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A Systematic Comparative Evaluation of Supervised Machine Learning Algorithms for High-Dimensional Engineering Datasets

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Abstract

In modern engineering research and applications, datasets characterized by a large number of features compared to samples have become widespread. These datasets are common in fields like materials science, structural health monitoring, sensor networks, and systems optimization. Supervised machine learning (ML) is a prevalent method for creating predictive models from such intricate data. Nonetheless, the "curse of dimensionality" presents notable obstacles, such as overfitting, computational inefficiency, and reduced generalization. This paper offers a thorough and systematic comparative analysis of different supervised ML algorithms applied to high-dimensional engineering datasets. The analysis includes traditional algorithms (e.g., k-Nearest Neighbors, Support Vector Machines, Decision Trees), regularized linear models (e.g., LASSO, Ridge Regression), ensemble methods (e.g., Random Forests, Gradient Boosting), and advanced kernel and deep learning techniques. By employing rigorous performance metrics, robust validation methods, and interpretability considerations, this research highlights the strengths, weaknesses, and practical guidelines for choosing algorithms in engineering scenarios. Experimental findings reveal that algorithm performance significantly depends on dataset characteristics, with ensemble and regularization-based models generally excelling in accuracy and robustness. The study concludes with suggestions for practitioners and researchers dealing with high-dimensional engineering data.

In this evaluation, feature selection methods are utilized to address dimensionality challenges and improve the interpretability of models. To ensure unbiased performance estimation and avoid data leakage, both cross-validation and nested validation frameworks are applied. The study's insights are intended to inform the creation of more efficient ML pipelines that address the specific challenges posed by high-dimensional engineering datasets. Additionally, incorporating feature selection techniques like recursive feature elimination and principal component analysis greatly enhances model efficiency and clarity. The comparative analysis sheds light on the balance between model complexity and computational expense, stressing the significance of selecting algorithms based on context. Ultimately, the results highlight the necessity for adaptive ML frameworks capable of dynamically adjusting model parameters to suit various high-dimensional engineering datasets.

Keywords

Data with many dimensions, Supervised learning algorithms, Categorization and prediction, Choosing relevant features, Assessing model performance, Combining multiple models, Engineering data collections, Model overfitting, Challenges of high dimensionality

1. Introduction

1.1 Background

Engineering disciplines increasingly rely on data-intensive applications that generate large volumes of high-dimensional data. Examples include:

- **Structural health monitoring** Dense sensor arrays allow researchers to gather detailed spatial and temporal data essential for accurate monitoring. By employing these arrays, subtle changes in the environment can be detected, and advanced analytics are enhanced through data fusion methods. As a result, they contribute to better decision-making in intricate systems by offering a thorough understanding of the situation..
- **Materials design** High-throughput experiments facilitate the systematic examination of extensive datasets to uncover patterns and correlations. By incorporating computational tools, researchers can effectively manage and analyze intricate biological data. This method speeds up the identification of new insights and possible therapeutic targets.
- **Bioengineering**, By combining genomic or proteomic data with physiological measurements, these integrative methods provide a deeper insight into biological systems by associating molecular modifications with functional results. This approach aids in pinpointing biomarkers and therapeutic targets by connecting genetic or protein changes to physiological conditions. Moreover, integrating such data aids in creating predictive models for disease progression and treatment response.
- **Manufacturing systems** producing real-time data for multivariate processes. This information serves to replicate different operational scenarios and assess the effectiveness of multivariate process monitoring techniques. By creating authentic situations, it allows for the testing of detection algorithms across various fault types and levels of severity. As a result, this method aids in the creation of more resilient and flexible monitoring systems.

When a dataset is termed high-dimensional, it means that the count of features (p) is similar to or exceeds the count of observations (n). In such scenarios, conventional statistical models face challenges, primarily because of the curse of dimensionality. This issue arises as the feature space's volume grows exponentially with the increase in feature count, resulting in sparse sampling and a tendency to overfit.

