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Abstract: Spatio-temporal evolutionary (STE) images are a class of complex dynamical systems that evolve over both space and time. With increased interest in the investigation of nonlinear complex phenomena, especially spatio-temporal behaviour governed by evolutionary laws that are dependent on both spatial and temporal dimensions, there has been an increased need to investigate model identification methods for this class of complex systems. Compared with pure temporal processes, the identification of spatio-temporal models from observed images is much more difficult and quite challenging. Starting with an assumption that there is no apriori information about the true model but only observed data are available, this study introduces a new class of multiscale lattice cell (MLC) models to represent the rules of the associated spatio-temporal evolutionary system. An application to a chemical reaction exhibiting a spatio-temporal evolutionary behaviour, is investigated to demonstrate the new modelling framework.

Keywords: Cellular neural networks, coupled map lattices, mutual information, orthogonal least squares, parameter estimation, spatio-temporal evolutionary systems.

1. Introduction

In the real world, spatio-temporal evolutionary (STE) phenomena is found in many diverse fields of science and engineering including biology, chemistry, ecology, geography, medicine, physics, and sociology (Kaneko 1993, Jahne 1993, Silva and Principe 1997, Astic et al. 1998, Bascompte and Sole 1998, Czaran 1998, Spors and Grinvald 2002, Dimitrova and Berezney 2002, Berezney et al. 2005, Dolak and Schmeiser 2005). To analyse or imitate STE phenomena, several efficient representations, for example the well known cellular automata (CA) (Wolfram 1994, Adamatzky and Bronnikov 1990, Adamatzky 1994, 1996, 2001, Ilachinski 2001), cellular neural networks (CNNs) (Chua and Yang 1988a, 1988b, Roska and Chua 1993, Chua et al. 1995, Crounse and Chua 1995, Thiran et al. 1995, Chua and Roska 2002), and coupled map lattice (CML) models (Kaneko 1989, 1993), have been proposed. In these representations, it is often assumed that the associated mathematical model structure, along with the model parameters, is known, so that the model can be used to describe or analyse some specific phenomena. However, the evolution laws associated with real-world STE phenomena may not always be completely known, and evolution rules need to be acquired from observed data of images or patterns. Hence, in recent years, the identification of spatio-temporal models from observed data has received much attention and several efficient identification methods and algorithms have been proposed, see for example Adamatzky and Bronnikov (1990), Adamatzky (1994, 1996, 1997), Sitz et al. (2003), Coca and Billings (2001), Mandelj et al. (2001), Billings and Coca (2002), Billings and Yang (2003), Yang and Billings (2003), Billings et al. (2006).

This study considers the spatio-temporal model identification problem, where it is assumed that there is no apriori information about the true model structure and only imaged data are available. Motivated by the successful applications of the wavelet-based multiscale and multiresolution analysis approach (Mallat 1989) in classical signal and image processing (Mallat 1998, Unser 1999), as well as in dynamical process modelling (Billings and Coca 1999, Billings and Wei 2005a, 2005b, Wei and Billings 2004a, 2004b, 2006, Wei et al. 2004, 2006), and also inspired by the easy tractability of conventional coupled map lattice models (Kaneko 1989, 1993), this study aims to introduce a novel multiscale lattice cell (MLC) model for STE system identification. Unlike in a typical wavelet-based multiscale or multiresolution dynamical modelling approach, where the elementary building blocks are strictly chosen to be some dyadic wavelets, in the new MLC model, the choice of the prototype functions are permitted to be very flexible, any functions including wavelets, B-splines and Gaussian type functions can be chose as the elementary building blocks as long as there is strong evidence that the functions possess desirable properties and can lead to a good model for a given modelling problem. In most existing wavelet models for dynamical systems, the scale and shift parameters are restricted to a dyadic lattice. Dyadic wavelet models are proved to be perfect for general static signal representation, in that dyadic wavelets, along with associated scale functions, can often form orthogonal (orthonormal) bases that play an important role in wavelet multiresolution analysis (MRA) (Mallat 1989, Daubechies

1992). An important property of an orthonormal decomposition is that the well known Pareval's theorem holds, that is, the energy of a signal is conserved, without any loss, in the wavelet coefficients. For the STE dynamical system modeling problem, where observations are often sparse in the problem space, however, a dyadic lattice may not usually be an optimal choice. In addition, data used in dyadic wavelet models for nonlinear dynamical systems often need to be compressed or normalised to [0,1], to simplify the associated modelling procedures (especially for the determination of the wavelet shift parameters) (Billings et al. 2006). Although data normalization is frequently used in many modelling approaches and can often simplify the associated modeling procedures, normalization may, at the same time, change the physical meanings of the signals to be modeled. This may be undesirable for some applications where variables are required to preserve their physical dimension. In the new MLC model, data normalisation procedures become unnecessary.

The MLC model is composed of a number of basis functions; the feature of each individual function is determined by three factors: the scale (dilation) parameter, the shift (translation) parameter, and the coefficient weighted on the associated function. For a chosen elementary building block (the prototype function), the task of MLC model identification involves as least three aspects: the determination of the scale and shift parameters; the determination of the model structure and complexity, that is, the determination of which and how many basis functions should be included in the model; and the estimation of the weight coefficients. A new simple unsupervised histogram-based clustering algorithm is introduced; this method can be used to determine the scale and shift parameters of individual functions that will be used to form an initial full MLC model; this full model is in general highly redundant. A forward orthogonal regression (FOR) learning algorithm (Billings and Wei 2007a, Wei and Billings 2007), implemented using a mutual information estimation method, is then applied to refine and improve the initial MLC model by removing redundant basis functions.

2. The MLC Model

In this study, the two-dimensional case, which has obvious physical meanings and is widely applied in practice, is taken as an example to illustrate how to construct an MLC model. For simplicity, only the zero-input (autonomous) case is considered here. In an autonomous STE system, no external input image is imposed, and the output image at any time t is due exclusively to the initial conditions and the evolution of the pattern. Model representations for these situations can easily be extended, in a straightforward way, to other more complex cases.

