Predicting Option Prices: From the Black-Scholes Model to Advanced Machine Learning Methods

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Introduction

Financial markets employ various sophisticated instruments to manage risk, enhance returns, and speculate on asset prices. Among these instruments, derivatives—financial contracts deriving their value from underlying assets such as stocks, bonds, indices, or commodities—play a pivotal role. Options, a significant class of derivatives, offer traders the right (without obligation) to buy (call) or sell (put) an asset at a specific price, known as the strike price, on (European) or before (American) a predetermined date. Options trading is integral to hedging strategies, portfolio diversification, risk management, and speculative endeavors (Hull, 2014).

A groundbreaking contribution to option pricing theory came with the introduction of the Black-Scholes (B&S) model by Fischer Black and Myron Scholes in 1973 (Black & Scholes, 1973). This model provided a closed-form analytical solution for pricing European-style options, premised upon several critical assumptions: (a) the underlying asset price follows geometric Brownian motion (b) markets are frictionless (absence of transaction costs and taxes) (c) volatility remains constant throughout the life of the option, and (d) the options can only be exercised at maturity (European-style). The B&S model incorporates several variables—underlying asset price (S), strike price (K), time until expiration (T), volatility of the underlying asset (σ), and risk-free interest rate (r). It revolutionized financial economics by introducing rigorous mathematical rigor into the field of derivatives pricing.

However, real-world financial markets seldom adhere strictly to these idealized assumptions. Volatility often varies significantly over the life of the option, market frictions such as transaction costs and taxes exist, and many actively traded options (particularly American-style) allow holders the flexibility to exercise the option at any time before maturity. Consequently, the limitations of the Black-Scholes model have spurred the development and implementation of more sophisticated pricing techniques to capture market dynamics more realistically.

Machine learning (ML) methods have recently become prominent alternatives due to their ability to handle large datasets, uncover complex nonlinear relationships, and adapt dynamically to market conditions. Unlike traditional models, ML algorithms are free from restrictive assumptions about data distribution, making them more suited to capturing the intricacies inherent in real-world financial data. Various ML methods, such as decision trees, random forests, gradient boosting algorithms, and neural networks, offer promising avenues for enhancing option pricing accuracy and reliability (Ke & Yang, 2019; D'Uggento et al., 2025).

Methods

The Black-Scholes Model

The mathematical formulation of the Black-Scholes model for European call options is

$$C = S\,\Phi(d_1) - Xe^{-rT}\Phi(d_2)$$

Where $d_1 = \frac{\log\left(\frac{S}{X}\right) + (r+\sigma^2/2)T}{\sigma\sqrt{T}}$ and $d_2 = d_1 - \sigma\sqrt{T}$.

Here, $\Phi(\cdot)$ denotes the cumulative distribution function (CDF) of the standard normal distribution, corresponding to the probabilistic interpretation underlying the model's assumptions.

Machine Learning Models

Several advanced ML algorithms have been explored in this study:

- **Decision Trees (DT)**: Structured models that use recursive binary partitions of data based on feature values, providing highly interpretable and intuitive predictive insights.
- **Random Forests (RF)**: Ensembles comprising numerous decision trees built from bootstrapped subsets of data, significantly reducing variance, improving prediction robustness, and mitigating overfitting issues.
- **Gradient Boosting (GB)**: Sequential ensembles where new decision trees iteratively correct residuals from preceding trees, thereby progressively improving model accuracy.
- **Neural Networks (NN)**: Inspired by biological neural structures, these consist of interconnected processing nodes organized into layers, highly adept at modeling intricate and nonlinear relationships within complex datasets.

This project specifically leveraged TensorFlow for neural network implementation initially (Part 1), while adopting PyTorch for subsequent exploration (Part 2).

