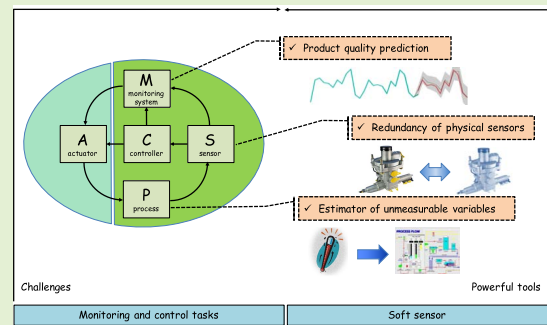


A Review on Soft Sensors for Monitoring, Control, and Optimization of Industrial Processes

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Abstract—Over the past twenty years, numerous research outcomes have been published, related to the design and implementation of soft sensors. In modern industrial processes, various types of soft sensors are used, which play essential roles in process monitoring, control and optimization. Emerging new theories, advanced techniques and the information infrastructure have enabled the elevation of the performance of soft sensing. However, novel opportunities are accompanied by novel challenges. This work is motivated by these observations and aims to present a comprehensive review of the developments since the start of the millennium. While a few books and review articles are published on the related topics, more focus on the most up-to-the-date advancement is put in this work, from the perspective of systems and control.

Index Terms—Soft sensor, soft sensing, process monitoring, optimization and control, industrial process.



I. INTRODUCTION

IN INDUSTRIAL processes, sensing enables the Silicon-based monitoring and control systems to gain access to the internal information about the operating statuses, the state trajectories, and the external variations reflected by the environmental factors. The traditional sensing devices are designed based on the physical laws require solid foundations and insights from natural science. Before their application in engineering systems, signal (energy) transformation and data-sampling are usually required. More recently, to improve

the interaction with the users and to provide intuitive context-related data, smart (intelligent) sensors with wireless communication capabilities and standalone processing functionalities are proposed. As observed from the industrial practice, numerous sensors and sensor networks are installed at various locations to collect the process data. They play an essential role as a part of the information infrastructure.

While we have seen evident increases in the availability of physical sensors, the collected yet underexploited raw data will eventually become data garbage without proper data analysis, information extraction and knowledge exploitation techniques [1]–[3]. Besides, it is neither economic nor beneficial to install sensors beyond requirement, because calibration and maintenance will lead to unnecessary workload and cost. As an alternative to the sensors implemented in the form of physical entities, soft sensors have become indispensable in the modern industry. The model-driven family of soft sensors is most commonly based on first principle models [4]. Nevertheless, when the necessary *a priori* knowledge is unavailable, or the modelling process is overcomplicated, the construction of soft sensors also depend on data-driven techniques. Specifically, soft sensors make the use of the underlying relations between the accessible process variables and provide readouts of the required physical quantities and/or the performance indices.

The development of soft sensors has been greatly facilitated by the achievements in data science, computing and communication technologies, statistical tools, and machine learning techniques. For instance, networking of large-scale systems and system-of-systems allows real-time information exchange. Geographically dispersed process data can be used to drive the

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soft sensors, and in turn, the outputs of the soft sensors can be used to drive the controllers and the process monitors [5]–[7]. Novel communication protocols and techniques help to make use of the communication bandwidth, and in the meantime, reduce the probability of package loss and the chance of external attacks.

In another aspect, to achieve better precision, reliability and adaptiveness, many complex models are adopted, the training and the online updating of which require much computing power. For instance, in a deep neural network, there can be thousands of parameters to be determined and optimized. Along with this, a colossal amount of historical data is fed to the construction and the validation of the soft sensors, from heterogeneous sources, most often with different sampling rates. Fortunately, the emerging computing techniques (e.g., cloud computing, fog computing, parallel computing, etc.) and database techniques provide novel solutions to dealing with the big data.

This work investigates the development of soft sensors over the past two decades. The significance of soft sensing, or rather, its irreplaceability, in improving the production safety and product quality management is discussed from the perspectives of system monitoring, control and optimization. For instance, it will be shown that soft sensors are not subject to the various physical constraints (such as the space for installation and the exposure to extreme working conditions). Additionally, it will be argued that many more unique potentials of the soft sensors will be magnified in the coming decade, where virtual instruments and digital avatars are the keys to elevate full life cycle management of the industrial processes.

Before the further use of the buzz words (“soft sensor” & “soft sensing”), the related terminologies are clarified and defined first to avoid confusion.

A. Terminology

The terminologies that are frequently used in literature can be grouped into two as shown in Fig. 1 (Different categories of “sensors”): (i) Soft sensor, virtual sensor [8], software sensors [9], soft sensing [10]; (ii) Physical/hardware based sensor [11].

Soft sensing refers to the approaches and the algorithms that are used to estimate or predict certain physical quantities or product quality in the industrial processes based on the available measurements and knowledge. Soft sensors are distinguished from the physical sensors in the way that they are implemented on computer software-based systems or embedded systems. In some limited cases, soft sensors can be regarded as the digital projections of the hardware sensing devices in the virtual space, whereas in many other cases, there is no physical counterpart. It is to be noted that soft sensors can overcome the constraint that some physical quantities cannot be measured accurately in the desired period of time.

In literature, soft sensors are also defined as:

- Mathematical models used to predict the behavior of real systems [12];
- The use of mathematical or statistical models to enrich the information measured by actual online sensors and offline sources such as laboratory data [9];

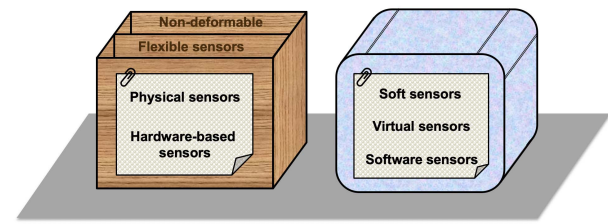


Fig. 1. Different categories of “sensors”.

- The combination of innovative sensor principles with modern methods of data analysis and modelling using process and product knowledge [13];
- The combination of analytical hardware data (from sensors, analytical devices, instruments and actuators) with mathematical models that create new real-time information about the process [14].

It should be emphasized that there are huge differences in the concept of flexible sensors and that of soft sensors discussed in this review. Flexible sensors generally refer to non-rigid or deformable physical sensors, such as wearable sensors [15].

