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Research Article

Enhancing Missing Values Imputation through Transformer-Based Predictive Modeling

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Abstract

This paper tackles the vital issue of missing value imputation in data preprocessing, where traditional techniques like zero, mean, and KNN imputation fall short in capturing intricate data relationships. This often results in suboptimal outcomes, and discarding records with missing values leads to significant information loss. Our innovative approach leverages advanced transformer models renowned for handling sequential data. The proposed predictive framework trains a transformer model to predict missing values, yielding a marked improvement in imputation accuracy. Comparative analysis against traditional methods—zero, mean, and KNN imputation—consistently favors our transformer model. Importantly, LSTM validation further underscores the superior performance of our approach. In hourly data, our model achieves a remarkable R2 score of 0.96, surpassing KNN imputation by 0.195. For daily data, the R2 score of 0.806 outperforms KNN imputation by 0.015 and exhibits a notable superiority of 0.25 over mean imputation. Additionally, in monthly data, the proposed model's R2 score of 0.796 excels, showcasing a significant improvement of 0.1 over mean imputation. These compelling results highlight the proposed model's ability to capture underlying patterns, offering valuable insights for enhancing missing values imputation in data analyses.

Introduction

In the ever-evolving data analysis landscape, the challenge of missing values within datasets is a formidable hurdle, impacting the reliability and efficacy of downstream applications [1]. Addressing this challenge has spurred the development of various imputation techniques, each attempting to reconcile the absence of data points with meaningful estimations. Traditional methods, such as zero imputation, mean imputation, and K-Nearest Neighbors (KNN) imputation, have long been employed. Yet, their efficacy is often limited in capturing complex dataset's intricate relationships and patterns.

Recognizing the shortcomings of conventional approaches and the imperative to preserve valuable information lost through record removal, this paper introduces an innovative method for missing values imputation. The proposed approach leverages the capabilities of advanced transformer models, which have exhibited exceptional performance in handling sequential data and contextual information. The transformer model is trained to predict missing values based on the inherent contextual dependencies within the dataset, offering a promising alternative to traditional imputation techniques [2]. Moreover, the utilization of transformer models in missing values imputation represents a paradigm shift from rule-based imputation methods to a more data-driven and adaptive approach [3]. By harnessing the power of self-attention mechanisms [4], the transformer model can effectively capture intricate relationships and dependencies across different features, leading to more accurate predictions of missing values.

This innovative approach is particularly advantageous when dealing with large and complex datasets, where conventional imputation techniques may struggle to capture the nuanced patterns inherent in the data. The transformer model's ability to consider global context and long-range dependencies ensures a holistic understanding of the dataset, enhancing its capacity to impute missing values in a manner that aligns with the underlying structure of the information [5]. Statistical imputation techniques employ conventional statistical methods, such as substituting missing values with the mean of available data and utilizing regression models [6-8].

In addressing missing data in short-term air pollutant monitoring with real-time PM2.5 monitors [9], univariate methods like Markov, random, and mean imputations prove superior, especially beneficial in resource-limited contexts. Furthermore, DACMI [10] addresses missing clinical data with a shared dataset,

revealing that models like LightGBM and XGBoost, coupled with careful feature engineering, excel in imputation performance, emphasizing the importance of balanced model complexity. In scRNA-seq, vital for studying single-cell transcription, addressing high-dimensionality and dropout values is crucial. This study [11] evaluates advanced imputation methods, providing insights for selecting appropriate approaches in diverse data contexts and aiding downstream functional analysis. Both the Self-Organizing Map (SOM) [12,13] and the MLP [14] represent additional ML techniques applied for the imputation of missing values.

Furthermore, studies employing the regression approach [15] implemented a novel method involving weighted quantile regression to estimate missing values within health data. In another article [16], the author introduced a comprehensive case regression approach for handling missing values, employing functional principal components. Iterative regression is used for effective imputation in multivariate data [17]. Another method Hot-deck imputation, matches missing values with complete values on key variables [18]. Research is conducted on expectation minimization in handling missing data using a dataset analyzing the effects of feeding behaviors among drug-treated and untreated animals [19]. Recognizing the insufficiency of merely deleting or discarding missing data [20], researchers often turn to employing multiple imputations. Multiple imputation involves leveraging the observed data distribution to estimate numerous values, reflecting the uncertainty surrounding the true value. This approach has predominantly been utilized to address the constraints associated with single imputation [21].

