Neural Networks-based Virtual Sensors Methodology

ANNA PEREZ-MENDEZ

LUIS NAVA-PUENTE Dpto. de Estadística Universidad de Los Andes Mérida, 5101 VENEZUELA

FRANCKLIN RIVAS-ECHEVERRÍA ELIEZER COLINA-MORLES Laboratorio de Sistemas Inteligentes Universidad de Los Andes Mérida, 5101 VENEZUELA rivas@ing.ula.ve ecolina@ing.ula.ve

Abstract: In this work a Methodology framework for implanting Virtual Sensors using Neural Networks will be presented, including the statistical analysis techniques that can be used for studying and processing the data. The proposed Methodology is based upon Software Engineering, Knowledge-based systems and neural networks methodologies. This methodological framework includes both technical and economical feasibility to build the virtual sensors and considers important aspects as the available computational platform, historical data files, data processing requirements such as filtering, pruning, set of variables that must be selected for the best performance of the virtual sensor, etc. There are also presented the statistical consideration and the corresponding techniques for data analysis and processing. The methodology includes techniques as principal components, cluster analysis, factorial analysis, etc.

Keywords: Virtual Sensors, Neural Networks, Statistical Analysis, Multivariate Analysis, Software Engineering.

1 Introduction

Nowadays there are new and stricter specification and restrictions for the behavior and for the Quality expected in industrial environments [2,6,8]. So, it is very important to have on-line measurement for quality levels and/or other variables that are critical for the performance of the process.

Many of the process quality variables that are important to evaluate, in order to satisfy productivity

levels and to guarantee the predefined specifications on the final product, are difficult to obtain due to the high costs of quality analyzers or because the complexity for having a mathematical mode[5,12].

Virtual sensors are an area of virtual instrumentation whose main objective is to generate indirect measurements of important variables using the information about past values of the variable or the measurements of other process variables that are related with the one desired to predict. Neural networks[2,9,11] have been one of the most used intelligent tool for designing and developing Virtual Sensors due to them accurate, modeling and Identification capabilities and easy for implantation.

This work is a generalization and a implantation of the methodology presented in [22] and organized as follows: Section 2 presents an introduction to artificial neural networks. Section 3 presents the methodology for implementing virtual sensors using neural networks. Finally, in section 4 we give some concluding remarks.

2 Neural Networks

Biological neurons are cells that constitute the principal elements of central nervous system[9,23]. Neurons are able to receive signals from other neurons, process that signals, generate nervous pulses and transmit them to other neurons. Each neuron possesses a cellular body (that contains the nucleus). In the cellular body are handled all the necessary activities for the neuron life. The neurons also possess a set of tubular extensions called dendrites, which are the signal receptors of neurons. Finally, the axon is the output connection used by the neuron in order to emit nervous signals. Figure 1 illustrates a biological neuron. The synapse is the union between one neuron's axon and other neuron's dendrite. In the synapses are concentrated all the learning capabilities of neural networks. Learning can be viewed as the process of finding the appropriate weights of the synaptic junctions.

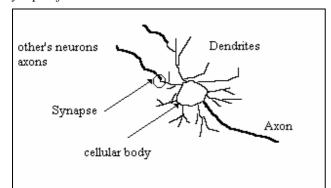


Figure 1. Biological Neuron

In the human brain, neurons are interconnected in complex spatial topologies in order to complete the central nervous system. A neuron operation can be explained as a process where the cell executes an addition of all the signals received via the dendrites. When this addition is bigger than a fixed value, the neuron changes to an excited condition and transmits an electric pulse using the axon. If the addition of the received signals is lower that the fixed value, the neuron remains in a inhibitory condition. This simplified model of the biological neurons is depicted in Figure 2.

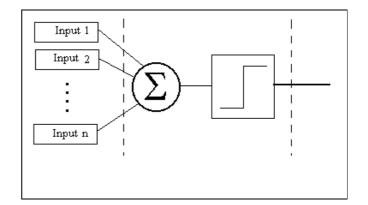


Figure 2. Artificial model of a neuron

The basic elements of most artificial neural networks are the adaptive linear neurons (Adalines). These adaptive neurons are composed of:

- A summing point of weighted inputs.
- A nonlinear activation function
- A learning algorithm.

Figure 3 presents an adaptive linear neuron.

