Wavelet Multiresolution Spatio-Temporal Modelling Using the Integro-Difference Equation

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Abstract

The Integro Difference Equation (IDE) is an increasingly popular model of spatio-temporal processes. Here we develop a Multiresolution Approximation (MRA) framework for the IDE based on semi-orthogonal cardinal B-spline wavelets. State and parameter estimation is approached in a Maximum Likelihood (ML) framework using the Expectation Maximisation (EM) algorithm. Examples are given to demonstrate the features of the model.

Index Terms

Dynamic spatio-temporal modelling, Expectation Maximisation (EM) algorithm, Integro-Difference Equation (IDE), Multiresolution Approximation (MRA), wavelets.

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I. INTRODUCTION

Complex spatio-temporal behaviour is found in many different systems such as aquatic ecosystems [1], meteorological forecasting [2], air pollution [3], soil temperature [4], thermal processes [5], disease spread [6] and real estate markets [7]. Spatio-temporal modelling aims to represent dynamic system behaviour across time and space.

Techniques for modelling spatio-temporal systems are generating growing interest, both in the applied and theoretical literature. Of particular interest are the class of dynamic spatio-temporal models, including Cellular Automata (CA) [8], Coupled Map Lattices (CMLs) [9], Lattice Dynamical Wavelet Neural Network (LDWNN) [10] and spatially correlated time series [11]–[13] which have all been used in a system identification context. The extent of the spatial interactions in these models is determined by a discrete neighbourhood structure.

Another such model is the Integro-Difference Equation (IDE). These models have received much attention in population ecology as models for the spatio-temporal spread of organisms [14], [15]. IDE models combine discrete temporal dynamics with a continuous spatial representation. The dynamics of this model are given by a spatial mixing kernel, which defines the mapping between the current spatial field and the previous spatial field. The IDE model can be applied to data sampled both regularly and irregularly in space due to the continuous representation of each spatial field. Estimating the underlying spatial field in time is of particular interest, and is not straightforward especially when the field displays structure at different spatial scales. Estimation of the underlying spatial field can be achieved by estimating the associated spatial mixing kernel from measured data, and then using this in a filtering framework.

Wikle [16] describes the IDE using a state-space formulation by decomposing the kernel and the field using a set of spectral basis functions. An alternative approach for the decomposition of the IDE was introduced in [17] where the resulting state and parameter space dimensions are independent of the number of observation locations. This is crucial not only for model parsimony but also has implications for studying systems observed at a high spatial resolution. In this method an Expectation-Maximisation

(EM) algorithm was used to estimate both the field and the kernel from the observed data. A similar approach is adopted by [18] which developed a model selection procedure by considering various spatial scales at which to represent the system.

Behaviour of the spatial field is often of interest at a variety of scales [19]–[22]. At each scale, an appropriate model should be adopted to adequately reflect the underlying phenomenon. The spatial field may have features at multiple scales either naturally or as a consequence of the measurement process [23] and hence modelling methods that represent the field at multiple scales are essential. Multiresolution Approximation (MRA) [24]–[26] provides such a modelling framework in which information at different scales can be represented simultaneously.

In practice, MRA can be implemented using different types of wavelet and scaling functions. Semi-orthogonal B-spline wavelets [27], [28] benefit from distinctive properties which are useful for system identification purposes. They are compactly supported and have a closed-form analytic expression which allows simple manipulations such as integration [29], [30]. This class of wavelets has been successfully applied in approximation schemes such as wavelet networks [31], [32] and wavelet based CML models [33].

In this paper a multiresolution approximation of the IDE based on the model proposed in [17] is presented. B-spline scaling and wavelet functions are used to decompose both the kernel and the spatial field. Maximum likelihood estimates of the derived parametric state-space model are obtained using the EM-based algorithm of [17]. In this model, the kernel and the spatio-temporal dynamics of the field are viewed at different spatial scales. Whereas in [18] different spatial scales were examined and one chosen, the work presented herein represents the system at a number of different spatial scales concurrently.

The rest of this paper is set out as follows: in Section 2, the IDE model is briefly reviewed and the MRA of the IDE is presented. Section 3 introduces the B-spline wavelet IDE model and provides necessary formulation to construct such a model in state-space. Section 4 briefly reviews the EM-based approach for parameter and state estimation. In Section 5, synthetic examples are given to demonstrate the ability of the developed MRA model in estimation of the hidden spatio-temporal field and the spatial mixing kernel. Finally conclusions are drawn in Section 6.

II. MRA OF THE IDE IN STATE-SPACE

The spatially homogeneous, linear IDE is given by

$$z_{t+1}\left(\mathbf{s}\right) = \int_{\mathcal{S}} k\left(\mathbf{s} - \mathbf{r}\right) z_t\left(\mathbf{r}\right) d\mathbf{r} + e_t\left(\mathbf{s}\right) \tag{1}$$

where $t \in \mathbb{Z}_0$ denotes discrete time, $\mathbf{s}, \mathbf{r} \in \mathcal{S} \subset \mathbb{R}^{n_S}$ are spatial locations in n_S-dimensional physical space, where $n_S \in \{1, 2, 3\}$. The continuous spatial field at time t and at location $\mathbf{s}$ is denoted $z_t(\mathbf{s})$. The model dynamics are defined by the homogeneous time invariant spatial mixing kernel, $k(\mathbf{s} - \mathbf{r}):$ $\mathbb{R}^{n_S} \to \mathbb{R}$ which maps the current spatial field to the next spatial field via the integral (1) and $e_t(\mathbf{s})$ is an *i.i.d.* disturbance such that $e_t(\mathbf{s}) \sim \mathcal{GP}(\mathbf{0}, \eta(\mathbf{s} - \mathbf{r}))$. Here $\mathcal{GP}(\mathbf{0}, \eta(\mathbf{s} - \mathbf{r}))$ denotes a zero mean spatial Gaussian process with covariance function $\eta(\mathbf{s} - \mathbf{r})$ [**?**]. The spatial field is observed by

$$\mathbf{y}_t = \mathbf{z}_t + \mathbf{v}_t \tag{2}$$

where the observation vector $\mathbf{y}_t = [y_t(\mathbf{s}_1) y_t(\mathbf{s}_2) \cdots y_t(\mathbf{s}_{n_y})]^\top$, compiled at n_y spatial locations and at time t, is corrupted by an i.i.d normally distributed zero-mean white noise $\mathbf{v}_t \sim \mathcal{N}(\mathbf{0}, \mathbf{\Sigma}_v)$ with $\mathbf{\Sigma}_v = \sigma_v^2 \mathbf{I}_{n_y}$. It is assumed here that $\mathbf{\Sigma}_v$ and $\eta(\mathbf{s} - \mathbf{r})$ are known. The superscript $\top$ denotes the transpose operator.