Moreover, another study [22] evaluates imputation methods for incomplete water network data, focusing on small to medium-sized utilities. Among the tested methods, IMPSEQ outperforms others in imputing missing values in cast iron water mains data from the City of Calgary, offering insights for cost-effective water mains renewal planning. The proposed one-hot encoding method by [23] excels in addressing missing data for credit risk classification, demonstrating superior accuracy and computational efficiency, especially in high missing-rate scenarios, when integrated with the CART model. Another work [24] proposes a novel imputation method for symbolic regression using Genetic Programming (GP) and weighted K-Nearest Neighbors (KNN). It outperforms state-of-the-art methods in accuracy, symbolic regression, and imputation time on real-world datasets. Conventional techniques for multiple imputations exhibit suboptimal performance when confronted with high-dimensional data, prompting researchers to enhance these algorithms [25,26]. Likewise, indications exist that exercising caution is advisable when applying continuous-based approaches to impute categorical data, as it may introduce bias into the results [27].

Motivated by the need for a comprehensive evaluation, we conduct extensive experiments to compare the performance of our transformer-based imputation against established methods. This comparison extends beyond conventional imputation techniques, encompassing zero [28], mean [29], and KNN imputations [30]. In the context of missing value imputation, it is noteworthy that addressing missing values is a common concern among researchers and data scientists. Recent research [31] thoroughly compares seven data imputation methods for numeric datasets, revealing kNN imputation's consistent outperformance. This contribution adds valuable insights to the ongoing discourse on selecting optimal methods for handling missing data in data mining tasks. Furthermore, we introduce an additional validation layer by subjecting the imputed data to scrutiny through Long Short-Term Memory (LSTM) networks [32]. This not only assesses the accuracy of imputation but also gauges the temporal coherence of the imputed values.

By undertaking this exploration, we aim to contribute valuable insights into the realm of missing values imputation, offering a nuanced understanding of the capabilities of transformer-based models. The observed improvements in imputation accuracy, particularly validated through LSTM analysis, underscore the potential of our proposed approach to address the persistent challenges associated with missing data. Through this work, we aspire to provide a robust foundation for future advancements in data preprocessing and analysis methodologies. These are the key contributions of the article:

- Introduced a novel missing values imputation approach using transformer models, deviating from traditional methods.
- Leveraging self-attention mechanisms, the transformer-based model provides a data-driven and adaptive solution for capturing intricate data relationships.
- Through a comprehensive comparative analysis, the transformer model consistently outperforms traditional imputation techniques like zero, mean, and KNN.
- The inclusion of LSTM validation adds a layer of scrutiny, evaluating not only imputation accuracy but also the temporal coherence of imputed values.
- The proposed model showcases robust performance across diverse datasets, demonstrating its efficacy in preserving data relationships and capturing variability.

Methodology

Handling missing values in datasets is a crucial challenge, particularly when predicting these values based on available data. Figure 1 outlines a comprehensive process for predicting missing values using a transformer model. In the initial step, we showcase an example dataset with missing values, highlighting the intricacies of the task. Moving to step two, we prepare the data for missing values imputation by segregating complete data for model training and reserving a test set for predicting missing data. Before arranging the data, each data sequence is assigned a unique identifier, ensuring traceability. Complete data features (f0, f3, f6, and f9) are repositioned on the right side in the third step. Subsequently, in step four, all complete rows are relocated to the top of the dataset.