In Part 1, we implement the NN1 model using TensorFlow consisting of an input layer with three nodes (corresponding to the three variables- moneyness, time to expiry and implied volatility), followed by three dense layers having 400 nodes each. The choice of activation function is Leaky ReLU with negative slope 0.01. The final output layer has a ReLU activation function. The model was compiled using the Adam optimizer at a learning rate of 0.01 trained on MSE loss over 1000 epochs.

In Part 2, we design and implement the NN2 model using PyTorch. This model consists of an input layer with 9 nodes. This is because in addition to the above three variables, we also considered polynomial features up to degree two, which results in 3^2 = 9 variables. The NN2 model consists of only a single dense layer of 50 nodes with ReLU activation. To compile the model, we used Stochastic Gradient Descent (SGD) optimizer with learning rate 0.05 trained on MSE loss for 5000 epochs.

Data Description

Data utilized in this analysis were sourced from OptionMetrics via Wharton Research Data Services (WRDS), a comprehensive repository renowned for detailed and high-quality historical financial data. The dataset encompasses extensive records of US-listed options and their corresponding underlying securities. Key variables utilized in the modeling process include:

- Current underlying asset price (S)
- Strike price (K)
- Time remaining until option expiration (T)
- Historical volatility (σ), computed from recent market trading activities

This dataset, covering both European and American option styles, facilitated extensive comparative analyses across diverse market conditions and option characteristics. Due to availability of more data points (~36000), we restrict our analysis to American-style options for the main part of the project relegating the analysis for European-style options with lesser data points (~8000) to the code in the Appendix.

Results

Model Performance Comparison

The predictive performances of the implemented models were evaluated using metrics such as MSE and RMSE providing clear indicators of accuracy against actual market observations:

Part 1: Deep learning vs Black-Scholes:

The neural network model NN1 demonstrated a substantial improvement over the traditional Black-Scholes approach, significantly reducing prediction errors (Ke & Yang, 2019). The NN1 model was able to achieve an MSE of 2053.03 on test data compared to the MSE of 11458.16 obtained using the B&S model. This signifies an approximately six-fold improvement in performance of the NN1 model compared to Black-Scholes.

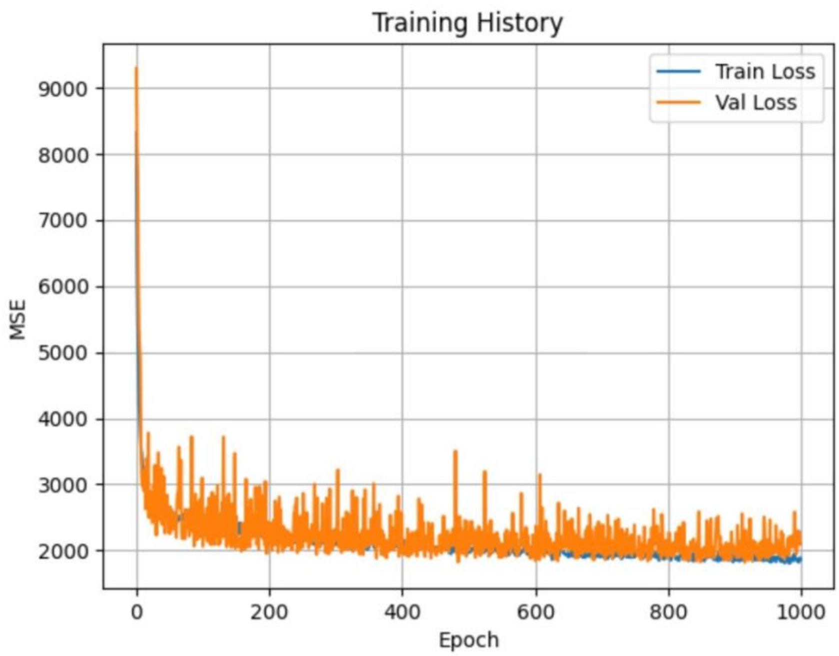

Figure 1: MSE Loss vs Epoch for NN1 model

Part 2: Comparative Analysis Across ML Models:

Random forests exhibited superior performance, achieving the lowest RMSE of 43.88. Neural networks followed closely with an RMSE of 49.68. Gradient boosting performed acceptably with an RMSE of 54.67, while decision trees (single tree) showed relatively inferior performance with RMSE of 60.97.

