Parameter uncertainty of chaotic systems

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Many physical processes, such as boundary layer turbulence or cloud microphysics, are represented in numerical weather prediction (NWP) models by physical parameterization schemes. These schemes contain closure parameters to express some unresolved variables by predefined parameters rather than by explicit modelling. The increasing complexity of NWP models makes it very demanding to optimally specify parameters values by manual techniques using limited samples of test forecasts. This may partly explain the increasing difficulties encountered in integration of new physical parametrizations schemes into model dynamics. Development of algorithmic tools to make statistical inference about the closure parameters would be helpful to facilitate and speed-up NWP model development. The same question of parameter optimization and uncertainty quantification is equally crucial for climate models. Additionally, the situation is complicated here by the challenge of unpredictability: due to chaoticity there is no unique solution for the long time model integrations, even with fixed model parameters, see, e.g., Ref.[1] for more discussion. Here we present recent methods for parameter estimation of chaotic systems, both for short-time and long-time situations.

Several approaches have been proposed for joint estimation of static parameters and dynamic state variables. It is relatively straightforward to augment the state vector in filtering applications with the static model parameters and treat them as artificial model states. A drawback is that parameter values tend to change from one filtering step to the next, in accordance with the changing atmosphere and observing network, although they are static or quasi-static. Moreover, filtering requires additional tuning parameters which may lead to bias for the model parameters Ref.[2]. Another way of employing the filtering approach is to construct a filter-based likelihood to be optimized with respect to the parameters Ref.[3]. For large systems such iterative optimization is prohibitively CPU demanding, however. For the same reason other approaches such as particle filtering are excluded in state estimation of large systems.

The idea of the EPPES concept Ref.[4], Ref.[5] is to create a 'CPU-free' NWP model parameter estimation by slightly modifying an existing EPS system: an operational ensemble prediction system is added with a functionality to perturb model parameters and to learn which ones tend to perform well. So the massive amount of model simulations of ensemble prediction would be utilized for on-line model optimization, practically without any additional CPU demand. The original EPPES concept is based on the steps, repeated for each assimilation window, of (i) sampling candidate parameter values from a Gaussian proposal distribution, (ii) launching each ensemble member of the prediction model with different candidate parameter values, (iii) evaluating the performance of the parameters against a cost function, and (iv) adapting the proposal distribution according to the parameter performance. The adaptation is done in a Monte Carlo way, based on the importance weights of the cost function values.

The approach was successfully applied to improve the performance of the already highly tuned IFS system in Ref.[6], Ref.[7]. The selection of the cost function, however, reveals a problem: while the performance of the model can be improved according to the criteria selected as part of the cost function, some other aspects of the prediction may deteriorate. This calls for a multicriteria optimization approach, where no relevant part of the model performance is allowed to converge towards unacceptable values. In Ref.[8] we apply an evolutionary optimization approach, the Differential Evolution (DE), for this purpose. Each assimilation window may be interpreted as a generation and the ensemble as the respective population. With slight modifications (due to the stochastic nature of the cost functions) the DE algorithm may then be employed to optimize the model parameters. The special requirements of various optimization criteria may be taken into account by, e.g., the desirability function method. Otherwise the implementation is similar to that with EPPES, in the sense that an existing EPS system is used, without any essential new CPU demand. As an optimization approach the DE version typically gives faster convergence, while the sampling-type original EPPES algorithm provides an uncertainty quantification for the parameter identification.

The closure parameters of a large scale climate model, ECHAM5, were studied in Ref.[9] using several summary statistics, such as temporal and spatial averages of the key balance factors of the climate, as the cost function. While parameter estimation was technically possible to perform, see Ref.[10] for the methods, the results remained inconclusive. The reason was the difficulty of selecting the cost function terms that would be sensitive enough with respect to the closure parameters. The standard way of estimating parameters of dynamical systems is based on the residuals between the data and the model responses, both given at the time points of the measurements. Supposing the statistics of the measurement error is known, a well defined likelihood function can be written. The maximum likelihood point is typically considered as the best point estimator, and it coincides with the usual least squares fit in the case of Gaussian noise. The full posterior distribution of parameters can be sampled by Markov chain Monte Carlo (MCMC) methods. The approach has become routine for the parameter estimation of deterministic models in Bayesian inference, see Refs.[11,13] for further references. The estimation of the parameters of chaotic models can not be performed in this way. After an initial time period where the system is predictable, the model responses, even with just slightly varying initial condition or some settings of a numerical solver employed, diverge so that the concept of a given model response at a given time point loses the meaning. The same effect can be seen when some infinitesimal changes to the model parameters are made. In this sense, there is no unique model trajectory corresponding to a fixed model parameter vector. But while all such trajectories are different, they approximate the same underlying attractor and should be considered in this sense equivalent. Here we discuss a statistical approach presented in Ref.[14] to quantify such "sameness" of trajectories, and to distinguish trajectories that are significantly different. The basic idea is to create a summary statistics that takes into account the geometry of the attractor, rather than using direct averages or other (linear) projections such as used in Ref.[9]. Various formulations of fractal dimensions have been developed to characterise the internal geometry of such attractors. Here we modify one of these, the so-called correlation dimension[15], to develop a way to quantify the variability of samples of an attractor by mapping the respective phase space trajectories onto vectors, whose statistical distribution can be empirically estimated. The distributions turn out to be Gaussian, which provides us a well defined statistical tool to compare the trajectories. We use the approach for the task of parameter estimation of chaotic systems. Other applications are pointed out as well.

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