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Adaptive soft sensor to estimate alite fraction in clinker production through quasi-ensemble PLS modelling

Mihnea Stefan[ab], Wilson R. Leal da Silva[b], Fabrizio Bezzo[a], Pierantonio Facco[a]*

[a] *CAPE*-Lab, Computer-Aided Process Engineering Laboratory, University of Padova, Department of Industrial Engineering, Via Marzolo 9, Padova, 35131, Italy
[b] Fuller Technologies, Scandiagade 8, 4, 2450, Copenhagen, Denmark
* Corresponding Author: pierantonio.facco@unipd.it.

ABSTRACT

Cement is regarded as the most widely used construction material worldwide; however, its production is also recognized as a major contributor to global CO_2 emissions. Strict control of cement quality is therefore required to prevent excessive consumption of raw materials and energy, which would otherwise increase the process environmental footprint. Cement quality is largely governed by clinker quality, which is primarily characterized by two quality control parameters: free-lime content and alite fraction. At present, these are characterized by costly and time-consuming laboratory analyses that are not optimal for real time process control and optimization. Hence, in this work, a soft sensor for the real-time estimation of the clinker alite fraction is proposed. The developed soft sensor is designed to adapt to process drifts and operating condition changes, capture nonlinear and dynamic behavior, and retain interpretability through a Partial Least Squares (PLS) modelling framework. To this end, a novel recursively adaptive local dynamic soft-sensing strategy (ALD-PLS) is introduced and implemented within a multi-model ensemble structure referred to as Quasi-Ensemble PLS (QE-PLS). Unlike conventional ensemble approaches, where model diversity is generated through data resampling or training–testing partitioning, the proposed framework constructs multiple sub-models using combinations of model hyperparameters, evaluated on the same evolving dataset. As a result, improved predictive accuracy and robustness are achieved, while estimation uncertainty is quantified. The proposed QE-PLS soft sensor is shown to outperform, in terms of R^2 and $RMSE$, PLS-based and single-instance implementations ALD-PLS for a similar task. The novel methodology is validated against data collected from an industrial cement production plant.

Keywords: Modelling, adaptive modelling, cement industry, ensemble modelling, PLS, soft sensing

1. INTRODUCTION

Cement is regarded as the most widely used construction material worldwide due to its scalability, affordability, and widespread availability. Nevertheless, cement production is recognized as a major contributor to global carbon emissions, accounting for ca. 8% of total anthropogenic CO_2 emissions [1]. Strict quality control is therefore required, since deviations in product quality may result in unnecessary consumption of raw materials and energy, increasing the overall environmental footprint of the process and product. Cement quality is largely governed by clinker quality, which is primarily controlled by two key indices, i.e. free-lime content and alite fraction, to mention a few [2]. At present, these are determined by laboratory analyses, which are costly and time-consuming, thus not optimal for real-time process monitoring, control, and optimization.

An alternative to laboratory measurements is provided by soft sensors, through which difficult-to-measure quality variables are estimated using data-driven models built from readily available process measurements, e.g. temperatures, pressures, and material flow rates [3]. In clinker production, real-time estimation of critical quality indices by soft sensors can support advanced control strategies and improved operational efficiency. However, research on soft sensing in the cement industry has remained limited, with most existing studies focusing on free lime and few addressing the alite fraction. Existing approaches can be grouped into three categories. First, black-box models, e.g. neural networks, have been associated with high predictive accuracy, while limited process interpretability has been provided [4]. Second, white-box Partial Least Squares (PLS)-based models have been employed to retain interpretability; however, performance has often been constrained by difficulties in capturing nonlinearity, dynamics, and process drifts typical of modern cement plants [5]. Third, mechanistic first-principles models have been characterized by both accuracy and interpretability, but high computational demand has frequently rendered their use impractical for real-time control and optimization [6].

In this work, the focus is on the real-time estimation of clinker alite fraction through an interpretable, adaptive soft-sensing strategy. In particular, PLS modelling has been adopted as the modelling strategy due to its robustness in handling collinearity and high-dimensional process data. A recursively adaptive PLS-based soft sensor has been proposed based on the established incremental PLS (I-PLS) strategy [7]. Process dynamics have been explicitly incorporated using lagged variables [8], while local modelling strategies have been employed to tailor the model to the prevailing data environment; improving predictive performance under nonlinear and non-stationary conditions. Such adjustments are needed since conventional PLS-based soft sensors do not adapt to evolving industrial conditions. In clinker production, non-stationarity, seasonal drifts, abrupt operating changes, and dynamic behavior have frequently been observed, often in association with multiple operating modes, thereby challenging static, global modelling approaches.