2.1 The lattice cell model

Assume that the 2-D image or pattern produced by an STE system, at the time instant t, consists of a $I \times J$ rectangular array of cells, $C^t(i, j)$, with Cartesian coordinates (i,j), i=1,2, …, I, j=1,2, …, J.

Following Chua and Roska (2002), let $S_r^t(i,j)$ be the sphere of influence of the radius r of cell $C^t(i,j)$, at the time instant t, defined as

$$S_r^t(i,j) = \{C^t(i,j) : \max_{1\le p\le I, 1\le q\le J} \{|i-p|, |j-q|\} \le r\} \tag{1}$$

where t=1,2, …, i=1,2, …, I, j=1,2, …, J, and r is a non-negative integer number indicating how many neighborhood cells are involved in the evolution procedure. The sphere $S_r^t(i,j)$ is sometimes referred to as the $(2r+1)\times(2r+1)$ neighbourhood. Let $s_{i,j}(t) \in \mathrm{R}$ be the state variable representing the cell $C^t(i,j) \in S_r^t(i,j)$. From the definition of $S_r^t(i,j)$, a total of $(2r+1)^2$ state variables are involved in (1), see Table 1, where the symbol $C(i,j)$ will be used to indicate cells at an arbitrary evolution time instant.

Let $s_{i,j}(t)$ be the (i,j)th cell to be updated at time t. A wide range of STE systems can be described by the discrete-time, discrete-space and continuous-state spatio-temporal difference equation of the form below

$$\begin{aligned} s_{i,j}(t) &= f(\mathbf{s}(t-1), \mathbf{s}(t-2), \mathrm{L}\ , \mathbf{s}(t-n_{lag})) \\ &= f(s_{i-r,j-r}(t-1), \mathrm{L}\ , s_{i,j}(t-1), \mathrm{L}\ , s_{i+r,j+r}(t-1), \mathrm{L}\ , \\ &\quad s_{i-r,j-r}(t-2), \mathrm{L}\ , s_{i,j}(t-2), \mathrm{L}\ , s_{i+r,j+r}(t-2), \mathrm{L}\ , \\ &\quad s_{i-r,j-r}(t-n_{lag}), \mathrm{L}\ , s_{i,j}(t-n_{lag}), \mathrm{L}\ , s_{i+r,j+r}(t-n_{lag})) \end{aligned} \tag{2}$$

where f is some nonlinear function, n_{lag} is the time lag, defined as a positive integer, indicating how many past images or patterns are involved in the evolution procedure, and $\mathbf{s}(t-k)$ is the state vector formed by the $(2r+1)^2$ state variables relative to the patterns at the time instant $(t-k)$ with k=1,2, …, n_{lag}, that is,

$$\mathbf{s}(t-k) = [s_{i-r,j-r}(t-k), \mathrm{L}\ , s_{i,j}(t-k), s_{i+r,j+r}(t-k)] \tag{3}$$

Table 1. The $(2r+1)\times(2r+1)$ neighbourhood

$C(i-r, j-r)$ x_1	…	$C(i-r, j)$ x_r	…	$C(i-r,j+r)$ x_{2r+1}
…	…	…	…	…
$C(i, j-r)$ $x_{r(2r+1)+1}$	…	$C(i,j)$ $x_{r(2r+1)+(r+1)}$	…	$C(i,j+r)$ $x_{(r+1)(2r+1)}$
	…		…	…
$C(i+r,j-r)$ $x_{2r(2r+1)+1}$	…	$C(i+r,j)$ $x_{2r(2r+1)+(r+1)}$	…	$C(i+r,j+r)$ $x_{(2r+1)\ (2r+1)}$

Note that the general lattice cell representation form (2) includes, as special cases, most typical coupled map lattice models. For convenience of description, introduce d single-indexed variables $x_k(t)$ as below

$$\mathbf{x}(t) = [x_1(t), x_2(t), \mathrm{L}\ , x_d(t)] = [\mathbf{s}(t-1), \mathbf{s}(t-2), \mathrm{L}\ , \mathbf{s}(t-n_{lag})] \tag{4}$$

where $\mathbf{s}(t-k) = [x_{1+(k-1)(2r+1)^2}(t), \mathrm{L}\ , x_{k(2r+1)^2}(t)]$ for k=1,2, …, n_{lag} . For the case n_{lag} =1, the description (4) is shown in Table 1. Also, let $y(t)$ represent the state variable $s_{i,j}(t)$ corresponding to the central cell $C^t(i, j)$. Then, Eq. (2) becomes

$$y(t) = f(\mathbf{x}(t)) = f(x_1(t), x_2(t), \mathrm{L}\ , x_d(t)) \tag{5}$$

In conventional coupled map lattice models, the nonlinear function f in model (2) is often assumed to be known as some deterministic function. However, for real-word complex STE systems, a pre-determined function f may not sufficiently characterise the underlying dynamics. It may be better to learn, from available real observations, an appropriate model for a given STE system. The task of STE system identification is to construct, based on available data, a model that can represent, as close as possible, the observed evolution behaviour. Unlike constructing static models for typical data fitting, the objective of dynamical modelling is not merely to seek a model that fits the given data well, it also requires, at the same time, that the model should be capable of capturing the underlying system dynamics carried by the observed data, so that the resultant model can be used in simulation, analysis, and control studies.

