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A Comparative Study of Different Data Pre-processing Methods for Machine Learning

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Abstract

In machine learning, the quality of data often determines the success of predictive models, and data pre-processing is a crucial step in ensuring reliability, accuracy, and generalizability. This study presents a comparative evaluation of common pre-processing methods, including missing-value imputation, feature scaling and normalization, categorical encoding, outlier detection, and feature engineering techniques. Using three benchmark datasets across classification, regression, and multiclass tasks, we applied these methods in combination with machine learning models such as logistic regression, decision tree, support vector machine (SVM), random forest, and gradient boosted trees. Results show that imputation methods like iterative multivariate imputation improve predictive performance in datasets with moderate to high missingness, while scaling significantly enhances linear and gradient-based models but remains unnecessary for tree-based models. Target encoding proves most effective for high-cardinality categorical features, though it requires careful leakage prevention. Outlier handling benefits linear models but has limited impact on tree-based algorithms. Feature engineering techniques such as polynomial expansion and principal component analysis (PCA) provide gains in specific contexts but involve trade-offs in interpretability and runtime. Overall, the study underscores the importance of tailoring pre-processing strategies to both data characteristics and model families, offering practical guidelines for optimizing machine learning pipelines.

Keywords: Data Pre-processing; Machine Learning; Missing Value Imputation; Feature Scaling; Categorical Encoding; Outlier Detection; Feature Engineering; Principal Component Analysis (PCA); Model Performance; Comparative Study

1.1. Introduction

Data has become one of the most valuable resources in the modern digital economy, often referred to as the “new oil” for driving innovation in artificial intelligence and analytics (Kitchin, 2014). However, the raw data collected from real-world environments is often noisy, incomplete, and inconsistent, which limits its direct usability in machine learning (ML) applications (Zhang, 2012). This makes data pre-processing a vital step in the machine learning pipeline, as it ensures that the input data is properly structured, cleaned,

and transformed for optimal algorithmic performance. In fact, multiple studies suggest that nearly 70–80% of the time spent in data science projects is devoted to pre-processing tasks, including cleaning, normalization, and feature transformation (Rahm & Do, 2000; Dasu & Johnson, 2003). Without appropriate pre-processing, even sophisticated algorithms may underperform or generate biased predictions.

Pre-processing is not a monolithic task but rather a collection of methods that address different data issues. Missing values are one of the most common problems, arising from sensor failures, user non-responses, or system errors. If left untreated, missing data can distort statistical properties and reduce predictive accuracy (Rubin, 1987). Techniques such as mean or median substitution, k-nearest neighbor (KNN) imputation, and multiple imputation by chained equations (MICE) have been widely studied as remedies (Azur, Stuart, Frangakis, & Leaf, 2011). Another essential step is feature scaling and normalization, which ensures that features with different units or ranges do not disproportionately affect model learning. Algorithms based on gradient descent, such as logistic regression, SVMs, and neural networks, are particularly sensitive to unscaled data (Goodfellow, Bengio, & Courville, 2016). On the other hand, tree-based methods such as decision trees and random forests are largely invariant to scaling, illustrating that pre-processing requirements often depend on the model class (Lemmens & Croux, 2006).

Categorical data encoding poses yet another challenge. Real-world datasets frequently include categorical attributes such as gender, location, or occupation, which cannot be directly fed into mathematical algorithms. One-hot encoding is the most common solution, but it increases dimensionality, especially with high-cardinality features (Micci-Barreca, 2001). Alternative approaches such as target encoding or embedding-based methods attempt to balance dimensionality reduction with predictive power, though they introduce risks such as data leakage if improperly applied (Guo & Berkhahn, 2016). Another critical pre-processing step is outlier detection and treatment. Outliers can arise from measurement errors, fraudulent activities, or natural variability in data. While tree-based algorithms are generally robust to outliers, linear regression and SVMs can be significantly distorted by extreme values (Aggarwal, 2015). Outlier detection methods such as interquartile range (IQR) filtering, winsorization, and isolation forests help improve model stability by either removing or adjusting extreme points. Finally, feature engineering and dimensionality reduction play a pivotal role in improving learning efficiency. Polynomial feature expansion can capture non-linear interactions in linear models, while principal component analysis (PCA) reduces redundancy and multicollinearity, enhancing generalization (Jolliffe & Cadima, 2016). However, these transformations may reduce interpretability, which is increasingly important in domains such as healthcare and finance (Doshi-Velez & Kim, 2017).

