Optimized Real-Time Soft Analyzer for Chemical Process Using Artificial Intelligence

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***Abstract*— This paper concerns application of data-derived approaches for analyzing and monitoring chemical process instruments, extracting product information, and designing estimation models for primary process variables, or difficult to measure in real-time variables. Modeling of process with an optimized classical neural network, the multi-layer perceptron (MLP) is discussed. Tennessee Eastman Process, a well-known plant wide process benchmark, is applied to validate the proposed approach. Investigations and several algorithms as step response test, Lipschitz number method and forward selection are used. The main advancement introduced here is that a hierarchical level responsible strategy is applied for selection of input variables and respective efficient time delays to attain the highest possible prediction accuracy of the neural network model for industrial process identification.**

Index Terms*— *Multi-Layer Perceptron, soft analyzer, Lipschitz number, Tennessee Eastman Process (TEP).

I. Introduction

During the last decade, modern process industries have made a lot of efforts to improve product quality, efficiency and safety credentials of operation in production plants by optimizing operation conditions. This would also be vital from economic point of view, for cost management. In this concept, efficient monitoring tools for supervising the processes, as well as assisting the design of advanced control strategies are crucial. Due to the uncertainty and complexity of industrial processes, mechanical models are often unavailable. Therefore, data-driven empirical models are viable alternatives [1]. Besides, despite the wide spread application of hardware analyzers, like gas chromatographs, in the industries such as chemical industry, they are usually expensive and difficult to maintain. Furthermore, the large measurement delay of hardware analyzers significantly degrades the corresponding control and other automation performance [2, 3]. To address this issue, empirical or soft sensor models, designed based on process operational data, are used along hardware analyzers to produce better estimation of process signals. This control scheme is called inferential control [4]. Application of more accurate physical sensors with high sample rating in advanced controlled processes can improve and assist system stability and controllability. The key factor in selecting the proper model is that the model must be capable of providing accurate predictions for key variables in order to improve process controlling signal characteristics.

Multi-layer perceptron (MLP), as a paradigm in artificial neural networks (ANNs), has been of interest as an empirical nonlinear model in the past decade [5-7]. In an MLP network, regarded as “black-box” model, detailed understanding of physicochemical phenomena underlying a process is unnecessary for the model development. Input–output nonlinear relationships are constructed solely based on historic process data and their performance depends on quality and size of the data, and structure of the model. The MLP-based soft-sensor uses logistic transfer functions and the parameters of the model (the number of hidden nodes and the connection weights) which are calibrated and optimized using a standard cross-validation scheme and the Levenberg−Marquardt method [8].

In this work, the design of a soft sensor for a planet wide chemical process is presented. The chemical process considered is Tennessee Eastman Process (TEP) was introduce in [9] and as a benchmark simulated process plant has been widely used for process control research. In most soft sensor designs the model structure and proper inputs are selected by use of process knowledge [10], otherwise by trial and error or exhaustive searches [11], which have uncertain answers and time consuming algorithms. Here we have used mathematical algorithm and tests in order to provide a comprehensive and much certain solution for selecting the most effective regressors for industrial soft sensor design.

On the other hand, most of process industries include huge number of I/O signals and employing all values as input increases model complexity and may lead to performance degradation. Thus, during modeling, input values and effective time shifts should be studied for relevancy with output to keep the model both simple and accurate. Several methods have been used to select the ideal dataset from I/O signals and their lagged matrices [12-14]. Lipchitz index is among the most accurate methods of delay estimation which, in this paper, is applied for input selection. Also, step response strategy is used here, along with Lipschitz number to get the optimum feedback for our understudy system.

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The remainder of this paper is organized as follows. In section 2 a new optimizing algorithm is introduced to improve soft sensor model structure. To have a well-tuned model for soft sensor, several techniques were introduced for selection of input variables and their respective efficient time delays. In section 3 a brief description is made on Tennessee Eastman process as considered process in this study. Case studies illustrating optimized soft-sensor development for the TEP as a chemical process benchmark are reported in section 4. Finally section 5 provides concluding remarks.

