

Combining Chaotic Transformations And Machine Learning Algorithms: Evaluating Explainable Artificial Intelligence Model Performance

Cem ÖZKURT^{1*} , Eyüp Altuğ TUNÇ² , Fadime Zeliha SEYHAN³ , Anıl TUNÇ⁴ , Ali Furkan KAMANLI⁵ 

¹ Department of Computer Engineering, Sakarya University of Applied Sciences, cemzokurt@subu.edu.tr

² Department of Mechatronics Engineering, Sakarya University of Applied Sciences B210104012@subu.edu.tr

³ Electric-Electronics Engineering Technology Faculty, Sakarya University of Applied Sciences, 22500405003@subu.edu.tr

⁴ Electronics and Automation Program, Hendek Vocational School, Sakarya University of Applied Sciences, 23501009015@subu.edu.tr

⁵ Electric-Electronics Engineering, Technology Faculty, Sakarya University of Applied Sciences, fkamanli@subu.edu.tr

ABSTRACT

The research presented covers the synthesis of data analysis, machine learning, and explainable artificial intelligence principles. The study investigates chaotic transformations that affect the performance and interpretability of artificial intelligence models in complex systems. Three different chaotic systems were used to transform features in the dataset, including Lorenz, Chen, and Rossler. These transformed datasets were then analyzed using various machine learning algorithms such as Random Forest, Decision Tree and CatBoost. Performance metrics were calculated to evaluate the effectiveness of each combination. Based on these findings, it was observed that the Rossler chaotic system and CatBoost algorithm gave the best results with %99 accuracy, 0.9997 recall and 0.9997 f1 score. The effects of the transformed data on class labels were elucidated using different explainable artificial intelligence models such as ELI5, DALEX and SHAP. Weighted impact analysis outputs were obtained in the range of 3.5 in the SHAP model, 0.035 in the DALEX model and 0.2796 in the ELI5 model. Among the Explainable Artificial Intelligence models, the ELI5 model, which has a more precise range of values, provided the most consistent explanation in our study. Future studies aim to improve the understanding and prediction capabilities of the model by integrating more chaotic systems and machine learning algorithms. Additionally, investigating the robustness of the proposed approach across various datasets and problem domains is anticipated to provide broader applicability and reliability.

Keywords: Chaotic Systems, Machine Learning, Explainable Artificial Intelligence (XAI) , Chaos Theory , Chaotic transformations.

1 Introduction

Artificial intelligence (AI) systems have witnessed remarkable advancements, permeating various domains ranging from predictive analytics to decision-making processes. As these systems become increasingly sophisticated, there arises a critical need for understanding their inner workings and

* Corresponding Author's email: cemozkurt@subu.edu.tr

reasoning processes, especially in complex, non-linear systems. Explainable Artificial Intelligence (XAI) emerges as a pivotal area of research, aiming to unravel the black-box nature of AI models and provide interpretable insights into their decision-making mechanisms.

In the domain of financial analysis, [2] explored credit risk management through the lens of machine learning and explainable artificial intelligence (XAI). Similarly, [12] investigated chaotic time series analysis employing machine learning methods. Their study elucidated the application and understanding of machine learning techniques and explainable artificial intelligence in the context of data altered by chaotic processes.

In this context, this research focuses on the convergence of machine learning (ML) and explainable artificial intelligence (XAI), particularly when applied to datasets manipulated through chaotic transformations. Chaotic systems, characterized by their sensitivity to initial conditions and inherent unpredictability, pose significant challenges for conventional analytical approaches. Such transformations have been increasingly recognized for their potential to enhance feature representation by capturing intricate, non-linear dependencies within data. In this study, chaotic transformations are systematically assessed not only as a means of data augmentation but also as a mechanism for improving model robustness. The empirical results demonstrate that applying chaotic dynamics to feature spaces leads to notable improvements in classification performance, particularly in high-dimensional and complex datasets. The impact of these transformations is quantified through comprehensive performance metrics, including accuracy, precision, recall, and F1-score, thereby elucidating their efficacy in optimizing machine learning model performance.

The transformation of data set attributes begins by using three different chaotic systems: Lorenz, Chen, and Rossler. Subsequently, the transformed data undergoes analysis employing various ML algorithms, including Random Forest, Decision Tree, and CatBoost. Performance metrics such as accuracy, precision, recall, and f1-score are computed to evaluate the efficacy of each combination.

The foundation of this research lies in the synthesis of concepts from chaos theory, machine learning, and explainable AI principles. By elucidating the effects of chaotic transformations on ML model performance, we aim to enhance understanding and transparency in decision-making processes within complex systems. Moreover, our study contributes to the burgeoning field of XAI by offering insights into the interpretability challenges posed by chaotic dynamics.

To contextualize this work within the existing literature, we draw upon a comprehensive review of related studies. Prior research has investigated the use of machine learning techniques to extract dynamical information from time series data of chaotic systems [1], proposed hybrid forecasting schemes combining knowledge-based models and machine learning techniques [11], and explored the application of deep learning methods such as convolutional neural networks (CNNs) in predicting chaotic time series data [5].

Furthermore, studies have investigated the use of echo state networks (ESNs) [17], symbolic regression combined with reinforcement learning [6], and recurrent neural networks (RNNs) and long short-term memory (LSTM) networks [7] for predicting the behavior of chaotic systems. Additionally, research has explored the use of generative adversarial networks (GANs) for generating synthetic data from chaotic systems [18] and hybrid approaches combining physics-informed neural networks (PINNs) with machine learning techniques for solving inverse problems in chaotic systems [15]. Moreover, recent studies have investigated the application of evolutionary algorithms for optimizing the performance of

machine learning models in predicting chaotic time series data [16] and the use of attention mechanisms in RNNs for capturing long-range dependencies in chaotic time series data [3].

