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An Iterative Orthogonal Forward Regression Algorithm

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Abstract -- A novel iterative learning algorithm is proposed to improve the classic orthogonal forward regression (OFR) algorithm in an attempt to produce an optimal solution under a purely OFR framework without using any other auxiliary algorithms. The new algorithm searches for the optimal solution on a global solution space while maintaining the advantage of simplicity and computational efficiency. Both a theoretical analysis and simulations demonstrate the validity of the new algorithm.

Index Terms: Iterative orthogonal forward regression, model structure detection, nonlinear system identification, orthogonal least squares

1. Introduction

The NARMAX (Nonlinear AutoRegressive Moving Average with eXogenous input) model and the associated Orthogonal Forward Regression (OFR) algorithm have been widely applied in nonlinear system identification including in the modelling of many engineering, chemical, biological, medical, geographical, and economic systems (Billings 2013). Variations of these algorithms have been developed for lumped and distributed parameter systems, time-invariant and rapidly time-varying systems, in the time, frequency and spatio-temporal domains. The OFR algorithm, which is also known as the OLS (Orthogonal Least Squares) or the FOLSR (Forward Orthogonal Least Squares Regression) algorithm, determines the model structure of nonlinear systems based on the ERR (Error Reduction Ratio) criterion without any a priori knowledge except for the specification of an initial model set.

However, under some extreme circumstances (for example non-persistently exciting inputs) the classic OFR algorithm can sometimes select some incorrect model terms (Billings and Wei 2007;

Mao and Billings 1997; Piroddi and Spinelli 2003; Sherstinsky and Picard 1996). Solutions are available which solve this problem (Billings 2013; Billings and Wei 2007; Li et al. 2006; Mao and Billings 1997; Wei and Billings 2008) but most of these methods involve combining the OFR algorithm with other routines. Contrary to the earlier approaches, this paper presents a new proposal to enhance the classic OFR without making any major conceptual changes. To clarify the difference with a standard OFR algorithm the new algorithm will be referred to as the iterative Orthogonal Forward Regression (iOFR) algorithm. The core ideas of the new algorithm are presented and it is shown that the new iOFR method can produce an optimal model under a revised but purely OFR-ERR framework. Another advantage of the new iOFR algorithm is that the new two-step iOFR does not require the initial model obtained at the first step to be an accurate model, which is different from most coarse-to-fine algorithms. This means the iOFR algorithm can start from an incomplete model and can still produce a complete optimal model.

The remainder of the paper is organised as follows. Section 2 briefly reviews the classic OFR algorithm. Section 3 introduces the new iterative OFR algorithm. A simple example is initially introduced to motivate the introduction of an iterative process to search for the optimal solution on a global solution space rather than a local space. Three illustrative examples are discussed in section 4. The first example shows that the iOFR can successfully eliminate any redundant terms and obtain a parsimonious model. The second example shows how the new iOFR algorithm can find the correct terms which may have been missed in earlier algorithms. The third example is used to illustrate the identification of the NARMAX model with noise terms using the new iOFR algorithm. Conclusions are finally drawn in Section 5.

2. NARMAX model and orthogonal forward regression

2.1 NARMAX model

A NARMAX model is essentially an expansion of the output with past inputs, outputs and noise terms. A wide class of nonlinear systems can be represented by a NARMAX model (Billings 2013; Leontaritis and Billings 1985) which can be defined as

$$y(k) = F\begin{pmatrix} y(k-1), y(k-2), \dots, y(k-n_y), u(k-d), u(k-d-1), \\ \dots, u(k-d-n_u), e(k-1), e(k-2), \dots, e(k-n_e) \end{pmatrix} + e(k)$$
(1)

where y(k), u(k) and e(k) are the system output, input, and noise sequences respectively; n_y , n_u , and n_e are the maximum lags for the system output, input, and noise; $F(\Box)$ is some nonlinear function; d is a time delay which is often set as d=1. Although both Volterra series and NARMAX models represent input-output relations, the Volterra series give an explicit representation while the NARMAX model gives an implicit representation, which is often of a much more compact form. A large class of systems can be described using the NARMAX model by selecting different forms of the functions F , for example the nonlinear DARX model (Shouche et al. 1998).

2.2 OFR algorithm

System identification based on the NARMAX model involves selecting the significant model terms from a full candidate term dictionary and then estimating the associated parameters in order to build a parsimonious model. The search for model subsets with minimum mean square error (MSE) can be approached in a straightforward manner by computing all possible regressions but the amount of computation required can be formidable, because the number of possible subsets increases exponentially. OFR offers an efficient procedure for finding the best subsets (Billings et al. 1988). The OFR algorithm involves a stepwise orthogonalisation of the regressors and a forward selection of the model terms based on the error reduction ratio (ERR) criterion (Billings 2013).

Specify an initial full model set $\mathbf{D} = \{\varphi_1, \varphi_2, \dots, \varphi_\kappa\}$, which is composed of a total number of κ candidate terms. Terms φ_i are linear or nonlinear functions of the input, output and noise. When the measurements of input, output, and noise are available, these functions can be evaluated and represented as the regression matrix

$$\boldsymbol{\Phi} = \begin{bmatrix} \boldsymbol{\phi}_1 & \boldsymbol{\phi}_2 & \cdots & \boldsymbol{\phi}_k \end{bmatrix}$$
(2)

where the column vectors $\boldsymbol{\phi}_i$'s are defined as $\boldsymbol{\phi}_i = [\varphi_i(1) \cdots \varphi_i(N)]^T$. By slightly abusing the notation, we sometimes use the column vector $\boldsymbol{\phi}_i$ to represent term φ_i and the regression matrix which includes all the columns to represent the term dictionary **D** in later discussions.

Because normally there is a lack of knowledge regarding the structure of function F in (1), the term dictionary is selected to be redundant and it is assumed that F can be expressed as a linear combination of a subset of **D**, that is $\mathbf{D}_{s} = \{\varphi_{s_{1}}, \varphi_{s_{2}}, \dots, \varphi_{s_{k_{s}}}\} \subset \mathbf{D}$, where $s_{i} \in \{1, 2, \dots, \kappa\}$, so that the model of system (1) can be represented by basis functions

$$\mathbf{y}(t) = \sum_{i=1}^{\kappa_s} \varphi_{\mathbf{s}_i}(t) \theta_i + \mathbf{e}(t)$$
(3)

where θ_i are the coefficients.

