Estimating Model Parameters with Ensemble-Based Data Assimilation: A Review

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Abstract

Weather forecast and earth system models usually have a number of parameters, which are often optimized manually by trial and error. Several studies have proposed objective methods to estimate model parameters using data assimilation techniques. This paper provides a review of the previous studies and illustrates the application of ensemble-based data assimilation to the estimation of temporally varying model parameters in a simple low-resolution atmospheric general circulation model known as the SPEEDY model. As shown in previous studies, our results highlight that data assimilation techniques are efficient optimization methods which can be used for parameter estimation in complex geophysical models and that the estimated parameters have a positive effect on short-to medium-range numerical weather prediction.

1. Introduction

State-of-the-art weather forecast and earth system models (hereafter numerical models) include a set of parameterizations to represent the effects of processes that cannot be fully resolved by the model equations, such as cloud microphysics, turbulence, radiation, and deep moist convection. These parameterizations formulate the effects of the unresolved scales as a function of the model variables on the basis of a simplification of the underlying physical processes. The link between the unresolved and resolved scales can be established on the basis of theoretical considerations or empirical laws derived from observations. In either case, a certain number of parameters appear in the equations that express the unresolved scale effects on the resolved scales. Some of the parameters (e.g., parameters related to the radiative scheme) have a direct physical interpretation and can be directly measured. However, other parameters that arise from the simplification of the underlying physical processes cannot be directly measured (e.g., numerical diffusion coefficients).

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Thus, the optimal values of some parameters are intrinsically uncertain.

The values of some parameters have a significant effect on model performance ranging from short-range forecasts to climate simulations (Stainforth et al. 2005). This indicates that the suboptimal setting of model parameters can account for a significant part of model errors. The optimal values for a set of parameters can be defined as the values that most efficiently reduce model errors in a certain metric. It should be noted that the optimal value for the parameters depends on the selected metric. In general, when dealing with an imperfect model, there is no single optimal value for a given parameter (Smith 2000). Moreover, in this case, there are no true model parameters but only optimal parameters, and the uncertainty represents our lack of knowledge about these optimal parameter values. Given the several sources of uncertainties associated with the parameterization of subgrid processes, an accurate, efficient, and objective way to estimate the optimal parameters is highly desirable.

Parameter estimation has several applications in the context of atmospheric and oceanic sciences. Some of these applications are listed below:

- Parameter estimation can contribute to adaptive model optimization, from short-to medium-range weather forecasts. Optimal parameters in numerical weather prediction (NWP) models can be a function of time and location. Parameter estimation can provide a flexible optimization tool to improve the forecast skill.

- Parameter estimation can provide an estimate of the uncertainty in the parameters from the available observations (See a companion paper, Ruiz et al. 2013b). This information can be used to design an ensemble forecast that includes perturbations in model parameters and also in the design of stochastic parameterizations (Hansen and Penland 2007).

- Climate models can be optimized using parameter estimation techniques. Climate simulations are less dependent on the initial conditions, and hence parameters play an important role in the performance of the model (Stainforth et al. 2005).

Parameter estimation is a complex problem which needs an efficient and objective methodology that can account for all the sources of parameter sensitivity at a reasonable computational cost. Moreover, dealing with the large number of degrees of freedom and complexity of state-of-the-art numerical models is a challenge. As will be discussed extensively in this paper, data assimilation techniques have the potential to provide a solution to this complex parameter estimation problem. Several studies have shown that data assimilation techniques applied to the parameter estimation problem have the potential to reduce model errors in applications ranging from high-resolution forecasts (Tong and Xue 2008) to large-scale decadal variability representation (Zhang 2011), and even in the simulations of current and future climate (Annan et al. 2005) with atmosphere, ocean, and land models as well as coupled models. These studies have demonstrated the relevance of parameter estimation techniques and have reinforced the idea that a significant part of model errors may be associated with a suboptimal set of some model parameters.