Note, however, that the proposed models' predictive performance was found to depend on a relatively large number of interdependent hyperparameters, including the number of latent variables and the dynamic lag structure, whose optimal values vary over time and operating conditions. Thus, the models' hyperparameters have been allowed to vary within physically and statistically meaningful bounds - instead of being fixed a priori. As a result, a new methodology based on a multi-model structure that is inspired by ensemble learning principles has been developed, resulting in an ensemble over model structures, not calibration datasets. This novel strategy is referred to as Quasi-Ensemble PLS modelling. To prove its predictive superiority the performance of QE-PLS, in terms of estimation R^2 and $RMSE$, is compared to that of its components, I-PLS and ALD-PLS.

2. MATERIALS AND METHODS

The proposed novel soft-sensing methodology was developed and validated using industrial data collected from a cement production plant. In this section, the clinker production process is briefly described, followed by an overview of the dataset and preprocessing steps, and a detailed presentation of the modelling framework adopted in this work.

2.1 Clinker production process

Cement is produced by grinding clinker together with supplementary cementitious materials and gypsum. Clinker itself is obtained by thermally processing a raw meal composed mainly of limestone and clay. The raw meal is preheated in a multistage cyclone tower, partially calcined in a precalciner, and subsequently fed into a rotary kiln where clinker formation occurs. The hot clinker is then rapidly cooled to preserve the formed alite phase [10]. A schematic representation of the clinker production process is shown in Figure 1.

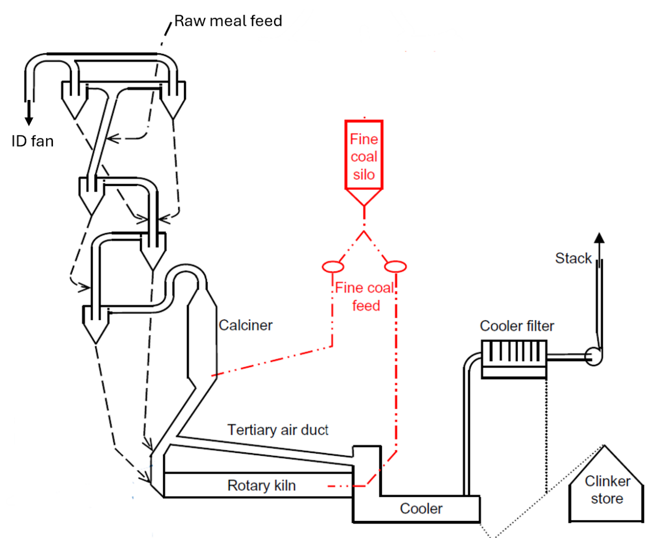

Figure 1. Clinker production process; adapted from [10].

2.2 Dataset preprocessing

The dataset used in this study comprises 74 process variables and the corresponding product quality measurements in terms of alite fraction. For confidentiality reasons, the dataset origin (cement plant) and the description of individual variables cannot be disclosed. All process variables were recorded at a nominal sampling interval of 1 min. While process variables were continuously measured, the alite fraction was obtained through laboratory analysis at a lower frequency (ca. once per hour). Hereafter, the process variables and the alite fraction are referred to as the **X**-block and the **y**-vector.

Data preprocessing steps include: (i) removal of missing values, sensor decoupling periods, and unphysical measurements; and (ii) outlier detection and removal based on Q (SPE) residuals and Hotelling's T^2 statistics [11], exceeding twice their respective 95% confidence limits in PLS modelling. This resulted in a final dataset spanning ca. two months of operation, where $\mathbf{X}$ has the dimension of $[N_{observations} \times V_{variables}] = [826 \times 74]$ and **y** of $[N_{observations} \times 1] = [826 \times 1]$.

