Computational Statistics and Data Analysis xx (xxxx) xxx–xxx

Contents lists available at ScienceDirect

Computational Statistics and Data Analysis

journal homepage: www.elsevier.com/locate/csda

Approximation error approach in spatiotemporally chaotic models with application to Kuramoto–Sivashinsky equation

J.M.J. Huttunen [a,b,*], J.P. Kaipio [c,a], H. Haario [d,e]

[a] Department of Applied Physics, University of Eastern Finland, P.O. Box 1627, 70211 Kuopio, Finland
[b] Nokia Technologies, Karaportti 4, 02610 Espoo, Finland [1]
[c] Department of Mathematics, University of Auckland, Private Bag 92019, 1142 Auckland, New Zealand
[d] Department of Mathematics and Physics, Lappeenranta University of Technology, P.O. Box 20, 53851 Lappeenranta, Finland
[e] Finnish Meteorological Institute, P.O. Box 503, Helsinki FI-00101, Finland

HIGHLIGHTS

- The applicability of Bayesian approximation error methods to chaotic state evolution problems has not been investigated previously.
- We have applied Bayesian approximation error approach to the state and parameter estimation problems induced by the Kuramoto–Sivashinsky (KS), which has also been referred to as the "simplest" chaotic PDE.
- The results suggest that the nonstationary BAE is a potentially feasible approach for reduced order chaotic models. The accuracy of the state estimates is comparable to that of respective non-reduced order model.

ARTICLE INFO

Article history:
Received 19 April 2017
Received in revised form 9 January 2018
Accepted 28 January 2018
Available online xxxx

Keywords:
Nonstationary inverse problems
State estimation
Filtering
Spatiotemporal chaos
Chaotic models
Bayesian approximation error approach

ABSTRACT

Model reduction, parameter uncertainties and state estimation in spatiotemporal problems induced by chaotic partial differential equations is considered. The model reduction and parameter uncertainties induce a specific structure for the state noise process, and also modify the observation noise model. The nonstationary Bayesian approximation error approach (BAE) is employed to construct the state evolution and observation models. Earlier results have shown that the effects of severe model reduction and parameter uncertainties can be handled with the nonstationary BAE. The applicability of BAE to chaotic state evolution problems has not been investigated previously. The Kuramoto–Sivashinsky equation is considered with noisy measurements and, in addition, the related state space model identification problem is also considered. The results suggest that the nonstationary BAE is a potentially feasible approach for reduced order chaotic models and, when feasible, the accuracy of the state estimates is comparable to that of respective non-reduced order model.

1. Introduction

A large class of state estimation problems is induced by partial differential equations (PDE) that govern the underlying physical phenomena. Examples of such phenomena include (heat) transfer, chemical reaction kinetics, structural vibrations

* Correspondence to: Nokia Bell Labs, Karakaari 7, 02610 Espoo, Finland.
E-mail addresses: jmhuttun@gmail.com (J.M.J. Huttunen), jari@math.auckland.ac.nz (J.P. Kaipio), heikki.haario@lut.fi (H. Haario).

[1] Present address.

https://doi.org/10.1016/j.csda.2018.01.015

and wave propagation in general. The tasks, on the other hand, include state estimation (of variables that are not directly observed), state space identification (estimation of time-invariant parameters of the PDE's) and control.

The standard approach to derive the state evolution model is to use a semi-discrete scheme to turn the PDE's into (often large) systems of ODE's and equip the discretized models with a more or less trivial state noise model. Typically, the model for the state noise process is a mutually independent identically distributed noise model, that is, the covariance is modelled as a scaled identity matrix. As long as there are no model uncertainties (e.g. unknown/inaccurate variables that are not modelled as unknown) and the discretization is relatively accurate such that discretization errors are negligible (compared to the inherent state and observation noise processes), such trivial state noise models may yield feasible state estimates, that is, the true state and parameters are supported by the (posterior) distribution estimate. The relatively accurate models are, however, often computationally prohibitively complex, and reduced order models have to be used.

It has been found that, under significant model reduction and model uncertainties, trivial state noise models can give infeasible or significantly misleading estimates for the state and the state model parameters. The central problem is then how to model the state noise process such that the noise processes represents the error due to the model reduction. The Bayesian approximation error (BAE) approach was introduced in Kaipio and Somersalo (2005, 2007) to provide a systematic method to construct statistical structure for such noise processes. The approach was originally applied to handle discretization errors in problems such as electrical impedance tomography and deconvolution. Lately, BAE has also been extended to deal with more general modelling errors such as treating anisotropic scattering in optical tomography (Heino et al., 2005), unknown boundary data on computational truncation boundaries (Lehikoinen et al., 2007), unknown nuisance parameters (Kolehmainen et al., 2011; Nissinen et al., 2009; Lehikoinen et al., 2010; Huttunen et al., 2014), and the approximation of the radiative transfer model with a simpler diffusion model in optical tomography (Tarvainen et al., 2010).