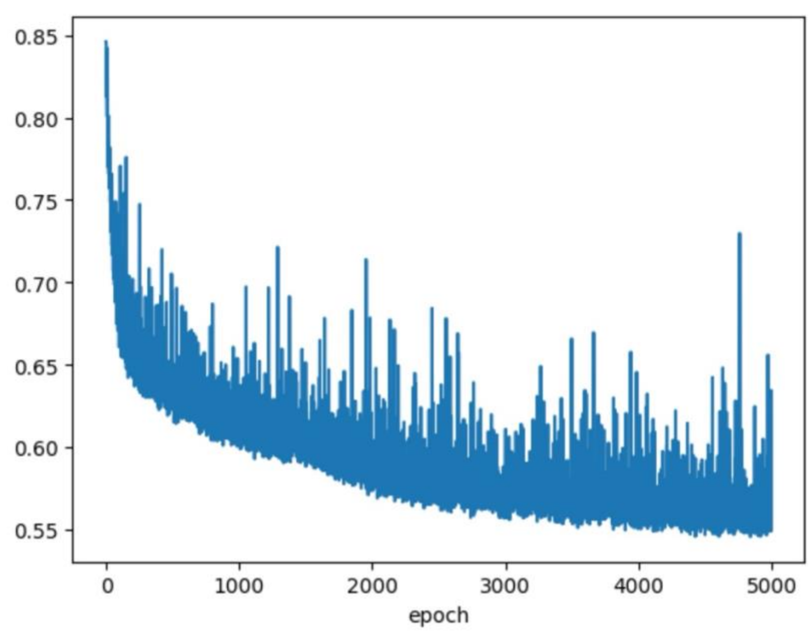

Figure 2: MSE Loss vs Epoch for NN2 model

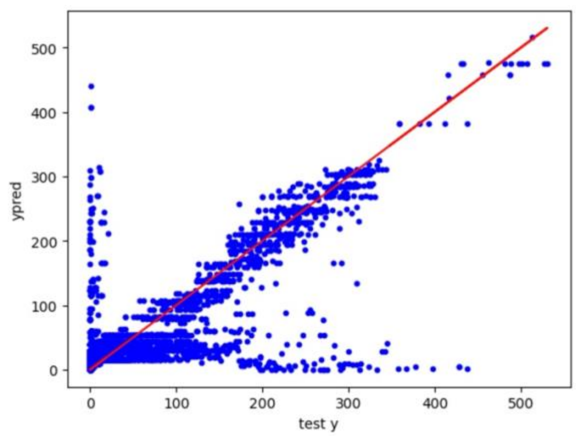

Figure 3: Predicted vs actual values for single tree with 236 bottom nodes

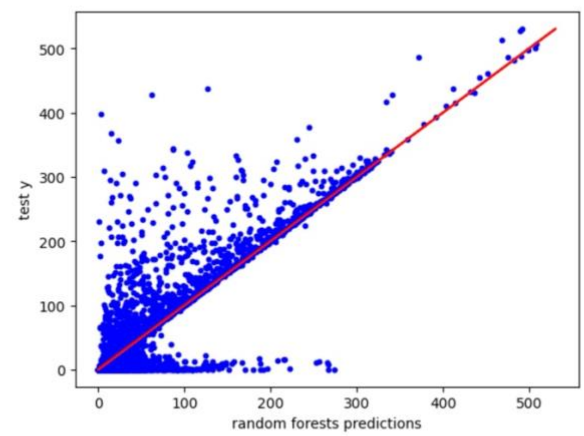

Figure 4: Predicted vs actual values for random forest model with 1000 estimators