Step five reveals the division of the dataset into X-data and Y-data, forming the basis for training the model. In step six, we

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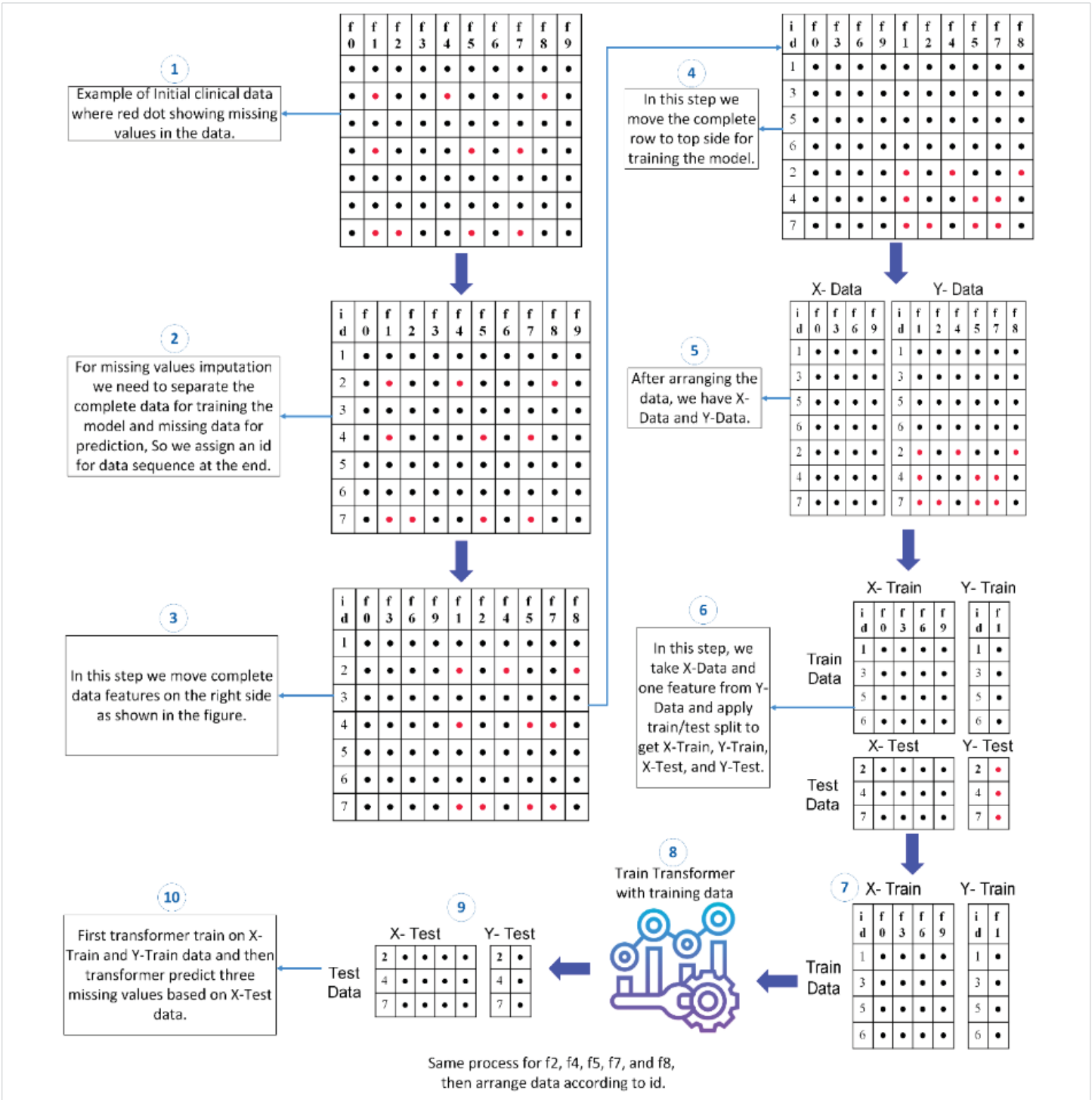

Figure 1: A detailed process of preparing data for the Transformer for missing values prediction.

select the complete X-Data and the target feature f1 from Y-Data, which contains missing data. Utilizing the train-test split on X-Data and Y-Data (f1), we generate X-Train, Y-Train, X-Test, and Y-Test. In step seven, the train data is prepared for our proposed prediction model, providing a complete set for training the Transformer model.

