Non-asymptotic State Estimation of Linear Reaction Diffusion Equation using Modulating Functions

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Abstract: In this paper, we propose a non-asymptotic state estimation method for the linear reaction diffusion equation with general boundary conditions. The method is based on the modulating function approach utilizing a modulation functional in time and space. This results in a signal model control problem for a system of auxiliary PDEs in order to determine the modulation kernels. First, the algorithm is mathematically derived and then numerical simulations are presented for illustrating the good performance of the proposed approach and demonstrating the efficient implementation scheme.

Keywords: State Estimation, Modulating Functions, Partial Differential Equations, Non-asymptotic Estimation.

1. INTRODUCTION

State estimation for systems modeled by partial differential equations (PDEs) is an important problem in many applications. These include e.g. control, medical imaging, seismic imaging, oil exploration and computer tomography (Cameron et al., 2007). Many methods have been proposed to solve this problem, most of them converge asymptotically and are usually based on observers. For instance, adaptive and iterative observers have been proposed by Orlov and Bentsman (2000), recursive observers based methods have been introduced in (Moireau et al., 2008). Different other types of observers have been proposed for coupled dynamical cascade systems including Ordinary Differential Equations (ODE) and PDEs for example in (Susto and Krstic, 2010), (Tang and Xie, 2011). More recently, a boundary observer has been designed by Hasan et al. (2016), for a coupled system of hyperbolic dynamical cascade systems with measurements at the boundary to estimate the states of the system using the Volterra integral transformation.

It is known that most of the observer based estimation methods provide asymptotic convergence, i.e. the estimated state will converge to the real state when time goes to infinity. However in many situations, it is desirable to have an estimator which converges in finite time. Finite time convergence estimators which are also known as non-asymptotic estimators have been studied and designed for finite dimensional systems. Different methods exist, for instance, sliding mode observers and modulating functions. In this paper, we propose a finite time state estimation approach for PDEs. Our approach is based on the so-called modulating function (MF), introduced in the early 1950s by Shinbrot (Shinbrot, 1957), to be used for parameters identification of ODEs. The extension of this method was given by Perdreaulville and Goodson (1966) for constant and space varying parameters identification of PDEs using distributed measurements. Later, this approach was extended to the estimation of spatial derivatives using finite difference scheme (Fairman and Shen, 1970). Then, in 1997, Co and Ungarala (1997) adapted the method towards real-time parameter identification for ODEs. The Modulating Function Based method (MFBM) has been applied for parameters and source estimation of one dimensional PDEs (Asiri and Laleg-Kirati, 2017), for fault detection (Fischer and Deutscher, 2016). It has also been extended for state and parameters estimation of linear and some nonlinear dynamic systems (Jouffroy and Reger, 2015), for unknown inputs and parameters estimation for fractional-order ODEs (Belkhatir and Laleg-Kirati, 2017) and fractional-order PDEs (Aldoghaither et al., 2015) and for the estimation of the fractional-order derivatives of noisy signals in (Liu et al., 2014), (Liu and Laleg-Kirati, 2015). The method has been combined with optimization based methods for the joint estimation of the fractional differentiation order and the parameters of fractional-order ODEs (Belkhatir...
and Laleg-Kirati, 2018) and PDEs (Aldoghaither et al., 2015). Moreover, the modulating functions method has been reformulated in terms of a Volterra integral operator in Pin et al. (2017), for the identification of the amplitude, frequency and phase of a biased sinusoidal signal. However, so far no work has been done on the state estimation of PDEs using MFBM.

The MFBM features several important advantages. Respective algorithms may converge non-asymptotically, i.e. in finite time. The method usually is formulated in a deterministic and continuous time framework, which makes it applicable directly to the usual models in control. Another feature is that estimates of parameters and states may be generated through integration, without resorting to the explicit differentiation of the system measurements. This provides some robustness against noise and numerical stability of the algorithm. Furthermore, approximating the derivatives of the measurements, which are usually noisy, is avoided. The inherent FIR filter structure of the method allows to obtain the estimates in finite time, requiring only moderate computational burden. In the MFBM, neither initial nor boundary conditions are needed. Generally speaking, the direct problem does not have to be solved.