B. Scope and Structure of This Article

In this article, we would like to mainly explore the answers to the following questions about soft sensors and soft sensing.

- (Q1) What is the general procedure to construct a soft sensor applicable to the industrial processes?
- (Q2) How can soft sensors be used to help with the monitoring, control and optimization of industrial processes?
- (Q3) Are there any popular areas of soft sensing applications?
- (Q4) What are the major differences in design for different application scenarios?
- (Q5) What advancement have been made during the past twenty years? What challenges are still existing? What are the promising future directions?

This article is structured as follows. The next section introduces the related surveys and reviews. Section III elaborates the general procedures necessary for soft sensor construction. Section IV summarizes the common problems and advancement in the available solutions. Afterwards, Section V presents a summary of the state-of-the-art applications to the industry, and VI discusses the open challenges and the future directions.

II. RELATED REVIEW WORKS

A few books and review/survey type of articles can be seen in literature that discuss soft sensors and the approaches to their design. However, there is no work that presents a comprehensive review of the progress over the past two decades (2000–2020) and an outlook for the coming decades or giving answers to the questions proposed in the previous section. Some of the existing review-type literature is limited by the time-span of investigation. For instance, in the book [Soft Sensors for Monitoring and Control of Industrial Processes] published in 2007 [16], over 60% of its references are before

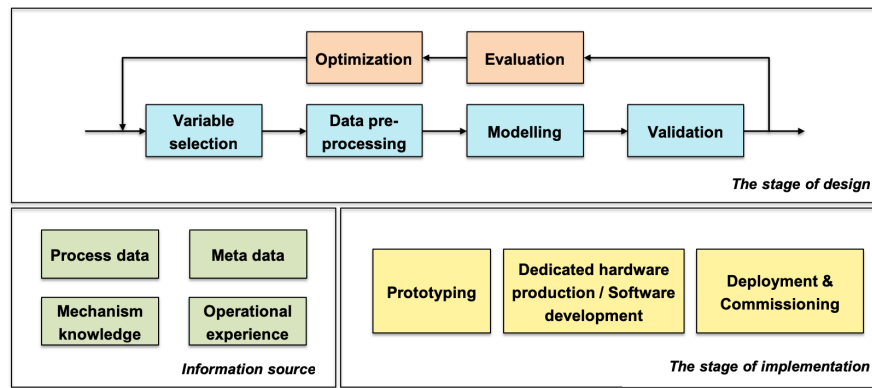


Fig. 2. Construction procedure for a soft sensor.

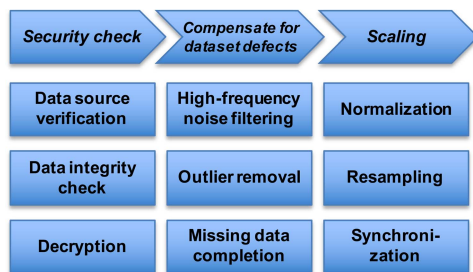


Fig. 3. Data preprocessing tasks.

2000, and only 3% are later than 2005. Many of the approaches described therein have, since then, been replaced or improved by novel techniques. In the review [11], only 10% are published within the past five years. In [17], all of the referred work is dated before 2015, most of which are the preliminary results published at conferences.

In another aspect, some review articles discuss specific categories of modelling approaches or focus on specific application areas. For instance, Chapter 2 of the recently published book [12] only covers deep learning-based approaches; In [17], only the regression-based approaches are investigated. The articles [11], [14] and [13] focus only on the applications to polymer processing, the upstream bioprocesses, and the food & beverage processes, respectively.

Based on the fruitful innovative outcomes by senior researchers and learning from the existing review work, this article presents the current industrial practices and the most significant advancement over twenty years and introduces the state-of-the-art research where novel techniques inject fresh blood into this field of study. In the meantime, the most classical and influential papers, published even if over twenty years ago, are cited whenever necessary.

III. PROCEDURES FOR SOFT SENSORS CONSTRUCTION

One of the major efforts of this work lies in finding the answers to the question “How can soft sensors be used to help with monitoring, control and optimization of industrial processes?” Bearing this in mind, we must first clarify what the most significant system specifications are and design parameters for such purposes. To this end, before diving into

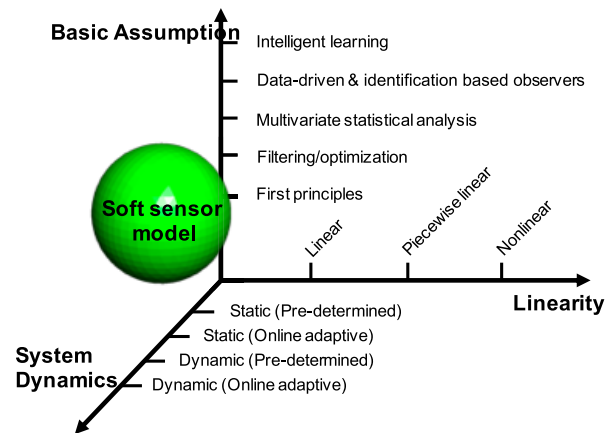


Fig. 4. Dimensions for categorization.

the procedures for soft sensor construction, the application-related key factors and the performance evaluation indices are firstly discussed.

A. Key Factors and Performance Evaluators

Although soft sensors can be designed to generate variable estimations or key performance predictors online, the design procedure can hardly be carried out in a goal-oriented manner to directly meet the key requirements and technical specifications in monitoring, control and optimization (MCO). Instead, it is more of the job of the design engineers of the specific sub-tasks to achieve these specifications based on the available soft sensing data. What they can do is to put forward the requirements for the design specifications of the soft sensors.

In Table I, the differences in the targets of MCO and those of soft sensor design are highlighted. It can be seen that despite the wide variety of sub-tasks and the application scenarios, there are some common factors to characterize the design specifications. Based on the rightmost column of Table I, the answer to “What are the significant performance indices and criteria used for the evaluation and the validation of the soft sensors” is explored.

