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Parameter estimation using chaotic time series

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ABSTRACT

We show how the response of a chaotic model to temporally varying external forcing can be efficiently tuned via parameter estimation using time series data, extending previous work in which an unforced climatologically steady state was used as the tuning target. Although directly fitting a long trajectory of a chaotic deterministic model to a time series of data is generally not possible even in principle, this is not actually necessary for useful prediction on climatological time-scales. If the model and data outputs are averaged over suitable time-scales, the effect of chaotic variability is effectively converted into nothing more troublesome than some statistical noise. We show how tuning of models to unsteady time series data can be efficiently achieved with an augmented ensemble Kalman filter, and we demonstrate the procedure with application to a forced version of the Lorenz model. The computational cost is of the order of 100 model integrations, and so the method should be directly applicable to more sophisticated climate models of at least moderate resolution.

1. Introduction

Parameter estimation has risen to prominence in geophysical research in recent years due to its relevance to the topical problem of climate prediction (Andronova and Schlesinger, 2001; Gregory et al., 2002; Knutti et al., 2002; Murphy et al., 2004). The behaviour of a coupled ocean–atmosphere model on climatological time-scales is highly dependent on the details of parametrizations which cannot be precisely determined from theory or direct observations. As well as determining the forecast mean, it is also the uncertainty in parametrizations that generates the range of uncertainty in climate model forecasts (at least for a given scenario of external forcing, the determination of which is primarily a socio-economic rather than geophysical question). Therefore, probabilistic parameter estimation methods are an important tool in the understanding of climate change.

Recently, Annan et al. (2004) have introduced an efficient method for multivariate parameter estimation in non-linear models, based on an augmented ensemble Kalman filter (EnKF; Evensen, 2003). This has successfully been applied to a range of models including the Lorenz model (Annan and Hargreaves, 2004) and a coupled two-dimensional atmosphere–three-dimensional ocean Earth System Model (Hargreaves et al., 2004). The method bypasses both the ‘curse of dimensionality’ (Bellman, 1961) and chaotic hypersensitivity to small parameter perturbations (Lea et al., 2000) that have handicapped previous attempts at parameter estimation in climate modelling.

In these recent applications of the EnKF, however, the model was only tuned to a steady-state climatology, and the integrations were performed without time-varying external forcing. Although this is a useful first step in ensuring that a model provides a reasonable approximation to reality, it ignores any information concerning the rate of externally forced climate change that may be contained in time series of observational data. This is clearly less than ideal, especially because it is the magnitude and rate of anthropogenically forced change of the future climate which we particularly wish to estimate. Evidence regarding this is contained in the recent historical record and can, at least in principle, be used to constrain estimates of future climate change (Gregory et al., 2002; Knutti et al., 2002).

Although full time series of observational data are frequently used as a qualitative check on model output (e.g. Tett et al., 1999, 2000; Stott et al., 2000, 2001; Levitus et al., 2001; Hansen et al., 2002; Johns et al., 2003; Sun and Hansen, 2003), and methods such as optimal fingerprinting have also been used to distinguish quantitatively between natural variability and forced response (Hegerl and Allen, 2002; Allen and Stott, 2003), these data have rarely been used to directly tune climate models in an objective manner. In Knutti et al. (2002) and Gregory et al. (2002), a time series of observations was condensed to a single value, the net change in ocean heat content over the O(40)-yr time series, and the direct sampling Monte Carlo methods they used are only possible for low-dimensional estimation problems

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using simple models due to the large number of simulations required. Multivariate parameter estimation with sophisticated climate models is a significantly more demanding task, and it is this gap that we hope to fill with the efficient method described here.

Over climatological time-scales, it is not possible, even in principle, to select the initial conditions and/or parameters of a deterministic chaotic model in order to make its trajectory match a long time series of real observational data within the observational errors, because such an 'ι-shadowing trajectory' (Gilmour, 1998; Smith and Gilmour, 1998) does not exist. Even when a perfect model is used for idealized tests, tuning model parameters by the use of time series data has generally been found to be a rather intractable problem (Pisarenko and Sornette, 2004). However, when we wish to predict the climatological response to some imposed forcing, then in fact there is no need for the trajectory of the model to closely track that of historical observational data in all its chaotic detail; indeed, by definition, the climatological response is that statistical component which is independent of the precise initial conditions. Therefore, all that we can require is that the climate of the model (under suitable external forcing) matches historical observations smoothed over suitable climatological time-scales. Even so, brute force approaches to this problem, based on exhaustive multifactorial or randomized exploration of parameter space, are prohibitively expensive unless the number of parameters to tune is extremely small. In this short paper, we show how the EnKF method can readily be extended in order to use time series data to efficiently tune the response of a model to slowly varying external forcing.

