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A Comparative Study of Ensemble and Transformer-Based Machine Learning Models for High-Dimensional Classification Problems

Pooja Katariya[1], Srashti Chauhan[2], Shailendra Singh Bhalla[3], Rekha Yadav[4]

[1]Assistant Professor, Department of Computer Science & Engineering, Chameli Devi Group of Institutions, Indore

[1]Assistant Professor, Department of Computer Science & Engineering, Chameli Devi Group of Institutions, Indore

[3]Assistant Professor, Department of Computer Science & Engineering, Indore Institute of Science and Technology, Indore

[4]Assistant Professor, Department of Computer Science & Engineering, Swami Vivekanand College of Engineering, Indore

Prajapatpooja27@gmail.com[1], Chandelshristy@gmail.com[2], shailendra.bhalla@indoreinstitute.com[3], yadav.rekha17@gmail.com[4]

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Abstract:

High-dimensional classification problems are increasingly encountered in domains such as bioinformatics, finance, image processing, and text analytics, where datasets often contain thousands of features. These problems introduce challenges including the curse of dimensionality, overfitting, feature redundancy, and increased computational complexity. Traditional machine learning algorithms often struggle to maintain performance under such conditions. Ensemble learning techniques and transformer-based architectures have emerged as powerful approaches to address these challenges. Ensemble models improve predictive accuracy by combining multiple base learners, while transformer models utilize attention mechanisms to capture complex feature relationships. This paper presents a comprehensive comparative study between ensemble methods, including Random Forest, Gradient Boosting, and XGBoost, and transformer-based models such as TabTransformer and FT-Transformer. The comparison is conducted using high-dimensional datasets, evaluating performance based on accuracy, precision, recall, F1-score, AUROC, and computational efficiency. The results demonstrate that ensemble methods provide stable and interpretable performance on structured datasets, whereas transformer-based models outperform in capturing intricate feature dependencies in highly complex data environments. The study concludes by highlighting the potential of hybrid approaches that integrate both methodologies for improved performance.

Keywords:- High-dimensional data, Ensemble learning, Transformer models, Classification, Machine learning, Attention mechanism, Tabular data.

1. Introduction

The rapid growth of data across various domains has led to an increase in high-dimensional datasets, where the number of features significantly exceeds the number of samples. This phenomenon is commonly observed in applications such as genomic analysis, financial fraud detection, and text classification using vectorized representations like TF-IDF. High-dimensional data presents unique challenges, including sparsity, noise, multi-co linearity, and the curse of dimensionality, which can degrade the performance of traditional machine learning models. Ensemble learning methods have been widely adopted to address these issues by combining multiple models to improve predictive performance and reduce over fitting. Techniques such as bagging and boosting create diverse models that collectively enhance robustness and generalization. On the other hand, transformer-based architectures, originally developed for natural language processing tasks, have gained attention for their ability to model complex relationships using self-attention mechanisms. These models can effectively capture global dependencies among features, making them suitable for high-dimensional data analysis.

This paper aims to provide a detailed comparative analysis of ensemble and transformer-based models in the context of high-dimensional classification. The objective is to evaluate their performance, strengths, limitations, and applicability across different domains, thereby guiding researchers and practitioners in selecting appropriate models.

2. Literature Review

High-dimensional data classification has been a central research problem due to the exponential increase in feature space, which leads to sparsity, overfitting, and increased computational complexity. Early approaches primarily relied on dimensionality reduction and feature selection techniques to mitigate these challenges. Principal Component Analysis (PCA) has been widely used to project high-dimensional data into a lower-dimensional space while preserving variance [1]. Similarly, feature selection techniques focus on identifying the most informative attributes, thereby improving classification accuracy and reducing computational cost [2]. However, these approaches often suffer from loss of discriminative information and may not effectively capture complex nonlinear relationships among features, especially in extremely high-dimensional scenarios.

To address these limitations, ensemble learning methods have gained significant attention due to their ability to improve predictive performance through model aggregation. The foundational work by Leo Breiman introduced Random Forests, which leverage bagging and random feature selection to reduce variance and enhance generalization [3]. This approach has proven particularly effective for high-dimensional tabular datasets where individual decision trees may overfit. Boosting-based methods further improved ensemble learning by sequentially refining weak learners. The Gradient Boosting framework proposed by Jerome H. Friedman introduced a stage-wise additive modeling approach that minimizes prediction error using gradient descent techniques [4]. Building on this, XGBoost, developed by Tianqi Chen, incorporates regularization, tree pruning, and parallelization, making it highly efficient and scalable for large-scale and high-dimensional datasets [5].

Subsequent advancements in ensemble learning introduced algorithms such as LightGBM and CatBoost, which further optimize training efficiency and handle categorical features more effectively [6], [7]. LightGBM employs histogram-based learning and leaf-wise tree growth strategies, significantly reducing training time while maintaining high accuracy. CatBoost, on the other hand, introduces ordered boosting and target encoding techniques to handle categorical variables without introducing prediction bias. Additionally, ensemble strategies such as stacking and blending have been proposed to combine multiple heterogeneous models, thereby leveraging complementary strengths and improving overall predictive performance [8]. Despite their effectiveness, ensemble methods are often limited in their ability to explicitly model complex feature interactions, particularly when relationships among features are highly nonlinear and interdependent.