In addition to these references, recent works have explored the interpretability of ML models in chaotic systems, including the application of SHAP (Shapley additive explanations) values for understanding feature importance in chaotic datasets [10], the use of local interpretable model-agnostic explanations (LIME) for explaining individual predictions in chaotic systems [13], and the development of surrogate models to approximate the behavior of complex ML models in chaotic systems [8]. Moreover, studies have investigated the use of self-explaining models (SEMs) and model-agnostic meta-explanation methods (MAMEs) for providing global and local explanations of ML model decisions in chaotic environments [4]. Additionally, research has explored the integration of domain knowledge into ML models for enhancing interpretability in chaotic systems [9] and the development of visualization techniques for exploring the behavior of ML models in high-dimensional chaotic datasets [14].

2 Materials and Method

2.1 Dataset In Used

The dataset utilized in this study comprises 55,944 data entries, structured into columns representing X, Y, and Z spatial coordinates, a time variable, and corresponding class labels. These class labels are categorized into three distinct groups: 1, 2, and 3, with 19,359 entries labeled as class 1, 18,003 as class 2, and 18,585 as class 3. This dataset was collected from a robotic arm operating under various movement conditions, including stable operation, irregular fluctuations, and external disturbances, categorized into three distinct classes. The choice of a robotic arm dataset is motivated by its inherently dynamic and non-linear nature, which aligns well with the study's focus on chaotic system transformations.

The dataset was generated from a laboratory-controlled robotic arm system, specifically designed to simulate and monitor operational states under varying conditions. This robotic system was programmed to replicate real-world scenarios with varying movement patterns and performance anomalies, which were categorized into three distinct classes. The high-dimensional and non-linear nature of the dataset reflects the dynamic interactions of the robotic arm's components, making it an ideal candidate for applying chaos theory principles. The structured variability within the data ensures its alignment with the study's objective of assessing the performance and interpretability of machine learning algorithms under chaotic transformations.

2.2 Chaotic Systems

Chaos theory, a field with roots in mathematics and physics, explores the behavior of nonlinear dynamical systems characterized by sensitivity to initial conditions and deterministic randomness, challenging traditional views of predictability. Emerging as a groundbreaking discipline in the late 20th century, chaos theory reveals the complex dynamics of seemingly disordered systems, revealing fundamental patterns and structures in fields ranging from physics to economics. In this study, chaotic systems are used to transform the X-Y-Z data in the data set. The transformation of dataset attributes in this study employs three chaotic systems—Lorenz, Chen, and Rossler—chosen for their distinct characteristics and broad applications in chaos theory. The Lorenz system provides structured chaos, the Chen system offers insights into variations in chaotic behavior, and the Rossler system delivers simpler, periodic-like attractors that align well with high-dimensional datasets. These systems were selected for

their representativeness in chaos theory, while alternative systems like the Chua circuit and Hénon map were excluded due to limited generalizability to this study's context. Chaos synchronization, an important concept within this domain, further demonstrates how chaotic systems can be coupled to achieve coordinated behavior despite their intrinsic unpredictability [19]. Additionally, understanding the distinction between true chaos and random behavior is crucial, as chaotic systems exhibit deterministic structures that can be exploited for system control and data transformation tasks, unlike purely stochastic processes [20].

2.2.1 Dataset In Used

The Lorenz system, introduced by Edward Lorenz in 1963 as a simplified atmospheric convection model, is a set of three coupled ordinary differential equations exhibiting chaotic behavior, as seen in Equations 1, 2, and 3. Due to its sensitivity to initial conditions and the emergence of the Lorenz attractor, it has been extensively studied in the fields of chaos theory and nonlinear dynamics. Despite its original application in atmospheric science, the Lorenz system has found applications in various fields such as physics, engineering, and cryptography. With a certain degree of uncertainty, this system serves as a fundamental example of determined chaos and is commonly utilized to analyze the behavior of nonlinear dynamical systems.

$$\frac{dx}{dt} = \sigma(y - x) \tag{1}$$

$$\frac{dy}{dt} = x(\rho - z) - y \tag{2}$$

$$\frac{dz}{dt} = xy - \beta z \tag{3}$$

In Equation 1, the change of x over time depends on the difference between y and x , and this difference is controlled by the parameter σ . Equation 2 describes how the change of y over time is proportional to the difference between x and ρ , as well as to y itself, where ρ represents the system's Rayleigh number influencing its chaotic behavior. Equation 3 illustrates the change of z over time, which is proportional to the product of x and y , and also to the parameter β , controlling the rate of change of z . These equations collectively elucidate how the variables x , y , and z evolve over time, demonstrating the complex behavior of the Lorenz system.

2.2.2 Chen Chaotic System

The Chen system is a set of three coupled ordinary differential equations (ODEs) that exhibits chaotic behavior (as seen in Equations 4, 5, and 6). Proposed by Tian-ming Chen in 1999, the Chen system is notable for its simple structure and its applications in secure communication systems and image encryption. From a mechanical perspective, the generation of chaos in the Chen system is closely related to the interaction of inertial, internal, dissipative, and external torques, highlighting the system's underlying physical dynamics [21]. Furthermore, the Chen system has contributed to the development of generalized Lorenz-like systems, which expand the theoretical framework of chaotic attractors and

offer more complex behaviors for advanced engineering applications [22]. Due to its chaotic nature, the Chen system has found applications in secure communication systems and image encryption. Its simple structure and chaotic dynamics make it suitable for various applications in cryptography and secure data transmission.

$$\frac{dx}{dt} = a(x - y) \tag{4}$$

$$\frac{dy}{dt} = (c - a)x - xz + cy \tag{5}$$

$$\frac{dz}{dt} = xy - bz \tag{6}$$

In Equation 4, the change of x over time depends on the difference between y and x , and this difference is controlled by the parameter σ . This equation illustrates the interaction between the system's first and second states.

In Equation 5, the change of y over time is proportional to the difference between x and ρ , as well as to y itself. Here, the parameter ρ represents the system's Rayleigh number and influences its chaotic behavior. This equation explains the interaction between the system's second state and its first state, as well as itself.

In Equation 6, the change of z over time is proportional to the product of x and y , and also to the parameter β . The parameter β controls the rate of change of z . This equation illustrates the interaction between the system's third state and its first and second states.