In this paper, we propose a method for the finite-time state estimation of PDEs using available measurements. We investigate the modulating functions approach, in particular on a reaction diffusion equation with general boundary conditions. The paper is organized as follows: In Section 2, we introduce the problem and review some required preliminaries on modulating functions. Section 3 provides a study of the state estimation for the reaction diffusion equation, using modulation functions, where an appropriate model for the modulating function is proposed. In Section 4, the solvability of the proposed modulating function’s model is discussed. Section 5 validates our method resorting to simulation results.

2. PRELIMINARIES

In this section, we present the definition of the modulating functions and some of its useful properties. Then we formulate the main problem to be discussed in this paper.

Classically, the modulating function for ODEs is defined in the following way (Aldoghaither et al., 2015):

**Definition 1. (Modulating Function).** A function \( \varphi \in C^k([a,b],\mathbb{R}) \) is called a modulating function of order \( k \) with \( k \in \mathbb{N}^+ \) if and only if

\[
\varphi^{(i)}(a) = \varphi^{(i)}(b) = 0, \quad i = 0, 1, \ldots, k - 1. \tag{1}
\]

An extension to distributed systems can be obtained by defining the kernel function in the time and spatial domain (Fischer et al., 2018), (Fischer and Deutscher, 2016):

**Definition 2. (Modulation Functional).** The state modulation functional is defined by

\[
M[h] = \int_t^{t-T} \int_0^L m(z, \tau - t + T) h(z, \tau) dz d\tau. \tag{2}
\]

where \( h : [0,L] \times \mathbb{R}_0^+ \rightarrow \mathbb{R} \) and \( m : [0,L] \times [0,T] \rightarrow \mathbb{R} \) is the modulating function to be constructed.

For simplicity, denote

\[
\langle m, h \rangle_{\Omega,t} := M[h],
\]

where \( \Omega := [0,L] \) and \( I := [t-T,t] \) with receding horizon length \( T > 0 \). If the integration only concerns the temporal or spatial variable, \( \langle m, h \rangle_{\Omega} \) and \( \langle m, h \rangle_{I} \) are used.

### 2.1 Problem Statement

We consider the following linear reaction-diffusion equation with constant diffusion rate, dissipation rate and a non-identically vanishing reaction function:

\[
\begin{aligned}
&c_t(x,t) = D c_{xx}(x,t) - \nu c(x,t), \\
&c(0,t) = u(t), \quad c_x(L,t) = 0,
\end{aligned}
\]  

where \( t \geq 0, x \in [0,L], y(t) \) is the input signal and \( c_0(x) \) represents the unknown initial conditions.

The objective of this paper is to extend the well-known modulating functions approach for obtaining the state estimate \( \hat{c}(x,t) \) for the considered class of parabolic PDEs at all time and all position using some boundary measurements. To this end, the solution of the linear PDE (3) is represented as a function series of the form

\[
c(x,t) = \sum_{j=1}^{\infty} C_j(t) \phi_j(x) \tag{4}
\]

where \( \phi_j \) are basis functions of the spatial domain \( X = \{ f : \Omega \rightarrow \mathbb{R} \ | \ |f|_\infty < \infty \} \) and orthonormal with respect to the weighted inner product \( \langle f,g \rangle_v = \int_0^L v(x)f(x)g(x)dx \).

### 3. MODULATING FUNCTIONAL METHOD FOR STATE ESTIMATION

In this section, the MF based method is proposed for the considered reaction diffusion equation.

