Interpretable Soft Sensors using Extremely Randomized Trees and SHAP

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Abstract: Tree-based models are easy to implement and have been widely used in various fields. However, tree-based models have limitations in industrial process applications since the vast majority of tree-based models are prone to over-fitting. In addition, the internal structure of a tree-based model is very complex and the output of the model is also difficult to explain, which makes its application in industrial soft sensors very challenging. The purpose of this work is to build accurate and interpretable soft sensors for industrial processes. First, a robust tree ensemble model, extremely randomized trees, is used to build accurate soft sensors. Then, an interpretable machine learning algorithm, Shapely additive explanation, is used to infer the global and local contributions of each feature to the predictions. Finally, the effectiveness of the proposed algorithms is validated on real industrial fluid catalytic cracker unit data.

Keywords: Interpretability, SHAP, Extremely Randomized Trees, Soft Sensor

1. INTRODUCTION

In modern industrial processes, it is necessary to monitor a large number of critical variables that are closely related to the process's safety and economic benefits (Gopaluni et al. (2020)). These critical variables are called quality variables. However, some quality variables are difficult or expensive to measure by sensors in real-time, which poses challenges for the monitoring and control of industrial processes. To achieve real-time monitoring of quality variables, data-driven soft sensors are proposed to estimate quality variables from easily measured process variables (Zhu et al. (2020)).

With the booming development of big data and computing power, tree-based models (including decision trees (Kotsiantis (2013)), random forests (Ho (1995)), light gradient boosting machine (Ke et al. (2017)), extremely randomized trees (Geurts et al. (2006)), etc.) have been widely used in various fields. Compared with traditional statistical models, tree-based models are easy to understand and implement, and the accuracy of the models is improved by leaps and bounds. During the past decade, almost all winners of Netflix competitions, Kaggle competitions, etc., utilized ensemble tree models in their solutions.

However, these algorithms have limitations in industrial process applications since modern industrial processes are often characterized by high dimensions, multi-collinearity, and strong noise (Cao et al. (2022)). The vast majority of tree-based models are prone to over-fitting due to the characteristics of industrial processes. For example, the well-known decision tree algorithm recursively splits the training data based on the decision nodes. The optimal split is determined by maximizing the certain score function. The score function is sensitive to the training data. Some minor modifications to the original dataset result in an entirely different decision tree, which makes it difficult to generalize.

The decision tree is fairly easy to understand and implement. However, just one tree is not enough to produce valid results. The random forest consists of many decision trees, and there is no relationship between different decision trees. It randomly selects features for each decision tree, then averages the result (regression) or performs a majority voting (classification). A large number of uncorrelated decision trees will produce more accurate predictions than a single decision tree. But, some recent studies have shown that random forests are easily overfitted in the presence of noise(Biau (2012)).

To further avoid over-fitting, extremely randomized trees (ET) is proposed. ET is a tree-based ensemble method that uses a different type of decision tree compared to the random forest. It is superior to the random forest in terms of generalization and has outstanding performance when having redundant and noisy features. ET is similar to random forests but more robust and faster since stronger

randomization when splitting its decision tree node. We will describe the ET in detail in section 2.

Although tree-based ensemble models have achieved good results in many fields, there are little attention has been paid to explaining their predictions. These models have a common problem: the internal structure is very complex, which is difficult for humans to understand. The output of the model is also difficult to explain, which makes its application in some areas related to life safety or important decision-making very risky. Due to the risk-sensitive nature of industrial processes, the reliability and stability of soft sensors are necessary for industrial applications. The interpretation of soft sensor predictions can increase the reliability and stability of soft sensors. Therefore, it is crucial to understand the mechanism of the model and the important factors that affect the decision-making of the model through model interpretation (Du et al. (2019)).

