Virtual Instruments Based on Stacked Neural Networks to Improve Product Quality Monitoring in a Refinery

4 Author(s)

L. Fortuna ; P. Giannone ; S. Graziani ; M.G. Xibilia

View All Authors

Abstract:
A virtual instrument, based on neural networks, for the estimation of octane number in the gasoline produced by refineries is introduced. The stacking approach is proposed to improve the estimation performance of the instrument. The validity of the proposed approach has been verified by comparison with the performance of traditional modeling techniques. The proposed virtual instrument can be used during the maintenance phases of hardware devoted to the measurement of the octane number

Published in: Instrumentation and Measurement Technology Conference, 2005. IMTC 2005. Proceedings of the IEEE

Date of Conference: 16-19 May 2005

Date Added to IEEE *Xplore*: 13 March 2006

Print ISBN: 0-7803-8879-8

Print ISSN: 1091-5281

INSPEC Accession Number: 8968022

DOI: 10.1109/IMTC.2005.1604500

Publisher: IEEE

Conference Location: Ottawa, Ont., Canada

SECTION 1
Introduction

Quality standards and environmental issues in industrial plants, and in particular in refineries, require the development of huge monitoring networks using both high-cost on-line measurement devices and when possible, suitable models producing real-time estimates of unmeasured quantities on the basis of available operational data [1], [2], [3], [4], [5].

Among modeling strategies, first principles models require a deep knowledge of the physical and chemical phenomena involved in the process and seldom guarantee a sufficient accuracy with a reasonable modeling effort.

On the contrary, empirical models, or data-driven models, producing reliable real-time estimates of process variables on the basis of their correlation with other relevant system variables are being largely used [1], [2], [3], [4].

Though, both linear statistical methodologies and nonlinear strategies have been proposed to estimate empirical models prediction algorithms are usually developed through nonlinear identification techniques to deal with the peculiar nonlinearities of processes.

Obtained models can be used alone as a valuable, low-cost alternative to expensive sensors, or they can work in parallel with hardware devices allowing model-based techniques to be adopted for the development of fault detection schemes [6]. Moreover, they can take the place of sensors which have been taken off for maintenance, to keep control loops working properly and to guarantee product specifications without undertaking conservative production policies, which are usually too expensive. Such models used as part of Virtual Instruments should easily be implemented on existing hardware and should be easy to re-tune when operational conditions or system parameters undergo major changes. Finally, the use of Virtual Instruments can allow real-time estimates to be performed, thus overcoming the delay introduced by slow hardware devices (e.g. gas-chromatographs) and eventually improving the performance of control algorithms. The desired process models are usually determined on the basis of all the information available about the process, i.e. analytical considerations technologist knowledge, and trial and error identification strategies. For industrial processes, and in particular for refineries, due to the complexity of the nonlinear phenomena involved and the great amount of historical operational data available, Multi Layer Perceptrons (MLP) have been widely and successfully used to this end [7], [8].

The possibility to monitor product quality in refinery by using a Virtual Instrument whose core is a combination of neural networks, generally known as a stacked neural network, is investigated. In particular the possibility to efficiently estimate the research octane number (RON) by using a number of measured input quantities, in gasoline produced by a powerformer unit is considered. The estimation is required from the plant technologists in order to replace on line measuring devices during planned maintenance actions.

Data used to derive the models were collected by measuring devices installed at a large refinery in South Italy, during a period lasting about 45 days with a sampling period of 3 min (corresponding to about 20000 samples, after invalid Data elimination).

SECTION II.
The Plant

Data collected from a Powerformer Unit, by using available hardware have been considered for the development of the virtual instrument introduced in this paper.

The Powerformer Unit, receives as input the Heavy Virgin Naphtha (HVN) flow coming from the Naphtha Splitter bottom. The output flow of the plant, that feeds the Deetanizer and Debutanizer distillation columns, is a liquid high in research octane number (RON) which contains aromatic composites, hydrogen oil gas, and liquefied petroleum gas (LPG).

The RON value of the powerformed gasoline is used to monitor the product quality and to control the powerforming process.