Hence system identification based on the measurements involves the determination of the model structure and the estimation of the parameters. However the determination of the structure and the estimation of the parameters are coupled with each other. The significance of a term in a model depends on the estimated parameters while the estimation of the coefficients depends on the model structure. Using a traditional forward regression algorithm, all the coefficients in a model need to be re-estimated when a new term is added. Hence the evaluation of the contribution of a newly added term to the model is computationally intensive because of the matrix inversion involved in the coefficient re-estimation. However, the structure detection and the parameter estimation can be successfully decoupled when all the terms are orthogonal to each other.

Data collected from 1 to N yields the matrix form of equation (3)

$$\mathbf{y} = \boldsymbol{\Phi}_{s} \boldsymbol{\Theta} + \boldsymbol{\Xi}. \tag{4}$$

An orthogonal decomposition of Φ_s is given as

$$\mathbf{\Phi}_{\rm s} = \mathbf{W}\mathbf{A} \tag{5}$$

Here **A** is a $\kappa_s \times \kappa_s$ unit upper triangular matrix and

$$\mathbf{W} = \begin{bmatrix} \mathbf{w}_1 & \cdots & \mathbf{w}_{\kappa_s} \end{bmatrix}$$
(6)

is a N× κ matrix with orthogonal columns which satisfy

$$\left\langle \mathbf{w}_{i}, \mathbf{w}_{j} \right\rangle = \begin{cases} d_{i} > 0, & i = j \\ 0, & i \neq j \end{cases}$$
(7)

where $\langle \cdot, \cdot \rangle$ denotes the inner product defined on space \mathbf{R}^{N} , that is $\langle \mathbf{w}_{i}, \mathbf{w}_{j} \rangle = \mathbf{w}_{i}^{T} \mathbf{w}_{j} = \sum_{k=1}^{N} w_{i}(k) w_{j}(k)$.

Equation (4) can then be written as

$$\mathbf{y} = \mathbf{W}\mathbf{g} = \sum_{i=1}^{\kappa} \mathbf{w}_i \mathbf{g}_i + \mathbf{\Xi}$$
(8)

The coefficient of each term $\,g_{i}\,$ can be calculated individually as

$$\mathbf{g}_{i} = \frac{\langle \mathbf{w}_{i}, \mathbf{y} \rangle}{\langle \mathbf{w}_{i}, \mathbf{w}_{i} \rangle}.$$
(9)

In the OFR algorithm a criterion called the error reduction ratio (ERR) has been introduced to measure the significance of the model terms in the description of system (1) and to determine the model structure by selecting all the significant terms. The error reduction ratio ERR_i due to term w_i is defined as

$$\operatorname{ERR}_{i} = \frac{g_{i}^{2} \langle \mathbf{w}_{i}, \mathbf{w}_{i} \rangle}{\langle \mathbf{y}, \mathbf{y} \rangle} = \frac{\langle \mathbf{w}_{i}, \mathbf{y} \rangle^{2}}{\langle \mathbf{w}_{i}, \mathbf{w}_{i} \rangle \langle \mathbf{y}, \mathbf{y} \rangle},$$
(10)

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It is worth noting that the ERR criterion evaluates the contribution of a term considering both the form of the term and also the associated coefficients, which is essentially different from the orthogonal projection or inner product criterion used by the Projection Pursuit and Matching Pursuit algorithms (Huber 1985; Mallat and Zhang 1993; Pati et al. 1993), where the effects of the coefficients has not been considered.

When all the terms are orthogonal with each other the values of ERR of the terms in a model satisfy

$$1 = \sum_{i=1}^{\kappa_s} ERR_i + \frac{\langle \mathbf{e}, \mathbf{e} \rangle}{\langle \mathbf{y}, \mathbf{y} \rangle}$$
(11)

where the last term on the right hand side of the equation represents the noise-to-signal ratio.

The error reduction ratio offers a simple, effective, and intuitive means of selecting a subset of significant terms from a large number of candidate terms in a forward regression manner. By applying the OFR algorithm and the ERR criterion, the contribution of a term can be evaluated avoiding reestimating all the coefficients. At each step, a term which produces the largest value of ERR₁ among the candidate terms is selected, and the selection procedure is terminated at κ_s step when

$$1 - \sum_{i=1}^{\kappa_s} ERR_i < \rho \tag{12}$$

where ρ is a desired tolerance, and this leads to a subset model of κ_s terms. In the application of the OFR-ERR algorithm, various criteria, such as AIC (Akaike Information Criterion), BIC (Bayesian Information Criterion), and other statistical tests, can be used to aid the termination of the term selection (Billings and Chen 1989).

To summarise, the standard orthogonal forward regression algorithm consists of the following steps:

(i) Sufficiently excite the system and measure the inputs and outputs of the system;

(ii) Specify an initial full model set of κ candidate terms and the value of ρ ;

(iii) Compute the values of the ERR for each of the κ candidate terms and select the term which gives the largest value of ERR into the model as the first term;

(iv) At the k th ($k \ge 2$) stages compute the values of the error reduction ratio for each of the (κ -k+1) remaining candidate terms by assuming that each is the k th term in the selected model and perform the corresponding orthogonalisation; The term that gives the largest value of the error reduction ratio is then selected into the model as the k th term. If condition (12) is satisfied, finish the process and go to (v). Otherwise set k = k+1 and repeat step (iv);

(v) The final model contains κ_s terms and the parameter estimates can be calculated using a least squares formulae.

