Interpretable Soft Sensors using Extremely Randomized Trees and SHAP

Liang Cao[1], Xiaolu Ji[1], Yupeng Li[1], Lim Siang[2], Yankai Cao[1], Vijay Kumar Pedriedla[1], Jin Li[2],Bhushan Gopaluni[1]

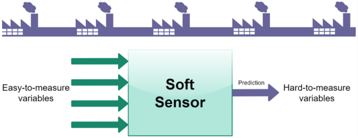
1. The University of British Columbia, Canada

2. Parkland Corporation, Canada

IFAC 2023

Soft Sensors

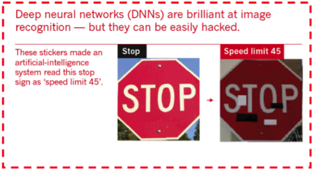
- A soft sensor is a mathematical model that uses measurable variables X to estimate the difficult-to-measure variables Y.
- The variables Y are usually related to product quality/process safety, and hence important.
- Machine learning is the dominant approach used in building soft sensors.

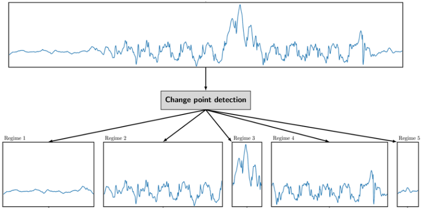


$$\boxed{Y = f(X)}$$

Motivation: Why Ensemble Tree Models?

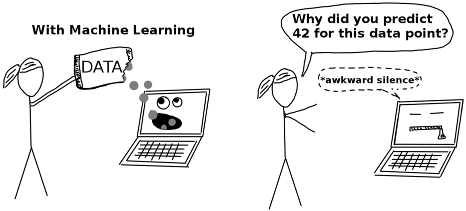
- Most machine learning models perform well with high signal-to-noise ratio scenarios, but fail to high noise samples (adversarial examples).
- Industrial process are extremely noisy, noise may come from changing operating conditions, measurement errors, or the introduction of unnecessary variables.
- Ensemble tree based models are robust to noise and outliers. Almost all winners of competitions, utilized tree-based ensemble models in their solutions.





Motivation: Why Model Interpretability?

- Industrial processes involve risk-sensitive tasks, any accidental situation can lead to disastrous consequences.
- It is not enough to get the prediction (the what). The model must also explain why it came to the prediction (the why) and how to intervene the process with the prediction (the how).
- Most machine learning models are black-box models, difficult to interpret their behavior in relation to the process variables.



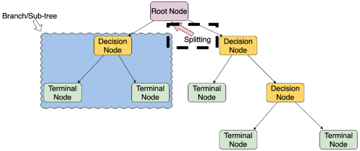
Motivation

Research Problem

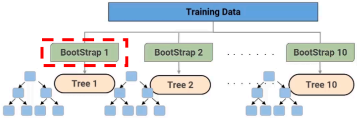
- How do we build accurate and robust soft sensors?
- How do we explain soft sensor predictions?
- Our goal is to design soft sensors that provide accurate and robust predictions as well as good interpretations.

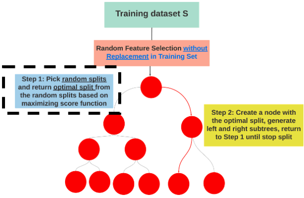
Extremely Randomized Trees

Decision Tree

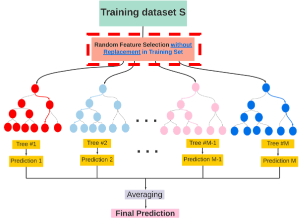


Random Forest





Single Tree of Extremely Randomized Trees



Extremely Randomized Trees

Extremely Randomized Trees

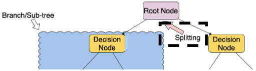
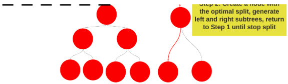
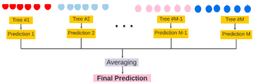


Table 1. Comparison of different tree methods

	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





Extremely Randomized Trees

Pros

- ✓ Faster Computation
- ✓ Robust to Noise and Outliers
- ✓ More Diverse Decision Trees
- ✓ Lower Risk of Overfitting

Cons

- ✗ Complex Internal Structure
- ✗ Hard to Interpret

Explainable Model

- It is difficult to (mathematically) define interpretability.
- A (non-mathematical) definition: Interpretability is the degree to which a human can understand the cause of a decision.
- An Explainable Model is one that can accurately estimate the contribution of each input feature to the model predictions.

$$y = \beta_0 + \sum_{i=1}^{m} \beta_i x_i$$

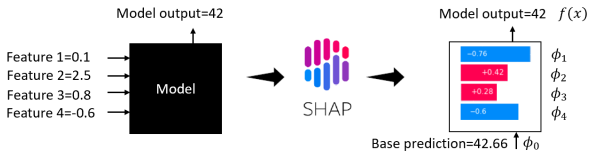
$$y = \frac{1}{K} \sum_{k=1}^{K} \sum_{i=1}^{m} w_{ki} f_{ki}(x_i)$$

Explainable Model: SHAP (Shapley additive explanation)

- Lloyd S. Shapley proposed the idea of Shapley value to interpret model prediction based on game theory and won Nobel Prize in Economics 2012.
- SHAP is an algorithm used to explain the output of any complex machine learning models.