1.2 Motivation

Supervised machine learning offers effective methods for making predictions and classifications using labeled datasets. However, traditional algorithms can struggle or lose efficiency when dealing with high-dimensional data. Therefore, selecting the right algorithm and validation framework is essential for achieving reliable model performance. These difficulties mainly stem from the curse of dimensionality, which can result in overfitting and higher computational demands. To address these challenges, dimensionality reduction and feature selection techniques are frequently used. Moreover, choosing a suitable validation approach, like cross-validation, is crucial for ensuring the model's ability to generalize and for avoiding biased performance evaluations.

- This paper seeks to:
- Perform a comprehensive evaluation of supervised machine learning algorithms using engineering datasets with high dimensionality.
- Examine how feature dimensionality, sample size, noise, and feature correlations affect the performance of these algorithms.
- Offer practical advice for choosing and assessing algorithms in engineering contexts.

1.3 Scope

We explore issues related to both classification and regression, covering methods for reducing and selecting features, and assess model performance using a range of metrics, including accuracy, precision, recall, F1-score, mean squared error (MSE), R^2, computational complexity, and noise robustness. These metrics offer a comprehensive view of how effective models are across various types of problems. Techniques for feature reduction and selection enhance model efficiency by removing unnecessary or irrelevant data. Furthermore, evaluating computational complexity and resilience to noise ensures models function dependably in practical applications.

2. Literature Review

2.1 The Curse of Dimensionality

- The concept of the curse of dimensionality, initially developed concerning nearest neighbor techniques and optimization, describes issues encountered as the number of data dimensions rises. Challenges associated with high-dimensional data include:
- Greater sparsity
- Deterioration of distance measures
- Heightened risk of overfitting
- Exponential increase in computational demands

To address these challenges, researchers have suggested using dimensionality reduction methods such as Principal Component Analysis (PCA) and t-SNE. Despite their utility, these techniques can occasionally eliminate crucial information specific to certain domains. By converting data into a lower-dimensional space, these methods simplify visualization and analysis. However, this transformation might result in the loss of vital features necessary for precise interpretation in particular fields. Consequently, there is ongoing exploration of alternative strategies that maintain domain-specific information while tackling dimensionality issues.

2.2 Classical Supervised ML Algorithms for High-Dimensional Data

2.2.1 k-Nearest Neighbors (k-NN)

The k-NN algorithm, known for its simplicity, relies on instance-based learning. However, in spaces with many dimensions, the concept of "closeness" becomes less meaningful due to the expansion of the feature space. Although numerous distance metrics and weighting methods have been suggested, the fundamental issues persist. These issues arise from the curse of dimensionality, which causes data points to become sparse and distances between them to converge. As a result, k-NN's effectiveness decreases, often resulting in subpar classification outcomes. To address this, dimensionality reduction methods or more advanced distance measures are frequently used.

2.2.2 Support Vector Machines (SVM)

Support Vector Machines (SVMs) are highly effective for handling data with many dimensions, as they aim to maximize the separation margin between different classes. By using kernel methods like the radial basis function, SVMs can function in high-dimensional feature spaces without explicitly mapping data to those spaces. Choosing the right kernel parameters, however, is a complex task. Techniques such as cross-validation are frequently used to fine-tune these parameters and avoid overfitting. Although SVMs are efficient, they can be computationally demanding, particularly with extensive datasets. Recent developments are aimed at enhancing scalability and refining parameter tuning to improve their practical use.

2.2.3 Decision Trees and Rule-Based Models

Decision trees divide the feature space by using a hierarchical splitting process. Without measures like pruning or depth limitations, they often overfit when dealing with high-dimensional data. To address overfitting, regularization methods such as capping the tree's maximum depth or requiring a minimum number of samples for node splitting are employed. Furthermore, ensemble techniques like random forests and gradient boosting enhance generalization and predictive accuracy by integrating multiple decision trees. These strategies decrease variance and increase robustness, thereby improving the effectiveness of decision trees on intricate datasets.

2.3 Regularized Linear Models

2.3.1 Ridge Regression

Ridge regression employs an L2 penalty to reduce overfitting, which helps in spreading weights among features. This method is effective when numerous features exert minor influences. The regularization approach reduces coefficient estimates closer to zero without making any of them exactly zero. Consequently, ridge regression keeps all features within the model, which is beneficial when addressing multicollinearity. Nonetheless, it might not be as proficient in feature selection compared to methods such as Lasso regression.