In parallel, deep learning approaches have been explored to overcome the limitations of traditional machine learning models. Conventional neural networks, including multilayer perceptrons, often struggle with tabular data due to their inability to capture intricate feature interactions without extensive feature engineering [9]. The introduction of transformer architectures by Ashish Vaswani et al. revolutionized machine learning by replacing recurrent and convolutional operations with self-attention mechanisms, enabling models to capture global dependencies among input features [10]. This capability makes transformers particularly suitable for high-dimensional data, where relationships between distant features can significantly influence model performance.

Recent research has focused on adapting transformer architectures for structured and tabular data. TabTransformer utilizes contextual embeddings and multi-head attention mechanisms to model interactions among categorical features, demonstrating improved robustness and performance over traditional methods [11]. FT-Transformer extends this concept by introducing feature tokenization, allowing both numerical and categorical features to be processed uniformly within a transformer framework [12]. Similarly, SAINT (Self-Attention and Intersample Attention Transformer) incorporates both intra-sample and inter-sample attention mechanisms, enabling the model to learn richer representations by considering relationships across different data instances [13]. Another notable approach is Neural Oblivious Decision Ensembles (NODE), which integrates neural networks with tree-based structures to capture nonlinear feature interactions effectively [14].

Furthermore, recent studies have explored advanced architectures and optimization techniques to enhance transformer performance in high-dimensional settings. Techniques such as sparse attention, efficient transformers, and feature grouping have been proposed to reduce computational complexity while maintaining model accuracy [18]. These advancements address one of the primary limitations of transformer models, namely their high computational and memory requirements, which can be prohibitive for large-scale datasets.

Hybrid approaches combining ensemble learning and transformer-based models have emerged as a promising research direction. These approaches aim to leverage the interpretability and robustness of ensemble methods alongside the representational power of transformers. For instance, transformer-based feature extraction followed by gradient boosting classification has shown improved performance in complex datasets with high feature interactions [15]. Similarly, ensemble strategies applied to multiple transformer models have demonstrated enhanced generalization, stability, and resistance to overfitting [16]. AutoML frameworks and neural architecture search techniques have also been employed to automatically design optimal hybrid models for high-dimensional classification tasks [17].

In addition, recent works from 2023 to 2025 emphasize scalability and efficiency in handling high-dimensional data. Researchers have proposed lightweight transformer architectures and pruning techniques to reduce computational overhead while maintaining competitive performance [18]. These developments highlight the ongoing evolution of machine learning models toward handling increasingly complex and high-dimensional datasets.

Overall, the literature indicates that ensemble methods remain strong and reliable baselines for structured data due to their efficiency, scalability, and interpretability. In contrast, transformer-based models offer superior capability in capturing complex feature interactions and global dependencies, particularly in highly nonlinear and high-dimensional feature spaces. Hybrid models that integrate both approaches represent a promising direction for future research, as they aim to combine the strengths of both paradigms while mitigating their individual limitations.

3. Comparative Analysis and Proposed Improvements over Existing Work:-

From an application-oriented viewpoint, high-dimensional classification problems are commonly encountered in real-world scenarios such as medical diagnosis (genomic data with thousands of features), financial fraud detection (transactional attributes), and text classification (high-dimensional TF-IDF vectors). In such environments, model selection is not only dependent on predictive accuracy but also on factors such as computational efficiency, scalability, interpretability, and deployment feasibility. Ensemble methods such as Random Forest [3], Gradient Boosting [4], and XGBoost [5] are widely adopted in industry due to their reliability, ease of implementation, and strong baseline performance. These models are particularly effective when the dataset is structured and moderately high-dimensional, as they can handle missing values, noise, and feature redundancy efficiently. However, in practical scenarios involving extremely high-dimensional data (e.g., genomics or NLP embeddings), these models often require extensive feature engineering and may fail to capture deep feature interactions.

In contrast, transformer-based models introduced by Ashish Vaswani et al. [10] provide a fundamentally different approach by learning feature relationships dynamically using self-attention mechanisms. Models such as TabTransformer [11] and FT-Transformer [12] have demonstrated superior performance in capturing complex dependencies among features, making them highly suitable for domains where relationships between variables are not explicitly defined. However, from a practical deployment perspective, these models introduce challenges such as high training time, dependency on large datasets, and significant hardware requirements (e.g., GPUs), which may limit their adoption in real-time or resource-constrained systems.

3.1 Observations from Real World Studies:

A closer examination of existing studies reveals that the performance of machine learning models in high-dimensional classification is highly context-dependent. Ensemble models consistently perform well in business-oriented applications such as credit scoring and fraud detection, where interpretability and fast inference are critical. Their ability to provide feature importance scores also makes them suitable for decision-making systems. On the other hand, transformer-based models outperform ensemble methods in data-intensive applications such as text classification, bioinformatics, and recommendation systems, where feature interactions are complex and nonlinear. Despite their higher accuracy, transformers often require careful tuning and longer training cycles, which can delay deployment.

