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Methods for Plant Data-Based Process Modeling in Soft-Sensor Development

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There has been an increased use of soft-sensors in process industry in recent years. These soft-sensors are computer programs that are used as a relatively cheap alternative to hardware sensors. Since process variables, which are concerned with final product quality, cannot always be measured by hardware sensors, designing the appropriate soft-sensor can be an interesting solution. Additionally, a soft-sensor can be used as a backup sensor, when the hardware sensor is in fault or removed due to maintenance or replacement. Soft-sensor is based on the mathematical model of the process. Since industrial processes are generally quite complex, a theoretical modeling approach is often impractical, expensive or sometimes even impossible. Therefore, process model building is based on measured data. This approach significantly gets complicated if only plant data, taken from the process database, are available. In this paper the most popular methods for plant data-based modeling that appeared in the last two decades are summarized and briefly explained. Apart from giving a short survey of the most important papers, tips about choosing the appropriate methodology for process model building are also provided.

Key words: Data-based process modeling, Plant data, Soft-sensor, Modeling methods overview, Papers overview

Metode modeliranja na pogonskim podacima za razvoj soft-senzora. U posljedne vrijeme moguće je uočiti povećano korištenje soft-senzora u procesnoj industriji. Soft-senzori su računalni programi koji su jeftina alternativa hardverskim senzorima. Budući da su procesne veličine povezane s kvalitetom izlaznog proizvoda često nemjerljive, razvoj soft-senzora može biti zanimljivo rješenje. Nadalje, soft-senzor se može koristiti kao zamjena za hardverski senzor kada je on u kvaru ili nedostaje uslijed održavanja ili zamjene. Soft-senzor se temelji na odgovarajućem matematičkom modelu procesa. Kako su industrijski procesi najčešće vrlo složeni, teorijski pristup modeliranju procesa često je nepraktičan, vrlo skup, a ponekad čak i nemoguć. Iz tog razloga, izgradnja modela procesa često se temelji na mjernim podacima. Ovaj pristup se značajno usložnjava ako su na rapolaganju samo pogonski podaci, preuzeti iz procesne baze podataka. U ovom radu su ukratko opisane postojeće metode za modeliranje procesa na temelju pogonskih podataka koje su se pojavile u posljednja dva desetljeća. Osim toga, ukratko su izloženi najznačajniji radovi, a dane su i smjernice za odabir pogodne metode za izgradnju modela procesa.

Ključne riječi: modeliranje procesa na temelju podataka, pogonski podaci, soft-senzor, pregled metoda za modeliranje, pregled radova

1 INTRODUCTION

Requirements regarding final product quality, production efficiency, process safety and environment pollution are continuously increasing in the process industry. These aspects can be addressed by installing monitoring and control systems in the industrial plants which are based on measurements of different process variables (Fig. 1). Performance of the monitoring and control systems heavily depends on the quality of the measurements.

Problems with tight control and optimization appear when important process variables, which give information about the final product quality, cannot often be measured by a sensor or the measurements are too expensive and/or not reliable enough so that are not used. The value of these difficult-to-measure variables is often determined by laboratory analysis based on the samples taken from the process. This kind of measurement is performed periodically, with a long time delay in obtaining information, so continuous monitoring of the final product quality and introduction of automatic control are not possible [1].

Since most of the process variables are measured by hardware sensors, their accuracy, availability and sampling frequency are the most important factors for successful process monitoring and control. However, sometimes information obtained from sensor can be useless or even completely absent due to several causes:

- different sensor faults,
- data acquisition system fail,
- sensor removal due to its maintenance or replacement,
- sensor's very low sampling frequency (e.g. gas chromatographs, NIR analyzers).

This can negatively affect process monitoring and control which can result in increased production costs, lower product quality or even dangerous situations for plant personnel or environment [2].

In order to improve system reliability, process monitoring and control, soft-sensors (intelligent sensors) are often used. The main applications of soft-sensor is on-line estimation of difficult-to-measure variables and process monitoring where soft-sensor is used to raise alarm when the process starts to significantly deviate from normal conditions. Besides that, soft-sensor is often used as a back-up for a hardware sensor. This requires that appropriate diagnostic algorithms are implemented that will detect and identify faulty sensor. These diagnostic procedures are often categorized as soft-sensors, too.

Problems, which appear in soft-sensor development, were firstly explored in the field of chemometrics [3]. After that, many papers dealing with different types of soft-sensors and several overviews of this area were published. In [4] a comprehensive overview of data-driven soft-sensors in the process industry is given which does not deal with mathematical background of the methods. In [2] focus is mainly on real industrial applications, with minor attention to theoretical issues. Overview of the various soft-sensor modeling methods through different aspects is given in [5]. Very brief overview of data-based techniques is given in [1] with discussion about control loops with soft sensors.

