

## ESTIMATION OF NO<sub>x</sub> EMISSIONS IN THERMAL POWER PLANTS USING ENG-GENES NEURAL NETWORKS

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**Abstract:** This paper investigates neural network based estimation of NO<sub>x</sub> emissions in a thermal power plant, fed with both oil and methane fuels. Two types of neural network namely a novel 'eng-genes' architecture and a Multilayer Perceptron (MLP) have been developed, both being optimised using genetic algorithms. Due to the local nature of the NO<sub>x</sub> generation process, operational information on the burner cells of the combustion chamber has been considered. Neural networks, with different numbers of hidden nodes have been tested on a set of three-dimensional data of the simulated combustion chamber. It is shown that, the proposed 'eng-genes' neural network can produce accurate estimations with better generalisation performance than MLP.  
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**Keyword:** power generation, pollution, estimation, neural networks, genetic algorithms.

### 1. INTRODUCTION

Nitrogen oxides (NO<sub>x</sub>) emissions, produced by combustors and engines, have harmful effects on both the environment and human health. Strict legislations have been introduced recently in many industrial countries to restrict such pollutant emissions. As a consequence, both theoretical and experimental research has been done to explore various NO<sub>x</sub> emission reduction techniques (Li, Thompson, Wieringa, et al, 2003; Muzio and Quartucy, 1997; et al).

With respect to thermal power plants, technologies may be grouped into two categories, namely combustion modification and post combustion. Advanced operation and control techniques for emission reduction fall into the first category. These techniques control and optimise essential operational parameters to affect the shape of the fireball and the

temperature distribution in the combustion chamber thus reducing the NO<sub>x</sub> formation rate. Detailed measurements of temperature and major reagents concentrations in the combustion chamber are normally used to characterise the NO<sub>x</sub> formation process. However, as these intermediate variables are normally not measurable, NO<sub>x</sub> emissions are often estimated using a model which relates various operational inputs and measurements to the NO<sub>x</sub> emission outputs. A number of models have been studied for different thermal power plants, including coal-fired (Li, Thompson and Peng, 2004), oil-fired (Li and Thompson, 1996), and both oil- and methane fired (Ferretti and Piroddi, 2001).

NO<sub>x</sub> formation is a highly complex process, which can often be described by a set of partial and ordinary differential equations (PDEs and ODEs), based on chemical and physical laws (De Soete, 1975). To estimate NO<sub>x</sub> emissions by solving these

equations needs computational fluid dynamics (CFD) codes in one-, two-, or three- dimensions (Visona and Stanmore, 1996). Given clear boundary conditions, a three-dimensional CFD simulator with fine meshes can produce a solution of nearly 90% accuracy (Stopford, 2002). Generally speaking, the CFD method needs significant computing facility and is quite time-consuming. Therefore it is mainly used in new plant design and optimisation of operational settings, not suitable for real-time plant optimisation and control.

Due to the highly nonlinearity in the combustion process, simple linear models based on the input/output relations are not suitable for plant optimal operation and control (Li, Thompson and Peng, 2004). Nonlinear regression models have been developed so far to improve the model performance as well as the model transparency (Li, Thompson and Peng, 2004), the model complexity has however not been significantly reduced. As universal approximators, artificial neural networks (ANN) such as the Multi-Layer Perceptron (MLP) and radial basis functions (RBF) networks have been widely used in the industry, including application in NO<sub>x</sub> emissions in thermal power plants (Ferretti and Piroddi, 2001). However the neural model transparency has not been addressed and its generalisation performance can not be guaranteed.

In this paper, neural networks based estimation of NO<sub>x</sub> emissions in a thermal power plant fed with both oil and methane fuels, is studied. The focus is on the estimation accuracy, model robustness and model complexity. Two types of neural network - a novel 'eng-genes' neural network and a conventional MLP have been built. An integrated GA-based optimisation platform has been developed for network optimisation (Li, *et al*, 2003). The two networks, with different number of hidden nodes have been tested on a set of three-dimensional data of the simulated combustion chamber. The problem under study here appears to be a good benchmark for NO<sub>x</sub> emission estimation, as essential local information for NO<sub>x</sub> formation in the combustion chamber such as the cell temperature and mass flows of fuel and air for each burner cells, are all available.