We emphasize at the outset that in this paper we deliberately ignore some significant issues that could hamper attempts at practical application. In reality, models are imperfect, and both the models and data may contain significant unforced variability on multiyear time-scales that would have to be accounted for (e.g. Levitus et al., 2000, but note also Gregory et al., 2004). In principle, this could perhaps be addressed by the use of off-diagonal terms in the error covariance matrix; however, estimating these might not be easy. In any case, our purpose here is simply to illustrate the existence of an efficient method by which these time series could potentially be utilized to greater advantage than has heretofore been the case.

2. Model and data

The Lorenz model (Lorenz, 1963) is a computationally simple chaotic system of three variables which has frequently been used as a demonstration tool in climate research. Palmer (1999) modified the basic model by the addition of an external forcing term, which he used to illustrate the qualitative nature of the response that might be expected from a small perturbation to a non-linear system (e.g. anthopogenic forcing of the Earth's climate). We use his model to demonstrate how the forcing can be efficiently determined from a time series of observations.

The equations for the forced Lorenz model are given by

$$x' = \sigma(y - x) + f \cos\theta \tag{1}$$

$$y' = rx - y - xz + f \sin\theta \tag{2}$$

$$z' = xy - bz \tag{3}$$

where σ, b and r take the standard values 10, 8/3 and 28, respectively, and f and θ give the strength and direction of the forcing. The response of the model is rather insensitive to the choice of θ, so we fix this at the arbitrarily selected value of 70°. When projected on to the *x–y* plane, the unforced model's state vector oscillates chaotically around two symmetrical unstable fixed points $(x, y) = \pm(3\sqrt{8}, 3\sqrt{8})$. When a modest positive forcing $f > 0$ is applied, the model's behaviour seems qualitatively similar over integrations of at least several characteristic time periods, but in fact the model state is biased towards one part of the attractor. If averaged over a sufficiently long interval, the model's projection into the *x–y* plane is biased towards the positive quadrant, as shown in Palmer (1999); a negative forcing has the opposite effect. This bias can be quantified by, for example, calculating the mean value of *x* over a sufficiently long interval, which for $|f| \leq 5$, increases in near-linear proportion to the strength of the forcing. For sufficiently strong forcing, the model behaviour changes qualitatively and so we apply the limit $|f| \leq 5$ throughout this paper.

We will use this model as a simple simulacrum for a climate model, with *x* taking the place of global temperature, and *f* corresponding to the variation in radiative forcing due to natural and anthropogenic causes. We define a 'year' of model integration as 1000 time units. Of course, this model cannot provide a realistic simulation of the real climate, and our experiment is merely intended to illustrate how a time series of data can be used to tune a chaotic model that is subject to slowly varying forcing. Nevertheless, we make the arbitrary decision to use realistic forcing. The four dominant sources of variability in radiative forcing are described and estimated in Crowley (2000), and consist of volcanic dust, solar variability, anthropogenic greenhouse gases (GHGs; predominantly CO_2) and sulphate aerosols. The annually averaged estimated values for the radiative forcing effect of these factors for the years 1949–1998 are plotted in the top half of Fig. 1. The volcanic forcing is highly variable and is dominated by the major eruptions of El Chichon (1982) and Mt Pinatubo (1991). The GHG forcing shows a strong upward trend, the sulphate aerosols a smaller negative trend, and the solar output exhibits a much lower variability on a decadal time-scale. However, although these factors can be directly measured, significant uncertainty remains as to their conversion into effective radiative forcings of the Earth's climate system (Houghton et al., 2001; Gregory et al., 2002). We treat these uncertainties as a priori unknown but temporally fixed multiplicative factors by which the four given time series of forcing terms are scaled.

