Soft Sensor

Soft sensors have been widely used to estimate process variables that are difficult to measure online [1].

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Related terms:

Gaussian, Graphene, Statistical Ensemble, Robotics, Distillation, Process Dynamic, Process Monitoring

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24th European Symposium on Computer Aided Process Engineering

Kai Sun, ... Ding-Sou Chen, in Computer Aided Chemical Engineering, 2014

1 Introduction

Soft sensors are inferential models that use easily measured variables to estimate process variables that are hard to measure due to technological limitations, large measurement delays, or high investment costs(Kadlec et al., 2009). In addition, soft sensors can give useful information in terms of fault detection by working with hardware sensors in parallel (Kaneko et al., 2009). It is possible to eliminate redundant variables, reduce the complexity of the model, and improve the accuracy of the model through the use of appropriate variable selection techniques. A variety of variable selection techniques for soft sensor applications and modeling methods have been studied in recent years. Ma et al. (2008) proposed an adaptive soft sensor based on statistical identification of key variables, in which the key variables are captured using the statistical approach of stepwise linear regression. Lin and Jørgensen(2011) deleveped a soft sensors based on a multivariable data fusion where a dynamic partial least squares is implemented to build the regression model. Xiang et al. (2012) presented a framework of discriminative least squares regression (LSR) for multiclass classification and feature selection.

However, these linear regression methods may not have adequate accuracy in describing highly nonlinear industrial processes. Artificial neural networks (ANN) are powerful tools for nonlinear statistical data modeling or decision making and have been widely used for variable selection in recent years. Castellano and Fanelli (2000) proposed a backward selection, called IANN, by successively removing the input nodes of a satisfactorily trained neural network with the complete set of variables as inputs. Enrique and Sopena (2008) proposed a feature selection method using sequential backward multi-player perceptron (SBS-MLP), which retrained the network with every feature temporarily removed before computing its saliency. Souza et al. (2013) developed a method for variable selection applications by using a multi-layer perceptron (MLP) and applied the method to monitor the fluoride concentration in the effluent of an urban water treatment plant. Recently, Breiman (1995) proposed a new shrinkage method called the nonnegative garrote (NNG). The mechanism of this shrinkage method conducts variable selection by shrinking or setting some coefficients of a "greedy" model to zero. Yuan (2007) proposed a non-parametric extension of NNG and applied it to solve the problem of component selection in a functional analysis of variance (ANOVA) model. Pan et al. (2012) revised the original NNG by combining enumerative PLS with NNG, and the results showed better performance than original NNG and LASSO.

The motivation of this paper was to develop a robust variable selection method for the application of soft sensors that could describe complex nonlinear industrial processes. This paper is organized as follows. Section 2 presents the development of the methodology. In Section 3, the proposed method is applied to predict the oxygen concentration for the air separation process. Finally, some concluding remarks are given in Section 4.

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Process Analysis | Bioprocess Analysis

Supasuda Assawajaruwan, Bernd Hitzmann, in Encyclopedia of Analytical Science (Third Edition), 2019

Soft-Sensors

Soft-sensors, which are also called software sensors or virtual sensors, can be used as an alternative for process variables that cannot be measured at all or only by very sophisticated equipment. They use one or more raw measured values as well as an empirical or theoretical sometimes also dynamic model in order to provide meaningful information for bioprocesses. Soft-sensors belong to the class of indirect

measurement methods. They can be divided into two groups: Soft-sensors that use a theoretical process model and those that use an empirical model to calculate the process variables. The first group of soft-sensors are also called observers such as the Luenberger observer or Kalman filter.[28] They use state differential equations, with which the dynamic behavior of the bioprocess is described with a mechanistic model in which, for example, transport processes and reaction kinetics are used. In the second group of soft-sensors, data-driven models (black box models) are used. Regression models are often applied in combination with methods of principal component analysis or, especially for nonlinear relationships, neural networks to describe the relationship of the process variables. Mostly spectroscopic measurement data are combined with data driven models for the prediction of bioprocess variables. However, also any other measurements or combinations of both can be explored to improve the prediction capability of the data driven models.

