Improved Model Identification for Nonlinear Systems Using A Random Subsampling and Multifold Modelling (RSMM) Approach

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Abstract: In nonlinear system identification, the available observed data are conventionally partitioned into two parts: the training data that are used for model identification and the test data that are used for model performance testing. This sort of 'hold-out' or 'split-sample' data partitioning method is convenient and the associated model identification procedure is in general easy to implement. The resultant model obtained from such a once-partitioned single training dataset, however, may occasionally lack robustness and generalization to represent future unseen data, because the performance of the identified model may be highly dependent on how the data partition is made. To overcome the drawback of the hold-out data partitioning method, this study presents a new random subsampling and multifold modelling (RSMM) approach to produce less biased or preferably unbiased models. The basic idea and the associated procedure are as follows. Firstly, generate K training datasets (and also K validation datasets), using a K-fold random subsampling method. Secondly, detect significant model terms and identify a common model structure that fits all the K datasets using a new proposed common model selection approach, called the multiple orthogonal search algorithm. Finally, estimate and refine the model parameters for the identified common-structured model using a multifold parameter estimation method. The proposed method can produce robust models with better generalization performance.

Keywords: Cross-validation, model structure/subset selection, nonlinear system identification, parameter estimation, random resampling, split-sample.

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1. Introduction

A mathematical model of a nonlinear dynamical system is usually defined by two properties: the model structure and the associated model parameters. The central task in any nonlinear system identification task is to construct, based on available observations, a suitable model structure using some specified elementary building blocks, and then to calculate the associated model parameters using some linear or nonlinear parameter estimation algorithm. Take the commonly used linear-in-the-parameters regression modelling problem as an example, where a linear regression model is employed to describe the underlying system, and where candidate model terms or regressors are formed by some linear or nonlinear combinations of lagged input and output variables. The initial full regression model may be very complex and will typically include a great number of candidate model terms and some efficient model structure selection procedures, using either the best subset or stepwise search methods, will need to be performed to determine which model terms are important and should be included in the model. The forward stepwise regression method, especially the well known orthogonal forward regression (OFR) type methods (Billings et al. 1989b, Chen et al. 1989), have been widely employed in recent years for model structure identification of nonlinear dynamical systems (Leontaritis and Billins 1987, Billings et al. 1989a, Billings and Chen 1989, Chen et al. 1992, Zhu and Billings 1993, 1996, Billings and Zhu 1994, Aguirre and Billings 1994, 1995a, b, Chen et al. 1996, Billings and Chen 1998, Correa et al. 2000, Harris et al. 2002, Hong et al. 2003a,b,c, Wei et al. 2004, Tsang and Chan 2006, Truong et al. 2007).

Conventionally, the available observational dataset is often partitioned into two parts: the training data that are used for model identification including parameter estimation, and the test data that are used for model performance testing. The main advantage of this sort of 'hold-out' or 'split-sample' data partitioning method is that it is convenient and the associated model identification procedure is in general easy to implement. Notice, however, that the division of the training and test data using the 'hold-out' method, for model identification, may sometimes be subjective and models produced by the once-partitioned single training dataset may occasionally be biased, because the identified model structure and the estimated model parameters can be highly dependent on how the given dataset was partitioned. The most useful approach, to overcome the drawbacks of the hold-out method for nonlinear dynamical modelling, is to introduce cross-validation, which has been extensively applied in conventional linear regression and related models (Allen 1974, Stone 1974, Golub et al. 1979, Shao 1993), into the model identification procedures (Stoica et al. 1986, Ljung 1987). In fact, leave-one-out (LOO) cross-validation has been introduced for model parameter estimation of nonlinear regression models (Hansen and Larsen 1996, Myles et al. 1997, Monari and Dreyfus 2002) and for model construction of linear-in-the-parameters regression models for nonlinear dynamical systems (Hong et al. 2003a, b, c, Chen et al. 2004). It has been shown that by incorporating the LOO cross-validation in the OFR procedure, the resultant algorithms can often produce efficient sparse models for nonlinear

identification problems using the linear-in-the-parameters regression form of models (Chen et al. 2004). Recent applications of the forward or backward orthogonal selection algorithms, assisted by the LOO criterion, can be found in Truong et al. (2007) and Hong and Mitchell (2007). A variation of the conventional LOO criterion for model subset selection of nonlinear systems can be found in Billings and Wei (2007). An attractive advantage of LOO for dealing with linear least squares problems is that, a closed form solution is available to calculate the associated LOO criterion from the results of a single least-squares fit to all training samples.

It has been shown that although LOO cross-validation produces almost unbiased estimates for the expected generalisation error (Stone 1974, Efron and Tibshirani 1993), the associated variance may be very large (Efron 1983, Breiman 1996). Another drawback of the LOO cross-validation is that it is unstable with respect to small perturbations in the data, that is, a slight data perturbation may lead to a drastic change in the resultant regression models (Breiman 1996). Furthermore, LOO cross-validation also has some more subtle deficiencies in model subset selection. For example, it has been shown (Shao 1997) that for linear regression models, LOO is asymptotically equivalent to the AIC and Mallow's C_p criteria; however, leave-v-out cross-validation, is asymptotically equivalent to Schwarz's Bayesian information criterion (BIC), for some specifically chosen v. It is known that, with the same subset selection procedure, the number of model regressors chosen by using the AIC criterion is always greater than that chosen by using the BIC criterion. Results from numerous simulations have shown that while AIC tends to produce badly overfitted models with a small number of training samples, BIC can still work well (Hurvich and Tsai 1989, Shao and Tu 1995). This suggests that leave-v-out cross-validation, with some appropriately chosen values for v, should provide better results, for linear regression models. In fact, Breiman and Spector (1992) found that, for subset selection and evaluation in linear regression modeling, leaving out 10% to 20% of the data gave better results than LOO.

With the aforementioned observations and keeping in mind that prediction accuracy is often the 'gold standard' for model identification, this study aims to present a new random subsampling and multifold modelling (RSMM) approach to produce robust models with better generalization properties. The implementation of the RSMM method consists of three stages. The first stage involves data resampling, which is quite similar to K-fold random cross-validation. At this stage, K training datasets are independently generated; each dataset contains a certain number of data points that are randomly selected from a specified dataset. Corresponding to each training dataset, a validation dataset can be obtained by removing the training data points from the whole measured dataset. The second stage involves the detection of common significant model terms and the identification of a common model structure that fits all the K datasets. A new common model selection approach, called multiple orthogonal search (MOS) algorithm, is proposed to achieve the target of this stage. The objective of the third stage is to refine the associated model, by applying a multifold parameter estimation approach to the identified common-structured model, to produce some improved estimates of the

model parameters.

The paper is organised as follows: In section 2, the linear-in-the-parameters regression model is briefly presented. In section 3, the three stages are presented in detail. Some examples are provided in section 4, to demonstrate how well the new proposed RSMM approach works on model identification of nonlinear systems. The paper ends with summary in section 5, where some comments are given.

2. The Linear-In-The-Parameters Model

Consider the identification problem for nonlinear systems given N_0 pairs of input-output observations, $\{(u(t), y(t)) : t = 1, 2, \cdots, N_0\}$, where $u(t)$ and $y(t)$ are the observations of the system input and output, respectively. The relationship between the input and the output of a wide class of nonlinear systems can formally be described using the NARX (Nonlinear AutoRegressive with eXogenous inputs) model below (Leontaritis and Billings 1985, Pearson 1995, 1999, Ljung 2001)

$$y(t) = f(y(t-1), \cdots, y(t-n_y), u(t), \cdots, u(t-n_u)) + e(t) \tag{1}$$

where f is some nonlinear function, n_u and n_y are the maximum lags in the input and output, respectively, and $e(t)$ is an independent identical distributed noise sequence.

The function f is in general unknown and needs to be identified from given observations of the system. The task of system identification is thus to find, from the given data, a nonlinear approximator $\hat{f}$ that can represent the true (but unknown) function f. Generally, the identified model should not only fit the observed data accurately, but also possess good generalization properties, meaning that the model is capable of capturing the underlying system dynamics, so that the model can be used for simulation, prediction, and control. One commonly used approach, for effectively reconstructing the nonlinear function f, is to construct a nonlinear approximator $\hat{f}$ using some specific types of basis functions including polynomials, radial basis functions, kernel functions, splines and wavelets (Leontaritis and Billings 1987, Chen and Billings 1992, Brown and Harris 1994, Murray-Smith and Johansen 1997, Cherkassky and Mulier 1998, Liu 2001, Harris et al. 2002, Wei and Billings 2004, Billings and Wei 2005a). More often, models constructed using these methods can easily be converted into a linear-in-the-parameters form, which is an important class of representations for nonlinear system identification, because compared to nonlinear-in-the-parameters models, linear-in-the-parameters models are simpler to analyze mathematically and quicker to compute numerically.

Let $d = n_y + n_u$ and $\mathbf{x}(t) = [x_1(t), x_2(t), \cdots, x_d(t)]^T$ with

$$x_k(t) = \begin{cases} y(t-k) & 1 \le k \le n_y \\ u(t-(k-n_y)) & n_y + 1 \le k \le d \end{cases} \tag{2}$$

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A general form of the linear-in-the-parameters regression model is given as

$$y(t) = \hat{f}(\mathbf{x}(t)) = \sum_{m=1}^{M} \theta_m \phi_m(t) + e(t) = \boldsymbol{\varphi}^T(t)\boldsymbol{\theta} + e(t) \tag{3}$$

where M is the total number of candidate regressors, $\phi_m(t) = \phi_m(\mathbf{x}(t))$ ($m=1,2, \ldots, M$) are the model terms generated, in some specified way, by the elements of the 'input' (predictor) vector $\mathbf{x}(t)$, θ_m are model parameters, and $\boldsymbol{\varphi}(t) = [\phi_1(\mathbf{x}(t)), \cdots, \phi_M(\mathbf{x}(t))]^T$ and $\boldsymbol{\theta}$ are the associated regressor and parameter vectors, respectively. Notice that in most cases the initial full regression equation (3) might be highly redundant, some of the regressors or model terms can thus be removed from the initial regression equation without any effect on the predictive capability of the model, and this elimination of the redundant regressors usually improves the model performance. Generally, only a relative small number of model terms need to be included in the regression model for most nonlinear dynamical system identification problems. An efficient model term selection algorithm is thus highly desirable to detect and select the most significant regressors.