2.3 Partial Least Squares (PLS)

Partial Least Squares (PLS) regression was selected due to its effectiveness in handling highly correlated, high-dimensional industrial data. All PLS models were built using the NIPALS algorithm [12]. Equations 1-4 represent the model formulation and estimation formulae.

$$\mathbf{X} = \mathbf{T}\mathbf{P}^{\mathrm{T}} + \mathbf{E} \tag{1}$$

$$\mathbf{Y} = \mathbf{U}\mathbf{Q}^{\mathrm{T}} + \mathbf{F} \tag{2}$$

$$\mathbf{U} = \mathbf{T}\mathbf{B} \tag{3}$$

$$\hat{\mathbf{y}}_{\mathrm{new}} = \mathbf{x}_{\mathrm{new}}\mathbf{W}(\mathbf{P}^{\mathrm{T}}\mathbf{W})^{-1}\mathbf{B}\mathbf{Q}^{\mathrm{T}} \tag{4}$$

where, $\mathbf{X}, \mathbf{Y}$ refer to the predictor and response matrices, $\mathbf{T}$ and $\mathbf{U}$ the scores matrices, $\mathbf{P}$ and $\mathbf{Q}$ the loadings matrices, and $\mathbf{E}$ and $\mathbf{F}$ the residual matrices resulted from the decomposition of the predictor and response blocks. Besides, $\mathbf{W}$ represents the weights matrix, $\mathbf{B}$ the regression coefficients vector, and $\mathbf{x}_{\mathrm{new}}$ the new observation vector while $\hat{\mathbf{y}}_{\mathrm{new}}$ the estimation for the corresponding response.

However, an adjustment to classical PLS is needed, since it is inherently linear and static. In particular, models are calibrated once and, subsequently, applied without adaptation, rendering them incapable of accounting for the frequent process drifts and operating mode changes – typical of industrial clinker production. Hence, an adaptive modelling strategy – described as follows – is required to overcome these limitations.

2.4 Incremental update strategy PLS

The incremental recursive updating strategy for PLS [7] is adopted to enable model adaptation over time. Specifically, at each time instant, a PLS model is recalibrated using all available historical data, and the current process observation is projected to estimate the corresponding alite fraction. Once the true measurement becomes available, it is incorporated into the historical dataset and the procedure is repeated.

While this recursive approach allows for tracking process changes, it suffers from two drawbacks: (i) as the dataset size grows, diminishing influence on the recalibrated model is exerted by the new observations, reducing adaptivity; and (ii) increasing computational cost due to repeated recalibration on an ever-growing dataset. These limitations motivate the proposal of a local adaptive dynamic PLS framework (see Section 2.6), where a similarity-based selection of historical samples is used to maintain model relevance and estimation accuracy.

2.5 Lagged variables PLS

The standard PLS framework is extended by lagged-variables PLS through augmentation of the **X**-block with time-shifted versions of the process variables, enabling the model to capture process dynamics and temporal autocorrelation [8]. In classical dynamic PLS, the augmented **X**-block is formed by concatenating copies of the original variables shifted by predefined time lags.

In this work, a modified lag-construction strategy is adopted for the adaptive local dynamic PLS framework (Section 2.6). Specifically, instead of generating lagged variables from the main modelling dataset, lagged information is extracted from the higher-resolution 1-minute dataset (Section 2.2). This helps incorporate the dynamic information present at finer time scales, while the main **X**–**y** modelling dataset remains aligned with the lower sampling frequency of the alite measurements (ca. one hour).

As for lagged variables, they are constructed by selecting a lag spacing W, defining the time shift between consecutive lags. In the main dataset, for each sample at time t, process variable observations at times $t - W, t - 2W, \dots, t - R$ are retrieved from the 1-minute dataset and horizontally concatenated to form the augmented **X**-block. Thus, the total number of lags added in the dynamic X-block reads R/W.

Altogether, this approach enables the incorporation of dynamic process information without increasing the temporal resolution of the primary dataset and forms the basis for the adaptive local modelling strategy described as follows.

2.6 Proposed methodology: adaptive local dynamic PLS (ALD-PLS)

The proposed methodology integrates I-PLS, dynamic lagged-variable methods, and local modelling into a unified adaptive local dynamic PLS (ALD-PLS) strategy. The objective is to retain the adaptability and interpretability of PLS while overcoming the limitations of static global models when applied to non-stationary, dynamic industrial processes. A schematic overview of the methodology is provided in Figure 2.