The paper is organised as follows. A brief introduction to the novel 'eng-genes' network is given in section 2. The integrated platform for neural network optimisation is discussed next in section 3. Section 4 introduces the NO<sub>x</sub> benchmark problem and gives results on the performance of the two neural network paradigms. Section 5 gives the concluding remarks.

## 2. 'ENG-GENES' NETWORKS

Various types of neural networks, e.g. Multi-layer perceptrons (MLPs), radial basis functions (RBFs),

and wavelet networks have been proposed and widely applied to modelling and control of industrial processes and non-linear dynamic systems. It has been proved that these networks can approximate a wide range of functions to an arbitrary degree of accuracy under certain conditions, based on the Kolmogorov's superposition theorem. However, conventional neural models carry little physical knowledge about the system. Although researches has been done to employ hybrid modelling, where both neural networks and first principle models are used together as complementary components, little has been done so far to incorporate 'a priori' physical knowledge into the neural model to improve its transparency and performance.

The 'Eng-genes' method takes a different approach by extracting some fundamental functions – namely 'eng-genes', from 'a priori' engineering knowledge about the plant, while retaining the neural network structure. These fundamental functions or 'eng-genes' are used as the activation functions in the hidden or output layers. The 'eng-genes' reflect the unique nonlinearity existing in the engineering system and may be regarded as analogous to the genes in the human neural system. It is natural then to construct and code these genes, and their associated structure into appropriate chromosome representations. Given a suitable fitness function, using evolutionary approach such as the genetic algorithm, a population or multiple populations of chromosomes will evolve for a certain number of generations through selection, mutation and reproduction to finally produce a neural model best-fitting the system. This approach is therefore named 'eng-genes' - an abbreviation of 'engineering genes'.

Like the MLP network, the 'eng-genes' network can have more than one-hidden layer, and the simplest one-hidden layer 'eng-genes' network for a multi-input single-output (MISO) system can be formulated as

$$y_k = \theta_0 + \sum_{i=1}^p \theta_i \varphi_i(\mathbf{u}_k; \mathbf{c}_i) \quad (1)$$

where

$$\varphi_i = \begin{cases} \psi_1(\mathbf{u}_k; \mathbf{c}_i), m_0 = 1 < i \leq m_1; \\ \psi_2(\mathbf{u}_k; \mathbf{c}_i), m_1 < i \leq m_2; \\ \vdots \\ \psi_q(\mathbf{u}_k; \mathbf{c}_i), m_{q-1} < i \leq m_q = p \end{cases}$$

are 'eng-genes' or some fundamental functions identifiable from physical and chemical laws for the system under study, ( $m_j - m_{j-1}$ ) is the number of hidden neurons with the same  $j$ th type of 'eng-genes',  $\psi_j, j = 1, \dots, q$  are the activation functions for the neural nodes,  $\mathbf{c}_i$  is the vector of associated parameters (weights and bias) of the  $i$ th neuron,  $\mathbf{u}_k$  is the vector of input to the neural model. Obviously

(1) can be easily extended to networks with multiple layers for multi-input multi-output systems (MIMO).

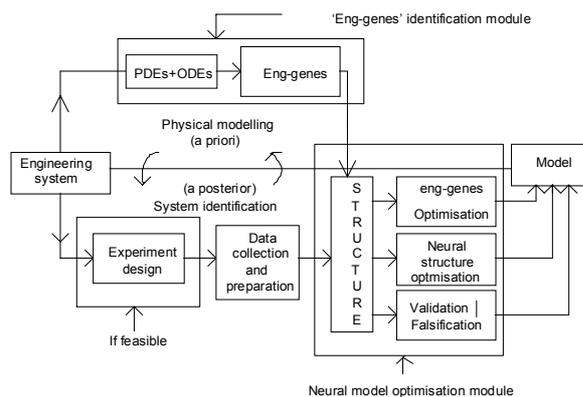


Fig. 1 'Eng-genes' method for nonlinear system modelling

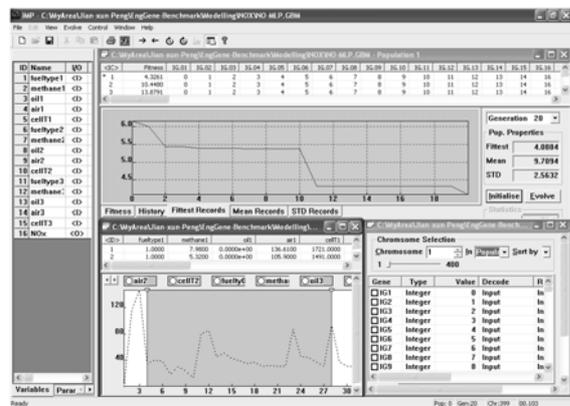


Fig. 2 Screen snapshot of the work space from the optimisation tool for neural modelling