3. The Random Subsampling and Multifold Modelling Approach

The random subsampling and multifold modelling (RSMM) approach consists of three steps: random subsampling, common model structure identification and model parameter estimation.

3.1 Random subsampling

Random resampling methods, including cross-validation, bootstrapping and jackkniffing (Devijver and Kittler 1982, Efron and Gong 1983, Efron and Tibshirani 1993), have been widely applied for data analysis and nonparametric modelling tasks. This study, however, employs a K-fold random subsampling method to generate, from a set of chronologically recorded observations, a number of training and validation datasets, which are to be used for model identification including parameter estimation of nonlinear systems.

Consider the model identification problem for a nonlinear dynamical system, where N_0 pairs of observations, $\{(\mathbf{x}(t), y(t)) : t = 1, 2, \cdots, N_0\}$, are available. Following the conventional routine of the 'hold-out' method, the N_0 data pairs are first split into two parts: the training dataset consisting of the first N data pairs, and the test dataset consisting of the remaining $N_0 - N$ data pairs. Let $B = \{\xi_t : t = 1, 2, \cdots, N\}$ and $T = \{\xi_t : t = N+1, \cdots, N_0\}$, where $\xi_t = (\mathbf{x}(t), y(t))$ is the t-th sample (observation pair). Following the idea of conventional cross-validation, samples in the dataset B can be resampled as follows:

- K-fold cross-validation. The dataset B is split, along the coordination of the sampling index t, into K subsets, with roughly equal data length (number of samples). The hold-out method is then repeated K times, and at each time, one of the K subsets is used as a validation set and the other

K-1 subsets are used as a training set.

- *K*-fold random subsampling. The dataset *B* is randomly partitioned into *K* different subsets; each subset contains a certain number of samples that are randomly selected (without replacement) from *B*. Each of the *K* subsets is successively used as a validation set.

Note that the two *K*-fold resampling methods above are slightly different in detail in that the splitting in the first case works on ordered data, while in the second case it works on randomly permuted data. Although from a statistical point of view these two sampling methods are equivalent, it is important to distinguish these two cases when the data comes from a dynamical system because the order of the samples is important for dynamical signals. This study considers the *K*-fold random subsampling method, which is implemented as below.

- Step 1. Let $\Gamma_0 = \{1,2,\cdots,N\}$ and $\Gamma = \{i : i \in \Gamma_0\}$ be a random permutation of Γ_0. Divide the index set Γ into *K* different parts, $\Gamma_1, \Gamma_2, \cdots, \Gamma_K$, where each part is roughly with the same size.

- Step 2. Let $V_k = \{\xi_t : \xi_t \in B, t \in \Gamma_k\}$ and $B_k = B \setminus V_k = \{\xi_t : \xi_t \in B, t \in \Gamma \setminus \Gamma_k\}$, with *k*=1,2, …,*K*. Each B_k is used as a training set and each V_k is used as a validation set.

For the given N_0 pairs of samples $\{\xi_t = (\mathbf{x}(t), y(t)) : t = 1,2,\cdots,N_0\}$, both the associated training dataset $B = \{\xi_t : t = 1,2,\cdots,N\}$ and the *K* training sets $B_1, B_2, \cdots, B_K$, along with the *K* validation sets $V_1, V_2, \cdots, V_K$, will be used to identify an appropriate regression model of the form (3) for the relevant dynamical system. This will be achieved with a new multiple orthogonal search algorithm (MOS) below.

3.2 The multiple orthogonal search algorithm for model selection

From the above discussion, it is known that all the datasets $B_1, B_2, \cdots, B_K$ and $V_1, V_2, \cdots, V_K$ come from the same dynamical system. These datasets should thus share, in theory, the same model structure, as well as the same model parameters. At the moment, however, the common model structure is not yet known and needs to be identified from these given datasets.

Let the number of samples in the training dataset B_k be N_k, and denote these N_k samples by $\{\xi_{k,t} = (\mathbf{x}_k(t), y_k(t)) : \xi_{k,t} \in B_k, \quad t = 1,2,\cdots,N_k\}$. The objective is to identify a common-structured sparse model, for the given system, from the following multiple regressions

$$y_k(t) = \sum_{m=1}^{M} \theta_{k,m} \phi_m(\mathbf{x}_k(t)) + e_k(t) = \sum_{m=1}^{M} \theta_{k,m} \phi_{k,m}(t) + e_k(t) \tag{4}$$

where $\phi_{k,m}(t) = \phi_m(\mathbf{x}_k(t))$, with *k*=1,2, …, *K*, *m*=1,2, …, *M*, and *t*=1,2, …, N_k. These equations can be expressed using a compact matrix form below

$$\mathbf{y}_k = \Phi_k \boldsymbol{\theta}_k + \mathbf{e}_k \tag{5}$$

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where $\mathbf{y}_k = [y_k(1), \cdots, y_k(N_k)]^T$, $\boldsymbol{\theta}_k = [\theta_{k,1}, \cdots, \theta_{k,M}]^T$, $\mathbf{e}_k = [e_k(1), \cdots, e_k(N_k)]^T$, and $\Phi_k = [\boldsymbol{\varphi}_{k,1}, \cdots, \boldsymbol{\varphi}_{k,M}]$ with $\boldsymbol{\varphi}_{k,m} = [\phi_{k,m}(1), \cdots, \phi_{k,m}(N_k)]^T$ for $k=1,2, \ldots, K$ and $m=1,2,\ldots, M$.

3.2.1 Multiple orthogonal search (MOS) for model term selection

The multiple orthogonal search (MOS) method, which can be considered as an extension of the well known orthogonal forward regression (OFR) type algorithms (Billings et al. 1989, Chen et al. 1989), is developed to select a common-structured sparse model from the multiple regressions given by (4) and (5). Let $I = \{1,2,\cdots,M\}$, and denote by $D = \{\phi_m : m \in I\}$ the dictionary of candidate model terms. For the kth training dataset B_k, the dictionary D can be used to form a dual dictionary $\mathrm{D}_k = \{\boldsymbol{\varphi}_{k,m} : m \in I\}$, where the mth candidate basis vector $\boldsymbol{\varphi}_{k,m}$ is formed by the mth candidate model term $\phi_m \in D$, in the sense that $\boldsymbol{\varphi}_{k,m} = [\phi_m(\mathbf{x}_k(1)), \cdots, \phi_m(\mathbf{x}_k(N_k))]^T$ ($k=1,2, \ldots, K$). The common model term selection problem is equivalent to finding, from the dictionary $D = \{\phi_m : m \in I\}$, a subset $\{\phi_{s_1}, \phi_{s_2}, \cdots, \phi_{s_n}\} \subset D$ (generally $n << M$), so that $\mathbf{y}_k$ ($k=1,2, \ldots, K$) can be satisfactorily approximated using a linear combination of $\{\boldsymbol{\varphi}_{k,s_1}, \boldsymbol{\varphi}_{k,s_2}, \cdots, \boldsymbol{\varphi}_{k,s_n}\} \subset \mathrm{D}_k$ as

$$\mathbf{y}_k = \theta_{k,1}\boldsymbol{\varphi}_{k,s_1} + \cdots + \theta_{k,n}\boldsymbol{\varphi}_{k,s_n} + \mathbf{e}_k \tag{6}$$

The MOS algorithm selects significant model terms in a forward stepwise way, one model term at each search step. Initially, let $\mathbf{r}_{k,0} = \mathbf{y}_k$ ($k=1,2, \ldots, K$). For $k=1,2, \ldots, K$ and $j=1,2, \ldots, M$, calculate

$$\mathrm{err}^{(1)}(k, j) = |\cos(\mathbf{y}_k, \boldsymbol{\varphi}_{k,j})|^2 = \frac{(\mathbf{y}_k^T \boldsymbol{\varphi}_{k,j})^2}{(\mathbf{y}_k^T \mathbf{y}_k)(\boldsymbol{\varphi}_{k,j}^T \boldsymbol{\varphi}_{k,j})} \tag{7}$$

and define

$$s_1 = \arg\max_{1 \le j \le M} \left\{ \frac{1}{K} \sum_{k=1}^{K} \mathrm{err}^{(1)}(k, j) \right\} \tag{8}$$

Notice that $\mathrm{err}^{(1)}(k, j)$, as the squared cosine of the angle between the involved vectors $\mathbf{y}_k$ and $\boldsymbol{\varphi}_{k,j}$, provides a measurement of the similarity between the associated vectors, and can be used to measure the correlation dependence of $\mathbf{y}_k$ on $\boldsymbol{\varphi}_{k,j}$. The most significant common vectors, with respect to all the designed signals $\mathbf{y}_k$ ($k=1,2, \ldots, K$), can be determined by maximising (8). Notice also that $\mathrm{err}^{(1)}(k, j)$ can be explained as the error reduction ratio (ERR) that is introduced by including the mth basis vector $\boldsymbol{\alpha}_{k,m} = \boldsymbol{\varphi}_{k,s_m}$ into the kth regression model; see Billings et al. (1989) and Chen et al. (1989)

for a detailed explanation of ERR. From (7) and (8), the first significant common model term can be selected as the s_1th element, ϕ_{s_1}, in the dictionary D. Accordingly, the first significant basis vector for the kth regression model is thus $\boldsymbol{\alpha}_{k,1} = \boldsymbol{\varphi}_{k,s_1}$, and the associated orthogonal basis vector can be chosen as $\mathbf{q}_{k,1} = \boldsymbol{\varphi}_{k,s_1}$. The model residual for the kth regression model, related to the first step search, is given as

$$\mathbf{r}_{k,1} = \mathbf{r}_{k,0} - \frac{\mathbf{y}_k^T \mathbf{q}_{k,1}}{\mathbf{q}_{k,1}^T \mathbf{q}_{k,1}} \mathbf{q}_{k,1} \tag{9}$$

