

# Evolutionary Multi-objective Optimization Design of a Butane Content Soft Sensor<sup>\*</sup>

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**Abstract:** Industrial processes must be well equipped with a variety of sensors to maintain a desired quality. However, some variables cannot be easily measured due to different causes, such as acquisition and/or maintenance costs and slow acquisition time. This situation leads to a lack of real-time information in the process, which could lead to lower quality in the final product. One of such processes is the debutanizer column, where butane content measurement is highly delayed. To enable online prediction of such variables, available information from the process can be used to estimate predictive models, known as soft sensors. To this end, data-driven techniques can be used, such as statistical and machine learning. However, such techniques usually take into account a single metric when estimating the models, and there are multiple factors that play an important role when designing a soft sensor, such as stability and accuracy. To cope with such a situation, this paper proposes a multi-objective optimization design procedure, where feature selection and ensemble member combination are performed. Therefore, the multi-objective differential evolution algorithm with spherical pruning (spMODE-II) is initially employed for building a pool of non-dominated linear support vector regression (SVR) models. Subsequently, the same evolutionary algorithm is applied for selecting the weights of the previously generated models in a weighted combination ensemble. In a final multi-criteria decision making stage, a preferred ensemble is selected using the preference ranking organization method for enrichment of evaluations (PROMETHEE). Results indicate that the proposed approach is able to produce a highly stable and accurate butane content soft sensor for the debutanizer column.

*Keywords:* Soft sensor, Machine learning, Ensemble learning, Evolutionary algorithms, Multi-objective optimization, Chemical industry, Chemical sensors, Monitoring.

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## 1. INTRODUCTION

Industrial processes must be well equipped with a variety of sensors to maintain a desired quality. Although it is not difficult to acquire sensors for temperature, pressure, and humidity, there exist several situations where not all variables can be easily measured. Such variables are denominated hard-to-measure, and the cause to a difficult measurement can be associated to a high sensor acquisition (or maintenance) cost or slow acquisition time. This scenario leads to a lack of real-time information in the process (Souza et al., 2016). One of such processes is the debutanizer column, where the butane content measurement is highly delayed, demanding solutions for online prediction (Fortuna et al., 2005, 2007).

To alleviate such a problem, industry and academy started using available information from the process to create

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predictive models, known as soft sensors (Kadlec et al., 2009). Such models can be estimated through statistical and machine learning techniques (Souza et al., 2016), which usually train a model by optimizing a single metric. However, there are multiple factors that play an important role when building a predictive model, such as accuracy and stability (Ribeiro et al., 2019).

To build a soft sensor that takes into account stability and accuracy, this work employs a multi-objective optimization design (MOOD) procedure for building ensemble models. The proposed procedure is composed of two multi-objective problems (MOPs), one designed for building a pool of diverse support vector regressors (SVRs) (Boser et al., 1992; Cortes and Vapnik, 1995) through feature selection, and other for selecting the weights of each resulting SVR in a weighted average ensemble model. The multi-objective differential evolution with spherical pruning (spMODE-II) algorithm (Reynoso-Meza et al., 2014) is applied to optimize both problems, and the preference ranking organization method for enrichment evaluation (PROMETHEE) (Brans and De Smet, 2016) is used for aiding the selection of a preferred non-dominated ensemble.

ble. To the best of the authors knowledge, this is the first application of such tools to develop a soft sensor. Results indicate the creation of a highly accurate and stable butane content soft sensor for the debutanizer column.

The remainder of this paper is organized as follows: Section 2 introduces the problem, related work and the generation of features; Section 3 details the proposed MOOD procedure for soft sensor development; Section 4 reveals the experimental procedure and achieved results, which are discussed in Section 5; Finally, the paper is concluded with some final remarks and future work.

## 2. DEBUTANIZER COLUMN

Fortuna et al. (2005, 2007) introduced the debutanizer column as a soft sensor problem, composed of one hard-to-measure and seven easy-to-measure variables. The system is part of a refinery process, and online prediction is desired for improving quality monitoring and control of the plant. Figure 1 illustrates the block scheme of such system.