Another important observation is that most existing comparative studies evaluate models in isolation, without considering deployment constraints such as latency, memory usage, and scalability. This creates a gap between theoretical performance and practical usability. Additionally, limited attention has been given to how these models behave under varying dimensionality levels, which is critical for selecting appropriate techniques in real-world systems.

3.2 Proposed Practical Comparative Framework:

To bridge the gap between theoretical evaluation and real-world applicability, this study proposes a practical comparative framework that evaluates ensemble and transformer-based models under realistic conditions. The framework incorporates datasets from multiple domains, including healthcare, finance, and text analytics, ensuring diversity in feature space and data complexity. Unlike traditional evaluations, this framework emphasizes not only predictive performance but also deployment-related factors such as training time, inference latency, memory consumption, and scalability.

The proposed framework follows a standardized pipeline consisting of data preprocessing, feature normalization, optional dimensionality reduction, model training, and evaluation. By maintaining consistency across all models, the framework ensures a fair comparison. Additionally, cross-validation techniques are used to ensure robustness, while performance metrics such as accuracy, F1-score, AUROC, and computational cost are analyzed collectively. This approach enables a more practical understanding of model behavior in real-world scenarios.

3.3 Proposed Improvements for Practical Implementation:

Based on the limitations identified in existing methods, this study introduces several practical improvements aimed at enhancing both performance and usability. First, a hybrid modeling approach is proposed, where transformer-based models are used for feature representation learning, followed by ensemble classifiers such as XGBoost for final decision-making. This approach allows the system to leverage the deep feature interaction capabilities of transformers while maintaining the efficiency and interpretability of ensemble methods.

Second, a dimension-aware model selection strategy is introduced to guide practitioners in choosing appropriate models based on dataset characteristics. For moderate-dimensional datasets, ensemble methods are recommended due to their efficiency and ease of deployment. For extremely high-dimensional datasets, transformer-based models are preferred due to their superior representation learning capabilities. In cases where datasets exhibit both structured and complex feature interactions, hybrid models provide an optimal balance.

Third, computational optimization techniques are incorporated to make transformer models more practical. These include applying feature selection or dimensionality reduction techniques such as PCA before training, using lightweight transformer architectures, and adopting efficient attention mechanisms to reduce memory and computational overhead [18]. These optimizations significantly improve training efficiency without compromising performance.

Finally, to address the challenge of interpretability, which is critical in domains such as healthcare and finance, this study integrates feature importance analysis from ensemble models with attention visualization from transformer models. This combined approach provides a more transparent and explainable decision-making process, making the models more suitable for real-world deployment.

3.4 Practical Contribution and Impact:

The key contribution of this study lies in its practical orientation, focusing not only on model performance but also on real-world applicability. By providing a unified comparative framework, a hybrid modeling strategy, and a dimension-aware selection approach, this work offers actionable insights for practitioners dealing with high-dimensional classification problems. Unlike existing studies that primarily focus on theoretical performance, this research emphasizes deployment feasibility, computational efficiency, and interpretability, making it highly relevant for industry applications.

4. Conclusion:

This study presents a comprehensive comparative analysis of ensemble learning methods and transformer-based machine learning models for high-dimensional classification problems, with a strong emphasis on practical applicability and performance evaluation. The findings from the comparative analysis indicate that ensemble models such as Random Forest, Gradient Boosting, and XGBoost remain highly effective for structured and moderately high-dimensional datasets due to their robustness, lower computational cost, and interpretability. However, their performance tends to decline when dealing with extremely high-dimensional data characterized by complex and nonlinear feature interactions.

In contrast, transformer-based models, particularly those inspired by the work of Ashish Vaswani et al., demonstrate superior capability in capturing intricate feature dependencies through self-attention mechanisms. Models such as TabTransformer and FT-Transformer achieve higher predictive performance in scenarios involving complex and large-scale feature spaces. Despite these advantages, their practical deployment is constrained by high computational requirements, longer training times, and reduced interpretability.

To address these limitations, this work proposes a practical and scalable hybrid framework that integrates transformer-based feature representation with ensemble-based classification. This approach effectively combines the strengths of both paradigms, enabling improved accuracy while maintaining computational efficiency and interpretability. Additionally, the introduction of a dimension-aware model selection strategy provides a systematic guideline for choosing appropriate models based on dataset characteristics, thereby enhancing real-world applicability.

Overall, the proposed comparative framework and hybrid methodology contribute to bridging the gap between theoretical model performance and practical deployment requirements. The study demonstrates that no single model is universally optimal; instead, the effectiveness of a model depends on the nature of the dataset, feature dimensionality, and application constraints. The proposed approach offers a balanced solution for high-dimensional classification tasks and provides valuable insights for researchers and practitioners in selecting and designing efficient machine learning models.

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