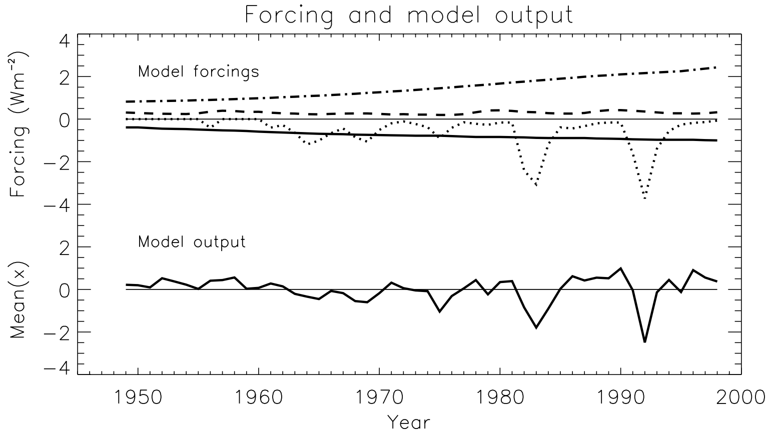

Fig. 1. Radiative forcings (top) and model output (bottom). Thick solid, dotted, dashed and dot-dashed lines in the top plot show aerosol, volcanic, solar and GHG forcings, respectively. The thick solid line in the lower plot shows annually averaged model output when forced as described in the text. Thin horizontal lines indicate zero.

Thus, the total forcing term takes the form

$$f(t) = \alpha_1 f_1(t) + \alpha_2 f_2(t) + \alpha_3 f_3(t) + \alpha_4 f_4(t)$$

where f_i are the individual constituents of the total forcing, and α_i are be determined. Although these parameters are simple scalings on the external forcing, arbitrary internal parameters of a more complex model (e.g. those which affect the cloud feedback), which control the response to forcing, could equally well be tuned by the method outlined in Section 3. In order to demonstrate the technique, we perform an identical twin test, generating a synthetic time series of data by selecting the four scaling factors independently from the normal distribution $N(\mu, \sigma) = N(1.5, 0.25)$ (the selected values were, in order, 1.4, 1.5, 1.1 and 1.1 to two significant figures) and integrating the model for a period of 51 yr, with the first year being a spin-up from random initial conditions. Observations are made at intervals of one time unit, with independent observational errors drawn from $N(0, 1)$. The results are not sensitive to these choices unless either the observational error or sampling interval is dramatically increased. The output from this integration is plotted in the lower half of Fig. 1. The dominant features in the model output are the two large troughs in the latter part of the run due to the two massive volcanic eruptions mentioned previously, despite which there is a small positive anthropogenically forced trend over the whole time series. We now show how these data can be used to determine the parameters by which they were generated.

3. Method for assimilation of time series data

The Kalman filter (Kalman, 1960) is an optimal filter for linear systems. Given a model forecast state $\mathbf{m}^{\mathrm{f}}$ with error covariance matrix $\mathbf{P}^{\mathrm{f}}$, observations $\mathbf{o}$ (which are valid at the forecast time) with their error covariance matrix $\mathbf{R}$, the analysis state $\mathbf{m}^{\mathrm{a}}$ is calculated by

$$\mathbf{m^a} = \mathbf{m^f} + \mathbf{P^f H^T}(\mathbf{H P^f H^T} + \mathbf{R})^{-1}(\mathbf{o} - \mathbf{H m^f}), \tag{4}$$

where $\mathbf{H}$ is the measurement operator that maps the model to observations, and the analysis error covariance matrix $\mathbf{P}^{\mathrm{a}}$ is given by

$$\mathbf{P^a} = \mathbf{P^f} - \mathbf{P^f H^T}(\mathbf{H P^f H^T} + \mathbf{R})^{-1}\mathbf{H P^f}. \tag{5}$$

The EnKF uses an ensemble of model states as an efficient Monte Carlo approximation to the mean and covariance matrix of the model state. A full description and an extensive list of applications are given in Evensen (2003), and it is notable that although the method is only provably optimal in the case of a linear system and limit of infinite ensemble size, in practice it can usually handle substantial non-linearity, and a modest ensemble size of about 100 members has usually been found to be adequate across a wide range of problems. One simple extension of the method is to augment the model state with parameter values, in order that the parameters themselves are also estimated along with the state variables. Here we augment the model state with the four coefficients α_i. A standard implementation of the EnKF would involve an analysis step at each time that observations became available. After the full time series of data are assimilated, the ensemble members should hopefully sample the joint posterior parameter distribution. However, in practice this approach to parameter estimation often gives rather poor results when attempted with highly chaotic models, even in simple identical twin tests such as this. The failure of the method manifests itself as a convergence of the parameter values to distributions that are inconsistent with the truth (commonly termed filter divergence), as shown by Kivman (2003). In his research, a particle filter delayed, but ultimately did not prevent, this failure from occurring. Our implementation of this sequential trajectory-fitting approach using the EnKF for our parameter estimation problem also results in a qualitatively similar (although quantitatively less severe) failure which is not presented here. Of course, the apparent limitations of these and other methods do not necessarily mean that they cannot be developed to solve parameter estimation problems of this type. Rather, the presentation here of one possible solution is just a demonstration that the problem is in principle tractable rather than a claim to be the best possible method.