2.2 The new MLC model

Inspired by the idea behind the traditional coupled map lattice models, the present study employs an additive model structure to approximate the nonlinear function (5)

$$y(t) = \hat{f}(\mathbf{x}(t)) + e(t) = f_1(x_1(t)) + f_2(x_2(t)) + \mathrm{L}\ + f_d(x_d(t)) + e(t) \tag{6}$$

where $f_i(\cdot)$ are some univariate nonlinear functions that need to be identified, and $e(t)$ is some modelling error that can be treaded as an independent identical distributed noise sequence. One commonly used approach, for effectively reconstructing the nonlinear functions $f_i(\cdot)$, is to construct a nonlinear approximator $\hat{f}_i$ 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, Aguirre and Billings 1995, Murray-Smith and Johansen 1997, Cherkassky and Mulier 1998, Harris et al. 2002, Wei and Billings 2004a, 2004b, Billings and Wei 2005a, 2005b). 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. The present study, however, employs a family of shifted multiscale basis functions to approximate the nonlinear maps $f_1, f_2, \mathrm{L}\ , f_d$ in (6).

Now take a wavelet-based approximation as an example. Let ψ be a chosen mother wavelet. Consider the family

$$\psi(x;b,a) = \psi\left(\frac{x-b}{a}\right) \tag{7}$$

where $a \in \mathrm{R}^+$, $b \in \mathrm{R}$, and the wavelet ψ is admissible. The admissibility condition is depicted using the Fourier transform $\hat{\psi}(\xi)$ of the function ψ as $C_\psi = \int_{-\infty}^{\infty} \xi^{-1} \left|\hat{\psi}(\xi)\right|^2 d\xi < \infty$ (Daubechies 1992). Each of these d functional components $f_i(x_i)$ can now be represented as

$$f_i(x_i(t)) = \sum_k \sum_j w_{k,j}^{(i)} \psi(x_i(t); b_{k,j}^{(i)}, a_{k,j}^{(i)}) \tag{8}$$

where $a_{k,j}^{(i)}$ and $b_{k,j}^{(i)}$ are pre-determined scale and shift parameters, and $w_{k,j}^{(i)}$ are the associated weight coefficients. Equation (6) can now be written as

$$\begin{aligned} y(t) &= \hat{f}(\mathbf{x}(t)) + e(t) = \sum_{i=1}^{d} f_i(x_i(t)) + e(t) \\ &= \sum_{i=1}^{d} \sum_k \sum_j w_{k,j}^{(i)} \psi(x_i(t); b_{k,j}^{(i)}, a_{k,j}^{(i)}) + e(t) \end{aligned} \tag{9}$$

This is the initial full MLC model for the associated STE system (2). In this model the scale and shift parameters $a_{k,j}^{(i)}$ and $b_{k,j}^{(i)}$ are restricted to a pre-specified non-dyadic lattice, which is directly determined by using the information given by the original observation dataset. The weight coefficients $w_{k,j}^{(i)}$, however, need to be estimated by solving the associated regression equation problem.

Some realization issues, relative to the construction of the MLC model (6), include:

- The determination of the scale and shift parameters $a_{k,j}^{(i)}$ and $b_{k,j}^{(i)}$.
- The initial full model (9) is often redundant, so a key problem involves how to refine and improve the model to produce a parsimonious model with good generalisation properties.
- The estimates of the weight coefficients $w_{k,j}^{(i)}$ are highly dependent on the given estimation dataset of the observations. A second key problem is how to effectively estimate the weight coefficients.

3. The Determination of the Shift and Scale Parameters

3.1 The Histogram-Based Grouping Algorithm

Consider a given time series $\{x(t): t = 1,2,\text{L}\ ,N_0\}$. Let $x_{\min} = \min\{x(t)\}_{t=1}^{N_0}$, $x_{\max} = \max\{x(t)\}_{t=1}^{N_0}$ and $R = [x_{\min}, x_{\max}]$. Now the objective is to partition all the data points in the time series $\{x(t)\}$ into K groups. The grouping criterion and the associated partitioning procedure are as follows:

- Divide the interval R into k equally-spaced sub-intervals (bins); the kth bin is defined as $R_k = [r_k, r_{k+1})$ for k=1,2, …, K-1, and $R_k = [r_k, r_{k+1}]$ for k=K, where $r_k = x_{\min} + (k-1)h$ and $h = (x_{\max} - x_{\min})/K$ (h is referred to as the bin width).
- If $x(t) \in R_k$, then the t-th data point is included in the kth bin.
- Denote the number of data points contained in the kth bin R_k by g_k.

These are the basic ideas of the commonly used histogram method. However, the determination of the bin width and bin number K is still an open issue in histogram analysis (Wade 1997). The famous Sturges' rule (Sturges 1926), which has been used in default in some popular languages and software, suggests that the total bin number be chosen to be $K = 1 + \log_2(N_0)$. It has been pointed out (Scott 1992) that the Sturges' rule is more of a number-of-bins rule rather than a bin-width-oriented rule itself, and it has been shown (Scott 1992) that the bin width produced by the Sturges' rule leads to an over-smoothed histogram, especially when the number of samples is large. Based on a well-established theory (Scott 1992), two cross-validation (CV) criteria has been derived for bin width choice. The biased CV and unbiased (least squares) CV functions are given below

$$\text{BCV}(h(K)) = \frac{5}{6N_0 h(K)} + \frac{1}{12N_0^2 h(K)} \sum_{k=1}^{K-1} (g_{k+1} - g_k)^2 \tag{10}$$

$$\text{UCV}(h(K)) = \frac{2}{(N_0 - 1)h(K)} - \frac{N_0 + 1}{N_0^2 (N_0 - 1)h(K)} \sum_{k=1}^{K} g_k^2 \tag{11}$$

where $h(K) = (x_{\max} - x_{\min})/K$ is the bin width of K partitions. The bin width for the associated dataset is defined to be the one that minimises the BCV or UCV vriteria. These cross validation criteria can be used to determine the scale and shift parameters of the associated basis functions.

3.2 Choice of the Shift and Scale Parameters

For a given time series $\{x(t): t = 1,2,\text{L}\ ,N_0\}$, assume that a total of K groups have been determined using the above histogram-based grouping algorithm, and let c_k be the centre (midpoint) of the kth interval R_k. In the present study, wavelet shift parameters are chosen to be these K centres.