Availability: While any sensing device or measuring instrument requires a minimum time to give outputs, it is acceptable as long as two conditions are met: (i) the sampled-data system

TABLE I
COMPARISON OF THE SPECIFICATIONS OF CONVENTIONAL DESIGN AND SOFT SENSOR DESIGN

Task	Sub-task	Application scenarios of the soft sensor (Section V-A)	Example key design requirement and technical specification	Soft sensor factors
Process monitoring	Fault detection	1,2	Delay in the detection time	1) Availability (sampling rate, time-delay, missing rate, etc.) 2) Reliability (estimation/prediction accuracy, range of error, probability of error, etc.) 3) Trustworthiness (data source, data integrity, confidentiality, etc.)
			False alarm rate	
			Fault detection rate/miss detection rate	
	Detailed fault information	1,2	Fault classification (precision, recall, sensitivity, ROC, AUC, etc.)	
			Fault identification accuracy	
			Fault isolation accuracy	
Performance degradation estimation	3	Key performance indicator estimation accuracy		
		Remaining useful life prediction accuracy		
Control	Stabilization	1,2	Stability margin	
	Tracking		Tracking error	
	Constraints		Overshoot	
			Bounds for the control command	
			Nonlinearity (deadzone and output saturation)	
Optimization	Parameter optimization	1,2,3	Optimized values of the loss function	
	Scheduling	3	Availability of raw materials and devices	
	Supply chain management		Total cost/profit	

respects the Nyquist-Shannon sampling theorem, i.e., in order to restore the analog signal free from distortion, the sampling frequency should be no less than twice the maximum frequency in the analog signal spectrum; and (ii) the delay is negligible compared to the system dynamics and will not lead to notable performance degradation.

As a novel data source for MCO purposes, soft sensors must provide stably available outputs. It should be noted that the availability issue is quite different from that of physical sensors because, at the online stage, the soft sensors are driven by a set of variables which are also measured online, rather than by the perception of the environment. Therefore, the problems of synchronization, multi-rate, and heterogeneous data have to be considered. Usually, the rate of giving soft sensing outputs cannot exceed the lowest sampling rate among the dependent data sources, and the nominal time-delay of the soft sensor is determined by the sum of the longest delay of each physical sensor or measuring instrument, the transmission (network communication) delay, and the online computational time (algorithm efficiency).

Reliability: It is important that the outputs (estimations and predictions) of the soft sensors do not deviate far from the true values. As reported in [16], the performance of some predictive models degrades promptly due to error propagation, such as the moving average model and the nonlinear moving average model. For MCO applications, it would lead to disasters if the accuracy cannot meet the design specifications: there will be miss detections in case of faults, and the closed-loop control system cannot be stabilized.

Regarding the evaluation of the soft sensors, apart from the average accuracy, it is sometimes more important to check the distribution of the errors, the frequency of unacceptable errors, as well as whether there are bounding values. In another aspect, it is favorable for the soft sensors to give quantitative

or qualitative self-evaluations as the degree of reliability as a supervisory output, which provides an additional reference for the fault diagnosis systems and the control systems. Technically, this requires the models to be designed in the framework of the probability theory. Furthermore, albeit long time-delay, whenever there are physical sensors available to directly measure the corresponding outputs of the soft sensors, corrections and adaptation should be carried out, which is the only chance for online calibration.

The reliability of the soft sensors also indicates the robustness against the performance degradation in the data sources. Specifically, when one or more dependent measurements are biased readouts (lack of precision) or outliers (wrong data), the soft sensor should not be sensitive to them. Besides, soft sensing depends on the well-functioning of all other data sources. If faults occur at the related physical sensors, it is expected that the soft sensor can identify the situation and in turn help to alert the corresponding faulty data source. This is essential for blocking the propagation of faults.

Trustworthiness: The trustworthiness issue is raised here because of the increasing risks of external attacks to the cyber-physical system (CPS) based industrial processes, and the popularized practice of distributed and networked deployment of the sensors (sensor networks).

Nowadays, CPS security is not only a task in the ICT (Information and Communication Technologies) sector but also a novel challenge in the systems and control domain. If the communication channels are compromised, soft sensors will be driven by malicious external signals, which can present a colossal problem to the overall safety of the monitored or control systems. Especially, concealed attacks such as replay attack and false data injection attack must be identified before the soft sensing outputs are controlled by illegal parties. Therefore, in order to ensure credibility, soft

sensors, when using data from external sources, need to verify the data source, examine the data integrity and confidentiality (when applicable).

Other Factors: During the design of soft sensors, one must also consider the overheads relating to the computational load, the memory footprint, the storage space, as well as the required communication bandwidth.

B. General Procedure

Since the construction of a soft sensor for practical use involves many engineering problems, most of the innovative research articles only focus on one or a few parts, rather than reporting the complete design procedure in detail. It is also worth to note the decisive role of the design targets (technical specifications from the clients, based on practical demands) in the selection of appropriate approaches for modelling.

In this part, a generic and complete procedure for soft sensor construction is introduced. As shown in Fig. 2 (Construction procedure for a soft sensor), the construction of a soft sensor includes the stages of data/information collection (information source), design and implementation.

Information Source: The availability and the quality of the four categories of information sources constitute the basis of the subsequent tasks. First of all, there must be a pool of historical process data, especially the measurements from other available hardware sensors. When a subset is considered useful for soft sensing, the online measurements from the corresponding sensors will be used to drive the soft sensor. Associated with the process data, the metadata describes the dataset (e.g., the data property) and clarifies how they can be interpreted. At the design stage, the system/process knowledge, e.g., in the forms of physical principles and chemical reaction equations, will greatly contribute to the tasks of variable selection and data preprocessing. Furthermore, the operational experience from the field operators and maintenance experts is an additional source of information, which may be valuable for all the subsequent steps. As suggested in [16], “Without any expert help or physical insight, a soft sensor design can become an unaffordable task and data can be only partially exploited. The task requires the cooperation of soft sensor designer and plant experts, in the form of meetings and interviews.”

The Stage of Design: This stage is dedicated to transforming the available data and knowledge into an applicable tool, i.e., the soft sensor, in the form of algorithmic approaches. In recent years, although some fruitful research outputs are reported in the literature that solve the specific sub-tasks (as in the top block of Fig. 2), little change is observed in terms of the overall routine for soft sensor design. In fact, the one presented here is very much aligned with those reviewed recently ([11]), five years ago ([17]), and even a decade ago ([4]). For this reason, in this article, we only highlight some major differences and novel challenges, whereas the basic concepts of the widely-recognized steps are not repeated. Moreover, “Variable selection” and “modelling” are not presented here, as they will be discussed in Sections IV-B and IV-C, respectively.