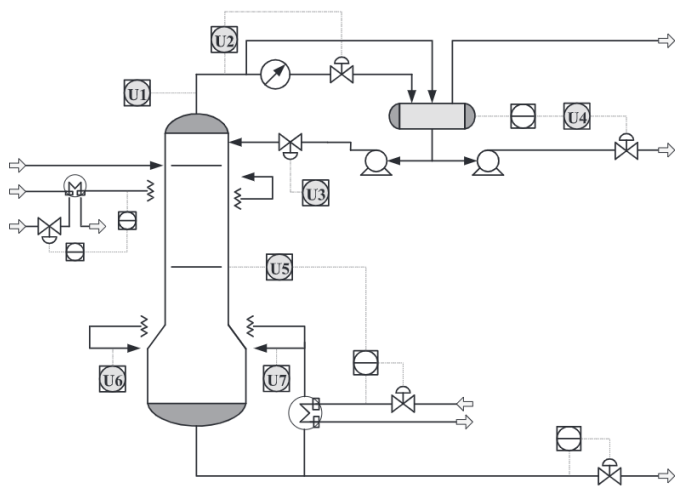


Fig. 1. Schematic of the debutanizer column (Fortuna et al., 2007), adapted by Shao et al. (2014).

The hard-to-measure variable is the butane (C4) content in the bottom flow of the column. According to Fortuna et al. (2005), such variable is indirectly analyzed on the overheads of a deisopentanizer column by a gas chromatograph. Therefore, there is a constant delay between 30 and 75 minutes in the acquisition of the C4 content. Since this variable depends exclusively on the debutanizer operating conditions, seven easy-to-measure variables can be used for estimating the desired variable. Table 1 indicates the inputs and output of this problem.

Table 1. Variables in the debutanizer column.

Variables	Description
Inputs	$u_1$ Top tray temperature
	$u_2$ Top pressure
	$u_3$ Reflux flow
	$u_4$ Flow to next process
	$u_5$ 6th tray temperature
	$u_6$ Bottom temperature
	$u_7$ Bottom temperature
Output	$y$ Butane content

Fortuna et al. (2007) made a data set available<sup>1</sup>, which contains 2394 samples and the eight variables. The sample time is considered as 15 minutes, and the delay for output acquisition is 45 minutes (Shao et al., 2014). Different solutions for this problem are presented below.

Ge and Song (2010) make use of just-in-time (JIT) learning to develop the soft sensors. In total, three models are analyzed: partial least squares (PLS), SVR, and least squares (LS)-SVR. When testing different number of samples (delays) with the JIT approach, 1000 samples are used for testing the models. LS-SVR, SVR, and PLS attained correlation coefficients ( $R^2$ ) of 0.9132, 0.6897, and 0.4035, respectively. Similar works have been performed with principal component regression (PCR) (Ge, 2014) and gaussian process regression (GPR) (Ge, 2016), achieving root mean squared error (RMSE) values around 0.15 and 0.06, respectively.

Selection of variables and lags is performed by Souza and Araújo (2011), where mutual information (MI) and  $R^2$  criteria are compared. Subsequently, LS-SVR is employed for online prediction. The experiment is made using 298 samples in the test set, and the available features are the seven inputs ( $u_1(k)$  to  $u_7(k)$ ) and their fourth and eighth delays ( $k - 4$  and  $k - 8$ ). Lower general and regularized RMSE values of 0.0461 and 0.0750 are achieved when using MI. Such feature selection criteria also attains a  $R^2$  value of 0.9626. However, a lower mean absolute error (MAE) of 0.3129 is obtained by employing feature selection with  $R^2$ .

Local PLS is employed by Shao et al. (2014) in a test set composed of 744 samples. Different from other works, Shao et al. (2014) use the delayed hard-to-measure butane content ( $y(k - 4)$ ,  $y(k - 5)$ , and  $y(k - 6)$ ) in addition to the easy-to-measure variables. Final results on the test set achieve RMSE, relative RMSE, and MAE values of 0.01058, 0.156, and 0.0419, respectively.