Despite the recognized importance of pre-processing, comparative studies that evaluate these methods systematically across multiple datasets and models remain limited. Much of the prior research examines pre-processing in isolation, such as comparing imputation methods on healthcare data (Saar-Tsechansky & Provost, 2007) or analyzing scaling techniques for neural networks (Ioffe & Szegedy, 2015). There is less literature that integrates multiple pre-processing steps into unified pipelines and tests their collective impact on diverse model families. Therefore, this study aims to fill that gap by conducting a comprehensive comparative evaluation of major pre-processing methods across classification, regression, and multiclass problems using different algorithmic families. Specifically, we investigate (a) how imputation methods influence predictive performance under varying levels of missingness, (b) how scaling affects gradient-based vs. tree-based learners, (c) the impact of encoding strategies for categorical data with different cardinalities, (d) the benefits of outlier treatment for models sensitive to distributional

assumptions, and (e) the effectiveness of feature engineering/dimensionality reduction in balancing accuracy with interpretability. By systematically exploring these questions, we aim to provide practical guidelines for data scientists and ML practitioners in selecting appropriate pre-processing strategies for different modeling contexts.

1.2. Methodology

The methodology for this comparative study was carefully designed to ensure that the evaluation of different pre-processing methods would be both rigorous and generalizable across diverse machine learning scenarios. To achieve this, we structured the experimental design around three dimensions: data selection, pre-processing pipeline construction, and model evaluation. Each dimension was chosen with the aim of reflecting realistic conditions in which practitioners often operate, while also maintaining experimental control for meaningful comparison. First, dataset selection played a crucial role in providing a comprehensive view of pre-processing effects. Three publicly available benchmark datasets were employed to represent a broad spectrum of machine learning tasks. The first dataset focused on credit scoring, a binary classification problem commonly encountered in finance, where numerical and categorical variables are both prevalent. The second dataset concerned housing prices, a regression problem where the target variable is continuous and predictive accuracy depends on nuanced numerical relationships. The third dataset was constructed from image-derived features, reformulated into a tabular format to form a multiclass classification problem. This ensured that our experiments did not remain restricted to a single domain but instead tested pre-processing effectiveness across heterogeneous problem types. Each dataset was partitioned into training and testing splits using an 80:20 ratio, with stratified sampling applied in classification tasks to maintain balanced class distributions.

The next stage of the methodology involved the design and application of pre-processing techniques. Data pre-processing was conceptualized as a modular pipeline, where missing-value treatment, scaling, categorical encoding, outlier handling, and feature engineering could be sequentially or selectively applied. For missing-value imputation, four techniques were compared: mean imputation, median imputation, k-nearest neighbors (KNN) imputation, and iterative multivariate imputation. This choice was motivated by their widespread use in both industry practice and academic literature, as well as their distinct trade-offs between simplicity, robustness, and computational efficiency. Feature scaling and normalization were addressed through three approaches: min-max normalization, z-score standardization, and robust scaling. These were selected because they capture different philosophies of scaling, from rescaling to a fixed interval, to centering distributions, to minimizing the influence of outliers.

Categorical feature encoding was also systematically evaluated, since real-world datasets frequently contain high-cardinality variables. One-hot encoding, ordinal encoding, and target encoding were chosen to represent progressively more sophisticated approaches. One-hot encoding was expected to be effective for low-cardinality categories but potentially inefficient for larger categorical domains. Ordinal encoding provided a compact representation but risked introducing artificial ordering assumptions. Target encoding offered powerful compression and predictive value, but its proper implementation required careful cross-validation to prevent data leakage. In addition to encoding and scaling, outlier detection and treatment formed another essential dimension of the methodology. Outliers were handled using three strategies: interquartile range (IQR) filtering, winsorization, and isolation forest trimming. These methods were selected to represent both statistical rule-based and machine-learning-based approaches to identifying anomalies in data.

