NNARX Model of the PEMFC Used Neural Network Pruning Model Structure

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Abstract—The paper presents a nonlinear modeling of the PEMFC using Neural Network Auto-Regressive model with eXogenous inputs (NNARX) approach. The Multilayer Perception (MLP) network is applied to evaluate the structure of the NNARX model of PEMFC. The NNARX model structure is according to the Optimal Brain Surgeon (OBS) methodology to indicate the significant network structure. The validity and accuracy of NNARX model are tested by one step ahead relating output voltage to input current from measured experimental of PEMFC. The results show that the obtained nonlinear NNARX model based on OBS technique can efficiently approximate the dynamic mode of the PEMFC and model output and system measured output consistently.

Index Terms—PEMFC, NNARX, Optimal Brain Surgeon (OBS), Neural Network (NN)

I. INTRODUCTION

Fuel Cell (FC) technologies development and commercialization motivation is concerned with increasing environment and resource issues. Polymer Electrolyte Membrane Fuel Cell (PEMFC), as a renewable energy source, is one of the most promising fuel cells due to their compact modular, high efficiency and good stability. Because of its advantage, PEMFC is demanded as a dependable power sources for many application such as distributed power generation and automobile [1], [2].

PEMFC is an extremely complex nonlinear multi-input and multi-output and coupled dynamic system. The performance of PEMFC can be represented by a current-voltage relation that is influenced by levels of internal influential parameters such as gas flow channel design, stoichiometric flow rate, and others. All these parameters have strong impacts on PEMFC performance, and are related to each other by nonlinear behaviors. The inner working processes are accompanied with liquid, vapor, gas-mixed transportation, heat conduction and electrochemical dynamic reaction. For such kind of nonlinear system of PEMFC, yet there is no standardized procedure neither to estimate a matching mode structure nor to select a suitable types of models. During the last several decades, various mechanism models of PEMFC, based on mass, energy and momentum conservation laws, has received much attention in an attempt to better understand the phenomena occurring within the cell, and a variety of mechanism models have been established in previous research [3], [4]. In open literatures, these models characteristics focused on FC operating condition such as temperature effects, reaction gas transportation phenomena, heat management, etc. Each parameter with according to the operating conditions will exert different effects to improve the performance and define quantitative determination whether the effects of operating factors are necessary on the PEMFC. These models are very useful for analyzing the transient characteristic, but they are too complicated to be used for control system design.

For the purpose of dynamic control of real system in future work, precise dynamic characteristic model of the PEMFC are necessary. However, no matter what kind of models, there must be some errors between the models and real performance of the PEMFC because assumptions and approximations are made in modeling for computing simplify. In order to improve the accuracy of mechanism models and make the models reflect the actual PEMFC performance better, it is necessary to mode the structure of the models using nonlinear model approach. Most dynamic systems can be better described by nonlinear models, which are able to present the whole behavior of
the system during the all operating condition [5]-[7].
Motivated by this need, an attention has been paid to identification of nonlinear dynamical systems. The nonlinear dynamic systems behavior has made the employ of Artificial Neural Network (ANN) for the modeling task in recent decades [8], [9]. In addition, all the numerical studies have proven the Multilayer Perceptron (MLP) neural networks match very well for nonlinear system identification. In the process of training neural network, the regularization can be generalizing the trained model.

In this work, a nonlinear model approach, consisting of a Neural Network Auto-regressive model with eXogenous inputs (NNARX) approach is adopted to model the nonlinear dynamic of the PEMFC. The paper organized as follows: Section II gives a description of NNARX model approach. Section III presents the results of modeling of PEMFC based on NNARX approach. Section IV is the conclusion. The proposed nonlinear modeling of the PEMFC based NNARX approach procedure is graphically summarized in Fig. 1.

The goal of this work is to optimize a neural network architecture based on multilayer perceptrons by eliminating non-useful weights and bias and to improve its generalization in the performance of PEMFC. To achieve aims we used an algorithm called Optimal Brain Surgeon (OBS) to perform the pruning. The approach to network pruning is based on the information on second order derivatives of the error surface in order to determine the weights or bias that can be removed without performance degradation.