By using 1197 testing samples on the problem, Pani et al. (2016) test multiple linear regression (MLR), PCR, and artificial neural networks (ANNs), while Siddharth et al. (2019) tests regression trees and adaptive neuro fuzzy inference system (ANFIS). On the one hand, Pani et al. (2016) attain MAE, RMSE and  $R^2$  values of 0.055, 0.076, and 0.856 using ANNs, respectively. On the other hand, Siddharth et al. (2019) obtain a MAE of 0.048 with regression tree, while obtaining RMSE and  $R^2$  scores of 0.0672 and 0.8829 with ANFIS, respectively.

Pan et al. (2019) make use of dynamic and static learning, while employing a mixed integer genetic algorithm for variable selection and weighting of the inputs and 6 delays. For the dynamic scenario, 597 samples are used for testing, achieving RMSE and  $R^2$  scores of 0.0121 and 0.9942, respectively. For the static scenario, using 598 samples, RMSE and  $R^2$  scores of 0.0452 and 0.9187 are attained, respectively.

Finally, Marchioro et al. (2019) performed evolutionary instance and feature selection on both SVRs and decision trees for the debutanizer problem. The test data set is composed of the last 20% samples, and genetic algorithm

<sup>1</sup> Available in: [http://www.springer.com/cda/content/document/cda\\_downloaddocument/9781846284793\\_material.zip?SGWID=0-0-45-349600-p168288081](http://www.springer.com/cda/content/document/cda_downloaddocument/9781846284793_material.zip?SGWID=0-0-45-349600-p168288081)

has been used for optimizing the models. As a result, the SVR with instance selection achieves the best RMSE score of 0.0979.

### 2.1 Feature Engineering

In this work, feature engineering is performed for generating additional features from the ones already available. Similar to previous works, the delayed signals are used. However, new signal processing and statistical features are also generated. The new features are described below, given the seven inputs  $u_i(k)$  and output  $y(k)$  at the current sample  $k$ .

**Signals and delays.** In addition to the current input values, a total of 8 lags are used for each input signal. Also, 4 lags are used for the output signal, starting from the fourth lag. Therefore, the initially created features are

$$X_u(k) = \{u_i(k-l), \forall i, l \in \mathbb{Z} : l \in [1, 7], l \in [0, 8]\} \quad (1)$$

$$X_y(k) = \{y(k-m), \forall m \in \mathbb{Z} : m \in [4, 8]\} \quad (2)$$

where  $i$  is the signal number,  $l$  is the lag value for the input, and  $m$  is the lag value for the output. This results in a total of 68 available features.

**Differences.** For each of the previously generated features ( $X_u(k)$  and  $X_y(k)$ ), the difference to the previous sample is also considered a feature, computed as follows.

$$X_{du}(k) = X_u(k) - X_u(k-1) \quad (3)$$

$$X_{dy}(k) = X_y(k) - X_y(k-1) \quad (4)$$

**Statistical.** Mean, standard deviation, minimum and maximum values are also computed for the original signals. All of these features are created considering a window of  $w = 30$  samples. Such features are computed as follows.

$$X_{\bar{u}}(k) = \left\{ \sum_{n=0}^{W-1} u_i(k-n)/W, \forall i \in \mathbb{Z} : i \in [1, 7] \right\} \quad (5)$$

$$X_{\delta}(k) = \left\{ \sqrt{\sum_{n=0}^{W-1} (u_i(k-n) - X_{\bar{u}i}(k))^2 / (W-1)}, \right. \\ \left. \forall i \in \mathbb{Z} : i \in [1, 7] \right\} \quad (6)$$

$$X_{max}(k) = \left\{ \max_{n=0}^{W-1} u_i(k-n), \forall i \in \mathbb{Z} : i \in [1, 7] \right\} \quad (7)$$

$$X_{min}(k) = \left\{ \min_{n=0}^{W-1} u_i(k-n), \forall i \in \mathbb{Z} : i \in [1, 7] \right\} \quad (8)$$