Assuming $z_t(.)$ and $k(.)$ are square-integrable functions, MRA of the one-dimensional IDE can be obtained by expanding both the field and the kernel in the integral (1) in terms of the translations and dilations of a scaling function $\phi(s)$ and a mother wavelet $\psi(s)$. For the one-dimensional kernel this is given by,

$$k(s - r) = \sum_{l \in \mathbb{Z}} \alpha_{j_0, l} \phi_{j_0, l}(s - r) + \sum_{j \geq j_0}^{\infty} \sum_{l \in \mathbb{Z}} \beta_{j, l} \psi_{j, l}(s - r) \tag{3}$$

In this expansion, $\alpha_{j_0, l}$ are the approximation coefficients at the lowest scale j_0 and $\beta_{j, l}$ represent the detail coefficients at different scales j, with $\phi_{j, l}(s) = 2^{\frac{j}{2}} \phi(2^j s - l)$ and $\psi_{j, l}(s) = 2^{\frac{j}{2}} \psi(2^j s - l)$. Integers j and l are called scale and translation parameters accordingly. The one-dimensional field can similarly be decomposed as

$$z_t(s) = \sum_{l \in \mathbb{Z}} x_{t, j_0, l} \phi_{j_0, l}(s) + \sum_{j \geq j_0}^{\infty} \sum_{l \in \mathbb{Z}} \check{x}_{t, j, l} \psi_{j, l}(s) \tag{4}$$

where $x_{t, j_0, l}$ and $\check{x}_{t, j, l}$ are the coefficients of the expansion at time t. A two-dimensional MRA can be implemented using 2-D scaling and wavelet functions built up using the tensor-product approach [34], [35]. We write the 2-D scaling function as

$$\phi_{j, \mathbf{l}}(s_1, s_2) = \phi_{j, l_1}(s_1) \phi_{j, l_2}(s_2) \tag{5}$$

and three 2-D wavelet functions $\psi^{(n)}(\mathbf{s})$ where $n = 1, 2, 3$ as

$$\psi_{j, \mathbf{l}}^{(1)}(s_1, s_2) = \phi_{j, l_1}(s_1) \psi_{j, l_2}(s_2) \tag{6}$$

$$\psi_{j, \mathbf{l}}^{(2)}(s_1, s_2) = \psi_{j, l_1}(s_1) \phi_{j, l_2}(s_2) \tag{7}$$

$$\psi_{j, \mathbf{l}}^{(3)}(s_1, s_2) = \psi_{j, l_1}(s_1) \psi_{j, l_2}(s_2) \tag{8}$$

for $j \in \mathbb{Z}$ and, $\mathbf{l} \in \mathbb{Z}^2$, where $\psi_{j,\mathbf{l}}^{(1)}, \psi_{j,\mathbf{l}}^{(2)}$ and $\psi_{j,\mathbf{l}}^{(3)}$ extract fine features of the 2-D field at vertical, horizontal and diagonal orientations respectively. This can be generalised to d-dimensional MRA by introducing the scaling function

$$\phi_{j,\mathbf{l}}(s_1, s_2, \cdots s_d) = \phi_{j,l_1}(s_1)\phi_{j,l_2}(s_2) \cdots \phi_{j,l_d}(s_d) \tag{9}$$

$$j \in \mathbb{Z}, \quad \mathbf{l} \in \mathbb{Z}^d$$

and $2^d - 1$ wavelet functions $\psi^{(n)}(\mathbf{s})$, $n = 1, \cdots, 2^d - 1$ with a procedure similar to the 2-D case. Using these basis functions, multi-dimensional MRA of the kernel and the field can be obtained by

$$k(\mathbf{s} - \mathbf{r}) = \sum_{\mathbf{l} \in \mathbb{Z}^d} \alpha_{j_0, \mathbf{l}} \phi_{j_0, \mathbf{l}}(\mathbf{s} - \mathbf{r})$$

$$+ \sum_{j \geq j_0}^{\infty} \sum_{\mathbf{l} \in \mathbb{Z}^d} \sum_{i=1}^{2^d - 1} \beta_{j,\mathbf{l}}^{(i)} \psi_{j,\mathbf{l}}^{(i)}(\mathbf{s} - \mathbf{r}) \tag{10}$$

$$z_t(\mathbf{s}) = \sum_{\mathbf{l} \in \mathbb{Z}^d} x_{t,j_0,\mathbf{l}} \phi_{j_0,\mathbf{l}}(\mathbf{s}) + \sum_{j \geq j_0}^{\infty} \sum_{\mathbf{l} \in \mathbb{Z}^d} \sum_{i=1}^{2^d - 1} \check{x}_{t,j,\mathbf{l}}^{(i)} \psi_{j,\mathbf{l}}^{(i)}(\mathbf{s}) \tag{11}$$