**Theorem 3.** Consider the problem given in (3). If there exists a series of modulating functions \( m^k(x,\sigma) \) with \( k = 1,2,\ldots,N \) for \( N \in \mathbb{N} \) that satisfies the system

\[
\begin{aligned}
m_x^k(x,\sigma) &= -Dm_{xx}^k(x,\sigma) + \nu m^k(x,\sigma), \\
m_{\sigma}^k(x,\sigma) &= 0, \\
m^k(x,\sigma) &= 0, \quad \sigma = T, \tag{5}
\end{aligned}
\]

for \( \sigma \in [0,T] \) and \( x \in \Omega \), then the state can be estimated \( \hat{c}(x,t) \approx \bar{c}(x,t) \) for all \( t \geq T \) and for all positions \( x \) by

\[
\bar{c}(x,t) = \sum_{j=1}^{N} \hat{C}_j(t) \phi_j(x) = \sum_{j=1}^{N} \Lambda_j[y,u] \phi_j(x) \tag{6}
\]

with approximation order \( N \in \mathbb{N} \) and the resulting time modulation operators \( \Lambda_j \) as derived from (14).

**Proof.** We start by applying a series of modulating functionals defined in (2) for \( k = 1,\ldots,N \) to the PDE in (3) which leads to:

\[
\langle m^k,c_\tau \rangle_{\Omega,I} = D \langle m^k,c_{xx} \rangle_{\Omega,I} - \nu \langle m^k,c \rangle_{\Omega,I} \tag{7}
\]

We have by temporal integration by parts:

\[
\langle m^k,c_\tau \rangle_{\Omega,I} = D \langle m^k,c_{xx} \rangle_{\Omega,I} - \nu \langle m^k,c \rangle_{\Omega,I} \tag{7}
\]
\[
\langle m^k, c_\tau \rangle_{\Omega,I} = \int_{t-T}^{t} \int_{0}^{L} m^k(x, \tau + T - t)c_\tau(x, \tau)dxdt = -\int_{t-T}^{t} \int_{0}^{L} m^k\tau(x, \tau + T - t)c(x, \tau)dxd\tau + \int_{0}^{L} m^k(x, T)c(x, t)dxdt - \int_{0}^{L} m^k(x, 0)c(x, t - T)dxdt.
\]

Under the assumptions that
\[
\begin{align*}
\langle m^k(x, \sigma) \rangle_{\sigma=0} &= 0 \quad \forall x \in [0, L], \\
\langle m^k(x, \sigma) \rangle_{\sigma=T} &= \Phi^k(x) \quad \forall x \in [0, L],
\end{align*}
\]
we get
\[
\langle m^k, c_\tau \rangle_{\Omega,I} = -\langle m^k, c_\tau \rangle_{\Omega,I} + \langle \Phi^k, c_\tau \rangle_{\Omega,I},
\]
where \( \Phi^k \) is an arbitrary function that we suppose not identically equal to zero in order not to lose the desired estimated state and which is represented as an arbitrary weighted orthonormal basis \( \{\phi_i\}_{i \in \mathbb{N}} \) of \( X \) as
\[
\Phi^k(x) = v(x) \sum_{i=1}^{N} M_i^k \phi_i(x),
\]
and hence,
\[
\langle \Phi^k, c_\tau \rangle_{\Omega,I} = \sum_{i=1}^{N} M_i^k \phi_i \langle c_\tau, \phi_i \rangle_{\Omega,I} = \sum_{i=1}^{N} C_i(t) M_i^k.
\]
This assumption guarantees that the extra term from the temporal integration by parts (9) vanishes by utilizing the respective state series expansion (4). The state can be estimated by isolating the coefficients \( C_i(t) \). On the other hand, using integration by parts twice over \( \Omega \) and the boundary conditions and the measurements in (3), we have for the spatial derivative term in (7):
\[
\begin{align*}
\langle m^k, c_{xx} \rangle_{\Omega,I} &= \int_{t-T}^{t} \int_{0}^{L} m^k(x, T - t + \tau)c_{xx}(x, \tau)dxd\tau \\
&= \int_{t-T}^{t} \int_{0}^{L} m^k(L, T - t + \tau)c(L, \tau)dxd\tau - \int_{t-T}^{t} \int_{0}^{L} m^k(0, T - t + \tau)c(0, \tau)dxd\tau \\
&\quad + \int_{t-T}^{t} \int_{0}^{L} m^k(L, T - t + \tau)c_2(L, \tau)dxd\tau - \int_{t-T}^{t} \int_{0}^{L} m^k(0, T - t + \tau)c_2(0, \tau)dxd\tau \\
&= \langle m^k_{xx}, c \rangle_{\Omega,I} - \langle m^k_{x}, c \rangle_{L} + \langle m^k_{xx}(0), c \rangle_{0} + \langle m^k_{x}(0), c \rangle_{0} - \langle m^k_{xx}(0), c \rangle_{0} - \langle m^k_{x}(0), c \rangle_{0} - \langle m^k_{xx}(0), c \rangle_{0} - \langle m^k_{x}(0), c \rangle_{0}.
\end{align*}
\]