The 'eng-genes' modelling procedure, summarised in Fig. 1, is described as follows:

- Step 1. Establish the fundamental mechanisms of the engineering system. Typically these will consist of a set of first principle laws expressed in ODEs or PDEs.
- Step 2. From these extract fundamental static functions or 'eng-genes'.
- Step 3. Data acquisition and pre-processing, generally through experimental tests or selection from real-time operational data from the plants.
- Step 4. Optimisation of the 'eng-genes' network using genetic algorithms, or for simple applications using LM method for neural training.
- Step 5. Validate the model.

*Remark 1:* The eng-genes are some fundamental static nonlinear functions, such as exponential, polynomial, rational, trigonometry, or Gaussian functions, which are uniquely identifiable from the system first principle laws. Like conventional neural networks, this neural structure can be used for modelling both dynamic and static nonlinear systems.

*Remark 2:* A number of eng-genes may be extracted from first principle laws however, only a few may be predominant while the others can have little impact. The most significant eng-genes will be selected and optimised using genetic algorithms.

### 3. INTEGRATED OPTIMISATION PLATFORM FOR NEURAL NETWORKS

Unlike conventional MLP networks for which the activation functions in all hidden nodes are of the same type, an 'eng-genes' network may have different functions resulting in heterogeneous network. Optimisation of the weights and parameters in the activation functions for the two network paradigms can be quite complex.

The authors have developed user-friendly integrated optimisation C++ software for MLP, RBF and 'eng-genes' networks. In this software, a mixed coding scheme is employed for representing a chromosome. The first half of each chromosome composes integer genes representing the indexes of all hidden nodes in the network structure. The second half composes floating genes representing synaptic weights and parameters to be identified for the integer genes. Advanced techniques for genetic algorithms have been employed to improve the GA performance (Li *et al* 2003). A snapshot of screen from the software package is shown in Fig. 2. The main characteristics of this interactive modelling tool are:

- 1) Flexibility. The user may select any data segment for modelling from a sliding window.
- 2) Visualisation. Different "views" are designed for the network optimization process:
  - Project view: allows the user to access all relevant information and parameters for network construction.
  - Data view: plots and displays training data, and users can select any data segment for network training and validation.
  - GA population view: displays, in graphical or text format, the population/sub-populations and their properties during the evolution process.
  - GA chromosome view: displays a selected chromosome in its decoded form.
  - Validation view: displays the network estimation performance of any chosen chromosome for any data set.
- 3) All GA solutions can be transferred to the Matlab workspace, and the model performance can be reproduced in Matlab workspace.

### 4. NEURAL MODELLING OF NO<sub>x</sub> EMISSIONS

#### 4.1 General description of the thermal power plant

In this study, the 320 MW unit of a power plant of Tavazzano (Italy) is considered (Ferretti and Piroddi, 2001). Nine front burners and nine back burners are

placed on the walls, at three levels, in the lower part of the furnace, allowing combustion of both oil and methane. Recycling gases enter the furnace only at the bottom. The schematic view of the chamber in the front is illustrated in Fig. 3. The whole volume of the combustion chamber, of dimensions  $37.65\text{m} \times 10.1\text{m} \times 10.1\text{m}$ , has been simulated using 4059 cells. This choice represents a trade-off between accuracy and numerical efficiency.