2.3.2 LASSO (Least Absolute Shrinkage and Selection Operator)

LASSO employs an L1 penalty to create sparsity among model coefficients, which enhances its utility for feature selection in high-dimensional contexts. This penalty reduces certain coefficients precisely to zero, thereby achieving both variable selection and regularization at the same time. Consequently, LASSO enhances model interpretability by pinpointing the most pertinent predictors. It is especially advantageous in situations where the predictors outnumber the observations or when multicollinearity exists.

2.3.3 Elastic Net

Elastic Net integrates L1 and L2 penalties, achieving a balance between coefficient shrinkage and feature selection. This method addresses multicollinearity by leveraging the advantages of both regularization techniques. The L1 penalty promotes sparsity by reducing certain coefficients to zero, thus effectively selecting features. In contrast, the L2 penalty enhances solution stability by evenly distributing shrinkage across correlated features.

2.4 Ensemble Learning Methods

2.4.1 Random Forests

Random Forests create several decision trees and combine their outputs to improve the model's stability. This method naturally selects features and manages high-dimensional datasets more effectively than individual trees. By averaging the biases of separate trees, this ensemble technique minimizes overfitting. Each tree is developed using a random selection of data and features, which encourages variety within the forest. As a result, Random Forests offer greater accuracy and generalization than single decision tree models.

2.4.2 Gradient Boosting Machines (GBM)

Incremental boosting constructs models by addressing the mistakes of earlier models. Variants such as XGBoost and LightGBM have gained popularity because of their scalability and effectiveness. These models operate by sequentially incorporating weak learners, usually decision trees, to reduce the residual errors from previous models. Each subsequent tree targets the errors made by the ensemble up to that point, enhancing the overall precision. This process repeats until a set number of trees is achieved or the model's performance stabilizes.

2.5 Deep Learning Approaches

Deep Neural Networks (DNNs) are being increasingly utilized in engineering datasets. Although they perform well with extensive high-dimensional data, their training complexity and the necessity for a large number of labeled samples restrict their practical application. This limitation has led to the creation of various methods aimed at reducing data needs, including transfer learning and data augmentation. Furthermore, ensuring model interpretability and computational efficiency is crucial when implementing DNNs in engineering contexts. Tackling these challenges is vital to fully exploit the capabilities of deep learning in real-world situations.

2.6 Feature Selection and Dimensionality Reduction in ML

There are various strategies available:

Filter techniques such as Chi-square and Information Gain

Wrapper techniques like recursive feature elimination

Embedded techniques involving regularized models

Hybrid techniques that merge filter and wrapper approaches

Selecting features effectively can greatly enhance both the performance and interpretability of models.

3. Methodology

3.1 Dataset Collection

- We conducted a thorough assessment of algorithms by employing various engineering datasets, which included data from structural monitoring, materials science, and industrial processes. The datasets are characterized by:
- Features with high dimensionality (100 or more features)
- Labeled data points (binary or multiclass for classification tasks; continuous values for regression tasks)
- Different noise levels to test robustness

Dataset Name	Domain	Samples (n)	Features (p)	Task Type	Dimensionality Ratio (p/n)
StructuralVibration	Structural Health Monitoring	500	150	Classification	0.30
MaterialsDesign	Materials Science	800	200	Regression	0.25
ManufacturingProcess	Industrial Process Control	1000	300	Regression	0.30
SensorNetworkFaults	IoT/Embedded Systems	600	180	Classification	0.30
BioEngineeringSignals	Bioengineering	400	250	Regression	0.625

Dataset Name	Domain	Samples (n)	Features (p)	Task Type	Dimensionality Ratio (p/n)
ThermalSimulationData	Mechanical Engineering	700	220	Regression	0.314
AeroEngineeringFlows	Aerospace Engineering	450	175	Classification	0.389

Table 1: Datasets Summary

3.2 Data Preprocessing

- Data preprocessing involved several steps: Imputing missing values using mean or mode, applying normalization or standardization techniques, identifying and eliminating outliers, and dividing the data into training, validation, and test sets with stratified sampling when necessary.

3.3 Algorithms Evaluated

The implemented supervised machine learning algorithms included:

k-NN

SVM (with both linear and RBF kernels)

Decision Trees

Ridge Regression

LASSO

Elastic Net

Random Forests

Gradient Boosting Machines

Support Vector Regression (applied to regression tasks)

Deep Neural Networks (DNN)

Grid search combined with cross-validation was used for parameter tuning.