At each time t, the modelling procedure is carried out according to the following update paradigm:

1. **Step 1:** data from time 1 to $t-1$ are used to construct a global dynamic PLS model, where the **X**-block consists of the lag-augmented process variables and the **y**-vector the corresponding alite fraction measurements. The construction of the dynamic **X**-block requires the selection of a proper lag W and the maximum lag range R (Section 2.5). The global model is built using A_g latent variables.
2. **Step 2:** the current observation of the $V = 74$ online process variables at time t, represented in its dynamic lagged-variable form, is projected into the global PLS

score space.

3. **Step 3:** Euclidean distances between the score vector of the current point and those of all historical samples are computed, and the L closest historical points are selected. These samples are considered the most relevant local neighborhood for modelling the current process state.
4. **Step 4:** using the selected L samples, a local dynamic PLS model is constructed with A latent variables.
5. **Step 5:** Variable Importance in Projection (VIP) indices [13] are calculated for each predictor in the dataset. Predictors with VIP < 1 are subsequently removed [13], and the local dynamic PLS model is recalibrated using the reduced predictor set.
6. **Step 6:** the current observation at time t is projected onto the score space of the refined local PLS model, and the alite fraction is estimated.

The abovementioned local modelling strategy ensures that estimations are based on the most relevant historical data while maintaining robustness against irrelevant or degenerate predictors.

2.7 Quasi-Ensemble PLS Modelling

The predictive performance of the proposed methodology depends on a set of critical hyperparameters (Section 2.6) summarized in Table 1. Note that the choice of hyperparameters is interdependent.

Table 1. Hyperparameters of the proposed ALD-PLS.

Hyperparameter	Description
L	size of similarity neighborhood
A	number of LVs of the local PLS model
A_g	number of LVs of the global PLS model
W	lag frequency (time shift of the variables between two consecutive lags)
R	maximum time shift considered

Instead of selecting a single optimal hyperparameter configuration, a multi-model strategy inspired by ensemble learning [9] was adopted. In contrast to classical ensemble approaches, where diversity is generated through resampling or partitioning of the dataset, the proposed framework constructs diversity through different combinations of model hyperparameters evaluated on the same evolving dataset. This approach is referred to as Quasi-Ensemble PLS modelling (QE-PLS).

All possible combinations of hyperparameters values in reasonable ranges are selected to build the sub-models of the Quasi-Ensemble (QE). The selected values of the hyperparameters, selected through heuristics, are shown in Table 2. For each sub-model, the ALD-PLS is executed, yielding an independent estimation of the alite fraction at each time point.

The QE estimation is obtained by averaging the sub-model outputs, while the associated estimation uncertainty is quantified through the standard deviation in the estimation. Specifically, for the i-th observation, the ensemble mean and standard deviation are given by Equations (5-6):

$$\hat{y}_i = \bar{y}_i = \frac{1}{M}\sum_{j=1}^{M} \hat{y}_i^{(j)} \tag{5}$$

$$\sigma_i = \sqrt{\frac{1}{M}\sum_{j=1}^{M}\left(\hat{y}_i^{(j)} - \bar{y}_i\right)^2} \tag{6}$$

where, $\hat{y}_i^{(j)}$ denotes the estimation of the i-th sample produced by the j-th sub-model, and M is the total number of sub-models in the QE; M =3840 in the present case.