The three-dimensional discretization of the combustion chamber was directly used to compute  $\text{NO}_x$  emissions, while an average over the same ten cells of the early one-dimensional model was considered for the sake of thermal exchange and power generation modelling. Examination of the  $\text{NO}_x$  flow rate fields from the three-dimensional model showed that the fields were quite uniform along the horizontal coordinates and the generation of  $\text{NO}_x$  was limited to the sections containing three burners (3, 4, 5) (Ferretti and Piroddi, 2001). The observation was even more evident when the incremental generation of  $\text{NO}_x$  along the vertical coordinate was examined. This fact can be interpreted as follows (Ferretti and Piroddi 2001) - generation of  $\text{NO}_x$  occurs at the burners, where the highest temperatures are reached, by reaction of the nitrogen contained both in fuel (fuel  $\text{NO}_x$ ) and in air (*thermal* and *prompt*  $\text{NO}_x$ ). Since the temperature rapidly decreases when exiting from the zones of the burners, no new generation of  $\text{NO}_x$  takes place, while the reaction of  $\text{NO}_x$  destruction is equally inhibited. Based on the above analysis of the local  $\text{NO}_x$  generation characteristics, the prediction of  $\text{NO}_x$  generation then can be based on correlations relating  $\text{NO}_x$  flow rate to the external *local* inputs to the burners such as oil, methane and air flow rates and a suitable “mean” temperature.

The three dimensional model of the combustion chamber has been simulated under different conditions, and a comprehensive set of data has been collected. A total of 35 simulation experiments were performed, ranging from a load of 140 MW to a load of 320 MW as follows:

- 11 at different load levels with methane fuel only;
- 14 at different load levels with oil fuel only; and
- 10 in various mixed-fuel combustion situations.

From each simulation experiment, operational data relating to the burner cells has been considered:  $f$  - the fuel type, 1 for oil, 2 for methane;  $w_{f,i}$  and  $w_{a,i}$  inlet flow rates of fuel and air for each cell (kg/s);  $w_{\text{NO}_x,i}$  - the local  $\text{NO}_x$  production rate (g/s);  $T_i$  - aggregated cell temperature (K). The index  $i$  ( $i=1,2,3$ ) refers to the specific burner cell that contributed most significantly to the  $\text{NO}_x$  production. The overall  $\text{NO}_x$  production rate was assumed equal to the sum of the three local production terms in the burner cells.

#### 4.2 Neural network construction and training

In this study all the above-mentioned local inputs to the burner cells and the cell temperatures were used as network inputs to estimate the overall chamber  $\text{NO}_x$  output (see Fig. 4). The data from the 35 simulation experiments was split into two parts, one containing 30 experiments for neural network learning, and the remaining 5 experiments for generalisation testing or validation of the networks. The statistics of the  $\text{NO}_x$  emissions in the training and validation data sets are listed in table 1.

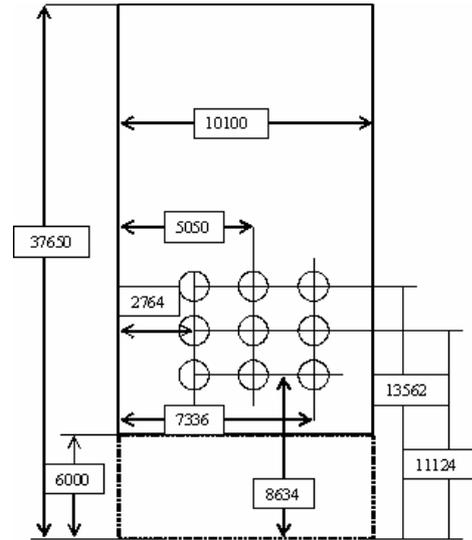


Fig. 3 Schematic view of the chamber in the front (Ferretti and Piroddi, 2001)

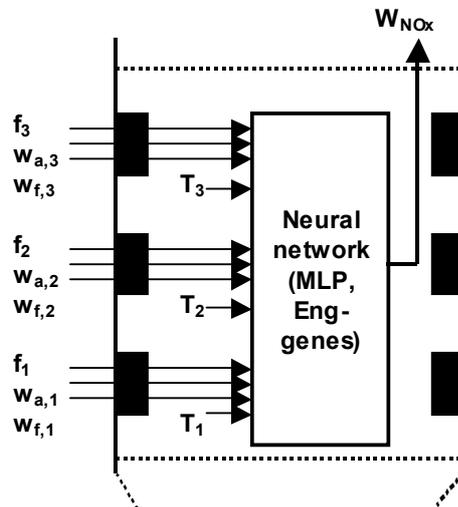


Fig. 4 Neural network structure for chamber learning

Table 1 Statistics of the  $\text{NO}_x$  emissions in the two data sets (g/s)