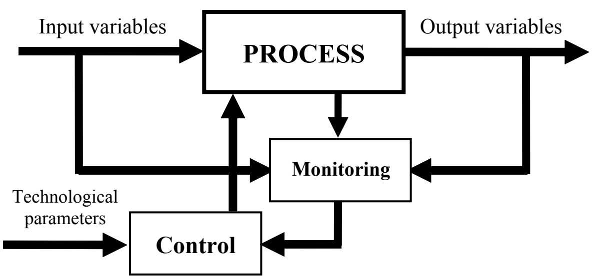

Fig. 1. Process monitoring and control

In this paper we tried to summarize and briefly explain the most popular mathematical methods for plant data-based modeling that appeared in the last two decades. In Section 2 the procedure for soft-sensor development is explained. Section 3 gives overview of the most popular methods for model building with their advantages and drawbacks, followed by popular case studies which can be found in the literature in Section 4. Section 5 deals with tips for choosing appropriate method for process model building. The paper is concluded in Section 6.

2 PLANT DATA-BASED MODELING

Soft-sensor is based on appropriate mathematical model which connects easy-to-measure variables (e.g. flows, temperatures, pressures) with the output variable which can be difficult-to-measure variable (e.g. viscosity) or state of the process (process within specification or process out of specification). In practice, the model is usually not available, so it has to be built. There are two approaches:

- first principles modeling (theoretical modeling),
- data-based modeling (data-driven or empirical modeling).

The first approach is based on deriving equations describing the physical and chemical principles. Since industrial processes are often very complex, this approach is often impractical, time-consuming, requiring great process knowledge and effort and sometimes it is even impossible. While it gives great insight about process, it often results in insufficiently accurate model parameters. The second approach is used whenever there is not enough a-priori knowledge about process. This type of modeling generally produces models which are simpler and which better describe input-output relationship than first principles models. Also, it is applicable to different types of processes.

In data-based modeling, obtaining the process model is based on the measured data. There are two ways in which data can be gathered:

- through specially designed experiment (experimental data),
- through normal plant operation (plant data, historical data).

Advantage of the first approach relies on the fact that, if the experiment is carefully planned, data can be very informative since all process modes can be activated and the presence of disturbances and errors in the data can be reduced to minimal possible extent. Additionally, if output variable is sampled with high frequency, classical methods developed in the field of process identification can be used [6]. However, conduction of the experiment is sometimes not allowed or it is very expensive.

Modern industrial plants are often equipped with a large number of sensors which measure different process variables. These measured data, acquired through couple of

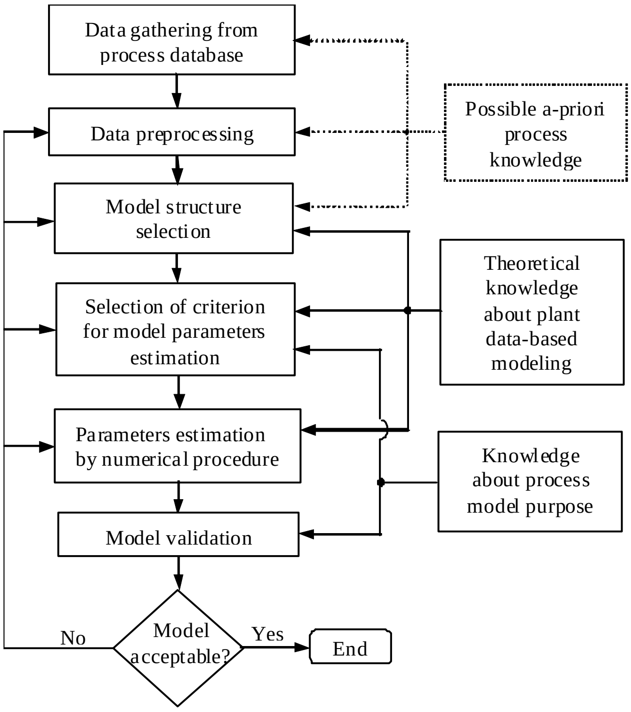

Fig. 2. Flow chart of plant data-based modeling procedure

years and accumulated in the process database, can be a useful source of information for model building. Modeling based on measured data taken from the process database is generally quite economical but it is not a trivial task since this data have "data rich, information poor" property and contain lots of different impurities which additionally complicate model building.

Data-based process modeling procedure based on data taken from process database is presented in Fig. 2. When measured data are acquired in the raw form, they often contain a lot of "impurities" as a result of different disturbances, malfunctions, degradation and errors in sensors and data acquisition system. Besides that, only some of measured variables are important for modeling procedure. Therefore, data preprocessing, which includes variable selection, data de-noising, outlier detection and missing value replacement, is an important part of the modeling procedure [2,4,7]. After that, it is necessary to choose the appropriate model structure. The next step is the definition of the criterion for model parameters estimation followed by estimation of the model parameters from the data by appropriate numerical procedure. If the built model satisfies the requirements, modeling procedure is finished. However, this is a rare situation in practice and modeling is often done through several iterations. Selection of proper model structure and criterion for parameter estimation are not trivial tasks and deserve special attention since these issues have great impact on the overall soft-sensor quality.