Based on process experts' knowledge the following variables that influence the RON value were selected:

- reactorS temperature $(\mathrm{u}_1, \mathrm{u}_2, \mathrm{u}_3, \mathrm{u}_4)$;
- input flow (u_5);
- pressure value at the top of the Debutanizer $(\mathrm{u}_6$;

Also, a suitable number of regressors were fixed for each input quantity, on the basis of both correlation analysis and considerations on system physics, resulting in the following model structure:

$$\begin{aligned}\hat{y}(k)=f(&u_1(k), u_1(k-3), u_1(k-5), u_2(k), u_2(k-5),\\ &u_3(k), u_3(k-4), u_3(k-5), u_4(k), u_4(k-5),\\ &u_5(k), lk(k-1), u_6(k), u_6(k-1))\end{aligned} \tag{1}$$

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where $\hat{y}(k)$ is the estimation of RON k-th sample and $f(.)$ is an adequate function.

It is to be observed that, taking into account the necessity to estimate the model output in (temporary) absence of any measuring device for the RON only MA models have been considered for the development of virtual instruments.

SECTION III.
The Linear Model for RON Estimation

For matters of comparison linear models have been also taken into account. In particular, in accordance with (1), the following linear model was considered:

$$\begin{aligned}\hat{y}(\mathrm{k}) = {} & \mathrm{a}_1\mathrm{u}_1(\mathrm{k}) + \mathrm{a}_2\mathrm{u}_1(\mathrm{k}-3) + \mathrm{a}_3\mathrm{u}_1(\mathrm{k}-5) + \mathrm{b}_1\mathrm{u}_2(\mathrm{k}) + \\ & + \mathrm{b}_2\mathrm{u}_2(\mathrm{k}-5) + \mathrm{c}_1\mathrm{u}_3(\mathrm{k}) + \mathrm{c}_2\mathrm{u}_3(\mathrm{k}-4) + \mathrm{c}_3\mathrm{u}_3(\mathrm{k}-5) + \\ & + d_1\mathrm{u}_4(\mathrm{k}) + \mathrm{d}_2\mathrm{u}_4(\mathrm{k}-5) + \mathrm{e}_1\mathrm{u}_5(\mathrm{k}) + \mathrm{e}_2\mathrm{u}_5(\mathrm{k}-1) + \\ & + \mathrm{f}_1\mathrm{u}_6(\mathrm{k}) + \mathrm{f}_2\mathrm{u}_6(\mathrm{k}-1) + \mathrm{h} \end{aligned} \tag{2}$$

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where $\{\mathrm{a}_1, \mathrm{a}_2, \mathrm{a}_3, \mathrm{b}_1, \mathrm{b}_2, \mathrm{c}_1, \mathrm{c}_2, \mathrm{c}_3, \mathrm{d}_1, \mathrm{d}_2, \mathrm{e}_1, \mathrm{e}_2, \mathrm{f}_1, \mathrm{f}_2, \mathrm{h}\}$ is a set of multiplicative coefficientS to be searched for.

In Fig. 1 the performance of the linear model, where coefficients were obtained by using the LMS approach, is showed. In particular the acquired RON values are compared with the corresponding linear model estimations. Though the linear model follows the trend of real time series, the model accuracy was considered not satisfactory form the plant technologists and this was considered to be a consequence of the plant nonlinearity that cannot be modeled by using the model (2).

In the next sections nonlinear models developed to improve prediction capabilities are described. All considered nonlinear models exploit the modeling capabilities of Multi Layer Perceptrons (MLPs) with one hidden layer, with nonlinear activation function, and linear activation function for the output layer.

