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Direct Parameter Identification of Distributed Parameter Systems

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Abstract
A new direct approach to identifying the parameters of distributed parameter systems
from noise corrupted data is introduced. The model of the system which takes the form of a set
of linear or nonlinear partial differential equations is assumed known with the exception of a
set of constant parameters. Using finite difference approximations of the spatial derivatives the
original equation is transformed into a set of ordinary differential equations. The identification
approach involves smoothing the measured data and estimating the temporal derivatives using
a fixed interval smoother. A least squares method is then employed to estimate the unknown
parameters. Three examples that illustrate the applicability of the proposed approach are
presented and discussed.

1 Introduction
A large number of physical processes can be modelled by partial differential equations and
in many cases the partial differential equation (PDE) governing such systems can be derived
using the basic laws of physics or chemistry. The estimation of the unknown parameters of
the infinite-dimensional system however, involves comparing the measurements made on the
system with the solutions of the equations. The system parameters are then identified such
that the model can reproduce the observed dynamical behaviour as closely as possible with
respect to a chosen performance criterion.

Although the parameter estimation problem for distributed systems has been studied
and is well documented (see the survey papers of Goodson and Polis (1978), Kubrusly (1977),
Banks and Kunish (1989)), many of the methods available in the literature have been designed
to solve a particular identification problem where a number of restrictive assumptions apply.
The use of such approaches to solve a general more complicated parameter estimation problem
is therefore limited and often impossible. Examples of such limiting assumptions which confine
many identification methods to particular classes of distributed systems include knowledge of
the initial and boundary conditions, a linear form of the partial differential operators, a certain
number of measurement locations and of data samples available from these locations.

In this context the present paper proposes an original approach to the parameter identifi-
cation problem of distributed parameter systems which imposes only mild restrictions regarding
the observed system. The proposed approach can deal for example with systems described by
general, linear or nonlinear PDE's the form of which is known a priori. The method does not
require knowledge of the initial or boundary conditions. Also the number of measurement locations required is very small, depending on the order of the partial differential equation and of the number of spatial coordinates (two locations for one-dimensional first order PDE’s, three locations for one-dimensional second order PDE’s etc).

The approach taken here involves the use of finite difference approximations to convert the original set of PDE’s into a set of ordinary differential equations. By exploiting the regularity of the solution with respect to the time variable a fixed interval Kalman smoother is implemented to smooth the output data and estimate the additional time derivatives which appear in the differential equations. Finally, the unknown parameters can be estimated directly from the data using simple least squares or other optimisation schemes.

The proposed method is implemented and tested under the assumption that the parameters which relate to specific physical properties of the distributed system, such as conductivity, resistivity, charge density, stiffness or damping properties, diffusion or convection parameters, can be assumed constant over the operating range. However, the time-varying parameter identification problem, not discussed in this paper, can also be solved by the same approach with minimum additional effort.

2 System description

Assume that the system under consideration is governed by a general linear or nonlinear PDE which take the form

\[ F\left( \frac{\partial^l u}{\partial t \partial^{j_1} x_1 \ldots \partial^{j_n} x_n}, \ldots, u, t, x, \theta \right) = f_\theta(t, x) \]  

where \( u(x, t) \) is the dependent variable \( x = (x_1, x_2, \ldots, x_m) \in \Omega \subset \mathbb{R}^m \) is the vector of spatial variables, \( t \) denotes time, \( \theta \) is the vector of unknown constant parameters, \( l = j + \sum_{k=1}^m j_k \), \( F(\cdot) \) and \( f_\theta(\cdot) \) are known linear or nonlinear functions. The boundary and initial conditions for equation (1) are,

\[ B(u)_{x \in \partial \Omega} = u_\Omega(x, t), \quad T(u(x, 0)) = u(x) \]  

which are assumed unknown in the parameter estimation procedure. In equation (2) \( B \) is the differential operator which operates on the boundary \( \partial \Omega \) of the spatial domain \( \Omega \) and \( T \) is a differential operator evaluated at \( t = 0 \) providing the initial conditions of \( u \) and of time derivatives of \( u \).