3 METHODS FOR MODEL BUILDING

Measured data, acquired from process database, after preprocessing step can be presented as *m* input variables collected in the matrix $\mathbf{X} \in \Re^{n \times m}$ and the vector of output variable $\mathbf{y} \in \Re^{n \times 1}$ (in the case of MISO model) where *n* is number of available samples. Data-based process model building is in fact a search for an approximating function $\boldsymbol{f}_m : \Re^m \to \Re$ which approximates the unknown natural functional dependence of the output process variable on the selected input variables. A function with a finite-dimension vector of parameters is commonly used for the approximating function, so the model can be represented as:

$$\hat{y} = \boldsymbol{f}_m(\mathbf{x}, \boldsymbol{\Theta}), \tag{1}$$

where $\mathbf{x} \in \Re^{1 \times m}$ is a sample of input variables, $\boldsymbol{\Theta}$ vector of parameters of the approximating function $\boldsymbol{f}_m(\cdot)$ (i.e. process model) and $\hat{y}$ is model output. From the mathematical point of view, searching for the approximation function from the available data is the ill-posed problem since there is infinite number of possible approximating functions [8]. The most important feature of the soft-sensor is its prediction capability. Therefore, functions which will generalize well have to be chosen. Usually there is no prior knowledge about the process, which could be used in the model structuring, so a general model structure is used. For the approximating function, a function which is the sum of several functions is usually used:

$$\boldsymbol{f}_m(\mathbf{x}, \boldsymbol{\Theta}) = \sum_{k=1}^{K} \boldsymbol{\nu}_k(\mathbf{x}, \boldsymbol{\Theta}_k), \tag{2}$$

where $\boldsymbol{\nu}(\cdot)$ is basis function and *K* is total number of basis functions. Model structuring is therefore reduced to the selection of the basis functions type and model dimension. Choosing optimal model dimension plays important role since it affects bias-variance trade-off (i.e. model prediction capabilities) [9].

For the chosen model structure its parameters $\boldsymbol{\Theta}$ have to be determined from the limited data set. In the prediction model building, the parameters are usually determined by regression, in which all model parameters are estimated based on minimization of output error of approximation. Plant data have undesirable features which make classical regression techniques inefficient in optimal model parameters estimation [3]:

- highly dimensional input space,
- highly correlated input space,

- presence of different errors and disturbances.

There are plenty of various modeling methods that can be used for process model building from the plant data. Mathematical unification of the empirical methods is given in [9], where the common framework is introduced, which allows easy comparison of different methods from diverse fields such as chemometrics, statistics or artificial intelligence. Using similar point of view, methods which are usually used for soft-sensor model development will be discussed in the following subsections.

3.1 Multivariate statistical methods

Methods that were developed in the field of multivariate statistics analysis are widely used in the plant data-based modeling to improve linear regression modeling due to their simplicity and clear mathematical background. Hereby, input space is at first projected into a lower dimensional subspace, and the regression is performed on these new (latent) variables which are obtained from the projection [10]. Hence, the model (2) can be represented as a composition of two functions:

$$\hat{y} = \boldsymbol{f}_m(\mathbf{x}, \boldsymbol{\Theta}) = \boldsymbol{f}_r\left(\boldsymbol{\varphi}_j(\mathbf{x}; \boldsymbol{\alpha}_j); \boldsymbol{\beta}\right) \; j = 1, 2, ..., J, \tag{3}$$

where $\boldsymbol{\varphi}(\cdot)$ input space into the latent space projection function, $\boldsymbol{f}_r(\cdot)$ latent space into the output projection function, J is number of latent variables and α, β are model parameters. Apart from the selection of the appropriate functions and dimension J, this model structure also requires definition of two separate criteria for parameter estimation. In that way more control is taken over trade-off between bias and variance of the prediction error [10].

Principal Component Analysis (PCA) is often used as a method for soft-sensor model building. Mathematical and statistical properties of the PCA can be found in [11]. Basically, it is linear projection of the original input space. Directions of projection $\boldsymbol{\alpha}_j$ (also called loadings) are obtained by maximizing variations in the input space:

$$\max_{\boldsymbol{\alpha}_j}\left[\operatorname{var}(\mathbf{X}\boldsymbol{\alpha}_j)\right], \tag{4}$$

so the normalized matrix $\mathbf{X}$ can be decomposed as follows:

$$\mathbf{X} = \hat{\mathbf{X}} + \mathbf{E} = \mathbf{Z}\mathbf{A}^{\mathrm{T}} + \mathbf{E}, \tag{5}$$

where $\mathbf{Z} \in \Re^{n\times J}$ is orthogonal matrix (so called scores or latent variables), $\mathbf{A} \in \Re^{m\times J}$ is orthonormal matrix (loading matrix) containing directions of projection $\boldsymbol{\alpha}_j$ (often called principal components - PCs), $\mathbf{E} \in \Re^{n\times m}$ represents unmodeled variations (residuals) and J is number of latent variables. Directions of projection can be computed by eigenvalue decomposition of the covariance matrix $\mathbf{X}^{\mathrm{T}}\mathbf{X}$ [11] or by NIPALS algorithm [12].