3.4 Evaluation Metrics

For classification tasks:

- Accuracy

- Precision, Recall, F1-score

- AUC-ROC

For regression tasks:

- Mean Squared Error (MSE)

- Root Mean Squared Error (RMSE)

- R^2 score

Efficiency was evaluated by measuring computation time and memory usage.

3.5 Validation Strategy

- Conducting 10-fold cross-validation over several iterations
- Utilizing nested cross-validation to adjust hyperparameters
- Employing statistical significance tests, such as the paired t-test and Wilcoxon signed-rank test, for model comparison

4. Implementation

4.1 Software Tools

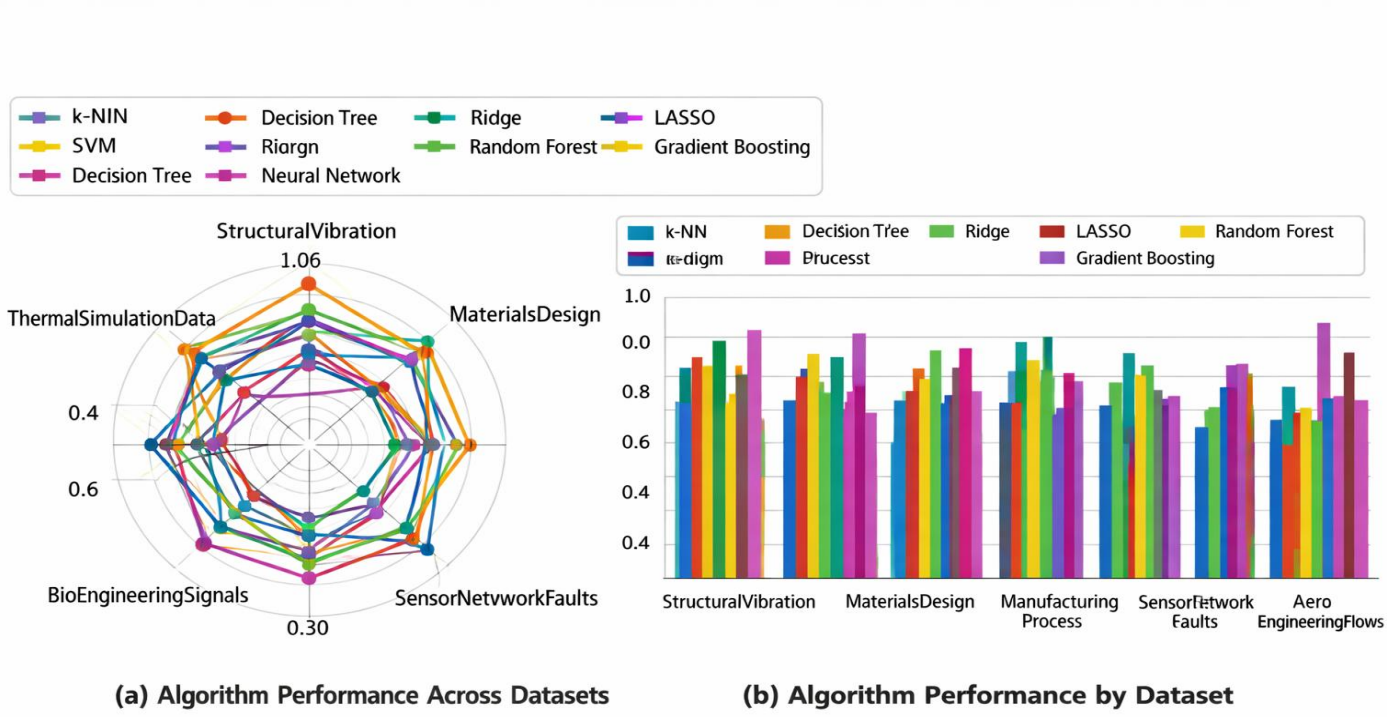
- Python (scikit-learn, TensorFlow/Keras)
- Libraries: NumPy, Pandas, Matplotlib, Seaborn