In this paper, a review of the objective techniques used for parameter estimation in numerical models is presented, with particular emphasis on the techniques based on data assimilation methods. The implementation of one of these techniques is illustrated using the local ensemble transform Kalman filter (LETKF, Hunt et al. 2007) with the SPEEDY model (Molteni 2003). In the experiments presented in this work, we restrict ourselves to the ensemble Kalman filter (EnKF) methods that could be implemented in operational data assimilation cycles at a relatively low computational cost. This paper is organized as follows. Section 2 presents a review of data assimilation techniques for the parameter estimation problem in NWP and climate prediction. Section 3 describes the implementation of parameter estimation in the EnKF framework and presents some experiments with a simple atmospheric general circulation model (GCM). Finally, Section 4 summarizes the conclusions of this study.

2. Review of parameter estimation methods using data assimilation

2.1 Objective methods for parameter estimation

The typical number of parameters that can be adjusted in a numerical model is at least $O(10^2)$ without considering spatial variability. Thus, the cost of naively exploring the entire parameter space for optimizing the model performance is prohibitive. If the evaluation of the model performance for each set of parameters is conducted over a long period of time, the associated computational cost would be even larger. In a typical modeling process, most parameters are fixed at preset values, and only a small number of parameters are tuned manually and subjectively.

During the last few decades, considerable effort has been devoted to the development of robust and objective methodologies for parameter estimation for large and complex systems like the ones used in numerical weather and climate predictions (Jarvinen et al. 2010, Liu et al. 2005, Severijns and Hazeleger 2005, Jackson et al. 2004). In these studies, a measure was defined to objectively quantify model performance, for instance, a cost function that penalizes model errors based on the root mean square error (RMSE) of the model output. If all model runs share the same initial condition and are performed for the same period, the cost function is only a function of the parameters that are being estimated. Therefore, changes in the total error (cost function) can only be attributed to changes in model errors associated with different parameter values. Most of these studies used minimization methods to find the optimal set of parameters that gives the minimum of the cost function, i.e., the parameters that produce the lowest model error. Simplified methods such as the simplex method (Press et al. 1992) may require several evaluations of the cost function, which in this context, means conducting several simulations with the model. These methods provide an alternative to the manual tuning of model parameters. They can obtain optimal parameters by objectively comparing the model outputs with observations. However, nonlinear model responses may produce multiple local minima in the cost function (Posselt and Bishop 2012), and thus sophisticated optimization algorithms are required to find the global minimum corresponding to the optimal parameters. Such optimization algorithms are usually too expensive computationally to be employed in sophisticated models with many degrees of freedom. In certain applications, a parameterization scheme can be optimized offline (i.e., without being coupled with the entire model). This substantially reduces the computational cost associated with the parameter estimation, allowing the use of more sophisticated algorithms (Pulido et al. 2012, Posselt and Bishop 2012, Golaz et al. 2007).

2.2   Parameter estimation and data assimilation

Most data assimilation techniques are based on an efficient implementation of the minimization of a cost function, which depends on a large number of variables, typically $O(10^7)$. In the classical data assimilation problem, an a priori estimate of the state of a system (usually a short-range forecast) is combined with a set of observations to produce an optimal estimate of the state. Data assimilation techniques can be extended to estimate the optimal model parameters in addition to the system state. Most parameter estimation techniques based on data assimilation use an augmented state vector, i.e., extension of the state space by adding the parameters to be estimated so that the parameters are treated as state variables in the data assimilation system. In this way, when the cost function is minimized, the optimum values for the state variables and parameters are obtained. Parameters are usually assumed to be constant during the model integration so that the parameter values only change in the data assimilation step. Evensen 1998 gives a theoretical framework for the parameter estimation problem using data assimilation techniques. In this framework, the spatial and temporal variability of the parameters can be considered. The model bias estimation problem is thus discussed as a particular case of parameter estimation. Inclusion of the parameters in the state vector can significantly modify the dynamical properties of the model. Even for a linear model, if the model includes products between parameters and state variables, the augmented state will behave as a nonlinear model (Yang and Delsole 2009). Another source of nonlinearity is the presence of on-off switches in the parameterizations. In that case, the sensitivity to the parameters may be nonsmooth. Therefore, a highly nonlinear model response to parameter changes may exist.