**Detrending.** Finally, the detrended input signals are also generated. This is computed by subtracting the moving average from the current sample, detailed as follows.

$$X_{u-\bar{u}}(k) = \{u_i(k) - X_{\bar{u}i}(k), \forall i \in \mathbb{Z} : i \in [1, 7]\} \quad (9)$$

The final feature vector is composed of all the  $S = 171$  previously generated features, as follows.

$$X(k) = X_u(k) \| X_y(k) \| X_{du}(k) \| X_{dy}(k) \| X_{u-\bar{u}}(k) \\ \| X_{\bar{u}}(k) \| X_{\delta}(k) \| X_{max}(k) \| X_{min}(k) \| X_{u-\bar{u}}(k) \quad (10)$$

Next, it is necessary to find a predictor  $f(\cdot)$  that approximates  $y(k)$  by operating over the features  $X(k)$ , in the form of  $\hat{y}(k) = f(X(k))$ . The following section details the proposed approach for this task.

## 3. EVOLUTIONARY MULTI-OBJECTIVE FEATURE SELECTION AND ENSEMBLE COMBINATION

This section details the proposed MOOD procedure for soft sensor development. First, an evolutionary algorithm generates a pool of regressors by minimizing error's bias and variance through feature selection of linear SVRs. Next, the same evolutionary algorithm selects the weights of each of the non-dominated SVR in an ensemble approach. Finally, a multi-criteria decision making tool is employed for aiding the selection of a preferred final ensemble.

This section is organized as follows: First, the SVR feature selection MOP is detailed, followed by the ensemble member combination MOP. Then, the evolutionary algorithm is presented. Finally, the multi-criteria decision making step is described.

### 3.1 Multi-objective Feature Selection

The first MOP focus on building a diverse pool of SVR regressors, as illustrated in Figure 2. To this end, feature selection is performed for minimizing three objectives. The problem can be mathematically formulated as follows.

$$\min_{\theta} \mathbf{F}(\theta^f) = [F_{MAE}(\theta^f), F_{\sigma^2}(\theta^f), F_f(\theta^f)] \quad (11)$$

subject to

$$\theta_s^f \in \{0, 1\}, \forall s \in \mathbb{Z} : s \in [1, \dots, S] \quad (12)$$

where

$$F_{MAE}(\theta^f) = \sum_{k=1}^K |e(k)|/K \quad (13)$$

$$F_{\sigma^2}(\theta^f) = \sum_{k=1}^K (e(k) - \bar{e})^2 / (K-1) \quad (14)$$

$$F_f(\theta^f) = \sum_{s=1}^S \theta_s^f \quad (15)$$

$$\bar{e} = \sum_{k=1}^K e(k)/K \quad (16)$$

$$e(k) = y(k) - \hat{y}(k) \quad (17)$$

being the objectives MAE ( $F_{MAE}(\theta^f)$ ), error' variance ( $F_{\sigma^2}(\theta^f)$ ), and number of used features ( $F_f(\theta^f)$ ). In the decision vector  $\theta^f$ ,  $\theta_s^f$  is the selection of feature  $s$  in a data set with  $S$  features. Additionally,  $e(k)$  is the error between the real ( $y(k)$ ) and predicted ( $\hat{y}(k)$ ) values at sample  $k$ , in a set with  $K$  samples.