In general, the mth significant model term ϕ_{s_m} can be chosen as follows. Assume that at the $(m-1)$th step, $(m-1)$ significant model terms, $\phi_1, \phi_2 \cdots, \phi_{m-1}$, have been selected. Let $\boldsymbol{\alpha}_{k,1}, \boldsymbol{\alpha}_{k,2}, \cdots, \boldsymbol{\alpha}_{k,m-1}$ be the associated basis vectors for the kth regression model, and assume that the $(m-1)$ selected bases have been transformed into a new set of orthogonal vectors $\mathbf{q}_{k,1}, \mathbf{q}_{k,2}, \cdots, \mathbf{q}_{k,m-1}$ via a standard Gram–Schmidt orthogonal transformation. Let

$$\mathbf{p}_{k,j}^{(m)} = \boldsymbol{\varphi}_{k,j} - \sum_{s=1}^{m-1} \frac{\boldsymbol{\varphi}_{k,j}^T \mathbf{q}_{k,s}}{\mathbf{q}_{k,s}^T \mathbf{q}_{k,s}} \mathbf{q}_{k,s} \, , \; j \in J_m \tag{10}$$

where $J_m = \{j : 1 \le j \le M, j \ne s_t, 1 \le t \le m-1\}$. For $k=1,2,\ldots,K$ and $j \in J_m$, calculate

$$\mathrm{err}^{(m)}(k,j) = |\cos(\mathbf{y}_k, \mathbf{p}_{k,j}^{(m)})|^2 = \frac{(\mathbf{y}_k^T \mathbf{p}_{k,j}^{(m)})^2}{(\mathbf{y}_k^T \mathbf{y}_k)[(\mathbf{p}_{k,j}^{(m)})^T \mathbf{p}_{k,j}^{(m)}]} \tag{11}$$

and define

$$s_m = \arg\max_{1 \le j \le M} \left\{ \frac{1}{K} \sum_{k=1}^{K} \mathrm{err}^{(m)}(k,j) \right\} \tag{12}$$

Similar to $\mathrm{err}^{(1)}(k,j)$ given by (7), $\mathrm{err}^{(m)}(k,j)$ here provides an indicator to show the correlation dependence of $\mathbf{y}_k$ on $\mathbf{p}_{k,j}^{(m)}$, and the most significant common vectors can be determined by maximising (12). The mth significant common model term can then be selected as the s_mth element, ϕ_{s_m}, in the dictionary D. Accordingly, the mth significant basis vector for the kth regression model is thus $\boldsymbol{\alpha}_{k,m} = \boldsymbol{\varphi}_{k,s_m}$, and the associated orthogonal basis vector can be chosen as $\mathbf{q}_{k,m} = \mathbf{p}_{k,s_m}^{(m)}$. The model residual for the kth regression model, related to the mth step search, is given as

$$\mathbf{r}_{k,m} = \mathbf{r}_{k,m-1} - \frac{\mathbf{y}_k^T \mathbf{q}_{k,m}}{\mathbf{q}_{k,m}^T \mathbf{q}_{k,m}} \mathbf{q}_{k,m} \tag{13}$$

Notice that $\mathrm{err}^{(m)}(k,s_m)$ can be explained as the error reduction ratio (ERR) (Billings et al. 1989, Chen et al. 1989) that is introduced by including the mth basis vector $\boldsymbol{\alpha}_{k,m}=\boldsymbol{\varphi}_{k,s_m}$ into the kth regression model. The criterion (12), by maximizing the sum of the ERR values, relative to all the K data sets, guarantees that the variation of the outputs in all the K data sets can be explained by including the model term ϕ_{s_m}, with the highest percentage, compared with selecting any other candidate model term $\phi \in D = \{\phi_m : m \in I\}$. The quantity

$$\mathrm{AERR}(m) = (1/K)\sum_{k=1}^{K}\mathrm{err}^{(m)}(k,s_m) \tag{14}$$

is referred to as the mth average (or overall) error reduction ratio (AERR).

Subsequent significant vectors can be selected in the same way step by step. Once the first (m-1) basis vectors $\boldsymbol{\alpha}_{k,1},\boldsymbol{\alpha}_{k,2},\cdots,\boldsymbol{\alpha}_{k,m-1}$ (respectively the associated orthogonalized vectors $\mathbf{q}_{k,1},\mathbf{q}_{k,2},\cdots,\mathbf{q}_{k,m-1}$) have been determined, then these (m-1) vectors together with the mth vector $\boldsymbol{\alpha}_{k,m}=\boldsymbol{\varphi}_{k,s_m}$ (respectively the orthogonalized vector $\mathbf{q}_{k,m}=\mathbf{p}_{k,s_m}^{(m)}$) , can explain the variation in the outputs of the K data sets with a higher percentage than by including any other candidate vectors. This step-by-step forward selection algorithm is a non-exhaustive search method, and may not always produce the global optimal solution. For most problems, however, this algorithm usually produces satisfactory and nearly optimal results.

From the above orthogonal procedure, it is known that the vectors $\mathbf{r}_{k,m}$ and $\mathbf{q}_{k,m}$ are orthogonal, thus

$$\| \mathbf{r}_{k,m} \|^2 = \| \mathbf{r}_{k,m-1} \|^2 - \frac{(\mathbf{y}_k^T\mathbf{q}_{k,m})^2}{\mathbf{q}_{k,m}^T\mathbf{q}_{k,m}} \tag{15}$$

By respectively summing (13) and (15) for m from 1 to n, yields

$$\mathbf{y}_k = \sum_{m=1}^{n}\frac{\mathbf{y}_k^T\mathbf{q}_{k,m}}{\mathbf{q}_{k,m}^T\mathbf{q}_{k,m}}\mathbf{q}_{k,m} + \mathbf{r}_{k,n} \tag{16}$$

$$\| \mathbf{r}_{k,n} \|^2 = \| \mathbf{r}_{k,n-1} \|^2 - \frac{(\mathbf{y}_k^T\mathbf{q}_{k,n})^2}{\mathbf{q}_{k,n}^T\mathbf{q}_{k,n}} = \| \mathbf{y}_k \|^2 - \sum_{m=1}^{n}\frac{(\mathbf{y}_k^T\mathbf{q}_{k,m})^2}{\mathbf{q}_{k,m}^T\mathbf{q}_{k,m}} \tag{17}$$

Equation (16) shows that $\mathbf{y}_k$ can be approximated using a set of orthogonal vectors $\{\mathbf{q}_{k,1},\mathbf{q}_{k,2},\cdots,\mathbf{q}_{k,n}\}$, which are transformed from the original vectors $\{\boldsymbol{\varphi}_{k,s_1},\boldsymbol{\varphi}_{k,s_2},\cdots,\boldsymbol{\varphi}_{k,s_n}\}\subset D_k$. The norm $\| \mathbf{r}_{k,n} \|^2$, or some associated variations, is often used to form a criterion to determine the model complexity (model size) in some conventional identification procedure, where observed data are partitioned using the 'hold-out' method. In this study, however, the model complexity will be determined using the BIC criterion and this will be described in 3.2.3.

3.2.2 Parameter estimation of individual models

It is easy to verify that the relationship between the selected bases $\{\boldsymbol{\varphi}_{k,s_1}, \boldsymbol{\varphi}_{k,s_2}, \cdots, \boldsymbol{\varphi}_{k,s_n}\} \subset \mathrm{D}_k$ and the associated orthogonal bases $\mathbf{q}_{k,1}, \mathbf{q}_{k,2}, \cdots, \mathbf{q}_{k,n}$, for the kth data set, is given by

$$\mathbf{A}_{k,n} = \mathbf{Q}_{k,n}\mathbf{R}_{k,n} \tag{18}$$

where $\mathbf{A}_k = [\boldsymbol{\varphi}_{k,s_1}, \boldsymbol{\varphi}_{k,s_2}, \cdots, \boldsymbol{\varphi}_{k,s_n}]$, $\mathbf{Q}_{k,n}$ is an $N_k \times n$ matrix with orthogonal columns $\mathbf{q}_{k,1}, \mathbf{q}_{k,2}, \cdots, \mathbf{q}_{k,n}$, and $\mathbf{R}_{k,n}$ is an $n \times n$ unit upper triangular matrix whose entries are calculated during the orthogonalization procedure. The unknown parameter vector, denoted by $\boldsymbol{\theta}_{k,n} = [\theta_{k,1}, \cdots, \theta_{k,n}]^T$, for the regression with respect to the original vectors, can be calculated from the triangular equation $\mathbf{R}_{k,n}\boldsymbol{\theta}_{k,n} = \boldsymbol{\gamma}_{k,n} = [g_{k,1}, \cdots, g_{k,n}]^T$, where the elements of $\boldsymbol{\gamma}_{k,n}$ are given by $g_{k,m} = (\mathbf{y}_k^T \mathbf{q}_{k,m})/(\mathbf{q}_{k,m}^T \mathbf{q}_{k,m})$ for $m=1,2, \ldots, n$.