It is known that wavelet basis functions are compactly supported or nearly compactly supported. For example the B-splines and associated wavelets (Chui 1992, Unser et al. 1993, User 1999) are compactly supported, while the Gaussian and the Mexican hat (or Marr) wavelets (Daubechies 1992, Billings and Wei 2005a) are nearly compactly supported. Hence, to the wavelet transform (7), for any scale and shift parameters a and b, there must exist a positive number δ such that

$$|\psi(x;b,a)| = \left|\psi\left(\frac{x-b}{a}\right)\right| \approx 0, \text{ for } \left|\frac{x-b}{a}\right| \geq \delta \tag{12}$$

For example, for the 1-D Mexican hat wavelet $\psi(x) = (1-x^2)\exp(-x^2/2)$, $|\psi(x)| \leq 0.0001$ for $|x| \geq \delta = 5$. Thus, for a fixed shift parameter b, the scale parameter a should not be chosen too small, because a very scale will 'disable' many useful data points. On the other hand, the scale parameter a should not be chosen too large, because a very large scale could make the associated functions become too smooth to capture detailed dynamics of the signal.

From the above discussion, the shift and scale parameters b and a are chosen as follows:

- The number of wavelet shift parameters is chosen to be K, where K is defined using the histogram-based grouping algorithm.
- The K shift parameters b_1, b_2, L, b_K are chosen to be the centres of the K bins (groups).
- For each shift parameter b_k, allocate a total of J scale parameters to the associated basis functions, denote these scale parameters by a_1, a_2, L, a_J, where $a_j = 2^j a_0/4$ for j=1,2, …, J and $a_0 = h(K)/\sqrt{2K}$.

Here, the idea of choosing $a_0 = h(K)/\sqrt{2K}$ comes from Haykin (1999), where it is suggested that the scale (bandwidth) parameter be chosen as $\sigma = \max_{1 \leq i < j \leq K} \{|b_i - b_j|\}/\sqrt{2K}$. Applying the above procedure to equation (6), yields,

$$\begin{aligned} y(t) &= \sum_{i=1}^{d}\sum_{k=1}^{K_i}\sum_{j=1}^{J} w_{j,k}^{(i)} \psi(x_i(t); b_k^{(i)}, a_j^{(i)}) + e(t) \\ &= \sum_{i=1}^{d}\sum_{k=1}^{K_i}\sum_{j=1}^{J} w_{k,j}^{(i)} \psi\left(\frac{x_i(t) - b_k^{(i)}}{a_j^{(i)}}\right) + e(t) \end{aligned} \tag{13}$$

where $a_j^{(i)}$ and $b_k^{(i)}$ are the scale and shift parameters, relative to the ith variable $x_i(t)$. In model (14), it is assumed that the time series $\{x_i(t)\}$ produced by the ith variable $x_i(t)$ has been partitioned into K_i groups, and thus a total of K_i shift parameters are involved for the variable $x_i(t)$; for each of these shift parameters, there are a total of J scale parameters associated with the wavelets. Therefore, the

initial full wavelet model (14) contains a total of $M = J(K_1 + \mathrm{L} + K_d)$ basis functions. Model (14) can easily be converted to a linear-in-the-parameters form below

$$y(t) = \sum_{m=1}^{M} \theta_m \phi_m(t) + e(t) = \boldsymbol{\varphi}^T(t)\boldsymbol{\theta} + e(t) \tag{14}$$

where $\phi_m \in \{\psi(x_i; b_k^{(i)}, a_{k,j}^{(i)}) : i = 1,2,\mathrm{L}\ ,d; k = 1,2,\mathrm{L}\ ,K_i; j = 1,2,\mathrm{L}\ ,J\}$, θ_m are model parameters, and $\boldsymbol{\varphi}(t) = [\phi_1(t),\mathrm{L}\ ,\phi_M(t)]^T$ and $\boldsymbol{\theta}$ are the associated regressor and parameter vectors, respectively. Notice that in most cases the initial full regression equation (14) 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 relatively 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.

4. Model Refinement Using the Forward Orthogonal Regression Algorithm

Let $\boldsymbol{\varphi}_m = [\phi_m(1),\mathrm{L}\ ,\ \phi_m(N)]^T$ be a vector formed by the mth candidate model term in the initial full model (15), where m=1,2, …, M. Let $D = \{\boldsymbol{\varphi}_1,\mathrm{L}\ ,\boldsymbol{\varphi}_M\}$ be a dictionary composed of the M candidate bases. From the viewpoint of practical modelling and identification, the finite dimensional set D is often highly redundant. The model refinement problem amounts to finding, from the vector dictionary D, a full dimensional subset $D_m = \{\mathbf{p}_1,\mathrm{L}\ ,\mathbf{p}_m\} = \{\boldsymbol{\varphi}_{i_1},\mathrm{L}\ ,\boldsymbol{\varphi}_{i_m}\}$, where $\mathbf{p}_k = \boldsymbol{\varphi}_{i_k}$, $i_k \in \{1,2,\mathrm{L}\ ,M\}$ and k=1,2, …, m (generally $m << M$), so that $\mathbf{y}$ can be satisfactorily approximated using a linear combination of $\mathbf{p}_1, \mathbf{p}_2, \mathrm{L}\ , \mathbf{p}_m$ as below

$$\mathbf{y} = \beta_1 \mathbf{p}_1 + \mathrm{L} + \beta_m \mathbf{p}_m + \mathbf{e}_m \tag{15}$$

where $\mathbf{e}_m$ is the associated model residual vector.