If the soft-sensor is used for on-line prediction of the difficult-to-measure variable then Multiple Linear Regression (MLR) is usually performed on the latent variables in order to obtain β model parameters. In that case, model (3) is called Principal Component Regression (PCR) and can be written as:

$$\hat{y} = \sum_{j=1}^{J} \beta_j \sum_{i=1}^{m} \alpha_{ij}\, x_i. \tag{6}$$

Prediction of the difficult-to-measure variable can help in detection of the quality problem but rarely in identifying root causes [13]. Therefore, very often methods used in the field of statistical process monitoring (SPM) are focused on the easy-to-measure variables, not only quality variables. When PCA is used for process monitoring, two statistics, namely Squared Prediction Error (SPE) and T2 statistics are used to detect abnormal situation in the process (sensor and process faults):

$$\mathrm{SPE}(\mathbf{x}) = \left\|(\mathbf{I} - \mathbf{A}\mathbf{A}^{\mathrm{T}})\mathbf{x}\right\|^2, \tag{7}$$

$$\mathrm{T}^2(\mathbf{x}) = \mathbf{x}^{\mathrm{T}}\mathbf{A}\boldsymbol{\Lambda}^{-1}\mathbf{A}^{\mathrm{T}}\mathbf{x}, \tag{8}$$

where $\boldsymbol{\Lambda}$ is a diagonal matrix containing J largest eigenvalues of the covariance matrix. Control limits can be determined for these two statistics such that their violation indicates abnormal process conditions [13].

Disadvantages of the PCA are inability to model nonlinear relationships and model (6) can sometimes have poor prediction properties because the input-output relation is not taken into consideration when parameters α are determined. To overcome the latter drawback, Partial Least Squares (PLS) method was developed [12]. The PLS presents an important extension of the PCA technique when it is used in prediction model building because PLS criterion for parameter estimation takes into account not only variation in the input space, but also correlation between input and output variables:

$$\max_{\boldsymbol{\alpha}_j}\left[\operatorname{corr}^2(\mathbf{y}, \mathbf{X}\boldsymbol{\alpha}_j)\operatorname{var}(\mathbf{X}\boldsymbol{\alpha}_j)\right]. \tag{9}$$

Directions of projection can be found through eigenvalue decomposition of matrix $(\mathbf{X}^{\mathrm{T}}\mathbf{Y})^{\mathrm{T}}(\mathbf{X}^{\mathrm{T}}\mathbf{Y})$, by NIPALS algorithm or by SIMPLS algorithm [14]. Partial Least Squares Regression model (PLSR) has equal structure like PCR model (equation (6)), but often has better prediction capabilities [3]. Like PCA, PLS can be used to detect abnormal changes in process by monitoring three statistics, namely, $\mathrm{SPE_x}$, $\mathrm{SPE_y}$ and T^2.

In [15] Continuum Regression (CR) is presented which is a generalization of the existing methods of the multivariate analysis, so that PCR, PLSR and MLR are just special cases of the CR method. This generalization is based on criterion for α parameter estimation that includes the so-called continuum parameter which provides more control over bias-variance tradeoff.

3.2 Artificial neural networks

Artificial Neural Networks (ANNs) are very popular techniques in data-based modeling for nonlinear model building. ANNs have appealing properties such as universal approximation and generalization ability. However, they often require high ratio between number of samples and number of model parameters (weights) in order to achieve successful parameter estimation, which results in high computational demands. Many different types of ANNs and algorithms for parameter estimation (learning) were developed. Comprehensive overview of ANNs and their mathematical background is given in [8].

One of the most popular ANN is MultiLayer Perceptron (MLP). MLP with one nonlinear hidden layer and linear output layer has the following structure:

$$\hat{y} = \sum_{j=1}^{J} \beta_j \boldsymbol{\varphi}_j(\mathbf{x}) \; = \; \sum_{j=1}^{J} \beta_j \, \boldsymbol{\psi}_j \left(\sum_{i=1}^{m} \alpha_{i\,j} \, x_i \right) + \beta_0 \,, \tag{10}$$

where β_0 is a bias term and $\boldsymbol{\psi}_j(\cdot)$ are activation functions that have sigmoid shape. In fact, this model has nonlinear input space projection with linear regression in the second part of the model (3). All models parameters are calculated according to the following criterion:

$$\min_{\alpha,\beta} \left(||\mathbf{y} - \hat{\mathbf{y}}||^2 \right) . \tag{11}$$

The most popular algorithm for simultaneous parameter estimation is error backpropagation algorithm [8].

The other very popular ANN is Radial Basis Function Network (RBFN). Like MLP, RBFN is also universal approximator. However, while MLP constructs global approximation of the input-output relationship, RBFN constructs local approximation [9]. RBFN is composed of nonlinear hidden layer and linear output layer where regression is performed on the latent variables obtained by nonlinear input transformation. In the hidden layer radial basis functions are used as activation functions. The most popular activation function is Gaussian function [8]. In that case, RBFN model has the following structure:

$$\hat{y} = \sum_{j=1}^{J} \beta_j \exp\left(-\frac{1}{2\sigma_j^2} \sum_{i=1}^{m} (x_i - \mathrm{t}_{ij})^2 \right) + \beta_0 \,, \tag{12}$$

where $\mathbf{t}_j$ and σ_j are centers and widths of the basic functions. The most popular approach for parameter estimation is combined learning [16]. In the first step parameters $\mathbf{t}_j$ and σ_j are determined (usually by k-means algorithm and P-nearest neighbors heuristic), followed by estimation of output weights by the minimization of the model approximation error:

$$\min_{\beta} \left(||\mathbf{y} - \hat{\mathbf{y}}||^2 \right) . \tag{13}$$

There are also other popular algorithms such as Orthogonal Least Squares (OLS) [17].

