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Systematic physics constrained parameter estimation of stochastic differential equations

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ABSTRACT

A systematic Bayesian framework is developed for physics constrained parameter inference of stochastic differential equations (SDE) from partial observations. Physical constraints are derived for stochastic climate models but are applicable for many fluid systems. A condition is derived for global stability of stochastic climate models based on energy conservation. Stochastic climate models are globally stable when a quadratic form, which is related to the cubic nonlinear operator, is negative definite. A new algorithm for the efficient sampling of such negative definite matrices is developed and also for imputing unobserved data which improve the accuracy of the parameter estimates. The performance of this framework is evaluated on two conceptual climate models.

1. Introduction

In many areas of science the inference of reduced order hybrid dynamic-stochastic models, which take the form of stochastic differential equations (SDE), from data is very important. For many applications running full resolution dynamical models is computationally prohibitive and in many situations one is mainly interested in large-scale features and not the exact evolution of the fast, small scale features, which typically determine the time step size. Thus, reduced order stochastic models are an attractive alternative. Examples are molecular dynamics (Horenko et al., 2005), engineering turbulence (Heinz, 2014) and climate science (Franzke et al., 2005; Franzke and Majda, 2006; Kondrashov et al., 2006).

The inference of such models has been done using non-parametric methods (Siegert et al., 1998; Friedrich et al., 2000; Crommelin and Vanden-Eijnden, 2006) from partial observations. These non-parametric methods need very long time series for reliable parameter estimates and can be used only for very low-dimensional models because of the curse of dimension. More importantly, they do not necessarily obey conservation laws or stability properties of the full dimensional dynamical system. In many areas of science one can derive reduced order models from first principles (Majda et al., 2009; Pavliotis and Stuart, 2008) such that certain fundamental properties of the full dynamics are still valid. These methods provide us with parametric forms for the model fitting. Physical constraints then not only constrain the parameters one has to estimate but they can also ensure global stability. Thus, there is a need for systematic physics constrained model and parameter estimation procedures (Peavoy, 2013; Majda and Harlim, 2013).

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For instance, the climate system is governed by conservation laws like energy conservation. Based on this energy conservation property the normal form of stochastic climate models has been derived by Majda et al. (2009) using the stochastic mode reduction procedure (Majda et al., 1999, 2001, 2008; Franzke et al., 2005; Franzke and Majda, 2006). This procedure allows the systematic derivation of reduced order models from first principles. This normal form provides a parametric form for parameter estimation from partial observations which we will use in this study.

The fundamental form of climate models is given by

$$\frac{d\mathbf{z}}{dt} = F + L\mathbf{z} + B(\mathbf{z}, \mathbf{z}), \tag{1}$$

where $\mathbf{z} \in \mathbb{R}^N$ denotes the N-dimensional state vector, F the external forcing, L a linear and B a quadratic nonlinear operator. The nonlinear operator B is conserving energy $\mathbf{z} \cdot B(\mathbf{z}, \mathbf{z})$. For current climate models N is of the order of 10^6–10^8. This shows that running complex climate models is computationally expensive. But for many applications like extended-range (periods of more than 2 weeks), seasonal and decadal climate predictions one is only interested in the large-scale circulation of the climate system and not whether there will be a cyclone over London on a particular day next year. The large-scale circulation can successfully be predicted using reduced order models (Selten, 1995; Achatz and Branstator, 1999; Franzke et al., 2005; Franzke and Majda, 2006; Kondrashov et al., 2006).

The stochastic mode reduction procedure (Majda et al., 1999, 2001, 2008) provides a systematic framework for deriving reduced order climate models with a closure which takes account of the impact of the unresolved modes on the resolved modes. In order to derive reduced order models one splits the state vector $\mathbf{z} = \binom{\mathbf{x}}{\mathbf{y}}$ into resolved $\mathbf{x}$ and unresolved $\mathbf{y}$ modes. The stochastic mode reduction procedure now enables us to systematically derive a reduced order climate model which only depends on $\mathbf{x}$

$$d\mathbf{x} = \left(\tilde{F} + \tilde{L}\mathbf{x} + \tilde{B}(\mathbf{x}, \mathbf{x}) + M(\mathbf{x}, \mathbf{x}, \mathbf{x})\right) dt + a(\mathbf{x}, \boldsymbol{\sigma}) d\mathbf{W}, \tag{2}$$

where M denotes a cubic nonlinear term, W is the Wiener process and σ the diffusion parameters.

In this study we will develop a systematic Bayesian framework for the efficient estimation of the model parameters using Markov Chain Monte Carlo (MCMC) methods from partial observations. We are dealing with partial observations because we now only have knowledge of the few resolved modes $\mathbf{x}$ and are ignorant about the many unresolved modes $\mathbf{y}$.

Stochastic climate modeling is a complex problem and empirically estimating the parameters poses several problems. First, the nonlinearity of climate models requires an approximation of the likelihood function. While it can be shown that this approximation converges to the true likelihood, this is not necessarily the case for real world applications. Here we develop a MCMC algorithm for the first time for stochastic climate models and demonstrate that this algorithm performs well. Second, the nonlinearity of the problem causes the space of parameters leading to stable and physical meaningful solutions to become small as the dimension of the problem increases. We show that a lot of the posterior mass is on parameter values which lead to solutions exploding to infinity in finite time. To solve this problem we derive global stability conditions. These conditions take the form of a negative definite matrix. Hence, we devise a novel sampling strategy based on sampling non-negative matrices. We show that this sampling strategy is computationally efficient and leads to stable solutions.

In Section 2 we introduce stochastic climate models and derive conditions for global stability. Previous studies have shown that reduced climate models with quadratic nonlinearity experience unphysical finite time blow up and long time instabilities (Harlim et al., 2014; Majda and Yuan, 2012; Majda and Harlim, 2013; Yuan and Majda, 2011). Here we use the normal form of stochastic climate models (Majda et al., 2009) and derive sufficient conditions for global stability for the normal form of stochastic climate models. These normal form stochastic climate models have cubic nonlinearities. The here derived stability condition is more general than the one in Majda et al. (2009). In Section 3 we develop a Bayesian framework for the systematic estimation of the model parameters using physical constraints. Here we develop an efficient way of sampling negative-definite matrices. Without this constraint the MCMC algorithm would produce about 40% unphysical solutions which is clearly very inefficient. Here we also demonstrate that for these kinds of SDEs imputing data improves the parameter estimates considerably. In Section 4 we demonstrate the accuracy of our framework on conceptual climate models. We summarize our results in Section 5.

2. Stochastic climate models and global stability

Here we study the following D dimensional normal form of stochastic climate models (which has the same structural form as Eq. (2), see Majda et al., 2009):

$$dx_i = \left(\alpha_i + \sum_{j=1}^{D} \beta_{i,j} x_j + \sum_{j+1}^{D} \sum_{k=1}^{j} \gamma_{i,j,k} x_j x_k + \sum_{j=1}^{D} \sum_{k=1}^{j} \sum_{l=1}^{k} \lambda_{i,j,k,l} x_j x_k x_l\right) dt \tag{3a}$$

$$+ \sum_{j=1}^{D} a_{i,j} dW_j + \sum_{j=1}^{D} \sum_{k=1}^{j} b_{i,j,k} x_j dW_k, \tag{3b}$$