A geometric interpretation of the above procedure has been given by Chen, Billings & Luo (1989). Consider y as a vector in the N dimensional Euclidean space \mathbf{R}^{N} where $\{\phi\}$ are κ linearly independent vectors in this space. Each of the vectors can be spanned into a one dimensional subspace of \mathbf{R}^{N} . Denote the subspace which is spanned by ϕ as $S(\phi)$. At the first step, the ERR's for each ϕ measure the orthogonal projections of y onto each of the subspaces. The subspace $S(\phi_{i})$ which gives the maximal projection is determined and the corresponding term ϕ_{s_1} is selected as the first term which is denoted as w_1 . At the second step, consider the orthogonal projections of y onto a two dimensional space $S\{\phi_{s_1}, \phi\}$ which is spanned by ϕ_{s_1} and each of the remaining $(\kappa - 1)$ vectors ϕ_{s_1} where $i \in \{1, 2, \dots, \kappa\} \setminus \{s_i\}$. Since at each step ϕ_i has been orthogonalised into w_i , the orthogonal projection of y onto $S\{\phi_{k_i},\phi_{i_j}\}$ can be determined by evaluating the orthogonal projection of y onto w_i . The term ϕ_{s_2} which spans the subspace $S\{\phi_{s_1},\phi_{s_2}\}$ on which the orthogonal projection of y reaches the maximum is selected as the second term. The orthogonalised vectors $\{\mathbf{w}_1, \mathbf{w}_2\}$ comprise an orthogonal basis of the subspace $S\{\phi_{s_1}, \phi_{s_2}\}$. At the kth step, the orthogonal projections of y onto k-dimensional subspaces are considered. The selected term ϕ_{s_k} and the previous k-1 terms span the subspace $S\left\{\phi_{s_1},\phi_{s_2},\cdots,\phi_{s_{k-1}},\phi_{s_k}\right\}$ on which the projection of **y** is maximal.

Compared to traditional forward regression methods, the OFR algorithm is computationally efficient because it successfully avoids the re-estimation of the parameters and evaluates the contribution of each term individually. The OFR is also extremely sufficient in the term selection. At the kth step the regression analysis are preformed on the orthogonal complement of the subspace spanned by the previous k-1 terms. This successfully eliminates the information redundancy in the model and produces a parsimonious model. Accordingly, the OFR can in most cases obtain the optimal solution with only forward selection rather than stepwise regression. However, the classic OFR algorithm may occasionally give a suboptimal model because of the information overlap among the nonorthogonal terms. For example, a wrong term can be selected at the first step because the term carries the information from more than one correct term. This often happens at the first step because the terms have not been orthogonalised. In this paper, a new iterative OFR algorithm will be introduced to solve this problem, to improve the performance of the classic OFR algorithm, and to provide a relatively simple and easy to use algorithm for term selection in complex dynamic models.

3. Iterative orthogonal forward regression

Following the discussion in the previous section, the OFR algorithm selects at each step the best term which comprises an optimal subspace with the existing terms. However optimal choices at every step cannot always guarantee a global optimum. Although the classic OFR algorithm is always very efficient, OFR can sometimes produce a suboptimal solution rather than an optimal one (Billings et al. 1989). This happens because the candidate terms in the initial term dictionary are not orthogonal with each other and the information which is represented by these terms overlaps with each other. The value of the ERR may therefore depend on the order in which the corresponding term enters the model.

In this section, a very simple example is first studied in detail to explain why the basic OFR algorithm sometimes converges to a local optimum. Consider the problem of the regression of a vector β using three linear independent vectors α_1 , α_2 , and α_3 in a three-dimensional space. Define the regression matrix $\mathbf{\Phi}$ as

$$\boldsymbol{\Phi} = \begin{bmatrix} \alpha_1 & \alpha_2 & \alpha_3 \end{bmatrix} = \begin{bmatrix} 1 & 3 & 2.1 \\ 2 & 2 & 1.8 \\ 3 & 1 & 2.1 \end{bmatrix}, \quad \boldsymbol{\beta} = \begin{bmatrix} 2.3 \\ 2.2 \\ 2.1 \end{bmatrix}.$$
(13)

It is easy to show that vector β in this example is actually a linear combination of vectors α_1 and α_2 , satisfying

$$\beta = 0.5\alpha_1 + 0.6\alpha_2. \tag{14}$$

Equation (14) gives the model which represents the accurate relationship between β and the independent vectors.

Figure 1 shows the geometric representation of the four vectors in a three-dimensional Euclidian space. Observe that vector β is closer to α_3 than to the other vectors although β actually stays in the plane spanned by α_1 and α_2 . This is because vector α_3 can be decomposed as

$$\alpha_3 = 0.5\alpha_1 + 0.5\alpha_2 + \alpha_3^{\perp} \tag{15}$$

where $\alpha_3^{\perp} = [0.1 - 0.2 \ 0.1]^{\mathsf{T}}$. Vector α_3 is actually composed of two components: the component which lies in the plane spanned by α_1 and α_2 and a small component α_3^{\perp} which is perpendicular to the plane and has no contribution to the explanation of the dependent vector β . Hence vector α_3 possesses both the information of α_1 and the information of α_2 .



Fig 1 The geometric relations of the vectors in (13)

The standard OFR process is to find a sequence of nesting subspaces $S_1 \subset S_2 \subset \cdots \subset S_{\kappa_s}$ step by step. Each subspace S_k which is spanned by the (k-1) vectors from S_{k-1} and a new selected vector from the regression matrix is optimal at each step. Here optimal means the orthogonal projection of \mathbf{y} on \mathbf{S}_k is maximal. In order to decouple the contribution of each term to the total projection, the k-th term is orthogonalised to the (k-1) terms selected in the earlier steps so that the projection can be calculated stepwise. The k orthogonal terms form a k-dimensional orthogonal basis of space \mathbf{S}_k . Denote the sum

of the ERR values at the k-th step as $SERR_k = \sum_{i=1}^k ERR_i$. The sum of the ERR values represents a normalised measurement to the projection. Mao and Billings (1997) argued that when using the orthogonal algorithm to detect the model structure, previously selected terms can influence the selection of later terms. Therefore the detection of a minimal model structure can be considered as a search for the optimal orthogonalisation path which is defined as the order in which candidate terms are orthogonalised into the regression equation.

In order to analyse the effects of orthogonalisation paths, all the possible orthogonalisation paths are listed in Table 1. For this example, there are a total number of 6 different orthogonalisation paths in which three terms can be orthogonalised into a model.

	Pat	h 1	Pat	h 2	Pat	h 3	Pat	h 4	Pat	h 5	Pat	h 6
No.	Terms	ERRs										
1	α_1	83.02	α_1	83.02	α_2	88.21	α_2	88.21	α_3	99.37	α3	99.37
2	α_2	16.98	α3	16.40	α_1	11.79	α3	11.39	α_1	0.06	α_2	0.23
3	α_3	0	α_2	0.58	α3	0	α_1	0.40	α_2	0.57	α_1	0.40
SERR		100%		100%		100%		100%		100%		100%

Table 1 ERRs along the six different orthogonalisation paths for eq. (14)

Along the six different paths, the orthogonalised terms form six different orthogonal bases which are shown in Fig 2. Projecting β on each of the orthogonal bases, the ERR values are given in Table 1.