Data preprocessing covers a variety of tasks, corresponding to different dataset properties. In other words, it is somewhat

oriented to specific practical applications. Fig. 3 summarizes the common data preprocessing tasks into three requirements, namely, for security check, for scaling, and the compensation of dataset defects. Among them, the security check is emphasized due to the trend of using soft sensors for cyber-physical systems. The trustworthiness of the data from external sources, e.g., the third-party devices, must be verified. Besides, in case that network-based communication is compromised or exposed to cyber-attacks, the integrity of data should be examined at the data-processing stage to prevent potential misinterpretation. Furthermore, in the case of confidential data, encryption and decryption techniques are also required.

The difference of validation and evaluation lies in the testing items: validation only focuses on the primary design specifications while evaluation gives the full report of the multi-dimensional performance of the soft sensor, such as those introduced in the previous subsection. Based on the evaluation results, optimization techniques can be introduced to improve (e.g., by fine-tuning) the model parameters, and the whole design process forms a close loop until the design specifications can be met.

The Stage of Implementation: This stage aims to transform the algorithmic approaches obtained from the design stage into electronics-based solutions, in the form of either executable software algorithms (software applications) or dedicated hardware implementation. Prototype development and testing are required for batch applications, such as in distributed power grids and automotive applications. Furthermore, deployment and commissioning are required to ensure that the soft sensor is working as expected and the communication channels are properly established, before using the outputs for monitoring and control purposes.

In the future, when cyber-physical systems become the most popular industrial practice, people will also see a trend that the stakeholders of the industrial processes tend to contract the soft sensor construction projects to standalone companies and seek for third-party technical supports such as dedicated hardware production and software development, as well as consultation services, rather than build an expert team by themselves. In turn, this will facilitate the process of commercialization and creating added values of the related techniques.

IV. COMMON PROBLEMS AND ADVANCEMENT IN SOLUTIONS

This section first reviews the common problems in soft sensor design. Since many of the solutions suggested in previous review articles reflect the situation a decade ago, in this part we put special focus on presenting the latest techniques that lead to further advancement to problems encountered at that time. Additionally, emerging technologies and industrial demands have led to new challenges and promoted new research directions.

A. Quality of Data

As have been discussed in Section III-B, data collection is the basis of the data-driven methods. The quality of the historical data has a direct influence on the performance of

the soft sensors. Data collection in the industrial processes sometimes suffers from problems like sampling time, missing data, outliers, and so forth. As a result, the data are not directly applicable to soft sensor modelling.

1) Sampling Rate: In industrial systems, it is common that heterogeneous types of variables have different sampling rates. Some physical quantities can be measured by highly sensitive devices, thus having high sample rates. Some critical variables are difficult to measure, thus having low sampling rates. To deal with this, the traditional approach is resampling, including down-sampling and up-sampling.

The former may lose some of the useful process information while the latter may lead to poor model performance due to the interpolation of the sparsely available quality data. An alternative is to model the multi-rate data by the finite impulse response model [18] and use the output to approximate the unmeasurable variables. This approach avoids excluding the samples. More recently, data fusion techniques are adopted. In [19], an extension of the modified track-to-track fusion approach is proposed. The state estimations of two independent Kalman filters are fused optimally, one of which deals with the slow sampling rate and the varying delay.

2) Missing Data: This happens when no value is stored for one or more variables in an observation. Under the condition that the proportion of the missing values is small, the time instances containing missing data can be removed with listwise or pairwise deletion approaches. Alternatively, the missing values can be imputed employing mean substitution, hot-deck substitution, regression substitution, conditional distribution-based substitution and multiple imputations [2]. It is worth to note that the more recently developed multiple imputation approach has better performance than single imputation in most cases. The most studied multiple imputation approach is based on probabilistic principal analysis [20]. Nevertheless, it has a heavy computational load.

Two other approaches employed to deal with missing data are expectation maximization [21] and maximum likelihood [22], which assume the missing data are subject to a certain distribution. Additionally, an autoencoder is employed to reconstruct the missing data in [23]. Based on this, several modern approaches have been developed, such as extreme learning machine autoencoder [24] and supervised variational autoencoders [25]. The limitation of using the autoencoders is in the size of the auto-associative neural networks.

3) Outliers: Outliers refer to the measurements that deviate from the typical and the meaningful range of the variables. Many popular outlier detection approaches are based on the statistical properties of the historical data. The 3σ rule is one of the simplest solutions, which assumes the variables subject to normal distribution. However, its performance is unsatisfactory in the case of multivariate outliers. The correlation among variables needs to be considered by multivariate approaches.

Multivariate approaches can be categorized into the distance-based, the density-based and the proximity-based ones [2]. Distance-based approaches treat the samples that are far from the center of data distribution as outliers using, for instance, Mahalanobis metric. However, the Mahalanobis distance-based approach can only be used to describe Gaussian

clusters. Density-based approaches estimate the distribution and identify outliers that locate at the low-density regions. Examples include the Parzen window, C-means and the Gaussian mixture model [26]. The Parzen window approach is easy to implement whilst sensitive to the choice of the initial cell volume. When applying the C-means approach, the cluster number need to be defined based on the knowledge of the experts. The Gaussian mixture model approach is able to deal with non-Gaussian data. However, its performance deteriorates in case of very high dimensional data. As for the proximity-based approaches, the similarity in data with their neighbors is considered. Popular solutions include k-nearest neighbor [27], local outlier factor [28] and angle-based outlier factor [29]. The K-nearest neighbor approach removes a proportion of observations of large distances, thus losing the information therein. The performance of the local outlier factor approach is heavily dependent on the number of nearest neighbors, and the angle-based outlier factor approach is not suitable for large dataset.

Although there are many available solutions, there are some limitations as well. First, strong assumptions to the dataset make them poor in the generalization capability. Second, most solutions are time-consuming due to the need to calculate metrics between all data. This is especially notable in the case of high dimensional data. Third, the results still have to be validated by process experts to reduce false detection.