Equations (10) and (11) are infinite series expansions. For practical implementation, (10) and (11) must be truncated at some level j, therefore we have

$$k(\mathbf{s} - \mathbf{r}) \approx \boldsymbol{\theta}^\top \boldsymbol{\lambda}(\mathbf{s} - \mathbf{r}) \tag{12}$$

$$z_t(\mathbf{s}) \approx \boldsymbol{\mu}(\mathbf{s})^\top \mathbf{x}_t \tag{13}$$

where the unknown parameter vector $\boldsymbol{\theta} \in \mathbb{R}^{n_\theta}$ and the unknown state vector $\mathbf{x}_t \in \mathbb{R}^{n_x}$ are defined as

$$\boldsymbol{\theta}^\top = \begin{bmatrix} \boldsymbol{\alpha}_{j_0}^\top & \boldsymbol{\beta}_{j_0}^\top & \boldsymbol{\beta}_{j_0+1}^\top \cdots \boldsymbol{\beta}_j^\top \end{bmatrix} \tag{14}$$

$$\mathbf{x}_t^\top = \begin{bmatrix} \mathbf{x}_{t,j_0}^\top & \check{\mathbf{x}}_{t,j_0}^\top & \check{\mathbf{x}}_{t,j_0+1}^\top \cdots \check{\mathbf{x}}_{t,j}^\top \end{bmatrix} \tag{15}$$

and where the kernel approximation coefficient vector $\boldsymbol{\alpha}_{j_0}$ and the field approximation coefficient vector $\mathbf{x}_{t,j_0}$ comprise all the coefficients $\{\alpha_{j_0,\mathbf{l}} : \mathbf{l} \in \mathbb{Z}^d\}$ and $\{x_{t,j_0,\mathbf{l}} : \mathbf{l} \in \mathbb{Z}^d\}$ respectively. The kernel detail coefficient vectors $\boldsymbol{\beta}_j$ and the field detail coefficient vectors $\check{\mathbf{x}}_{t,j}$ are defined by

$$\boldsymbol{\beta}_j^\top = \begin{bmatrix} \boldsymbol{\beta}_j^{(1)\top} & \boldsymbol{\beta}_j^{(2)\top} \cdots \boldsymbol{\beta}_j^{(2^d-1)\top} \end{bmatrix} \tag{16}$$

$$\check{\mathbf{x}}_{t,j}^\top = \begin{bmatrix} \check{\mathbf{x}}_{t,j}^{(1)\top} & \check{\mathbf{x}}_{t,j}^{(2)\top} \cdots \check{\mathbf{x}}_{t,j}^{(2^d-1)\top} \end{bmatrix} \tag{17}$$

where the vector $\boldsymbol{\beta}_j^{(i)}$ contains all the coefficient $\left\{ \beta_{j,\mathbf{l}}^{(i)} : \mathbf{l} \in \mathbb{Z}^d \right\}$ and the vector $\check{\mathbf{x}}_{t,j}^{(i)}$ contains all the coefficient $\left\{ \check{x}_{t,j,\mathbf{l}}^{(i)} : \mathbf{l} \in \mathbb{Z}^d \right\}$. The vector of the kernel scaling and wavelet functions $\boldsymbol{\lambda} : \mathbb{R}^{n_s} \to \mathbb{R}^{n_\theta}$ and the vector of the field scaling and wavelet functions $\boldsymbol{\mu} : \mathbb{R}^{n_s} \to \mathbb{R}^{n_x}$ are defined by

$$\boldsymbol{\lambda}^\top (\mathbf{s} - \mathbf{r}) = \begin{bmatrix} \boldsymbol{\phi}_{j_0}^\top (\mathbf{s} - \mathbf{r}) & \boldsymbol{\psi}_{j_0}^\top (\mathbf{s} - \mathbf{r}) & \boldsymbol{\psi}_{j_0+1}^\top (\mathbf{s} - \mathbf{r}) \\ & \cdots & \boldsymbol{\psi}_{j}^\top (\mathbf{s} - \mathbf{r}) \end{bmatrix} \tag{18}$$

$$\boldsymbol{\mu}^\top (\mathbf{s}) = \begin{bmatrix} \boldsymbol{\phi}_{j_0}^\top (\mathbf{s}) & \boldsymbol{\psi}_{j_0}^\top (\mathbf{s}) & \boldsymbol{\psi}_{j_0+1}^\top (\mathbf{s}) \cdots \boldsymbol{\psi}_{j}^\top (\mathbf{s}) \end{bmatrix} \tag{19}$$

Each vector of basis functions on the right hand-side of (18) and (19) are constructed in a way similar to their corresponding weight vectors in (14) and (15). Note that the identified IDE model will approximate the underlying spatio-temporal dynamics at different spatial scales. In this way both macroscopic and microscopic behaviour of the system can be represented simultaneously.

The state-space representation of the spatio-temporal IDE proposed in [17] is derived for an arbitrary set of basis functions and hence this derivation can be applied using scaling and wavelet basis functions. Let

$$\boldsymbol{\Lambda}_x = \int_{\mathcal{S}} \boldsymbol{\mu} (\mathbf{s}) \boldsymbol{\mu} (\mathbf{s})^\top d\mathbf{s} \tag{20}$$

$$\boldsymbol{\Lambda}_\theta = \iint_{\mathcal{S}} \boldsymbol{\mu} (\mathbf{s}) \boldsymbol{\theta}^\top \boldsymbol{\lambda} (\mathbf{s} - \mathbf{r}) \boldsymbol{\mu} (\mathbf{r})^\top d\mathbf{r} d\mathbf{s} \tag{21}$$

where $\boldsymbol{\Lambda}_x, \boldsymbol{\Lambda}_\theta \in \mathbb{R}^{n_x \times n_x}$. The spatial IDE model in (1) and (2) can be represented as linear state-space model of the form

$$\mathbf{x}_{t+1} = \mathbf{A} (\boldsymbol{\theta}) \mathbf{x}_t + \mathbf{w}_t \tag{22}$$

$$\mathbf{y}_t = \mathbf{C} \mathbf{x}_t + \mathbf{v}_t \tag{23}$$

where

$$\mathbf{A} (\boldsymbol{\theta}) = \boldsymbol{\Lambda}_x^{-1} \boldsymbol{\Lambda}_\theta \tag{24}$$