Advancing further, at step eight, the transformer undergoes comprehensive training using the entirety of the available data. In the subsequent step nine, the adeptly trained model takes on the task of predicting missing values within the X-Data. The imputed f1 feature is seamlessly integrated back into the X-Data, initiating a cascading effect as subsequent missing values are accurately predicted. This iterative refinement persists until the entirety of missing values is meticulously filled.

In the culminating step, the dataset is meticulously organized, preserving its inherent structure by adhering to initially assigned

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IDs. This methodical approach not only ensures the seamless integration of imputed values but also maintains the overall integrity and coherence of the dataset. In essence, our methodology provides a structured and systematic solution, navigating the intricacies of missing value imputation using a transformer model.

Proposed model validation

After the missing data imputation process finished using our suggested transformer-based prediction model, a thorough validation was carried out. During the validation stage, we aimed to assess how well our suggested model performed in comparison to other widely used imputation techniques, such as zero, mean, mode, and KNN imputation. We used these various imputation methods to produce five sets of imputed data. We validated each imputation model using Long Short-Term Memory (LSTM) networks to evaluate its effectiveness thoroughly. The LSTM network was fed the imputed data from all five models, including our suggested transformer-based imputation, as shown in Figure 2. Our objective was to conduct a comprehensive comparison and evaluation of the overall performance and forecast accuracy for each imputed dataset. Notably, the results consistently demonstrated the superior performance of our proposed transformer-based prediction-based imputation model when pitted against other, less intricate imputation techniques. This underscores its robust predictive capabilities in effectively managing missing values within the dataset.

The validation procedure, when juxtaposed with conventional imputation techniques, serves as a testament to the resilience and efficacy of our proposed model. The outcomes not only showcase its superiority but also affirm its ability to outperform fewer complex alternatives.

Results and analysis

Table 1: A detailed comparative analysis of the Imputation techniques.

FE Data	P Measure	Zero Imputation	Mean imputation	Mode Imputation	KNN Imputation	Proposed Model Imputation
Hourly Data	R2 score	0.233	0.647	0.437	0.765	0.96
	MAE	0.058	0.113	0.075	0.037	0.036
	MSE	0.006	0.02	0.008	0.003	0.003
	RMSE	0.077	0.141	0.089	0.055	0.055
	MAPE	1.2	0.92	1.01	0.83	0.423
Daily Data	R2 score	0.391	0.556	0.471	0.791	0.806
	MAE	0.066	0.051	0.059	0.048	0.028
	MSE	0.009	0.008	0.0073	0.004	0.003
	RMSE	0.077	0.095	0.055	0.045	0.045
	MAPE	0.93	0.85	0.89	0.47	0.32
Monthly Data	R2 score	0.251	0.696	0.698	0.419	0.796
	MAE	0.023	0.051	0.029	0.038	0.025
	MSE	0.001	0.003	0.002	0.004	0.001
	RMSE	0.032	0.055	0.045	0.063	0.032
	MAPE	1.13	0.89	0.891	1.01	0.523

Table 1 examines the imputation performance across three datasets: hourly energy consumption data, daily energy consumption data, and monthly energy consumption data; the R2 score emerges as a critical metric for evaluating the effectiveness of various imputation methods. The proposed imputation model yields a noteworthy R2 score of 0.96 in hourly data, showcasing a substantial improvement of 0.195 over the next best method, KNN imputation. This enhancement underscores the proposed model's ability to capture underlying patterns within the data, outshining traditional techniques such as zero, mean, and mode imputation. Similarly, the proposed model's R2 score of 0.806 in daily data outperforms the KNN imputation by 0.015, demonstrating a notable superiority of 0.25 over the mean imputation. Moving to monthly data, the proposed model's R2 score of 0.796 excels, showcasing a significant improvement of 0.1 over mean imputation and an even more substantial gain of 0.359 over mode imputation.