3.3 Support vector machines

A Support Vector Machine (SVM) is a supervised learning method based on statistical learning theory and structural risk minimization [18]. It gained on popularity in the recent time because it does not suffer from local minima and overfitting problems that frequently occur in ANN learning. Like ANN, SVM is also universal approximator of any multivariate function to any desired degree of accuracy.

The Support Vector Regression (SVR) model can be also treated as model (3). The input space is first projected to the latent space (feature space) via nonlinear transformation $\boldsymbol{\varphi}(\cdot)$ (similar to ANN) and then the linear regression is performed in the latent space:

$$\hat{y} = \; \boldsymbol{f}(\mathbf{x}, \boldsymbol{\beta}) = \sum_{j=1}^{J} \beta_j \boldsymbol{\varphi}_j(\mathbf{x}) \; + \mathrm{b} \,, \tag{14}$$

where b is bias term. Trade-off between approximation error and generalization performance is achieved by minimization of the following criterion:

$$\min_{\beta} \left(\frac{1}{2} \left\| \boldsymbol{\beta} \right\|^2 + C \sum_{i=1}^{n} |y_i - \boldsymbol{f}(\mathbf{x}_i, \boldsymbol{\beta})|_{\varepsilon} \right) , \tag{15}$$

where C is a penalty factor. The first part of equation (14) minimizes the so-called Vapnik-Chervonenkis dimension of the model (and consequently the generalization error) and the second part is the so-called Vapnik ε-sensitive loss function which minimizes the approximation error of the model [19]. Therefore, SVM based soft-sensors often achieve better prediction capabilities than ANN based.

While (15) is in fact an optimization of the quadratic problem with inequality constraints, in soft-sensing applications Least Squares SVM (LS-SVM) are usually used where quadratic loss function in (15) and equality constraints are employed [20].

3.4 Hybrid methods

Hybrid methods are another group of popular methods that combine some of already mentioned methods (see Fig. 3). Hybridization exploits good properties of the methods that are combined which often results in more accurate process models.

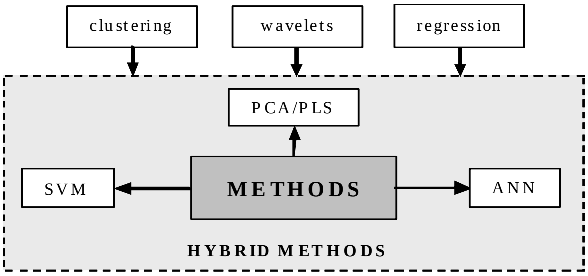

Fig. 3. Modeling methods used in soft-sensor development

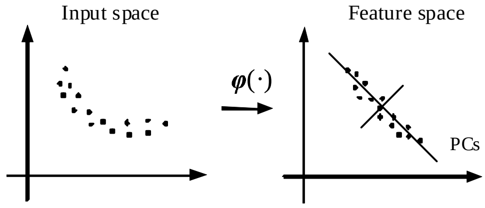

Fig. 4. Illustration of kernel PCA

3.4.1 Nonlinear PCA

The main disadvantage of the PCA is its inability to model nonlinear relationships between variables. Nonlinear PCR model for difficult-to-measure process variable estimation can be obtained by applying nonlinear regression on the latent variables obtained by minimizing criterion (4). In [21] neural network is trained on the variables obtained by the input projection with the PCA method – resulting method is often called NNPCR. More general method was developed in [10] where CR method was combined with MLP.

Nonlinear PCA methods that can be used for process monitoring was developed in [22,23]. However, these approaches rely on the use of associative neural networks which involves nonlinear optimization procedure and are rarely used.

In the recent time there is increased use of kernel PCA (KPCA) due to advances in the theoretical background of the kernel methods [24]. KPCA combines nonlinear input transformation $\boldsymbol{\varphi}(\cdot)$ like in SVM and PCA which searches for PCs in the feature space (see Fig. 4):

$$\max_{\boldsymbol{\alpha}_j} \left[\mathrm{var}\left(\boldsymbol{\varphi}(\mathbf{X}) \boldsymbol{\alpha}_j \right) \right] . \tag{16}$$

In that way, nonlinear model is obtained which can cope with nonlinear processes more successfully than the classical PCA model. In comparison to other nonlinear PCA techniques, KPCA requires only the solution of an eigenvalue problem without any nonlinear optimization because it utilizes so-called kernel trick [24]. Additionally, the number of PCs doesn't need to be defined in advance. Process monitoring is based on the monitoring of the same statistics like in PCA (i.e. SPE and T^2) but in the feature space [25].