	Min	Max	Mean	STD
Training	13.49	146.54	48.38	30.07
Validation	25.69	65.91	44.29	15.39

**4.2.1 Eng-genes network optimisation.** The first step in ‘eng-genes’ network construction was to extract the ‘eng-genes’ from the chemical and physical equations for the NO<sub>x</sub> generation. It is understood that three NO species are formed during the combustion process: fuel NO, thermal NO, and prompt NO (De Soete, 1975). Analysis of the formation mechanism of these three NO species (Li, Thompson and Peng, 2004) shows that the generation rates follows both (i) Arrhenius behaviour,  $k = Ae^{(-E_a/RT)}$ , where  $k$  is the reaction rate,  $A$  is a constant,  $E_a$  is the activation energy,  $R$  is the universal gas constant, and  $T$  is the temperature; and (ii) non-Arrhenius behaviour, where the fundamental function in form of  $x^c$  appears in these equations. Therefore, in this work, two static fundamental nonlinear functions or ‘eng-genes’ were used in the network construction -  $\varphi_1 = e^{(c_1/(x+b_1))}$  and  $\varphi_2 = (x+b_2)^{c_2}$ , where  $c_1, b_1, c_2, b_2$  are parameters to be optimised and  $x$  is the extended action potential for the neurons, i.e. the sum of weighted inputs plus bias.

One hidden layer ‘eng-genes’ networks with 5, 10 and 15 hidden nodes were developed. Optimisation of the ‘eng-genes’ networks was performed on the training data set containing 30 experimental tests, and the networks was then used to predict the NO<sub>x</sub> output over another unseen data set containing 5 unused experimental tests. Each network was optimised for 200, 400, and 600 generations. The population size in the genetic algorithms was 400. An elitist scheme was employed in the genetic optimisation and, in each generation, the 8 best chromosomes were retained. The network learning performance and the validation performance of the three ‘eng-genes’ networks, optimised for three different generations, are listed in table 2. Here the RMSE was defined as

$$RMSE = \left( \frac{\sum_{i=1}^N (NO_x(k) - \overline{NO_x(k)})^2}{N} \right)^{\frac{1}{2}} \quad (2)$$

where  $NO_x(k)$  is the measured NO<sub>x</sub>,  $\overline{NO_x}$  the network estimation,  $N$  is size of the data set.

**Table 2 Performance (RMSE) of the ‘eng-genes’ networks**

		200 gen	400 gen	600 gen
5 nodes	Training	1.75	1.25	1.11
	Validation	2.32	1.89	1.70
10 nodes	Training	0.80	0.54	0.47
	Validation	1.58	1.20	1.05
15 nodes	Training	0.46	0.15	0.10
	Validation	1.46	1.70	1.76

**Table 3 Performance (RMSE) of MLP networks**

		200 gen	400 gen	600 gen
5 nodes	Training	1.05	0.837	0.78
	Validation	10.39	11.66	11.75
10 nodes	Training	0.78	0.39	0.30
	Validation	2.78	2.98	2.74
15 nodes	Training	0.27	0.14	0.11
	Validation	3.217	3.47	3.87

**4.2.2 MLP network construction and optimisation.** Similarly, MLP networks with 5, 10 and 15 hidden nodes were also produced using the same learning and validation data sets. The learning performance and the validation performance of the three MLP networks are listed in table 3, when the MLP networks were optimised for 200, 400 and 600 generations separately. From the results in tables 2 and 3, it is clear that both the ‘eng-genes’ and MLP networks are able to produce satisfactory estimation of NO<sub>x</sub> emissions in the thermal plant using only one-layer network with a relatively small number of hidden nodes (between 5 to 15 nodes). Among all the networks listed in tables 2 and 3, the eng-genes network with 10 hidden nodes is able to give the best performance over the validation data set when it is trained for 600 generations (see Fig. 5 and Fig. 6) while keeping fairly satisfactory training accuracy.

Furthermore, the ‘eng-genes’ network is able to give a high accurate estimation of NO<sub>x</sub> output over the training data with a far better generalisation performance over the validation data than the MLP network.