Fig 2 Six different orthogonal bases for eq. (14)

An optimal model means the smallest model which includes all the correct terms. In the language of the ERR framework, an optimal model includes the smallest number of terms but produces the largest sum of ERR values. In this example, the optimal model is composed of the two correct terms α_1 and α_2 . The classic OFR algorithm searches for a solution along a path where the sum of the ERR's increases at the fastest speed. In this example, although vector β is on the plane spanned by α_1 and α_2 , the first term that will be selected by the OFR algorithm is α_3 because α_3 is the term which is mostly close to β and gives the largest projection, see Fig 1. Therefore, the OFR will orthogonalise the regressors along path 6 in Table 1, $\alpha_3 \rightarrow \alpha_2 \rightarrow \alpha_1$. However following path 6 the obtained model is not optimal. When a specific tolerance is taken, for example, $\rho = 0.50\%$, a correct term will be missed along path 4, and 6 while a redundant term will be selected along path 2 and 5. However along both paths $\alpha_1 \rightarrow \alpha_2 \rightarrow \alpha_3$ and $\alpha_2 \rightarrow \alpha_1 \rightarrow \alpha_3$, the search process produces an optimal model which consists of two correct terms for any tolerance less than 10%. This means that along a correct orthogonalisation path the algorithm will be much more robust, to yield optimal results, and the cutoff is much more obvious and easier to select.

In a forward regression process, since the terms are selected one by one into a model, all the orthogonal paths comprise a solution tree. At the first step, there are κ options $\phi_1, \dots, \phi_{\kappa}$ which represent the κ direct child nodes of the root node. These direct child nodes divide the whole tree into κ branches and each of the branches is also of a tree structure. There are $(\kappa - 1)$ options at the second step and $(\kappa - 2)$ options at the third step, and so on. There are a total number of κ ! different orthogonalisation paths. A forward regression method starts from the common root node and selects terms one by one from an upper layer to a lower layer. The ERR values assign a weight for each branch of the tree. Each path from the root node to a leaf node represents a complete orthogonalization path along which a corresponding model can be obtained. For the example under consideration, the solution tree is shown in Fig 3.



Fig 3 Solution tree of a forward regression algorithm for eq. (14)

For a globally optimal solution, we would need to search on the whole tree and evaluate all the solutions on the different branches. Observe that there are many opportunities to find a correct solution by exhausting all the paths on the solution tree. For a correct model which consists of m terms there are a total number of m! different perturbations, where (·)! represents the factorial operation, and each represents a correct solution on different branches of the solution tree. There are a total number of m! optimal solutions on the tree. These optimal solutions can only happen on the paths which start from a correct term. Hence only the sub-trees which start from a correct term need to be considered when searching for an optimal solution. In the above example, there are two optimal orthogonalisation paths and only the branches starting from α_1 and α_2 may include the optimal solution.

A classic OFR algorithm can occasionally search along a wrong orthogonalisation path by picking a wrong term in the first steps. As a result, the search process will be along a wrong path and produce a sub-optimal model. From the root node, a searching process can be forced onto a certain sub-tree by fixing the first term before the searching process proceeds. Therefore an intuitive idea is to use the OFR algorithm to search on each of the sub-trees. A sub-optimal model is obtained on each sub-tree. Compare these obtained models and choose the best one as the final result. The optimal model will be in these sub-optimal models. Remember that there are a total number of m! opportunities to find a optimal model. However search on all the sub-trees is not necessary because any search path starting

from a wrong term will never give an optimal model. Therefore, only the sub-trees starting from a correct term need to be considered. However, it is unknown which term is a correct term. Nevertheless a suboptimal model can always be a good starting point for the search for an optimal solution. It is reasonable to assume that a suboptimal model consists of a majority of correct terms and a few incorrect terms. Therefore an iterative learning algorithm can be proposed to find an efficient and intuitive solution to this problem. The new iterative OFR algorithm consists of the following steps.

- i). Preset a tolerance ρ and apply the standard OFR algorithm on the whole term dictionary Φ to produce a suboptimal term set $\Phi_s = \{ \phi_{s_1} \ \phi_{s_2} \ \cdots \ \phi_{s_{n_s}} \};$
- ii). Select a small number $\Delta \rho$ as an amendment to the tolerance in the first step (see Remarks 2 for the choice of $\Delta \rho$);
- iii). Select one of the terms ϕ_j ($j = s_1, s_2, \dots, s_{\kappa_s}$) in Φ_s as a preselected first term and search the other terms on the term set $\Phi \setminus \{\phi_i\}$ to construct a suboptimal solution satisfying $1 \sum \text{ERR}_i < \rho + \Delta \rho$;
- iv). Repeat iii) for all the ϕ 's in Φ_s and obtain κ_s suboptimal models;
- v). Compare the obtained κ_s suboptimal models and choose the best one as the final model Φ_{op} .

NARMAX models which typically include highly correlated unknown noise terms can be identified by following the iterative procedure below. Because the noise terms are not know<u>n</u> a priori the model prediction errors (residuals) will be used to approximate the noise terms.

- i). Assume the noise terms are zero and identify the model which does not included the noise terms using the iOFR algorithm.
- ii). Produce the prediction errors using the best model obtained in step i).
- iii). Use the residuals as the noise terms and construction the new term dictionary in which the delayed noise terms are included.
- iv). Identify the full NARMAX model from the dictionary obtained in step iii) using the iOFR algorithm.

v). Repeat steps ii) - iv) until a satisfying model obtained. At each time the residuals are calculated based on the new identified model. Validate the model.

Remarks:

1) The searching process can be further iterated by selecting Φ_{op} as the suboptimal solution Φ_s in step i) and repeating steps ii) ~ v) for a better result. This time only terms in the set $\Phi_s - \Phi_{op} : \{ \phi | \phi \in \Phi_{op}, \text{ and } \phi \notin \Phi_{op} \}$ need to be considered. However further iterations are often not needed. An optimal solution may be found in the first iteration because the OFR algorithm itself is powerful in searching for an optimal solution but more steps may be needed in some cases.

