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Identification of Partial Differential Equation Models for Continuous Spatio-temporal Dynamical Systems

L. Z. Guo and S. A. Billings

Department of Automatic Control and Systems Engineering
University of Sheffield
Sheffield, S1 3JD
UK

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Guo, L. Z. and Billings, S. A.

Department of Automatic Control and Systems Engineering
University of Sheffield
Sheffield S1 3JD, UK

Abstract

The identification of a class of continuous spatio-temporal dynamical systems from observations is presented in this paper. The proposed approach is a combination of implicit Adams integration and an orthogonal least squares algorithm, in which the operators are expanded using polynomials as basis functions and the spatial derivatives are estimated by finite difference methods. The resulting identified models of the spatio-temporal evolution form a system of partial differential equations. Examples are provided to demonstrate the efficiency of the proposed method.

1 Introduction

The identification of spatio-temporal dynamical systems has received a lot of attention recently. This has mainly been driven by the need to determine high quality models, which can be used as a basis for analysis and control of this class of systems with high accuracy. Although partial differential equation (PDE) or coupled map lattice (CML) models for such systems can sometimes be derived by analytic modelling methods, often a large number of assumptions have to be made in order to obtain such models. There is a need to use identification methods to refine, update and validate these models. The identification of CML models of spatio-temporal dynamical systems has been extensively studied over the past few years. Various methods for the identification of local CML models from spatio-temporal observations have already been proposed (Billings and Coca 2002, Mandelj, Grabec and Govekar 2001, Marcos-Nikolaus, Martin-Gonzalez and Sóle 2002, Grabec and Mandeji 1997, Parlitz and Merkwirth 2000). Coca and Billings (2002a,b,c) have also investigated identifying finite element discrete time models of distributed parameter systems based on observations of the evolution of the system and the forcing function. But there are many instances where it would be valuable to be able to determine continuous models such as a system of PDEs to describe continuous spatio-temporal systems. Obviously such models may easily be related to the original system parameters that can provide a clear physical explanation. In this paper, the problem of identifying PDE models for a class of continuous spatio-temporal dynamical systems is investigated.

The identification of PDE models of continuous spatio-temporal systems has been studied by several authors (Coca and Billings 2000, Fioretti and Jetto 1989 Voss, Bunner, and Abel 1998, Travis and White 1985, Phillipson 1971, Niedzwecki and Liagre 2003). However most of these studies assume that the form of the PDE equations is known up to a set of constant parameters. In this paper a novel approach is used to reconstruct the system of PDEs for unknown continuous spatio-temporal dynamical systems. This new approach represents one of the first algorithms to determine the PDE model terms, and estimate the unknown parameters, from a given spatio-temporal data set. The approach can be regarded as the inverse of the classical Adam-Moulton method for the numerical solution of differential equations, that is, the operator of the evolution is estimated from the observed values of the system variables. By using implicit Adams integration, a system of algebraic equations can be obtained for the underlying continuous spatio-temporal system that is discrete in time. The advantages of the Adams-Moulton method over Euler integration is that the former should provide a better fit for less data than the latter, and the latter works well only when the sampling interval is small which might amplify any possible noise. By adapting system identification techniques, the continuous operator can then be estimated. This is achieved by using a polynomial estimation of the operator and an orthogonal least squares algorithm (Chen, Billings, and Luo 1989).

The paper is organised as follows. Section 2 introduces the basic idea of the proposed approach and presents the derivation of the system of algebraic equations by using Adams-Moulton formula. The identification algorithm is given in section 3. Section 4 illustrates the proposed approach, and finally conclusions are given in section 5.

2 Problem description

Assume that the evolution of the continuous spatio-temporal dynamical system under consideration is governed by a system of partial differential equations as follows

$$\dot{y} = f(y, y', y'', \cdots, y^{(l)}), x \in \Omega, t \in T \tag{1}$$

where $y(x,t) \in R^n$ is the independent variable of the system, The dot $\cdot$ denotes the time derivative of y and the prime $'$ denotes the spatial derivatives of y. $t \in T$ denotes time and $x \in \Omega \subset R^m$ denotes the spatial variable. $f(\cdot)$ is a unknown nonlinear function. Note that the time and spatial variables t and x do not appear in f directly. This indicates that the system under consideration is time and spatial invariant. The initial and boundary conditions for eqn.(1) are