Assume that the system measurements are recorded at sampling instants \([0 \Delta t \ldots n \Delta t]\) using a finite number of sensors distributed over the spatial domain. In practice the output will be corrupted by measurement noise. Denote \( X = \{x_k\} \) to be the vector of sensor locations, and \( u_k = [u(k, 1) \ldots u(k, n \Delta t)] \) the output vector recorded from the \( k \)th sensor, the noisy observation vector from the \( k \)th sensor can then be defined as

\[ z_k = u_k + e_k \]  

where \( e_k = [e(k, 1) \ldots e(k, n \Delta t)] \) is the measurement noise vector associated with the \( k \)th sensor.
Using finite differences equation (1) can be converted into a set of ordinary differential equations. It follows that for each sensor located inside the spatial domain \( \Omega \) we can write a differential equation which has the following general form

\[
F\left( \frac{d^i u \Delta t^{-j} u}{dt^j \Delta x_1 \ldots \Delta x_n}, \ldots, u, t, x, \theta \right) = f_n(t, x)
\]  

(4)

This results by replacing the partial derivatives with respect to the spatial variables by finite difference approximations. In order to estimate the parameter vector \( \theta \) the signal and the corresponding time derivatives involved in equation (4) have to be estimated initially.

An efficient solution to numerical differentiation of noisy signals which uses a fixed-lag Kalman smoother to accomplish this task was proposed by Fioretti and Jetto (1989). With a few modifications the same approach is implemented here to obtain accurate estimates of the output signals and of the time derivatives directly from noisy measurements. If equation (4) is linear-in-the-parameters \( \theta \) the parameter vector \( \theta \) can be estimated using the least-squares method. Whenever the parameters enter equation (4) in a nonlinear fashion an alternative method, such as gradient-descent optimisation scheme can be used.

3 Data smoothing and differentiation

In many practical situations a certain degree of regularity can be assumed for the output \( u(x, t) \). In particular the smoothing and differentiation algorithm employed in this paper assumes \( u(x, t) \) to be a \( C^p \) function with respect to the time variable. In particular when \( p = \infty \) the solution \( u(x, t) \) is continuously differentiable infinitely often with respect to the time variable \( t \).

Under these assumptions, for the output signal recorded from the \( k \)th sensor \( u_k(t) \) it is possible to define a state vector \( U_k(t) \) composed of the signal \( u_k(t) \) and the derivatives \( \frac{d^j u_k(t)}{dt^j} \), \( j = 1, \ldots, N, N < p \) (Fioretti and Jetto, 1989). By differentiating \( U_k(t) \) with respect to time it is possible to write the following continuous state-space equations.

\[
\dot{U}_k(t) = DU_k(t) + G \frac{d^{N+1} u_k(t)}{dt^{N+1}}
\]  

(5)

where \( D \) is the \((N+1) \times (N+1)\) matrix

\[
D = \begin{bmatrix}
0 & 1 & 0 & \ldots & 0 & \ldots \\
0 & 0 & 1 & \ldots & 0 & \ldots \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
0 & 0 & 0 & \ldots & 1 & \ldots \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots 
\end{bmatrix}
\]  

(6)

and \( G = [0 \ldots 0 1]^T \) is a \((N+1)\)-dimensional vector.

Assuming \( \Delta t \) to be the sampling time, the discrete state space equations associated with (5) have the following form

\[
U_k(t + \Delta t) = AU_k(t) + W(t)
\]  

(7)
where $A$ is the state transition matrix

$$A(\Delta t) = \begin{bmatrix}
1 & \Delta t & \Delta t^2/2! & \ldots & \Delta t^N/N! & \ldots \\
0 & 1 & \Delta t & \ldots & \Delta t^{(N-1)}/(N-1)! & \ldots \\
& \vdots & & & \vdots & \\
0 & 0 & 0 & \ldots & 1 & \ldots \\
& & & & &
\end{bmatrix}$$

(8)

Because in normal situations $u_k(t)$ is the only signal available for measurement, the measurement equation for the $k$th sensor can be written as

$$z_k(t) = HU_k(t) + e_k(t) = u_k(t) + e_k(t)$$

(9)

where $H = [1 \ldots 0]$ is a $(N+1)$-dimensional vector and $e_k(t)$ represents measurement noise.