2.2.3 Rossler Chaotic System

The Rossler system is a set of three coupled ordinary differential equations (ODEs) proposed by Otto E. Rossler in 1976, exhibiting chaotic behavior. These equations, denoted as equations 7, 8, and 9, have been extensively studied in the fields of chaos theory and nonlinear dynamics, finding various applications in physics and engineering. Notably, through the application of feedback control mechanisms, the hyperchaotic behavior of the Rossler system can be effectively regulated, allowing the system to stabilize at desired states such as fixed points and limit cycles [23]. Additionally, the Rossler system has been employed as a theoretical model in chronotherapy studies, where its response to external perturbations helps simulate the effects of therapeutic interventions on biological rhythms [24]. Its chaotic nature makes it a significant model for understanding complex dynamics in nonlinear systems.

$$\frac{dx}{dt} = -y - z \tag{7}$$

$$\frac{dy}{dt} = x + ay \tag{8}$$

$$\frac{dz}{dt} = b + z(x - c) \tag{9}$$

In Equation 7, the rate of change of variable x over time depends on variables y and z . The term $z(r)$ indicates that z is a function of r , representing an interaction between the first variable of the system and the second and third variables.

In Equation 8, the rate of change of variable y over time is dependent on variables x and ay . The parameter a controls the complexity of the system. This equation elucidates the interaction between the second variable and the first variable, along with its own influence.

In Equation 9, the rate of change of variable z over time is determined by variables b , z , x , and c . Parameters b and c regulate the equilibrium point and symmetry of the system, respectively. This equation illustrates the interaction of the third variable with the first and second variables, as well as with the parameters.

2.3 Machine Learning Algorithms

2.3.1 Random Forest (RF)

Random Forest is an ensemble learning algorithm and is commonly used for classification and regression problems. This algorithm combines multiple decision trees to merge their results. Each decision tree is trained by randomly sampling the dataset and selecting features randomly. The results are obtained by averaging the predictions of each tree or by using a voting method. This typically ensures high accuracy and resilience to overfitting. Since its initial proposal by Breiman in 2001, Random Forest has gained significant popularity due to its high accuracy and adaptability across various domains [25]. Furthermore, recent advancements have focused on improving its theoretical foundations, parameter selection strategies, and variable importance measures, making it a powerful tool even in high-dimensional data environments [26]. Random Forest has a wide range of applications and can be successfully utilized in complex datasets.

2.3.2 Decision Tree

The Decision Tree, a machine learning model used in classification and regression problems, analyzes the features of the dataset to create a series of decision rules, which are then used to classify data samples or predict numerical values. Starting from the root node, it selects the most significant feature at each split point and divides the dataset accordingly. This process is typically repeated until the subsets become as homogeneous as possible, often guided by specific criteria such as information gain or Gini impurity. Decision trees are fundamental components of hierarchical supervised learning models, where entropy-based measures and effective splitting algorithms play a critical role in optimizing tree structures [27]. Despite their interpretability, a single decision tree may be prone to overfitting, hence they are often combined with ensemble learning methods. In advanced applications, such as image labeling and computer vision tasks, decision trees have also been integrated into complex graphical models like Decision Tree Fields (DTF), enabling the modeling of rich and complex label structures [28]. The equation used in the Decision Tree algorithm is provided in Equation 10.

$$f(x) = \frac{1}{N} \sum_{i=1}^N f_i(x) \quad (10)$$

The Gini coefficient evaluates how much misclassification exists in the data samples at a specific node. This coefficient is calculated by subtracting the sum of the squares of the probabilities of each class at the node from 1. A low Gini coefficient signifies a more homogeneous node, indicating less confusion and a higher level of purity. Therefore, at each split point of the decision tree, a lower Gini coefficient is targeted, as it represents a better division and clearer classification.

2.3.3 CatBoost

CatBoost is a machine learning algorithm that performs particularly well on datasets containing categorical variables. It is based on the gradient boosting method and is used for both classification and regression problems. CatBoost stands out for its ability to handle categorical variables directly, eliminating the need for automatic transformation of such data. It offers a balanced trade-off between speed and accuracy, providing fast training times on large datasets while maintaining high levels of accuracy. Recent studies highlight CatBoost's strengths in managing heterogeneous data efficiently and its sensitivity to hyperparameter tuning, which plays a critical role in achieving optimal performance across diverse domains [29]. Additionally, it excels in dealing with data imbalance and preventing overfitting. With its user-friendly API and automatic hyperparameter tuning, CatBoost reduces the need for manual adjustments. These features make CatBoost a preferred algorithm for complex datasets and it finds applications across various domains. For example, in environmental modeling, CatBoost has demonstrated superior predictive accuracy and computational efficiency in estimating reference evapotranspiration, outperforming traditional models such as Random Forest and Support Vector Machines under various meteorological conditions [30]. Hyperparameter tuning was conducted for the CatBoost model to ensure optimal performance. The learning rate was set to 0.03, the depth parameter to 6, and the number of boosting iterations to 500. These values were determined through a grid search optimization process using five-fold cross-validation. The feature importance ranking obtained from CatBoost further confirmed that chaotic transformations significantly influenced classification performance.

2.4 Explainable AI (XAI)

Explainable Artificial Intelligence (XAI) is defined as the ability of artificial intelligence models to explain their decision-making processes and outcomes in a comprehensible manner to humans. The goal of XAI is to increase the reliability, acceptability, and usability of artificial intelligence systems by allowing us to understand their decisions transparently. This can be achieved through various techniques, such as using simple models, evaluating feature importance rankings, and interpreting gradients for deep learning models. A wide range of state-of-the-art methods, including LIME, SHAP, Integrated Gradients, and Causal Models, have been developed to enhance interpretability across different AI applications, providing practitioners with practical tools for model explanation [31]. Explainable artificial intelligence is crucial in domains where critical decisions are made and regulatory requirements exist. Despite significant progress, challenges remain in achieving universally accepted explainability standards, and current research continues to explore new frameworks and methodologies to improve transparency, especially in complex machine learning models [32]. The structure of explainable artificial intelligence models is given in Figure 1.