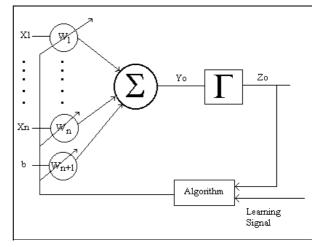


Figure 3 Adaptive linear neuron

From Figure 3 it can be obtained the following expressions:

$$Y_0(t) = \sum_{i=1}^n W_i(t) X_i(t) + W_{n+1}(t)b$$
(1)

$$Z_o = \Gamma(Y_0) \tag{2}$$

Neural networks power and representation capabilities depend on interconnectivity between the neurons and the learning algorithm used for updating the interconnection weights. The different existing learning methods can be grouped in two categories:

- Supervised learning
- Non-supervised learning

In supervised learning, there exist a "teacher" that gives to the neural network the desired output and the algorithm tries to minimize the difference between the desired output and the one given by the network. An example of this kind of algorithms is the popular "Backpropagation learning Algorithm". On the other hand, the non-supervised learning algorithms consist of a local information-based auto-organization process, that doesn't requires and external "teacher".

3 Virtual sensors and neural networks

Virtual sensors constitute a novel area of virtual instrumentation, whose principal mission is to perform indirect measurements of process important variables using historical data of the desired variable and some other variable that affects its performance. Some authors have defined virtual sensors as: "... the numerical prediction or estimation of a desired system state given other related physical signals such that the output of the virtual sensor estimates the true state in real time, on-line in an open-loop configuration"[8].

Virtual sensors are some times designed for working in parallel with a physical sensor in order to evaluate its performance, but they can be used also for having online estimation of the desired measurement.

Virtual sensors are widely used because they are just computer programs that can be change or updated when it is necessary. Virtual sensors using neural networks can be designed in order to learn the laboratory tests results (See figure 4) or to learn the signals given by a physical sensor (Figure 5).

During the last years, neural networks-based virtual sensors [2,5,8] have been widely used in industrial environments because of it potentiality for identifying complex nonlinear dynamical systems and for having appropriate results in different situations

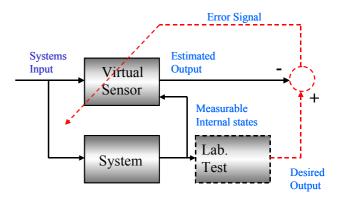


Figure 4. Virtual sensor learning using the Laboratory test results

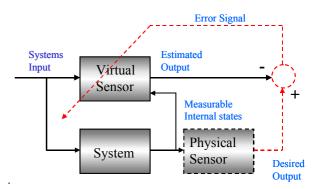


Figure 5. Virtual sensor learning using the Physical sensor results

3.1. Methodology for implementing Virtual Sensor using Neural Networks.

The following Methodology is based upon Software Engineering, Knowledge-Based Systems and Neural Networks Methodologies. It includes both technical and economical feasibility for building the virtual sensors and considers important aspects concerning computational platform, data processing, virtual sensor requirements, etc. It also considers the computational nature of virtual sensors and is very complete but easy to follow because of it structure based on stages, steps and phases. The proposed methodology description is presented next:

Stage 1: Analysis and description of the problem: In this stage it is analyzed the environment and characteristics of the problem and studies the feasibility for developing a virtual sensor using neural networks.

- Step 1.1.- General description of the problem:

1.1.1.- Familiarization with the process selected for using a Virtual Sensor.

1.1.2.- Detailed definition of the problem to be solved using Expert Systems.

- Step 1.2.- Feasibility analysis for developing a neural network-based virtual sensor: In this step the conditions for developing the virtual sensor are verified considering all the requirements given by a neural network application.
- Step 1.3.- Familiarization with the computational environment where is located the data that will be used by the virtual sensor and revision of the data acquisition process.
- Step 1.4.- Variable Analysis: In this step it is detailedly studied all variables involved in the process, that affects the behavior (directly or indirectly) of the wanted to estimate variable. It should be used statistical techniques for detecting: outliers, required transformation, variables relation, descriptive statistics, etc. It also should be evaluated the possibility for applying multivariate statistical analysis techniques or cluster analysis for patterns and variables reduction.

Stage 2: Requirements Specifications: In this stage it is revised the global requirements of the virtual sensor to be developed considering: final users, functional requirements, desired formats, etc.

- Step 2.1.- Definition of the final users for the virtual sensor to be designed: In this step it is defined the final users for the virtual sensor, the kind of information need for each of the users, users requirements, etc.
- Step 2.2.- Information and Equipment requirements: It is evaluated the information

requirements (updating period) and the equipment requirements (hardware and software interconnection requirements, computer platform required, etc.).