Most parameters cannot be directly measured; hence, they might be estimated through correlations between parameters and state variable errors. This is analogous to the case of state variables that are not directly observed but can be estimated from the observations of other state variables that are somehow coupled to the observed state variables. If the error covariance between the observed variables and a parameter is significant, the parameters have a strong influence on the observed variables. Then, the parameter can be accurately estimated from the observations. In this case, it is said that the parameter is identifiable (Navon 1997). If the observed variables are weakly correlated with the parameter value, the parameter cannot be estimated well. In this case, there are two possibilities: either the parameters do have a significant impact on model performance but not on the observed variables or the model sensitivity to changes in the parameters is weak. In the latter case, the model performance is not sensitive to the parameter values, and therefore parameter estimation is not essential.

The covariances between observed variables and

parameters can be highly state dependent. For instance, in the case of the parameters associated with the convective scheme, the spatial structure of the error covariances between the parameters and observed variables is highly dependent on the activation of the convective scheme. Data assimilation techniques that consider the state dependence of error covariances are necessary for the simultaneous estimation of the model state and parameters. Examples of these techniques include the four-dimensional variational (4D-Var) schemes, EnKF, and particle filters (PFs).

2.3   Parameter estimation based on variational data assimilation

At the beginning of a certain time period, 4D-Var data assimilation schemes seek the model state whose evolution produces the closest fit to the background state and the observations within the time window. This is achieved by minimizing the cost function that measures the differences between the model state and the observations within the time window and those between the model state and a prior estimate of the system state at the beginning of the time window. The cost function is based on the maximum likelihood and usually on the assumption that the errors in the state variables at the beginning of the time window are Gaussian (this last hypothesis can be relaxed, for example, see Fletcher and Zupanski 2007). The minimization of the cost function requires the gradient of the cost function, which is computed by means of the adjoint model (Errico 1997).

The variational data assimilation technique can be extended to find both the initial condition and a set of parameters that minimize the cost function. Navon 1997, Gong et al. 1998, Zhu and Navon 1999, Pulido and Thuburn 2005, and Bocquet 2011, among many others, have used the 4D-Var technique to estimate model parameters. The adjoint model has to include the model sensitivity to the parameters. Navon 1997 presented a review of parameter estimation using variational techniques. Zhu and Navon 1999 successfully performed a simultaneous estimation of the atmospheric state and three model parameters using the full-physics adjoint of a GCM in a perfect model scenario. They examined the impact of parameter estimation on short-range forecasts and determined it to be positive. In this work, the spatial or temporal dependence of the parameters was not considered. In this regard, Pulido and Thuburn 2005, 2006 used a 4D-Var approach to estimate the spatial distribution of the forcing associated with the gravity wave drag in the middle atmosphere. 4D-Var provides an accurate estimation of the spatial and temporal distribution of an unknown missing forcing term in the momentum equations, allowing detection of the regions and times of the year where the gravity wave drag in the middle atmosphere is more significant.

The 4D-Var technique is a promising approach for parameter estimation. However, the extension of the adjoint models to include parameter sensitivity may require considerable effort depending on the complexity of the model and the parameterizations. The success of 4D-Var depends on the geometry of the cost function. If the model response to the parameters is strongly nonlinear, the cost function may have multiple local minima or a shape that significantly increases the convergence time of most minimization algorithms. In this case, the minimization may fail to find the global minimum. However, this should be attributed to a limitation of the minimization algorithm rather than to a limitation of the method formulation. This issue is also present in the estimation of state variables because of the nonlinear dynamics of geophysical systems such as the ocean and the atmosphere.

Another issue that appears in the simultaneous estimation of the state and parameters using variational data assimilation and that is common to other methods such as the EnKF is that the uncertainty in the value of the parameters is not known a priori and it is needed to define the background error covariance matrix of the augmented state.