3.2.3 Model size determination

Model selection criteria are often established on the basis of estimates of prediction errors, by inspecting how the identified model performs on future (never used) data sets. Several criteria, for example, the Akaike information criterion (AIC) (Akaike 1974), the Bayesian information criterion (BIC) (Schwarz 1978), the minimum description length (MDL) (Rissanen 1978), the generalised cross-validation (GCV) (Golub et al. 1979), and many variants (Miller 1990, Hansen and Yu 2001, Stoica and Selen 2004), are available to determine the model complexity or model size (number of regressors). In this study, however, one variation of the conventional BIC (Efron and Tibshirani 1993) is considered, and this given as below

$$\mathrm{BIC}(p) = \left[1 + \frac{p\ln(N)}{N-p}\right]\mathrm{MSE}(p) = \left[1 + \frac{p\ln(N)}{N-p}\right]\frac{\mathrm{RSS}}{N} \tag{19}$$

where $\mathbf{y}$ is the observed (or desired) output sequence of length N, MSE and RSS represent the mean-squared-error and the residual sum of squares, respectively, corresponding to the choice of the model of p terms. The relationship between MSE and RSS is defined as $\mathrm{MSE}(p) = \mathrm{RSS}(p)/N = \|\mathbf{r}_p\|^2/N$, where $\mathbf{r}_p$ represents the associated model residual.

Now consider again the multiple (K-fold) regression modelling problem discussed in the previous section. The present study uses a weighted average information criterion to determine the number of common model terms. The weighted average BIC is given by

$$\mathrm{WABIC}(p) = \alpha\mathrm{WABIC}^{(\mathrm{Train})}(p) + (1-\alpha)\mathrm{WABIC}^{(\mathrm{Val})}(p) \tag{20}$$

where α is a constant satisfying $0 \le \alpha \le 1$, $\mathrm{WABIC}^{(\mathrm{Train})}(p)$ and $\mathrm{WABIC}^{(\mathrm{Val})}(p)$ respectively represent

the values of the associated weighed average information criterion, corresponding to the model of p terms, calculated by applying the BIC to the relevant training and validation data sets as below

$$\text{WABIC}^{(*)}(p) = \frac{1}{K}\sum_{k=1}^{K}\text{BIC}_k^{(*)}(p) \tag{21}$$

where '*' indicates either 'Train' or 'Val', meaning that $\text{BIC}_k^{(*)}(p)$ and $\text{WABIC}^{(*)}(p)$ are calculated from either the training datasets $B_1, B_2, \cdots, B_K$, or the validation datasets $V_1, V_2, \cdots, V_K$. The subscript k in $\text{BIC}_k^{(*)}(p)$ indicates that the criterion is for the kth model and is associated with the kth training and validation data set.

3.3 Model parameter estimation and refinement

Assume that a total of n common model terms, $\{\omega_m(\mathbf{x}(t))\}_{m=1}^{n} = \{\phi_{i_m}(\mathbf{x}(t))\}_{m=1}^{n} \subset D$, have been selected by applying the multiple orthogonal search (MOS) algorithm to the associated training dataset B that consists of N data pairs, $\{(\mathbf{x}(t), y(t)) : t = 1, 2, \cdots, N\}$. The common-structured model can then be described as

$$y(t) = \sum_{m=1}^{n}\beta_m\omega_m(\mathbf{x}(t)) + e(t) = \sum_{m=1}^{n}\beta_m\omega_m(t) + e(t) \tag{22}$$

3.3.1 Ridge regression

Let Φ be the design matrix associated with (22), $\mathbf{y}$ the output vector, and $\boldsymbol{\beta} = [\beta_1, \beta_2, \cdots, \beta_n]^T$ the model parameter vectors. The least squares estimator of the model parameter vector $\boldsymbol{\beta}$ is then given by

$$\hat{\boldsymbol{\beta}}_{\text{LS}} = (\Phi^T\Phi)^{-1}\Phi^T\mathbf{y} \tag{23}$$

Note that the least squares method may occasionally produce very poor estimates of the regression coefficients when it is applied to non-orthogonal data (Montgomery et al. 2001), meaning that the absolute value of the least squares estimates may be too large and that they are very unstable, that is, their magnitudes and signs may change considerably given a different sample (Montgomery et al. 2001). This stems from the requirement that the estimate $\hat{\boldsymbol{\beta}}_{\text{LS}}$ be an unbiased estimator of $\boldsymbol{\beta}$. One way to alleviate this problem is to drop the requirement that the estimator of $\boldsymbol{\beta}$ be unbiased by using ridge regression, a penalised least squares method originally proposed by Hoerl and Kennard (1970a,b) . The ridge estimator $\hat{\boldsymbol{\beta}}_{\text{Rig}}$ is defined as

$$\hat{\boldsymbol{\beta}}_{\text{Rig}} = (\Phi^T\Phi + \lambda\mathbf{I})^{-1}\Phi^T\mathbf{y} \tag{24}$$

where $\lambda \geq 0$ is some constant. Hoerl and Kennard (1976) proposed to use the following iterative

estimation procedure to determine the ridge biasing parameter λ.

- Step 0: Calculate

$$\lambda_0 = \frac{n\hat{\sigma}_{\mathrm{LS}}^2}{\hat{\boldsymbol{\beta}}_{\mathrm{LS}}^T\hat{\boldsymbol{\beta}}_{\mathrm{LS}}} \tag{25}$$

where

$$\hat{\sigma}_{\mathrm{LS}}^2 = \frac{1}{N-n}(\mathbf{y} - \Phi\hat{\boldsymbol{\beta}}_{\mathrm{LS}})^T(\mathbf{y} - \Phi\hat{\boldsymbol{\beta}}_{\mathrm{LS}}) \tag{26}$$

- Step k ($k \geq 1$): Calculate

$$\lambda_k = \frac{n\hat{\sigma}_{\mathrm{LS}}^2}{\hat{\boldsymbol{\beta}}_{\mathrm{Rig}}^T(\lambda_{k-1})\hat{\boldsymbol{\beta}}_{\mathrm{Rig}}(\lambda_{k-1})} \tag{27}$$

where $\hat{\boldsymbol{\beta}}_{\mathrm{Rig}}(\lambda_{k-1})$ is the ridge estimator corresponding to the biasing parameter λ_{k-1}.

Results from our own simulation studies have shown that the above iterative estimation procedure converges very fast, and in most cases the biasing parameter λ_k becomes unchanged (a constant) after only three or five steps.

3.3.2 *K*-Fold estimation

This study proposes using a *K*-fold parameter estimation approach to obtain more robust estimates of the model parameters. Either the least squares (23) based or the ridge regression (24)-(27) based *K*-fold estimation approach can be used to achieve this objective. Taking *K*-fold ridge regression as an example, the associated procedures can be briefly summarised as follows:

- Step 1: Apply the *K*-fold random subsampling method to the associated training dataset *B*, to generate *K* subsets $\Omega_1, \Omega_2, \cdots, \Omega_K$, each roughly containing say 90% data samples in *B*.

- Step 2: Apply the ridge regression to the training dataset *B*, and let the resultant ridge estimator be $\hat{\boldsymbol{\beta}}_{\mathrm{Rig}}^{(0)}$.

- Step 3: Apply the ridge regression to these *K* subsets $\Omega_1, \Omega_2, \cdots, \Omega_K$. Let the resultant ridge estimator, relative to the *k*th dataset Ω_k, be $\hat{\boldsymbol{\beta}}_{\mathrm{Rig}}^{(k)}$, with *k*=1,2, …, *K*.

- Step 4: The average of the *K*+1 ridge estimators, defined as $\hat{\boldsymbol{\beta}}_{\mathrm{KF}} = (\sum_{k=0}^{K} \hat{\boldsymbol{\beta}}_{\mathrm{Rig}}^{(k)})/(K+1)$, is chosen as the model parameter vector of the associated model.

4. Examples and Applications

Two examples are provided to demonstrate the application of the proposed random subsampling and multifold modelling (RSMM) approach. The data used in the first example are simulated from some low-order nonlinear models; the objective is to illustrate how well the RSMM approach works

on improving the model parameter estimates for nonlinear models, where the model structure is assumed to be known. The data used in the second example are for a wild type of fly, called Drosophila; this example involves a real-world nonlinear input-output system identification problem.

4.1 Improved parameter estimates with known model structure

Consider two models given below

$$M_1: \quad x(t) = 0.8x(t-1) - 0.6x(t-2) + 0.8u(t-1) - 0.4u^2(t-1) + 0.6u^3(t-1) - 0.7u^4(t-1) \qquad (28a)$$

$$y(t) = x(t) + \varepsilon(t) \qquad (28b)$$

$$M_2: \quad x(t) = u(t-1) + 0.5u(t-2) + 0.4u(t-1)u(t-2) - 0.2u^2(t-1)u(t-2) \qquad (29a)$$

$$y(t) = x(t) + \varepsilon(t) \qquad (29b)$$

where $u(t)$ is the input, $y(t)$ is the output, $x(t)$ is the state, and $\varepsilon(t)$ is the additive noise signal. The properties of $u(t)$ and $\varepsilon(t)$, along with some simulation conditions, are described in the details later. The objective here was to identify, from given observations of the system input and output, the model parameters. The systems were simulated and the associated input-output observations were recorded; these observations were then used for model parameter estimation, under an assumption that the model structure was known but the model parameters were unknown.