B. Variable and Feature Selection

There is a colossal number of variables in modern large-scale industrial processes. Some variables are highly correlated with the target variables while the others are useless for soft sensor construction. An appropriate selection procedure will reduce the model development effort, simplify the model structure, and improve the soft sensing performance. With the aid of system experts and some reliable automatic tools, two aspects are usually considered: determine a criterion to assess the most useful feature subset; employ a search strategy for a suitable variable subset. Three different approaches that try to achieve this are briefly reviewed below.

1) Ranking-Based Approaches: Ranking-based approaches calculate the relevance of each variable to the target variable using, e.g., the correlation coefficient or mutual information [30]. Then, a subset of variables is selected by comparing the scores to a threshold. In [31], an efficient feature selection algorithm is proposed based on normalized mutual information. However, the estimation of multidimensional probability density function leads to heavy computational load. Most recently, improvement is achieved by the integration of Tabu Search into the approach. Falling into a local minimum is thus avoided [32].

2) Wrapper Approaches: Wrapper approaches make selections according to the generalization performance of the models that are trained using different subsets of variables. The key is to reduce the computational burden (unacceptably large number of subsets) with a search procedure. Sequential feature selection and the genetic algorithm are the potential choices in this respect [33]. It is interesting to notice that, recently, efforts are made in combining the wrapper approaches and

TABLE II
COMPARISON OF SINGLE AND MULTIPLE IMPUTATION

Approaches		Advantages	Disadvantages
Single imputation	Mean substitution	Efficient and unbiased estimation	Distortion in variances and correlations
	Hot-deck substitution	Good variance estimation	Missing records
	Regression substitution	Inherited from the regression models	Distortion in variances and correlations
	Conditional distribution	Alleviate the distortion problem	Constraint in the distributions
Multiple imputation		Better performance	Computationally intensive

the ranking-based approaches. Good performance in specific applications has been reported in [34], [35]. The drawback lies in that each time a subset of variables needs to be evaluated, a regression model has to be constructed.

3) Embedded Approaches: Embedded approaches incorporate feature selection as a part of the training process. A typical class of algorithms that follow this idea is the regularization-based ones with a penalty term [36]. In [37], regularization is applied to the neural networks. A penalty function is defined to weaken the influence of the useless variables. Another solution first uses all the inputs to train the model. Then, the irrelevant variables are removed sequentially according to the result of a sensitivity analysis [38]. Similar to the wrapper approaches, the model is retained each time the variables need to be evaluated.

In addition to the above, unsupervised approaches have received increasing attention in recent years [39]–[41]. Comparisons are made in [42], [43] on the partial least squares (PLS) related approaches.

C. Model Selection and Model Construction

There are various categories of approaches for soft sensor modelling. Each class is based on different assumptions and applies to specific system types. Fig. 4 shows a three-dimensional space that can cover a wide range of soft sensors, designed during the past twenty years.

According to linearity, the model type can be categorized into linear models, piecewise linear models and nonlinear models (e.g. nonlinear autoregressive with exogenous input model, neural networks, Bayesian network, fuzzy model and wavelet model) [44]. Generally, linear models are considered first. If the performance is unsatisfactory, piecewise linear models shall be tried before seeking for solutions by the nonlinear ones. Based on the Monte Carlo study, it was shown in [45] that reliable criterion for model selection includes the Bayesian information criteria and the Geweke-Meese criteria. Moreover, nonlinear function estimation is another strategy to quantify the nonlinearity degree in the process variables [46].

In another aspect, the selection of the soft sensor model should also be appropriate to **the system dynamics**. In some industrial processes, the variables of interest show a static relationship with the available measurement variables. However, the dynamic characteristics must be considered when there is a non-negligible correlation in time (time series) and in states (state-dependent) [47]. That is one of the major issues to be considered during model selection, between, for instance, the multivariate statistical analysis-based model construction approaches and the observer/filter-based approaches.

The strategies to deal with variations in the operational point and the external environmental factors can be grouped into two. Pre-determined switching laws based on pattern recognition have been extensively studied. It is simple and effective when the variations to be considered are finite (thus the switching regions are finite) [48]. Otherwise, online adaptive strategies tend to be more robust in the case of continuous (infinite) and unexpected variations.

In the following, soft sensing model construction will be categorized **according to different basic assumptions**.

1) Multivariate Statistical Analysis: The basic assumption is the existence of some consistent statistical features, such as constant variance, covariance and some latent structures. Many basic approaches have been reviewed in [11], [17], [49]. For instance, a robust improvement of PLS was proposed in [50], [51]. In [52], recursive PLS model was fused with wavelet coefficient matrices to represent different frequency. Recently, an open-source toolbox was published [42] where many tools are available for basic multivariate statistical analysis.

2) Data-Driven and Identification Based Observers: The basic assumption is the existence of the system states. Model-based observers have been well-studied in modern control theory, where system matrices are known (calculated using accurate models based on physical principles. For complex industrial processes, this is sometimes infeasible due to the need for comprehensive knowledge. Black-box system identification provides an alternative. System matrices are solved offline using dedicatedly designed excitation signals and the corresponding outputs and will remain unchanged at the online stage [53]. In contrast, data-driven observers rely only on process data and are more easily extended for online update and adaptation [54], [55].

3) Machine Learning: The basic assumption is that the outputs are uniquely determined by the nonlinear projection of the inputs, or the dynamics of the systems mimic some natural behavior. In most scenarios, the quality and the quantity of the training dataset governs the modelling performance.

In recent years, intelligent algorithms, especially the deep learning techniques, have boosted the development of soft sensors. To capture the abstract features, deep structures based on the convolutional neural network, deep brief network and autoencoders have been extensively studied [56], [57]. For time series data, long short-term memory networks and its modifications (such as gated recurrent unit) are the most popular tools [58], [59]. As for the traditional machine learning approaches (e.g., support vector regression), for soft sensor applications, they are usually integrated with the optimization

procedures, such as random forest and generic algorithm [60], [61].