It is easy to see that assuming $e_k(t)$ to be a white noise sequence, equations (7) and (9) have a suitable form for Kalman filter implementation. In particular, the fixed interval smoother described in Anderson and Moore (1979) provides an optimal solution to state estimation. The state vector in this case consists of the measured output and the unobserved higher order derivatives. The remaining $(N+1)^{th}$ derivative of $u^k(t)$ in equation (5) will be treated as white noise so the term $W(t)$ in (7) is a white noise sequence with the covariance matrix $Q$. It can be shown (Fioretti and Jetto, 1989) that the generic element of $Q$ is given by

$$q_{ij} = \sigma_w^2 \frac{\Delta t^{2m+3-(i+j)}}{(m+1-i)!(m+1-j)!(2m+3-(i+j))}$$

(10)

with $\sigma_w^2$ given by

$$\sigma_w^2 = \frac{q_N}{3\Delta t}$$

(11)

The quantity $q_N$, which formally represents the remainder of the Taylor series expansion of order $N$ of the signal, can be approximated as

$$q_N = \frac{M \Delta t}{\pi} \frac{\omega_c^{N+2}}{4} \exp(\omega_c \Delta t)$$

(12)

In equation (12) $M$ is the upper bound for the amplitude spectrum of the signal and $\omega_c = 2\pi f_c$ is such that $f_c$ defines a cut-off frequency above which the power spectral density of the observation signal is negligible. In practice by computing the FFT and the power spectral density $P_w$ of the measured signals both $M$ and $f_c$ can be determined directly from data.

The fixed interval smoother was implemented here as a combination of two Kalman filters one running forward in time and one moving backwards (Meditch, 1973). The state transition matrices will be $A$ for the filter moving forward and $A^{-1}$ for the backward moving filter.

If $Y_k = \{z_k(t_1), z_k(t_2), \ldots, z_k(t_n)\}$ is the set of available observations consider

$$Y_k(t_i) = \{z_k(t_1), z_k(t_2), \ldots, z_k(t_i)\}$$

(13)

$$Y_k^+(t_i) = \{z_k(t_i), z_k(t_{i+1}), \ldots, z_k(t_n)\}$$

(14)
the sets of "past and present" and "future and present" observations at a given instant $t_i = i\Delta t$.

The smoothed state estimate at each time instant which represents the minimum variance estimate given all the data, past and future, is given by the well known formulas

$$\hat{z}_k(t_i) = (P_1^{-1} + P_2^{-1})^{-1}(P_1^{-1}\hat{z}_{k,1}(t_i) + P_2^{-1}\hat{z}_{k,2}(t_i))$$  \hspace{1cm} (15)$$
$$P = \text{cov}(\hat{z}_k - z_k) = (P_1^{-1} + P_2^{-1})^{-1}$$  \hspace{1cm} (16)

where

$$\hat{z}_{k,1}(t) = \mathcal{E}\{z_k(t_i)|Y^-_k(t_i)\}$$  \hspace{1cm} (17)

denotes the filter running forward in time and

$$\hat{z}_{k,2}(t) = \mathcal{E}\{z_k(t_i)|Y^+_k(t_i)\}$$  \hspace{1cm} (18)

denotes the estimate produced by the filter running backwards in time and $P_1$ and $P_2$ are the covariance matrices corresponding to the forward and backward filters.

If the data sequence is short the two filters can be run forward and backwards a few times in order to achieve convergence. In this case at the end of each run the covariance matrices associated with each filter are interchanged and so are the final state estimates. In this way the final estimates of the forward filter become initial conditions for the filter running backwards and vice-versa.

The key assumption when smoothing is performed is that the forward-time and backward-time system descriptions are equivalent so that the filters can cooperate by combining in an optimal way the estimates obtained from two independent sets of measurements $Y^-_k(t_i)$ and $Y^+_k(t_i + 1)$ (Lewis, 1986).

If however the signal or the associated derivatives have isolated discontinuities, eventually one of the models will fail to correctly describe the signal at that point. In this case it is possible to allow only one of the filters to produce the estimate, instead of combining them, by using an additional decision rule (Niedźwiecki and Sethares, 1995). In principle this could provide a solution when the underlying signals have isolated singularities.