Overall, these results consistently highlight the proposed

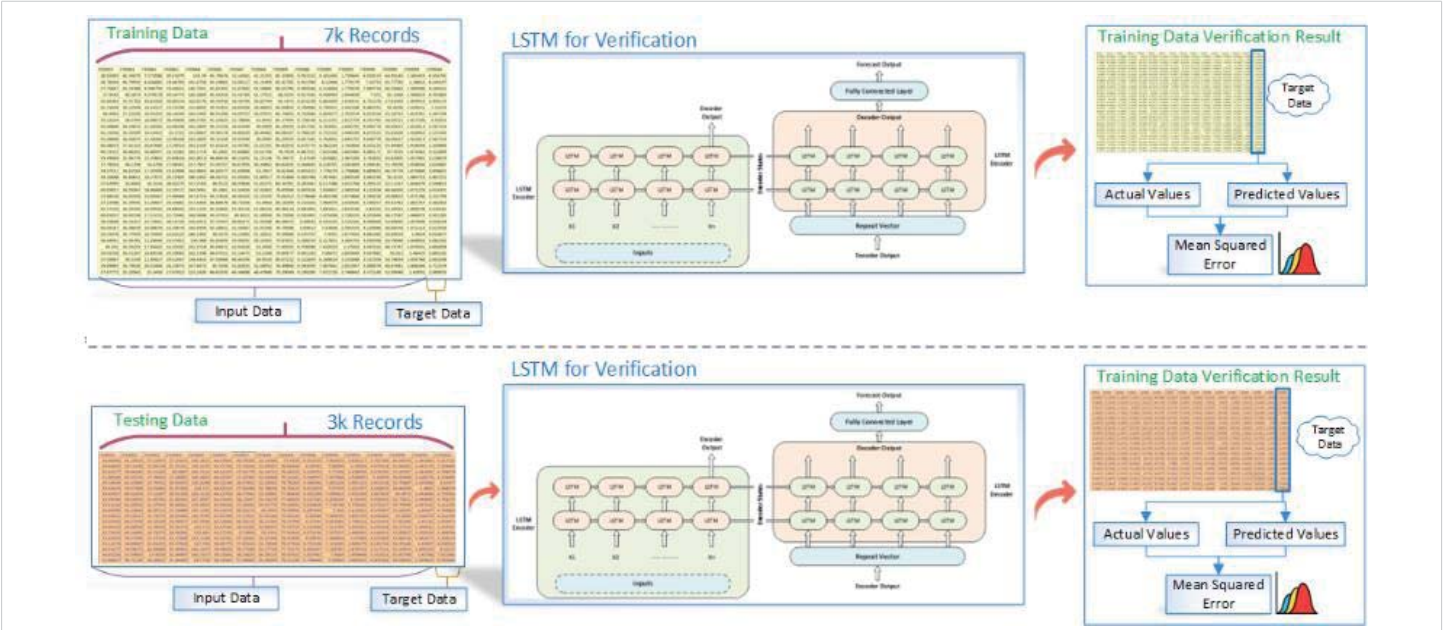

Figure 2: Validation process of the Imputed data using LSTM.

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model's effectiveness in preserving data relationships and capturing variability across diverse datasets, positioning it as a robust choice for imputing missing values when accurate modeling of underlying data patterns is crucial. A visual analysis of the r2 score for the selected imputation method is illustrated in Figure 3.

Beyond R2 scores, an in-depth analysis of other error metrics further solidifies the superiority of the proposed imputation model, as shown in Figure 4. In hourly consumption data, the model's Mean Absolute Error (MAE) of 0.036 is notably lower than that of other methods, reflecting its ability to predict missing values with minimal deviation accurately. This trend continues in daily and monthly consumption data, where the proposed model consistently achieves the lowest MAE values, indicating superior imputation accuracy. Similarly, examining Mean Squared Error (MSE) and Root Mean Squared Error (RMSE) across all datasets, the proposed model consistently outperforms alternative methods. The observed reductions in MAE, MSE, and RMSE collectively underscore the robustness of the proposed model in minimizing imputation errors. These comprehensive findings suggest that, beyond R2 scores, the proposed imputation model consistently excels across various error metrics, affirming its efficacy in accurately filling missing data and offering a comprehensive solution for handling diverse datasets with absent values.