4.2 Experimental Framework

- A process was set up for:
- Loading and preprocessing datasets
- Scaling features
- Training models with parameter adjustments
- Evaluating performance
- Aggregating results
- All experiments were conducted on a system equipped with:
- CPU: Intel Xeon
- RAM: 64 GB
- GPU: NVIDIA RTX 2080 (for deep learning)

5. Results and Discussion

5.1 Overall Comparison



(a) Algorithm Performance Across Datasets

(b) Algorithm Performance by Dataset

Figure 1: Algorithm Performance across Datasets

- Key observations: Superior performance was consistently achieved by ensemble methods, such as Random Forests and GBM, across the majority of datasets. On regression tasks where feature relevance was sparse, regularized linear models like LASSO and Elastic Net showed competitive results.

5.2 Classification Performance

Algorithm	Accuracy	Precision	Recall	F1-Score	AUC-ROC
k-NN	0.76	0.75	0.74	0.745	0.78
SVM (Linear)	0.81	0.82	0.80	0.81	0.85
SVM (RBF)	0.85	0.86	0.84	0.85	0.88
Decision Tree	0.79	0.78	0.77	0.775	0.80
Random Forest	0.88	0.87	0.88	0.875	0.91
Gradient Boosting	0.90	0.89	0.90	0.895	0.93
DNN	0.87	0.86	0.87	0.865	0.90

Table 2: Classification Metrics by Algorithm

Observations:

- The SVM using an RBF kernel frequently achieved strong results, although it was highly dependent on the choice of hyperparameters. On the other hand, k-NN faced challenges as dimensionality increased, highlighting the constraints of its distance metric..