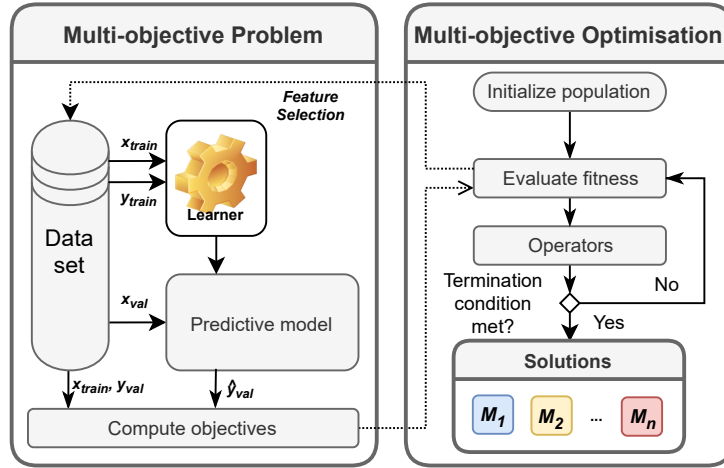


Fig. 2. The multi-objective feature selection method, adapted from Ribeiro and Reynoso-Meza (2019).

### 3.2 Multi-objective Ensemble Member Combination

The second MOP focus on combining the diverse pool of SVR regressors, as illustrated in Figure 3. Therefore, ensemble member weighting is performed for minimizing two objectives. Thus, the problem can be mathematically formulated as follows.

$$\min_{\theta^e} C(\theta^e) = [C_{MAE}(\theta^e), C_{\sigma^2}(\theta^e)] \quad (18)$$

subject to

$$0 \leq \theta_c^e \leq 1, \forall c \in \mathbb{Z} : c \in [1, C] \quad (19)$$

where

$$C_{MAE}(\theta^e) = \sum_{k=1}^K |e_{ens}(k)|/K \quad (20)$$

$$C_{\sigma^2}(\theta^e) = \sum_{k=1}^K (e_{ens}(k) - \bar{e}_{ens})^2 / (K - 1) \quad (21)$$

$$\bar{e}_{ens} = \sum_{k=1}^K e_{ens}(k) / K \quad (22)$$

$$e_{ens}(k) = y(k) - \sum_{c=1}^C \hat{y}_c(k) \cdot \theta_c^e \quad (23)$$

being the objectives once again MAE ( $C_{MAE}(\theta^e)$ ) and error's variance ( $C_{\sigma^2}(\theta^e)$ ). In the decision vector  $\theta^e$ ,  $\theta_c^e$  is the weight of model  $c$  in from a pool with  $C$  models. Additionally,  $e_{ens}(k)$  is the error between the real ( $y(k)$ ) and ensemble's output ( $\hat{y}_{ens}(k)$ ) values at sample  $k$ , in a set with  $K$  samples.

### 3.3 Multi-objective Optimization Algorithm

The spMODE-II (Reynoso-Meza et al., 2014) is employed for optimizing both MOPs. To this end, the algorithm is configured with a population of 50 individuals, 100 generations, a crossover ratio of 20%, and a scaling factor of 50%. This evolutionary algorithm presents desirable

convergence, diversity, and pertinence characteristics, and has been used with success for optimizing anomaly detection (Ribeiro and Reynoso-Meza, 2019) and time-series forecasting (Ribeiro et al., 2019) models.

### 3.4 Multi-criteria Decision Making

After the multi-objective ensemble member combination, a final preferred model is found by selecting the best ranked ensemble according to a multi-criteria decision making tool. The PROMETHEE (Brans and De Smet, 2016) is employed for such task, where significant and insignificant differences are defined for computing the criteria's outranking flows for each solution. Table 2 presents the (in)significance values, based on the objectives (MAE and error's variance) calculated for an ensemble with  $C$  equal weights. The decision variable  $\theta^{ref}$  for this scenario is demonstrated below:

$$\theta_c^{ref} = 1/C, \forall c \in \mathbb{Z} : c \in [1, C] \quad (25)$$

Table 2. Matrix with (in)significant differences for aiding the selection of a preferred ensemble.

I/S differences matrix		
Objective	I	S
$C_{MAE}(\theta^e)$	$0.01 \cdot C_{MAE}(\theta^{ref})$	$0.5 \cdot C_{MAE}(\theta^{ref})$
$C_{\sigma^2}(\theta^e)$	$0.01 \cdot C_{\sigma^2}(\theta^{ref})$	$0.5 \cdot C_{\sigma^2}(\theta^{ref})$

## 4. EXPERIMENT AND RESULTS

This section details the experiments and the achieved results. The first subsection explains the experimental procedure, where the proposed MOOD procedure is employed to develop a soft sensor for the debutanizer column. The next subsection brings the qualitative results with tables and figures.