A factor which clearly determines the accuracy of the estimates is the order of the signal model used. In theory the estimation error tends to zero monotonically with $N$, the largest order of the derivatives considered if data is sampled sufficiently fast relative to the frequency band of the signal. In practice, $N = 6, ..., 9$ can be chosen with good results. A value for $N$ which is too large will generally slow down the computation and also increase the risk of numerical instability.

The fixed-interval smoother can be applied to obtain the optimal state estimate, in particular the output $u_k$ and the higher order derivatives of $u_k(t)$ with respect to time which appear in equation (4). The Kalman smoother can also be used to smooth the outputs of the neighbouring sensors which are used to compute the finite difference approximations of the spatial derivatives in (1).

Assuming that equation (4) is linear-in-the-parameters a suitable form which allows $\theta$ to be estimated using simple least-squares, can be derived. Alternatively other optimisation algorithms can be used to determine the unknown parameters.
4 Simulation Results

The following three examples are intended to test the proposed parameter estimation approach.

4.1 Example 1

In this example the following model studied in (Hara et al., 1988) is considered

\[
\frac{\partial^2 u(x,t)}{\partial t^2} + C \frac{\partial^2 u(x,t)}{\partial x^2} = -\exp(-x)\cos(2t), \quad (x \in [0,1], t \in [0,1])
\]  

(19)

When \( C = 3.0 \) the solution \( u(x,t) \) of (19) is

\[
 u(x,t) = \exp(-x)\cos(2t)
\]  

(20)

Using finite differences the partial differential operator with respect to the spatial variable is replaced for \( z = x_k \) by a second-order centred difference approximation

\[
\frac{d^2 u_k(t)}{dt^2} = -C \frac{u_{k-1}(t) - 2u_k(t) + u_{k+1}(t)}{\Delta x^2} - \exp(-x)\cos(2t)
\]  

(21)

where \( \Delta x \) is the step size of the data sampled along the \( x \) axis and \( u_{k-1}(t) = u(x_k - \Delta x, t) \), \( u_k(t) = u(x_k, t) \) and \( u_{k+1} = u(x_k + \Delta x, t) \) are the outputs recorded from the sensors located at \( x = x_k - \Delta x \), \( x = x_k \) and \( x = x_k + \Delta x \) along the \( x \) axis.

The data set used to perform the identification procedure was generated by sampling the outputs \( u_{k-1}(t) \), \( u_k(t) \) and \( u_{k+1}(t) \) every \( \Delta t = 0.01s \). The estimation procedure was performed for different values of the step size \( \Delta x \) in order to test the sensitivity of the estimated parameters with respect to this variable.

For each value of \( \Delta x \) the resulting data sequences consisted of 1000 data points each. To make the simulation more realistic three uncorrelated white noise sequences with zero mean and variance \( \sigma^2 = 0.002 \) were added to the outputs. The resulting simulation data is plotted in Fig.1.

![Figure 1: Example 1: Simulated noisy data: \( x_k = 0.5 \), \( \Delta x = 0.25 \) and \( \sigma^2 = 0.002 \)](image-url)
A Kalman smoother with $N = 9$, the model order, implemented as described in Section 3 was used in each case to provide accurate estimates of $u_k(t)$, $u_{k-1}(t)$, $u_{k+1}(t)$, Fig.2, and $\frac{d^2 u_k(t)}{d t^2}$, Fig.2, at each sampling instant. As noted in Section 3, the values of $M$ and $f_c$ which appear in equation (12) were determined experimentally by computing the FFT and the power spectral density $P_\omega$ of the output signals. In particular, $f_c$ was selected such that $P_\omega < \rho$ for $f > f_c$. Numerical experiments have shown that by choosing the threshold $\rho$ around $(0.2\% - 0.5\%) P^{\text{max}}_\omega$ good estimates of the cut-off frequency $f_c$ and indirectly of the parameter $\sigma^2_\omega$ can be obtained.