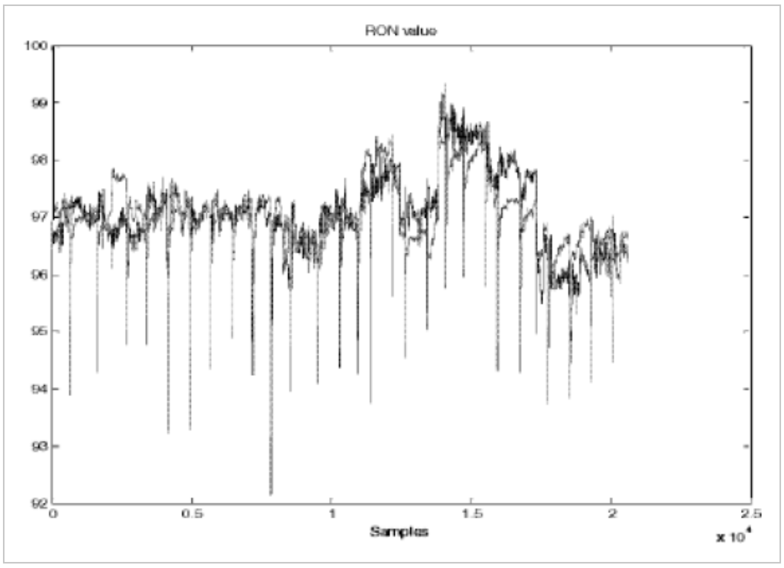

Fig. 1
Acquired RON values (solid line) and their linear estimation (dotted line).

SECTION IV.
Stacked Neural Networks Based

Stacked Neural Networks Based Virtual Instrument

Recently several strategies have been proposed to improve the performance of models, based on combining a set of neural networks [9], [10] [11], [12], [13]. In fact, during the training process, a number of candidate neural models is usually obtained, each of them with different architectures and/or training patterns and/or different initial weights. Generally only one neural network is chosen among candidates to model the system under investigations.

Since each network can behave differently in different regions of the II. space, a combination of different models can improve the overall prediction capability. A combination of different neural models is usually called 'stacking'. Stacked generalization is a generic term referring to any strategy for feeding information from one set of generalizers to another, before forming the final guess [9]. When a set of neural network models are combined the combination is called a 'stacked neural network'. The various approaches proposed in literature feature different strategies to select and combine the neural models.

A number of different stacking approaches have been considered to combine the 'best' neural predictors. In particular, combination strategies of MLPs based on simple average, the least squares approach and a nonlinear combination strategy, based on a cascade of neural networks, has been taken into account.

Neural networks considered in this paper differ either for the patterns used MODEL during the training phase or for the number neurons in the MODEL layer.

The performance of the different models have been compared by using one set of testing patterns.

A scheme of the generic stacking structure is shown in Fig. 2. Regressors in Fig. 2 were chosen on the basis of Eqn. (1), and each MLP produces an estimation of the octane number.

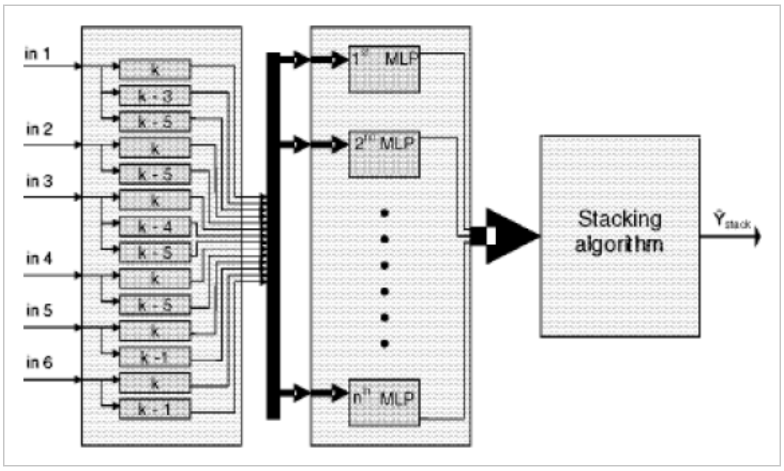

Fig. 2
The stacking structure adopted to estimate the octane number.

Let $\hat{y}_i$ be the vector of the estimated output from the i-th neural preaictor. The estimation proposed from the stacked network is:

$$\widehat{y}_{stack} = g\left(\widehat{y}_1, \widehat{y}_2, \cdot\cdot, \widehat{y}_i, \cdot\cdot, \widehat{y}_n, W\right) \tag{3}$$

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where W is a matrix of weighting parameters to be searched for an $g(.)$ is the stacking function. The number of MPLs used to realize the stacked network was determined by searching for the maximum of the correlation coefficient between the octane number an its estimation.