### 4.1 Experimental Procedure

First, it is necessary to process the data set. Initially, the available data set is engineered with the new features from Section 2.1. Subsequently, it is split in half into

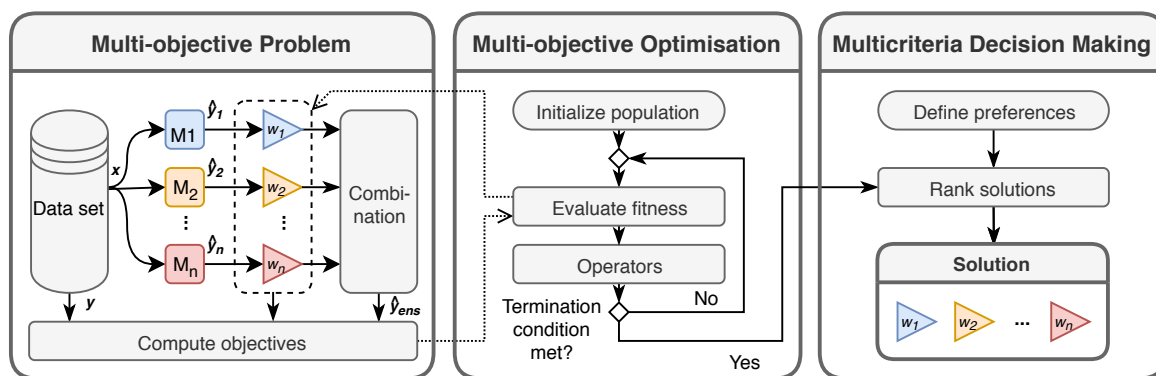


Fig. 3. The multi-objective ensemble member combination method, adapted from Ribeiro and Reynoso-Meza (2019).

development and test sets (1197 sequential samples each). Later, the development set is randomly split into training (60%), validation<sub>1</sub> (20%), and validation<sub>2</sub> (20%).

The training set is used for generating the pool of SVR models (with linear kernel), while the validation<sub>1</sub> set is employed for evaluating the models under the feature selection optimization problem. Next, the validation<sub>2</sub> set is applied for assessing the performance of the ensembles in the member combination optimization problem.

After the two MOPs, a set of non-dominated ensembles is returned, and a final preferred ensemble is selected with the aid of PROMETHEE (first ranked ensemble). Finally, the test set is employed for assessing the performance of the selected ensemble, and the results are shown in the next subsection.

#### 4.2 Results

This subsection brings the results for the debutanizer column problem. First, Figure 4 illustrates the results on the test data set. Next, Table 3 displays the qualitative results. Finally, Table 4 details the selected ensemble with the base models' corresponding weights.

Figure 4 plots the butane content signal (black bold line) and the estimated soft sensor (grey dashed line). Additionally, the error for each sample is shown in a lower subplot. It is important to notice how the soft sensor signal follows the real variable correctly, presenting maximum errors of approximately 10 around sample number 400.

Despite showing interesting results in the plot, it is also important to qualitatively analyze the performance of the soft sensor. Table 3 shows the RMSE, MAE, error's variance ( $\sigma^2$ ) and standard deviation ( $\sigma$ ), and the correlation coefficient ( $R^2$ ) for the estimated model computed on the test set.

Table 3. Qualitative results of the butane content soft sensor.