The input-output description of the models (28) and (29) was assumed to be known as below

$$y(t) = \boldsymbol{\varphi}^T(t)\boldsymbol{\beta} + \varepsilon(t) \qquad (30)$$

where $\boldsymbol{\varphi}(t)$ is the regressor vector that will be used to form the associated design matrix, and $\boldsymbol{\beta}$ is the model parameter vector. For the models (28) and (29), the vector $\boldsymbol{\varphi}(t)$ is respectively given as

$$\boldsymbol{\varphi}(t) = [x(t-1), x(t-2), u(t-1), u^2(t-1), u^3(t-1), u^4(t-1)]^T,$$

and

$$\boldsymbol{\varphi}(t) = [u(t-1), u(t-2), u(t-1)u(t-2), u^2(t-1)u(t-2)]^T,$$

while the true parameter vector $\boldsymbol{\beta}$ for the models (28) and (29) is respectively given by $\boldsymbol{\beta} = [\beta_1, \beta_2, \cdots, \beta_6]^T = [0.8, -0.6, 0.8, -0.4, 0.6, -0.7]^T$ and $\boldsymbol{\beta} = [\beta_1, \beta_2, \beta_3, \beta_4]^T = [0.1, 0.5, 0.4, -0.2]^T$.

4.1.1 Experiments for model M_1

The input $u(t)$ was uniformly distributed on $[-1, 1]$, and the noise $\varepsilon(t) \sim N(0, \sigma^2)$. Four cases, corresponding to $\sigma = 0.0106, 0.1071, 0.3374$ and 0.5979, were considered. These enable the signal-to-

noise ratio (SNR) to be roughly 40, 20, 10 and 5dB, respectively. Simulations and Monte-Carlo experiments were carried out by performing the procedures below:

- For each case, the model was simulated 200 times
- At each time of simulation, a data set containing 500 input-output data points was collected.
- For each of the 200 datasets, the ordinary least squares algorithm was used for parameter estimation.
- For each of the 200 datasets, the *K*-fold parameter estimation procedure, described in section 3.3, was performed for parameter estimation, where *K* was chosen to be 10.

Let $\hat{\beta}_p^{(q)}$ be the estimate of the *p*th parameter $\hat{\beta}_p$, produced from the *q*th dataset using either the ordinary least squares algorithm or the *K*-fold parameter estimation method, where *p*=1,2,3,4,5,6, and *q*=1,2,3, …, 200. This study uses the following three statistics to measure the performance of the parameter estimates for a known model structure.

- The mean (or average)

$$\hat{\beta}_p^{\text{mean}} = \frac{1}{200}\sum_{q=1}^{200}\hat{\beta}_p^{(q)} \tag{31}$$

- The standard deviation

$$\hat{\beta}_p^{\text{dev}} = \left[\frac{1}{200}\sum_{q=1}^{200}[\hat{\beta}_p^{(q)} - \hat{\beta}_p^{\text{mean}}]^2\right]^{1/2} \tag{32}$$

- The mean of the total relative error

$$\hat{\beta}_p^{\text{MTRE}} = \frac{1}{200}\sum_{q=1}^{200}\left(\frac{1}{6}\sum_{p=1}^{6}\left|\frac{\hat{\beta}_p^{(q)} - \beta_p^{(q)}}{\beta_p^{(q)}}\right|\right)\times 100\% \tag{33}$$

The three statistics associated with the above four cases are listed in Table 1.

4.1.2 Experiments for model M_2

The input *u*(*t*) was an AR(2) process of the form $u(t)=1.6u(t\text{-}1)\text{-}0.6375u(t\text{-}2)+0.16w(t)$, and the noise $\varepsilon(t)$ was of the form $\eta(t) = 0.75\eta(t-1) + cw(t)$, where with $w(t) \sim N(0,1)$ and *c* is a constant. Four cases, corresponding to c=0.01, 0.1, 0.25 and 0.5, were considered. These make the signal-to-noise ratio (SNR) to be roughly 40, 20, 10 and 5dB, respectively. The same simulations and Monte-Carlo experiments, as described for the previous model M_1, were carried out, and the associated results are shown in Table 2. From the results given in Tables 1 and 2, it can be concluded, in a statistical and an asymptotical sense, that:

- When the SNR is high, both the ordinary least squares algorithm and the *K*-fold estimation methods can provide very good parameter estimates, with low standard deviations and low total relative errors.
- The variance of the parameter estimates produced by the ordinary least squares algorithm is much greater than that produced by the *K*-fold estimation methods.
- The total relative errors of the parameter estimates produced by the ordinary least squares algorithm is much greater that that produced by the *K*-fold estimation method.
- The variance of the parameter estimates produced by the *K*-fold ridge regression is less than that produced by the *K*-fold least squares method.
- The total relative errors of the parameter estimates produced by the *K*-fold ridge regression are comparable with those produced by the *K*-fold least squares method.

Table 1 Comparisons of the parameter estimates produced by the ordinary least squares algorithm and by the *K*-fold RSMM method, for the model given by (28)

SNR	Parameter estimates and the associated performance							
	Method		β_1	β_2	β_3	β_4	β_5	β_6	MTRE (%)
40dB	Mean	LS	0.7998	-0.5999	0.8002	-0.3999	0.5998	-0.7002	0.4563%
		KLS	0.7999	-0.5999	0.8003	-0.4002	0.5997	-0.6998	0.0561%
		KRR	0.7999	-0.5999	0.8003	-0.4003	0.5997	-0.6997	0.0566%
	Dev	LS	0.0005	0.0005	0.0031	0.0046	0.0048	0.0067	
		KLS	0.0001	0.0001	0.0005	0.0008	0.0007	0.0012	
		KRR	0.0001	0.0001	0.0005	0.0008	0.0007	0.0012	
20dB	Mean	LS	0.7855	-0.5868	0.7999	-0.4008	0.6004	-0.7015	5.0218%
		KLS	0.7857	-0.5870	0.8006	-0.4003	0.5995	-0.7023	1.0798%
		KRR	0.7856	-0.5869	0.8007	-0.4039	0.5989	-0.6970	1.1937%
	Dev	LS	0.0048	0.0046	0.0287	0.0478	0.0438	0.0691	
		KLS	0.0007	0.0007	0.0047	0.0078	0.0061	0.0109	
		KRR	0.0007	0.0007	0.0046	0.0076	0.0060	0.0107	
10dB	Mean	LS	0.6789	-0.4908	0.7968	-0.4262	0.0611	-0.6711	19.6064%
		KLS	0.6784	-0.4901	0.8055	-0.4293	0.5898	-0.6664	8.2488%
		KRR	0.6773	-0.4893	0.8057	-0.4545	0.5847	-0.6274	10.3088%
	Dev	LS	0.0166	0.0159	0.0915	0.1531	0.1391	0.2209	
		KLS	0.0025	0.0021	0.0153	0.0186	0.0237	0.0266	
		KRR	0.0025	0.0020	0.0144	0.0156	0.0222	0.0227	
5dB	Mean	LS	0.5130	-0.3458	0.8076	-0.4456	0.5858	-0.6612	34.3088%
		KLS	0.5117	-0.3459	0.8117	-0.4266	0.5789	-0.6929	17.0049%
		KRR	0.5097	-0.3443	0.8106	-0.4856	0.5654	-0.5971	20.9344%
	Dev	LS	0.0274	0.0283	0.1554	0.2260	0.2321	0.3225	
		KLS	0.0044	0.0038	0.0276	0.0457	0.0420	0.0699	
		KRR	0.0044	0.0038	0.0236	0.0307	0.0356	0.0500	
	LS: Ordinary least squares algorithm; KLS: LS based *K*-fold parameter estimation; KRR: Ridge regression based *K*-fold parameter estimation;								

Table 2 Comparisons of the parameter estimates produced by the ordinary least squares algorithm and by the *K*-fold RSMM method, for the model given by (29).

SNR	Method		β_1	β_2	β_3	β_4	MTRE (%)
40dB	Mean	LS	0.9998	0.5001	0.4000	-0.2000	0.3393%
		KLS	0.9998	0.5002	0.4001	-0.2000	0.0619%
		KRR	0.9998	0.5002	0.4001	-0.2000	0.0622%
	Dev	LS	0.0056	0.0055	0.0009	0.0006	
		KLS	0.0016	0.0014	0.0002	0.0001	
		KRR	0.0016	0.0014	0.0002	0.0001	
20dB	Mean	LS	1.0000	0.4993	0.3995	-0.1997	3.8751%
		KLS	1.0014	0.4967	0.3995	-0.1995	0.4562%
		KRR	0.9998	0.4980	0.3995	-0.1995	0.4174%
	Dev	LS	0.0508	0.0475	0.0096	0.0064	
		KLS	0.0064	0.0094	0.0017	0.0011	
		KRR	0.0064	0.0093	0.0017	0.0011	
10dB	Mean	LS	1.0049	0.4941	0.4021	-0.2004	10.3419%
		KLS	1.0035	0.4964	0.4038	-0.2002	1.2701%
		KRR	0.9942	0.5039	0.4036	-0.1998	1.1024%
	Dev	LS	0.1315	0.1252	0.0253	0.0174	
		KLS	0.0197	0.0209	0.0045	0.0021	
		KRR	0.0191	0.0203	0.0045	0.0020	
5dB	Mean	LS	1.0182	0.4852	0.4001	-0.2005	20.1103%
		KLS	0.9991	0.4909	0.4011	-0.1977	2.2415%
		KRR	0.9996	0.5165	0.4006	-0.1962	2.7484%
	Dev	LS	0.2514	0.2499	0.0480	0.0306	
		KLS	0.0412	0.0342	0.0065	0.0054	
		KRR	0.0376	0.0305	0.0065	0.0054	

4.2 Fruit fly modelling

The fruit fly insect dataset contains 1000 experimental data points for a wild type of fruit fly, called Drosophila. The system input was the response of the photoreceptors (PR: mV), and the output was the response of the large monopolar cells (LMCs, mV). The relationship between the input and the output in the fruit fly experiment is complex, because in addition to the response from the photoreceptors, several other factors may also affect the output response of the large monopolar cells. The objective here was to find a model that reflects, as closely as possible, the relationship between the response of the photoreceptors (the input) and the response of the large monopolar cells (the output), to facilitate the analysis and understanding of the associate behaviour of this kind of insect.