In the case of the linear stacking approaches Eqn. (3) reduces to:

$$\widehat{y}_{stack} = \sum\nolimits_{i=1}^{n} w_i \widehat{y}_i \tag{4}$$

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The simplest approach (called in the following stacking method 1) suggested in literature is basei on a simple average of the available neural predictions. In this case the weights w_i in Eqn. (4) are $w_i = 1/n (i = 1, \cdot\cdot, n)$.

The MSE_OLC (Mean Square Error_Optimal Linear Combination) approach (called in the following stacking method 2) is based on deriving the weights w_i, which minimize the MSE between the actual plant output an its estimation obtained by Eqn. (4), by using a Least Square approach.

The last approach (called stacking method 3) is basei on the attempt to exploit the interpolation capabilities of simple NNs with one hidden layer to combine the outputs $\hat{y}_i$ of each MPL to estimate the actual output y. The estimation of of the octane number, produced by each MLP, was used to train a set of MLPs with hyperbolic tangent activation function for hidden neurons, while the corresponding recorded vector of RON values was used as desired output.

SECTION V.
Experimental Results

The performance of the various stacking strategies was checked by using a validation data set never used for the training of the MPLs. In the case of stacking method 1, it was found that three MLPs gave the best results as it can be observed in Fig. 3. It reports the correlation coefficient value between the octane number an its estimation as a function of the number of stacked MLPs.

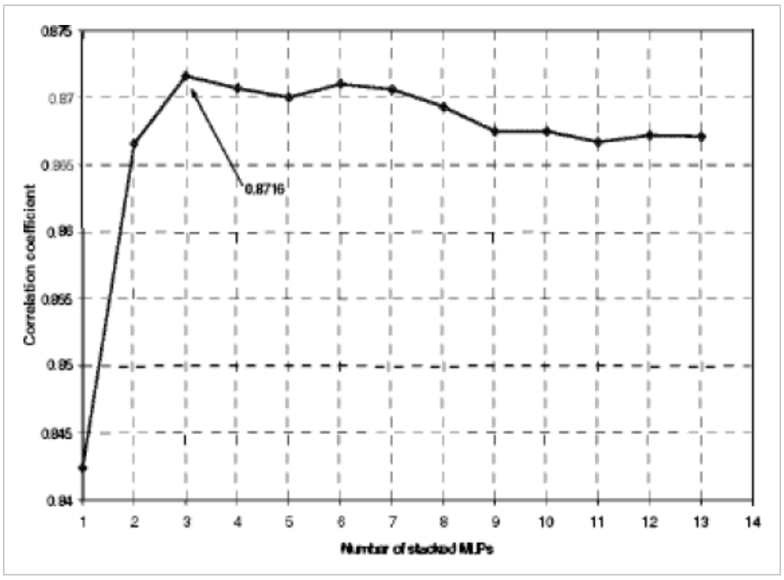
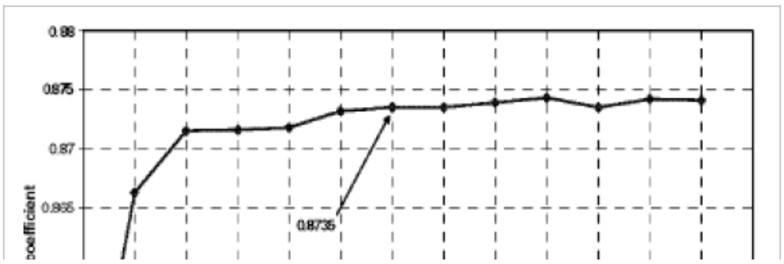


Fig. 3
Correlation coefficient value for stacking method 1 as a function of the number of stacked MLPs. Best performance were obtained by using 3 MLPs.

The same approach was used for the stacking method 2. Obtained results are showed in Fig. 4. In this case considering more than seven MLPs in the stacking structure did not gave any significant improvement in the model estimation capability. For this reason seven MLPs were considered the optimum number of the MSE_OLC stacking strategy.