with boundary conditions (3) and under the assumption
\[
m^k(x, \sigma)_{|x=0} = 0 \quad \forall \sigma \in [0, T].
\]

By plugging (9) and (10) into (7), we obtain
\[
\begin{align*}
-\langle m^k, c \rangle_{\Omega,I} + \sum_{i=1}^{N} C_i(t) M_i^k &= D(m^k_{xx}, c)_{\Omega,I} + D(m^k_{x}(0), u)_{L} - D(m^k_{x}(L), y)_{I} - \nu(m^k, c)_{\Omega,I}.
\end{align*}
\]

The most trivial way to simplify (12) is to choose the modulation function \( m^k(x, t) \) as a function that satisfies the following adjoint reaction diffusion equation:
\[
m^k(x, \sigma) = -Dm^k_{xx}(x, \sigma) + \nu m^k(x, \sigma),
\]
similar to the case in Fischer and Deutscher (2016). Thus, using (13), (12) becomes
\[
\begin{align*}
\sum_{i=1}^{N} C_i(t) M_i^k &= D(m^k_{xx}(0), u)_{I} - D(m^k_{x}(L), y)_{I}.
\end{align*}
\]

This system of equations is solvable if for each modulating function \( m^k(x, t) \) the coefficients \( M_i^k \) are forming a full rank matrix. By inverting the relation (14), one obtains the estimation result \( C_i(t) = \Lambda_k[y, u] \) dependent on the measurement and input signal.

In the next part, we will discuss the solvability of (5) to check if there exists at least one modulating function \( m^k(x, t) \) that satisfies the required conditions.

## 4. SOLVABILITY OF THE MODULATING FUNCTION SYSTEM

From the former considerations, the following modulating function specifications have been formulated in (5), that is
\[
\begin{align*}
\langle m^k, c \rangle_{\sigma=0} &= 0, \\
\langle m^k, c \rangle_{\sigma=T} &= \Phi^k(x), \\
\langle m^k, c \rangle_{|x=0} &= 0,
\end{align*}
\]
where \( x \in \Omega, \sigma \in [0, T] \). Note that beside the initial condition there is a final time state condition which has to be forced by signal construction. As there is still a spatial condition missing due to the second order with respect to space, an additional degree of freedom can be introduced in the following way:
\[
\begin{align*}
\langle m^k_{xx}, c \rangle_{\Omega,I} - \langle m^k_{x}, c \rangle_{L} + \langle m^k_{xx}(0), c \rangle_{0} + \langle m^k_{x}(0), c \rangle_{0} - \langle m^k_{xx}(0), c \rangle_{0} - \langle m^k_{x}(0), c \rangle_{0} - \langle m^k_{xx}(0), c \rangle_{0} - \langle m^k_{x}(0), c \rangle_{0}.
\end{align*}
\]

with the boundary input \( \eta_k : [0, T] \rightarrow \mathbb{R} \) which can be used for signal model control to fulfill the specifications.