and

$$\mathbf{C} = \begin{pmatrix} \boldsymbol{\phi}_{j_0} (\mathbf{s}_1) & \boldsymbol{\phi}_{j_0} (\mathbf{s}_2) & \cdots & \boldsymbol{\phi}_{j_0} (\mathbf{s}_{n_y}) \\ \boldsymbol{\psi}_{j_0} (\mathbf{s}_1) & \boldsymbol{\psi}_{j_0} (\mathbf{s}_2) & \cdots & \boldsymbol{\psi}_{j_0} (\mathbf{s}_{n_y}) \\ \boldsymbol{\psi}_{j_0+1} (\mathbf{s}_1) & \boldsymbol{\psi}_{j_0+1} (\mathbf{s}_2) & \cdots & \boldsymbol{\psi}_{j_0+1} (\mathbf{s}_{n_y}) \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{\psi}_{j} (\mathbf{s}_1) & \boldsymbol{\psi}_{j} (\mathbf{s}_2) & \cdots & \boldsymbol{\psi}_{j} (\mathbf{s}_{n_y}) \end{pmatrix}^\top$$

and where

$$\mathbf{w}_t = \mathbf{\Lambda}_x^{-1} \int_{\mathcal{S}} \boldsymbol{\mu}(\mathbf{s}) \, e_t(\mathbf{s}) \, d\mathbf{s} \tag{25}$$

is a vector valued, zero-mean normally distributed white noise process with covariance given by (Lemma 1, Appendix)

$$\mathbf{\Sigma}_w = \mathbf{\Lambda}_x^{-1} \mathbf{\Pi} \mathbf{\Lambda}_x^{-\top} \tag{26}$$

and

$$\mathbf{\Pi} = \iint_{\mathcal{S}} \boldsymbol{\mu}(\mathbf{s}) \, \eta(\mathbf{s} - \mathbf{r}) \, \boldsymbol{\mu}(\mathbf{r})^{\top} \, d\mathbf{r}d\mathbf{s} \tag{27}$$

By substituting the parameter vector $\boldsymbol{\theta}$, the state vector $\mathbf{x_t}$, the vector of kernel basis functions $\boldsymbol{\lambda}$ and the vector of field basis functions $\boldsymbol{\mu}$ in (20-27), the state-space representation of the multiresolution approximation of the IDE can be achieved. It should be noted that the complexity of the model is independent of the number of observation locations, providing more flexibility in handling high resolution data.

III. B-SPLINE WAVELET IDE MODEL

Multiresolution approximation can be implemented using different classes of scaling and wavelet functions. In order to determine the matrices $\mathbf{\Lambda}_x$ and $\mathbf{\Lambda}_\theta$ convolution and inner product expressions of the basis functions need to be computable. B-spline wavelet and scaling functions are particularly convenient in the above decomposition as their convolution and inner product expressions can be found analytically.

The mth order cardinal B-spline scaling function is defined by the recurrence relation [27]

$$\begin{aligned} N_m(s) &= (N_{m-1} * N_1)(s) \\ &= \int_0^1 N_{m-1}(s-r)\,dr \quad m > 1 \end{aligned} \tag{28}$$

Here $*$ denotes the convolution operator and $N_1(s)$ is the characteristic function of the unit interval $[0,1)$

$$N_1(s) = \begin{cases} 1 & \text{if } 0 \le s < 1, \\ 0 & \text{elsewhere} \end{cases} \tag{29}$$

In order to compute the integrals (20) and (21) we need to be able to calculate the convolution and inner product of B-spline scaling functions. Equation (28) can be rewritten as $(m-1)$ times convolution of indicator function with itself

$$N_m(s) = \underbrace{(N_1 * N_1 * \cdots * N_1)}_{m-1 \quad \text{convolutions}}(s) \tag{30}$$

then by using the associativity property of the convolution operator, it is clear that

$$N_m(s) * N_{m'}(s) = \overbrace{(N_1 * \cdots * N_1)}^{m-1 \quad \text{convolutions}}(s) * \overbrace{(N_1 * \cdots * N_1)}^{m'-1 \quad \text{convolutions}}(s)$$
$$\underbrace{}_{m+m'-1 \quad \text{convolutions}}$$
$$= N_{m+m'}(s) \tag{31}$$

This result can be used to show that (Lemma 2, Appendix)

$$\langle N_m(s-l_1), N_{m'}(s-l_2)\rangle = N_{m+m'}(m+l_1-l_2)$$
$$= N_{m+m'}(m'+l_2-l_1) \tag{32}$$

where $\langle .,. \rangle$ denotes the inner product.

The mth order compactly supported B-spline wavelet function is defined as [27]

$$\varphi_m(s) = \sum_{n=0}^{3m-2} q_n N_m(2s-n) \tag{33}$$

with the coefficients given by:

$$q_n = \frac{(-1)^n}{2^{m-1}} \sum_{l=0}^{m} \binom{m}{l} N_{2m}(n-l+1) \quad 0 \leq n \leq 3m-2 \tag{34}$$

By exploiting properties (31) and (32) the integrals (20) and (21) can be computed. In order to calculate elements of $\mathbf{\Lambda}_x$ and $\mathbf{\Lambda}_\theta$, scaling and wavelet basis functions should be expanded in terms of N_m at the appropriate scale. It is important to note that B-spline scaling and wavelet functions possess the following orthogonality properties [28]:

$$\langle \psi_{m;j_1,l_1}(s), \psi_{m;j_2,l_2}(s)\rangle = 0 \quad \text{for} \quad j_1 \neq j_2 \tag{35}$$

$$\langle \phi_{m;j_1,l_1}(s), \psi_{m;j_2,l_2}(s)\rangle = 0 \quad \text{for} \quad j_1 \leq j_2 \tag{36}$$

Where the subscript m is introduced to $\phi_{j,l}(s)$ and $\psi_{j,l}(s)$ to indicate the mth order B-spline scaling and wavelet functions. In the two dimensional case, the convolution integral can be factorised as follows,

e.g.