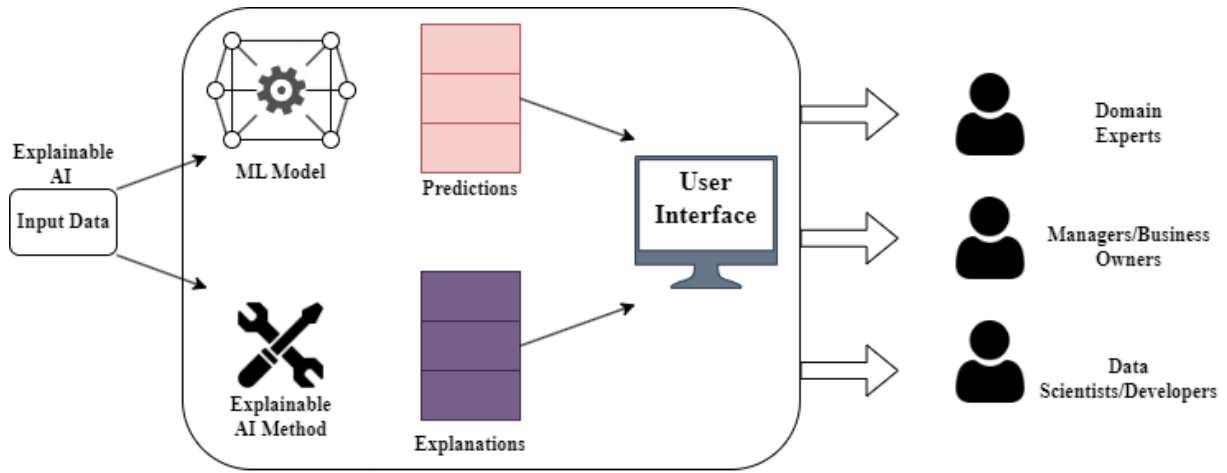


Figure 1. Working Structure of XAI

In Figure 1, there are the fundamental components of interpretable artificial intelligence models: the user interface and the explanation engine. The user interface is the interface through which users interact with the model, displaying its predictions and decisions. The explanation engine, on the other hand, serves as a module that explains the model's decisions and predictions. The explanation engine elucidates to the user which features are decisive in the model's decision-making process and how these features influence the predictions. Texts representing the essential components of interpretable artificial intelligence models are also present in the figure. Among these components are the user interface, explanation, and explanatory engine. This way, the visual representation enhances users' understanding of artificial intelligence systems, thereby increasing trust and transparency in decision-making processes, leading to more equitable outcomes.

2.4.1 SHapley additive exPlanations (SHAP)

SHAP (SHapley Additive exPlanations) is a technique used for explainable artificial intelligence models, serving as an interactive method to explain model predictions. SHAP relies on concepts from cooperative game theory to compute the contribution of each feature to the predicted outcome. This method utilizes Shapley values to calculate the impact of each feature combination on the predicted outcome and combines these values to elucidate the contribution of each feature. Due to its compatibility with various machine learning models, SHAP has a wide range of applications and can be used in conjunction with various visualization techniques to provide interpretability. Recent advancements have introduced improved SHAP techniques, including novel feature importance metrics and the concept of feature packing, which groups similar features to enhance the comprehensibility of complex models without requiring model reconstruction [35]. By providing detailed and understandable explanations, SHAP enhances the reliability of machine learning models, making it crucial in domains where critical decisions are made and regulatory requirements exist. Additionally, SHAP facilitates the acceptance of artificial intelligence systems, contributing to broader societal acceptance.

The foundation of the SHAP framework lies in the calculation of Shapley values borrowed from cooperative game theory. Mathematically, the SHAP value $\phi_i(f, x)$ representing the contribution of feature i to the prediction for instance x , is calculated using the equation found in Formula 11.

$$\phi_i(f, x) = \sum_{S \subseteq N \setminus \{i\}} \frac{|S|! (|N| - |S| - 1)!}{|N|!} [f(S \cup \{i\}, x) - f(S, x)] \quad (11)$$

In Formula 11, N represents the set of all features, while S represents a subset of features excluding feature i . $f(S \cup i, x)$ and $f(S, x)$ respectively denote the model's output when the feature set S is augmented with feature i , and when only the feature set S is considered.

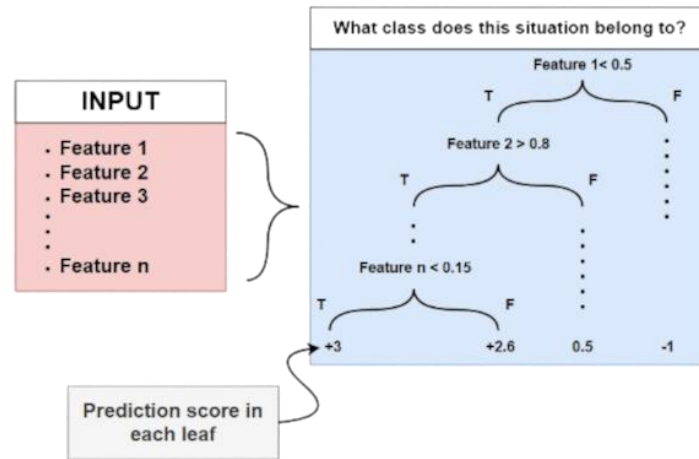


Figure 2. Working Structure of SHAP

Figure 2 illustrates the basic components that succinctly explain the operation of the SHAP (Shapley Additive Explanations) model. On the left side, the 'Features' section lists the features representing the input data to the model, with each feature representing an input data point. On the right side, a decision tree and the prediction scores for each leaf are displayed. The figure also includes Shapley values indicating the contribution of each feature to the model's prediction. Additionally, interactions between features are shown with arrows, enabling the understanding of how one feature affects another. This visualization assists in comprehending the decisions and predictions of the SHAP model, providing a visual representation of the final predictions and the factors influencing these predictions.