Interpretable machine learning is a popular field of current and future machine learning research (Murdoch et al. (2019)). In this work, an interpretable model is one that can accurately estimate the contribution of each input feature to the model predictions. Shapley value is a concept based on the game theory proposed by economist Lloyd Shapley (Kuhn and Tucker (2016)). Its core idea is to fairly distribute the contributions of each player in a game, and then explain the black-box machine learning model from both global and local levels. If the Shapley value attribution is represented as a linear additive feature model, then it will be Shapley additive explanations (SHAP) model (Lundberg and Lee (2017)). It has a wide variety of applications as well as solid theoretical guarantees (consistency, local accuracy, and missingness) (Molnar (2020)). In this work, We use SHAP to explain ET-based soft sensor predictions, where the player is the input to the soft sensor, the game is the prediction of the soft sensor, and the SHAP value is the contribution of each input to the prediction.

This work aims to establish robust and interpretable industrial soft sensors based on extremely randomized trees and SHAP. The remaining part of this article is organized as follows. In Section 2, detailed explanations of extremely randomized trees and SHAP are given. In Section 3, novel robust and interpretable inferential sensors are put forward, with detailed implementation procedures and analysis. Section 4 presents a case study on the real fluid catalytic cracker (FCC) unit data to verify the effectiveness of the proposed method. Section 5 closes the paper with a summary.

2. METHODS

2.1 Extremely Randomized Trees

Define S as $n \times p$ matrix, n as the number of training samples, p as the number of features, M as the number of trees, K as the number of features that are selected at each node, y as the output label and n_{min} as the minimum sample size for splitting a node.

ET is a tree-based ensemble method for supervised machine learning problems. Fig. 1 shows the structure of ET.

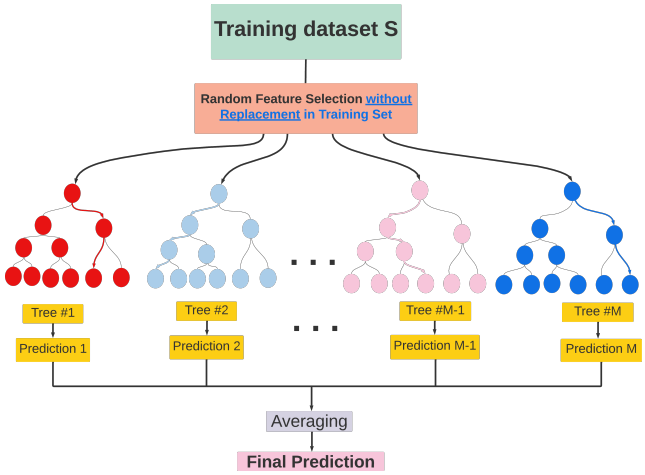

Fig. 1. Extremely Randomized Trees structure

To build ET, the first step is to create M decision trees. Different from random forests, the sampling for each tree is random, without bootstrap replacement. The usage of the full original training dataset (no bootstrap) can minimize the bias of ET. Then, K features among p features are selected randomly to develop ET. The value of K affects the randomness of the tree. In general, the smaller K is, the more random the tree is.

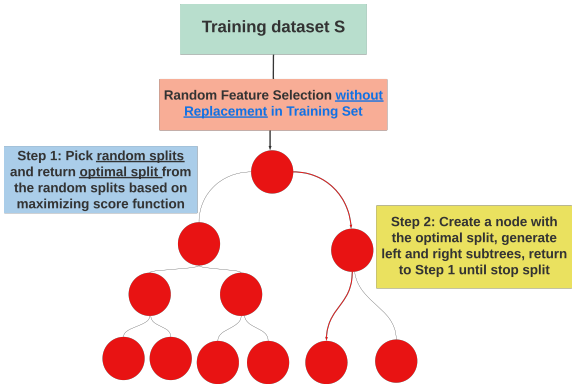

Fig. 2. Singe tree structure of Extremely Randomized Trees

As we know, the traditional decision tree directly calculates the optimal split using entropy or information gain. Entropy is a measure of the uncertainty of a random variable and the information gain represents the degree of uncertainty reduction in the output y with knowing certain feature X. The definition of entropy and information gain can be given as follows:

$$\begin{aligned} &P\left(X=x_i\right)=p_i, i=1,2,\cdots,n \\ &H\left(X\right)=-\sum_{i=1}^{n} p_i log p_i \\ &H\left(y \mid X\right)=\sum_{i=1}^{n} p_i H\left(y \mid X=x_i\right) \\ &IG\left(y,X\right)=H\left(y\right)-H\left(y \mid X\right) \end{aligned} \tag{1}$$

where p is the probability of random variable X, $H\left(X\right)$ is the entropy of random variable X, $H\left(y \mid X\right)$ is the conditional entropy of y given X, $IG\left(y,X\right)$ is the information gain.

Different from the traditional decision tree, every single tree of ET randomly selects the optimal feature and divides the training data into subsets. They are done recursively until all training data subsets are correctly assigned or the sample size in subsets is smaller than n_{min}. Fig. 2 shows the structure of each tree in ET. The algorithm picks random splits and then returns the optimal splitting feature from the random splits based on maximizing score function. Here, the score function in ET regression is defined as follows:

$$Q = \frac{var\{y \mid S\} - \frac{|S_l|}{S} var\{y \mid S_l\} - \frac{|S_r|}{S} var\{y \mid S_r\}}{var\{y \mid S\}} \quad (2)$$

where S_l and S_r represent the two subsets (left subset and right subset) of S that correspond to the split s, $var\{y \mid S\}$ is the variance of y in S. This score function is also called relative variance reduction. In fact, the construction of a tree is a method of dividing the space with a hyperplane. Random splits make the trees more diversified and robust since the optimal split (optimal hyperplane) in random forests may overfit the original dataset.

In this section, we introduce extreme random trees and design a robust soft sensor with ET. Fig. 3 gives the flowchart of an ET-based soft sensor. We also discuss the advantages of extremely randomized trees over random forests and decision tree. Table 1 summarizes the differences and similarities of decision trees, random forests, and extremely randomized trees.

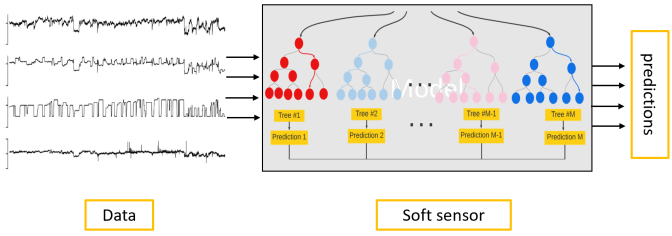

Fig. 3. An ET-based soft sensor

Table 1. Comparison of different tree methods

	ET	RF	DT
Number of trees	Many	Many	1
Decision node	Random features	Random features	All features
Split	Random split	Optimal split	Optimal split
Bootstrapping	No	Yes	NA
Variance	Low	Medium	High

The decision path of a tree is a straightforward interpretable approach, but for large-scale ensemble tree models, the decision path is too complicated. If the ensemble model needs to be interpreted, the decision path of each tree needs to be combined, and the results will become difficult to understand. Therefore, we need additional methods to interpret ensemble tree models.

2.2 SHAP (Shapley Additive exPlanations)

The potential impact of explanations for tree-based machine learning models is widespread. The goal of interpretation is to distribute the contribution of each feature to the prediction. The Shapley value uses game theory ideas to assign feature contributions. Its main advantage is providing a consistent and fair solution. For the results predicted by multiple features, since there may be interactions between each feature, the Shapley value of a feature i is the weighted average contributions under all feature combinations.

The Shapley value of feature i is defined as follows:

$$\phi_i(f,x) = \sum_{S' \subseteq p \backslash i} w_x(S') \left[f\left(S' \cup \{i\}\right) - f(S') \right] \quad (3)$$

where f is the black box model, x is the input data, $\phi_i(\bullet)$ is the Shapley value of feature i under model f, p is the number of input features, S' is a subset of the features. For $w_x(S') = \frac{|S'|!(p-|S'|-1)!}{p!}$, the denominator $p!$ represents all possible feature combinations; the numerator $|S'|!(p-|S'|-1)!$ means the appearance times of $S' \cup \{i\}$ in all $p!$ combinations; $f\left(S' \cup \{i\}\right) - f(S')$ indicates the expected marginal contribution of feature i in one combination.