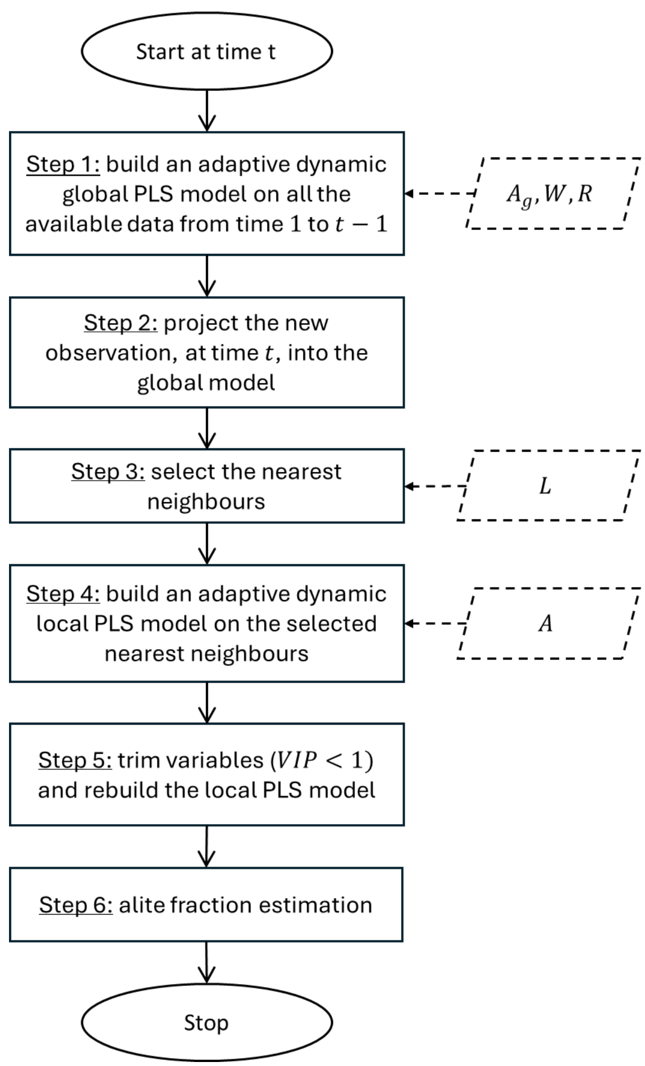

Figure 2. Schematic of the ALD-PLS at time t.

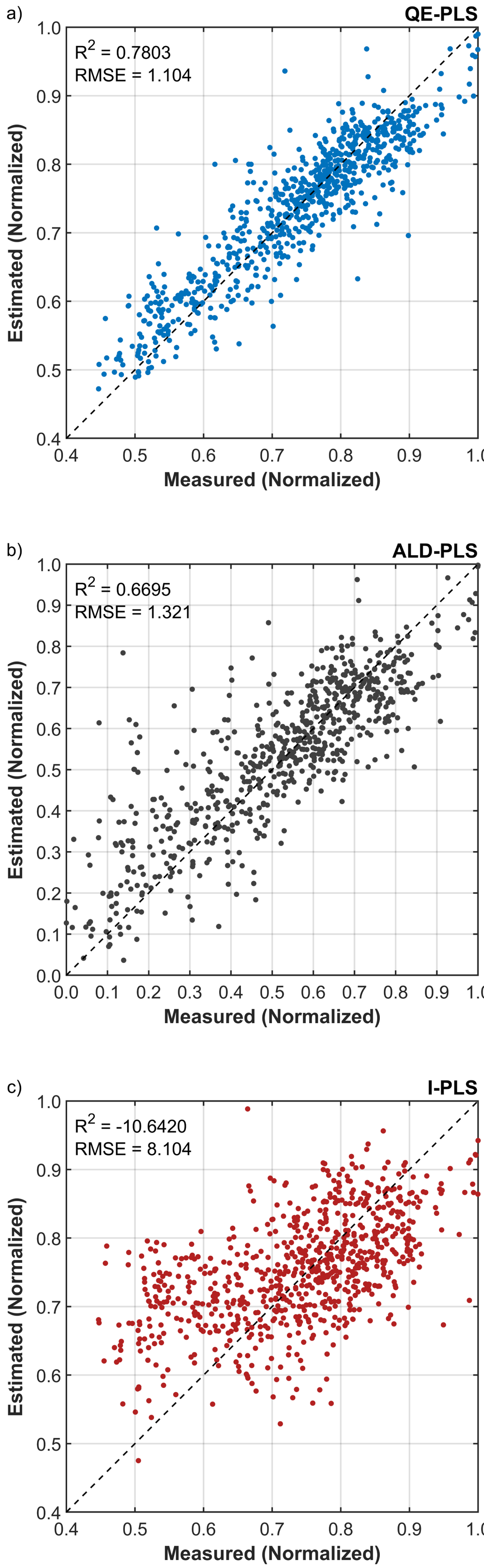

Figure 3. Parity plot of predicted alite fraction vs measured alite fraction: a) QE-PLS, b) ALD-PLS and c) I-PLS.

Based on σ_i, approximate 95% confidence intervals for the final estimations are computed as $\bar{y}_i \pm 2\sigma_i$. The QE-PLS allows the proposed soft sensor to remain robust to hyperparameter uncertainty and process variability, while simultaneously providing predictive uncertainty estimates without requiring explicit probabilistic modelling.

Table 2. Selected hyperparameters ranges.