Although fitting every chaotic detail of the model to that of the time series does not appear to be possible, we note that this is not in fact necessary or even particularly desirable in order to make meaningful predictions of climate change. Any infinitesimal discrepancy between the true and model states will rapidly grow during the forecast interval, and on climatological time-scales, the oscillations of model and truth around their climatological means will be wholly independent of each other. For this reason, it is the climatological statistics which are of primary interest, and (by definition) these are essentially independent of the initial conditions except perhaps in pathological cases. Lea et al. (2000) showed that by averaging the model's output over an adequately long time-scale, the effect of the chaotic dynamics can be considered as nothing more than a random sampling error caused by the limited precision with which the statistics of a finite integration interval approximate the true climatology of the model. This sampling error is for all practical purposes indistinguishable from Gaussian stochastic noise and scales inversely in proportion to the square root of the averaging interval. Although those experimental results were generated with the Lorenz model, the sensitive dependence of chaotic models to the initial conditions, together with the central limit theorem, implies that the same ideas will apply in the general case. Furthermore, the sampling errors on consecutive disjoint intervals are independent, so long as the averaging interval is long relative to the characteristic time-scale of chaotic dynamics of the model. Therefore, the chaotic variability can be treated as simple independent observational errors on the temporally averaged observations.

We choose here to average our observations over intervals of 1 yr. For our definition of 1 yr as 1000 time units in the Lorenz model, the standard error on the mean of one year's worth of observations of x is approximately 0.3 units, which value we use as the observational error in the assimilation scheme (the true observational error makes a negligible contribution to this value). Using a much shorter year would result in the noise of the climatological sample swamping the signal of the forcing time series. The total external forcing over the first 6 yr of the model integration in Fig. 1 has very small variability, so the model output over this interval indicates the variability due to this random sampling noise.

In order to assimilate climatological observations, we need to augment the model state with appropriate climatological diagnostics. Because we are not only interested in the posterior parameter values, but also wish to check how well the model reproduces the historical time series with these parameter values, we treat the problem as a smoother rather than filter. This means updating all of the previous output from the model (as well as the current state) in the light of new measurements, so that information propagates backwards as well as forwards in time. Evensen and Leeuwen (2000) explain in some detail how this can be readily achieved with essentially the same analysis algorithm as the EnKF, by merely augmenting the current model state with a history of model output, which is thereby automatically updated by new observations. They also prove that the final estimate of model state (including parameters, in our case) is not affected by this modification to the standard Kalman filter algorithm. In our example, we only need to augment the set of tunable parameters with the series of annually averaged observations to generate a vector of 54 values for each ensemble member, and perform the analysis in a single step at the end of the integration using the 50 annual observations of the identical twin output. The model state itself is not needed for the analysis. By using this method, the full time series of climatological values and parameters are updated in a mutually consistent manner by the analysis routine, and we do not need to repeat the 50-yr integration with the posterior parameter estimates in order to generate a consistent hindcast. The computational costs are still dominated by the 100-member ensemble integration, as is usual for EnKF applications.

We choose deliberately ignorant priors of the form $\alpha_i \in N(1, 1)$ in order to investigate to what extent the data alone can constrain the parameter values. As mentioned previously, the magnitude of total forcing was capped at 5, this being approximately the level at which the response to forcing becomes significantly non-linear. The output from the prior ensemble is plotted at the top of Fig. 2. The ensemble mean is reasonably close to the data, although the upward trend in the time series appears slightly too shallow, as are the volcanic troughs. More importantly, the width of the ensemble is very broad, reflecting our prior ignorance of the parameter values.