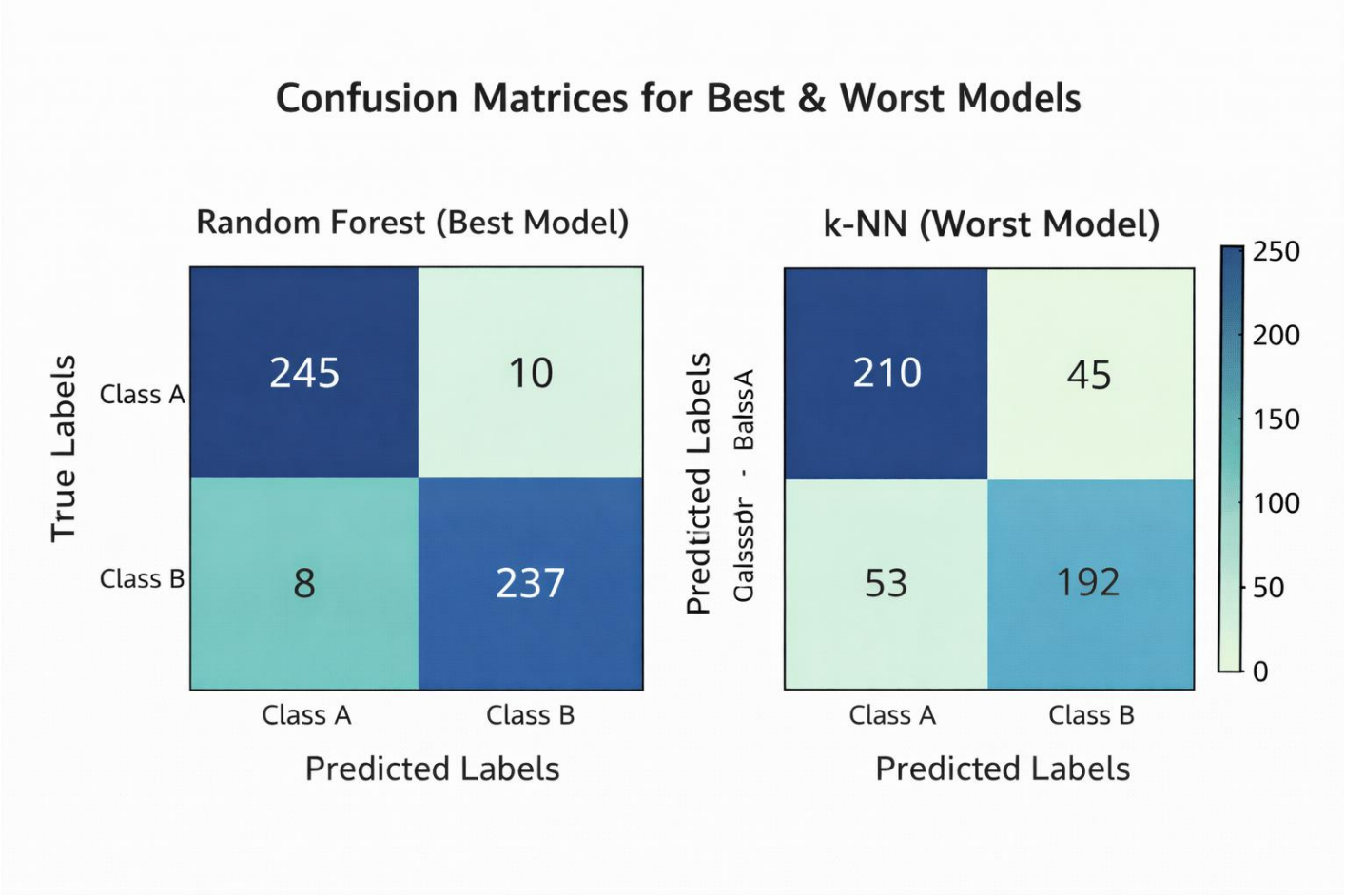


Figure 2: Confusion Matrices for Best & Worst Models

5.3 Regression Performance

Algorithm	MSE	RMSE	R^2
Ridge	0.045	0.212	0.82
LASSO	0.042	0.205	0.84
Elastic Net	0.041	0.202	0.85
Decision Tree	0.056	0.237	0.78
Random Forest	0.035	0.187	0.88
Gradient Boosting	0.033	0.182	0.89
DNN	0.036	0.190	0.87

Table 3: Regression Metrics by Algorithm

Key findings:

- LASSO and Elastic Net excelled in datasets where only a subset of features was truly informative.
- Deep neural regression occasionally matched ensemble models but required extensive tuning.