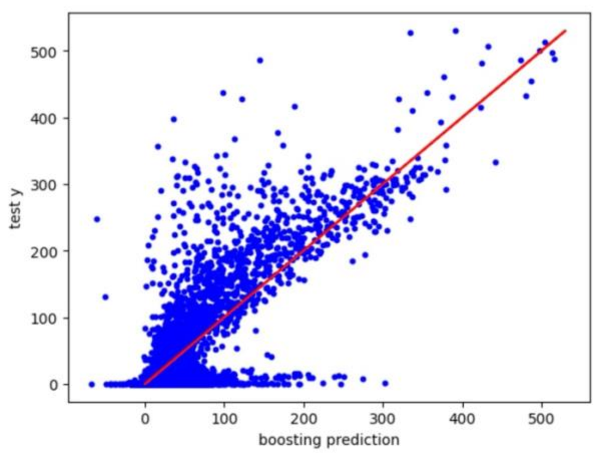

Figure 5: Actual vs predicted values for gradient boosting with 1000 estimators

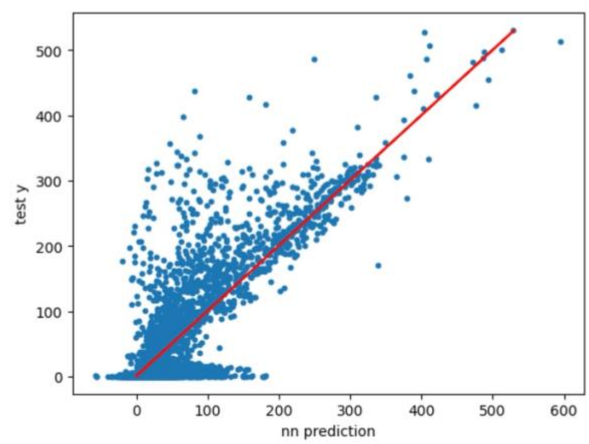

Figure 6: Predicted vs actual values for NN2 model

The models can be ranked according to their performance based on their RMSE values:

1. Random Forest with 1000 estimators (43.88)
2. Neural Network NN2 after 5000 epochs (49.68)
3. Gradient Boosting with 1000 estimators (54.67)
4. Decision Tree with 236 leaf nodes (60.97)