The orthogonal least squares (OLS) algorithm (Billings et al. 1989, Chen et al. 1989,) can be used to determine model basis functions (model terms). In this study, however, a variation of the OLS algorithm, called the forward orthogonal regression (FOR) algorithm, implemented using a mutual information method (Billings and Wei 2007a, Wei and Billings 2007), is employed for model refinement. Assume that $\mathbf{x}$ and $\mathbf{y}$ are two random discrete variables, with alphabet X and Y, respectively, and with a joint probability mass function $p(x, y)$ and marginal probability mass functions $p(x)$ and $p(y)$. The mutual information $I(\mathbf{x}, \mathbf{y})$ is the relative entropy between the joint distribution and the product distribution $p(x)p(y)$, given as (Cover and Thomas 1991)

$$I(\mathbf{x},\mathbf{y}) = \sum_{x\in \mathsf{X}} \sum_{y\in \mathsf{Y}} p(x,y) \log\left(\frac{p(x,y)}{p(x)p(y)} \right) \tag{16}$$

The mutual information $I(\mathbf{x},\mathbf{y})$ is the reduction in the uncertainty of $\mathbf{y}$ due to the knowledge of $\mathbf{x}$, and vice versa. Mutual information provides a measure of the amount of information that one variable shares with another one. If $\mathbf{y}$ is chosen to be the system output (the response), and $\mathbf{x}$ is one regressor in a linear model, $I(\mathbf{x},\mathbf{y})$ can then be used to measure the coherence of $\mathbf{x}$ with $\mathbf{y}$ in the model. Several algorithms have been proposed to estimate mutual information from observed data, see for example Moddemeijer (1989, 1999), Darbellay and Vajda (1999), and Paninski (2003) and the references therein.

Detailed discussions about the utility of the mutual information for model term selection can be found in Billings and Wei (2007a) and Wei and Billings (2007). Now, let $\mathbf{p}_1, \mathbf{p}_2, \mathrm{L}\ , \mathbf{p}_n$ be the n selected linearly independent basis vectors after the nth step search, and let $\mathbf{q}_1, \mathbf{q}_2, \mathrm{L}\ , \mathbf{q}_n$ be a group of orthogonal vectors, generated from the vectors $\mathbf{p}_1, \mathbf{p}_2, \mathrm{L}\ , \mathbf{p}_n$, by means of some orthogonal transformation. Following Billings et al. (1989), Chen et al. (1989), the error reduction ratio (ERR), produced by including the nth basis vector $\mathbf{q}_n$, or equivalently by including $\mathbf{p}_n$, is defined as

$$\mathrm{ERR}_n = \frac{\gamma_n^2 \| \mathbf{q}_n \|^2}{\| \mathbf{y} \|^2} \tag{17}$$

where $\gamma_n = < \mathbf{y}, \mathbf{q}_n > / \| \mathbf{q}_n \|^2$. ERR can be used to measure the significance of individual model terms in that it provides an index indicating the contribution made by each selected individual model term to explain the total variance in the desired output signal.

Let $\mathbf{e}_n$ be the residual vector produced at the nth search step. Similar to in the OPP algorithm, the model residual vector $\mathbf{e}_n$ can be used to form a criterion to terminate the search procedure. Following the suggestion in Billings and Wei (2007b), the following adjustable prediction error sum of squares (APRESS), also referred to as the adjustable generalised cross-validation (AGCV), will be used to monitor the regressor search procedure

$$\mathrm{APRESS}_n = \frac{\mathrm{MSE}(n)}{(1-\lambda n/N)^2} \tag{18}$$

where $\mathrm{MSE}(n) = \| \mathbf{e}_n \|^2 / N$ is the mean-square-error that is associated to the model of n model terms. The number of regressors (wavelet functions) will be chosen as the value where APRESS arrives at a minimum. Billings and Wei (2007b) suggest that the adjustable parameter λ be chosen between 5 and 10.

Following Billings and Wei (2007a) and Wei and Billings (2007), the mutual information based forward orthogonal regression (FOR) algorithm, is briefly summarised below.

The FOR-MI algorithm:

Step 1**:** Set $U_1 = \{1,2,\mathrm{L}\ ,M\}$;

for j=1 to M

$\mathbf{q}_j^{(1)} = \boldsymbol{\varphi}_j$;

$I^{(1)}[j] = MI(\mathbf{r}_0, \mathbf{q}_j^{(1)})$; // Calculate the mutual information for all

// candidate basis vectors.//

end for

$\mathrm{l}_1 = \arg\max_{i \in U_1}\{I^{(1)}[i]\}$; $V_1 = \{\mathrm{l}_1\}$;

$\mathbf{p}_1 = \boldsymbol{\varphi}_{\mathrm{l}_1}$; $\mathbf{q}_1 = \mathbf{p}_1$; $\gamma_1 = \dfrac{<\mathbf{y}, \mathbf{q}_1>}{\| \mathbf{q}_1 \|^2}$; $\mathbf{r}_1 = \mathbf{r}_0 - \gamma_0 \mathbf{q}_1$;

$\mathrm{ERR}[1] = \dfrac{\gamma_1^2 \| \mathbf{q}_1 \|^2}{\| \mathbf{y} \|^2}$; $\mathrm{APRESS}[1] = \dfrac{1}{(1-\lambda/N)^2} \dfrac{\| \mathbf{r}_1 \|^2}{N}$;

Step n, $n \geq 2$ **:**

For n=2 to M

$U_n = U_{n-1} \setminus V_{n-1}$;

for $j \in U_n$

$\mathbf{q}_j^{(n)} = \boldsymbol{\varphi}_j - \sum_{k=1}^{n-1} \dfrac{<\boldsymbol{\varphi}_j, \mathbf{q}_k>}{\| \mathbf{q}_k \|^2} \mathbf{q}_k$;

$I^{(n)}[j] = MI(\mathbf{r}_{n-1}, \mathbf{q}_j^{(n)})$; //Calculate the mutual information for all

// for all candidate basis vectors.//

//{if $\| \mathbf{q}_j^{(n)} \|^2 \leq \varepsilon$, set $I^{(n)}[j] = 0$ }//

end for (end loop for j)