Critical discussion

In this study, we have demonstrated the superior efficacy of transformer models over traditional methods like zero mean and KNN imputation, particularly in handling accuracy and context in missing data. However, the performance of these models varies with different data types and sizes, highlighting potential limitations in scalability and applicability to diverse datasets. Comparative analysis suggests that while transformers excel in interpreting sequential data, they may not be the most suitable choice for simpler or smaller datasets. The practical applications of

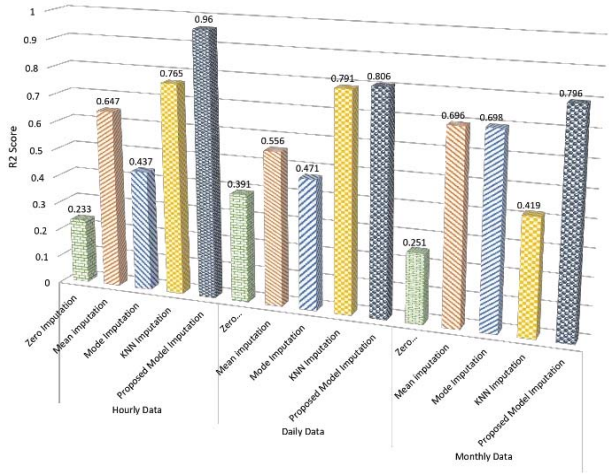

Figure 3: R2 score analysis for the selected imputation methods.

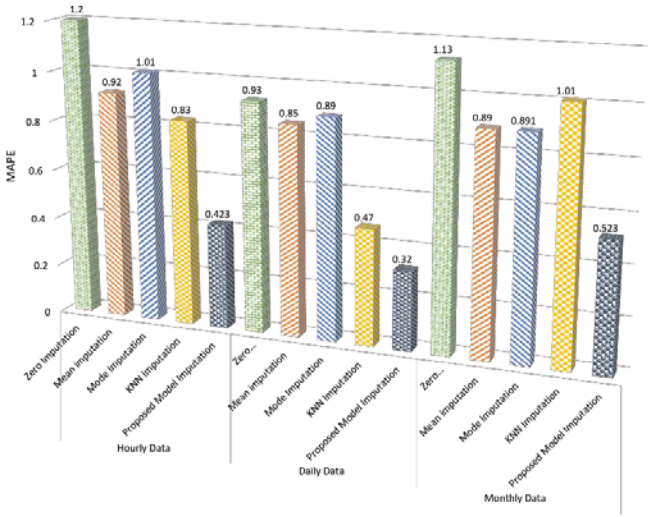

Figure 4: MAPE analysis for the selected imputation methods.

our model are promising, yet they are accompanied by challenges in computational demands and ethical considerations, especially in sensitive sectors like healthcare and finance. The generalizability of our model across various types of missing data and its application across different fields remains an area ripe for further research and validation.

Future studies should focus on integrating advanced machine learning techniques to enhance the robustness and applicability of our model. Additionally, while the use of LSTM networks for validation is beneficial, alternative methods might provide a more comprehensive evaluation. It is crucial to acknowledge that the quality of imputation has a significant impact on the predictive accuracy of models, particularly in fields where data integrity is crucial. Our findings highlight the importance of continuous development in imputation methods, keeping pace with evolving data complexities and advancements in AI. This research contributes to the broader understanding of missing data imputation, setting a foundational stage for future innovations in predictive modeling.

Conclusion

This paper introduces a novel transformer-based prediction model to handle the critical problem of dataset missing value imputation. By methodically explaining the process, we demonstrated a comprehensive strategy that outperformed conventional imputation strategies, such as zero imputation, mean imputation, and KNN imputation. The suggested model demonstrated exceptional prediction powers by capturing complex patterns in sequential data. Our model significantly outperformed alternative imputation techniques after extensive validation using LSTM networks, highlighting its effectiveness and resilience. The present study significantly contributes to advancing missing values imputation approaches by providing a detailed comparative analysis of transformer-based and conventional methods. In light of the difficulties associated with missing data, the suggested approach closes a large gap in the literature and offers a viable path toward more trustworthy data analysis.

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