4) *Filtering (Kalman Filter)*: The condition for the adoption of Kalman filter and extended Kalman filter is that the knowledge about certain stochastic properties of measurements and noises are available. As optimal state estimators, they are usually derived from the models constructed based on the practical process to deal with noises [62], [63]. In [18], the Kalman filter was adopted as the core of a data fusion algorithm to deal with multi-rate sampling problem. More recently, an unscented Kalman filter was proposed for fast-sampled measurements while a modified form (delay-dependent variable step-ahead prediction) was used for slow-sampled measurements [64].

5) *First Principle Models*: The condition that this type of models is feasible is to have sufficient knowledge about the underlying principles of physics, chemistry and even biology. The construction activities must be case-oriented. In complex scenarios, finite element analysis is usually necessary. Typical first principle models are based on the principle of Conservation of Energy [8], [64], the principle of material balance [65], as well as kinematics and system dynamics [66]. In most soft sensor publications, first principle models are rarely used directly, but rather are usually integrated with other data-driven models or calibration procedures [67].

D. Soft Sensor Maintenance

The performance of soft sensors degrades over time when drifting and variations occur in the industrial processes. There is limited information contained in the historical data (at least with a limited period of time) that can be used to construct soft sensors. Considering this, the online operational data and the contextual data that can characterize the evolution of the processes are the necessary sources of information. Unlike physical sensors which usually go through scheduled calibration, frequent examination and periodic replacement, there still is no consensus on how to maintain soft sensors for long-term functioning.

Continuous adaptation methods can avoid the problems caused by fixed models. To achieve this, sample selection can be applied to select the most relevant data samples while sample weighting contributes to changing the degree of importance of the samples dynamically according to, for instance, the time of measurement. These strategies can easily be combined with the modelling methods based on, e.g., principal component analysis and artificial neural networks [68]. Typical solutions proposed recently include just-in-time learning [69], [70], iterative learning [71], incremental learning [72], and ensemble learning [52], [73]–[76]. Adaptive data-driven soft sensing approaches based on various machine learning techniques have been compared in [68].

V. STATE-OF-THE-ART IN SOFT SENSOR APPLICATIONS

In this section, a categorization of the soft sensor application scenarios is firstly presented. It is shown that the applications fall into at least 10 different purposes. After that, the applications to the practical areas, as well as several real-world deployment cases are introduced.

A. Application Scenarios

1) *Virtual Redundancy of Physical Sensors*: While the outputs of the soft sensors can be used for the monitoring, control and optimization of the whole process, soft sensor itself can be regarded as a nominal system or a fault-free digital twin of a real sensing device (when exists). In this context, soft sensors are also called observers, filters, state estimators, or predictors in the disciplines of control and fault diagnosis. By examining the difference in the outputs of the physical entities and their virtual counterparts, the healthy status of the physical sensors including well-functioning, material ageing, software errors and hardware failure can be determined with the aid of fault detection, fault classification and fault identification techniques [8], [16], [54]. Through this capability, periodic maintenance can be cancelled or reduced, which can be consequential for the case of remotely and distributed installed sensors. Therefore, the soft sensors can be applied in the following scenarios:

- i) Online diagnosis of the hardware-based sensors.
- ii) Temporary backups for physical sensors during routine maintenance.
- iii) Digital twin of a physical sensor, characterizing the full life cycle and covering the stages of design, manufacturing, commissioning, deployment, operation, maintenance, and disposal.

2) *Estimator for Unmeasurable Physical Quantities*: Each physical sensing device has a designed range, precision and sampling rate for measurements. For instance, the clinical thermometer can usually give readouts between 35 °C and 42 °C. However, there are practical demands for many industrial processes to operate in unusual conditions; such as extremely high pressure, extremely high temperature or extremely low temperature. It is also not rare to see some processes working under a wide range of and frequent variations. In another aspect, the large-scale systems like dams and power grids must also depend on mathematical tools to compensate for the unreachable order of magnitude of the physical sensors. As a result, soft sensors become the only possibility to gain process knowledge and carry out online monitoring and control in these cases.

In a drilling process, the primary task is to perceive the downhole circumstances and detect, in a timely manner, whether a part of the mechanical structure, most importantly the drill, is broken. However, high pressure and high temperature pose severe challenges to the use of downhole sensors. In today's engineering practice, the flow rate of the volume of the drilling fluid that enters and returns from the wellbore is used as an alternative for monitoring and control purposes. Due to the existence of the mixed cuttings and gas squeezed in the drilling fluid, the performance of the physical flow meters can be degraded. To deal with this, soft sensors for the flow rate estimation are designed based on the upstream level data collected by ultrasonic equipment and the corresponding reference data [77]. The necessity of soft sensor application due to the similar reason is also demonstrated in the blast furnace iron making process [74], shaft furnace roasting process [10], etc.

In the waste water treatment processes, the ammonia concentration is a key variable for the control and evaluation of the removal performance of the harmful substances. While ammonia concentration can be determined by some commercial-off-the-shelf devices such as in-situ ion selective electrodes and ex-situ analyzers, these high-end yet error-prone instruments require frequent maintenance by skilled staff. A more economical alternative was reported in [78]. The authors explained the possibility of using cheaper sensors (pH and oxidation-reduction potential) to construct soft sensors to achieve the same goal. More recently, the reliability of the soft sensors is improved in a way that compensate for the drift of the pH sensors: in [79], qualitative features (the minima and maxima of the pH difference signal) are suggested to be included in the design.

In summary, the soft sensors play a significant role in the following scenarios:

- iv) In extreme operation condition that exceeds the limit of the physical sensors.
- v) When implementation of some physical sensors is economically unacceptable or undesirable.

Furthermore, it is also easy to see the value of soft sensors in the following cases:

- vi) Infrequent and/or delayed measurement by hardware sensing devices ([64]).
- vii) Requirement for non-invasive measurement.
- viii) There is no space or load for the installation of the physical sensors (e.g., spacecraft).