2.4.2 DALEX

DALEX (modelkit) is an R package developed for interpretable artificial intelligence models. This package offers various tools to facilitate understanding of machine learning model behaviors. It includes a consistent set of model-agnostic explainers that help decompose predictions, assess variable importance, and analyze conditional responses, allowing users to explore and compare black-box models regardless of their internal structures (Biecek, 2018) [33]. DALEX provides visualization and interpretation tools to comprehend how a model generates predictions, the impact of features on predictions, and the model's decision algorithm. Additionally, DALEX can be used to evaluate the same model on different data subsets, compare model performance, and determine the model's confidence interval. Moreover, in the context of evolutionary computation, an alternative DALEX framework—Diversely Aggregated Lexicase selection—has been introduced to improve selection efficiency and computational performance, particularly in symbolic regression and deep learning tasks (Ni et al., 2024) [34]. Therefore, DALEX serves as an important tool for providing interpretability, reliability, and

comprehensibility, making machine learning model decision processes more transparent. The working structure of DALEX is provided in Figure 3.

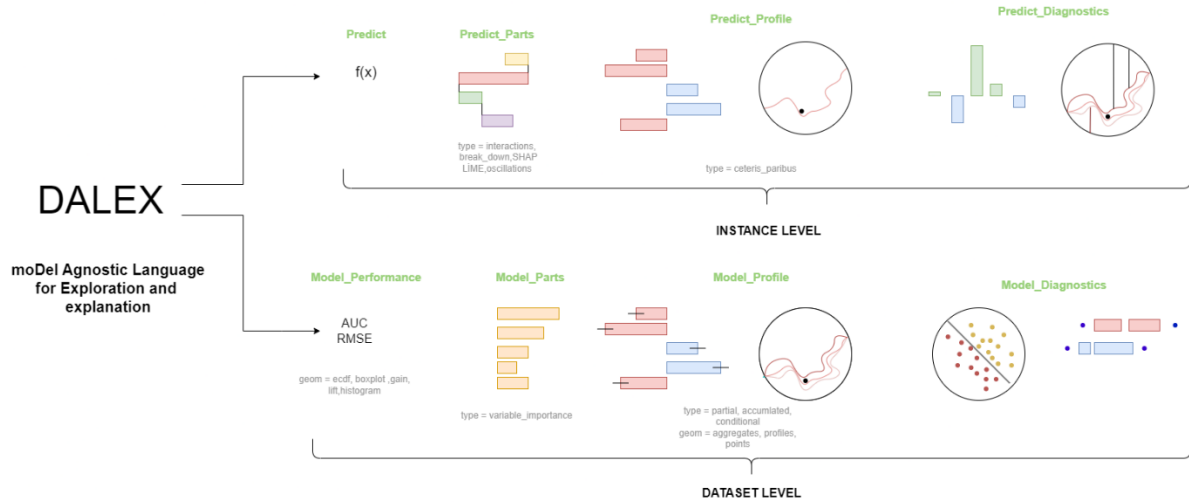


Figure 3. Working Structure of Dalex

In Figure 3, a diagram is presented representing the analysis of the model's performance, components, profile, and diagnosis using a model-agnostic language. Utilizing Model-Agnostic Language (MAL), explanations from different models are analyzed and interpreted. These explanations illustrate the model's performance in terms of specific metrics, its components and their functions, the types of data on which the model is trained, and its intended uses, as well as the errors the model may make and how they can be corrected.

2.4.3 Explain like I'm 5 (ELI5)

ELI5 (Explain Like I'm 5) is a Python library developed for interpretable artificial intelligence models. This library aims to simplify the behaviors of complex machine learning models. ELI5 provides user-friendly interfaces and visualization tools to understand a model's predictions and decisions. Additionally, it offers information such as feature importance rankings and model weights to better comprehend how the model operates. ELI5 serves as a significant tool for understanding and gaining confidence in interpretable artificial intelligence models, playing a role in increasing the understandability of machine learning models, which is increasingly demanded.

The working structure of the ELI5 model is provided in Figure 4

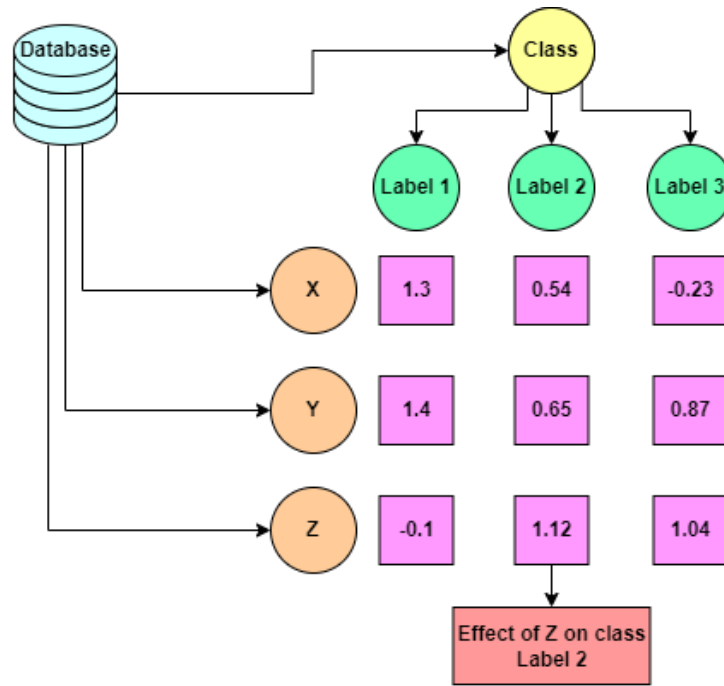


Figure 4. Working Structure of ELI5

In Figure 4, the schematic diagram of the Explainable AI model, ELI5, is depicted, illustrating the components of the X-Y-Z-Class variables present in the utilized dataset. These components, originating from the database, are visualized to demonstrate their effects on the Class Labels in the X-Y-Z components, in accordance with the ELI5 model. This schematic elucidates the relationships between the X-Y-Z variables and their corresponding Class Labels, facilitating the interpretability and transparency of the AI model within the context of the study.