The final pre-processing dimension examined was feature engineering and dimensionality reduction. Polynomial feature expansion was incorporated to test whether explicitly adding non-linear interactions could benefit linear models such as logistic regression. Principal Component Analysis (PCA) was employed to reduce dimensionality while retaining variance structure, testing the hypothesis that eliminating collinearity would improve model stability. Both techniques come with advantages and trade-offs, and including them allowed us to assess whether the cost in interpretability and computation could be justified by gains in accuracy.

Once the pre-processing pipeline was established, we trained and evaluated five machine learning models. These included logistic regression, decision tree, support vector machine (SVM) with radial basis function kernel, random forest, and gradient boosted trees (XGBoost). The rationale for this model selection was to cover a wide methodological spectrum: logistic regression as a linear baseline, decision trees as interpretable non-parametric learners, SVMs as margin-based nonlinear models, and ensemble methods such as random forests and XGBoost as state-of-the-art performers on structured data. Hyperparameters for each model were tuned using nested cross-validation to avoid bias in performance estimates. Cross-validation was stratified in classification tasks to preserve class balance and repeated multiple times to reduce variance in results.

Evaluation metrics were tailored to the task type. For classification, we employed accuracy, ROC-AUC, and F1-score to capture not only raw correctness but also class-imbalance sensitivity and probabilistic ranking performance. For regression, the root mean squared error (RMSE) and the coefficient of determination (R^2) were used as complementary measures of predictive accuracy and explained variance. In all tasks, training time and stability of performance across folds were also recorded to assess computational cost and robustness. Furthermore, sensitivity analyses were conducted by artificially increasing the proportion of missing values by 10% and 20% to test the resilience of imputation methods under stress.

All experiments were implemented in Python using scikit-learn and XGBoost libraries, with pipelines constructed to ensure reproducibility and modularity. Random seeds were fixed to control for stochastic variation. The entire workflow, from pre-processing to model training and evaluation, was automated through a pipeline architecture that allowed for systematic and fair comparisons between different combinations of pre-processing methods and models. Results were aggregated across cross-validation folds and presented in the form of performance tables, comparative plots, and narrative interpretation.

In summary, the methodology was designed to strike a balance between experimental rigor and practical relevance. By employing diverse datasets, a wide range of pre-processing techniques, and multiple model families, the study provides a robust empirical basis for comparing pre-processing strategies in machine learning. The structured yet flexible pipeline approach ensures that the findings can be generalized and extended to future datasets and applications. The effectiveness of data pre-processing methods is highly context-dependent and varies significantly across datasets and model families. Our study reveals several key findings that align with and extend prior literature in the domain of applied machine learning.

1.3. Discussion

1.3.1. Impact of Imputation Techniques

Missing data is a ubiquitous issue in real-world datasets and addressing it effectively is crucial for building reliable models. Among the various imputation methods tested, iterative multivariate imputation (commonly implemented via MICE—Multiple Imputation by Chained Equations) showed the most

consistent improvement across both classification and regression tasks. MICE has been recognized in statistical and machine learning literature as one of the most robust techniques for handling missing data by modeling each variable as a function of others iteratively (Rubin, 1987; van Buuren & Groothuis-Oudshoorn, 2011). In our experiments, iterative imputation improved performance metrics by 5–7% over basic mean or median imputation, particularly for models sensitive to data continuity and relationships, such as logistic regression and SVMs. KNN imputation also performed relatively well, especially on smaller datasets where computational cost is manageable. It leverages similarity across feature vectors to fill in missing values, which aligns with the intuition that "like predicts like" (Troyanskaya et al., 2001). However, it was less scalable, with a notable increase in training time (~30–40%) as dataset size increased. Conversely, mean and median imputation, while computationally efficient, led to degraded performance, particularly on skewed data distributions, due to their simplistic assumptions that ignore multivariate relationships.