Hyperparameter	Range
L	30:10:60
A	1:1:8
A_g	1:1:10
W	30 minutes
R	2:2:24 hours

2.8 Performance Metrics

In this work the performance metrics used to assess the quality of the proposed soft sensor are the determination coefficient, R^2, and the root mean square error, $RMSE$; i.e.:

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2} \quad (7)$$

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2} \quad (8)$$

where, y_i is the i-th elements of the **y** measurements, $\hat{y}_i$, the estimation for that element, $\bar{y}$ the mean alite fraction data, and n the number of samples in the **y** dataset.

3. RESULTS

The proposed methodology was applied to the pre-processed **X** and **y** datasets (Section 2.2). The resulting alite fraction estimations are shown in the parity plot of Figure 3 a). The QE-PLS soft sensor achieved an R^2 of 0.7803 and a $RMSE$ of 1.1037. Considering the intrinsic variability of the alite fraction measurements, this indicates an accurate and reliable predictive performance.

To further assess the proposed approach, a comparative study was conducted against two state-of-the-art PLS-based soft-sensing strategies, i.e.: (i) a standard incremental update PLS model, i.e. I-PLS (Section 2.4), and (ii) a single instance of the adaptive local dynamic PLS model, i.e. ALD-PLS, corresponding to one sub-model of the QE. The corresponding parity plots for a single instance of the ALD-PLS and the I-PLS are presented in Figure 3 b) and 3 c), respectively.

The comparative study results are listed in Table 3. They indicate that the QE-PLS model outperforms both I-PLS and ALD-PLS models on R^2 and $RMSE$. Besides, QE-PLS is shown to improve the performance of ALD-PLS sub-models, demonstrating the benefit of aggregating estimations across multiple hyperparameter configurations. Such improvement highlights the ability of the QE framework to enhance robustness and adaptability when modelling the nonlinear and dynamic behavior of alite fraction data in industrial clinker production.

Table 3. Comparison of the estimation performance of tested models on predicting alite fraction.

Model	R^2	*RMSE*
QE-PLS	0.7803	1.1037
ALD-PLS	0.6695	1.3212
I-PLS	-10.6420	8.1038

The tested models were evaluated on a laptop equipped with a 13th Gen Intel Core i9-13900H processor (2.60 GHz), 32 GB RAM, and MATLAB R2024b. Under this configuration, I-PLS showed the lowest computational cost, requiring milliseconds for the estimation of one observation, compared with deciseconds for ALD-PLS and a few minutes for QE-PLS. Thus, I-PLS was much faster than ALD-PLS and QE-PLS. This trend is consistent with the increasing complexity of the models; notably, QE-PLS comprises 3840 ALD-PLS sub-models, which explains its substantially higher runtime. Although this computational burden is a limitation of the proposed soft sensor, the method remains suitable for quality control, since the current laboratory-based reference measurements are acquired only once per hour.

4. CONCLUSIONS & FUTURE WORK

In this work, a soft-sensing framework for the real-time estimation of clinker alite fraction was proposed. The results obtained for the industrial case study (clinker production) indicate that the proposed adaptive PLS-based soft sensor is capable of effectively capturing the nonlinear and dynamic behavior of the alite fraction under realistic operating conditions.

In addition, a novel modelling strategy, i.e. Quasi-Ensemble PLS (QE-PLS), was introduced. The proposed strategy constructs multiple sub-models using different combinations of model hyperparameters evaluated on the same evolving dataset. The QE-PLS framework was shown to outperform both classical incremental PLS (I-PLS) models and single-instance adaptive local dynamic PLS (ALD-PLS) models, demonstrating improved predictive accuracy and robustness.

Despite the achieved favorable performance, the proposed QE-PLS framework entails a relatively high computational cost due to the evaluation of several sub-models. Hence, future work shall focus on reducing computational requirements through optimization of the hyperparameter combination space, as well as through the investigation of more advanced parallelization and asynchronous execution strategies. Besides, further validation will allow for assessing the generalizability and robustness of the proposed approach. Finally, the inherent interpretability of the PLS-based framework will be exploited to support process understanding, anomaly detection, and explainability in industrial process monitoring and control applications.

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6. AUTHOR IDENTIFIERS

Author ORCIDs:
Stefan M.: 0009-0006-2898-4023
Leal da Silva W. R.: 0000-0001-9895-5128
Bezzo F.: 0000-0003-1561-0584
Facco P.: 0000-0001-8383-6783

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