The BAE approach has been extended to nonstationary state estimation and identification problems (Huttunen and Kaipio, 2007b, a; Huttunen et al., 2010). It was shown that the nonstationary BAE approach is capable of yielding feasible estimates. In all of the studies, state evolution models were, however, non-chaotic.

In the context of chaotic state evolution models, the state estimation approach and different nonlinear extensions of Kalman filter (Kalman, 1960; Adams and Fournier, 2003) have been successfully applied to several types of chaotic problems. For example, the ensemble Kalman filter (EnKF) (Evensen, 1994) was applied to estimate the parameters in Lorenz model in Annan and Hargreaves (2004) and several filtering approaches for turbulent chaotic systems were considered in Majda and Harlim (2012). The local ensemble transform Kalman filter (a version of EnKF) was applied to spatiotemporally chaotic Rayleigh–Bénard convection in Cornick et al. (2009). For Kalman filter algorithms for determining the optimal closure parameters in climate models, see for example Annan et al. (2005) or Hakkarainen et al. (2012). Furthermore, if the state variable is still a very high dimensional one, such as in weather prediction, 4DVAR type approaches (see e.g. Fisher and Andersson, 2001; Rabier et al., 2000; Dimet and Talagrand, 1986) are conventionally employed.

There are also attempts to take care of model and approximation errors caused by the model reduction in data assimilation problems. For example, Janjic and Cohn (2006) considers errors due to unresolved scales (features that cannot be represented using the low-dimensional state) caused by model reduction in atmospheric data assimilation problems. Model errors caused by approximation of fast (often chaotic) components in climate models are considered, for example, in Mitchell and Gottwald (2012), Gottwald and Harlim (2013) and Berry and Harlim (2014). However, all of these consider specific model reduction related to ordinary differential equations, that is, they do not model the spatiotemporal (covariance) structure of the related PDE's. The main advantage of BAE is that it is a systematic approach to compute a (normal) model for the mean and covariance of the state noise process. We note, in particular, that the mean of the state noise process is generally non-zero, in contrast to the conventional assumptions of the state noise process.

Our aim is to give a preliminary assessment of the feasibility of the BAE approach to chaotic problems. In particular, we study the state and parameter estimation problems induced by the Kuramoto–Sivashinsky (KS) equation which has also been referred to as the "simplest" chaotic PDE (Brummitt and Sprott, 2009). We apply the BAE approach proposed in Huttunen et al. (2010) to the state estimation and identification problems related to the KS equation. The approach is here used to handle errors due to model reduction and misspecification of model parameters, which are common in data assimilation problems (Cane et al., 1995; Dee, 1991; Voutilainen et al., 2007). The BAE approach to state estimation and identification problems leads to a modification of (extended) Kalman filter.

The rest of the paper is organized as follows. In Section 2, we formulate the state estimation and state space model identification for the Kuramoto–Sivashinsky equation. In Section 3, we give a brief review of state estimation, extended Kalman filter (EKF) and the nonstationary Bayesian approximation error approach. Section 4 discusses numerical experiments and a discussion is given in Section 5.

2. Kuramoto–Sivashinsky equation: the state estimation and identification problems

We consider the Kuramoto–Sivashinsky (KS) equation. The KS equation was first developed to model waves in the Belousov–Zhabotinsky reactions (Kuramoto and Tsuzuki, 1976). In addition, the KS equation has been applied, for example, to model instabilities of the plane front of a laminar flame (Sivashinsky, 1977, 1980), and to flows of thin liquid films (Sivashinsky and Michelson, 1980; Chang, 1986; Chen and Chang, 1986; Shlang and Sivashinsky, 1982). The instabilities of the KS equation have also been extensively studied analytically and numerically (Kudryashov, 1990; Kevrekidis et al., 1990; Papageorgiou and Smyrlis, 1991; Smyrlis and Y, 1996).

Please cite this article in press as: Huttunen J.M.J., et al., Approximation error approach in spatiotemporally chaotic models with application to Kuramoto–Sivashinsky equation. Computational Statistics and Data Analysis (2018), https://doi.org/10.1016/j.csda.2018.01.015.