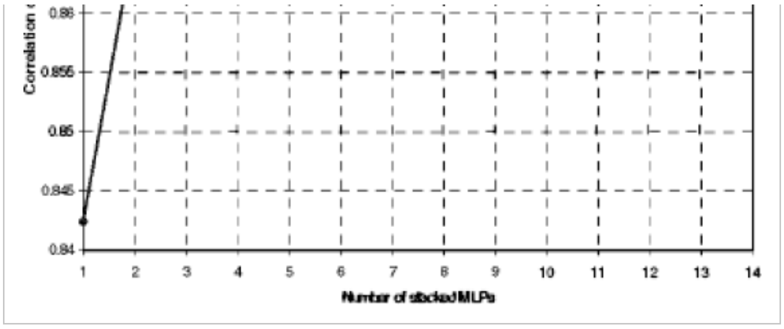


Fig. 4
Correlation coefficient value for stacking method 2 as a function of the number of stacked MLPS. Seven MLPS were considered the optimum number of the MSE_OLC stacking strategy.

Tab. I Comparison of the performance of different modeling strategies. Results referring to linear models and single MLP nonlinear models are reported for matter of comparison.

	Correlation coefficient	Residual mean value	Residual standard deviation
Linear model	0.7738	-9.07*10^{-5}	0.473
Single MLP	0.8424	0.00015	0.4027
Stacking method 1	0.8716	0.00016	0.3661
Stacking method 2	0.8735	0.0058	0.3638
Stacking method 3	0.8741	0.0057	0.3623

Finally a one hidden layer MLP with hyperbolic tangent activation function for hidden neurons and linear activation function for the output neuron was used to realize the stacking strategy. In this case a further parameter to be fixed is the number of hidden neurons in the stacking network. Different numbers of MLPs were considered to obtain the vector $\hat{y}_i$ and for each vector a different number of hidden neurons was taken into account in the stacking network. Obtained results are showed in Fig. 5. It is possible to observe that best results were obtained when the outputs of four MLPs were combined by using a stacking network with five hidden neurons for each MLP.

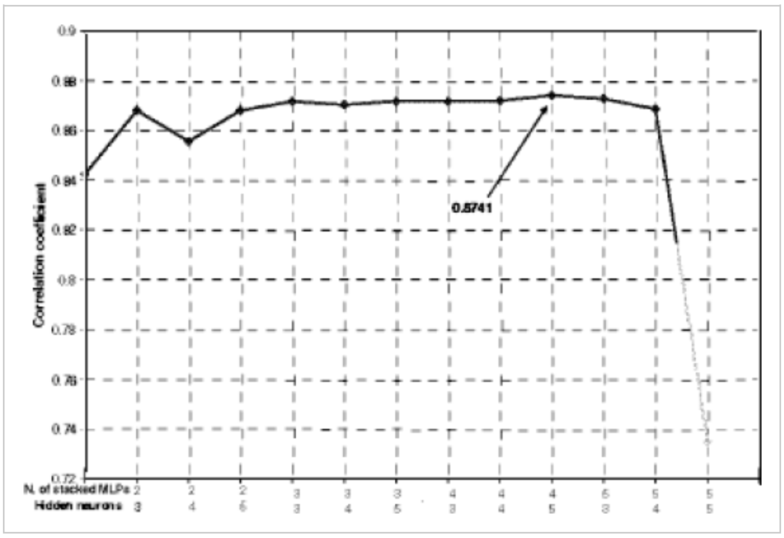


Fig. 5
Correalation coefficient value for stacking method 3 as a function of the number of stacked MLPs and of the number of hidden neurons in the staking neural network. Best results were obtained when the outputs of four MLPs were combined by using a stacking network with five hidden neurons for each MLP.

Result obained by using the described modling strategies are summarized in Tab. I.

For matter of comparison, in the second row of Tab. I are shown the best performances that were obtained by using the linear model (2), while the third row reports results obtained by using a single MLP based nonlinear model. In particular, Tab. I reports the correlation between acquired hidden data and the corresponding RON estimations. Also, both the mean value and the standard hidden deviation of the model residual are reported.