![Figure 2](image1.png)

**Figure 2:** Example 1: Smoothed output data (dashed) superimposed on the simulated noise-free data (cont): $x_k = 0.5$, $\Delta x = 0.25$ and $\sigma^2 = 0.002$

![Figure 3](image2.png)

**Figure 3:** Example 1: Estimated (dashed) and true (cont) second-order derivative of $u(0.5, t)$
<table>
<thead>
<tr>
<th>Step Size</th>
<th>Sensor Location</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta x$</td>
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<tr>
<td>0.45</td>
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<tr>
<td>0.25</td>
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</tr>
</tbody>
</table>

Table 1: Example 1: Estimates of $C$ for different sensor locations $x_k$ and step sizes $\Delta x$

The smoothed signals were subsequently used in equation (21) to estimate the unknown parameter $C$. The results which are summarised in Table 1 compare favourably with the results reported elsewhere (Hara et al., 1988; Sagara et al., 1991) where different techniques were employed.

4.2 Example 2

Another system which was studied by Hara et al (1988)

\[
\frac{\partial^2 u(x,t)}{\partial t^2} - \frac{\partial^2 u(x,t)}{\partial x^2} = f(x,t), \quad (x \in [0,1], t \in [0,1])
\]  
(22)

was also used to test the new parameter estimation approach.

In equation (22) $f(x,t)$ was given by

\[
f(x,t) = 13 \exp(-x) \cos(1.5t) - 9.32 \exp(-0.5x) \cos(2.1t)
\]  
(23)

The solution of the system described by (22) and (23) is

\[
u(x,t) = 4 \exp(-x) \cos(1.5t) + 2 \exp(-0.5x) \cos(2.1t)
\]  
(24)

In this example, the system model was assumed to be described by the second-order partial differential equation

\[
\frac{\partial^2 u(x,t)}{\partial t^2} + C_2 \frac{\partial^2 u(x,t)}{\partial x \partial t} + C_3 \frac{\partial^2 u(x,t)}{\partial x^2} + C_4 \frac{\partial u(x,t)}{\partial t} + C_6 u(x,t) = f(x,t)
\]  
(25)

Using finite differences this partial differential equation can be transformed into the following ordinary differential equation

\[
\frac{d^2 u_k(t)}{dt^2} + \frac{C_2}{\Delta x} \left[ \frac{d u_k(t)}{dt} - \frac{d u_{k-1}(t)}{dt} \right] + C_3 \frac{u_{k-1}(t) + u_{k+1}(t) - 2u_k(t)}{\Delta x^2} + C_4 \frac{d u_k(t)}{dt} + C_6 u_k(t) = f(x_k,t)
\]  
(26)
where $u_{k-1}(t) = u(x_k - \Delta x, t)$, $u_k(t) = u(x_k, t)$, $u_{k+1}(t) = u(x_k + \Delta x, t)$. 1000 data points for each output variable, sampled every $dt = 0.01s$ and contaminated by white noise with variance $\sigma^2 = 4 \times 10^{-4}$ were used for the identification.

The identification was again performed using different values for the step size $\Delta x$ and for different sensor positions $x_k$. In each case a fixed interval smoother with $N = 9$ was applied first and then the parameters were estimated using least-squares. The results are summarised in Table 2. The accuracy of the estimates also compare favourably with that achieved using spline functions (Hara et al., 1988).

The results obtained in Examples (1) and (2) illustrate that by applying the proposed method, accurate estimates of the parameter vector associated with a distributed parameter system can be obtained directly from noise corrupted data. For the examples considered, the numerical simulations have shown that the estimates are not very sensitive to the sensors locations. With respect to the distance between the sensor locations which is equivalent to the step size used to discretise the partial differential equation along the spatial variable, only a small deterioration of the accuracy of the parameter estimates can be noticed especially in Example 2 as the discretisation step is reduced.

In general however, the choice of sensor locations in the spatial domain will be dictated by practical considerations and observability requirements. While practical circumstances may place restrictions on the choice of measurement locations, it is essential to ensure that for a particular choice of measurement variables and locations the distributed system is observable, that is, given the measurements $z(t)$ the solution $u(x, t)$ is uniquely determined within the spatial domain $\Omega$. From this point of view the proposed method is quite flexible as it does not require a special sensor configuration in the spatial domain. More on this topic can be found in a number of papers which address the sensor location and the observability problem in more detail (Wang and Fung, 1964; Goodson and Klein, 1970; Goodson and Polis, 1978).

### 4.3 Example 3

The final example considered here involves estimating the parameters of a nonlinear partial differential equation. Many methods available in the literature assume a linear form of the partial differential equation describing the distributed parameter system. From this point of view this example emphasises the applicability of the proposed method to nonlinear distributed systems.