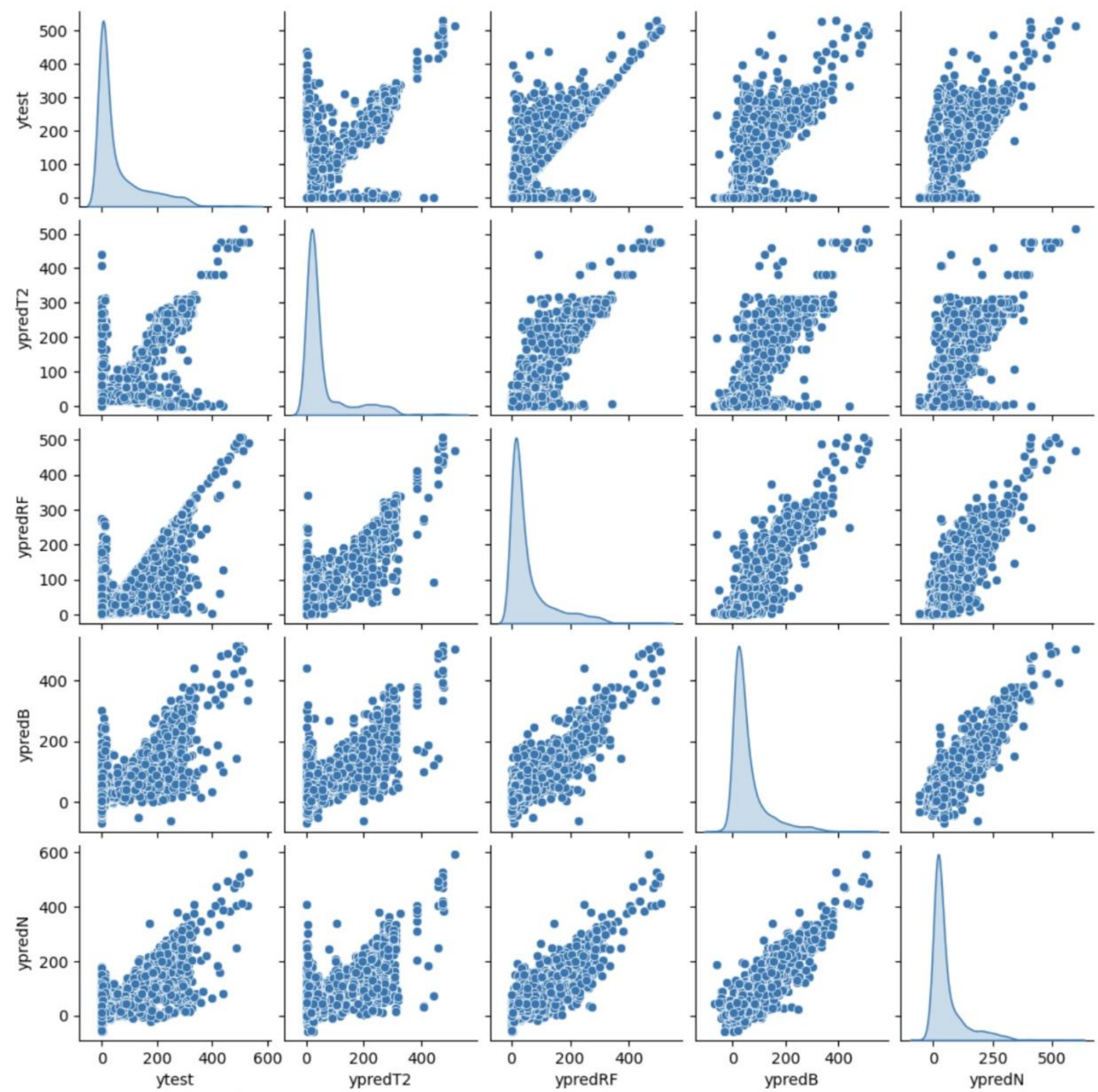

Figure 7: Pairwise comparison plots showing the relationships between actual test option prices (ytest) and predicted option prices from various models: Decision Trees (ypredT2), Random Forests (ypredRF), Gradient Boosting (ypredB), and Neural Networks (ypredN). Each scatter plot illustrates how closely each model's predictions align with actual market prices, with diagonal distributions showing individual prediction distributions. The Random Forest and Neural Network models demonstrate tighter clustering around the ideal diagonal line, indicating superior predictive accuracy compared to Decision Trees and Gradient Boosting.

Observations and Insights

- ML techniques consistently outperformed the traditional B&S model, particularly under dynamic market conditions.
- Random forests showcased exceptional robustness, leveraging ensemble learning to effectively handle complex decision landscapes inherent in financial markets.

- Neural networks displayed notable flexibility, particularly when augmented with comprehensive financial features, indicating their capability in managing extensive, high-dimensional data (D'Uggento et al., 2025).

Conclusion and Future Scope

This comprehensive analysis highlights significant limitations of traditional financial models such as Black-Scholes when confronted with the complexities and dynamics of real-world markets. Conversely, machine learning models, particularly random forests and neural networks, demonstrate significant potential due to their accuracy, flexibility, and robustness.

Future research could benefit from investigating advanced deep learning architectures, including recurrent neural networks (RNNs) and transformer-based models, capable of capturing temporal dependencies and sequential market dynamics. Further exploration into directly modeling bid-ask spreads would also enhance insights into liquidity dynamics and market microstructure.

References

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