4. Results from the identical twin test

The lower half of Fig. 2 shows the output of the ensemble Kalman smoother. The posterior hindcast gives a very close fit to the data. The four posterior parameter values are given by (1.3 ± 0.2, 1.7 ± 0.6, 0.9 ± 0.3, 1.0 ± 0.5) which are consistent with the true values and substantially narrower than the prior distributions. The volcanic forcing has been significantly constrained by the distinctive shape of the forcing and data, but the effect of solar forcing (which is very small and varies relatively little) is much less well defined. The GHG and aerosol forcings are more interesting. Although they are both much larger forcings than the solar variability, and vary by more than a factor of 2 over the hindcast interval, they also remain rather uncertain. The mean value of α_3 is also slightly degraded, which is probably due to the sampling error of the small ensemble. There is, however, a substantial correlation between these two scaling parameters across the ensemble members, with a Pearson correlation coefficient of 0.9 (the next largest pairwise correlation between the scaling parameters is 0.3). Examining the time series of the input forcings in Fig. 1, we can see that both GHG and aerosol forcings have very similar shapes (but opposite signs), showing a steady increase in magnitude through the time interval. It is not surprising therefore that their scaling coefficients cannot be simultaneously constrained by the single time series of data, because the effects of increasing both of their scaling coefficients

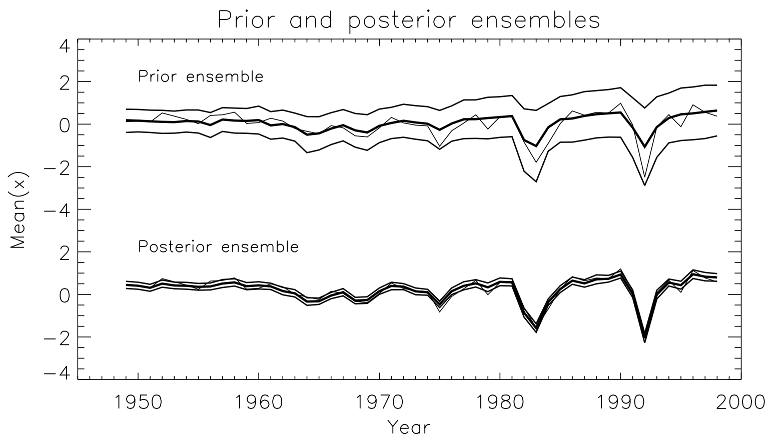

Fig. 2. Prior (top) and posterior (bottom) ensemble output. For each plot, the thickest line is the ensemble mean, the two medium width lines indicate the one standard deviation width and the thin line shows the model data from Fig. 1.

simultaneously will largely cancel out. Although the model used here is in no way realistic, this ambiguity between the effects of GHG and aerosols is known to pose a significant difficulty in the attribution of recent climate change (Houghton et al., 2001).

Despite the chaotic nature of the model, the relationship between the tunable parameters and model output is highly linear. In fact, the occasional truncation of the forcing to $|f| \leq 5$ is the only detectable source of non-linearity. Therefore, because the EnKF maintains linear balance in the calculation of the posterior, the posterior parameter and climate estimates are highly consistent, as can be demonstrated by integrating the ensemble over the same interval, this time using the posterior parameter values during the integration. The results from this (not shown) are very similar to the posterior estimates, with a marginally broader ensemble width being the only sign of numerical inaccuracy. For more complex problems, the Gaussian approximation to the error structure implicit in the Kalman filter equations may introduce significant inaccuracy, especially if the prior is much broader than the posterior. In this case, the iterative approach presented in Annan et al. (2004) and Annan and Hargreaves (2004) will improve the accuracy and self-consistency of the output, at the cost of requiring multiple integrations over the full time interval. There may, of course, be other approaches which would achieve higher accuracy at lower computational cost.

5. Conclusions

We have demonstrated how time series data can be used efficiently to constrain parameters in a chaotic model. The method relies on the averaging of the chaotic observational data and model output over sufficient intervals that the high-frequency chaotic dynamics can be treated as stochastic noise, following which the ensemble Kalman filter (or smoother) can be used in a very similar manner to the steady-state applications previously presented. Any practical application with geophysical data would have to address the important issue of model error, which is not addressed here, and there also may not be such a clear cut-off point between high-frequency chaos and low-frequency climate change as in this toy example. These problems could be expected to limit the accuracy of parameter estimates, but at least the method outlined here may have the potential to address this parameter estimation problem in a computationally efficient manner.

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