3.4.2 Nonlinear PLS

As with the nonlinear PCA, there are several papers dealing with nonlinear PLS (NLPLS). In the pioneer work [26], a quadratic function is used between latent variables and output variable. Among several methods [27,28], nonlinear PLSR model based on ANN (NNPLS), that was proposed in [29], is mostly used in soft-sensor development. It combines linear PLS and neural network with sigmoid activation functions in a way that input space is firstly projected by minimizing criterion (9) and then nonlinear regression is performed on the obtained latent variables by minimizing criterion (13).

3.4.3 Multiple-model method

It is well known that ensemble of models can have better prediction capabilities in comparison with single model [30]. In Multiple-Model (MM) method, data are divided into different sub-domains and local sub-models are constructed over every domain. In that way, instead of using a single global model, number of simpler models are developed which are then combined to obtain prediction or state of the process. This often results in more accurate soft-sensor when modeling highly nonlinear processes because different clusters can be recognized in the space of the process data which correspond to different operating states of the process [31].

One of MM method that can be used for process monitoring is Multiscale PCA (MSPCA) [32]. This method combines wavelet analysis and PCA. While PCA decorrelates measurements, wavelet analysis extracts deterministic features and approximately decorrelates autocorrelated measurements. More precisely, in MSPCA measurements are decomposed by wavelet analysis. Obtained coefficients at each scale are then used to develop PCA model for each scale independently. Resulting sub-models are then combined. Therefore, MSPCA can be more efficient in process monitoring than classical (single scale) PCA.

When building soft-sensors for on-line estimation of the difficult-to-measure variable, MM are developed by clustering input space by some method followed by regression on the obtained clusters $\mathbf{X}_1, ..., \mathbf{X}_p$. Output of the MM is

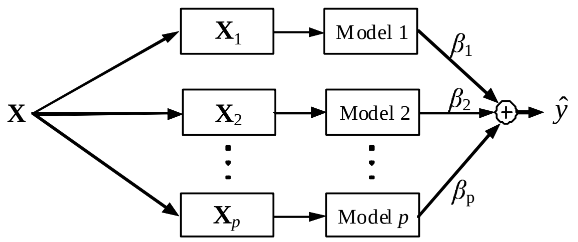

Fig. 5. Multiple-model method

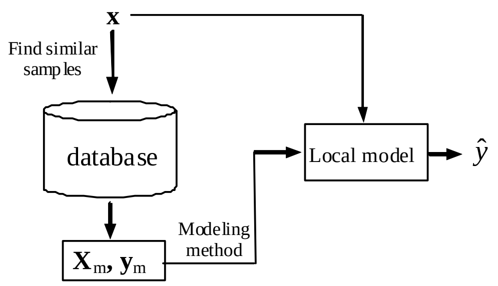

Fig. 6. Just-in-time learning method

weighted sum of the sub-model outputs as shown in Fig. 5:

$$\hat{y} = \sum_{i=1}^{p} \beta_i \hat{y}_i \tag{17}$$

where p is number of sub-models, β_i are weight factors and $\hat{y}_i$ are sub-models predictions. Input space is usually clustered by k-means or fuzzy clustering method and sub-model parameters are obtained by regression methods such as fuzzy Takagi-Sugeno modeling, ANN or SVR.

Another approach for nonlinear process modeling that emerged in recent years is Just-In-Time Learning (JITL) (also known as locally weighted learning, lazy learning or model-on-demand) [33,34]. In JITL, when prediction of the output variable $\hat{y}$ based on input sample **x** is needed, local model is dynamically built from the similar samples stored in database (see Fig. 6).

Local model building is based on input-output samples ($\mathbf{X}_m$,$\mathbf{y}_m$) that are chosen according to some nearest neighborhood criterion and some already mentioned modeling method. Obtained model is only valid for the operating condition characterized by the current query data. After prediction model is discarded and the new model has to be built when new sample **x** is acquired. Strictly speaking, method is not MM since only one model is used for prediction but has similar localization feature. The method seems promising for soft-sensor model building since it has inherently adaptive feature.

3.5 Adaptive methods

Since most industrial processes are time-varying, soft-sensor performance will start to deteriorate after some time. To maintain soft-sensors performance through a longer period of time, model parameters have to be retuned in an on-line manner by adaptive methods such as recursive PCA [35] and recursive PLS [36]. However, adaptive methods are out of the scope of this paper and some of them are only mentioned in the Section 4.

4 REPORTED APPLICATIONS OF THE SOFT-SENSORS IN PROCESS INDUSTRY

In this section, a list of published papers dealing with soft-sensors model building and applications in the process industry is given in chronological order of their appearance in the literature. Since there is vast number of papers published in last two decades, only interesting and notable ones are presented according to the authors' opinion with the accent on the latest papers.

In [37] ARMAX type soft-sensor is used for prediction of biomass concentration in an industrial polymerization reactor, product composition of large industrial distillation tower and melt flow index on an industrial polymerization reactor.

In [38] are proposed relative sensitivity ratio tables to select relevant input variables and method for removing redundant samples from data set. The NNPLS method is used for modeling catalytic reforming system.

