Optimisation on the Least Squares Identification of Dynamical Systems with Application to Hemodynamic Modelling

*Yi Pan, *Ying Zheng, *Sam Harris, †Daniel Coca, *David Johnston, *John Mayhew and †Stephen Billings

Abstract—Dynamic modelling using the traditional least squares method with noisy input/output data can yield biased and sometimes unstable model predictions. This is largely because the cost function employed by the traditional least squares method is based on the one-step-ahead prediction errors. In this paper, the model-predicted-output errors are used in estimating the model parameters. As the cost function is highly nonlinear in terms of the model parameters, the particle swarm optimisation method is used to search for the optimal parameters. We will show that compared with model predictions using the traditional least squares method, the model-predicted-output approach is more robust at dealing with noisy input/output data. The algorithm is applied to identify the dynamic relationship between changes in cerebral blood flow and volume due to evoked changes in neural activity and is shown to produce better predictions than that using the least squares method.

I. INTRODUCTION

The objective of system identification is to find a suitable model to approximate the input/output relationship from a set of observed data. Linear regression models, as a subset of linear-in-parameters models, are an important class of representations for system identification and have been widely used. One important feature of linear regression models is that they are easy to apply, simple to analyze mathematically and to interpret physically. At the centre of the linear regression models is the least squares algorithm. The unknown parameters in the regression model are usually estimated by minimising the sum of squares of errors between the observed and the model predicted responses. The least squares algorithm uses the one-stepahead (OSA) predictions as the model predicted response, and hence the cost function is a quadratic function of the unknown parameter vector and the optimisation can be done with ease.

Unlike the OSA prediction, the model predicted output (MPO) which is generated by the past model predicted output and input data is a more conservative measure of model prediction. It is usually applied in the final stage of the system identification process as an important tool of assessing the performance of the obtained model [3]. Because the cost function based on the MPO errors is highly nonlinear with respect to the unknown model parameters, the MPO method is rarely used for parameter estimation in linear regression models.

*Department of Psychology, Sheffield University, United Kingdom

In the present study, a new parameter estimation method is proposed by minimising a nonlinear cost function based on MPO errors. Model parameters are directly optimised using the particle swarm optimisation [4] method which searches the global optimal parameter estimates over complex parameter spaces for the associated nonlinear cost function. Particle swarm optimisation is a stochastic, populationbased algorithm for solving nonlinear optimisation problems. Compared with other evolutionary computation techniques, particle swarm optimisation has several attractive properties. It has memory, so knowledge of good solutions are retained by all particles. It also has constructive cooperation between particles.

The proposed parameter estimation method is applied to estimate the dynamical relationship between the changes of cerebral blood flow (CBF) and cerebral blood volume (CBV) due to evoked changes in neural activity. The results show that the proposed parameter estimation method based on MPO errors is superior to the least squares estimation based on the OSA errors.

II. MATERIALS AND METHODS

A. Experimental Data

The data presented here are reworked from [6] [10]. The experimental procedures for concurrent measurement of cerebral blood flow (CBF) and volume (CBV) are described in greater detail in [6]. They are briefly reviewed here.

Urethane anesthetised Hooded Lister rats were used (300- 400g). Electrical stimulation of the whisker pad was delivered with intensity 1.2 mA and an individual pulse width of 0.3 ms. The duration of the stimulation is 2s with the stimulus onset at 8s after the start of each trial, with stimulus frequencies 1, 2, 3, 4 and 5Hz. Changes in CBF were measured using laser-Doppler flowmetry, with a sampling rate of 30Hz, while changes in CBV were measured using optical imaging spectroscopy (OIS) with a sampling rate of 7.5Hz. To establish the dynamic coupling between CBF and CBV, we down-sampled CBF to 7.5Hz and used the time series of normalised changes in CBF and CBV defined as

$$
\Delta f = \frac{CBF - CBF_0}{CBF_0}, \Delta v = \frac{CBV - CBV_0}{CBV_0}
$$

where the subscript 0 denotes baseline values. Data were averaged over 5 animals. Fig.1(a) shows the time series of normalised changes in CBF and the accompanying changes in CBV at stimulus frequency of 3Hz. The black bar denotes the onset period of the electrical stimulus. Fig.1(b) shows the same two time series but both normalised to have a maximum

This work was supported by the Engineering and Physical Sciences Research Council (EPSRC), U.K.

[†]Department of Automatic Control and Systems Engineering, Sheffield University, United Kingdom

of unity. This figure demonstrates the well-known feature that the CBF time series returns to baseline much quicker than that of CBV [2] [9].