Stage 3: Cost, time and resources analysis: It is estimated the working hours and resources needed for developing the virtual sensor. With that estimation it is possible to calculate the approximate cost of the system. In this stage it is also done the activities plan for developing the virtual sensor.

Stage 4: Data requirements: In this stage there are selected the inputs that are going to be given to the neural network. It also contemplates the signal preprocessing and pruning using statistical techniques in order to solve the identified problems in step 1.4.

- Step 4.1.- Data processing and learning set selection: In this step, the variables selected as possible inputs for the neural network are processed. Outliers detection is done using graphical or formal tests, it is selected the appropriate transformation functions for those variable that require a transformation for having a symmetric behavior. It can be also consider performing a principal components analysis or factorial analysis in order to reduce the number of patterns or variables to be used in the training phase. For selecting the data sets to be used for training and proving the neural networks, it can be used a random sampling procedure.
- Step 4.2.- Hardware and Software specifications: In this step, it is specified the hardware and software needed; considering the data processing given in the preceding step. It is selected the computational tools required.

Stage 5: Virtual Sensor Design using Neural Networks: In this stage a virtual sensor preliminary design is done. It is considered the selected and processed variables in step 4.1.

- Step 5.1.- Neural Networks training: In this step it is trained the neural network using the variables and patterns selected in step 4.1. It is important to select the neural network topology (inputs and outputs number, number of hidden layers, number of neuron in each layer, activation functions, etc). It is also important to select the learning algorithm to be used for updating the interconnecting weights.

- Step 5.2.- Neural Network model Verification: It is important to validate the obtained neural network model for the virtual sensor. It is used the proving set of data for verifying the performance of the trained neural networks with different inputs as the used in the learning phase.

Stage 6: Design of the computational tool for implementing the virtual sensor: It is carefully designed each of the modules that are going to be used by the computational tool, including internal and external interconnections with programs and equipments.

Stage 7: Neural network-based virtual sensor implantation: This is the last stage of developing the virtual sensor. In this stage it is implanted the whole system and start the depuration and prove phase. It is important to verify the results given by the neural network in order to fix any possible problem. It can be also decided to train again the neural network.

Stage 8: Actualization and maintenance of the system: This stage lasts during all the operative life of the system. It should be consider any changes to the process and any new requirements for the developed system.

4 Virtual sensor for Estimation of gasoline quality using neural networks

In this section it will be presented an industrial application of the proposed methodology, using the most important stages. It was designed a virtual analyzer for estimating the quality of a Houk type gasoline obtained in a catalytic cracking unit.

Stage 1: Analysis and description of the problem:

- Step 1.1.- General description of the problem: Oil companies, expends lots of money and work in order to guaranty the process performance and the quality requirements of the products to be obtained. The refinement process is very complex and is divided in sections or units. In the catalytic cracking unit of the refinery plant there are measured more than 180 chemical and physical variables. In this unit it is obtained different products from the crude as: alcohols, gas oils, gases, different kinds of gasoline, etc. The mission of this unit is to break the carbon chains in order to obtain lighter ones, which are more commercially attractive. The Houk gasoline is obtained from the plate 33 of the catalytic cracking unit. The quality of the Houk gasoline may be expressed in terms of it final point temperature (temperature when the total evaporation of the gasoline in a lab test occurs).

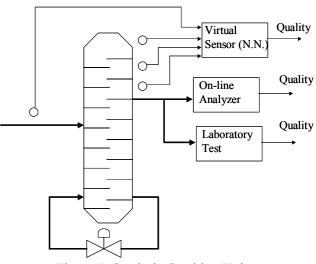


Figure 5. Catalytic Cracking Unit

The work consists in obtaining and estimation of the final point temperature of the Houk gasoline in order to obtain an on-line estimation of the quality of the product (that is obtained using laboratory analysis only two or three times a day).

Step 1.2.- Feasibility analysis for developing a neural network-based virtual sensor: According to the characteristics of the problem, and considering that the variable to be estimated possesses functional relations with other variables that are measured periodically, that there exists a lot of historical data; it is possible to construct a neural networks-based virtual sensor for estimating the Houk Gasoline Quality.