Results reported in Tab I, suggest that best performances were obtained by using stacking strategy 3. For this reason results obtained with this structure are shown in more details. In particular, in

3. For this reason results obtained with this structure are shown in more details. In particular, in Fig. 6a the comparison between octane number and its estimation obtained by using the staking strategy 3, are showed. Also, in Fig 6b, the 4-plot analysis of the residual is showed [14].

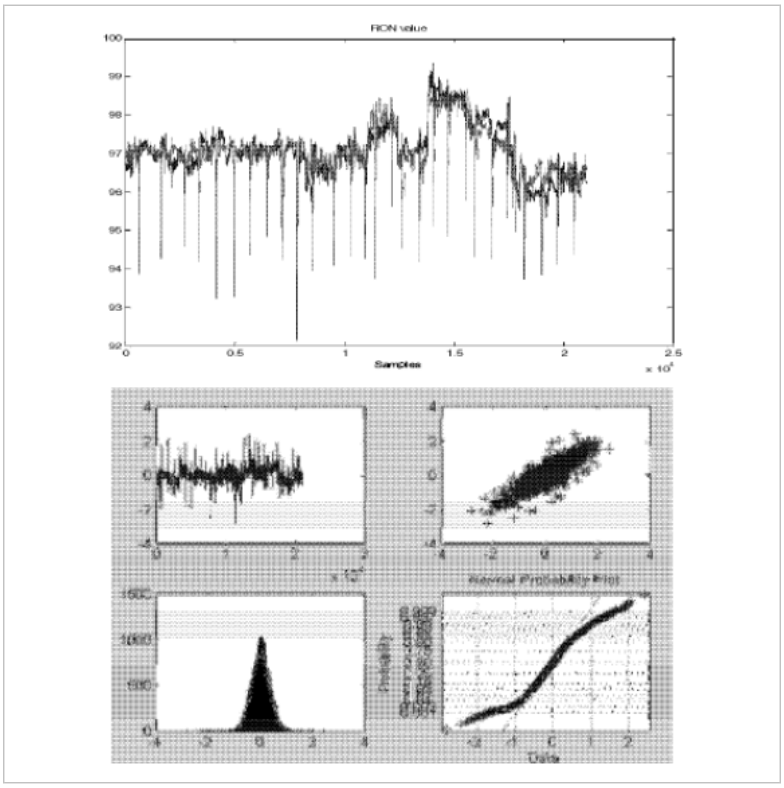


Fig. 6
RON estimation obtained by using the staking strategy 3: a) RON acquired values (solid line) and their estimations (dotted line); b) 4-plot analysis of the model residual.

SECTION VI.
Conclusions

In the paper a virtual instrument, based on stacked neural networks, is proposed for the estimation of the product quality in refineries. In particular the RON value of gasoline produced by a Powerformer Unit is taken into account.

The proposed virtual instrument has been designed in order to be used when instruments generally available for the measurement of RON are temporarily off line for maintenance reasons.

Validation of the proposed approach by using experimental data shows that the proposed virtual instrument over performs both traditional linear data driven models and models based on a single neural network.

ACKNOWLEDGEMENTS

The authors would like to thank Dr. M. Sinatra and Dr. P. De Bartolo at ERG Raffineria Mediterranea s.r.1 (ERGMED), Syracuse, Italy., for their helpful support.

Keywords

IEEE Keywords
Instruments, Neural networks, Intelligent networks, Refining, Petroleum, Hardware, Industrial plants, Particle measurements, Delay estimation, Stacking

INSPEC: Controlled Indexing

virtual instrumentation, chemical variables measurement, computerised monitoring, estimation theory, neural nets, petroleum, petroleum industry

INSPEC: Non-Controlled Indexing
gasoline refineries, virtual instruments, stacked neural networks, product quality monitoring, octane number estimation

Author Keywords
quality coontrol, industrial plants, modeling, neural networks

Authors

L. Fortuna
Università degli Studi di Catania, DIEES, Viale A. Doria 6 95125, Catania
ITALY - tel: +390957382327

P. Giannone
Universita degli Studi di Catania

S. Graziani
Universita degli Studi di Catania

M.G. Xibilia

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