Fig. 1. Time series of CBF and CBV at stimulus frequency of 3Hz. (a) Normalised changes ∆*f* and ∆*v* ; (b) changes in CBF and CBV normalised to have maximum of unity.

B. Identification Methods

Consider the following linear-in-parameter discrete model for a SISO (Single Input Single Output) dynamical system,

$$
y(t) = \sum_{i=1}^{m} \theta_i f_i(u(t-1),...,y(t-1),...) + \varepsilon(t),
$$
 (1)

where $u(t)$, $y(t)$ are input and output variables respectively, $\varepsilon(t)$ is the additive noise on the output measurements. The model terms $f_i(.)$, $i = 1,...,m$ in (1) can be linear or nonlinear combinations of the input/output variables.

Given an identified model in the form of (1), the corresponding OSA output prediction and errors are defined as below,

$$
y^{(osa)}(t) = \sum_{i=1}^{m} \hat{\theta}_i \hat{f}_i(u(t-1), ..., y(t-1), ...)
$$

\n
$$
e^{(osa)}(t) = y(t) - y^{(osa)}(t)
$$
\n(2)

where $\hat{\theta}_i, \hat{f}_i(.)$, $i = 1,...,m$ denote the estimated parameters and model terms respectively.

Similarly, the corresponding MPO and associated prediction errors in (3) are defined in the following equation.

$$
y^{(mpo)}(t) = \sum_{i=1}^{m} \hat{\theta}_i \hat{f}_i(u(t-1),...,y^{(mpo)}(t-1),...)
$$

\n
$$
e_t^{(mpo)}(t) = y(t) - y^{(mpo)}(t)
$$
\n(3)

Comparing these two definitions given in (2) and (3), it can seen that $y^{(mpo)}(t)$, which is simulated by the past model predicted output $y^{(mpo)}(t-1)$,... and input data is more realistic in assessing the performance of the model prediction capabilities. The OSA predicted output defined in (2), which uses the past output measurements $y(t-1)$,... instead, shows single step prediction capability only.

It is well known that the least-squares estimate of the model parameter θ_i is derived by minimizing the following cost function.

$$
\hat{\theta}_i^{(OSA)} = arg \min_{\theta} \sum_{t} \left(e^{(osa)}(t) \right)^2
$$

$$
= arg \min_{\theta} \sum_{t} \left(y - \sum_{i=1}^{m} \theta_i f_i(u(t-1), ..., y(t-1), ...) \right)^2 \tag{4}
$$

In (4), the OSA prediction error $e^{(\cos a)}(t)$, which is also referred to as the regression error, has a linear relationship with the parameter θ .

It can also be seen from (3) that the MPO error $e^{(mpo)}(t)$ is a nonlinear function of the parameter ^θ. This is illustrated in the following example.

Consider a simple discrete linear system with two parameters *a* and *b*.

$$
y(t) = ay(t-1) + bu(t) + \varepsilon(t), t = 1, 2, ...,
$$
 (5)

When the system is driven by an impulse function $\delta(t)$ as the input, the model predicted output and the corresponding error with the estimated \hat{a} and \hat{b} can be obtained in the following compact form.

$$
y^{(mpo)}(t) = \frac{\hat{b}}{1 - \hat{a}^t}
$$
 (6)

$$
e^{(mpo)}(t) = y(t) - \frac{\hat{b}}{1 - \hat{a}^t}
$$
 (7)

In (7), unlike the OSA error, the MPO error is a nonlinear function of the parameter \hat{a} although the regression model (5) is linear in parameters. As a key criterion of assessing the identified model, the following equation based on the MPO error is much preferred to produce accurate parameter estimates than using the cost function defined in (4).

$$
\hat{\theta}^{(MPO)} = arg \min_{\theta} \sum_{t} \left(e^{(mpo)}(t) \right)^2 \tag{8}
$$

Due to the nonlinear relationship in (7), the estimation of parameter θ_i using the nonlinear cost function (8) becomes a nonlinear optimisation problem. To solve this problem, a nonlinear optimisation method called particle swarm optimisation [4] was used to search for the global optimal values of the associated model parameters.