As we mentioned before, when the Shapley value is represented as a linear additive feature model, the model prediction will become a sum of individual feature contributions. This is the definition of SHAP and can be shown as follows:

$$g(z') = \phi_0 + \sum_{j=1}^{p} \phi_j z'_j \quad (4)$$

where ϕ_0 is the base prediction without knowing any input information, usually the mean of output in training data. ϕ_j is the distributed contribution for feature j, $z' \in \{0,1\}$ is the subset features vector, 1 indicates that the corresponding feature is present while 0 is absent. Based on equation (3), we know that computing Shapley values is an NP-hard problem. In this work, a fast (polynomial-time) algorithm, TreeSHAP, is utilized to compute SHAP values for the ET-based soft sensor (Lundberg et al. (2018)). This is possible due to the structure of the tree-based model and the additivity of the Shapley values.

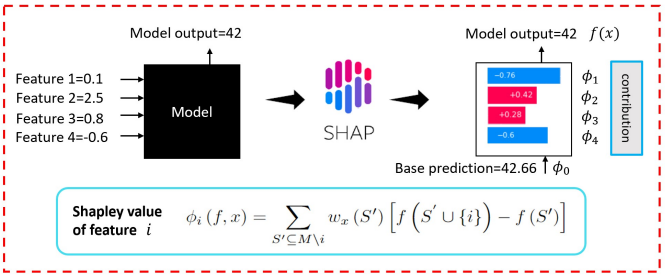

Fig. 4. An example of SHAP analysis

Fig. 4 shows an example of SHAP analysis, the black box model has 4 inputs and the output is 42. The base prediction is $\phi_0 = 42.66$. According to (3), the contribution of feature 1 is -0.76 and the contribution of feature 2 is +0.42, and so on and so forth. The sum of all individual contributions is equal to model output 42, which satisfies the definition of SHAP.

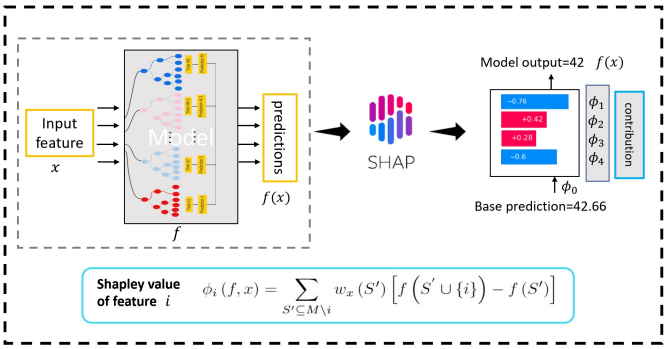

Fig. 5. The framework of proposed method

3. INTERPRETABLE SOFT SENSORS USING EXTREMELY RANDOMIZED TREES AND SHAP

Tree-based interpretable models have significant implications for industrial process monitoring, as interpretation helps operators and engineers understand, trust and use the model more effectively. In this work, we propose an accurate and interpretable soft sensor using ET and SHAP.

The framework of the proposed method is given in Fig. 5. The first step is data cleaning involving the removal of outliers and standardization of the cleaned data. Then, a robust and accurate ET soft sensor is developed with pretreated data. Finally, SHAP is used to accurately estimate the contribution of each input feature to the soft sensor predictions and the SHAP value is the contribution of the feature.

4. CASE STUDY

In this section, process data from the Parkland refinery in Burnaby, British Columbia, Canada, is used for case study. We focus on establishing a interpretable soft sensor for fluid catalytic cracker (FCC) unit. FCC is a core process in a refinery. It is an intermediate unit that processes the heavy hydrocarbons from crude oil and "cracks" them into smaller hydrocarbons, which can then be processed into a wide variety of different products (Su et al. (2021)). FCC unit consists of three main parts, namely the reactor, the regenerator and the fractionator, which can be seen in Fig. 6.