II. Tuning Soft sensor Model Structure

It is necessary to judiciously select the effective number of time delay for process variables in order to identify the considered output. Thus, Lipschitz delay estimation and step response algorithm were used in order to understand the proper value of the efficient time delay for process manipulated variables and setpoints.

A. Step response for delay estimation

Step response method is an open-loop, time domain approximation method. The input, output and noise signals are represented in this domain, i.e. in the basis where the basis functions are step functions $u(t-t_p)$. The efficient delay is estimated by measuring the time-delay to the start (the beginning of the rising part) of an estimated step response of the system. Since this can be done by thresholding these responses, these methods are also called thresholding methods [12].

In this method in order to estimate the most effective delay, a step signal with proper high signal-to-noise ratio (SNR) should be integrated with the studying signal in normal working operation. Step size is determined according to process information and step length should be longer than process settling time. Afterward, from the slope of the studying output response, the efficient time delay that the signal would affect studying output would be calculated. I/O dependencies, dominant process time constants, process gains, efficient size of lag time are obtained through the test which are needed in design of the soft sensor model.

B. Lipschitz number for delay estimation

The Lipschitz numbers method is used to identifying orders of input-output models [13, 15]. In [13], the method was improved in order to identify the most efficient delay of a signal in system identification purpose. Assuming that underlying model function f(x) is continuous and smooth and that sufficient input-output pairs (x_i,y_i), (i = 1,2,…, N) are available. Then Lipschitz quotient is defined by:

$$q_{ij}^{(n)} = \frac{\left|y_i - y_j\right|}{\left\|x_i - x_j\right\|_2}, \ (i \neq j)$$
$$= \frac{\left|y(i) - y(j)\right|}{\sqrt{(x_1(i)-x_1(j))^2 + \ldots + (x_n(i)-x_n(j))^2}} \ .(1)$$

$\left\|x_i - x_j\right\|_2$ is the Euclidean distance of two points x_i and x_j in the input space and $\left|y_i - y_j\right|$ is the distance between their corresponding outputs. The superscript n means that, in this case, all n significant variable delays are included in x. As f(x) is continuous, the Lipschitz condition says, that the Lipschitz quotient is bounded.

In order to reduce the influence of measurement noise, a weighted geometric mean of the p largest Lipschitz quotients is performed. This results in the so-called Lipschitz number,

$$q^n = \left(\prod_{k=1}^{p} \sqrt{n}\, q^{(n)}(k)\right)^{1/p} \cong \max_{i,j,(i \neq j)} (q_{ij}^{(n)}) . \qquad (2)$$

where $q^{(n)}(k)$ is the *k*th largest Lipschitz quotient among all $q_{ij}^{(n)}$ calculated for *n* input variables. The number of included quotients is recommended to be set to $p \in [0.01N, 0.02N]$ [13].

If the desired delayed variable is excluded from x, the Lipschitz number increases considerably. On the other hand, including redundant variables will not change the Lipschitz number significantly. Therefore to identify the desired most significant variable, two steps are taken:

1. Lipschitz number is calculated while including continuous delayed signal to the input set of x. This should be continued until there is no other significant decrease in Lipschitz numbers while adding more delayed variable to input set.
2. In the next step, conversely, latest delayed variables are excluded from the data set and the Lipschitz number trend is observed to find a significant increase in its value.

A special advantage of this method is its independency to the output sampling time, as desired most significant delay detection is only related to the sampling time of the input variable.

III. Tennessee Eastman Process

Tennessee Eastman process (TEP) is designed to be a realistic test problem for use in the testing of alternative regulatory and optimization strategies in process control. The process developed by Eastman Kodak Company in collaboration with University of Tennessee and proposed by Downs and Vogel [9]. The process model is available in Matlab Simulink at Ricker's homepage [16].

In TEP, there are 41 measured variables (22 variables provide continuous process measurements and 19 variables record the chemical compositions from gas chromatography) and 12 manipulated variables which are listed in TABLE I. The details on the process description are well explained in [9]. Among all of the 53 process variables, the compressor recycle valve, stripper steam valve and agitate speed are not manipulated, thus they have excluded in this case study.