2) The amendment $\Delta \rho$ of the tolerance often takes a small non-negative number. A tolerance ρ means the sum of ERR's of the selected terms in a model is no less than $(1-\rho)$. Hence the larger a tolerance ρ is, the less terms will be selected in the obtained model. A positive $\Delta \rho$ means $(\rho + \Delta \rho)$ is a stricter tolerance and the iterative process will eliminate some of the redundant terms to produce a smaller model. On the contrary, a negative $\Delta \rho$ means $(\rho + \Delta \rho)$ is a looser tolerance and the iterative process will select more terms into the model and produce a more accurate description. An increase of the tolerance by $\Delta \rho$ can significantly tighten the search process to produce a smaller model. At the same time a small $\Delta \rho$ will not expel the correct terms. For example, a good choice of the absolute value of $\Delta \rho$ can be the ERR value of the least significant term in Φ_s , that is, $\Delta \rho = \min \{ \text{ERR}(\phi) | \phi \in \Phi_s \}$. This follows because after all the correct terms have been selected, the remaining terms are considered as redundant terms and the corresponding contributions will be much smaller than the one with the smallest contribution in the suboptimal model. Since the new iOFR searches for solutions on several sub-trees in parallel and chooses the best model as the result it can be expected that the model which is obtained in the iterative process will be no worse than the suboptimal model in the first step when the tolerance is keeps kept unchanginged. Hence another often used selection of choice in $\Delta \rho$ is 0. When correct terms instead of the wrong terms are selected into

the model, the sum of ERR's will reach $(1-\rho)$ more quickly and a more parsimonious model is obtained.

3) In the classic OFR algorithm, the selection of the tolerance ρ is crucial for the identification of the model. Additionally, the selection of the tolerance is often problem-dependent. For example, the tolerance may depend on the noise level in the measurement of the input and output. A tight tolerance may expel some correct terms while a loose tolerance may cause overfitting of the data. In the classic OFR algorithm, a wrong term is selected in-to a model because the wrong term may include the information of more than one correct term and this becomes more significant at the first steps of the forward selection process. Selecting the wrong term into the model at an early stage will make the correct terms much less significant and the correct terms will be selected into the model later to compensate for the information which has been missed. When the remaining unexplained information is small and is comparable to the effects of noise, a slight change in the tolerance may lead to a different model the tolerance will become very sensitive. Hence accurate determination of the tolerance under which no correct terms will be missed can be difficult. This can be avoided by using the new iOFR algorithm. When any of these correct terms has been forced to be the first term, the contribution of the wrong term becomes much less significant because part of the information has been explained by the pre-determined-correct terms which has been selected in the previous steps. As a result, there is a much lesser possibility that the wrong term will be selected at the following steps. Along a correct orthogonalisation path all the correct terms will be significant and the OFR algorithm will be more robust to the value of the tolerance. This has been observed in the previous example where any tolerance which is not greater than 10% will lead to the correct model. Hence, the setting of the tolerance ρ can be relatively flexible in the new iOFR algorithm. This feature of the iOFR can be very useful in the identification of real systems.

4) <u>Unlike a coarse-to-fine algorithm which starts from a sub-optimal model and purely eliminates</u> redundant terms, In-the iterative stepsOFR algorithm, the search process is not operated search terms on the suboptimal set Φ_s but on the whole dictionary rather than on the suboptimal set Φ_s -except for the pre determined term ϕ_i . This enables the iOFR algorithm to select <u>find</u>-the correct terms which have been missed in the by the sub-optimal model which is obtained at <u>in</u> the first stage into the final model to<u>and</u> obtain a better solution. In other words, the new iOFR algorithm does not need the suboptimal model obtained at the first step to be a sufficient model. This will be observed in the example in Section 4.2.

The new iOFR algorithm may occasionally give a suboptimal solution since the algorithm only tries different routes at the first step and the remaining term selection could still follow a suboptimal trace. However this will happen with a very low probability. Firstly, the new iOFR searches the optimal model in parallel along several different paths on the whole solution tree. According to the previous discussion, there are a total number of m! opportunities to find the optimal model and hence the probability at which the iOFR can find the optimal solution will increase significantly. The improvement in the possibility to find the optimal solution will be discussed below. Secondly, along the different search paths the corresponding orthogonal basis will be quite different and the ERR's assigned to each term will change accordingly. The significant terms will then be selected into the term in a different order. This has been observed in the example given in Fig 2. To some extent, this process works like the heating process in a simulated annealing algorithm where the metal atoms in the material will be rearranged to build a better crystal structure in the cooling process. Finally, according to the previous discussion, the significance of a wrong term which may be selected in the first steps because it contains information from the correct terms will be greatly reduced when any of the correct terms has been firstly selected. In the selection of the remaining terms, the wrong term will be less likely to be selected although the search is still along the speediest increasing path of the sum of ERR values. Based on the above discussion, these are probably the best solutions available because the alterative full optimal search (Mao and Billings 1997) involves a huge computational overload that is just not feasible when studying real data sets where it is often necessary to try lags over the range 1-30 in the initial search. Noise model terms and MIMO (multi-input-multi-output) systems just further aggravate this problem.

We should ask what the probability is that the new iOFR algorithm will produce an optimal solution. Assume κ_1 terms in a $\kappa_2 - \kappa_2$ terms of the suboptimal model Φ_2 which were was obtained at the first stage-and are correct; the OFR algorithm can find an optimal solution with a probability of p along each path starting with a correct term. The iOFR algorithm will search the optimal solution along κ_s parallel paths. The probability that the iOFR will find the optimal solution on at least one path will be $1-(1-p)^{\kappa_1}$, which equals to one minus the probability that the iOFR fails to find the optimal solution <u>on all the paths</u>, seeing that the search along the $(\kappa_s - \kappa_1)$ paths which start with a wrong term will have no contribution for to the probability. The probability will be much higher than the probability of the single path search when κ_1 is large enough. For example, consider a suboptimal model which consists of $\kappa_s = 20$ terms in which $\kappa_1 = 10$ terms are correct terms. The iOFR algorithm searches for the optimal solution along 10 parallel paths at a probability of 50% on each path. It is easy to calculate that the probability that the iOFR algorithm will find the optimal solution is $(1-0.5^{10}) \approx 99.9\%$ which is much higher than the 50% succession probability of the single path search algorithm. In fact, the probability for the classic OFR to successfully find the optimal solution is much better than 50%. Even the classical OFR can produce an optimal solution in most cases except in some special situations.