The 1000 input-output data points, which are shown in Figure 1, were partitioned into two parts: the training data set consisting of the first 800 points, and the test data set consisting of the remaining 200 points. A Volterra series model was employed to describe the input-output relationship of the fruit fly data. The Volterra model is a special case of the linear-in-the-parameters form (3), where the 'input' (predictor) vector $\mathbf{x}(t)$ contains no lagged output $y(t-k)$, with $k \geq 1$. The input vector $\mathbf{x}(t)$ for the fruit fly data was chosen to be $\mathbf{x}(t) = [x_1(t), x_2(t), \cdots, x_{15}(t)]^T = [u(t-1), u(t-2), \cdots, u(t-15)]^T$, and the initial full model was chosen as
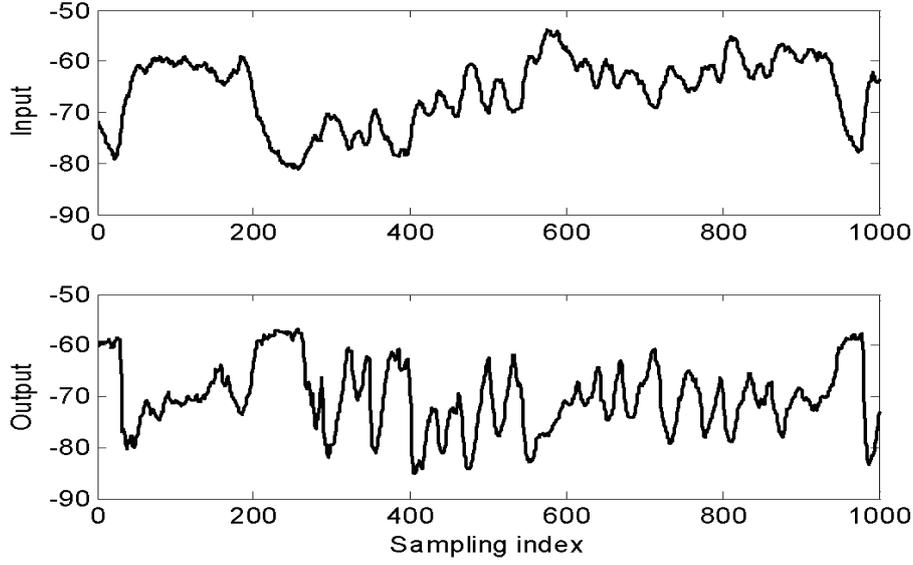
Fig. 1 The input and output signal for the fruit fly modelling problem.

$$y(t) = \theta_0 + \sum_{i=1}^{15} \theta_i u(t-i) + \sum_{i=1}^{15} \sum_{j=i}^{15} \theta_{i,j} u(t-i)u(t-j) + e(t) \tag{34}$$

A total of 136 candidate model terms were involved in the initial full model (34). A 10-fold random subsampling and multifold modelling (RSMM) approach, along with the weighed average BIC given by (20) where the weight coefficient α =0.5, was applied to the training dataset composed of the first 800 data points. For a comparison, the conventional orthogonal forward regression (OFR) algorithm, along with the BIC given by (19), was also applied to the same training dataset. The BIC and WABIC, shown in Figure 2, suggest that the model size for the OFR and RSMM produced models should be 13 and 12, respectively. The selected model terms for the two models are shown in Table 3, where individual model terms are ranked in the order that they entered into the model.

It can be seen from Table 3 that the performance of the RSMM produced model is slightly better than that produced by using the traditional hold-out method, in the sense that the RSMM produced model provides better predictive capability over the test dataset. More importantly, it can easily be noted that by using the *K*-fold ridge regression, the very large initial least squares estimates of the 8th coefficient 53.7965 has been significantly reduced, without deteriorating the model's generalisation properties. This is important because, from the discussion of the previous section, the ridge penalised model with shrinkage coefficients should be more robust. The model predicted output from the RSMM produced model is shown in Figure 3. Note that Figure 3 illustrates the model predicted output which is a much better indication of model performance than the one step ahead predicted output. The latter is virtually coincident with the data set.
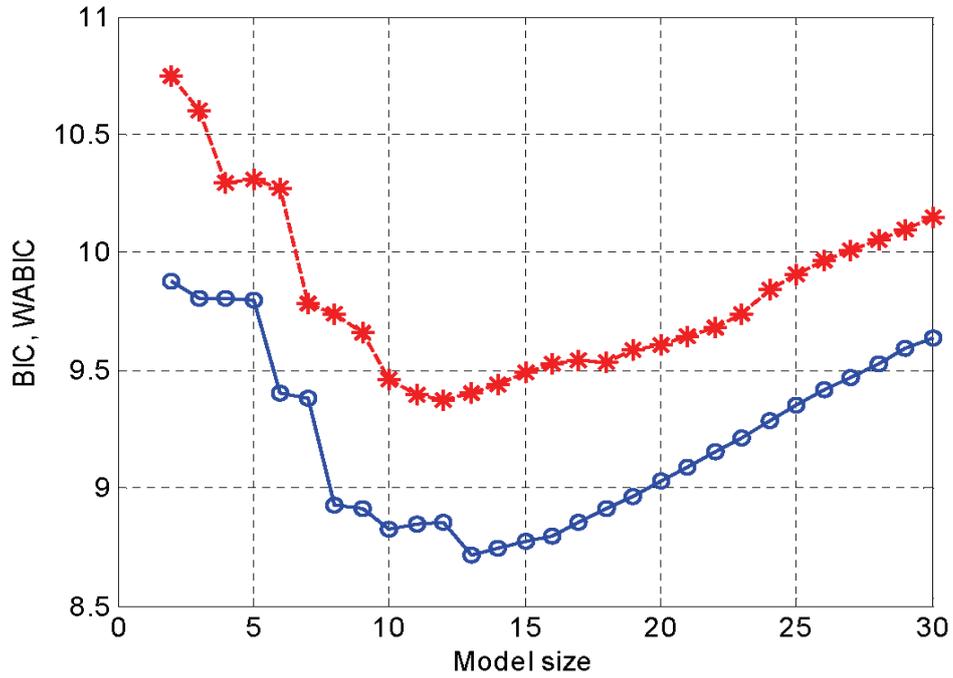
Fig. 2 The BIC for the OFR produced model (the circled-line) and the WABIC for the RSMM produced model (the stared-line) for the fruit fly modelling problem.

Table 3 Comparisons of the OFR and RSMM produced models for the fruit fly modeling problem.

| Index	OFR		RSMM			
	Model term	Parameter	Model term	Parameter		
				Initial (LS)	KLS	KRR
1	u(t-15)	0.399564	u(t-15)	0.439843	0.480600	0.141230
2	u(t-1)u(t-14)	-0.298695	u(t-1)u(t-14)	0.004403	0.004146	0.004584
3	u(t-7)u(t-14)	0.312272	u(t-8)u(t-10)	-0.003163	-0.003154	-0.002933
4	u(t-2)u(t-14)	0.015946	u(t-2)u(t-13)	0.012494	0.012462	0.012521
5	u(t-1)	3.397754	u(t-5)	0.390185	0.321670	0.916750
6	u(t-14)u(t-15)	-0.023164	u(t-1)u(t-5)	0.430601	0.426020	0.462471
7	u(t-1)u(t-13)	0.191000	u(t-1)u(t-15)	-0.091538	-0.089021	-0.084144
8	u(t-7)u(t-13)	-0.183164	const	53.796524	53.396613	0.062336
9	const	47.895010	u(t-1)	3.143354	3.159672	1.327320
10	u(t-1)u(t-1)	-0.059281	u(t-5)u(t-5)	-0.245837	-0.243192	-0.251918
11	u(t-1)u(t-5)	-0.001521	u(t-1)u(t-1)	-0.143858	-0.142570	-0.177004
12	u(t-1)u(t-7)	0.285200	u(t-5)u(t-15)	0.068354	0.066661	0.056249
13	u(t-7)u(t-7)	-0.208430				
	mse=5.3722; nrmse=0.3695;			mse=4.8159; nrmse=0.3498;	mse=5.0013; nrmse=0.3565;	mse=4.7537; nrmse=0.3475.
	LS: Ordinary least squares algorithm; KLS: LS based *K*-fold parameter estimation; KRR: Ridge regression based *K*-fold parameter estimation; The above MSE and NRMSE were calculated over the test dataset.					
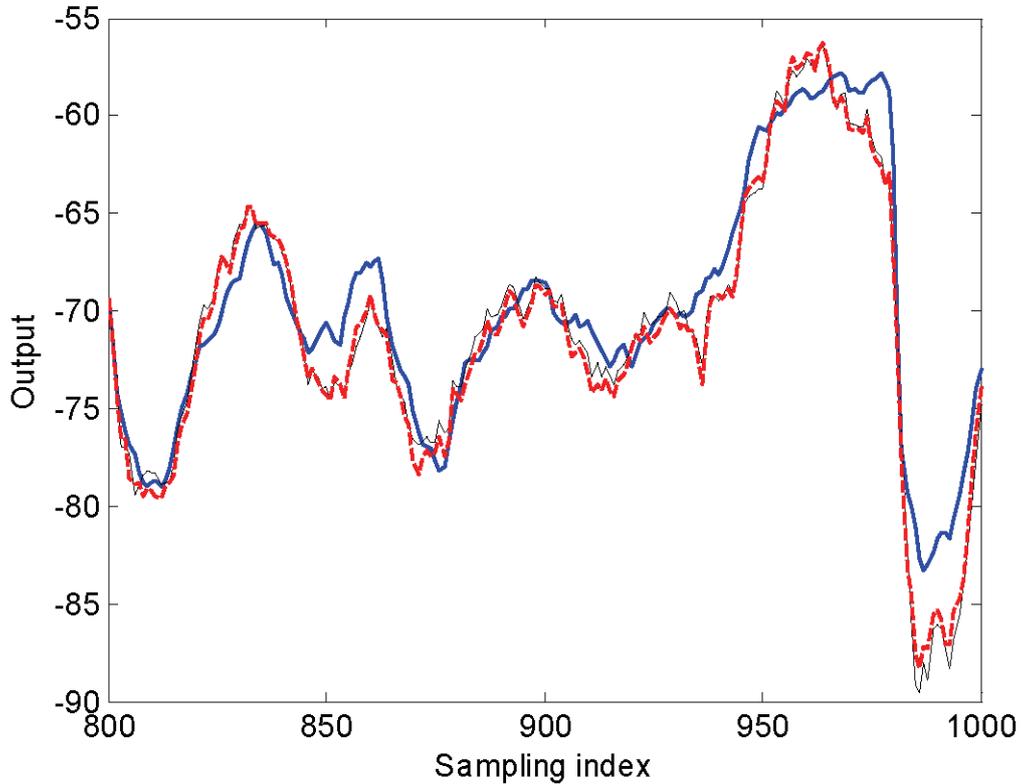
Fig. 3   A comparison of the model predicted output and the measurement for the fruit fly modelling problem. The thick solid line represents the measurement; the thick dashed line represents the model predicted output from the RSMM produced model; the thin solid line represents the model predicted output from the traditional hold-out method using the OFR algorithm.