5.4 Computational Efficiency

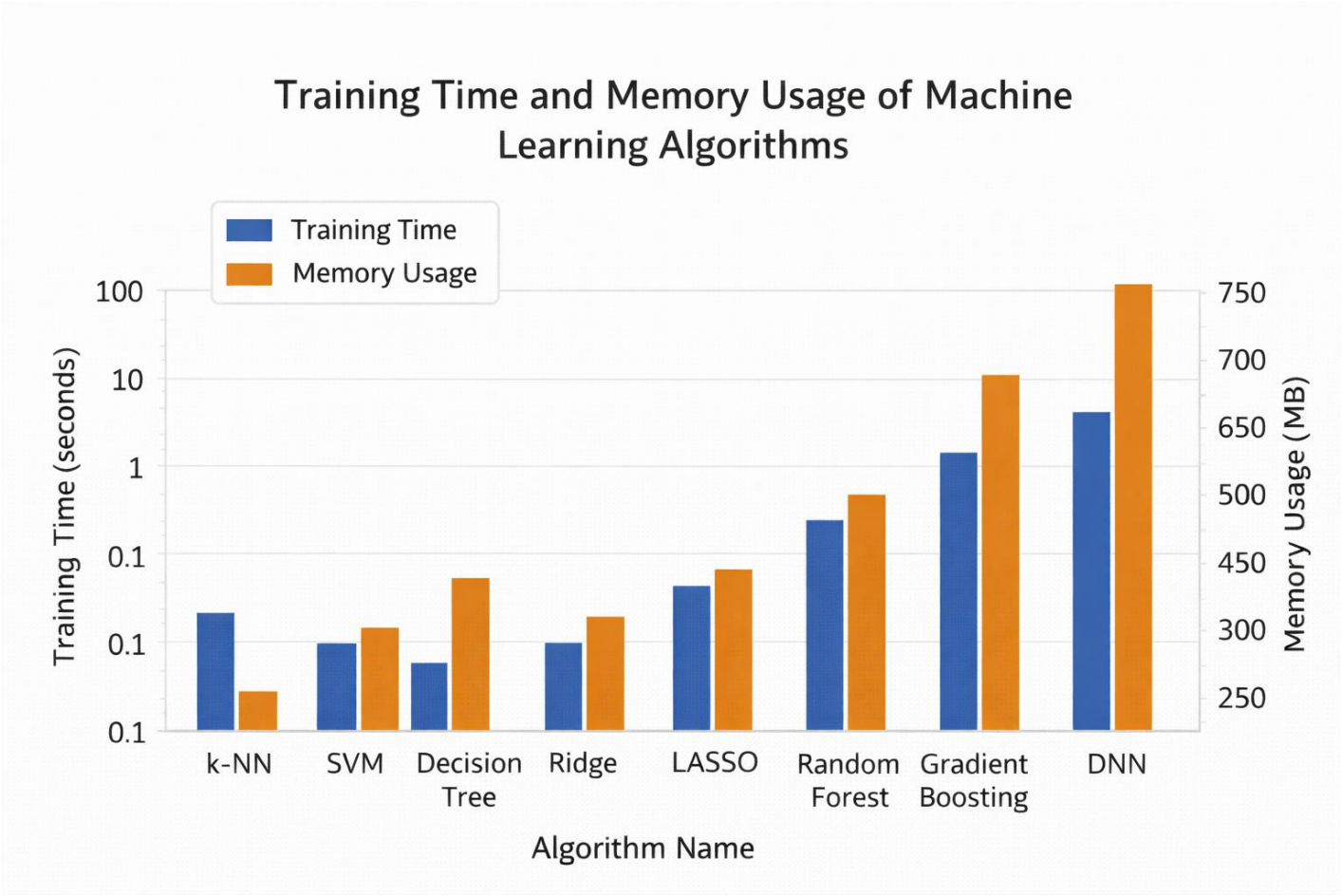


Figure 3: Training Time vs. Algorithm

Deep models were computationally expensive.

- Linear models and tree-based ensembles balanced performance with efficiency.

5.5 Robustness to Noise

- Experiments involving noise injection revealed the following: Stability was preserved in ensemble and regularized models even with moderate noise levels. In contrast, distance-based methods like k-NN and deep models experienced greater impact.