The new iOFR algorithm is also computationally efficient. As discussed in the paper (Mao and Billings 1997), there are a total number of κ ! orthogonalization orthogonalisation paths for a κ term dictionary, where (·)! represents the factorial operation. Searching for an optimal solution by exhausting all these paths is computationally just not practical. Applying the genetic algorithm assistant MMSD (Minimal Model Structure Detection) algorithm the search space can be reduced to a much more practical number which can still be a large number. Comparatively, in the new iOFR algorithm, the number of searching paths depends on the number of terms in the sub-optimal model obtained at the first stage which is much less than the size of the full dictionary, without mentioning the number of all the combinations. Consider the example in the Mao and Billings paper where 20 terms were included in the dictionary. An exhaustive search needs to evaluate 2.433×10¹⁸ paths; the

MMSD algorithm searches along 2×10^3 paths. Using the new iOFR algorithm, no more than 20 best searching paths which start from the terms in a suboptimal model need to be evaluated. Therefore it can be concluded that the new iOFR algorithm is very efficient. A discussion of the computational complexity of the classic OFR algorithm has been given in the references.

The performance of the new iOFR algorithm can be improved by appropriately increasing the number of parallel searches. For example, a smaller tolerance in the first stage will lead to a sub-optimal model with more terms and the global search at the second stage will be carried out on more parallel sub-trees. The iOFR algorithm can also be improved by increasing the number of the pre-selected terms where a subset instead of a term in Φ_s is pre-determined. The more correct terms are predetermined, the less possibly the wrong term will be selected into the final model. However, both improvements lead to an increase in computational complexity.

An alternative OFR algorithm has been proposed by Piroddi and Spinelli (2003) based on minimising the model predicted or simulated output rather than the one step ahead predictions. This is very similar to the algorithms by Billings and Mao (1998). The simulated output based algorithm has been shown to be effective where the data is grossly oversampled and where the input is badly designed and not persistently exciting. However, these solutions are hugely computationally expensive so that they cannot be realistically applied to complex models where searches over many lags, MIMO models, and noise are involved all of which are typical when dealing with real data sets rather than very simple simulated examples. The new iOFR offers a much simpler solution.

4. Test examples

Several examples will beare used to illustrate the new iOFR algorithm. While the literature is full of examples where the classical OFR algorithm works extremely well, each example below has been deliberately chosen from the small number of past results where the standard OFR has been shown to give non ideal results. In other words worst case examples are used below because on typical

examples where the data is sampled correctly and the input is persistently exciting the algorithm works perfectly every time.

4.1. A linear example

This linear example will beis used to show that the OFR algorithm can sometimes give a suboptimal model which includes redundant terms. But by applying an iterative process, the OFR algorithm is greatly improved and is able to produce an optimal solution. This example was taken from (Wei and Billings 2008).

Consider the system

$$y(k) = -1.7y(k-1) - 0.8y(k-2) + u(k-1) + 0.8u(k-2) + e(k)$$
(16)

where y(k), u(k), and e(k) represent the output, input and noise of the system. The input is uniformly distributed white noise u(k) ~ U(-1,1). The noise is normally distributed white noise e(k) ~ N(0,0.1²). A total number of 1000 input and output data are measured for the system identification. Define a candidate term dictionary which is composed of the delayed input and output terms $\Phi = \{y(k-1), y(k-2), y(k-3), y(k-4), y(k-5), u(k-1), u(k-2), u(k-3), u(k-4), u(k-5)\}$. Applying the classic OFR algorithm, the identified model is shown in Table 1. A total number of seven terms have been selected into the model which includes all the correct terms. However three redundant terms have also been selected.

No	Torms	EDD	Coefficients	Standard
110.	Terms	LIKKS	Coefficients	Deviation
1	y(k-1)	67.8218	-1.6982	0.02894
2	u(k-1)	26.6089	0.9994	0.00557
3	y(k-4)	2.8635	0.0017	0.01235
4	u(k-4)	0.5968	-0.0021	0.01396
5	u(k-3)	0.4825	0.0036	0.01325
6	u(k-2)	0.4121	0.7912	0.02944
7	y(k-2)	0.3908	-0.7992	0.03679
SERR		99.18		

Table 2 Results given by the standard OFR algorithm for system (16)

In this example the classic OFR algorithm gives an incorrect model because of under-sampling. System (16) can be considered as a discretisation of a second order system with a very low sampling frequency. The frequency response function and impulse response of system (16) (see Figure 4) show that the natural frequency of the system is around 0.45 Hz. The sampling frequency in this example is 1 Hz which is only about 2.2 times of the natural frequency. The severe under-damping in the system exasperates this problem. The impulse response shows that the system needs a long time to settle down and oscillates with a period about 2.2s. This means the response of the system will repeat every 2.2s (about 2 sampling intervals). Since the output is a convolution of the input with the impulse response function, y(k) may be of a similar pattern with y(k-2). This explains why y(k-4) may appear in the final model because the term looks like y(k-2) for this sampling and data case. The effect of sampling time on nonlinear system identification has been studied by Billings and Aguirre (1995), and Billings (2013).



Figure 4 Frequency response function and impulse response of system (16)

Taking each term in Table 2 as the first term and applying an OFR algorithm where $\Delta \rho = 0.3908$ % which is the least value of the ERR's in Table 2, yields the results of the iOFR process given in Table 3. Seven different models were obtained. Models 6 and 7 have the simplest structure where only four terms are used to produce the best SERR. Actually both models consist of four correct terms. Models 1, 2, 3, 4, and 5 missed the correct term y(k-2) under the amended tolerance ($\rho + \Delta \rho$) and produce a relatively smaller SERR. Therefore model 6 and model 7 are selected as the final results of the iOFR process. Notice that both models include the same terms with the same associated coefficients. All the

redundant terms in Table 2 have been successfully eliminated in the iterative process. The iOFR algorithm which starts from the results of a standard OFR process <u>gave gives</u> the optimal model.