4.3 Modelling the solar wind magnetosphere

The solar wind magnetosphere is a complex input-output dynamical nonlinear system, where the solar wind and the associated parameters play the role of the inputs and the geomagnetic indices can be considered as the outputs. The *Dst* index is an important parameter to measure the disturbance of the geomagnetic field in a magnetic storm. In this example, the magnetosphere system was considered to be a structure-unknown (black-box) dynamical system. The objective was to identify a mathematical model that can be used to forecast the *Dst* index. Following Wei et al. (2007), the magnetosphere system was treated to be a two-input and single output system, where the *Dst* index was the system output, and the solar wind parameter *VBs* and the solar wind dynamic pressure *P* were the two inputs. Figure 4 shows the measurements of the *Dst* index ('nT'), the solar wind parameter VB_s ('mV/m'), and the solar wind dynamic pressure *P* ('nPa'), measured for a period of 49 days, from day 230 to day 278, in the year 1998. The data points in figure 4 were recorded with a sampling interval *T*=1hour, thus there are a total of 1176 observations, with a time resolution of 1-hour, were involved.

20

These data points, which contain two intense storms on day 239 and day 268, respectively, were used for model identification.

For convenience of description, let $y(t) = Dst(t)$, $u_1(t) = VBs(t)$, and $u_2(t) = P(t)$. Following Wei et al. (2007), the significant model variables were chosen to be $\{y(t-i), u_1(t-j), u_k(t-k)\}$, with i=1,2, j=1,2,3,4, and k=1,2,3,4. The ten variables were then used to construct a mathematical model. Following the method given in Billings et al. (2007), the observations about the ten variables were clustered into 22 groups, where the corresponding geophysical centres are denoted by $\mathbf{c}_k = [c_{1,k}, c_{2,k}, \cdots, c_{10,k}]$ with k=1,2, ... ,22. Following Billings and Wei (2005b), a wavelet-ARX model below was considered

$$y(t) = f(\mathbf{x}(t)) + e(t) = \sum_{i=0}^{d} \theta_k x_k(t) + \sum_{k=1}^{N_c} \sum_{j=1}^{J} \theta_{j,k} \varphi(\mathbf{x}(t); \mathbf{c}_k, a_j) + e(t) \qquad (35)$$

where d=10, $\mathbf{x} = [x_0(t), x_1(t), x_2(t), \cdots, x_d(t)] = [1, y(t-1), y(t-2), u_1(t-1), \cdots, u_1(t-4), u_2(t-1), \cdots, u_2(t-4)]$, and φ is some wavelets defined as the tensor product of some one-dimensional functions as below
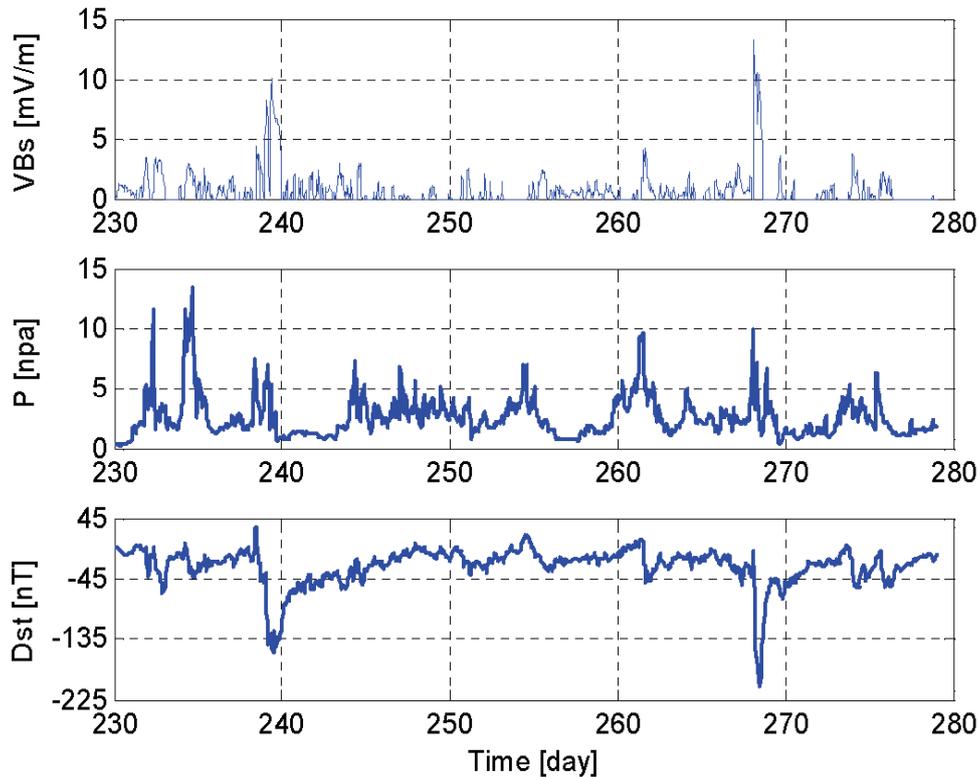

Fig. 4.   The two inputs (the solar wind parameter *VBs* and the dynamical pressure, *P*) and the output (the *Dst* index), measured for the period from day 230 to day 278, in the year 1998, with a sampling interval of 1-hour. A total of 1176 observations, with a time resolution of 1-hour, were involved.

$$\boldsymbol{\varphi}(\mathbf{x}(t); \mathbf{c}_k, a_j) = \prod_{i=1}^{d} \phi\left(\frac{x_i(t) - c_{i,k}}{a_j}\right) \qquad (36)$$

with $a_j = 2^j$ and ϕ being defined as the centralised and normalised 4th order cardinal B-spline

$$\phi(x) = \frac{3}{2} B_4(x+2) \qquad (37)$$

where the explicit expression of the ordinary 4th order cardinal B-spline B4(x) can be found in Billings and Wei (2006). The parameters involved in the wavelet-ARX model (35) were set to be: d=10, J=8, N_c=22, and thus a total of 187 candidate model terms were involved in the initial full model (35).

A 5-fold random subsampling and multifold modelling (RSMM) approach, along with the weighed average BIC given by (20) where the weight coefficient α =0.5, was applied to the training dataset composed of the 1176 data points. For a comparison, the conventional orthogonal forward regression (OFR) algorithm, along with the BIC given by (19), was also applied to the same training dataset. The BIC and WABIC, shown in Fig 5, suggest that the model size for the OFR and RSMM produced models should be 16 and 14, respectively. The selected model terms for the two models are shown in Table 4, where individual model terms are ranked in the order that they entered into the model, but have been rearranged for convenience of the comparison of the corresponding parameter estimates.
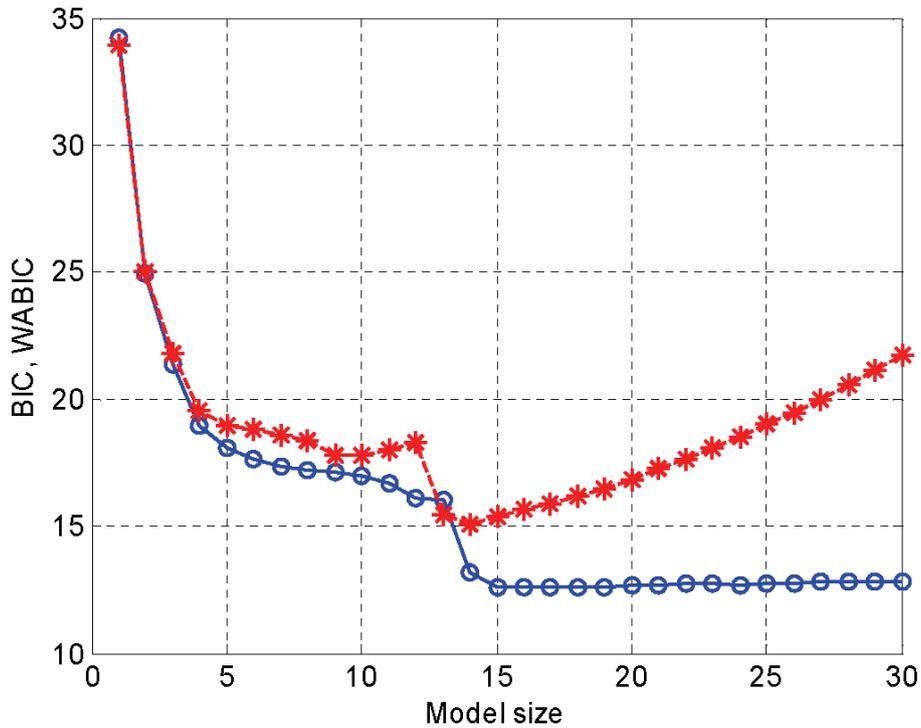

Fig. 5   The BIC for the OFR produced model (the circled-line) and the WABIC for the RSMM produced model (the stared-line) for the solar wind magnetosphere modelling problem.