3) Product Quality Prediction: The concept of soft sensor also covers the prediction of abstract features as well as qualitative or quantitative assessment indices in the industrial processes, for instance, the key performance indicators that characterize the final product quality. In wine production process, historical data and expert knowledge are required to adjust the timing and the quantity of the feeding of the components. However, this is an open-loop process. The final quality of the red wine cannot be learnt until the wine tasters give professional comments. Nevertheless, there are actually early hints and signs of potential quality degradation from the large amounts of process variables at different stages [80]. Following this assumption, soft sensors can be designed to give early predictions, using the multivariate statistical tools or the machine learning techniques. An interesting attempt was made in [81] where four-dimensional gradings made by the wine tasters were collected, namely, the presentation 15 points, fragrance 30 points, mouth feel 44 points, and subjective feeling 11 points, such that the overall wine quality is 100 points. Based on these evaluations and the corresponding process data, the soft sensors are trained as an alternative to human professionals, and beyond this, to give frequent online evaluations.

Soft sensors for other key performance indicators were studied in [50], [65], [70], [82], [83] (chemical production), [10], [52], [79], [84]–[86] (chemical processing), [47], [52], [70], [87]–[89] (petroleum refining), [67], [90], [91] (mechanical industry), [92] (drug industry), etc. In these examples, soft sensors:

- ix) Give early reports before time-consuming laboratory analysis (for early diagnosis and predictive maintenance).
- x) Monitor online/in real-time the quality and quantity of the final products and by-products.

B. Application Areas

Table III summarizes the soft sensor applications in industrial processes into several common areas. These examples are based on the articles published within the past decade (2010–2020), and can therefore reflect the latest research interests and the urgent practical needs. Corresponding to each industrial process, the specific physical quantities of sensing are listed. The symbols O_2 , CO , CO_2 , H_2S , and SO_2 are chemical symbols while the others denote surrogate symbols that are defined in the related references.

A major focus of study is on the chemical industry. To a great extent, this is due to the lack of applicable mechanism models in the chemical reactions—although some processes can be described by the chemical reaction equations, there are always side reactions accompanying the main reaction. Many of the side reactions are highly-complicated or even unknown. Furthermore, many chemical reactions are sensitive to the variation of external environmental factors, such as temperature, pressure, and the availability of the catalysts. As a result, solving the chemical equilibrium online in real-time is usually infeasible. On the other hand, the correlation among the reaction processes and among the process variables (including the reactants, the feed rates, the flow rates, temperature, pressure, the pH values, etc.) provides a solid theoretical foundation to the development of the soft sensors. In other words, the basic assumption on the dependency of the variables can be nicely satisfied, which is required by the multivariate analysis models, the regression models, and some (reduced-order) observers.

Among the soft sensor applications to the chemical industry, the most popular ones are the Tennessee Eastman process (TEP) and the debutanizer distillation column. TEP is an open and challenging chemical model simulation platform developed by the Eastman Chemical Company in the United States. It was designed to reflect the characteristics of the real-world chemical reaction process, and is now widely recognized as a benchmark in the areas of process control and fault diagnosis of complex industrial processes [93]. As shown in Table III, soft sensors were designed for the online estimation of different components in several TEP units. The extensively studied debutanizer distillation column was initially presented in [94] and soon afterwards included in the book [16]. It is a part of a desulfuring and naphtha splitter plant that is located at the Mediterranean Oil Refinery Company (ERG Raffineria Mediterranea S.R.L.) in Syracuse, Italy. In order to maximize the stabilized gasoline content in the liquefied petroleum gas splitter feed and to minimize the butane content in the naphtha splitter feed, soft sensors are required to provide real-time estimates of the butane concentration in gasoline and the gasoline concentration in butane [94].

In addition to the application to the chemical processes, there are also a number of practical needs in the mechanical sector. The most notable difference from the chemical industry

TABLE III
APPLICATION EXAMPLES OF SOFT SENSORS IN INDUSTRIAL PROCESSES

Industrial process		Innovative article		Reference	Dataset go public
Domain	Sub-domain	Specific application	Physical quantities of sensing		
Chemical industry	Chemical production	Vinylacetate-ethylene polymerization processes	Tensile strength of tile adhesive	[98]	Unknown
		Ammonia synthesis process	Content of O ₂	[99]	Unknown
			Content of residual CO and CO ₂	[99]	Unknown
			Concentration of CO ₂	[73]	Unknown
		Aluminum electrolysis	Concentration of alumina	[64]	Unknown
		Hydrocracking process	Content of silicon	[74]	Unknown
		Blast furnace ironmaking process	Initial boiling point of the diesel oil product	[9]	Unknown
		Bayer process (Purify bauxite into alumina, or aluminum oxide)	Strength of alumina crystal conglomerates refined from bauxite (A critical alumina quality parameter)	[50]	Unknown
			Component G in the purge gas	[70]	Yes
			Component B in the product stream	[65]	Yes
			Components D, E, and F in the product stream	[82]	Yes
			Component E in the purge gas	[100]	Yes
			Component F in the product stream	[83]	Yes
			Component C in the purge gas	[69]	Yes
	Chemical processing	Polyethylene production process	Melt index	[75][101][52]	Unknown
		Industrial sulfur recovery unit	Content of H ₂ S and SO ₂	[84]	Yes
			Concentration of H ₂ S and CO ₂	[85]	Yes
			Concentration of O ₂ in the effluent flow	[86]	Yes
		Wastewater treatment process: Benchmark Simulation Model No. 1	Amount of organic matter BOD ₅	[79]	Yes
			Qualitative evaluation of the pH differences	[10]	Unknown
	Petroleum refining	Mineral processing: shaft furnace roasting process	Recovery ratio of the magnetic tube	[47]	Unknown
		Debutanizer distillation column	Concentration of butane	[52][70][87-89][102]	Yes
		Crude refining process	Vapor pressure of the light naphtha	[103]	Unknown
	Thermodynamics	Multicomponent distillation process	Distillate composition	[77]	Unknown
Mechanical industry		Flow measurements of drilling fluid (Drilling of oil or gas well)	Volumetric flow of non-Newtonian fluids (The return flow of drilling muds)	[67]	Unknown
		Industrial hot strip mill	Thickness of the strip	[91]	Yes
		Industrial IsaMill	Size of the particle	[90]	Unknown
		Injection molding process	Weight of the final product	[104]	Yes
Renewable energy		Photovoltaic generation system	Solar irradiance	[105]	Unknown
		Pressurized water reactor (nuclear)	Flowrate of the feedwater	[106]	Unknown
Robotics		Unmanned aerial vehicle	Attitude of the vehicle	[107]	Unknown
		Soft robotics	Contact force and curvature	[108]	Unknown
		Soft robotics	Location of the contact pressure	[8]	Unknown
Building industry		Building ventilation units	Temperature, airflow and the speed of fan	[92]	Unknown
Drug industry		Penicillin production process	Concentration of the biomass and Penicillin	[80]	Yes
Food industry		Wine quality prediction	Wine quality (100 points) including Presentation (15 points) Fragrance (30 points) Mouth feel (44 points) Overall feeling (11 points)	[81]	Unknown

lies in the feature of the physical quantities of sensing: in most cases, soft sensors are constructed to meet the design requirement of high precision, which cannot (presently) be achieved by the physical sensors. These physical quantities include the volumetric flow, the strip thickness, the particle size, etc.