- Step 1.3.- Familiarization with the computational environment where is located the data that will be used by the virtual sensor and revision of the data acquisition process: The measurements of the processes variables are given by sensors that are located in different parts of the unit, the quality variables are measured using on-line analyzers and there are some other performance variables that are calculated using some computer algorithms. All this data is stored in databases.
- Step 1.4.- Variable Analysis: In the catalytic cracking unit there are some measured variables as: Temperatures, pressures, flows, and some calculated variables that are related with the desired quality. It has been used on-line analyzers and laboratory test for estimating the gasoline quality or final point temperature. The data acquisition system collects information about 183 variables. Some studies given by expert process engineers have determined that only 14 of those variables have some influence on the quality level. These 14 variables are quantitative and are measured using sensors or are calculated from other measured variables.

For the design of the virtual sensor, it was constructed a data matrix containing the obtained measurements of the temperature final point and the other important variables, selected by the experts, that can be used for estimating the quality variable. The obtained file contains 15 variables and 3721 observations for each variable. This data set needs to be processed in order to eliminate those patterns (observations) that are out of specifications or that present nonrandom behavior. Next table presents a briefly description of each of the variables:

	Min.	Max	X	S^2
PTO Q	28	252.95	227.98	1045.98
TP33	143.42	153.08	148.329	3.06552
TALIM	180.98	190.2	184.662	4.2435
PP33	1.20	1.29	1.25626	0.000223
VCBE	15.69	29.01	19.2361	1.5859
FSAL	214.13	522.36	377.135	3811.72
VCFQ	18.11	26.34	21.4979	1.1222
VCTP	8.15	16.45	13.1993	1.3304
TTOP	93.94	104.73	97.4146	4.503
TP34	132.21	141.95	137.53	3.701
TP32	145.98	155.23	151.24	3.650
TSAL	96.17	100.408	96.682	0.482
FALIM	839.81	1953.4	1511.4	21353.8
TFON	185.75	194.93	189.066	5.1234
PTOP	11.67	12.59	12.222	0.02628

	S	Range	S _{KP}	K
PTO Q	32.3416	224.62	93.521	201.079
TP33	1.751	9.66	-3.3643	-6.45
TALIM	2.0599	9.32	16.6123	-6.862
PP33	0.0149	0.08	-9.9121	-2.4676
VCBE	1.2593	13.32	26.8546	46.5912
FSAL	61.739	308.23	1.589	-13.4581
VCFQ	1.059	8.23	-0.634	-1.3553
VCTP	1.1534	8.3	-7.73	-2.4253
TTOP	2.122	11.79	10.731	-1.7121
TP34	1.924	9.74	-11.891	-2.056
TP32	1.9106	9.25	-9.889	-5.984
TSAL	0.6945	4.31	-16.1022	12.4015
FALIM	146.129	113.59	-6.061	-0.0497
TFON	2.2635	9.18	23.9817	-1.7934
PTOP	0.1621	0.92	-14.6441	-1.885

Next, it will be presented a briefly description of each of the selected variables:

- Final Point Temperature (Pto. Q): This is the quality variable that is going to be estimated using the virtual sensor, is a temperature value and is expressed in ⁰C. and should presents values between 220 y 247 ⁰C. In the table it can be seen that there exists values that are out of this specifications, so they may be excluded from the data set to be used.
- **Temperature on Plate 33 (TP33) :** This is a temperature variable and should present values between 144 and 154 ^oC. There also exist values under the specifications.
- Feeding crude temperature (TALIM): This is a temperature variable and should present values between 181 and 171 °C. There exist values under the specifications.
- **Pressure on Plate 33 (PP33):** This is a pressure variable and should present values between 1.25 and 1.29 PSI. There also exist values under the specifications.
- Adimensional Variable Calculated using the energy balance (VCBE): This variable is found using some operations over some other variables that are envolved in the energy balance. Doesn't have units and should present values between 16 and 24. There exist values under and over the specifications.
- Gasoline recolection flow (FSAL): This variable is measured in cubic meter per hour (mt³/hr) And Should present values between 219 and 515 mt³/hr. There also exist values Ander the specifications.