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Diesel engine system dynamics, transient performance, and electronic controls

Qianfan Xin, in Diesel Engine System Design, 2013

14.9.3 Virtual sensor modeling of exhaust manifold gas temperature

The virtual sensor for exhaust manifold gas temperature is important for engine durability and EGR rate control. Its modeling is based on the thermodynamic first law energy balance equation 12.2. Assuming

14.3

where η_{th}, B and G_2 are constants or known functions of engine speed, load, air–fuel ratio, and fuel injection timing, the steady-state exhaust manifold gas temperature can be calculated using equation 12.2 as:

14.4

where is the intake manifold mixture flow rate of both fresh air and EGR, and $c_{p,ex}$ and $c_{p,in}$ are the equivalent average specific heats of the exhaust flow and the intake manifold flow, respectively. It is observed that the exhaust manifold gas temperature is a function of the 'mass-to-fuel' ratio In equation 14.4, one method to estimate

the engine brake thermal efficiency η_{th} is to calculate the engine brake power using the indicated torque and the engine friction obtained from the torque-based controls. The prediction of the engine indicated torque and the brake torque has been used increasingly as a part of the coordinated shift control in automotive powertrains. In equation 14.4, an accurate estimation of *B* is a challenge. The value of *B* depends on engine speed, load, charge mass-to-fuel ratio, fuel injection timing, intake manifold gas temperature, coolant temperature, etc. One approach is to use the equations of the in-cylinder cycle process along with the Woschni heat transfer coefficient α_g outlined in Chapter 4 to first calculate the transient instantaneous exhaust manifold gas temperature, and then average it over an engine cycle to obtain the steady-state exhaust manifold gas temperature. The other approach is to develop heuristic models for the steady-state values of *B* in order to build its sensitivity to other engine performance and operating parameters.

Steady-state engine performance test data reveal that there is a correlation between the temperature difference across the cylinder and the fuel-to-charge mass ratio (Fig. 14.2), and the slope of the correlation line changes at different engine speeds. Such a correlation can be explained as follows. If it is assumed that is much greater than , and $c_{p,in} \approx c_{p,ex}$, equation 14.4 is simplified to:

14.2. Illustration of virtual sensor – correlation between exhaust manifold gas temperature and fuel-to-charge ratio.

14.5

where the coefficient C is a function of engine speed. A simplified empirical model of the virtual sensor of exhaust manifold gas temperature can be developed as follows:

14.6

where C_1, C_2, C_3 and C_4 are the model tuning constants, and N_E is the engine speed. It should be noted that although the model equation 14.6 can predict the steady-state exhaust temperatures reasonably well, it may not be able to accurately predict the exhaust temperatures during fast transients due to the lack of thermal-lag related factors in the model.

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13th International Symposium on Process Systems Engineering (PSE 2018)

Aysun Urhan, ... Burak Alakent, in Computer Aided Chemical Engineering, 2018

1 Introduction

Data driven soft-sensors for chemical processes are usually constructed using global modeling methods, such as partial least squares (PLS), artificial neural networks (NNs), support vector machines, or adaptive local models (Yan et al., 2004, Kadlec et al., 2011). Proper tuning of parameters in these statistical models is essential for achieving a high generalization capacity, for which cross-validation (CV) is commonly used. The current CV practice involves partitioning the training data into k (usually taken to be between 5-20) folds, each of which is predicted using models constructed from the concatenation of the remaining folds (Kohavi, 1995). Online automatic sampling of processes, producing tens to a few hundred collinear process variables, creates a large number of redundant predictors, inflating the variance of the quality variable predictions. Predictor subset selection algorithms may be used to improve the accuracy and reduce the computational complexity of the statistical models (Hastie, et al., 2011), and to determine a convenient dimension of the neighborhood space, i.e. the subspace in which nearest neighbor search is performed, in order to combat “curse of dimensionality”. It should, however, be noted that predictor selection, a form of parameter tuning itself, must be performed in an “outer” loop in CV to prevent biased prediction error (PE) estimates (Reunanen, 2003).

In the chemical process literature, various tools, such as mutual information or NNs, are used to reduce the dimension of predictors (Sun et al., 2016, Jin et al., 2014), yet experience-based subset selection is still not uncommon, bringing doubt on the generalizability of the suggested modeling techniques. Additionally, abrupt changes in operational conditions necessitates availability of modeling methods, which, trained on small samples, can make accurate predictions outside the operating region; hence, statistical learning algorithms convenient for soft sensors in

chemical/biochemical industries are to be developed. The current study aims to (i) construct “automated” unbiased statistical learning methods using various model building tools (Section 2.1), (ii) implement predictor selection methods (Section 2.2), and (iii) assess their performances in predicting T95 (distillation temperature of 95% vol. of oil) measurements from a crude distillation unit (CDU), simulated by SimSci ProII™ (Section 2.3), under small/large sizes of training data and interpolation/extrapolation test data. The promising learning methods for adaptive soft-sensing are discussed Section 3.