It should be noted that the 22 continuous output variables and 12 manipulated variables have the sampling interval of 1.8sec., while the other 19 composition measurements are sampled at the much longer period of 6 min (for reactor feed and purge gas analyzer) and 15min (for product analyzer). Thus the soft sensor is developed to predict them online. In this study, the continuous measurement variables and the manipulated variables are used as the inputs while the composition variables as outputs for the soft sensor modeling and estimation. One of the 19 component variables is selected for soft sensor development, which is the %G component in product stream.

TABLE I. MANIPULATED VARIABLES (XMV), PROCESS SETPOINTS, AND CORRESPONDING EFFICIENT TIME DELAYS, CALCULATED BY STEP RESPONSE AND LIPSCHITZ NUMBER ALGORITHMS.

Manipulated Variables	**Time Delay (hours)**		**Signal Description**
	Step Response	***Lipschitz number***	
XMV (1)	0.5	0.6	D Feed Flow (Stream 2)
XMV (2)	0.5	0.6	E Feed Flow (Stream 3)
XMV (3)	0.5	0.6	A Feed Flow (Stream 1)
XMV (4)	0.5	0.6	Total Feed Flow (Stream 4)
XMV (5)*	0.5	-	Compressor Recycle Valve
XMV (6)	0.5	0.5	Purge Valve (Stream 9)
XMV (7)	0.5	0.8	Separator Pot Liquid Flow (Stream 10)
XMV (8)	0.75	0.9	Stripper Liquid Product Flow (Stream 11)
XMV (9)*	0.5	-	Stripper Steam Valve
XMV (10)	0.5	0.7	Reactor Cooling Water Flow
XMV (11)	0.5	0.5	Condenser Cooling Water Flow
XMV (12)*	0.5	-	Agitator Speed
Product %G composition setpoint**	1	-	-
Product rate setpoint**	1	-	-

*as they are fixed in the studying control design, their efficient delay time only could be obtained from Step Response algorithm

**as process setpoint signals change slowly as process structure, their efficient time delay only investigated by Step Response algorithm

IV. THE SOFT SENSOR DESIGN OF THE QUALITY VARIABLE OF THE TEP

A. Efficient time delay estimation

Efficient time delay has estimated to identify the %G component in the product stream. Results from step response test and Lipschitz number algorithm are shown in TABLE I. With step response method, by exciting the candidate signals with proper integrated step signal, time variability and effective time delay of the signal can be diagnosed by observing the desired output trends. Although this is a simple and efficient technique for almost any signal efficient time delay estimation, the resolution of the results is affected by the output signal sample time. In this experiment, because the output signal has 0.25-h time, delay is partly estimated with this technique.

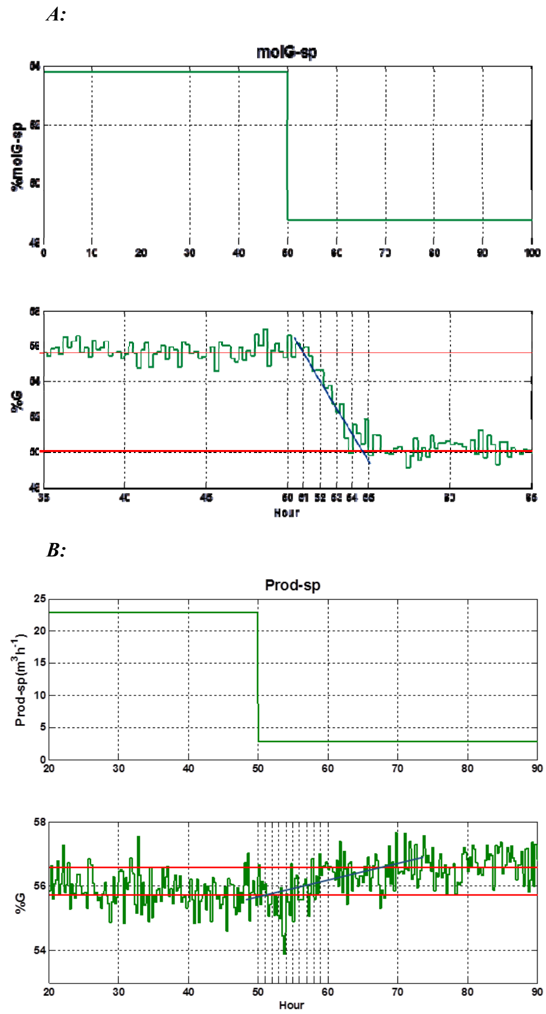

Fig. 1. Step response test on A: product %G composition and in B: product rate setpoint for efficient time delay estimation

Results of the step response test for two process setpoint signals are depicted in Fig 1 as an example of this study. A visual inspection is performed in order to estimate the effective time delay for every candidate process signal.