$$\phi_{m;j,\mathbf{l}}\left(s_1, s_2\right) * \psi_{m;j,\mathbf{l'}}^1\left(s_1, s_2\right) = \left[\phi_{m;j,l_1}\left(s_1\right) * \phi_{m;j,l_1'}\left(s_1\right)\right]$$
$$\times \left[\phi_{m;j,l_2}\left(s_2\right) * \psi_{m;j,l_2'}\left(s_2\right)\right]$$

(37)

The preceding factorisation can be also applied to the 2D-inner product integral. Non-zero quantities can be then expressed by

$$\left\langle\phi_{m;j,\mathbf{l}}\left(s_1, s_2\right), \phi_{m;j,\mathbf{l'}}\left(s_1, s_2\right)\right\rangle = \left\langle\phi_{m;j,l_1}\left(s_1\right), \phi_{m;j,l_1'}\left(s_1\right)\right\rangle$$
$$\times \left\langle\phi_{m;j,l_2}\left(s_2\right), \phi_{m;j,l_2'}\left(s_2\right)\right\rangle$$

(38)

likewise we can compute $\left\langle\psi_{m;j,\mathbf{l}}^1\left(s_1, s_2\right), \psi_{m;j,\mathbf{l'}}^1\left(s_1, s_2\right)\right\rangle$, $\left\langle\psi_{m;j,\mathbf{l}}^2\left(s_1, s_2\right), \psi_{m;j,\mathbf{l'}}^2\left(s_1, s_2\right)\right\rangle$ and $\left\langle\psi_{m;j,\mathbf{l}}^3\left(s_1, s_2\right), \psi_{m;j,\mathbf{l'}}^3\left(s_1, s_2\right)\right\rangle$.

Using these expansions it becomes straightforward to calculate the integrals (20) and (21). In this work, 4th order cardinal B-spline scaling and wavelet functions are used therefore, to compute the integrals (20) and (21) the 8th and 12th order B-spline values at integer points are required and can be found in [36].

IV. ESTIMATION OF THE MULTIRESOLUTION SPATIO-TEMPORAL IDE MODEL

A state-space representation of the IDE model allows the use of the Expectation Maximisation (EM) algorithm to infer both the kernel and the spatial field from the noise corrupted spatio-temporal data. In this context, the EM algorithm is a two part iterative algorithm that yields the maximum likelihood estimate of the spatial mixing kernel parameters and the posterior distribution of the field weights. In the M-step a lower bound $\mathcal{Q}\left(\boldsymbol{\theta}, \boldsymbol{\theta}'\right)$ of the complete-data log-likelihood $p\left(\mathbf{X}, \mathbf{Y} \mid \boldsymbol{\theta}\right)$, is maximised under the assumption of the system parameters being $\boldsymbol{\theta}'$ [37]. In the E-step, given an estimate of $\boldsymbol{\theta}$, filtering methods can be used to determine the posterior state sequence. Here we compare three techniques namely based on the Rauch Tung Striebel (RTS) smoother [38], Ensemble Kalman smoother (EnKs) [39] and a heuristic separable RTS smoother for state estimation problem. For the first method we modify the framework proposed in [17] by computing and storing the required elements prior to the iterative estimation algorithm,

the modified algorithm is computationally less demanding (see Appendix A). In Ensemble Kalman filter (EKf) an ensemble of model states, $\mathbf{X}_t \in \mathbb{R}^{n_x \times N} \sim \mathcal{N}(\mathbf{x}_t, \mathbf{P}_t)$ is propogated through the state equation to calculate the forecast estimates $\hat{\mathbf{x}}_t^f$ and the error covariance of the predicted model state, $\mathbf{P}_t^f$ where N is the number of ensemble members. Then the model state is updated to compute analysed estimates, $\hat{\mathbf{x}}_t^a$. This is important for model with high dimensional state space where standard Kalman filter is computationally infeasible to implement as the state covariance matrix needs to be stored and propogated in time. The EnKs updates the filtered ensembles at the current and all prior times every time a new set of measurements becomes available. The algorithm is given in Algorithm 1 for completeness. It is essential that the observations be also treated as an ensemble of random variables, $\mathbf{Y}_t$, having a distribution with mean equal to the observed value, $\mathbf{y}_t$ and covariance equal to $\mathbf{\Sigma}_v$ [40].

In the E-step, given an estimate of $\boldsymbol{\theta}$, the Rauch Tung Striebel (RTS) smoother can be employed to determine the posterior state sequence. It can be shown that [38], [41] every EM iteration increases the lower bound on the likelihood function and hence improving the state and parameter estimates. The stopping criterion is usually associated with either the change in the parameter estimates or the log-likelihood variation [37]. The stopping rule adopted herein is

$$\left(\parallel \mathbf{A} \parallel_F^{(i)} - \parallel \mathbf{A} \parallel_F^{(i-1)} \right) < \varepsilon \tag{39}$$

where ε is a threshold value and $\parallel \mathbf{A} \parallel_F^{(i)}$ and $\parallel \mathbf{A} \parallel_F^{(i-1)}$ are the Frobenius norm of the successive estimates of $\mathbf{A}$ matrices. It has been shown [17] that the state dimension is a critical factor in the complexity of the estimation procedure, however using the above decomposition, this is decoupled from the number of observation locations.

V. SIMULATION

In this section, we compare the performance of the different algorithms mentioned above on a synthetic example .....This section demonstrates the identification of the proposed IDE model. Primarily, the MRA of a synthetic model is demonstrated, which is able to represent the system at different spatial scales. In addition, the complexity of the field decomposition is shown to be independent to the number and spatial regularity of the observation locations. This allows the construction of parsimonious models using spatially dense observations, and demonstrates the utility of the approach to situations where the observations are not arranged on a regular lattice, i.e. sensor networks [42].