$\mathrm{l}_n = \arg\max_{j \in U_n}\{I^{(n)}[j]\}$; $V_n = \{\mathrm{l}_n\} \mathrm{U} \{\arg_{j \in U_n}(\| \mathbf{q}_j^{(n)} \|^2 < \varepsilon)\}$;

$\mathbf{p}_n = \boldsymbol{\varphi}_{\mathrm{l}_n}$; $\mathbf{q}_n = \mathbf{q}_{\mathrm{l}_n}^{(n)}$; $\gamma_n = \dfrac{<\mathbf{y}, \mathbf{q}_n>}{\| \mathbf{q}_n \|^2}$; $\mathbf{r}_n = \mathbf{r}_{n-1} - \gamma_n \mathbf{q}_n$;

$\mathrm{ERR}[n] = \dfrac{\gamma_n^2 \| \mathbf{q}_n \|^2}{\| \mathbf{y} \|^2}$; $\mathrm{APRESS}[n] = \dfrac{1}{(1-\lambda n/N)^2} \dfrac{\| \mathbf{r}_n \|^2}{N}$;

for k=1 to n

$r_{k,n} = \dfrac{<\mathbf{p}_n, \mathbf{q}_k>}{\| \mathbf{q}_k \|^2}$, for $k < n$; $r_{k,n} = 1$, for $k = n$;

end for (end loop for k)

end for (end loop for n)

The FOR algorithm provides an effective tool for successively selecting significant model terms (basis functions) in supervised learning problems. Terms are selected step by step, one term at a time. The inclusion of redundant bases, which are linearly dependent on the previous selected bases, can be efficiently excluded by eliminating the candidate basis vectors for which $\| \mathbf{q}_j^{(n)} \|^2$ are less than a predetermined threshold ε, say $\varepsilon \leq 10^{-10}$. Assume that a total of m significant vectors are selected, then the unknown parameter $\boldsymbol{\beta} = [\beta_1, \beta_2, \mathrm{L}\ , \beta_m]^T$, relative to the model (15), can easily be calculated

from the triangular equation $\mathbf{R}\boldsymbol{\beta}=\boldsymbol{\gamma}$, where R is an upper triangular matrix and $\boldsymbol{\gamma}=[\gamma_1,\gamma_2,\mathrm{L}\ ,\gamma_m]^T$ with $\gamma_i =< \mathbf{y},\mathbf{q}_i > / \| \mathbf{q}_i \|^2$ for i=1,2,…, m.

5. Applications

The new MLC modelling framework can be applied to identify some SPE phenomena, where the true models are unknown and the initial full model involves a great number of 'input' or 'independent' variables. To illustrate the application of the new modelling method, the Belousov-Zhabotinsky (Belousov 1959, Zhabotinsky 1964, Winfree 1972, Kuramoto 1984) reaction was considered here as an example.

The BZ reaction, as an excitable medium (Adamatzky 2001, 2004), is representative of an important class of chemical reactions exhibiting a spatio-temporal oscillatory behaviour. As a classical example of nonequilibrium thermodynamics, the BZ reaction provides an interesting chemical model of nonequilibrium phenomena, and the modelling and identification of these types of reactions is of extreme interest for theoretical analysis of such phenomena.

By adopting the recipe given by Winfree (1972), an experiment resulting in a thin layer BZ reaction was carried out in the laboratory, and a set of images were captured (sampled) with equal time intervals during the experiment, using a digital video camera that is connected to a PC via a USB socket. The sampled images were processed and saved as patterns with a resolution of 300 by 500 pixels. Some of these patterns are shown in Fig. 1.

The proposed MLC modelling framework was applied to these sampled images, and the objective was to identify a mathematical model for the BZ reaction. Details of the identification procedure are given below.

5.1 The initial model and the training data

Consider the model of the form (2), where the number of total model variables is determined by two factors: the radius of the neighbourhood, r, and the time lag, n_{lag} . In the present study, the two coefficients were chosen to be r=1, and n_{lag} =2. Thus, the model (2) involves a total of 18 model variables.

The state variable $s_{i,j}(t)$, at the present time instant t, was initially assumed to be associated with state variables in the past two adjacent neighbourhoods at the previous time instants t-1 and t-2. Any two patterns, at the abutting time instants t and t-1 are called an adjacent pattern group. For an arbitrary time instant, the data pair, $\{\mathbf{x}(t), y(t)\}$, where $\mathbf{x}(t)$ and $y(t)$ are defined by (4) and (5), is called a data pair. Notice that $\mathbf{x}(t)$ and $y(t)$ are also implicitly associated with the spatial location indices i and j (see Table 1). As a consequence, for any given time instant t, there would be a large number of data pairs available.