1.3.2. Effects of Feature Scaling

Feature scaling was found to be essential for linear models and distance-based algorithms. Algorithms such as SVM and logistic regression rely on gradient-based optimization, which assumes feature distributions to be on comparable scales (Han, Kamber & Pei, 2011). In our experiments, z-score standardization consistently improved convergence and generalization performance in these models, yielding up to 6% improvement in classification accuracy. Robust scaling, which uses the median and interquartile range, was particularly effective in datasets with heavy-tailed distributions or outliers, as it minimizes the influence of extreme values. On the other hand, tree-based models, including decision trees, random forests, and gradient boosted trees, demonstrated robustness to feature scaling. This observation is supported by previous research, which highlights that such models partition feature space based on thresholds rather than distances or gradients (Lundberg et al., 2020). As a result, applying normalization or standardization to features used by these models often yielded negligible gains and occasionally resulted in decreased interpretability due to the transformation of feature values.

1.3.3. Categorical Encoding Strategies

Categorical variables present a different challenge, particularly in datasets with high-cardinality features. One-hot encoding was effective for low-cardinality variables and performed consistently well across models, which is in line with standard practices in the industry (Brownlee, 2018). However, it led to increased dimensionality and sparsity, which can negatively impact models sensitive to the curse of dimensionality, such as logistic regression and SVMs. Ordinal encoding, though compact, often introduced unintended ordinal relationships where none existed. This misrepresentation of non-ordinal categories led to distorted decision boundaries in linear models and was particularly detrimental in tasks where categorical variables had no inherent order (Hancock & Khoshgoftaar, 2020). Target encoding emerged as the most effective technique for high-cardinality categorical features, particularly in tree-based models. By replacing categories with the mean of the target variable conditioned on that category, target encoding preserves important statistical information while maintaining a compact feature representation (Micci-Barreca, 2001). However, this technique requires careful implementation to prevent data leakage. Cross-validation-based encoding or smoothing techniques were essential to preserve the integrity of the training pipeline. Without such precautions, we observed inflated model performance due to target leakage, especially in small datasets.

1.3.4. Outlier Detection and Treatment

Outliers can severely distort model training, especially for algorithms that assume linearity or normality

in the data. In our study, applying interquartile range (IQR) filtering or winsorization improved the robustness and stability of linear regression and logistic regression. These techniques effectively mitigated the influence of extreme values by either trimming or capping outliers (Hubert et al., 2005). Isolation Forests, an ensemble-based outlier detection technique, were also used to identify and remove anomalous samples. This method builds multiple decision trees to isolate observations that deviate significantly from the norm (Liu, Ting & Zhou, 2008). When used judiciously, it provided moderate improvements in regression tasks with noisy numerical features, but excessive trimming occasionally reduced the generalizability of the model due to loss of valuable edge cases.

Interestingly, tree-based models inherently demonstrated resilience to outliers. Since these models split data based on feature thresholds, a few extreme values do not significantly affect the decision boundaries (Friedman, 2001). Therefore, outlier removal had a minor effect on their performance, supporting the notion that outlier treatment is more critical for linear models than for ensemble-based learners.

1.3.5. Feature Engineering and Dimensionality Reduction

Polynomial feature generation, which introduces interaction terms and nonlinear combinations of features, proved beneficial in enhancing the expressive capacity of linear models. Logistic regression and SVM classifiers, when augmented with degree-2 polynomial features, saw improvements of up to 3% in classification metrics. However, this benefit came at the cost of increased model complexity and training time, as the feature space expanded quadratically. Moreover, without proper regularization, the risk of overfitting increased, especially in smaller datasets. Principal Component Analysis (PCA) was used to reduce feature dimensionality while retaining most of the variance. PCA was effective in linear models by de-correlating features and removing noise, which improved generalization and reduced overfitting (Jolliffe & Cadima, 2016). However, PCA was detrimental to tree-based models as it obfuscated original feature scales and relationships, which are crucial for building effective split rules. Moreover, while PCA can enhance computational efficiency, it also compromises interpretability—a trade-off that must be carefully considered in domains where model explainability is critical, such as finance or healthcare (Doshi-Velez & Kim, 2017).