Algorithm 1 Ensemble Kalman smoother

1) Initialise:

$$\hat{\mathbf{x}}_0, \mathbf{P}_0$$

2) for $t \in \{0, \ldots, T\}$, calculate the state ensembles $\hat{\mathbf{X}}_t$ and the model errors ensemble $\mathbf{W}_t$ and propogate through the state equation:

$$\hat{\mathbf{X}}^f_{i,t+1} = \mathbf{A}\hat{\mathbf{X}}^a_{i,t} + \mathbf{W}_{i,t}$$

calculate the predicted state and the predicted covariance matrix

$$\hat{\mathbf{x}}^f_{t+1} = \frac{1}{N} \sum_{i=1}^{N} \hat{\mathbf{X}}^f_{i,t+1}$$

$$\mathbf{P}^f_{t+1} = \frac{1}{N-1} \sum_{i=1}^{N} \left(\hat{\mathbf{X}}^f_{i,t+1} - \hat{\mathbf{x}}^f_{t+1}\right) \left(\hat{\mathbf{X}}^f_{i,t+1} - \hat{\mathbf{x}}^f_{t+1}\right)^\top$$

3) compute $\mathbf{X}_4(t+1)$ and $\mathbf{X}_5(t+1)$ and the filtered state and the filtered covariance matrix:

$$\mathcal{K}_t = \mathbf{C}^\top (\mathbf{C}\mathbf{P}^f_{t+1}\mathbf{C}^\top + \mathbf{\Sigma}_v)^{-1}$$

$$\mathbf{X}_4(t+1) = \frac{1}{N-1} \sum_{i=1}^{N} (\hat{\mathbf{X}}^f_{i,t+1} - \hat{\mathbf{x}}^f_{t+1})^\top \mathcal{K}_t(\mathbf{Y}_{i,t+1} - \mathbf{C}\hat{\mathbf{X}}^f_{i,t+1})$$

$$\mathbf{X}_5(t+1) = \mathbf{I} + \mathbf{X}_4(t+1)$$

$$\hat{\mathbf{X}}^a_{t+1} = \hat{\mathbf{X}}^f_{t+1}\mathbf{X}_5(t+1)$$

4) compute the smooth ensemble for $t \in \{0, \ldots, T\}$

$$\hat{\mathbf{X}}^s_t = \hat{\mathbf{X}}^a_t \prod_{j=t+1}^{T} X_5(j)$$

A. One dimensional example

Consider the following homogeneous multiscale spatial mixing kernel

$$k\,(s-r) = -\phi_{4;0,-3}\,(s-r) + \phi_{4;0,-2}\,(s-r)$$

$$- 0.5\psi_{4;1,-6}\,(s-r) + 0.5\psi_{4;1,-3}\,(s-r) \tag{40}$$

The kernel and its decomposition are plotted in Fig.**??**. The dynamics associated with the IDE defined by (40) will be oscillatory and dissipative to initial conditions. The field is decomposed using scaling

functions $\phi_{4;0,k}$ and the associated wavelet functions $\psi_{4;j,k}$ with $j = 0, 1$. Observations are then generated from (20-27) for spatial domain defined as $\mathcal{S} = [0, 10]$ in response to an initial condition where $\Sigma_v = 0.2 \times \mathbf{I}_{n_y}$ and $\eta(s - r) = 2.5 \times \phi_{4,3,-2}(s - r)$. The response was sampled at 50 irregularly spaced random locations, at $t = 1, \cdots 400$. In order to estimate the spatial mixing kernel and the spatio-temporal field, the kernel and the field are decomposed using

$$k(s - r) = \sum_{l \in \mathbb{Z}} \alpha_{0,l} \phi_{4;0,l}(s - r) + \sum_{j=0}^{1} \sum_{l \in \mathbb{Z}} \beta_{j,l} \psi_{4;j,l}(s - r) \tag{41}$$

$$z_t(s) = \sum_{l \in \mathbb{Z}} x_{t,0,l} \phi_{4;0,l}(s) + \sum_{j=0}^{1} \sum_{l \in \mathbb{Z}} \check{x}_{t,j,l} \psi_{4;j,l}(s) \tag{42}$$

Note that the number of translation operations depends on the spatial range of the data. It follows that the total number of terms in (41) and (42) are 8 and 47 respectively. The estimated kernel in Fig.**??** is obtained for the cubic B-spline, with initial scale 0 and maximum scale 1. The EM algorithm is allowed to run for 30 iterations to avoid any issues regarding early stopping, though typically the change in $\| \mathbf{A} \|_F$ falls below 10^{-4} after less than 15 iterations. A total number of 500 estimation experiments are performed, where v_t and w_t are re-generated each trial.

The performance measure employed here is the Mean Integrated Squared Error (MISE) defined as

$$\mathbf{E} \left[\int_{\mathcal{S}} [e(s)]^2 \, ds \right] \tag{43}$$

where $e(s)$ is the error between the unknown function, $f(s)$ and its estimate, $\hat{f}(s)$. In this example the original kernel and the field are known and hence the integral in (43) can be computed analytically. For spatial mixing kernel we have

$$\int_{\mathcal{S}} [e(s)]^2 \, ds$$
$$= \left(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}} \right)^{\top} \left[\int_{\mathcal{S}} \boldsymbol{\lambda}(s) \boldsymbol{\lambda}(s)^{\top} \, ds \right] \left(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}} \right) \tag{44}$$