In the next method, Lipschitz algorithm solves the problem with numerical solution. Therefore here data needs to be rich enough to express the process behavior and training data is used in this algorithm. Some variables are fixed to their boundaries or have little changes, so this technique cannot be used for their delay estimation. For others, improvement in efficient time delay estimation resolution is observed in the results of TABLE I.

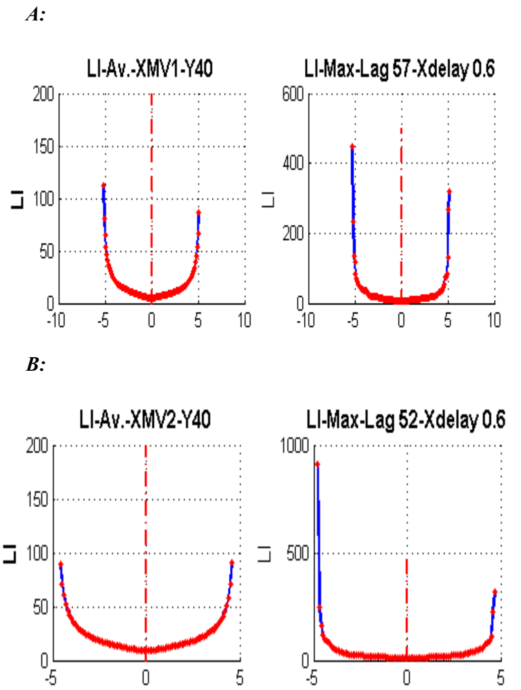

Fig. 2. Lipschitz number test on two Tennessee Eastman Process manipulated variables, A: XMV1 and B: XMV2

Lipschitz number test result on two process manipulated variable is brought here as an example in Fig. 2. It can be seen that while the efficient time delay is excluded from the variable set in the algorithm, the Lipschitz number would face a significant change in its value. In this figure, two Lipschitz number tests were plotted for each signal. One with maximum method (labeled with LI-Max) and the other with average method (labeled with LI-Av) to overcome the process noise. Horizontal axis is with 0.01 hour unit. 0.6-h is estimated for the efficient delay of both signals.

Although step response is a simple open loop test to understand the efficient time delay, but it's not possible for most closed loop process to perform this test on manipulated variables in their operation. Results are highly related to visual inspection of the operator to recognize the most efficient time delay for every candidate signal. Therefore Lipschitz is a powerful technique for this problem and can response with high precision while only needs training data which are available for most cases.

B. Input selection for soft sensor model

The input dataset of the proposed soft sensor model are the eight TEP variables with their proper delay time listed in TABLE I: four process input flow XMV1-4, XMV6 purge valve position, XMV7 separator pot liquid flow, product %G component setpoint and product flow rate setpoint. This input selection is made by conducting forward selection (FS) algorithm [8], input selection algorithm, and analysis of the process control structure while selecting most effective signals among the manipulated variables and process setpoints with their calculated effective delay.