$$g(y(0,t)) = y_i(x) \tag{2}$$

and

$$h(y(x,t)) = y_b(x,t), x \in \partial\Omega \tag{3}$$

For such a continuous spatio-temporal system, experimental measurements are often available in the form of a series of snapshots $y(x, n\Delta t)$, $n = 0, 1, 2, \cdots$, $x \in \Omega$, where Δt is the time sampling interval. In this paper, it is assumed that all the components of the vector $y(x,t) \in R^n$ at one location x are measurable otherwise some state space reconstruction techniques may be needed (Packard, Crutchfield, and Farmer 1980, Takens 1981, Sauer, Yorke, and Casdagli 1991). The objective is to determine the nonlinear function f in eqn. (1) from these discrete measured values. To this end, the implicit Adams-Moulton formula (Press, Flannery, Teukolsky, and Vetterling 1992) is used to obtain a discrete representation of eqn. (1). Consider a point x in the spatial domain Ω, let $y_n(x) = y(x, n\Delta t)$, then it follows

$$y_{n+1}(x) = y_n(x) + \int_{n\Delta t}^{(n+1)\Delta t} \dot{y}(x,t)dt = y_n(x) + \int_{n\Delta t}^{(n+1)\Delta t} f(y(x,t), y'(x,t), y''(x,t), \cdots, y^{(l)}(x,t))dt \tag{4}$$

The Adams-Moulton formula of order p is obtained by integrating a polynomial that interpolates $f_{n+1-j}(x), j = 0, 1, \cdots, p-1$, that is

$$y_{n+1}(x) = y_n(x) + \Delta t \sum_{j=0}^{p-1} \alpha_j f_{n+1-j}(x) \tag{5}$$

where $f_{n+1-j}(x) = f(y_{n+1-j}(x), y'_{n+1-j}(x), \cdots, y^{(l)}_{n+1-j}(x))$.

Note that eqn. (5) reduces to implicit Euler integration when $p = 1$. The advantages of Adams-Moulton integration over Euler integration is the former should provide a better fit for less data than the latter and the latter works well only when the sampling interval Δt is small which might amplify any possible noise.

Unlike the numerical problem, in our case $y_n(x), n = 1, 2, \cdots$, is given, and the task is to determine the nonlinear function f in eqn. (5). If the form of f is known then a least squares algorithm will often be sufficient to determine the parameters. However, when the form of f is unknown, it is necessary to expand f using a known set of basis functions or regressors belonging to a given function class. Typical regressor classes include polynomials, spline functions, rational functions, radial basis functions, neural networks, and wavelets. In this paper, the regressor class of polynomial functions is used. Approximating the nonlinear function f in (1) using the polynomial approximation space yields the following representation of (5)

$$y_{n+1}(x) = y_n(x) + \Delta t \sum_{j=0}^{p-1} \alpha_j \sum_{i=1}^{M} \beta_i \phi_{n+1-j}^i(x) \tag{6}$$

where M denotes the order of the polynomial, β_i is the coefficient of the ith polynomial term, and $\phi_{n+1-j}^i(x)$ is the corresponding monomial which is the product of different spatial derivatives of $y_{n+1-j}(x)$ at x. These spatial derivatives are difficult to measure in practice therefore they are replaced by their finite difference approximations when applying the identification algorithm. In principle, both the parameters α_j and β_i should be calculated during identification. For the sake of simplicity, the values of the α_j are the ones originally dictated by the Adams-Moulton formula. Therefore β_i are the only parameters that need to be determined.

Rewriting eqn. (6) in the form of linear-in-parameters β_i and replacing the spatial derivatives with their finite difference approximations yields

$$y(k, n+1) = y(k, n) + \sum_{i=1}^{M} \beta_i (\sum_{j=0}^{p-1} \Delta t \alpha_j \phi_{n+1-j}^i(k)) \tag{7}$$

Note that $\phi_{n+1-j}^i(k))$ contains some spatial neighbour terms of $y(k, n+1-j)$ like $y(k-1, n+1-j)$ and $y(k+1, n+1-j)$ etc. which depend on the highest order of the spatial derivatives. Therefore, eqn. (7) can be regarded as an implicit CML model representation of the continuous spatio-temporal dynamical system (1). It follows that the orthogonal least squares algorithm proposed by Chen, Billings, and Luo (1989) can be applied to select the suitable polynomial terms and to determine the corresponding coefficients.

3 Identification algorithm

Given a set of (candidate terms) basis functions from the polynomial regressor class, the objective of the identification algorithm is to select the significant terms from this set while estimating the corresponding monomial coefficients. In this paper, an Orthogonal Forward Regression algorithm (OFR) (Chen, Billings, and Luo 1989) is applied to a set of polynomial basis functions. The OFR algorithm involves a stepwise orthogonalisation of the regressors and a forward selection of the relevant terms based on the Error Reduction Ratio criterion (Billings, Chen, and Kronenberg 1988). The algorithm provides the optimal least-squares estimate of the polynomial coefficients θ.