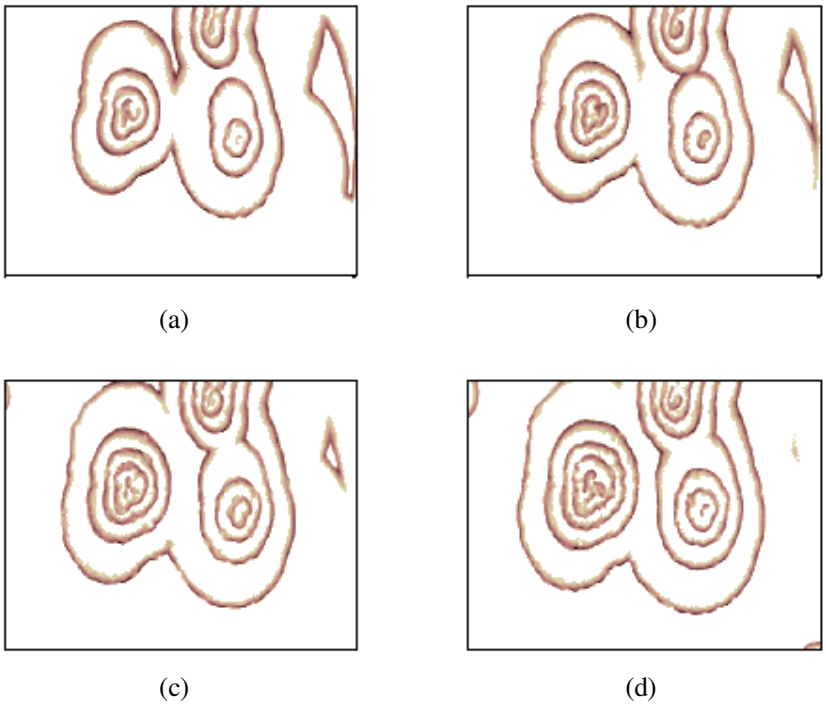


Fig. 1 Some snapshots for the BZ reaction at different time instants. The size of each template is 300×500 (300 pixels in the vertical direction and 500 pixels in the horizontal direction). (a) t=10; (b) t=20; (c) t=30; (d) t=40.

A training dataset, consisting of a total of N=6000 data pairs, $\{\mathbf{x}(k), y(k)\}_{k=1,2,\ldots,N}$, was generated for model identification, where $y(k)$ represents the value of the relevant central cell at the present time instant, and $\mathbf{x}(k)=[x_1(k), x_2(k),\mathrm{L}\ , x_{18}(k)]^T$ represent the values of the 18 involved cells on a squared lattice, at the previous time instants. Data pairs $\{\mathbf{x}(k), y(k)\}$ in the training dataset were randomly chosen from ten adjacent pattern groups that were also randomly selected from the first 40 sampled patterns.

5.2 Determining the shift and scale parameters

Note that all the involved 18 variables come from the same system; in a statistical sense, these 18 variables, as well as the 'output' variable $y(t)$, should obey the same distribution. Thus the 18 variables could be allocated the same shift parameters. It was noticed that the values of a great number of observations are exactly equivalent to the maximum value $y_{\max}$=255. Thus, the one shift parameter was in default chosen to be 255, and other shift parameters were determined by performing the histogram-

based grouping algorithms on the associated time series $\{y(t)\}$ with t=1,2, …, N, where data points whose values are exactly equivalent to $y_{\max}$, were excluded. The biased CV (BCV) criterion, shown in Fig. 2, suggests that the optimal number of groups for the associated dataset should be chosen as 8. Thus a total of 9 shift parameters $b_1, b_2, \mathrm{L}\ , b_9$ were chosen for the relevant dataset.

The Mexican hat wavelet function, defined as $\psi(x) = (1-x^2)e^{-x^2/2}$, was used as the elementary building block for constructing the MLC model, and the primary bandwidth for each group was chosen to be a_0 =6.25. For each shift parameter b_k, a total of 6 scales were to used to perform associated wavelet transforms; denote these scale parameters by $a_1, a_2, \mathrm{L}\ , a_6$, where $a_j = 2^{j-2}a_0$. The initial full MLC model was thus of the form

$$y(t) = \sum_{i=1}^{18}\sum_{k=1}^{9}\sum_{j=1}^{6} w_{k,j}^{(i)}\psi\left(\frac{x_i(t)-b_k}{a_j}\right) + e(t) \tag{19}$$

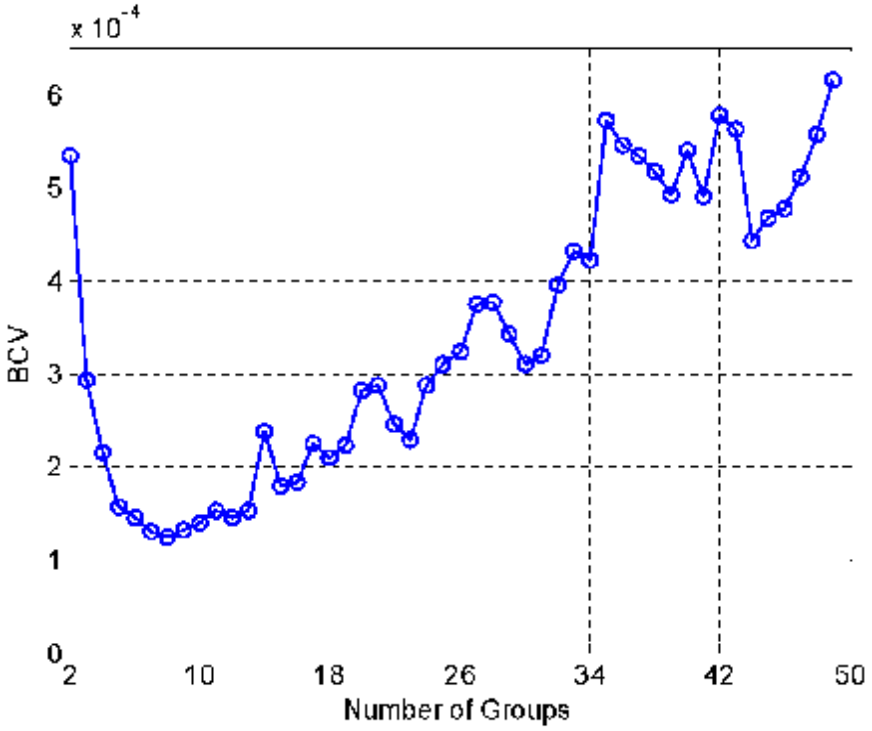


Fig. 2 The BCV criterion versus the number of groups, produced using the histogram-based clustering algorithm.