### 4.1 Time transformation

System (15) cannot be solved directly due to the noncausal nature of the adjoint operation in the distributed dynamics caused by the switch in sign of the time derivative. Therefore, we introduce a change of variables in time direction within the receding interval, i.e.
\[
\xi^k(x, \sigma) := m^k(x, T - \sigma), \quad \sigma \in [0, T]
\]
and then end up in the system representation
\[
\begin{align*}
\xi_k(x, \sigma) &= D_k \xi_k(x, \sigma) - \nu \xi_k(x, \sigma), \\
\xi_k(x, \sigma)|_{\sigma=0} &= \Upsilon_k(x), \\
\xi_k(x, \sigma)|_{\sigma=T} &= 0,
\end{align*}
\] (16)

where the new boundary input \( \tilde{\gamma}_k : [0, T] \to \mathbb{R} \) is introduced accordingly. Here, the parabolic auxiliary PDE can be solved analytically or numerically. The switch of initial and final time conditions results in a signal model stabilization problem where the initial profile \( m^k(x) \) is set and the boundary input \( \tilde{\gamma}_k \) is utilized for driving the system to zero before reaching the end of the horizon at \( \sigma = T \). Thus, all conditions specified can be fulfilled and the estimator relation (14) holds true.

The analytic solution can be calculated by applying separation of variables with trigonometric eigenfunctions:

\[
\xi_k(x, \sigma) = \sum_{i=0}^{\infty} \sin(\omega_i x) \left[ G_i e^{-\lambda_i^* \sigma} + \gamma_i(\sigma) \right] + x \tilde{\gamma}_k(\sigma),
\]

where
- \( \omega_i = (2i + 1) \frac{\pi}{2T} \) and \( \lambda_i = \nu + D \omega_i^2 \),
- \( G_i = \frac{2}{T} \int_{0}^{T} \sin(\omega_i x) |\phi_k(x) - x \tilde{\gamma}_k(0)| \, dx \),
- \( \gamma_i(\sigma) = \int_{0}^{\sigma} e^{\lambda_i(s-\sigma)} \left( \tilde{\gamma}_k(s) + \nu \tilde{\gamma}_k(s) \right) \, ds \).

This illustrates the modulating function shape as well as the signal model control impact. After constructing a sufficiently accurate solution \( \xi^k(x, \sigma) \) of system (16), either by analytical or numerical means, a back transformation is performed for obtaining the solution \( m^k(x, \sigma) \) of system (15). This allows realizing the final state estimation algorithm.

### 4.2 Implementation

First, the tuning parameters of receding horizon length \( T > 0 \) and the approximation order \( N \in \mathbb{N} \) have to be selected according to the desired robustness characteristics. Then, the initial condition function from (16) has to be selected. In order to guarantee a well conditioned system of equations (14), the following selection is made:

\[
M_k := \begin{dcases}
1 & : i = k \\
0 & : i \neq k
\end{dcases} \Rightarrow \Phi^k(x) = v(x) \phi_k(x),
\]

which generates a trivial system of equations due to the orthonormality property with respect to the weighted function basis of \( X \). Solving the transformed auxiliary problem (16), requires the positive definite weight \( v \) to be selected according to the boundary conditions and a signal model control strategy \( \tilde{\gamma}_k \) to be realized for stabilizing the system sufficiently fast. This is crucial for the final filtering characteristics of the observer. After calculating the \( N \) modulating function PDEs offline, the solutions are then related to the auxiliary system (15). This results in the final estimator relation for \( k = 1, \ldots, N \):

\[
\tilde{\epsilon}(t) = D \left( \langle m^k(0), u \rangle_T - \langle m^k(L), y \rangle_T \right)
\]

\[
= D \left( \int_{t-T}^{t} m^k(0, \tau - t + T) u(\tau) \, d\tau \right)
\]

\[
- \int_{t-T}^{t} m^k(1, \tau - t + T) y(\tau) \, d\tau \right)
\]

\[
=: \Lambda_k[y, u]
\]

\[
\end{equation}

and thus

\[
\tilde{\epsilon}(x, t) = \sum_{k=1}^{N} \tilde{\epsilon}(t) \phi_k(x) = \sum_{k=1}^{N} \Lambda_k[y, u] \phi_k(x),
\]

where only the time modulation operators \( \Lambda_k \) have to be implemented online. This can be realized as an FIR filter structure by discretizing the modulation integral like in the case of classical modulating function schemes such as in (Jouffroy and Reger, 2015). In Figure 1, the implementation scheme is illustrated in form of a block diagram. It demonstrates the real-time capability of the approach which ends up to be a simple LTI system combined with an output multiplication by the selected spatial basis functions. The computationally costly PDE solving process is performed prior to the implementation, directly after specifying the tuning parameters.