		Model 1			Model 2			Model 3			Model 4	
No.	Terms	ERRs	Coeffs									
1	y(k-1)*	67.8218	-1.081	u(k-1)*	23.8334	0.997	y(k-4)*	3.509	-0.2546	u(k-4)*	5.614	0.2622
2	u(k-1)	26.6089	0.997	y(k-1)	70.5972	-1.081	y(k-1)	66.7799	-1.081	y(k-1)	62.2166	-1.081
3	y(k-4)	2.8635	-0.2546	y(k-4)	2.8635	-0.2546	u(k-1)	27.0053	0.997	u(k-1)	26.8122	0.997
4	u(k-4)	0.5968	0.2622	u(k-4)	0.5968	0.2622	u(k-4)	0.5968	0.2622	y(k-4)	3.2483	-0.2546
5	u(k-3)	0.4825	-0.2354									
6	u(k-2)	0.4121	0.1748									
SERR		98.79			98.79			98.79			98.79	
		Model 5			Model 6			Model 7				
No.	Terms	ERRs	Coeffs	Terms	ERRs	Coeffs	Terms	ERRs	Coeffs			
1	u(k-3)*	8.9466	-0.3878	u(k-2)*	18.5449	0.7881	y(k-2)*	36.7635	-0.7941			
2	y(k-1)	59.2524	-1.2489	y(k-1)	49.3851	-1.6951	y(k-1)	32.6657	-1.6951			
3	u(k-1)	26.2424	0.9987	u(k-1)	26.6444	0.9992	u(k-1)	26.8377	0.9992			
4	y(k-3)	3.3286	0.3865	y(k-2)	4.6019	-0.7941	u(k-2)	2.9095	0.7881			
5	u(k-2)	1.2412	0.3418									
SERR		99.01			99.18			99.18				

Table 3 Results produced by iOFR algorithm for system (16)

* means the term is determined first.

4.2. A nonlinear example

This example is taken from (Mao and Billings 1997). System (17) has been widely used as a benchmark example for the study of variations of OFR algorithms and for comparisons of OFR with other algorithms (Baldacchino et al.). In this example, it will be shown that the iOFR can produce an optimum solution even when some correct terms are not selected in the first OFR step.

Consider the nonlinear system

$$y(k) = 0.2y^{3}(k-1) + 0.7y(k-1)u(k-1) + 0.6u^{2}(k-2) - 0.5y(k-2) -0.7y(k-2)u^{2}(k-2) + e(k)$$
(17)

The system is excited with a uniformly distributed white noise $u(k) \sim U(-1,1)$ and the output y(k) is disturbed by a normally distributed white noise $e(k) \sim N(0,0.1^2)$. A total number of 1000 input and output data were used for the system identification.

Up to third order polynomials of the delayed inputs and outputs {y(k-1), y(k-2), y(k-3), y(k-4), u(k-1), u(k-2), u(k-3)} were used to model the nonlinear system. A total number of 120 terms were included in the term dictionary $\mathbf{\Phi}$. Applying the OFR algorithm yields a five term model which is shown in Table 4. Notice that the model in Table 4 includes an redundant term y(k-4)u²(k-2) but misses a correct term y(k-2)u²(k-2).

No.	Terms	ERRs	Coefficients	Standard Deviation	
1	$y(k-4)u^{2}(k-2)$	36.2732	0.2922	0.02602	
2	y(k-1)u(k-1)	13.7147	0.6544	0.01528	
3	u ² (k-2)	11.3488	0.5134	0.009331	
4	y(k-2)	26.8516	-0.6743	0.01165	
5	y ³ (k-1)	3.3248	0.1949	0.009847	
SERR		91.513			

Table 4 Results produced by the standard OFR algorithm for system (17)

The nonlinear cross correlation model validation tests (Billings and Voon 1986; Billings and Zhu 1994) clearly show that the model is unacceptable as a sufficient model of system (17). Figure 5 shows that the cross correlation tests fail with two of the five cross correlations significantly outside the 95% confidence intervals. Notice that this model has been obtained by deliberately abusing the classic OFR algorithm to test the robustness of the new iOFR algorithm. In the application of the OFR algorithm, a-model validation is always adopted-conducted to aid the determination of the model size. An obtained model should be sufficient enough to pass all the model validations. For this example, an acceptable model can be obtained by increasing the number of terms until the model validations are-is satisfied.



Fig 5 Cross correlation model validation for example 4.2

Take the incorrect model in Table 4 as the starting point and apply the iOFR algorithm. Use each term in the previous model as the first term and employ the OFR algorithm to select the remaining terms until SERR satisfies a tolerance where $\Delta \rho = 0$. The new iOFR produced five different models. The results are shown in Table 5. All the five models have the same number of terms. However models 3 and 4 give a better SERR than the other three models. Compared with system (17), both models 3 and model 4 are composed of the correct terms and give an accurate representation of the original system. It is worth emphasising that the missed term $y(k-2)u^2(k-2)$ in Table 3 has now been correctly selected into the final model by the iOFR algorithm.

	Model 1			Model 2			Model 3		
No.	Terms	ERRs	Coeffs	Terms	ERRs	Coeffs	Terms	ERRs	Coeffs
1	$y(k-4)u^{2}(k-2)*$	36.2732	0.2922	y(k-1)u(k-1)*	13.7511	0.6544	u ² (k-2)*	24.7602	0.6004
2	y(k-1)u(k-1)	13.7147	0.6544	$y(k-4)u^{2}(k-2)$	36.2367	0.2922	y(k-2)	48.5816	-0.5124
3	u ² (k-2)	11.3488	0.5134	u ² (k-2)	11.3488	0.5134	y(k-1)u(k-1)	13.985	0.6828
4	y(k-2)	26.8516	-0.6743	y(k-2)	26.8516	-0.6743	$y(k-2)u^{2}(k-2)$	3.2488	-0.6683
5	y ³ (k-1)	3.3248	0.1949	y ³ (k-1)	3.3248	0.1949	y ³ (k-1)	3.4452	0.1983
SERR		91.513			91.513			94.0208	
	Model 4			Model 5					
No.	Terms	ERRs	Coeffs	Terms	ERRs	Coeffs			
1	y(k-2)*	29.8926	-0.5124	y ³ (k-1)*	0.9922	0.1949			
2	u ² (k -2)	43.4491	0.6004	$y(k-4)u^{2}(k-2)$	37.4213	0.2922			
3	y(k-1)u(k-1)	13.985	0.6828	y(k-1)u(k-1)	15.4601	0.6544			
4	$y(k-2)u^{2}(k-2)$	3.2488	-0.6683	y(k-2)	11.9572	-0.6743			
5	y ³ (k-1)	3.4452	0.1983	$u^2(k-2)$	25.6822	0.5134			
SERR		94.0208			91.513				

Table 5 Results produced by iOFR algorithm for system (17)

* represents the term is determined first.