Here, we are particularly interested in assessing the performance improvement as the scale of the details in MRA is increased. Performance based on (44) at different spatial scales and over 500 trials have been evaluated. The MISE of the model at $j = 0$ is 0.024 and reduces to 0.005 when $\psi_{4;1,k}$ terms are also included in the model, in fact estimation performance is improved by a factor of 4.8. The coarsest approximation of the kernel along with its approximation at $j = 1$ are illustrated in Fig.**??**. It can be seen that the model is able to estimate both slowly and rapidly varying segments of the kernel with very high accuracy. Field estimates at a selection of time instants are shown in Fig.**??**. It is clearly observed that the coarse and fine features of the original field have been captured accurately over regions where

observations are available. Observation locations are generated randomly, as shown in Fig. **??**. Assuming the observed field can be fully described by the decomposed IDE model, the variance of the field can be computed to express the uncertainty of the estimation, at each point in space and at time t we have

$$\text{Var}(\hat{z}_t(s_i)) = \boldsymbol{\mu}^\top(s_i)\mathbf{P}_{t|T}\boldsymbol{\mu}(s_i) \tag{45}$$

where $\mathbf{P}_{t|T}$ is the covariance matrix associated with the state estimates obtained from the RTS smoother. Variance based on (45) at each spatial location and at $t = 50$ is shown in Fig.**??**. The uncertainty of the estimation is higher at almost every spatial location at $j = 1$ compared to $j = 0$. This is to be expected as there are more wavelet basis functions at higher resolution and hence more associated weights need to be estimated. Peaks in the variance of the field coincide with regions where no observations have been made. Increasing the number of observation locations, or using equally spaced observation locations would reduce the variance of the field estimation.

B. Two dimensional example

In order to demonstrate the ability of the developed model in higher dimensions, a two dimensional IDE model with a single B-spline kernel $\phi_{4;0,\mathbf{l}}(s_1 - r_1, s_2 - r_2)$ and $\mathbf{l} = [-2, -2]^\top$ is used with parameter $\theta = 1$. In this example spatial region $\mathcal{S} = [0, 4]^2$ is simulated over $t = \{1 \cdots 200\}$ using 7 scaling and wavelet functions at $j = 0$ together with 24 wavelet functions at $j = 1$. Univariate cubic B-spline scaling and wavelet functions are used to generate 2-D basis functions using (5-8). A set of 250 random observation locations is used; $\boldsymbol{\Sigma}_v$ is taken the same as that in example 1 and $\eta(s_1 - r_1, s_2 - r_2) = 2.5 \times \phi_{4,3,\mathbf{l}}(s_1 - r_1, s_2 - r_2)$ where $\mathbf{l} = [-2, -2]^\top$. The histogram of the parameter estimates in Fig.**??** is generated using 500 runs of the EM algorithm. For comparison, snapshots for the original and the corresponding coarse and fine field estimates at time instants 5, 50 and 150 are illustrated in Fig.**??**-**??**. In addition, the MISE of the dynamic field at some time instants are presented in Table I. This shows that the multiresolution IDE model can estimate the spatio-temporal dynamics of the original system accurately. The accuracy of the estimation remains consistent over time. Performance is improved significantly at $j = 1$ compared to the case where $j = 0$.

VI. CONCLUSION

A multi-resolution approach to modelling spatio-temporal systems has been presented. This model is able to represent continuous-space, discrete-time dynamics at a number of spatial scales simultaneously. This ability greatly extends the class of system which the Integro-Difference Equation can represent.

TABLE I

MISE at particular scale between measured and estimated 2D-field at a particular time

Time	MISE	
	$j = 0$	$j = 1$
5	5.424	0.609
20	5.422	0.596
50	5.519	0.626
100	5.488	0.611
150	5.494	0.587

By decomposing both the spatial field and the spatial mixing kernel using a wavelet decomposition, it becomes possible to represent small scale details in the field at the same time as large scale details. This is an essential component of any practical spatio-temporal model, without which the model must be artificially separated into global and local modes a-priori.

The complexity of the model is not affected by the spatial resolution of the observation process, rather it reflects the underlying complexity of the system under study. Therefore, increasing the resolution at which the system is observed does not necessarily increase the complexity of the system identification problem. However the developed algorithm is sensitive to the state dimension, equivalent to the detail represented in the field, and hence intelligent approaches to reduce the number of basis functions is noted as future work.

By considering different levels of decomposition, the proposed approach could be used as a method of determining the appropriate scales of decomposition, within a model-selection framework. Combined with an approach to sparsely modelling spatial heterogeneity, such as boundary conditions, this would allow the application of this work to a real-world data set.

APPENDIX

Lemma 1: Consider the zero-mean process $e_t(s)$ with covariance as defined by (**??**) then

$$\mathbf{w}_t = \mathbf{\Lambda}_x^{-1} \int_{\mathcal{S}} \boldsymbol{\mu}(\mathbf{s}) \, e_t(\mathbf{s}) \, d\mathbf{s} \tag{46}$$

is a vector valued, zero mean normally distributed white noise process with covariance

$$\mathbf{\Sigma}_w = \mathbf{\Lambda}_x^{-1} \mathbf{\Pi} \mathbf{\Lambda}_x^{-\top} \tag{47}$$

and

$$\mathbf{\Pi} = \iint_{\mathcal{S}} \boldsymbol{\mu}\left(\mathbf{s}\right) \eta\left(\mathbf{s}-\mathbf{r}\right) \boldsymbol{\mu}\left(\mathbf{r}\right)^{\top} d\mathbf{r} d\mathbf{s} \tag{48}$$

Proof: Equation (46) is a linear function of $e_t(\mathbf{s})$ and hence $\mathbf{w}_t$ is also normally distributed. The expected value of $\mathbf{w}_t$ is given by

$$\begin{aligned} \mathbf{E}\left[\mathbf{w}_t\right] &= \mathbf{\Lambda}_x^{-1} \int_{\mathcal{S}} \boldsymbol{\mu}\left(\mathbf{s}\right) \mathbf{E}\left[e_t\left(\mathbf{s}\right)\right] d\mathbf{s} \\ &= 0 \end{aligned} \tag{49}$$