For a given candidate regressor set $G = \{\varphi_i\}_{i=1}^{M}$, the OFR algorithm can be outlined as follows

Step 1

$$I_1 = I_M = \{1, \cdots, M\}$$

$$w_i(t) = \varphi_i(t), \hat{b}_i = \frac{w_i^T y}{w_i^T w_i} \tag{8}$$

$$l_1 = arg \max_{i \in I_1}(\hat{b}_i^2 \frac{w_i^T y}{y^T y}) = arg \max_{i \in I_1}(err_i) \tag{9}$$

$$w_1^0 = w_{l_1}, c_1^0 = \frac{w_1^{0T} y}{w_1^{0T} w_1^0} \tag{10}$$

$$a_{1,1} = 1 \tag{11}$$

Step $j, j > 1$

$$I_j = I_{j-1} \backslash l_j - 1 \tag{12}$$

$$w_i(t) = \varphi_i(t) - \sum_{k=1}^{j-1} \frac{w_k^{0T} y}{w_k^{0T} w_k^0} w_k^0, \hat{b}_i = \frac{w_i^T y}{w_i^T w_i} \tag{13}$$

$$l_j = arg \max_{i \in I_j}(\hat{b}_i^2 \frac{w_i^T y}{y^T y}) = arg \max_{i \in I_j}(err_i) \tag{14}$$

$$w_j^0 = w_{l_j}, c_j^0 = \frac{w_j^{0T} y}{w_j^{0T} w_j^0} \tag{15}$$

$$a_{k,j} = \frac{w_k^{0T} \varphi_{l_j}}{w_k^{0T} w_k^0}, k = 1, \cdots, j-1. \tag{16}$$

The procedure is terminated at the M_s-th step when the termination criterion

$$1 - \sum_{i=1}^{M_s} err_i < \rho \tag{17}$$

is met, where ρ is a designated error tolerance, or when a given number of terms in the final model is reached.

The estimated coefficients are calculated from the following equation

$$\begin{pmatrix} \theta_{l_1} \\ \theta_{l_2} \\ \vdots \\ \theta_{l_{M_s}} \end{pmatrix} = \begin{pmatrix} 1 & a_{1,2} & \cdots & a_{1,M_s} \\ 0 & 1 & \vdots & a_{2,M_s} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix}^{-1} \begin{pmatrix} c_1^0 \\ c_2^0 \\ \vdots \\ c_{M_s}^0 \end{pmatrix} \tag{18}$$

and the selected terms are $\varphi_{l_1}, \cdots, \varphi_{l_{M_s}}$.

Variables	Terms	Estimates	ERR	STD
$y_1(k,n+1) - y_1(k,n)$	$y_2(k,n)$	-9.9965e-01	9.7963e-01	3.4379e-03
	$y_1(k,n)^2$	9.9902e-01	1.3584e-02	2.4631e-03
	$y_1(k,n)^3$	-9.9869e-01	6.7879e-03	2.1651e-05
	$y_1''(k,n)$	6.2418e-04	4.9108e-07	5.2295e-06
	$y_2(k,n)y_2'(k,n)$	-6.4475e-07	2.3719e-08	3.1966e-06
	$y_1(k,n)y_2(k,n)^2$	7.9923e-05	9.3988e-09	1.3483e-06
$y_2(k,n+1) - y_2(k,n)$	$y_1(k,n)$	3.9987e+01	9.9913e-01	5.7126e-03
	$y_2(k,n)$	2.0013e-01	8.7292e-04	7.0050e-05
	$y_2''(k,n)$	6.3113e-04	1.3585e-07	9.5098e-06

Table 1: The terms and parameters of the final model

4 Numerical simulation and analysis

Consider the following nonlinear reaction-diffusion system

$$\begin{aligned} \frac{\partial y_1(x,t)}{\partial t} &= d_1 \frac{\partial^2 y_1(x,t)}{\partial x^2} + y_1(x,t)^2 - y_1(x,t)^3 - y_2(x,t) \\ \frac{\partial y_2(x,t)}{\partial t} &= d_2 \frac{\partial^2 y_2(x,t)}{\partial x^2} + \delta y_1(x,t) - \gamma y_2(x,t) \end{aligned} \tag{19}$$

with $x \in \Omega = [0,1]$, and initial conditions

$$y_1(x,0) = y_2(x,0) = sin(\pi x) \tag{20}$$

and Dirichlet boundary conditions, that is, $y_1(0,t) = y_1(1,t) = y_2(0,t) = y_2(1,t) = 0$.

For the purpose of identification using the proposed approach, the PDEs (19) with parameters $d_1 = d_2 = 0.0006188, \delta = 40$ and $\gamma = -0.2$, were numerically solved by linearised θ-methods (Ramos 1997) with the time step $\Delta t = 0.01$, space step $\Delta x = 0.02$, and $\theta = 1/2$. The data are plotted in Fig.(1) and Fig.(2).