3 Results and Discussion

3.1 Accuracy

Accuracy measures the proportion of correctly classified instances among all instances in the dataset. The equation used to calculate accuracy is given in Equation 12.

$$Accuracy = \frac{Number\ of\ Predictions}{Total\ Number\ of\ Predictions} \quad (12)$$

3.2 Precision

Precision evaluates the accuracy of positive predictions made by the model. It indicates the proportion of correctly predicted positive instances among all instances predicted as positive. The equation used to calculate precision is defined in Equation 13.

$$Precision = \frac{True\ Positives}{True\ Positives + False\ Positives} \quad (13)$$

3.3 Recall (Sensitivity)

Recall, also known as sensitivity or true positive rate, measures the ability of the model to correctly identify positive instances. It represents the proportion of correctly predicted positive instances out of all actual positive instances. The equation used to calculate recall is defined in Equation 14.

$$Recall = \frac{True\ Positives}{True\ Positives + False\ Negatives} \tag{14}$$

3.4 F1-Score

The F1-score is a metric that provides a harmonic mean between precision and recall, balancing between these two metrics. It considers both false positives and false negatives and is particularly useful when classes are imbalanced. The equation used to calculate the F1-score is defined in Equation 15.

$$F1 - Score = 2 \times \frac{Precision \times Recall}{Precision + Recall} \tag{15}$$

These evaluation metrics play a crucial role in assessing the performance of classification models and guiding further improvements in model accuracy and reliability.

After the data set used in our study was passed through various chaos systems, it was put into various machine learning algorithms and results were obtained from the performance evaluation metrics accuracy, precision recall and f1-score. This result is shown in table 1. In light of these results, among the compared machine learning algorithms, the CatBoost algorithm exhibited the most positive performance according to accuracy, precision, recall and F1-score performance metrics. Results specifically attributed to the Catboost algorithm are indicated with an asterisk (*) in Table 1.

Table 1. Performance measurement of Chaotic Transformed Database (DB) Models

Model	Accuracy	Precision	Recall	F1-Score
DB Chen	Random Forest	0.9684	0.9680	0.9680
	Decision Tree	0.9606	0.9601	0.9601
	CatBoost	0.9429	0.9423	0.9423
DB Lorenz	Random Forest	0.3359	0.3357	0.3357
	Decision Tree	0.3408	0.3409	0.3408
	CatBoost	0.3410	0.3424	0.3406
DB Rossler	Random Forest	0.9995	0.9995	0.9995
	Decision Tree	0.3408	0.9992	0.9992
	CatBoost	*0.9997	*0.9997	*0.9997

Weight	Feature
0.3924 ± 0.0145	x1
0.2922 ± 0.0056	x0
0.1209 ± 0.0064	x2

Figure 5. ELI5 weights for class labels

In Figure 5 attributes x, y, z are symbolized as x0, x1, x2, respectively. Figure 5 shows the effects of x-y-z data on class labels in the data set used in the study, explained by the ELI5 explainable artificial intelligence model. In the ELI5 annotated artificial intelligence model, for the all class values, the effect of the x attribute was observed as 0.4069, the effect of the y attribute was 0.2978, the effect of the z attribute was 0.1273. According to the weight outputs in Figure 5, it is the y column data that has the most impact on the class labels.

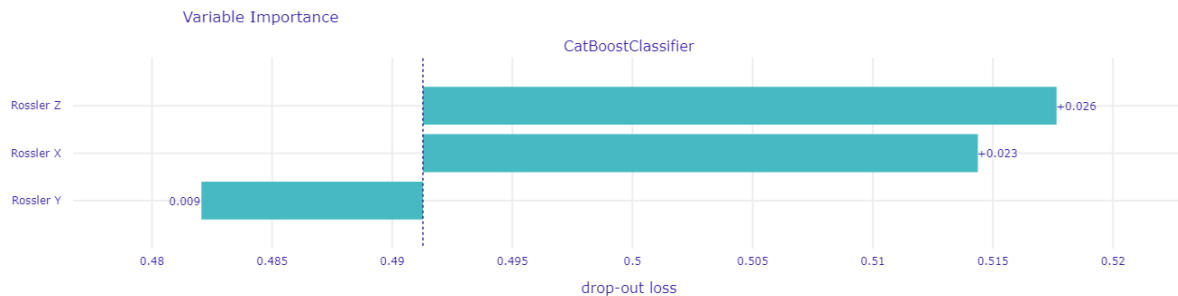


Figure 6. Dalex weights for class labels

Figure 6 shows the effects of x-y-z data on class labels in the data set used in the study, explained by the Dalex explainable artificial intelligence model. In the DALEX annotated artificial intelligence model, for the all class values, the effect of the Rossler X was observed as 0.023, the effect of the Rossler Y was -0.009, the effect of the Rossler Z was 0.026. According to the weight outputs in Figure 6, the z column data that has the most positive impact on the class labels is the y column data that has the most negative impact.