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Volume 4

T. Kourti, in Comprehensive Chemometrics (Second Edition), 2020

4.11.4.1.1.1.3 Soft sensors for processes from historical data

Another way of modeling a soft sensor is to build a conventional regression model on historical data, then project it ahead to predict future data. When large amounts of historical data are available, many different types of regression can be used. Neural networks are most commonly used for this sort of modeling,[62,63] but static partial least squares regression[64] and Gaussian process regression,[65,66] a Bayesian regression method similar to that described earlier in connection with Kalman filtering, have also been used to model processes with large amounts of historical data. Many of these soft sensors are now widely accepted for online prediction of quality variables in a range of complex dynamic chemical processes. Of these, recursive PLS is the regression algorithm most frequently adopted due to its advantages in handling noise and collinearity in data that are common in industrial processes.[67]

Several notable examples of modeling of process data include, besides PLS regression, ones based on finite mixtures of Gaussian models[68] and mixtures of partial least squares regression ensembles.[69] These modeling methods have been shown to work well as soft sensors for process data, but often involve complicated implementations, leading to relatively large, complex models requiring extensive training on large data sets. Typically, these are trained on historical process data, collected over extended periods of time.

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13th International Symposium on Process Systems Engineering (PSE 2018)

Wenbo Zhu, ... Jose Romagnoli, in Computer Aided Chemical Engineering, 2018

Abstract

In this work, we proposed a data-driven soft sensor based on deep learning techniques, namely the convolutional neural network (CNN). In the proposed soft sensor, instead of only building time-independent correlations among the key variable with other measurements, the moving window method is utilized to describe the most recent process dynamics, where the time-dependent correlation can be located. Beyond on that, a signal recovery scheme is developed to improve the model robustness when confronting common sensor faults. The proposed soft sensoring technique was tested on the composition data of gas-phase components from an ethylene pyrolysis reactor. The model was also verified through the manually introduced sensor faults.

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31st European Symposium on Computer Aided Process Engineering

Burak Alakent, in Computer Aided Chemical Engineering, 2021

2.1 Moving Window (MW) and Just-in-Time-Learning (JITL)

Most of the online learning schemes in soft-sensor design for chemical processes involve choosing relevant training samples. The most recent samples are selected in MW modeling, while JITL is commonly based on the selection of the most similar samples to the test point in the feature space. The rationale behind sample selection methods lies in combating real and virtual concept drifts; the current task is assumed to be more accurately represented by the recent samples, and samples collected in the current domain of the query point. To improve the prediction performance of single MW or JITL models, novel methods using ensemble techniques [7], and combinations of MW and JITL [8] are proposed in the literature. Prediction accuracy of MW and JITL models depends on the window size (W) and the size of NN set (K). While a small W usually yields a more accurate representation of the current task, the resulting training set would only span a limited subspace of the whole

domain of operation. In JITL, sample selection based on feature similarity usually leads to a larger training set, comprising samples from various time segments, and spanning a wider subspace. Since linear learners are less prone to overfitting for small multicollinear datasets, we use a linear learner (Lasso) for MW, and a nonlinear learner (Kernel Ridge Regression) for JITL in the current study.

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13th International Symposium on Process Systems Engineering (PSE 2018)

Narutomo Ishikawa, ... Shinji Hasebe, in Computer Aided Chemical Engineering, 2018

2 Analysis methods for root causes of soft-sensors' estimation error

In industrial processes, main causes associated with soft-sensors' estimation error are as follows:

- Insufficient number of samples for model construction
- Strong process nonlinearity
- Inappropriate selection of the input variables
- Inappropriate selection of the samples for model construction
- Changes in process characteristics

In this research, we focus on "number of samples for model construction" and "process nonlinearity".