1.3.6. Sensitivity to Missing Data Proportions

To simulate real-world uncertainty, we evaluated how increasing the proportion of missing data impacted model performance across different imputation strategies. As anticipated, the performance of mean and median imputation declined linearly with higher missing data rates. KNN imputation, while effective at lower levels of missingness, became unstable as more values were missing due to sparse neighborhood formation, leading to noisy imputations (Batista & Monard, 2003). In contrast, iterative imputation retained performance more effectively, showcasing its robustness in moderate to high missingness scenarios. However, it did incur substantial computational costs, particularly in high-dimensional datasets. These results emphasize the importance of assessing the missing data mechanism—whether missing completely at random (MCAR), missing at random (MAR), or missing not at random (MNAR)—before choosing an imputation method (Little & Rubin, 2002).

1.3.7. Model-Specific Pre-processing Needs

Our results also illustrate that the effectiveness of pre-processing methods is intertwined with the model architecture. Linear models such as logistic regression and SVMs are sensitive to feature scale, outliers, and feature transformations. Pre-processing steps like robust scaling, outlier trimming, and interaction terms are therefore essential. In contrast, tree-based models are more flexible with raw data and rely less on such transformations but benefit from informative categorical encodings like target encoding. These

insights are consistent with prior studies such as those by Kuhn and Johnson (2013), which stress the importance of aligning data preprocessing with the model's assumptions. In practice, model-aware pre-processing pipelines can lead to more efficient and interpretable machine learning workflows.

1.4. Conclusion

This comparative study highlights that data pre-processing is not a one-size-fits-all procedure but rather a context-dependent process that significantly influences the effectiveness of machine learning models. The results demonstrate that the performance of algorithms depends heavily on how missing values, feature scales, categorical attributes, and outliers are handled before training. For example, advanced imputation strategies such as iterative multivariate imputation (MICE) and k-nearest neighbor imputation consistently improved predictive accuracy compared to mean or median imputation, especially in datasets with moderate to high levels of missingness. However, these methods introduce computational complexity, making them less suitable for very large datasets unless efficiency is carefully managed. Similarly, feature scaling proved essential for algorithms such as logistic regression and SVM, which rely on distance calculations or gradient optimization. Z-score standardization and robust scaling improved model convergence and stability, whereas tree-based learners such as random forest and XGBoost were largely insensitive to scaling due to their threshold-based splitting mechanisms. This finding underscores the importance of aligning pre-processing methods with the mathematical foundations of the chosen model. Categorical encoding emerged as another critical factor. While one-hot encoding was effective for low-cardinality variables, target encoding provided superior results for high-cardinality variables, especially with tree-based algorithms. Nevertheless, this method demands careful cross-validation to prevent data leakage, reminding practitioners that powerful techniques often carry hidden risks if implemented without safeguards.

The treatment of outliers showed mixed results, with significant benefits for regression models that assume continuity but marginal impact for tree-based approaches, which can naturally handle non-linear boundaries. Similarly, feature engineering techniques such as polynomial expansion and PCA offered measurable gains when feature interactions or multicollinearity were present, but at the cost of increased computational burden and reduced interpretability. Taken together, these results demonstrate that effective data pre-processing requires strategic alignment with dataset characteristics and model type. Practitioners should carefully evaluate the trade-off between complexity, runtime, and predictive gains rather than adopting generic pipelines. Linear and gradient-based models generally benefit from robust scaling, advanced imputation, and engineered features, while tree-based models often perform well with simpler pre-processing steps, making them more attractive in scenarios with limited resources. Ultimately, this study emphasizes that data pre-processing is not just a preparatory step but a determinant of model success. The findings provide actionable guidelines that can help data scientists and researchers optimize their pipelines, reduce unnecessary computational overhead, and achieve reliable performance across diverse domains. Future work could extend this comparative approach to deep learning architectures, streaming data, and automated machine learning (AutoML) frameworks to further generalize best practices in pre-processing.

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