Metric	Value
RMSE	0.0187
MAE	0.0136
$\sigma^2$ (error)	0.0003
$\sigma$ (error)	0.0186
$R^2$	0.9944

Finally, Table 4 details the generated models, their features, and respective weight in the final ensemble. In total,

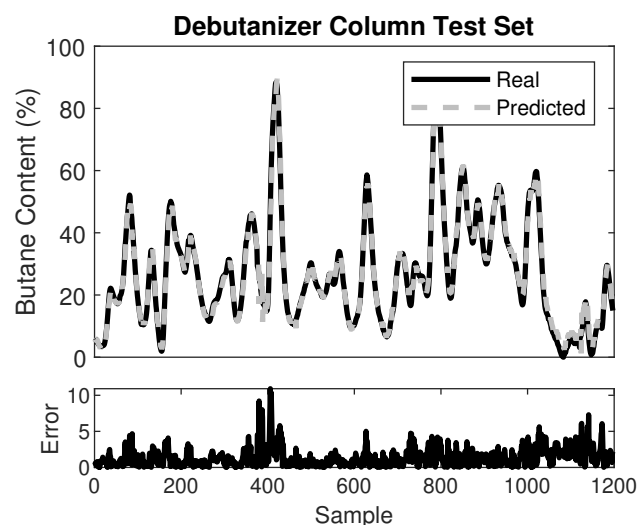


Fig. 4. Results on the test data set, composed of 1197 samples.

14 non-dominated SVRs are returned from the multi-objective feature selection problem. After the optimization of the multi-objective ensemble member combination and the multi-criteria decision making stage, the preferred ensemble discards five SVRs (numbers 5, 7, 9, 12, and 14). From the remaining base models, SVR 11 presents the highest weight (0.329), followed by SVR 6 (0.159), 4 (0.140) and 10 (0.105). Additionally, the 11 most used features, considering all SVR models, are:  $u_4(k-3)$ ,  $u_3(k-4)$ ,  $u_5(k-4)$ ,  $u_6(k-6)$ ,  $u_1(k-8)$ ,  $y(k-4)$ ,  $y(k-5)$ ,  $u_3(k-4) - u_3(k-5)$ ,  $y(k-4) - y(k-5)$ ,  $\max_{n=0}^{w-1} u_1(k-n)$ , and  $\max_{n=0}^{w-1} u_6(k-n)$ .

#### 5. DISCUSSION

The results from Section 4 indicate a proper soft sensor. However, it is also of interest to compare such results with the existing solutions found in literature. With a RMSE of 0.0187 and MAE of 0.0136, the proposed model achieves the best solution in comparison to any other model that deals with static models (Section 2). Also, despite achieving slightly higher RMSE and MAE values in comparison to some dynamic models (Shao et al., 2014; Pan et al., 2019), the proposed model achieves the best overall variance, with an  $R^2$  score of 0.9944. Therefore, the employed multi-objective optimization design procedure

Table 4. Weights of the selected SVR ensemble.

Model	Weight
SVR 1	0.054
SVR 2	0.070
SVR 3	0.034
SVR 4	0.140
SVR 5	0.000
SVR 6	0.159
SVR 7	0.000
SVR 8	0.087
SVR 9	0.000
SVR 10	0.105
SVR 11	0.329
SVR 12	0.000
SVR 13	0.014
SVR 14	0.000

for soft sensor development results in a highly accurate and stable model.

## 6. CONCLUSIONS

To develop a butane content soft sensor in a debutanizer column, this paper presents an evolutionary multi-objective feature selection and ensemble member combination method. To the best of the authors knowledge, this is the first application of such tools to develop a soft sensor. To this end, feature engineering is performed on the available data set, and new features are created. Next, the spMODE-II algorithm is employed for minimizing both the error's bias and variance of SVRs by performing feature selection. With the resulting set of non-dominated models, a novel optimization step is performed for minimizing the same objectives by selecting the weights of each SVR in a weighted ensemble. Finally, validation results are analyzed with PROMETHEE to select a preferred ensemble. Results on the debutanizer column indicate that the proposed approach is able to build a highly accurate and stable soft sensor.

Therefore, it is concluded that the application of MOOD procedures can benefit the development of the butane content soft sensor. Future work shall focus on the deeper analysis of the butane content problem and the development of soft sensors for different industrial plants. Additionally, new evolutionary algorithms and machine learning models for regression can be employed.

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