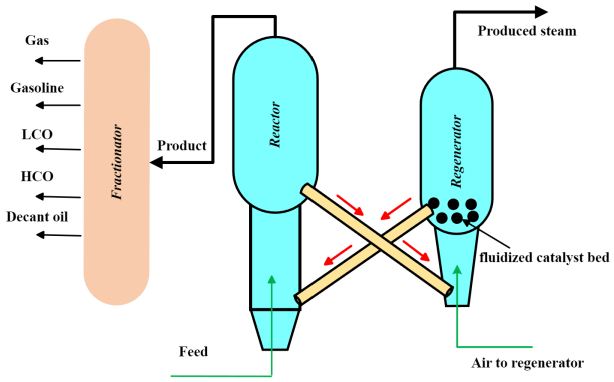

Fig. 6. A flow diagram of a Fluid Catalytic Cracking unit

The distillation temperature in the FCC fractionator is selected as the soft sensor output. 10 process variables that may impact the distillation temperature are selected based on process knowledge. We select 2076 samples from April 2018 to September 2022, of which the first 70% of the data (1453 samples) is used as the training set and the last 30% (623 samples) of the data is used as the test set. Considering confidentiality issues, we will not give the variable name and the magnitude of the variable. Fig. 7. shows the raw data after preprocessing.