In the past decade, a few applications have been reported in the domains of nuclear industry, smart buildings, drug production, and food industry. However, it should be noted that the application domains (sub-domains) and the value of the soft sensing techniques are more than what have been summarized here. Beyond the scope of this study, soft sensors have good potentials in medical care systems, automotive systems, and robotic systems.

C. Real-World Deployment Cases

Most of the existing research activities have been conducted as performance evaluation of soft sensors in laboratory setups (based on simulations) or with limited amounts of experimental data acquired from real plants. Only a few have been tested and verified on real systems and real plants. In this part, several real-world deployment cases are introduced.

Case 1: (2007, data-driven) A soft sensing scheme was proposed in [9] where an automated stepwise linear regression approach was used to find the relevant predictor variables. The soft sensor was adopted by the largest alumina refinery in Europe, RAAL (RUSAL Aughinish Alumina Ltd., located in southern Ireland). It replaced the previous statistical forecasting tool of RAAL, and was deployed to predict the strength of alumina crystal conglomerates—a critical alumina quality parameter in the Bayer process, and to forecast deviations off the normal operating conditions.

Case 2: (2010, model & data integrated) In [10], the authors proposed to combine the fuzzy mechanism model with a neural network compensator to online estimate the magnetic tube recovery ratio in the mineral processing. Data clustering techniques and a fast training algorithm were employed. The soft sensing approach was adopted by a metal company in Lanzhou, China, and plays a supervisory role as a reference value to monitor the shaft furnace roasting process.

Case 3: (2017, model-driven) In [91], the P80 particle size in a horizontally stirred mill (an industrial IsaMill) in Western Australia was estimated online. The proposed soft sensor is based on the random forest model. However, according to the observation over two months, it was pointed out that

recalibration is required to compensate for the frequent process drift in the mineral processing operations, owing to large variations in the feed.

Case 4: (2018, model & data integrated) The authors of [8] exploited the physical relationship inside the building ventilation units and constructed soft sensors based on simple linear and nonlinear regression models. The soft sensors are used to estimate the temperature, air flow, fan speed, and to diagnose faults in the heater energy meter. The developed soft sensors were tested on a real building for teaching—the Odense undervisning building 44 (OU44)—at the University of Southern Denmark, campus Odense, built in 2015.

VI. OPEN CHALLENGES AND FUTURE DIRECTIONS

Based on the above discussions, this section summarizes the open challenges to overcome and the future directions that are promising in the coming decade.

- Improving the autonomous capability (decision-making in design and self-validation): At present, several steps at the design and implementation stages rely on the assistance of human experts, such as model selection and feature selection. The performance of soft sensors has better guaranteed with the aid of the experts' knowledge and experience. However, this can be optimized in the future, to reduce the dependency on the designer skills. Although this direction has not been approached systematically and extensively today, it is inspiring to notice that there are some attempts reported. In [95], a probabilistic self-validating approach was proposed where unreliable data are identified and corrected. To deal with time-varying environment and operating conditions, authors in [96] proposed an online variable prediction approach where models are added or removed adaptively for improved ensemble performance; authors in [97] proposed to conduct automated validation to improve the accuracy and reliability of soft sensors, by integrating just-in-time models and relevant vector machine.

- Filling the gap between the laboratory outcome and the industrial practice: Due to the desire for good performance, algorithms developed for soft sensor design are usually complicated. However, a compromise in performance against computational efficiency is found to be unfavorable to meet the practical needs. As discussed in [13], although proven to be very effective in the academic domain, there are only few practical applications of evolutionary algorithms in the field of food and beverage production due to the heavy computational burden, especially the requirement of massive parallel implementation. In addition to the difficulties in online implementation, there are quite few practical cases reported as deployments in real industrial plants. As discussed in the previous section, most works are limited to simulations and laboratory-scale experiments. To improve this, further in-depth collaboration between the academia and the industry is required.

- Embedded in the integrated framework of control and optimization: Soft sensing is driven by process data online and in turn provides key information about the system. It is meaningful to expand the role if these estimations and predictions can be used in the close-loop for control and optimization

purposes. Compared with measurements from the sensors, the challenge of adopting soft sensing outputs lies in the strategy to ensure reliability in case of faults in the dependent variables, and to cut off the fault propagation path.

- Exploiting the potential of the deep learning techniques and other intelligent approaches: Deep learning is powerful in modelling highly complex nonlinear processes [12], [61]. However, several challenges still hinder its application to soft sensor design, for instance, the interpretability of the features extracted from data and the relationship with the outputs, the sensitivity to the network hyper-parameters, and the influence from the size of available training dataset.

VII. CONCLUSION

This review focuses on the key scientific problems in the design and implementation of soft sensors in the context of the modern industry. Based on an exhaustive investigation of the literature, it is dedicated to associating the studies reported over the past twenty years, and giving answers to the research questions proposed in Section I-B. While these questions are discussed whenever relevant, they are addressed mainly in the corresponding sections as follows: Q1 (III-B); Q2 (III-A, IV); Q3 (V); Q4 (IV, V-A); Q5 (Advancement: Discussed throughout the paper; Challenges and future directions: VI).

In the coming decade and beyond, apart from the efforts to overcome the aforementioned challenges, it is expected to witness more novel ideas, more advanced techniques and broader platforms where soft sensing plays an indispensable role in the monitoring, control and optimization of the industrial processes, not to mention the use in Digital Twins. The future of the soft sensing techniques is destined to be inspiring and exciting, no less that today looking back at the past.

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