2.4   Parameter estimation based on Kalman filter schemes

Another kind of data assimilation scheme is based on the Kalman filter (Kalman 1960) equations, which provides a way to explicitly compute the evolution of the state error covariances. The Kalman filter estimates the optimum state of a system using a prior estimate of the system state (typically a very short-range forecast) and a set of observations. The errors in the prior estimate of the system state are assumed to be Gaussian and the solution is obtained by seeking for the minimum variance in the analysis error. The original Kalman filter equations are optimum for linear models. For nonlinear models, a heuristic extension of the method known as the extended Kalman filter (EKF) can be used (Jazwinski 1970). In the EKF, the evolution of the state variable error covariances is computed using the tangent linear model. Although this method can be extended to incorporate the estimation of the parameters via the augmentation of the system state, the computational cost and memory

requirements associated with this scheme makes it only affordable for relatively small systems. Kondrashov et al. 2008 used the EKF for the simultaneous estimation of the model state and parameters in a simplified ocean-atmosphere coupled model. They performed a sequential estimation of parameters and initial conditions by a procedure similar to that in operational data assimilation systems. They reported positive feedback between the state and parameter estimations. Better parameter values reduce model errors and produce better state estimates, which in turn contribute to better parameter estimation. This work also shows that the EKF approach is adequate to accurately estimate the covariances between the state variables and some model parameters, producing an estimation of the optimal parameters that successfully reduces model errors. Carrasi and Vannitsem 2011 presented an efficient methodology to incorporate parameter estimation in a sequential EKF that does not require an extension of the adjoint model to perform the parameter estimation. The methodology was successfully tested for simple models under the perfect model assumption.

For nonlinear models with a large number of state variables, the EnKF (Evensen 1994) provides an affordable way to estimate the evolution of error covariances. In this case, an ensemble of forecasts is used to provide a prior estimate of the system state and its uncertainty (see Section 3 for further details). The error covariances among state variables are computed directly from the ensemble of forecasts. The forecast ensemble is obtained by perturbing the model initial conditions, and at the end of the data assimilation process, a new ensemble of initial conditions is obtained with the appropriate error covariances of the analyzed system state. In the case of simultaneous estimation of the model state and parameters, not only initial conditions but also model parameters are perturbed. In this way, the error covariances between model parameters and observed variables can be derived from the ensemble forecasts. The adjoint or tangent linear model is not required in this case; hence, the complexity associated with the implementation is significantly reduced. Another important advantage of EnKF-based methods is that the algorithms can be highly parallelized. As in the case of 4D-Var, some a priori knowledge of the uncertainty associated with the parameter values is needed. One of the main limitations of the Kalman filter framework is that posterior perturbations, which represent the uncertainty in the parameters, are linear combinations of the prior perturbations. Therefore, these algorithms cannot

capture nonlinear transitions in the shape of the probability distribution function (PDF) of the parameters (e.g., transition from one to multiple modes in the PDF) (Posselt and Bishop 2012).

Several studies have explored the implementation of the EnKF technique for parameter estimation (Anderson 2001, Annan et al. 2005, Hacker and Snyder 2005, Aksoy et al. 2006, Zupanski and Zupanski 2006, Orescanin et al. 2009, Koyama and Watanabe 2010, Tong and Xue 2008a, Skachko et al. 2009, Hu et al. 2010). Annan et al. 2005 and Annan and Hargreaves 2007 have proposed a parameter estimation method based on an EnKF to find the parameter values that produce the best representation of the system climatology in an intermediate complexity earth system model. The method employs an ensemble of relatively long model simulations for optimization on the climatological scale. This method only allows estimating time-independent parameters.

For a simple model, Yang and DelSole 2009 successfully estimated parameters that appear as additive terms in the model equations (additive parameters) as well as parameters that multiply the state variables in the model equations (multiplicative parameters). They showed that using the EnKF, the parameter estimation problem can be expressed as two separate estimations: one for the state variables and the other for the parameters. In particular, the implementation of parameter estimation within existing sequential data assimilation cycles based on the EnKF is straightforward.