A set of 100 spatio-temporal observations randomly selected among the data set was used for the identification. In the simulation, the highest order of the derivatives with respect to the spatial variables was set to be 3. The 3rd Adams-Moulton integration formula was used and the polynomial expansion of order 3 of the nonlinear function f was used. The identified terms and parameters using the orthogonal least squares algorithm are listed in Table (1), where ERR denotes the Error Reduction Ratio and STD denotes the standard deviations.

It can be seen that the ERR in Table (1) suggests that the terms $y_2(k,n)y_2'(k,n)$ and $y_1(k,n)y_2(k,n)^2$

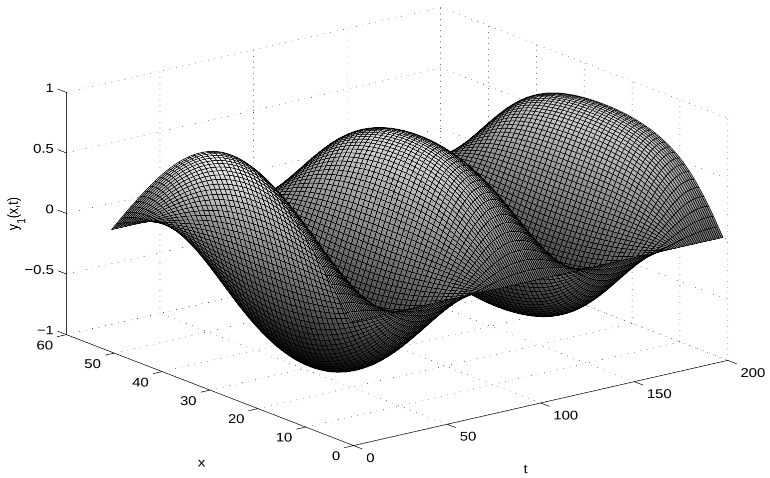

Figure 1: Data $y_1(x,t)$

make insignificant contributions to the reduction of the total errors and therefore can be removed, which results in the following identified continuous spatio-temporal dynamical model

$$\begin{aligned}\frac{\partial y_1(x,t)}{\partial t} &= 0.00062418\frac{\partial^2 y_1(x,t)}{\partial x^2} + 0.99902 y_1(x,t)^2 - 0.99869 y_1(x,t)^3 - 0.99965 y_2(x,t) \\ \frac{\partial y_2(x,t)}{\partial t} &= 0.00063113\frac{\partial^2 y_2(x,t)}{\partial x^2} + 39.987 y_1(x,t) - 0.20013 y_2(x,t)\end{aligned} \tag{21}$$

which indicates an excellent identified result. For the purpose of comparison, the parameters were also identified using an Euler integration representation, which results in the following model

$$\begin{aligned}\frac{\partial y_1(x,t)}{\partial t} &= -0.010797\frac{\partial^2 y_1(x,t)}{\partial x^2} - 1.5856 y_1(x,t)^2 + 0.95276 y_1(x,t)^3 - 0.99512 y_2(x,t) \\ \frac{\partial y_2(x,t)}{\partial t} &= -0.35994\frac{\partial^2 y_2(x,t)}{\partial x^2} + 42.641 y_1(x,t) - 0.012253 y_2(x,t)\end{aligned} \tag{22}$$

and which clearly shows that the proposed approach is superior to the Euler method.

5 Conclusions

A new approach for the identification of both model terms and the unknown parameters in PDE models of continuous spatio-temporal dynamical systems has been introduced. It has been shown that by combining the Adams integration and the OFR algorithm, a system of PDEs for

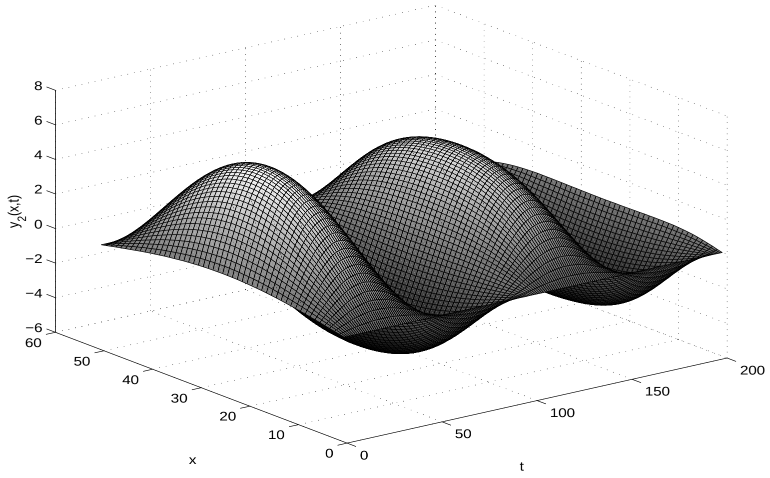

Figure 2: Data $y_2(x,t)$

the underlying continuous spatio-temporal system can be obtained. It is demonstrated that the proposed method is much better than the classic Euler integration approach.

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