### 5. SIMULATION EXAMPLE

In the following, system (3) is considered as a simple diffusion process with \( \nu = 0 \) and the boundary excitation \( u(t) := \sin(2\pi t) \). Figure 2 shows the input-output behavior as well as the resulting distributed state. For the receding horizon based state estimator, the interval length \( T = 1 \) is selected. An approximation order of \( N = 5 \) is realized for capturing the distributed state dynamics sufficiently accurate with the utilization of a polynomial basis function shape for \( \phi_k, k \in \{1, \ldots, N\} \) with respect to the weight \( v(x) = 20 \cdot x^2(1 - x)^2 \). In order to solve the respective auxiliary systems (16), the signal model controller is chosen as the boundary damping term

\[
\tilde{\gamma}_k(\sigma) := -\alpha \xi^k(1, \sigma), \quad \alpha > 0,
\]

which induces an additional decay rate that drives the already stable diffusion system sufficiently fast to zero at final time \( T \). This can be enhanced by selecting a different control strategy. The resulting time modulation kernels for the estimator relation (17) and the final implementation can now be calculated which was performed using a finite differences based solver. In Figure 3, example kernels for the sensor signal modulation are presented. These kernels act like signal weights with a certain filtering characteristics similar to the ODE case which was examined by
Figure 2. Simulation of diffusion process (3) with $\nu = 0$, distributed state $c(x, t)$, excitation $u(t)$ and measurement signal $y(t)$.

Figure 3. Measurement signal modulation kernels $m_k^x(1, \sigma)$ for operator $A_k$ from (17) with $k \in \{1, 2, 3\}$, $\sigma \in [0, T]$.

Preisig and Rippin (1993). Note that the information at the end of the receding horizon interval gets emphasized a lot more than older data. For lower order components, a longer time span with lower amplification is taken into account. Higher order terms receive a more significant weight for very recent data.

Now, the estimator (17) can be implemented. The state estimation result is shown in Figure 4 in direct comparison to the simulated state over the relevant time interval $[T, t_f] = [1, 2]$. The reconstructed state $\hat{c}(x, t)$ seems to match the simulated reference state $c(x, t)$ very accurately.

For further evaluation of the observer performance, the integral squared estimation error

$$V(t) = \int_0^L \left( (\hat{c}(x, t) - c(x, t)) \right)^2 dx$$

is illustrated in Figure 5. Indeed, it can be noted that the observation error stays on a very low level which demonstrates the functionality of the overall algorithm. However, some numerical error source remains. A truncation error results from the finite series expansion approach. Furthermore, a small deviation to the zero final condition of auxiliary system (16) due to insufficient signal model control could result in an error contribution from the unknown initial state condition at the beginning of the receding horizon interval.

6. CONCLUSION

This paper deals with a class of linear parabolic PDEs with known mixed BCs. The contributions of this paper is the development of a generalizable methodology for the modulating function based state estimation applied to distributed systems and thus, an expansion of the framework to a new problem class. Using boundary measurements as well as a filtering algorithm derived from auxiliary models...
for obtaining the modulating functions, the observation can be realized at arbitrary time and at all positions. The provided simulation results verify the overall functionality and beneficial properties of the approach.

After applying the modulating functions to distributed systems for source and parameter estimation, this work shows that the extension to observer design is feasible. In comparison to classical Luenberger-type PDE observers, no distributed system copy has to be solved in real-time due to the efficient implementation scheme from Figure 1. Operations with high computational cost, such as solving the auxiliary PDE and also the function series construction are performed offline in a preprocessing.

In general, the non-asymptotic modulation framework shows special robustness properties with respect to measurement noise and allows for an algebraic combination with disturbance reconstruction in order to design an adaptive identification algorithm.

A further direction would be to extend the proposed approach for two-dimensional PDEs as well as for unstable and nonlinear reaction terms. The next steps include a comprehensive performance comparison with similar approaches and the application to more practical scenarios.

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