Consider a diffusion process modelled by the following partial differential equation

$$\frac{\partial u(x, t)}{\partial t} = C_1 \frac{\partial u(x, t)}{\partial x} + C_2 u(x, t) + C_3 \frac{\partial^2 u(x, t)}{\partial x^2} + C_4 u(x, t)^3 + C_5$$  \hspace{1cm} (27)

with the following boundary and initial conditions.

$$\frac{du(1, t)}{dt} = 0, \quad u(0, t) = 2 \sin(10t)$$  \hspace{1cm} (28)
<table>
<thead>
<tr>
<th>Step Size $\Delta x$</th>
<th>Sensor Location $x_k = 0.45$</th>
<th>$x_k = 0.5$</th>
<th>$x_k = 0.55$</th>
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Table 2: Example 2: Estimates of $C_2$, $C_3$, $C_4$ and $C_6$ for different sensor locations $x_k$ and step sizes $\Delta x \left(\sigma^2 = 4 \cdot 10^{-4}\right)$. True values $C_2 = 0$, $C_3 = -1$, $C_4 = 0$ and $C_6 = 0$. 

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Using finite differences the partial differential equation can be replaced by a system of ordinary differential equations. In this example the resulting system of ordinary differential equations was integrated using a fourth-order Runge-Kutta routine with the step $\Delta t = 5 \cdot 10^{-4}$ to generate the simulation data. The parameters used in the simulation were $C_1 = -1$, $C_2 = -10$, $C_3 = 0.75$, $C_4 = -4$ and $C_5 = 3$. A relatively large step size $\Delta x = 0.05$ was used along the $x$ direction.

The ordinary differential equation corresponding to $x = x_k$ is as follows

$$\frac{du_k(t)}{dt} = -\frac{u_k(t) - u_{k+1}(t)}{\Delta x} - 10u_k(t) + 0.75 \frac{u_{k-1}(t) - 2u_k(t) + u_{k+1}(t)}{\Delta x^2} - 4u_k(t)^3 + 3 \quad (29)$$

where $u_{k-1}(t)$, $u_k(t)$ and $u_{k+1}(t)$ represent the outputs recorded from sensors located along the $x$ axis at $x_{k-1} = 0.2$, $x_k = 0.3$ and $x_{k+1} = 0.4$ respectively. The output sequences $u_{k-1}(t)$, $u_k(t)$ and $u_{k+1}(t)$ resulting after simulation consisted of 2000 data samples each. The sequences were down-sampled (decimated) by 2 and white noise with variance $\sigma^2 = 3.5 \cdot 10^{-5}$ was added to each output prior to performing parameter identification. The fixed interval smoother was then applied for the noisy output sequences, containing 1000 data points each, in order to smooth the data and estimate $\frac{du_k(t)}{dt}$.

The resulting signals were used to determine the unknown parameters in equation (29) by means of a least-squares algorithm. The estimated parameters $C_1 = -1.0719$, $C_2 = -9.6396$, $C_3 = 0.7257$, $C_4 = -3.8031$ and $C_5 = 2.8463$ are quite accurate given the relatively rough discretisation along the $x$ axis used initially to generate the simulation data.

5 Conclusions

A new direct approach to the identification of constant parameters in distributed systems directly from noisy observations has been introduced. The technique requires a knowledge of the form of the partial differential equations within a set of constant parameters but unlike most of the existing approaches the equations can be either linear or nonlinear and moreover the initial and boundary conditions do not need to be specified explicitly. The new method also requires only a small number of sensor locations to collect data for identification and this makes it particularly suitable for applications where technical or cost considerations prohibit using a large number of sensors.

The algorithm, which involves smoothing the original noisy output measurements and estimating the temporal and spatial derivatives involved in the model using a fixed interval smoother, was tested with excellent results using three simulated examples including a nonlinear distributed system.

The simulations performed show that the method is not sensitive to the choice of measurement locations and discretisation step along the spatial variable. Although in all the examples considered the distributed systems were one-dimensional, the method can also be applied to higher order systems the only difference being that additional sensor locations have to be used in order to be able to approximate all the spatial derivatives required.
References