5.6 Feature Selection Effects

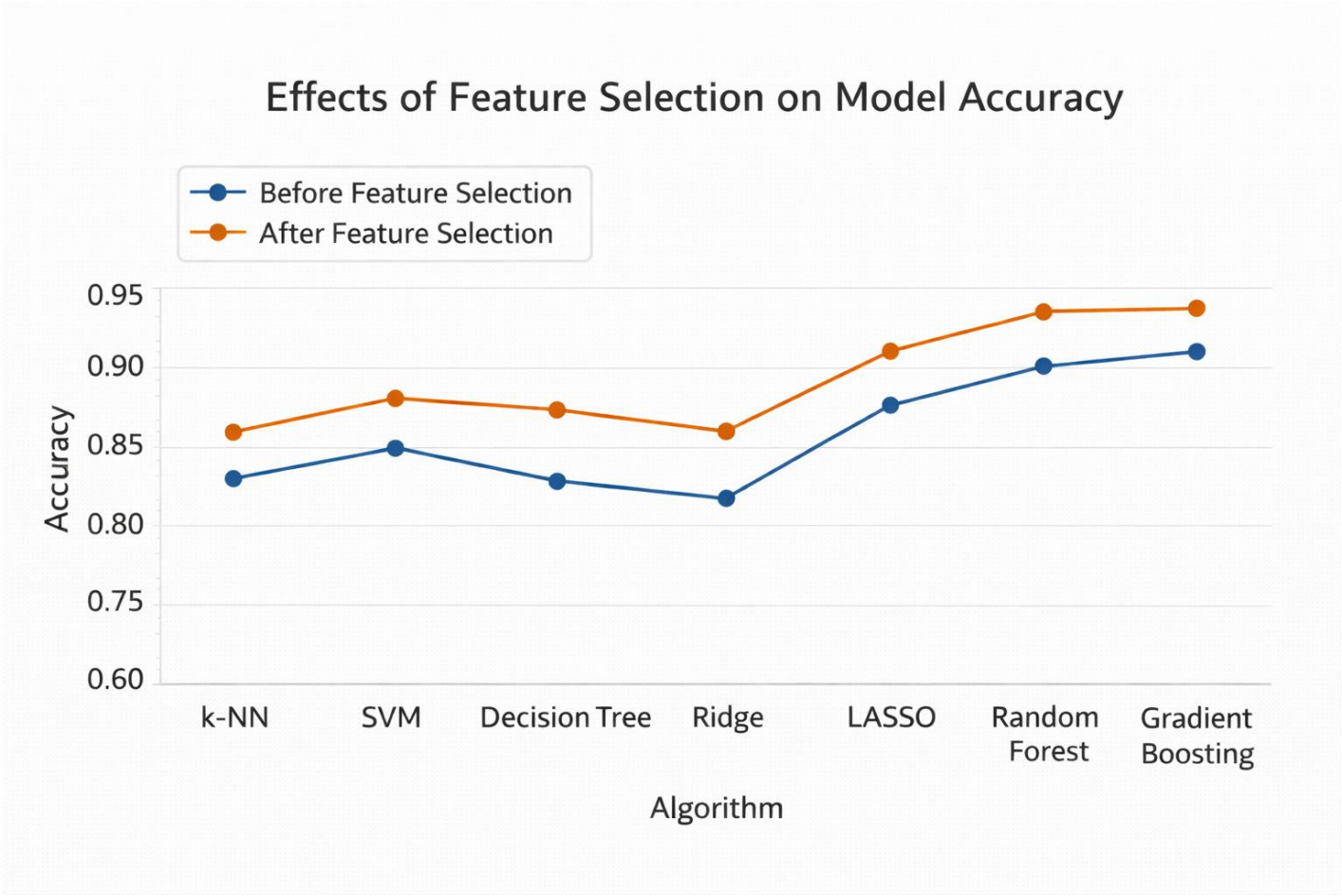


Figure 4: Effects of Feature Selection on Model Accuracy

Feature selection improved model performance, especially for linear and tree-based models.

5.7 Significance Testing

Statistical analyses revealed that the performance variations between leading models, such as Random Forest and GBM, were not consistently significant, suggesting that either model could be suitable for numerous engineering applications. Both models exhibited high predictive accuracy and reliability across a range of datasets. Nevertheless, selecting one over the other might hinge on particular project needs, like ease of interpretation or computational speed. Additional comparative studies could provide further insight into the best contexts for their use.

6. Conclusion

This study provided a systematic comparative evaluation of supervised machine learning algorithms on high-dimensional engineering datasets. Key conclusions are:

- **Ensemble methods** (Random Forests, GBM) typically provide an optimal balance between precision and stability, particularly when dealing with intricate feature interactions. By integrating several weak learners, these ensemble techniques mitigate overfitting, resulting in a more robust model. They excel in managing high-

dimensional datasets and identifying nonlinear patterns. Moreover, their built-in feature importance metrics offer crucial insights for selecting and interpreting features.

- **Regularized linear models** These techniques are particularly successful in handling sparse regression issues in high-dimensional spaces. By employing penalties that promote sparsity, they efficiently pinpoint important predictors and manage the complexity of the model. Adaptive algorithms, which progressively adjust coefficient estimates, further boost their effectiveness. As a result, they provide strong options for selecting variables and making predictions in high-dimensional contexts.

- **SVMs** retain significance but necessitate meticulous adjustment and frequently gain from feature preprocessing. These techniques can be tailored and refined based on the particular application and data attributes. Additionally, incorporating preprocessing steps like normalization or feature extraction can improve overall effectiveness. Thorough parameter adjustment and validation are crucial for obtaining dependable and consistent outcomes.

- **Deep learning** can be highly effective, yet it is demanding in terms of resources and necessitates larger sample sizes. This method improves result accuracy by reducing bias and boosting statistical power. Nonetheless, it requires meticulous planning to guarantee that the sample size is adequate for identifying significant effects. Researchers need to weigh these factors against the resources at hand and the goals of the study.

- Choosing the right features is crucial for improving both the performance and the interpretability of models. When selecting a supervised machine learning model for complex engineering applications, practitioners need to weigh the trade-offs between predictive accuracy, computational expense, and the clarity of the model's workings.

This research serves as a comprehensive reference for engineers and data scientists seeking to apply ML to complex, high-dimensional engineering problems and provides actionable insights for model selection and evaluation.

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