- Adimensional variable Calculated using crude phisico-chemical properties} (VCFQ): This variable is found using some operations over some phisico-chemical variables measured over the crude. Doesn't have units and should present values between 18 and 26. There exist values over the specifications.
- Variable Adimensional Calculada Basada en Temperaturas y Presiones (VCTP): This variable is found using some operations over some other tempersture and pressure variables. Doesn't have units and should present values between 10 0and 18. There exist values under and over the specifications.
- **Temperature on the Top of column (TTOP):** This is a temperature variable and should present values between 93 and 105 °C. There doesn't exist values out of the specifications.
- **Temperature on the Plate 34 (TP34):** This is a temperature variable and should present values between 133 and 143 °C. There also exist values out the specifications, but with small differences.
- **Temperature on Plate 32 (TP32):** This is a temperature variable and should present values between 147 and 157 °C. There also exist values under the specifications.
- Temperature of the gasoline at the end of the unit (TSAL): This is a temperature variable and should present values between 95 and 105 °C. There doesn't exist values out of specifications.
- Feeding crude flow (FALIM): This a flow variable ans should present values between 1000 and 2000 (mt³/hr). There exist values with smaller values than the especifications.
- Temperature at the bottom of the column (TFON): This is a temperature variable and should present values between 185 and 195 °C. There doesn't exist values under or over the specifications.
- **Pressure at the top of the unit (PTOP):** This is a pressure variable and should present values between 10 and 14 PSI. There doesn't exist values under or over the specifications.

Stage 2: Requirements Specifications:

Step 2.1.- Definition of the final users for the virtual sensor to be designed:

The system is going to be used by engineers and technicians working in the refinery plant and the

information they need id the numerical value of the final point of temperature.

Step 2.2.- Information and Equipment requirements:

The obtained prediction value for the quality variable should be stored in the databases every sampling time. It is required a system for acquiring the needed information from the databases and another system for storing the estimated value generated using the virtual sensor.

Stage 3: Cost, time and resources analysis: In this case it wasn't consider this stage, because it was a research program.

Stage 4: Data requirements:

Step 4.1.- Data processing and learning set selection:

Considering that from the previous stages it is determined that is appropriate the design and implantation of the virtual sensor using neural network, it is important to find the appropriate size for the learning and testing sets. For such a task it was used a random simple sampling using as parameter the set mean. For the sampling procedure, it was consider a maximum error of 15% and a confidence level of 97%, which determines a $Z_{\alpha/2} = 2,17$. The found size for the test or validation set was of 1056 observations and the size for the training set was1049.

Next, it was made an exploratory analysis for every variable. For selecting the input variables to the virtual sensor, it was performed a principal components analysis using all the 15 variables previously mentioned.

After the carefully study of all the variables, there were selected as virtual sensor inputs: PP33, VCBE, TP33, VCFQ, TP34, TP32. Some of these variables were mathematically transformed in order to promote symmetry.

For detecting atypical patterns or multivariate outliers, it was used the box-wisher diagram and normal probability graphics.

Stage 5: Virtual Sensor Design using Neural Networks:

Step 5.1.- Neural Networks training: For training the neural networks, there were selected three data sets. The first one is composed of the 14 variables initially selected. The second data set is form using the six statistically selected variables, and finally a data set using the same variables, but using the selected six mathematical transformation. The neural networks topologies that gave the best results are: 14 inputs, a hidden layer with 10 neurons with sigmoid activation function and a linear output for the first data set; 6 inputs, a hidden layer with 10 neurons with sigmoid activation function and a linear output for the second data set and finally a 6 inputs, a hidden layer with 8 neurons with sigmoid activation function and a linear output for the third data set

Step 5.2.- Neural Network model Verification:

For this step there were used data sets different that the ones used in the training step. The result are shown next:

- For the first data set (14 inputs): It was found an absolute mean error of 1.4535 and a correlation of 0.64.
- For the second data set (six inputs without transformations): It was found an absolute mean error of 1.3622 and a correlation of 0.75.
- For the third data set (six inputs with mathematical transformations): It was found an absolute mean error of 1.2234 and a correlation of 0.82.

It can be seen that the error is lower when the variable selection is done and even lower when a mathematical transformation is performed. On the other hand, the correlation results are better also when the selection is given and much better when transformation is done. So, it can be seen the obtained benefits using statistical techniques for variable selection, outlier analysis and mathematical transformations.

5 Conclusion

- In this work it has been proposed a methodological framework for implanting virtual sensor using neural network.
- Virtual sensors have become an important industrial tool, because they can be use for computationally estimating complex variable (usually quality variables) that otherwise should require very expensive equipments or laboratory tests that can consume many time before having a result.
- Neural networks have been used for designing virtual sensors due to its characteristics and capabilities for learning processes behaviors using historical data.
- The proposed methodology contemplates data processing requirements using statistical analysis in order to evaluate the selected

variables, eliminate redundant information, outliers eliminations, and mathematical transformations to be applied to some variables.

- In the designed virtual sensor for quality estimation, there were found improvement using the statistical analysis, because it use generate easier neural network topologies with better performance.

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