Table 4 Comparisons of the OFR and RSMM produced models for the solar wind magnetosphere modelling problem.

Index	OFR		RSMM			
	Model term	Parameter	Model term	Parameter		
				Initial (LS)	KLS	KRR
1	y(t-1)	1.093825	y(t-1)	1.076903	1.087722	1.207250
2	y(t-2)	-0.204097	y(t-2)	-0.224521	-0.229147	-0.247479
3	u1(t-1)	-1.528591	u1(t-1)	-1.414456	-1.406579	-1.204033
4	u1(t-2)	-3.119386	u1(t-2)	-3.250326	-3.253919	-3.050096
5	u1(t-3)	1.202844	u1(t-3)	1.325963	1.383175	1.618463
6	u1(t-4)	1.646110	u1(t-4)	1.488517	1.443757	1.610716
7	u2(t-1)	2.863310	u2(t-1)	2.776554	2.755978	2.587707
8	u2(t-2)	-4.033820	u2(t-2)	-4.017683	-3.991810	-4.299416
9	u2(t-3)	1.334032	u2(t-3)	1.372376	1.361874	1.628050
10	g(x, c15,a3)	8797.205872	g(x, c15,a3)	5062.882565	3124.930932	-243.470116
11	g(x, c15,a5)	-75.537995	g(x, c15,a4)	18.259092	4.687857	0.021499
12	g(x, c19,a5)	0.694249	g(x, c15,a5)	-72.298240	-67.466688	0.265323
13	g(x, c20,a5)	4.539476	g(x, c15,a6)	36.347918	35.197519	-0.204760
14	g(x, c20,a6)	-22.374429	g(x, c20,a7)	-17.417562	-16.452981	0.447423
15	g(x, c15,a7)	46.882333				
16	g(x, c20,a7)	-19.193810				
	Emax=57.43; Emean=1.95;			Emax =41.65; Emean =1.90;	Emax =40.97; Emean =1.87;	Emax =39.64; Emean =1.35.
	LS: Ordinary least squares algorithm; KLS: LS based *K*-fold parameter estimation; KRR: Ridge regression based *K*-fold parameter estimation; The function g in the second column indicates the function $\boldsymbol{\varphi}(\mathbf{x}(t);\mathbf{c}_k,a_j)$ defined by (36). Emax and Emean are defined by (38) and (39) respectively.					

It can be seen from Table 4 that the performance of the RSMM produced model is significantly improved compared with that produced by using the traditional hold-out method, in the sense that the RSMM produced model provides better predictive capability over the test dataset. More importantly, it can easily be noted that by using the *K*-fold ridge regression, the very large initial least squares estimates of the 10th coefficient has been significantly reduced, without deteriorating the model's generalisation properties. Again, this is important because, from the discussion of the previous section, the ridge penalised model with shrinkage coefficients should be more robust.

Note that the forecasts of strong storms ($Dst \leq 100$ nT) and larger storms ($Dst \leq 200$ nT) are particularly important in the solar wind magnetosphere modelling problem. In order to perform a stringent test on the identified model for such a problem, a test dataset containing a strong or large storm needs to be considered. To achieve this, a validation data set, which contains a large storm and which consists of 156 hourly sampled observations of the *Dst* index, the solar wind parameter VB_s and the solar wind dynamic pressure *P*, measured for a period of 6.5 days from day 223 to day 229 (12 hours for day 229), in the year 2000, was used to test the performance of the identified model. The model predicted output from the RSMM produced model is shown in figure 6. Note that the model

predicted output can reveal severe model deficiencies which would otherwise go undetected by one-step-ahead predictions.

To quantitatively measure and compare the performance of the identified models, the following two criteria were considered

$$E_{\max} = \max_{1 \le t \le T} \{ |y(t) - \hat{y}(t)| \} \tag{38}$$

$$E_{\text{mean}} = \frac{1}{T} \sum_{t=1}^{T} \frac{|y(t) - \hat{y}(t)|}{|y(t) - \bar{y}|} \tag{39}$$

where T is the data length of the test dataset, $\hat{y}(t)$ is the predicted value from the model, and $\bar{y}$ is the mean of the observations of the response $y(t)$ over the test dataset. The values for Emax and Emean, for the identified models, over the test dataset, were given in Table 4. It is clear from figure 6 and Table 4 that the proposed RSMM method, particularly the mutifold ridge regression based approach, produces significantly improved model estimation for the solar wind magnetosphere modelling problem, compared with the ordinary linear regression methods.
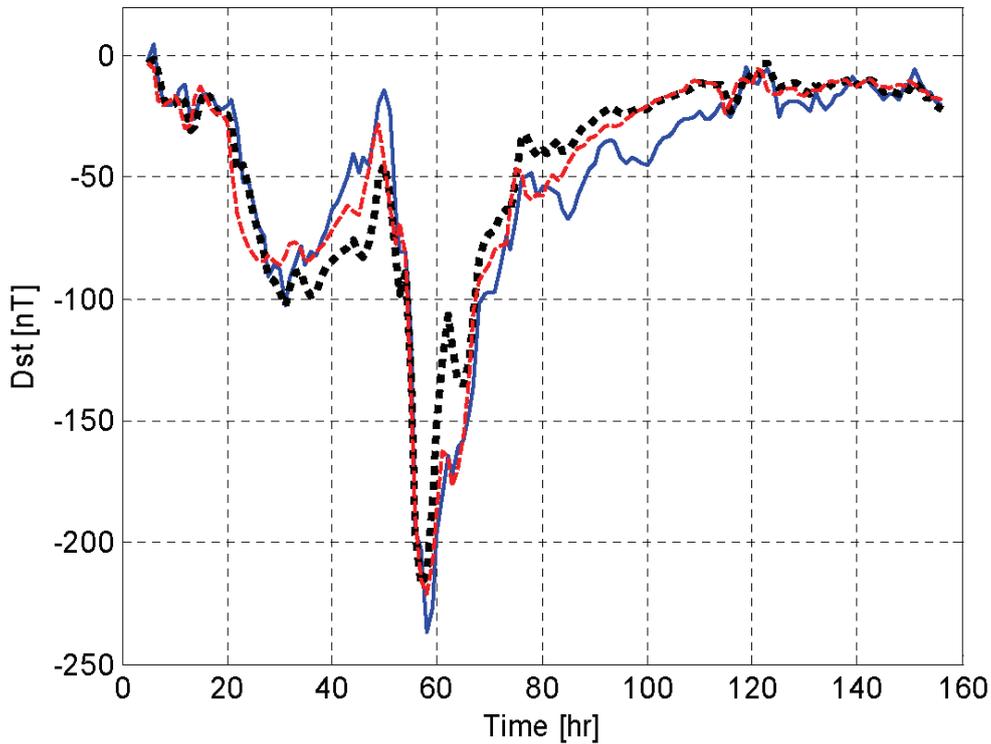

Fig. 6   A comparison of the model predicted output and the measurement for the solar wind magnetosphere modelling problem. The thick solid line represents the measurement; the thick dashed line represents the model predicted output from the RSMM produced model; the dotted-line represents the model predicted output from the traditional OFR algorithm.

5. Conclusions

The application of the new random subsampling and multifold modelling (RSMM) approach involves two steps: model term selection and model parameter refinement. As in other random sampling or bootstrapping methods, the information carried by a given data set can often be sufficiently exploited for model identification by means of the proposed multifold random subsampling approach. When the RSMM approach is applied to model structure selection, some kind of multiple search procedures, over a number of partitioned datasets, are inevitably involved. It would initially seem that the implementation of a multiple search is complex. Fortunately, however, the introduction of the new multiple orthogonal search (MOS) algorithm enables the realization of the associated multiple search to be quite convenient. It should be noted that the computation load of the RSMM algorithm involving K-fold subsampling will approximately be near to K times of that required by a single-time estimation algorithm which involves a single 'hold-out' dataset. But this does mean that the RSMM algorithm is time demanding, in fact for most real-world problems, the calculation of the associated RSMM procedure can be completed within just a few minutes. It should also be pointed out that the effect of the parameter K on the resultant model performance for general problems has not been studied in depth in this work; whether the resultant model performance can be improved by increasing the parameter K needs to be investigated further.

For convenience of description and illustration, the models involved in the first two examples were formed using polynomials, and the model involved in the third example was constructed using B-splines. However, it should be stressed that the RSMM approach can also be applied to any other parametric or non-parametric modelling problems where the initial full models can be written as a linear-in-the-parameters form.

The criterion used for model size determination in this study is a weighted average Bayesian information criterion (WABIC), where a weight coefficient needs to be provided. However, how to chose and optimise such a weight coefficient is still an open problem.

Acknowledgements

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