More recently, Aksoy et al. 2006, Koyama and Watanabe 2010, Kang 2009, Tong and Xue 2008a, and Hu et al. 2010 proposed methods for parameter estimation that can be implemented in a sequential data assimilation cycle to provide both optimal initial conditions and parameter values. Koyama and Watanabe 2010 introduced an extension of the EnKF that can be applied to the parameter estimation; this extension consists of two separate ensembles: one for the parameter estimation and the other for the state estimation. Using twin experiments with Lorenz 96 and a state-of-the-art GCM, they found that the technique successfully estimates several model parameters associated with different schemes and that the optimal parameters have a positive impact on the estimation of initial conditions as well as short to medium-range forecasts. They also showed that the technique can capture the temporal variability of the optimal parameters. Kang 2009 and Kang et al. 2011 used a parameter estimation technique based on the LETKF and successfully estimated the spatial

distribution and seasonal variation of CO_2 surface fluxes.

Hu et al. 2010 applied a parameter estimation methodology based on the EnKF to a mesoscale model and successfully estimated parameters related to the planetary boundary layer scheme using real observations. The parameter estimation led to a reduction of the model bias near the surface. These results show that parameter estimation can reduce model errors even for real data cases in which there are many other sources of model errors.

As shown in these studies, inclusion of parameter estimation within a data assimilation cycle has a positive feedback loop; namely, it improves the model itself and thus reduces model errors, and it reduces the analysis errors due to improvement in the short-range forecasts. Another advantage is that the optimal parameter uncertainty is explicitly included in the ensemble forecasts.

2.5   Parameter estimation based on particle filters

PFs (Van Leeuwen 2009, Doucet et al. 2000) have also been applied to estimate model parameters (Vossepoel and Van Leeuwen 2007, Kivman 2003, Ambadan and Tang 2005). PFs consider a general PDF without the Gaussian assumption and provide a more accurate estimation when the response of the model to the estimated parameters is strongly nonlinear, overcoming one of the main limitations of 4D-Var and the EnKF methods. Kivman 2003 and Ambadan and Tang 2005 performed experiments using a simple highly nonlinear model and showed that PFs outperform the EnKF, particularly for the estimation of model parameters. Vossepoel and Van Leeuwen 2007 used PFs to estimate the spatial distribution of a mixing parameter for an ocean GCM. They successfully reconstructed the main characteristics of the spatial distribution of this parameter as well as its uncertainty. They also found that the PDF associated with this parameter is strongly nonGaussian and might produce suboptimal estimations if other data assimilation techniques such as the EnKF and 4D-Var are employed. Results obtained with PFs are promising, particularly in terms of a better representation of the optimal parameter uncertainty under strongly nonlinear regimes. So far, an accurate estimation of the model state and parameters with most PFs requires a large number of particles (i.e., model simulations). Therefore, PFs are usually too expensive to be employed for operational data assimilation and/or parameter estimation in high-dimensional systems. However, recent developments suggest that PFs can be applied to realistic geophysical problems at an affordable computational cost (Van Leeuwen 2010). Alternatively, PF methods can be used only for estimating model parameters by implementing online algorithms such as the one proposed by Jarvinen et al. 2012 and Laine et al. 2012; thus, the dimension of the problem is significantly reduced. As stated before, this is true only when the two-or three-dimensional distribution of the parameters is not considered.

2.6   Parameter estimation and model errors

The data assimilation techniques for parameter estimation have also been used for the estimation of model errors. Model errors are among the most difficult issues in geoscience applications owing to the complexity of the models and the large number of variables involved. A review of methods to include the effect of model errors within data assimilation schemes is out of the scope of this paper. Since some studies attempted to estimate model errors as if they were parameters using the state augmentation approach, in this subsection, some techniques based on parameter estimation concepts that are used for model error estimation are discussed.

Dee and Da Silva 1998 and Dee and Todling 2000 presented a two-step analysis scheme that includes the online estimation of the spatial distribution of the forecast bias. Bias correction is applied after the model run and before the data assimilation step. The error covariance matrix for the bias is assumed to be the forecast error covariance matrix multiplied by a coefficient smaller than one. Thus, the estimated bias changes slowly with time.