In [39] an intelligent soft-sensor for batch digester quality prediction which is a combination of numerical, symbolic and graphical part, meta system, database and multimedia interface is described.

In [40] NNPLS model is used for monitoring NOx content of the exhaust gas in industrial heater. Sensor data analysis is performed by nonlinear PCA [22].

In [41] a soft-sensor based on Fuzzy-Neural-Net multimodel approach is proposed. More precisely, the soft-sensor is composed of fuzzy classifier and local models (ANNs) which outputs are weighted and combined to produce model output. The soft-sensor is used for prediction of propylene composition in a high purity distillation column.

In [42] PCA for sensor fault identification via reconstruction is introduced. A sensor validity index is proposed to determine status of each sensor. Method is applied to boiler process data.

In [43] multi-model approach, namely, fuzzy distributed radial basis function neural network is used as soft-sensor model. Input space is clustered by modified rival penalized competitive learning (RPCL) and learnt by distributed

RBFN. Proposed soft-sensor is used for propylene and propane composition prediction in a high purity distillation column.

In [44] recursively exponentially weighted PLS is proposed to cope with time-varying processes. The method is used for a simulated continuous stirred tank reactor control and for the prediction of different variables in an industrial mineral flotation circuit. The method outperformed recursive least-squares method (RLS).

In [45] an integrated framework known as self-validating inferential sensors is proposed where data from sensors are firstly validated by method proposed in [42], and then linear (PCR) or nonlinear models (NNPCR) are built. Method is applied to boiler NOx emission monitoring.

In [32] MSPCA is proposed for statistical process monitoring. MSPCA is applied to simulated examples and data acquired from industrial fluidized catalytic cracker unit simulator.

In [36] recursive sample-wise and block-wise PLS algorithms (RPLS) are proposed. Block-wise RPLS algorithm is further extended to a moving-window and forgetting factor adaptation schemes. RPLS is used for research octane number prediction of a catalytic reformer.

In [46] soft-sensors are used for particle size distribution estimation in a grinding plant when hardware sensor is unavailable due to calibration or its sharing among several parallel grinding lines. The soft-sensor are based on an ARMAX model structure that is determined by stepwise regression.

In [47] SPM monitoring by PCA is extended in the way that multidimensional fault detection, identification and reconstruction are proposed using a subspace approach. Necessary and sufficient conditions for fault detectability and reconstructability are derived for the PCA. Proposed methodology is applied to a simulated process to consider sensor and process faults.

In [28] the NNPLS method proposed in [29] is improved by the error-based input weights updating procedure. The method is applied to a simulated pH neutralization process and shows better modeling capabilities of nonlinear processes than the classical NNPLS.

In [48] dynamic PLS based on FIR model structure is used for simulated multicomponent distillation column modeling. The model is used for controlling product composition. It is found that the use of past measurements is effective for improving the accuracy of the estimation.

In [35] recursive PCA (RPCA) for adaptive process monitoring is presented. Additionally, the authors developed a complete adaptive monitoring algorithm that can deal with missing values and outliers. The method is applied to a rapid thermal annealing process in semiconductor processing.

In [49] nonlinear PCA from [23] is combined with nonlinear PLS [29] to form robust nonlinear PLS. Soft-sensor is used for composition estimation in high purity distillation column.

In [50] PCA/PLS is combined with locally weighted regression (LWR) to build local models. This methodology shows equal or better performances over PLS, NNPLS or ANN in modeling two real processes which exhibit strong nonlinear and relatively linear behavior: an industrial splitter column and an industrial crude column.

In [51] MLP based soft-sensor is used for the estimation of the composition variables in the hot metal and slag in a blast furnace.

In [52] adaptive MSPCA is used for monitoring wastewater treatment operation which exhibits time-varying behavior due to diurnal and seasonal changes.

In [53] MSPCA is applied for process monitoring. Method is applied for data sets obtained from gas phase tubular reactor process and industrial boiler system. It is able to detect and identify faults and abnormal events earlier than the conventional PCA approach.

In [54] several dynamical models (linear ARMAX, nonlinear ARMAX, PLS, wavelet based, fuzzy combinational, Takagi-Sugeno) are used for estimation of the concentrate grade in a rougher flotation bank.

In [55] RPLS proposed in [36] is revisited and further analyzed. Additionally, RPLS is integrated into multiblock PLS (MBPLS) to form recursive MBPLS. Proposed monitoring scheme is applied to a simulation of a fluid catalytic cracking unit and an industrial distillation process.

In [56] a new statistical method for process monitoring that uses independent component analysis ([8]) is proposed. The suggested method showed better monitoring performance than PCA on a simple multivariate process and the simulation benchmark of the biological wastewater treatment process.

In [25] a new nonlinear process monitoring technique based on KPCA is derived. The method was applied to same data sets like in [56].

In [57] a systematic framework for the development of soft-sensor is described. NNPCA based soft-sensor is used for estimation of "anchorage" of polymeric-coated substrates in the coating industry.

In [58] SVM and LS-SVM based soft-sensors are developed. Bayesian framework is used for the selection of the optimal model. Developed models are used for estimation of the freezing point of light diesel oil in a distillation column.