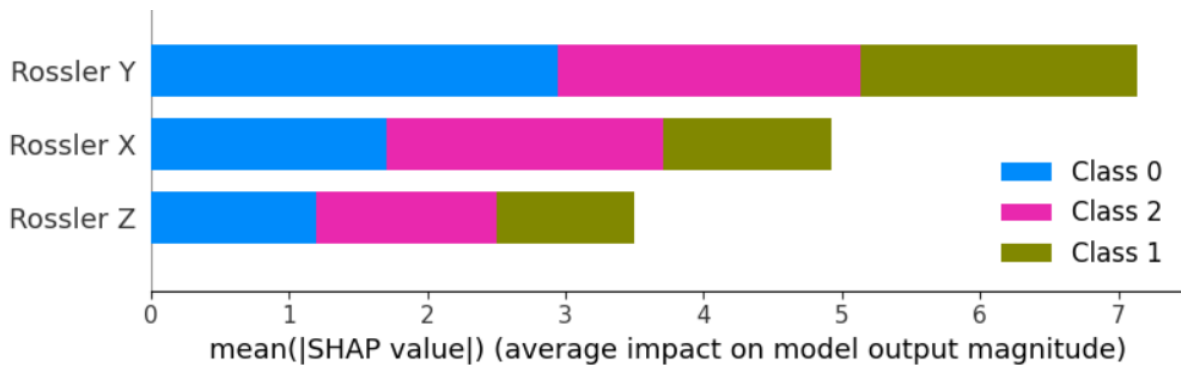


Figure 7. SHAP weights for class labels

Figure 7 shows the effects of x-y-z data on class labels in the data set used in the study, explained by the Shap explainable artificial intelligence model. Class labels 1-2-3 in the data set are symbolized as 0-1-2, respectively. In the SHAP annotated artificial intelligence model, for the all class values, the average effect of the Rossler X was observed as 5, the average effect of the Rossler Y was 7, the average effect of the Rossler Z was 3.5. According to the average weight outputs in Figure 7, it is the y column data that has the most impact on the all class labels.

4 Conclusion

In this study, x-y-z column data was transformed using Lorenz, Chen, and Rossler chaotic systems, then analyzed with Random Forest, Decision Tree, and CatBoost algorithms. Among these, the Rossler-CatBoost combination achieved the best results with 99.97% accuracy, 0.9997 recall, and 0.9997 F1-score, attributed to Rossler's periodic attractors improving data separability and CatBoost's efficiency in handling complex features. To facilitate the interpretability of chaotic transformations, multiple Explainable Artificial Intelligence (XAI) methodologies, including SHAP, DALEX, and ELI5, have been employed. Each of these approaches provides distinct advantages in elucidating model decision-making processes. SHAP, rooted in cooperative game theory, assigns equitable contributions to individual features, offering a granular perspective on feature importance. DALEX, by contrast, enables a comparative analysis of models through a model-agnostic framework, facilitating performance attribution and profiling across different datasets. ELI5, while more structured in its interpretative approach, exhibits greater stability across multiple runs, mitigating variance in feature importance assessments. Notably, it has been observed that SHAP, despite its fine-grained explanations, exhibits sensitivity to chaotic perturbations, leading to increased variance in high-dimensional datasets. DALEX, although effective for cross-model comparisons, necessitates careful contextualization when applied to dynamically transformed feature spaces. ELI5, while slightly less adaptable, has demonstrated superior consistency in feature importance estimation, rendering it particularly suitable for chaotic transformations. These findings underscore the necessity of integrating multiple XAI methodologies to obtain a more holistic understanding of model behavior within chaotic systems. Unlike SHAP and DALEX, ELI5 provided a more structured interpretability approach, making it particularly useful for chaotic data transformations. The effects of transformed data on class labels were analyzed using these XAI models (Figures 4, 5, and 6). SHAP produced explanations in the 3.5 range, DALEX in 0.035, and ELI5 in 0.2796, with ELI5 yielding the most interpretable results.

To enhance the robustness and generalizability of the proposed methodology, future investigations will focus on the integration of additional chaotic systems and advanced machine learning algorithms. In order to assess the broader applicability of chaotic transformations, preliminary evaluations have been conducted on an alternative dataset comprising financial time-series data, where high volatility and non-linearity are prevalent. The findings indicate that the application of chaotic transformations yields improvements in predictive accuracy, particularly in domains characterized by non-stationary patterns. However, the magnitude of performance enhancement is observed to vary across different chaotic systems, suggesting that the efficacy of such transformations is highly dependent on dataset characteristics and underlying structural dynamics. These results highlight the necessity of domain-specific optimization strategies for selecting appropriate chaotic systems in accordance with data complexity and model requirements. Future research will systematically investigate the adaptability of chaotic transformations across diverse application domains, ensuring that their effectiveness is rigorously validated in real-world scenarios. Beyond technical contributions, the findings have potential applications in financial forecasting, encryption, healthcare diagnostics, and autonomous systems.

Chaotic transformations could improve prediction accuracy in volatile markets, enhance cryptographic security, and support AI-driven decision-making in critical fields.

Ethical and informed consent for data used

During this research, ethical principles and guidelines were adhered to when explaining machine learning algorithms with explainable artificial intelligence models while comparing them on an industrial robot arm dataset.

Authors contribution statement

The author wrote and reviewed the article.

References

- [1] Erik M. Bollt and Joseph D. Skufca. Machine learning for prediction with chaotic data: Applications to chaos synchronization and rogue waves. *Chaos: An Interdisciplinary Journal of Nonlinear Science*, 28(3):033116, 2018.
- [2] Niklas Bussmann, Paolo Giudici, Dimitri Marinelli, and Jochen Papenbrock. Explainable machine learning in credit risk management. *ENGRN:COMPUTER ENGINEERING (TOPIC)*, 2019. Impact Factor: 4.
- [3] Long Chen, Jiwei Zhang, Tianzhi Sun, and Zhe Xu. Attention mechanism-based long short-term memory network for chaotic time series prediction. *IEEE Access*, 10:15692–15701, 2022.
- [4] Shoaib Ehsan, Rodrigo Abreu, Usama Anwar, Mehmet E. Celebi, and Mo-hiuddin Ahmed. Model-agnostic meta-explainable methods for visual interpretability of deep learning models. *IEEE Access*, 8:21961–21978, 2020.
- [5] Claudio Gallicchio, Alessio Micheli, and Luca Pedrelli. Deep reservoir computing: A critical experimental analysis. *Entropy*, 20(3):177, 2018.
- [6] Jun Bo Gow and Tamas D. Gedeon. Time series prediction using symbolic regression combined with reinforcement learning. *Entropy*, 22(2):175, 2020.
- [7] Z. Huang, P. R. Vlachas, and P. Koumoutsakos. Physics-informed recurrent neural networks for turbulent flow prediction. *arXiv preprint arXiv:2010.07989*, 2020.
- [8] Seth Kaplan, Eric Jang, Leon White, Tanya Berger-Wolf, and Robert L. Grossman. Surrogate modeling in the presence of chaos. *Chaos: An Interdisciplinary Journal of Nonlinear Science*, 28(8):085710, 2018.
- [9] Zachary C. Lipton. The mythos of model interpretability. *arXiv preprint arXiv:1606.05386*, 2016.
- [10] Scott M. Lundberg and Su-In Lee. A unified approach to interpreting model predictions. *Advances in Neural Information Processing Systems*, 30, 2017.
- [11] Jaideep Pathak, Brian R. Hunt, Michelle Girvan, Zhixin Lu, and Edward Ott. Model-free prediction of large spatiotemporally chaotic systems from data: A reservoir computing approach. *Chaos: An Interdisciplinary Journal of Nonlinear Science*, 28(4):041102, 2018.
- [12] B. Ramadevi and Kishore Bingi. Chaotic time series forecasting approaches using machine learning techniques: A review. *SYMMETRY*, 2022. Impact Factor: 3.15