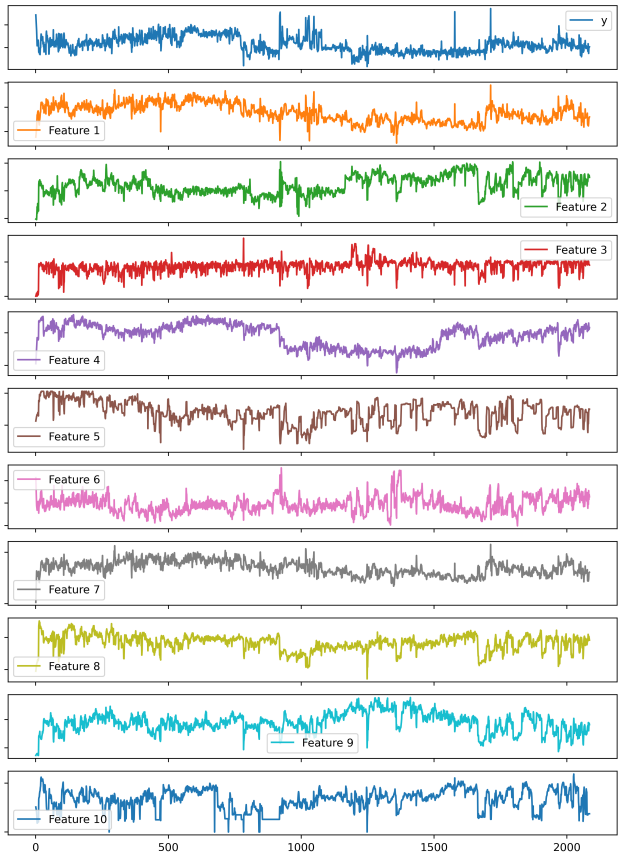

Fig. 7. Input and output data of the FCC unit

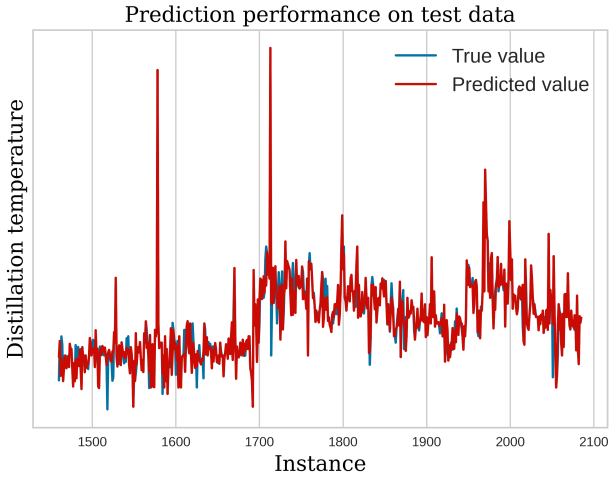

Fig. 8. The performance of ET soft sensor on test data

In this work, we use ET to construct soft sensors where the specific parameters are as follows: the number of trees

Table 2. Comparison of different soft sensors on test data

	RMSE	R^2
ET Regressor	3.8562	0.7932
Random Forest	4.0111	0.7771
Gradient Boosting Regressor	4.0301	0.7746
Huber Regressor	4.358	0.7367
Ridge Regression	4.4054	0.7311
Linear Regression	4.4067	0.7308
Neural networks (3 dense layers)	4.8609	0.6845
Lasso Regression	5.1631	0.6329
Elastic Net	5.3317	0.6093
Decision Tree Regressor	5.4937	0.5756

M is 100, the selected number of features K at each node is 5, and the minimum sample size for splitting a node n_{min} is 2. Fig. 8 gives the detailed prediction performance of the ET soft sensor on test data.

In order to verify the effectiveness of the proposed method, we also compare it with other machine learning methods, including Random Forest Regressor, Gradient Boosting Regressor, Huber Regressor, Ridge Regression, Linear Regression, Neural networks (3 dense layers), Lasso Regression, Elastic Net, and Decision Tree Regressor. Table 2 shows the performance of different soft sensors on test data. The results prove that the proposed ET soft sensor has the best performance (RMSE is 3.8562, R^2 is 0.7932). It should be noted that ET soft sensor has a larger improvement in performance compared to other tree-based methods, like Random Forest Regressor, Gradient Boosting Regressor, and Decision Tree Regressor, indicating that the proposed soft sensor is more accurate and robust.

Now we have a soft sensor of distillation temperature with excellent performance, but the problem is that the ET model itself has a complex structure, and it is difficult to know the inference process of the result from inside the model, usually only the predicted value is given, and the model is not interpretable at this time. Therefore, we need to use SHAP to enhance the interpretability of the model after the model is trained, and to mine the implicit information learned by the model.

SHAP can provide both global interpretation and local interpretation. Global interpretation refers to the interpretation of the entire model from input to output, from which we can understand the impact of each feature on the model. Fig. 9 displays the global interpretation of each input on the soft sensor prediction. Each instance is represented by a single dot on the feature row with the SHAP value (contribution) on the x axis. The sum of SHAP values is used to calculate the importance of the features, as shown on the y-axis. We can see that for all the data, the first and most important feature is feature 1; and for feature 1, the larger its feature value, the greater its contribution (positive correlation). Conversely, for feature 5, the smaller its feature value, the larger its contribution (negative correlation).

In addition to the global interpretation, we need to understand the variation in ET soft sensor predictions among specific instances. This type of explanation is called local interpretation. Local interpretation refers to explaining how the predictions change when the input values of an

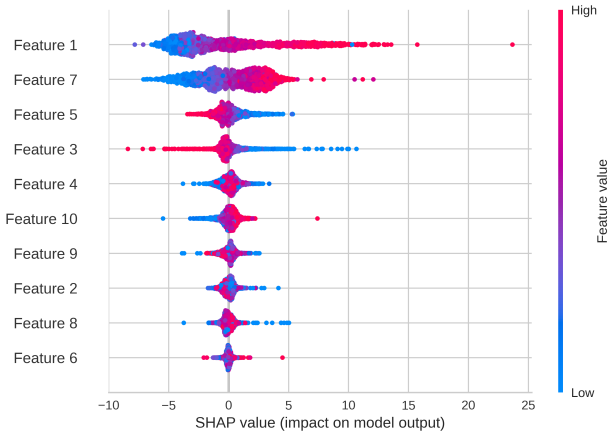

Fig. 9. Global interpretation of ET soft sensor

instance or a group of instances change. Fig. 10 shows the local interpretation of each instance on the ET soft sensor prediction. In this figure, $f(x)$ is the soft sensor prediction. For each individual prediction (column), the blue one means a negative contribution while the red one means a positive contribution. The darker the color, the greater the contribution.