In [59] JITL-PCA hybridization is used for process monitoring. Simulation results show that JITL-PCA outperforms both PCA and dynamic PCA in the monitoring of nonlinear static or dynamic systems.

In [60] soft-sensors based on nonlinear ARX model structure (implemented by MLP with one hidden layer) are used for predicting top and bottom product concentrations in the debutanizer distillation column. Soft-sensors were developed to overcome great time delay introduced by the corresponding gas chromatograph.

In [61] recursive nonlinear PLS algorithm is developed by combining linear PLS and RBFN and applied to a simulated pH neutralization processes and an industrial propylene polymerization process.

In [62] NNPLS is used for quality variables estimation in biological wastewater treatment process. To obtain dynamical models, NNPLS is integrated in FIR and ARX model structures.

In [63] an on-line dual updating strategy for PLS based soft-sensors is proposed, i.e. recursive PLS is combined with model output offset updating. The method is used for crystal particle size prediction in an industrial purified terephthalic acid purification process.

In [64] PLS based soft-sensor is used for melt flow index estimation in free radical polymerization process in autoclave reactor.

In [31] PCA is combined with fuzzy c-means and fuzzy Takagi-Sugeno modeling in order to develop a soft-sensor which is used for estimation of the melt flow index in the polyethylene process which is highly nonlinear and time-varying process. Proposed method showed better prediction capabilities than PLS, NNPLS and fuzzy PLS.

In [65] adaptive multiblock PCA is used for monitoring complex condensate fractionation process.

In [66] a new nonlinear multiscale method for process monitoring and fault diagnostics is proposed. The method combines multi-resolution analysis based on wavelets and KPCA. The method is applied to multivariate data obtained from a nonisothermal CSTR process.

In [67] a new adaptive local model based monitoring approach is proposed which combines JITL with LS-SVR. ICA-PCA is used to analyze process state. The method is applied to a numerical example from [23] and Tennessee Eastman benchmark process.

In [68] multi-model soft-sensor is developed by combining PCA, kernel fuzzy c-means clustering algorithm based on particle swarm optimization and neural network. The proposed modeling method is applied to an erythromycin fermentation process to estimate the biomass concentration.

In [69] a new method for soft-sensor model building is presented, which is based on JITL and correlation between measured variables (CoJITL). The proposed method is used for reactant concentration estimation in simulated CSTR and for aroma concentration estimation in cracked gasoline fractionator.

In [70] a numerically efficient and memory saving moving window KPCA is developed. The method is applied to a simulated nonlinear time-varying process and recorded data from an industrial distillation column.

In [71] LS-SVM is used for alumina powder flow estimation in the process of alumina conveying. The results show that LS-SVM based soft-sensor possesses higher precision accuracy and better generalization ability than RBFN based.

In [72] soft-sensor based on SVR with Akaike information criterion and genetic algorithm is used for concentrations of the biomass estimation in the erythromycin fermentation process. The proposed method outperforms ANN approach.

In [73] LS-SVR based soft-sensor is used for estimation of calcium-oxide content in the cement clinker calcination process.

5 TIPS FOR CHOOSING APPROPRIATE METHODOLOGY

When dealing with slightly nonlinear process, the user should firstly try with linear modeling methods, such as PLS, which is the mostly used method in soft-sensor model building. However, if process exhibits strong nonlinear behavior, nonlinear models will provide much better soft-sensor performance. The most popular methods are ANN and their combination with PCA and PLS. The multiple model approach can provide even better performance in this situation because it describes nonlinear behavior by several local sub-models. For process monitoring PCA is the mostly used approach. However, when dealing with highly nonlinear process this monitoring approach can be inefficient, leading to a number of false alarms. In that case, the user should try the KPCA method which appeared in the recent time.

Since heavy computational loads are not such problems anymore, due to ever-growing computing power, kernel based methods emerged as appealing methods for nonlinear model building. The most popular are SVM and LS-SVM based models which often achieve better performance than models based on multivariate statistical methods and ANN.

In the on-line application soft-sensor performance will probably gradually decrease, so the model will have to be retuned in an on-line manner. This issue should also be reconsidered when choosing a methodology for model building. Apart from the appropriate methodology, the user should be aware of the fact that model quality heavily depends on the data preprocessing step which in fact increase data "informativity" more or less.

6 CONCLUSION

Profit forces industries to run their processes more efficiently and safely. To enhance product quality and to reduce production costs, quality variables have to be measured which is sometimes difficult. Apart from ever-growing accent on the product quality, different government laws and regulations (e.g. Kyoto protocol) forces industries to reduce its impact on the environment. This often requires installation of expensive measurement devices (e.g. gas monitoring system), which are often unreliable and have high maintenance cost. Cheap solutions to the mentioned problems are soft-sensors which are used as estimators of important variables or for process monitoring. Soft-sensors are based on process model that is obtained from measured data. In this paper, commonly used methods for process model building based on plant data are discussed. The most interesting papers dealing with soft-sensors that appeared in the last two decades are shortly described. Tips for choosing appropriate methodology are also given. We believe that these points will help researchers in this field.

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