A. **NNARMAX Model**

A general linear system ARX empirical model can be described by the following equation:

\[
A(q^{-1}) y(k) = B(q^{-1}) u(k) + e(k)
\]  

where \(y(k)\) denotes the system output or autoregressive (AR) factor; \(u(k)\) is the system input or exogenous (X) factor, \(e\) is the white noise or disturbance and \(q^{-1}\) is the negative shift operator. The polynomials \(A(q)\) and \(B(q)\) are given by:

\[
A(q) = 1 + a_1 q^{-1} + \cdots + a_{n_a} q^{-n_a} \\
B(q) = b_0 + b_1 q^{-1} + \cdots + b_{n_b} q^{-n_b}
\]  

The model corresponding predictor:

\[
\tilde{y}(k|\theta) = -a_n y(k-1) - \cdots - a_1 y(k-n_s) + b_n u(k-n_x) + \cdots + b_1 u(k-n_x - n_z + 1)
\]  

is thus based regression vector:

\[
\vartheta(k) = [y(k-1), \ldots, y(k-n_s)u(k-n_x), \ldots, u(k-n_x - n_z + 1)]
\]  

where \(n_s\) is number of output poles; \(n_x\) is the number of input zeros and \(n_z\) is the system time delay. In order to estimate the parameter of nonlinear ARX model structure, the NN can be done. The neural network version of ARX model structure is defined as Neural Network ARX (NNARX). The NNARX model structure is presented in the Fig. 2. The relationship between input-output structures of NNARX model can be shown by:

\[
y(k) = g(\vartheta(k), \theta) + e(k)
\]  

- A. **NNARMAX Model**
- B. **NNARX Model**

II. **NEURAL NETWORK AUTO-REGRESSIVE MODEL WITH EXOGENOUS INPUTS (NNARX) MODELING APPROACH**

Modeling is an important issue in the process of parameter estimation. Auto-regressive eXogenous models have been employed extensively to represent the relationship of the system output with the system input in the present of noise in many linear systems. In the process of parameters estimation, the Levenberg-Marquardt (LM) algorithm is usually used in Neural Networks (NN) method. In order to meet a closer approximation to the real system, nonlinear ARX models are used, which are modeled by means of NN. The Multilayer Perceptron (MLP) network is one of the most studied members in the NN. The primary of MLP neural network reason is its ability to model simple as well as complex functional relationships. The LM algorithm minimizes the mean-square error of the prediction errors for the nonlinear ARX model, which is as particular case of a nonlinear Neural Network ARX model (NNARX), as described in after [10]-[13].
The One-Step-Ahead (OSA) prediction of the NNARX model structure is defined by:

\[ \hat{y}(k|\theta) = g[\varphi(k), \theta] \]  

(6)

where \( g \) is the function realized by the multilayer perceptron neural network method.

B. Multilayer Perceptron (MLP) Network

The Multilayer Perceptron (MLP) network is one of most used of the NN family; because of its capable simply represent complex function. The class of MLP NN meted with three layers: an input, an output and hidden layer. In the hidden layer \((j)\) of each neuron, the sums up of input data \( x_i \) after weighting them with strengths of the respective connections \( w_{ij} \) from the input layer and computed output \( y_j \) as a function of the sum:

\[ y_j = f(\sum_{i=1}^{k} w_{ij} x_i) \]  

(7)

where the function \( f() \) can be linear, threshold, sigmoid, hyperbolic tangent and radial basis. In this paper, hyperbolic tangent functions are considered for the neurons in the hidden layer and linear function for the output layer neurons, respectively. The output of the MLP presented:

\[ \hat{y}_j(w, W) = f(\sum_{i=1}^{k} W_{ji} f(\sum_{i=1}^{k} w_{ij} x_i + w_{i0}) + W_{o0}) \]  

(8)

where \( q \) is hidden neurons, \( w_{ij} \) between input and hidden neuron weighting; \( w_{i0} \) between hidden neuron and output weighting and \( m \) is input number. The weighting \( w \) and \( W \) of are the adjustable parameter of the network and determine through the training process. The sets of training inputs data \( u(t) \) and corresponding outputs \( y(t) \) defined:

\[ Z^x = \{[u(k), y(k)] | k = 1, \ldots, N\} \]  

(9)

The goal of training is to meet a mapping from the training data set to the set of possible weights \( Z^x \rightarrow \theta \), so that the network will produce the close to the true outputs \( y(k) \). The prediction error measurement is often described by a function required as the loss function. The general form can be depicted as:

\[ P_n(\theta, Z^x) = \frac{1}{2N} \sum_{i=1}^{N} e^2(x, \theta) \]  

(10)

In (10) is used to simplify differentiation when minimizing residual \( e(k, \theta) = y(k) - \hat{y}(k, \theta) \). \( Z^x \) is mean the training data set. The minimizing solution implements the Levenberg-Marquardt (LM) algorithm, due to its rapid convergence properties and robustness.