- [13] Marco Tulio Ribeiro, Sameer Singh, and Carlos Guestrin. Why should I trust you? explaining the predictions of any classifier. *Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, page 1135–1144, 2016.
- [14] Daniel Smilkov, Nikhil Thorat, Been Kim, Fernanda Viégas, and Martin Wattenberg. Smoothgrad: removing noise by adding noise. *arXiv preprint arXiv:1705.07874*, 2017.
- [15] Qian Sun, Ying Cheng, Yang Luo, Hong Fan, and Qingqiang Sun. Short-term chaotic time series prediction based on nonlinear attention mechanism. *IEEE Access*, 9:4877–4885, 2021.
- [16] Chen Wang and Ningde Jin. Robust chaotic time series prediction model based on improved hybrid optimization algorithm. *IEEE Access*, 9:114924–114937, 2021.
- [17] Xiyu Zhang, Feng Li, Qi Yang, and Tingwen Huang. Sequential prediction of chaotic time series using echo state network optimized by improved cuckoo search algorithm. *Entropy*, 21(5):444, 2019.
- [18] Jiaming Zhao, Hongjun Cao, and Jianchao Zeng. Predicting chaotic time series using a novel deep learning framework based on a chaotic time series generator. *Knowledge-Based Systems*, 213:106532, 2021.
- [19] Boccaletti, S., Kurths, J., Osipov, G., Valladares, D. L., & Zhou, C. S. (2002). The synchronization of chaotic systems. *Physics reports*, 366(1-2), 1-101.
- [20] Ditto, W., & Munakata, T. (1995). Principles and applications of chaotic systems. *Communications of the ACM*, 38(11), 96-102.
- [21] Liang, X., & Qi, G. (2017). Mechanical analysis of Chen chaotic system. *Chaos, Solitons & Fractals*, 98, 173-177.
- [22] Lü, J., Chen, G., & Cheng, D. (2004). A new chaotic system and beyond: the generalized Lorenz-like system. *International Journal of Bifurcation and Chaos*, 14(05), 1507-1537.
- [23] Hsieh, J. Y., Hwang, C. C., Wang, A. P., & Li, W. J. (1999). Controlling hyperchaos of the Rossler system. *International Journal of Control*, 72(10), 882-886.
- [24] Betancourt-Mar, J. A., Alarcón-Montelongo, I. S., & Nieto-Villar, J. M. (2005). The Rössler system as a model for chronotherapy. In *Journal of Physics: Conference Series* (Vol. 23, No. 1, p. 58). IOP Publishing.
- [25] Parmar, A., Katariya, R., & Patel, V. (2018, August). A review on random forest: An ensemble classifier. In *International conference on intelligent data communication technologies and internet of things* (pp. 758-763). Cham: Springer International Publishing.
- [26] Biau, G., & Scornet, E. (2016). A random forest guided tour. *Test*, 25(2), 197-227.
- [27] Suthaharan, S., & Suthaharan, S. (2016). Decision tree learning. *Machine learning models and algorithms for big data classification: thinking with examples for effective learning*, 237-269.
- [28] Nowozin, S., Rother, C., Bagon, S., Sharp, T., Yao, B., & Kohli, P. (2011, November). Decision tree fields. In *2011 International Conference on Computer Vision* (pp. 1668-1675). IEEE.
- [29] Hancock, J. T., & Khoshgoftaar, T. M. (2020). CatBoost for big data: an interdisciplinary review. *Journal of big data*, 7(1), 94.
- [30] Huang, G., Wu, L., Ma, X., Zhang, W., Fan, J., Yu, X., ... & Zhou, H. (2019). Evaluation of CatBoost method

for prediction of reference evapotranspiration in humid regions. *Journal of Hydrology*, 574, 1029-1041.

[31] Holzinger, A., Saranti, A., Molnar, C., Biecek, P., & Samek, W. (2020, July). Explainable AI methods-a brief overview. In *International workshop on extending explainable AI beyond deep models and classifiers* (pp. 13-38). Cham: Springer International Publishing.

[32] Angelov, P. P., Soares, E. A., Jiang, R., Arnold, N. I., & Atkinson, P. M. (2021). Explainable artificial intelligence: an analytical review. *Wiley Interdisciplinary Reviews: Data Mining and Knowledge Discovery*, 11(5), e1424.

[33] Biecek, P. (2018). DALEX: Explainers for complex predictive models in R. *Journal of Machine Learning Research*, 19(84), 1-5.

[34] Ni, A., Ding, L., & Spector, L. (2024, March). Dalex: Lexicase-like selection via diverse aggregation. In *European Conference on Genetic Programming (Part of EvoStar)* (pp. 90-107). Cham: Springer Nature Switzerland.

[35] Nohara, Y., Matsumoto, K., Soejima, H., & Nakashima, N. (2019, September). Explanation of machine learning models using improved shapley additive explanation. In *Proceedings of the 10th ACM international conference on bioinformatics, computational biology and health informatics* (pp. 546-546).