To illustrate the noise impact on the least squares based parameter estimates, the following simple linear system was simulated.

$$
y(t) = ay(t-1) + by(t-2) + cu(t-1) + du(t-2) + \varepsilon_y(t)
$$

$$
u(t) = 0.5 \exp^{(-0.1t)} sin(10t+1) + \varepsilon_u(t)
$$
 (9)

In (9), $\varepsilon_y(t)$ and $\varepsilon_u(t)$ are Gaussian white noise sequences with zero mean and variances $\sigma_{\varepsilon_v} = 0.007$, $\sigma_{\varepsilon_u} = 0.07$ respectively. The linear discrete model represented by (9) is simulated with model parameters chosen to be $a = 0.6, b =$ $0.2, c = 0.5$ and $d = -0.3$. Three different noise conditions associated with the input and output variables have been simulated. Comparisons of the parameter estimation results produced by least squares and nonlinear optimisation methods are given in Table I. It can be seen from this simple example that the parameter estimates obtained by the least squares method when the input data is corrupted by noise are not affected. However, the parameter estimates given by the least square method are seriously affected by the noise imposed on the output data. This shows that the identification of the linear regression model using the least squares method can be sensitive to the imposed noise although it is purely random white noise. Compared with the least squares estimates given by (4), model parameters estimated by nonlinear optimisation based on the error cost function (8) are significantly better and very close to the true values. This shows that the cost function defined on (8) is much more robust against noise imposed on the input/output data and directly reflects the prediction performance of the identified model.

III. RESULTS

The dynamic relationship between the normalised CBF and CBV is well known to be nonlinear [2][9] [7][16]. However a simple linear dynamic model was shown to be adequate at describing the relationship between the normalised changes in CBF (Δf) and that in CBV (Δv) [13]. Hence the starting point of our haemodynamic model is based on a linear discrete model with the model input as $u(t) = \Delta f(t)$ and the model output as $y(t) = \Delta v(t)$. It is worthwhile noting that both the input and the output are physiological measurements and are subject to physiological as well as measurement noise. After model term selection using orthogonal forward regression [8] [12], the following simple linear model was chosen:

$$
y(t) = a_1y(t-1) + a_2y(t-2) + b_1u(t-1) + b_2u(t-2)
$$
 (10)

The model parameters a_1 , a_2 , b_1 and b_2 were estimated using the OSA methodology (4) and the MPO methodology (8) and the model predicted outputs from both models are superimposed in Fig. 2. It can be seen that the model predicted output based on the MPO nonlinear optimisation method perform significantly better than those based on the least squares estimation using the OSA methodology. Particularly, as shown in Fig. 3(e), the model predicted output generated by the least squares estimation has become unstable.

The estimated model parameters in (10) using the two algorithms are compared in Table II. It can be seen that parameter estimates are different using the different algorithms, but the model prediction is better for the new algorithm which produced an excellent approximation for the observed CBV dynamics.

IV. DISCUSSIONS AND CONCLUSIONS

It has been observed and that the cost function used in the standard least squares method can not fully reflect the key requirements when the data contains noise on both the input and output. In the identification of linear regression models using the least squares method, as shown in the simulated example, the noise in the output can also make the parameter estimates seriously biased. However, this kind of identification problems can be handled by the nonlinear optimisation method, although computational costs are also increased. This proposed modelling approach has been successfully applied to obtain a linear dynamical model for the coupling between changes in CBF and changes in CBV. To fit a linear model to describe the dynamics of CBF changes and accompanying CBV changes without a priori information, the orthogonal forward regression model

Fig. 2. The model predicted Δ v of the identified linear dynamical model based on least squares estimation in response to the CBF changes with electrical stimuli delivered at: (a) 1Hz, (b) 2Hz, (c) 3Hz, (d) 4Hz, (e) 5Hz

selection method was initially applied to determine the linear model structure. In the following identification process, the associated model parameters were optimised based on the nonlinear cost function. Comparisons of model predicted output using the linear-in-parameter cost function and the nonlinear-in-parameter cost function showed the superior performance offered by the latter

V. ACKNOWLEDGMENTS

The authors gratefully acknowledge the supported by the Engineering and Physical Sciences Research Council (EPSRC), U.K.