Explainable Model: SHAP (Shapley additive explanation)

- SHAP is an algorithm used to explain the output of any complex machine learning models.
- Model-Agnostic: SHAP can interpret and compare different models in a consistent manner, regardless of their internal structures and operations.
- Post-Hoc Interpretability: SHAP offers interpretations after the model has been trained/ generated predictions.

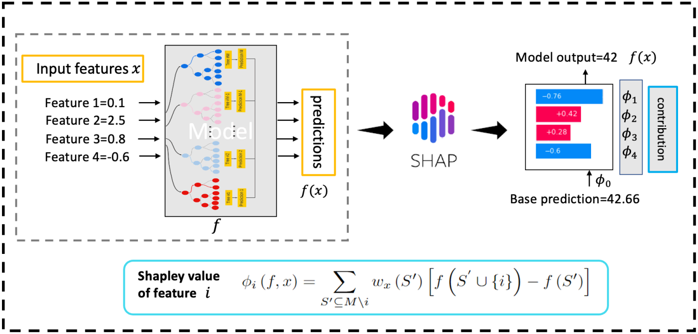


Shapley value of feature i

$$\phi_i(f,x) = \sum_{S' \subseteq M \setminus i} w_x(S')\left[f\left(S' \cup \{i\}\right) - f(S')\right]$$

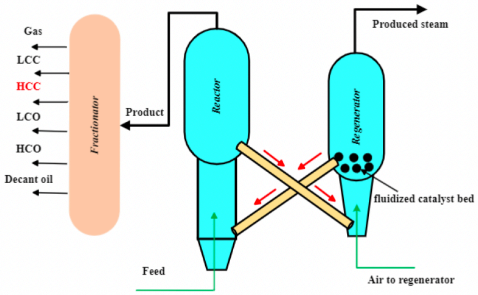
Explainable Soft Sensor Models - Summary

- An accurate and interpretable soft sensor using ET and SHAP is proposed.
- It has significant implications for industrial process monitoring, as interpretation helps operators and engineers understand, trust and use the model more effectively.



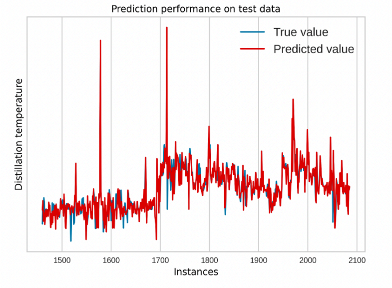
Canada Parkland Refinery Data

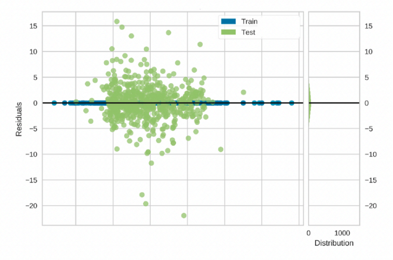
- Soft sensor data from Parkland refinery in Burnaby, British Columbia, Canada, is used for the case study.
- 2 years of data from a fluid catalytic cracking (FCC) unit, 10 process variables, 1 quality variable, 2076 samples, 70% for training, 30% for test.
- The objective is to provide an explanation for HCC gasoline 90% cut point predictions.



Results: Extremely Randomized Trees

The number of trees M is 100, the selected number of features K at each node is 5, and the minimum sample size for splitting a node is 2.





Results: Comparisons

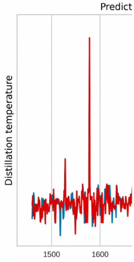
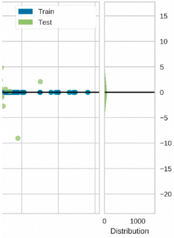
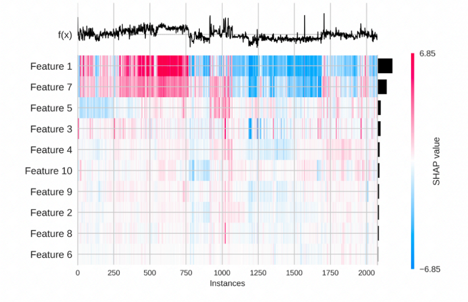


Table 2. Comparison of different soft sensors

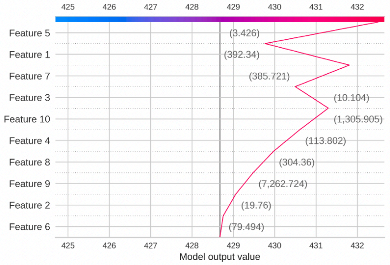
	RMSE	R^2
ET Regressor	3.8562	0.7932
Random Forest	4.0111	0.7771
Gradient Boosting Regressor	4.0301	0.7746
Huber Regressor	4.358	0.7367
Ridge Regression	4.4054	0.7311
Linear Regression	4.4067	0.7308
Neural networks (3 dense layers)	4.8609	0.6845
Lasso Regression	5.1631	0.6329
Elastic Net	5.3317	0.6093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



Results: Interpretation



Global/Local explanation: feature importance



Local explanation: feature attribution of 2000th sample

- This work presents a novel framework to build soft sensors and explain the predictions of soft sensors.
- The real-world commercial refinery case study validates the effectiveness of the proposed method.
- Model explanation is a promising research area that can offer significant benefits to the process industry.

✓ Extremely Randomized Trees to build accurate soft sensors.

✓ SHAP to interpret complex ensemble tree model by distributing the contribution of each feature.