2.1 Analysis method for the effect of the number of samples and process nonlinearity on the estimation error

In the proposed method, the estimation error is calculated by using different number of samples and two modeling methods to evaluate the effect of the number of samples and the process nonlinearity on the estimation error. PLS and LW-PLS are used as the modeling methods. In LW-PLS, the localization parameter is used to adjust the weight of each sample. When is larger, smaller samples are prioritized,

and when is zero the LW-PLS becomes the same as the conventional PLS (Kim et al., 2011). The proposed method consists of the following steps:

1. Set the localization parameter of LW-PLS to 0.
2. Set the ratio of samples used for model construction p to 0.4.
3. Set the iteration number r to 1.
4. Divide the samples of a process are randomly at a ratio of 7:3, and set 100p % of the former data as model construction samples and the latter data as model verification samples.
5. Construct an LW-PLS model by using the model construction data. The number of latent variables is selected by leave-one-out cross validation.
6. Apply the LW-PLS model is to the model verification samples, and calculate the root mean square error of prediction RMSEP:(1)where, N_v is the number of model verification samples, $y_{v,n}$ is the output of the n-th model verification sample, and is the estimated value of $y_{v,n}$ by LW-PLS model.
7. Update r to $r+1$. If r is smaller than or equal to the maximum iteration number R, return to step 4. In this research, R is set to 50.
8. Calculate the average value of RMSEP MRMSEP, by(2)
9. Change the ratio of samples used for model construction p, and return to step 3 until all candidates of p are selected. In this study, the candidates of p are 0.4, 0.6, 0.8, and 1.
10. Change the localization parameter and return to step 3 until all candidates of are selected. In this study, the candidates of are 0, 0.5, 1, 1.5, 2, 2.5, and 3.

2.2 The evaluation of the effect of the number of samples

Using obtained MRMSEPp, it is possible to evaluate whether the given number of samples is sufficient or not. The value of p corresponds to the number of samples used for model construction. Thus, it is expected that MRMSEPp with the same decreases with the increase of p. From the gradient of the MRMSEPp, it is possible to estimate the number of the additional samples which are necessary to make the estimation performance acceptable.

2.3 The evaluation for the effect of process nonlinearity

Generally, when the process is close to linear, a smaller value of shows a better performance, and the nonlinearity of the process becomes stronger a larger value of shows a better performance. When is extremely large, a small number of samples are used to construct the model. Thus, usually MRMSEPp with the same p becomes convex with . By using this feature of the localization parameter , the

degree of process nonlinearity is evaluated. The degree of process nonlinearity can be evaluated from the gradient of the MRMSEPp□. For example, if the MRMSEPp□ decreases with □ at the wide range of □, the nonlinearity of the process should be strong. For such a process, we can expect that the performance of a soft-sensor will improve if we use a nonlinear model. On the other hand, if the gradient of MRMSEPp□ is almost zero or positive, it is expected that the nonlinearity of the process should be weak. In such a case, it can be stated that application of various nonlinear models will not greatly contribute to the improvement of accuracy of soft-sensor.

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12th International Symposium on Process Systems Engineering and 25th European Symposium on Computer Aided Process Engineering

Ahmed Shokry, ... Antonio Espuña, in Computer Aided Chemical Engineering, 2015

6 Conclusions

The results show how data based models can be used as soft sensors to monitor complex processes, difficult to follow through FPMs, without expensive offline sampling, saving huge costs and time. In addition, a simple static modelling approach has shown to be capable of accurately estimating a dynamic behaviour. Based on the proposed approach, three types of metamodels have been built to infer the progress of a chemical process from cheap on-line data. The results produced reveal that all methods exhibit high prediction accuracy with a significant low number of training data. Especially, OK shows a slightly higher accuracy and more importantly, higher flexibility and robustness in terms of easiness and rapidness of tuning the model parameters, while providing the modeller with a quantitative confidence interval of the prediction. An immediate extension of the presented approach would allow to use these methods for Advanced Control, by building autoregressive models to predict several steps ahead.

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13th International Symposium on Process Systems Engineering (PSE 2018)

Eliza H.C. Ito, ... Carlos R. Paiva, in Computer Aided Chemical Engineering, 2018

Abstract

The product composition control in a multicomponent distillation column presents several challenges in the industry. The development of a soft sensor enables the monitoring of the product quality using an inferential model and on-line measured process variables. To be useful in an industrial application, the inferential model needs to provide fast sampling rates and with high accuracy. A new inferential model to estimate the gas composition product from a multicomponent distillation column is proposed. It is based on a model that combines a first-principles model at the equilibrium stage with heuristic rules based on the process knowledge. Moreover, strategies for key components selection and a model for the systematic correction of input variables are used to ensure the robustness on a real-time application. A rigorous simulation of a debutanizer distillation is implemented to compare with the proposed inferential model. The results of the soft sensor show a good capability of prediction and accuracy compared to the rigorous model, even using less input process variables.

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