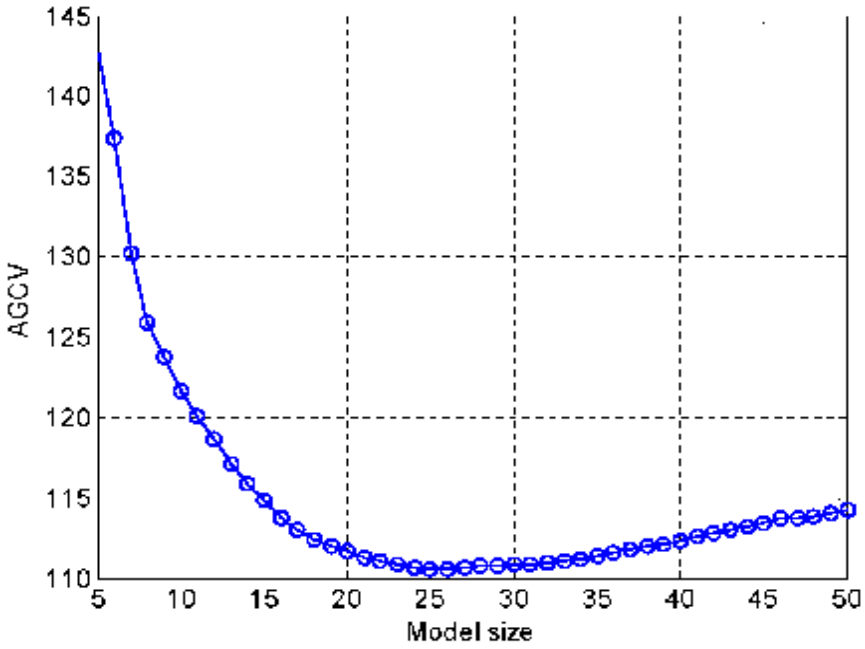
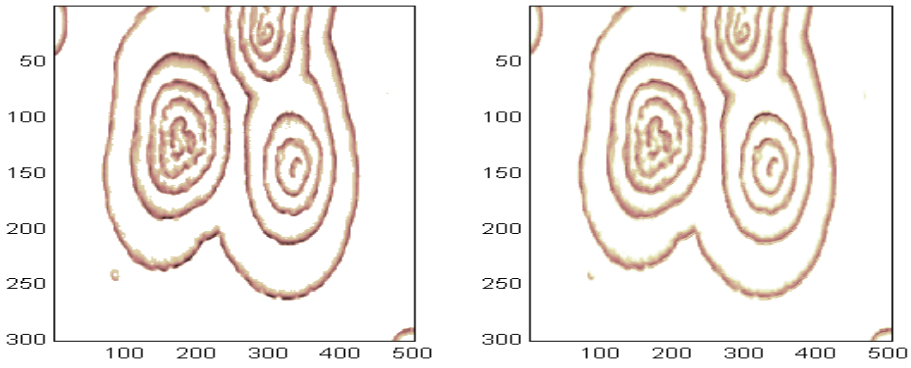


Fig. 3 The AGCV criterion versus the number of model terms (selected by using the FOR-MI algorithm).

5.3 Model refinement and performance evaluation

The initial full MLC model (19) contains a total of 972 model terms; most of the model candidate model terms may be redundant. The initial full model thus needs to be refined. The FOR-MI algorithm was performed, over the given training dataset, to select significant individual basis functions from the initial model (19). The adjustable generalized cross-validation (AGCV), defined by (18) and where the adjustable parameter $\lambda = 10$, suggests that a total of 26 basis functions should be included in the final model (see Fig. 3).

To evaluate the performance of the identified additive wavelet models, the short-term predictive capability of the models was inspected. Denote the observation of the image (pattern) measured at the time instant t by $X(t)$. The k-step-ahead prediction, denoted by $\hat{X}(t+k \mid X(t), X(t-1); f)$, where f represents the identified nonlinear function, is the iteratively produced result by the identified model, on the basis of $X(t)$ and $X(t\text{-}1)$, but without using information on observations for patterns at any other time instants. As an example, the measurements at the time instants t=41 and 42 were used to calculate the 1-step-ahead predictions for the values at the time instant t=43, and this is shown in Fig. 4.



(a) (b)

Fig. 4 Model prediction (one step ahead) for the BZ reaction at time instant t=43. (a) Real measurement at t=43; (b) Predicted image from the model.

To quantitatively measure the performance of the identified models, the 2-D normalised mean-square-error (NMSE), defined as below, was considered

$$\mathrm{NMSE}(t) = \frac{\sum_{i=1}^{I}\sum_{j=1}^{J} | s_{i,j}(t) - \hat{s}_{i,j}(t) |^2}{\sum_{i=1}^{I}\sum_{j=1}^{J} | s_{i,j}(t) - \bar{s}(t) |^2} \tag{20}$$

where $s_{i,j}(t)$ represent the observations at the time instant t, $\hat{s}_{i,j}(t)$ represent the corresponding predicted values from the given model, $\bar{s}(t)$ is the mean value of the patter at the time instant t, and I and J define the size of the associated patterns. The predicted values at t=43 were compared with the associated observations, and the normalised mean-square-error was calculated to be 0.0763.

From Fig. 4 and the NMSE value, it is clear that the identified MLC model can capture the main spatio-temporal evolution dynamics from these real laboratory BZ reaction. The identified model can provide very good short term predictions.

6. Conclusions

The multiscale lattice cell (MLC) model, by incorporating some multiscale approach into the traditional lattice cell model, provides an enhanced powerful representation for spatio-temporal evolutionary images. An initial full MLC model for a given model identification problem may involve a great number of basis functions. Experience has shown that in general only a relatively small number of basis functions are significant and need to be included in the model. Thus an efficient model term selection algorithm is necessary to produce a parsimonious model with good generalisation properties. Orthogonal least squares (OLS) type of algorithms, including the forward orthogonal regression aided

by mutual information (FOR-MI), have been proved to be quite effective for general model selection problems.

The MLC model identification procedure is performed on some scaled and translated basis functions, where two types of parameters need to be determined: the shift and the scale parameters. Although the present study provides some tips for choosing these parameters, optimisation of these parameters still need to be considered in a future study, to produce more efficient models for complex spatio-temporal systems.

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