Baek et al. 2006 implemented three different bias estimation algorithms in a simple model. In their study, the bias was treated as a parameter and the LETKF was used to estimate it. The magnitude of the variance of the bias error was assumed to be small and constant in time. The bias was augmented to the state vector and the augmented state error covariance matrix evolved according to the square root filter equations. This augmented state error covariance matrix included the covariances between errors in the state variables and in the bias. In that work, the size of the bias state was the same as the state space. Miyoshi 2005 tried to estimate the bias for a larger numerical model and found that the scheme leads to filter divergence. In that case, a low-order representation of the bias that can significantly reduce the number of parameters being estimated can be implemented (e.g., Miyoshi 2005, Zupanski and Zupanski 2006, Danforth et al. 2007). The main disadvantage of a reduced model error space is that it

requires some a priori knowledge about the model bias.

Zupanski and Zupanski 2006 used the maximum likelihood ensemble filter for the simultaneous estimation of the model state, some model parameters, and the bias. They found that estimating the model bias and model parameters reduced the analysis error. They proposed a different formulation for the bias. The bias is represented by model errors at each model time step. In this framework, the bias is estimated through the covariances between bias errors and errors in the state variables. Variational assimilation has also been used to estimate a model bias that is spread in the assimilation window; for example, Pulido and Thuburn 2008 estimated model errors as a forcing term in the momentum equations.

Several methods have been developed to account for model errors in 4D-Var. These methods are usually referred as weak constraint 4D-Var and involve an extension of the control space to include model parameters (Navon 2009, and references therein). Tremolet 2007 presented a weak constraint 4D-Var algorithm that relies on the augmentation of the state vector to include model errors within the assimilation window. This algorithm is also computationally efficient. Moreover, the estimation of the model error covariance matrix was also discussed. It was shown that using a model error covariance matrix with the same structure as the forecast error covariance matrix is not an appropriate choice.

Estimating optimal model parameters within a data assimilation scheme or estimating the model bias cannot account for all sources of model errors. For instance, limitations in the representation of complex physical processes using parameterizations cannot be corrected by finding optimal values for model parameters. This is why parameter estimation is potentially a good complement to other schemes that consider model errors within a data assimilation cycle. Further research is needed to assess how parameter estimation methods can be optimally combined with methods designed to represent other sources of model errors within a data assimilation cycle, such as adaptive inflation (Miyoshi 2011), additive inflation (Li et al. 2009), multi-model ensembles (Krishnamurti et al. 1999, Meng and Zhang 2007), stochastic physical tendencies perturbations (Buizza et al. 1999), and stochastic kinetic energy backscatter (Shutts 2005).

Several parameter estimation schemes have been developed and successfully tested, some of which can be applied to operational data assimilation systems at a relatively low computational cost. Most techniques have been tested independently; hence, there is little information about their relative strengths and weaknesses. Most of these tests have been performed using the twin experiment approach, in which the only source of model errors is assumed to be the error associated with the estimated parameters. There are, thus, many open questions with regard to the impact of parameter estimation in the presence of other sources of model errors.

In the next section, we discuss the implementation of parameter estimation in a data assimilation cycle based on the EnKF. The potential impact of parameter estimation on the improvement of the analysis and medium-range forecast is also discussed.

3. Sequential state and parameter estimation based on the EnKF

In a sequential data assimilation cycle, the system state is updated using the available observations at certain time intervals depending on the applications. Usually, global operational data assimilation systems assimilate observations every 6 h. Smaller scale applications, i.e., mesoscale and convective scale analysis, are usually performed using shorter assimilation cycles, typically from a few minutes to 1 h.

A sequential data assimilation cycle for state and parameter estimation based on the EnKF can be summarized in the following steps:

- The data assimilation cycle is started with an ensemble of augmented states, S_i^a being the $i - th$ ensemble member at the beginning of the assimilation cycle. The augmented state s contains the state variables and parameters, i.e., $s = [x x_p]$, where x is the state variable vector (as used in standard data assimilation) and x_p is a vector containing model parameters that are being estimated. $\bar{s}^a$ is the augmented state ensemble mean. S^a is an $N \times k$ matrix representing the augmented state ensemble perturbations, where N is the size of the augmented space (the total number of state variables plus the total number of estimated parameters) and k is the ensemble size. The $i - th$ column of S^a contains the $i - th$ ensemble perturbation.