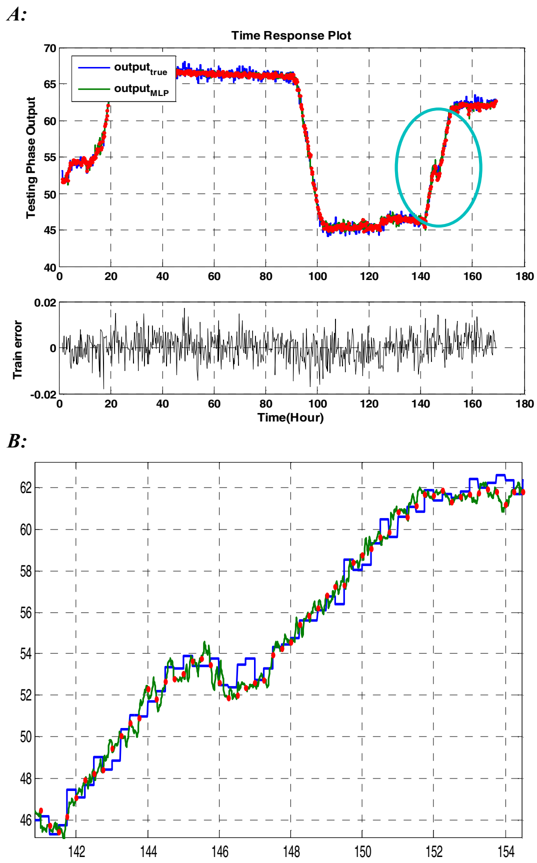

Fig. 3. Physical sensor and soft sensor response for validation data, B: is a closer look at the response – Blue line is physical sensor output, Green line is the soft sensor output, red dots are the soft sensor output in the physical sensor availability time

C. Training phase

Nonlinear model with one layer MLP structure is used in order to estimate the desired analyzer output. An optimal 23 hidden neuron number (HNN) has selected by semi cross validation technique [8], in which model response accuracy is investigated for validation data set which is non-trained part of process dataset.

During training phase, the weights and biases of the network are iteratively adjusted to minimize the MSE, the average squared error between the network outputs and the target outputs. The Levenberg - Marquardt (LM) algorithm, a well-known training algorithm for its fast convergence and small residual training error [8], is employed in this work.

Model has been trained by 168h process operation and 0.01h sample rate for data generation. Here the process is operating under the base case operating mode while a proper pseudo random binary sequence (PRBS) signal is introduced to the process in order to have full exciting dataset for identification purpose [17].

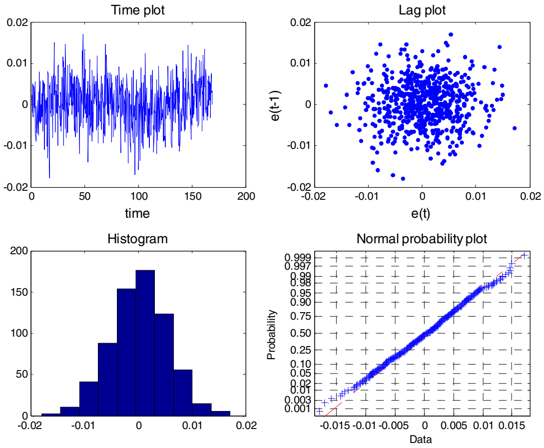

Fig. 4. 4-plot diagram for evaluating model performance in training phase

The result is shown in Figure 3-A, where the physical sensor output has estimated by soft sensor model with validation data. Here physical sensor output signal and soft sensor output is shown in the same diagram. Soft sensor error is calculated every 0.25-h which physical sensor data is available. In Figure 3-B, a closer look is made at the soft sensor response and its value is clarified by dots at the time physical sensor output is available.

In addition, a 4-plot validation figure [18] is used in order to validate soft sensor model performance in training phase and model response error characteristics have been investigated. Result of this investigation is shown in Figure 4, where error time response, lag, histogram and normal probability plots are visually monitored. It can be seen that all of the residual characteristics are similar to Gaussian noise characteristics, which means the model response error is the process noise and this model could have a good estimation of desired process output and eliminating the analyzer noise signal.

V. Conclusion

In this study a soft sensor is designed to overcome the process instrumental limitation made by analyzers in chemical process industry. In order to design such inferential instrument, a nonlinear artificial neural network, MLP, is used as soft sensor model. Several investigations made in order to introduce a novel improvement in model structure optimization. Therefore step response technique, Lipschitz number method and forward selection was applied in this study. Results show that the real-time inferential analyzer can be a good alternative for the former physical analyzer while significant improvement achieved in soft sensor response as it has optimized in the training phase. We showed that the designed soft sensor can perfectly estimate physical analyzer output and truly overcome with its output noise signal.

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