REFERENCES

- [1] B.M. Ances, E. Zarahn, J. H. Greenberg and J. A. Detre, Coupling of Neural Activation to Blood Flow in the somatosensory cortex of rats is time-intensity separable, but not linear, *Journal of Cerebral Blood Flow & Metabolism*,Vol. 20, 2000, pp. 92
- [2] R.B. Buxton, E.C. Wong and L.R. Frank, Dynamics of blood flow and oxygenation changes during brain activation: the balloon model, *Magnetic Resonance in Medicine*, Vol.39, 1998, pp.855-864.
- [3] S.A. Billings and Q.M. Zhu, Nonlinear model validation using correlation tests, *Int. J. Control*, Vol. 60, 1994, pp. 1107-1120.
- [4] M. Clerc, and J. Kennedy, The Particle Swarm-Explosion, stability, and convergence in a multidimensional complex space, *IEEE Transactions on Evolutionary Computation*, Vol. 6, 2002, 58-73.
- [5] K.J. Friston, A. Mechelli, R. Turner, and C. J. Price, Nonlinear response in fMRI: The balloon model, volterra kernels, and other hemodynamics, *NeuroImage*,Vol. 12, 2000, pp. 466-477.
- [6] M. Jones, J. Berwick, and J. Mayhew, Changes in Blood Flow, Oxygenation, and Volume Following Extended Stimulation of Rodent Barrel Cortex, *Neuroimage*, Vol. 15, 2002, 474-487.
- [7] Y. Kong and Y. Zheng and D. Johnston and J. Martindale and M. Jones and S. A. Billings and J. Mayhew, A Model of the Dynamical Relationship between Blood Flow and Volume Changes During Brain Activation, *Journal of Cerebral Blood Flow & Metabolism*, vol. 24, 2004, pp 1382-1392.
- [8] J. Leontaritis and S. A. Billings, Model selection and validation methods for non-linear systems. *International Journal of Control*, Vol.45, 1987, pp. 311-341.

TABLE I

MODEL PARAMETERS IN (9) ESTIMATED BY THE LEAST SQUARES AND NONLINEAR OPTIMISATION METHODS UNDER DIFFERENT NOISE CONDITIONS.

noise conditions	Input noise			Output noise			Input and output noise		
parameters	Val	OSA	MPO	Val	OSA	MPO	Val	OSA	MPO
a	0.60	0.60	0.60	0.60	0.31	0.65	0.60	0.39	0.55
	0.20	0.20	0.20	0.20	0.23	0.17	0.20	0.22	0.21
c	0.50	0.50	0.50	0.50	0.51	0.50	0.50	0.50	-0.50
	-0.30	-0.30	-0.30	-0.30	-0.19	-0.31	-0.30	-0.21	-0.29

TABLE II MODEL PARAMETERS IN (10) ESTIMATED BY LEAST SQUARES AND NONLINEAR OPTIMISATION METHODS WITH ELECTRICAL STIMULI DELIVERED AT 1HZ, 2HZ, 3HZ, 4HZ, 5HZ

- [9] J.B. Mandeville, J.J. Marota, C. Ayata, G. Zaharchuk, M.A. Moskowitz, B.R. Rosen and R.M. Weisskoff, Evidence of a Cerebrovascular Post-arteriole Windkessel with Delayed Compliance, *Journal of Cerebral Blood Flow & Metabolism*,Vol. 19, 1999, pp. 679-689.
- [10] J. Martindale, J. Mayhew, J. Berwick, M. Jones, C. Martin, D. Johnston, P. Redgrave and Y. Zheng, The Hemodynamic Impulse Response to a Single Neural Event, *Journal of Cerebral Blood Flow & Metabolism* Vol. 23, 2003, 546-555.
- [11] T. Rasmussen, N.H. Holstein-Rathlou and M. Lauritzen, Modelling neuro-vascular coupling in rat cerebellum: Characterization of Deviations from Linearity,*NeuroImage*,Vol. xx, 2009, pp. xxx-xxx. 1-930.
- [12] H. L. Wei and S. A. Billings and J. Liu, Term and variable selection for non-linear system identification. *International Journal of Control*, Vol. 77, 2004, pp. 86-110.
- [13] H.L. Wei and Y. Zheng and Y. Pan and D. Coca and L. M. Li and J. Mayhew and S. A. Billings, Model Estimation of Cerebral Hemodynamics Between Blood Flow and Volume Changes: A Data-Based Modelling Approach, *IEEE Trans. Biomedical and Engineering*,Vol. 56, 2009, pp. 1606-1616.
- [14] Y. Zheng and J. Martindale and D. Johnston and M. Jones and J. Berwick and J. Mayhew, A Model of the Hemodynamic Response and Oxygen Delivery to Brain, *NeuroImage*, vol. 16, 2002, 617-637.
- [15] Y. Zheng and D. Johnston and J. Berwick and D. Chen and S. Billings and J. Mayhew, A Three-compartment Model of the Hemodynamica Response and Oxygen Delivery to Brain, *NeuroImage*, vol. 28, 2005, 925-939.
- [16] Y. Zheng and J. Mayhew, A time-invariant visco-elastic windkessel model relating blood flow and blood volume, *NeuroImage*, *in press*.