and

$$\begin{aligned} \mathbf{\Sigma}_w &= \mathbf{E}[\mathbf{w}_t \mathbf{w}_t^{\top}] \\ &= \mathbf{\Lambda}_x^{-1} \mathbf{E}[\int_{\mathcal{S}} \boldsymbol{\mu}\left(\mathbf{s}\right) e_t\left(\mathbf{s}\right) d\mathbf{s} \int_{\mathcal{S}} \boldsymbol{\mu}\left(\mathbf{r}\right)^{\top} e_t\left(\mathbf{r}\right) d\mathbf{r}] \mathbf{\Lambda}_x^{-\top} \\ &= \mathbf{\Lambda}_x^{-1} \iint_{\mathcal{S}} \boldsymbol{\mu}\left(\mathbf{s}\right) \mathbf{E}[e_t\left(\mathbf{s}\right) e_t\left(\mathbf{r}\right)] \boldsymbol{\mu}\left(\mathbf{r}\right)^{\top} d\mathbf{r} d\mathbf{s} \mathbf{\Lambda}_x^{-\top} \\ &= \mathbf{\Lambda}_x^{-1} \iint_{\mathcal{S}} \boldsymbol{\mu}\left(\mathbf{s}\right) \eta\left(\mathbf{s}-\mathbf{r}\right) \boldsymbol{\mu}\left(\mathbf{r}\right)^{\top} d\mathbf{r} d\mathbf{s} \mathbf{\Lambda}_x^{-\top} \\ &= \mathbf{\Lambda}_x^{-1} \mathbf{\Pi} \mathbf{\Lambda}_x^{-\top} \end{aligned} \tag{50}$$

∎

Lemma 2: Let $N_m\left(s-l_1\right)$ and $N_{m'}\left(s-l_2\right)$ be shifted B-spline functions of order m and m' respectively. Then the inner product of $N_m\left(s-l_1\right)$ and $N_{m'}\left(s-l_2\right)$ can be calculated by

$$\begin{aligned} \langle N_m\left(s-l_1\right), N_{m'}\left(s-l_2\right)\rangle &= N_{m+m'}\left(m+l_1-l_2\right) \\ &= N_{m+m'}\left(m'+l_2-l_1\right) \end{aligned} \tag{51}$$

Proof: The support of $N_m\left(s\right)$ is $[0,m]$ and is symmetric with respect to $s = \frac{m}{2}$, i.e.

$$N_m\left(\frac{m}{2}+s\right) = N_m\left(\frac{m}{2}-s\right) \tag{52}$$

A direct consequence of (52) is

$$N_m\left(s\right) = N_m\left(m-s\right) \tag{53}$$

Therefore

$$\int_{-\infty}^{+\infty} N_m\left(s - l_1\right) N_{m'}\left(s - l_2\right) ds$$

$$= \int_{-\infty}^{+\infty} N_m\left(m - s + l_1\right) N_{m'}\left(s - l_2\right) ds$$

$$= \int_{-\infty}^{+\infty} N_m\left(m + l_1 - l_2 - u\right) N_{m'}\left(u\right) du$$

$$= \left(N_m * N_m'\right)\left(m + l_1 - l_2\right)$$

$$= N_{m+m'}\left(m + l_1 - l_2\right)$$

$$= N_{m+m'}\left(m' + l_2 - l_1\right)$$

∎

REDUCING THE COMPUTATIONAL COMPLEXITY

The state-space representation of the spatio-temporal IDE (22) and (23) has a quadratic $\mathcal{Q}$-function in a form of [17]

$$\mathcal{Q}\left(\boldsymbol{\theta}, \boldsymbol{\theta}'\right) = 2\boldsymbol{\theta}^\top \boldsymbol{v} - \boldsymbol{\theta}^\top \boldsymbol{\Upsilon} \boldsymbol{\theta} \tag{54}$$

which has a maximum at

$$\boldsymbol{\theta} = \boldsymbol{\Upsilon}^{-1} \boldsymbol{v} \tag{55}$$

where

$$\boldsymbol{\Upsilon} = \sum_{i,j,k,m=1}^{n_x} \left[\Xi_1\right]_{ij} \boldsymbol{\gamma}^{(k,j)} \left[\boldsymbol{\Lambda}_x^{-1} \Sigma_w^{-1} \boldsymbol{\Lambda}_x^{-1}\right]_{km} \boldsymbol{\gamma}^{(m,i)\top} \tag{56}$$

and

$$\boldsymbol{v} = \sum_{i,j=1}^{n_x} \left[\Xi_0 \Sigma_w^{-1} \boldsymbol{\Lambda}_x^{-1}\right]_{ij} \boldsymbol{\gamma}^{(j,i)} \tag{57}$$

where

$$\boldsymbol{\gamma}^{(i,j)} = \int_{\mathcal{S}} \left[\mu(s)\right]_i \left[\mathbf{M}(s)\right]_{:j} ds \tag{58}$$

and $\left[\mathbf{M}(s)\right]_{:j}$ denotes the jth column of $\mathbf{M}(s)$. The definitions of the Ξ_0 and Ξ_1 are the same as in [17]. Note that constant values with respect to $\boldsymbol{\theta}$ are ignored in (54). We define $n_x \times n_x$ block matrix $\mathbf{U}$ such that

$$\left[\mathbf{U}\right]_{i,j} = \boldsymbol{\gamma}^{(i,j)\top} \tag{59}$$

substituting (59) in (56) we get

$$\boldsymbol{\Upsilon} = \sum_{i,j=1}^{n_x} [\boldsymbol{\Xi}_1]_{i,j} [\mathbf{U}^{\mathsf{T}} \boldsymbol{\Lambda}_x^{-1} \Sigma_w^{-1} \boldsymbol{\Lambda}_x^{-1} \mathbf{U}]_{j,i} \tag{60}$$

and similarly substituting (59) in (56) we have

$$\boldsymbol{v} = \sum_{i,j=1}^{n_x} [\boldsymbol{\Xi}_0]_{i,j} [\Sigma_w^{-1} \boldsymbol{\Lambda}_x^{-1} \mathbf{U}]_{j,i} \tag{61}$$

with this substitution the second terms in (60) and (61) can be pre-calculated and stored. This lowers the comutational complexity of the estimation algorithm and provides a dramatic increase in estimation speed.

CROSS COVARIANCE MATRIX

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