Fig. 10. Local interpretation of ET soft sensor

To further show the interpretation of individual predictions, we choose the 1000th sample and the 2000th sample as examples for the analysis. The bottom of a waterfall plot starts as the base prediction (428.67), and then each row shows how the contribution of each feature moves the value from the base prediction to the ET soft sensor prediction.

As Fig. 11 shows, for the 1000th sample, the soft sensor prediction is 432.5. Feature 6 has the smallest contribution, moving only about 0.1 of the base prediction (428.67). Feature 5 has the largest contribution, moving about 3 of the base prediction (428.67). Similarly, as Fig. 12 shows, for the 2000th sample, the soft sensor prediction is 430.41. Feature 6 has the smallest contribution, moving only about -0.02 of the base prediction (428.67). Feature 7 has the largest contribution, moving about 2 of the base prediction (428.67). It is worth noting that the features that contribute most to the soft sensor predictions are different in 1000th sample (feature 5) and 2000th sample (feature 7), and this information is not available from the global interpretation.

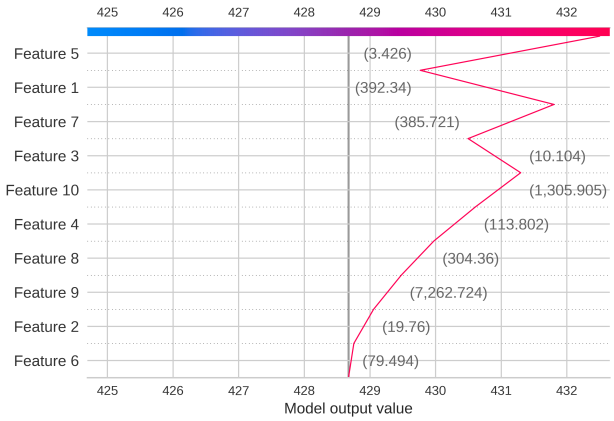

Fig. 11. Interpretation of ET soft sensor on 1000th sample

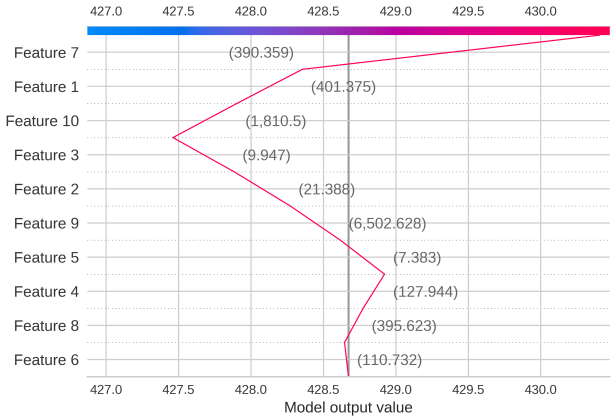

Fig. 12. Interpretation of ET soft sensor on 2000th sample

5. CONCLUSION

The objective of this work is to make process monitoring methods more robust, efficient, and interpretable. Due to the unique characteristics of industrial processes, we introduce the ET algorithm to build an accurate and robust soft sensor. By increasing the randomness in the modeling process, ET solves the overfitting to a certain extent. In addition, for the problem that the ensemble tree model is not interpretable, SHAP is used to interpret complex ET models from global and local perspectives. The proposed explainable soft sensors using ET and SHAP can greatly improve interpretability while maintaining high accuracy. The effectiveness of the proposed interpretable soft sensor is demonstrated with a real application to a commercial-scale FCC unit.

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