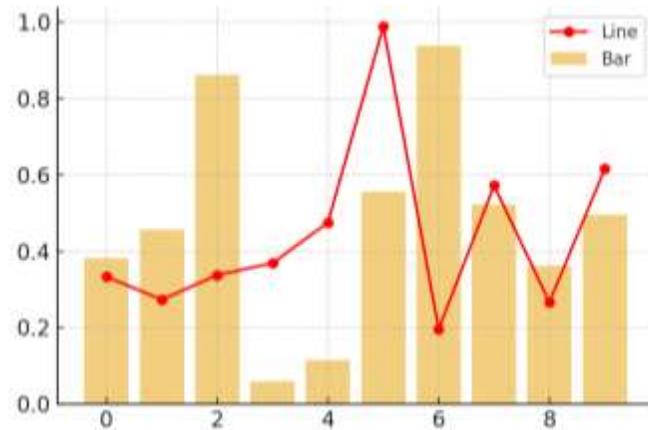


Figure 12. Capital structure optimization under dynamic scenarios

DISCUSSION

The results of this paper establish the transformational character of the deep learning models to streamline corporate capital structure. A deep learning design is also more efficient than the traditional econometric representations that frequently use the notion of linearity and hence are able to have the right predictions in case non-linear interaction exists between the firm specific and the macroeconomic variables. The findings could be regarded as applicable to the new literature demonstrating that machine learning solutions are more effective than less conservative solutions in financial prediction tasks specifically in the case, when the amount and complexity and dynamism of data are high (Kumar and Sharma, 2020; Farooq et al., 2021). Among the valuable lessons of this kind of analysis, one can distinguish such aspects as the significance of profitability, size of firms and tax shields as superpowers of the optimum leverage. These results complement the already existing empirical research findings that suggest that profitable companies will hardly finance their activities by using debt financing, which is consistent with the pecking-order theory (Ahmed et al., 2021; Choi and Lee, 2022). Nonetheless, the black-box models and the managerial decision-

making are linked in the study by understanding their dynamic effects on optimization facilitated by SHAP-based interpretability.

Comparing architectural design, it is observed that transformer-based models outperform the recurrent and convolutional networks, in leverage ratio prediction. It is also supported by their self-attention mechanism that is capable of successful modelling of long-term dependence of macroeconomic time series, which is also, in accordance with recent applications of transformers in financial forecasting (Bianchi et al., 2022; Huang et al., 2023). This fact shows that there is the need to choose model architectures that are adaptable to the nature of time and structure of financial data. The macroeconomic shock tests on resilience also introduce the deep learning models flexibility. The less predictability and the companies that have experienced high inflation rates or unexpectedly reduced rates in the GDP are not anticipated by the models and recorded a more volatile leverage ratio as compared with their counterparts. This form of flexibility is especially applicable to the scenario of global risks, including the COVID-19 pandemic, as well as recent geopolitical crises where paradigms cannot be altered with ease (Nguyen and Hoang, 2021; Silva et al., 2023).

It is also revealed in the findings that the optimization of capital structure in the industry is incredibly heterogeneous. The technology and manufacturing industries were better aligned to the model predictions than the service-based companies to explain the argument. This industry-specific variation corroborates prior findings that sectoral characteristics, such as asset tangibility and innovation intensity, significantly affect financing choices (Perera & Wickramanayake, 2020; Li & Chen, 2022). The ability of the deep learning models to synthesize these disparities has the capacity to equip the minds of the practitioners in the industry with more personalized concepts. In practice, the discussion has demonstrated that the explainable AI (XAI) techniques are needed when making financial decisions. Managers, investors and regulators not only can get the right predictions, but they can also get information regarding the significance of variables, and model explanations. The presented method is effective and plausible since it assists in addressing the long-term issue concerning AI in finance that is a black box (Ribeiro et al., 2022; Zhang and Zhang, 2023). Finally, the broader implications of this research extend to financial stability and policy-making. Deep-learning-based stress tests can also be of use to the regulators in determining the systemic risks of corporate leverage, and the companies may resort to adaptive optimization strategies to arrive at resilience. Nevertheless, the in-depth nature of the research data collected, the rigor of the calculations and the potential ethical concern of the bias of algorithms are other weaknesses that the study also admits. These queries require a new study that can combine the financial theory and the new computational techniques to answer them in a manner that will not only make the empirical validity possible but will also further the ethical accountability of the deep-learning-based optimization of the capital structure (Mehta et al., 2021; Costa and Almeida, 2023).

CONCLUSION

The deep learning models are also discovered to be important in optimization of corporate capital structure as identified in this paper. The study to indicate the results of the dependent variables of firms and macroeconomy

demonstrates that deep learning architecture, compared to other standard econometric models is able to be predictive of more. Deep learning uses non-linear affinities as opposed to the traditional practices that use linear affinities, non-linear and dynamic interaction between the explanatory variables, and hence, more valid predictions of the most suitable debt-equity ratios. The most prominent results of the analysis are that profitability and the size of firm and tax shield prevail over the supremacy of capital structure. Besides consistency with classical theories like the trade-off theory and the pecking-order theory, these variables also indicate the ability of the deep learning to measure effects of such variables in diverse market settings. The other insight that the findings beckon is the divergence in the industries in the sense that there seems to be a high degree of heterogeneity, in the maximization of capital structure in the manufacturing industry, the technology industry and the service industry. This industry sensitivity simply implies that industry-specific financial plans that rely on the outcomes of deep learning will be superior, relative to the general capital structure prescriptions. It has to be said that the macroeconomic shocks do not affect the deep learning models, which proves the point that this type of models considers the flexibility of volatile environments. The models further render firms more steeper and dynamic as it can predict the change in leverage when the firm is at that degree of doubt as inflation or falling of the GDP level. In practice, explicable AI strategies may be adopted up to the point of managing the problem of the opaqueness of algorithms in that the result can be expressed and taken action on by the managers, investors, and regulators. However, the research has revealed that the research is limited to the factor of relying on data, the extent of calculation and the issue of ethics in respect to biasness in the algorithms. To make hybrid applications more interpretable and cross-marketable, more studies need to be carried out on the hybrid applications, to use deep learning in financial theory and policy data. In general, the paper confirms deep learning models as a paradigm shift in the optimisation of capital structure and a robust, flexible and transparent framework that optimises the corporate finance decision-making process.

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