In both examples, the new iOFR algorithm produced optimal models which include all the correct terms and are of the simplest structure in a very efficient computational process. The iOFR algorithm worked well even when the first OFR step did not give a correct model as in the second example. Moreover, in both examples, the iOFR algorithm found optimal solutions on more than one searching path. This indicates that the new algorithm is significantly robust because the iOFR can still produce an optimal solution even when the algorithm fails on one of the parallel search paths.

4.3. A nonlinear example with noise modelling

This example is <u>taken</u> from <u>and uses the same settings in the Piroddi and Spinelli's paper with the</u> <u>same parameter settings</u> (Piroddi and Spinelli 2003). This example will be used to show that the iOFR algorithm can correctly identify an optimal model even when the systems are not persistently excited.

This example also illustrates the application of iOFR in identification of NARMAX models including delayed noise terms.

The system is given as follows

$$\begin{cases} w(k) = u(k-1) + 0.5u(k-2) + 0.25u(k-1)u(k-2) - 0.3u^{3}(k-1) \\ y(k) = w(k) + \frac{1}{1 - 0.8z^{-1}}e(k) \end{cases}$$
(18)

where u represents the input signal and y represents the observation of the output w. Both the input u(k) and the noise e(k) are Gaussian distributed white noise. It can be shown that the classic OFR algorithm can correctly select all the terms and produce an accurate model when the system is persistently excited. However, Piroddi and Spinelli argued that the classic OFR algorithm may incorrectly select autoregressive terms when the input signal is <u>less_not_rich_enough</u> in frequency components. Piroddi and Spinelli recommended an input which is generated by an AR process with two real poles between 0.75 and 0.9. Repeating Piroddi and Spinelli's simulation using an input signal which was generated by the following AR process.

$$u(k) = \frac{0.3}{1 - 1.6z^{-1} + 0.64z^{-2}} v(k)$$
(19)

where v(k) is Gaussian noise v(k) ~ N(0,1). The AR process has a repeat pole at 0.8 and the coefficient 0.3 is chosen to guarantee the input signal is at a reasonable level. Here the noise signal e(k) is a Gaussian distributed noise with a variance 0.02, that is, $e(k) \sim N(0,0.02)$. The results produced by the classic OFR algorithm are given in Table 6.

No.	Terms	ERRs	Coefficients	Standard Deviation	
1	y(k-1)	87.0633	0.4260	0.01436	
2	y(k-2)	6.9723	0.0131	0.004886	
3	u ³ (k-1)	1.1786	-0.3015	0.001741	
4	u ³ (k-2)	3.6867	0.1346	0.004265	
5	u(k-1)	0.1917	1.1097	0.0194	
6	$u^{2}(k-1)$	0.7733	0.1409	0.003438	
7	u(k-2)	0.0050	-0.2613	0.03052	
8	y(k-1)u(k-1)	0.0023	0.0034	0.003889	
9	y(k-2)u(k-1)	0.0053	0.0140	0.001935	
10	y(k-1)u(k-2)	0.0016	-0.0169	0.004702	
SERR		99.88			

Table 6 Results produced by the classic OFR algorithm for example 3

Observe that several incorrect autoregressive terms have been selected overwhelming the correct terms while a correct term u(k-1)u(k-2) was is missed. The new iOFR algorithm was employed to solve the problem. Each term in the model in Table 6 was selected as the pre-determined term and the remaining terms were selected in a model using a classic OFR algorithm. In this example, a total

number of 10 models were obtained. Three in the ten models give the same model which is the best model obtained under the given tolerance of 0.2%.

No.	Terms	ERRs	Coefficients	Standard Deviation
1	u ³ (k-1)	79.8101	-0.3002	0.000578
2	u(k-1)	14.4655	0.9686	0.01938
3	u (k-1)u(k-2)	5.3722	0.2485	0.001905
4	u(k-2)	0.1596	0.5413	0.01864
5	constant	0.0050	0.0477	0.009254
SERR		99.81		

Table 7 Model identified using the iOFR algorithm for example 3

Next we generated the residuals $\varepsilon(k) = y(k) - \hat{y}(k)$, where $\hat{y}(k)$ is the one-step-ahead prediction of the model in Table 7. Use-We then used the residuals to replace the noise terms. The new dictionary is composed of all the up to third order monomials of variables { u(k-1), u(k-2), y(k-1), y(k-2), $\varepsilon(k-1)$, $\varepsilon(k-2)$, $\varepsilon(k-3)$ }. The new iOFR is-was then used to identify the full NARMAX models form the constructed dictionary under the tolerance level 0.2%. This time -three of seven search paths gave the optimal solution which is shown in Table 8. All the terms in system (18) were successfully detected and the associated coefficients are close to the real values in the first time iteration for the noise model.

Standard ERRs Coefficients No. Terms Deviation 79.8129 -0.2995 1 u3(k-1) 0.000349 2 u(k-1) 14.4635 0.9647 0.012 3 u (k-1)u(k-2) 5.3719 0.2543 0.000933 0.1591 4 u(k-2) 0.5395 0.01156 ε(k-1) 5 0.1174 -0.7922 0.01968 SERR 99.92 ------

Table 8 Full model identified using the iOFR algorithm for example 3

5. Conclusions

Several algorithms have been proposed to enhance the OFR algorithm by introducing modified or add on algorithms, but the new iterative orthogonal forward regression algorithm improves OFR under a purely OFR framework. Very little extra programming is needed to implement the new iOFR algorithm which is also highly computationally efficient. The new iOFR improves the classic OFR in two ways: it eliminates the redundant terms in a suboptimal model to produce a more parsimonious model, and selects the correct terms to obtain an accurate system description. Because the new iOFR searches for the solution over the whole solution tree iOFR is capable of producing an optimal solution using simple search procedures and can be applied to estimate highly complex system models within a very efficient and intuitive framework.

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