For practical applications, even a simple one-hidden layer eng-genes network with 5 hidden neurons is able to produce satisfactory accuracy of estimation with good generalisation performance.

**Table 4 Performance of the ‘eng-genes’ network with 5 hidden nodes when evolved for 600 generations**

Data set	Max( err )	mean( err )	RMSE
Training	3.436	0.790	1.11
Validation	2.800	1.482	1.70

Table 4 lists the performance of the ‘eng-genes’ network with 5 hidden nodes when it is optimised by a genetic algorithm for 600 generations. In the 5 hidden nodes of the eng-genes network, four have  $\varphi_1$  as the activation function, one uses  $\varphi_2$ . For  $\varphi_1$ , the extended action potential can be regarded as a ‘pseudo’ temperature in the Arrhenius equation for combustion reaction rate. For  $\varphi_2$  the extended action potential can be regarded as a ‘pseudo’ temperature or ‘pseudo’ concentrations of chemical

reagents in non-Arrhenius behaviour of the combustion process for NO<sub>x</sub> production.

#### 4. CONCLUDING REMARKS

In this paper, neural network based estimation of NO<sub>x</sub> emissions in a thermal power plant, fed with both oil and methane fuels, has been studied for real-time plant operation and control. Two types of neural network, namely a Multilayer perceptron (MLP) and a novel 'eng-genes' network, with different numbers of hidden nodes, have been trained and validated on three-dimensional simulation data of the combustion chamber. It has been shown that even simple 'eng-genes' neural networks with a few hidden nodes can produce highly accurate estimations with desired generalisation performance. Moreover, as the two activation functions used in the 'eng-genes' networks are extracted from the fundamental physical and chemical laws for the NO<sub>x</sub> generation mechanisms, it is possible to use the resultant networks to derive some useful operation rules and for the training of the operators.

In this study, cell temperatures, which usually are difficult to obtain in real system, were used to estimate the NO<sub>x</sub> emissions. This was due to the fact that temperature information in the furnace is vital for accurate pollutant estimation. Future work will however explore the potential of 'eng-genes' network in estimating emissions without using cell temperature. The application of the 'eng-genes' network to real-time estimation of NO<sub>x</sub> emission and to plant optimisation and control will also be studied.

#### ACKNOWLEDGEMENTS

Dr K. Li wishes to acknowledge the financial support of the UK Engineering and Physical Sciences Research Council (EPSRC Grant GR/S85191/01).

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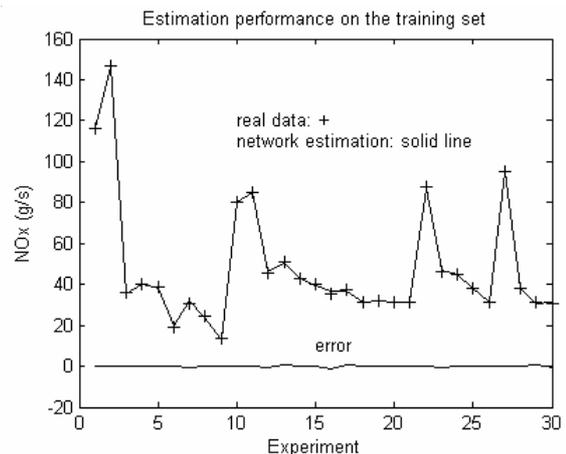


Fig.5. Estimation performance on the training data

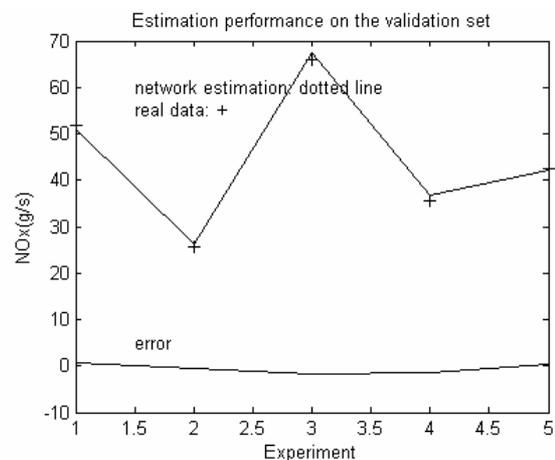


Fig.6. Estimation performance on the validation data