C. Optimal Brain Surgeon (OBS)

Parsimonious structures for neural network can be obtained by the process of pruning, that including in deleting insignificant weights and nodes. Once the network is simplified, problems related to overfitting disappear. The basic of the procedure is to estimate the increase in the training error when deleting weights using information in the second-order derivates of the error surface is constructed to evaluate the effect of weight deletion. The change in the cost function, assuming was found. The local minimum is nearly quadratic, can be approximated by [14]-[16]:

\[ \eta_j = \frac{y}{N} e^T H^{-1}(\theta) D \theta + \frac{1}{2} \frac{2}{H} \theta R(\theta) H^{-1}(\theta) e_j \]  

(11)

The method was according to the saliency for weight “\( j \)” is defined by:

\[ \partial P = \frac{1}{2} \partial w^T H \delta w \]  

(12)

where \( \delta w \) is the perturbation applied to the weight vector and \( H \) is the Hessian matrix. Lagrange multiplier can be used to solve the pruning problem:

\[ L = \partial P + \gamma (\varepsilon^T \delta w + w) \]  

(13)

Then, the Lagrange value can be compute optimized with respect to \( \delta w \), subject to the constraint that the jth weight is eliminated, called saliency \( L_j(w) \).

\[ L_j(w) = \frac{1}{2} w_j^2 \]  

(14)

where \( H^{-1} \) is the inverse of the Hessian matrix \( H \), and \( [H^{-1}]_j \) is the jjth element of the inverse matrix. The basis of the OBS is the calculation of the saliencies, that represent the change in training error resulting from the deletion of \( w_j \). Based on the saliencies of its weights, connections into the net are eliminated and all all remaining weights are reestimated. The retraining is done with the Levenberg-Marquardt method keeping the pruned weight equal to zero.

D. Evaluation of the Performance of the Models

The prediction results of the different models studied are presented in terms of Root-Mean-Square Error (RMSE) and absolute fraction of variance (\( R^2 \)) of prediction is define as:

\[ \text{RMSE} = \sqrt{\frac{(\hat{y} - y)^2}{n}} \]  

(15)

\[ R^2 = 1 - \frac{\sum_{i=1}^{N} (\hat{y} - y)^2}{\sum_{i=1}^{N} y^2} \]  

(16)

where \( y \), \( \hat{y} \) and \( n \) are the value of target, output and number of observations, respectively. Clearly, the best score for \( R^2 \) measure is 1 and for other measure is zero.

III. RESULTS AND DISCUSSION

In these work, the identification process was presented by the widespread mathematical software package MATLAB, provided by the MathWorks Inc. [17] The steady output voltage of power source of PEMFC is an
important. PEMFC experimental data was recorded during various step load of current [18], [19]. The data set was then split in two sets, one for training and remaining for validation. The NNARX model lags are the represented as the number of recurrent and previous connection fed back to the input layer. As regressor structure selection is used two past inputs (nb) and two past outputs (na) in this work. The MLP consisted of three layers (input, hidden and output layer). The sigmoid activation function was used in the hidden layer and linear activation function was used in the output layer. The combination of layers and activation functions are able to approximate any continuous functions, provided that they have sufficient hidden units. Fig. 3 shows the un-pruning model validation result, where the measures data is compared to the predicted data. From the results plot, the model output (OSA, One-Step-Ahead) displays over-fitting and not good agreement with the measured output.

<table>
<thead>
<tr>
<th>Net structure</th>
<th>Validation R²</th>
<th>Pruning R²</th>
<th>Validation RMSE</th>
<th>Pruning RMSE</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>0.951</td>
<td>0.903</td>
<td>0.0246</td>
<td>0.034</td>
</tr>
<tr>
<td>4</td>
<td>0.951</td>
<td>0.966</td>
<td>0.0223</td>
<td>0.0204</td>
</tr>
<tr>
<td>5</td>
<td>0.96</td>
<td>0.941</td>
<td>0.0223</td>
<td>0.0271</td>
</tr>
</tbody>
</table>

Using the pruning procedure it was possible to reduce the number of connections in all cases without performance degradation, but no significant improvement in the results was obtained. The evolution of the RMSE and R² in the validation set and pruning procedure in the optimization of the net structure in 4 is shown in Fig. 4.

The plot presented RMSE no little change until 17 connections increase the error sharply. The smaller RMSE in the pruning model was found when just three connections were present and the final net architecture is shown in Fig. 5.

To improve the generalization performance and over-fitting drawback, the OBS to pruning the network structure by eliminating insignificant weights and bias. The results presented in Table I show that the best results were found in net structure 4 and have better performance than other structure.

IV. CONCLUSION

In this paper, the new pruning approach based on Optimal Brain Surgeon (OBS) to determine the nonlinear
modeling structure of PEMFC is applied via Neural Network Auto-regressive model with eXogenous inputs (NNARX) has been proposed. The approach can be applied to determine redundant and insignificant network parameters. From the results of pruning procedure, the OBS algorithm can be efficiently and accurately indicate the optimal size and topology of net structure, and improve the performance of generalization and to avoid network over-fitting. In the future, some process of identification procedure or control scheme can be applied NNARX model based on OBS algorithm.

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REFERENCES

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