- Each ensemble member is propagated forward in time using the model. The model simulation corresponding to each ensemble member uses a different initial condition and a different set of parameters. Though the sensitivity to the perturbations in the initial conditions and in the parameters are propagated forward in time using

the nonlinear model, the Kalman filter equations assume that the error distribution is Gaussian. This is why the integration step should be short enough to guarantee that error growth from one assimilation step to the next is approximately linear. As an example, in the experiments presented later, the model integration time is 6 h. Usually, it is assumed that parameters remain constant during the model integration, i.e., a persistence model is assumed for the parameters.

- After the model integration, an ensemble of forecasts is obtained. Let s_i^f be the $i - th$ member of the forecast ensemble. $\bar{s}^f$ is the forecast ensemble mean and S^f the $N \times k$ forecast perturbation matrix. The forecast error covariance matrix can be estimated from the ensemble sample as follows:

$$P_s^f = \frac{1}{(k-1)}(S^f)(S^f)^T, \qquad (1)$$

where P_s^f is the augmented state forecast error covariance matrix. This matrix contains the covariances between the errors in different state variables and the cross-covariances between errors in the parameters and state variables. As stated before, observations of the state variables can provide information about the optimal parameters on the basis of these covariances.

- Observations can be optimally combined with the first guess in order to obtain the augmented state analysis (i.e., the optimal estimation of state variables and model parameters). The Kalman filter analysis equations (Jazwinski 1970) are used in this step:

$$\bar{s}_a = \bar{s}_f + K_g(y_o - h(\bar{s}_f)), \qquad (2)$$

where y_o is the observation vector, whose size is equal to the total number of observations to be assimilated (l), h is the observation operator, i.e., a function that maps the state space into the observation space. Usually, h can be a very complex function. K_g is an $N \times l$ matrix, usually referred as the Kalman gain matrix and is defined as follows:

$$K_g = P_s^f H^T (H P_s^f H^T + R)^{-1}, \qquad (3)$$

where H is the tangent linear model of the observation operator and R is the observation error covariance matrix. If h is linear, then $h(s_f) = H s_f$. In most applications, the parameters are not directly observed, so that $h(s_f) = h(x_f)$.

- The Kalman filter equations provide an estimate of the uncertainty of the augmented state after the assimilation of the observations:

$$P_s^a = (I - K_g H) P_s^f, \qquad (4)$$

where P_s^a is the estimated error covariance matrix for the augmented state analysis and I is the identity matrix of size $N \times N$. The new analysis perturbation matrix S^a that will be used in the next data assimilation cycle should satisfy the following relationship:

$$P_s^a = \frac{1}{(k-1)}(S^a)(S^a)^T. \qquad (5)$$

Different implementations of the EnKF may have a different way of computing the posterior perturbations. In the ensemble square root approach (Hamill and Whitaker 2002), the analysis perturbations are obtained using a square root factorization of the analysis error covariance matrix:

$$S^a = (k-1)(P_s^a)^{1/2}. \qquad (6)$$

A common issue of the ensemble-based data assimilation schemes is the lack of dispersion in the background and analysis ensembles in comparison to their actual errors. To avoid filter divergence associated with this particular issue, multiplicative inflation (Anderson and Anderson 1999) is usually applied to the state variables. If the number of ensemble members is small compared to the total number of variables in the augmented state, then sampling errors will affect the estimation of the forecast error covariance matrix. This can significantly degrade the analysis quality. Usually, to avoid this problem, the estimated covariance between two state variables is multiplied by a function of the physical distance between them. In this way, only the observations that are near a certain grid point can correct the value of the state variables at that point (Hunt et al. 2007). This procedure known as error covariance localization can be applied in several ways.

One important difference between parameter estimation and state-only estimation is that the parameters may be global, i.e., the parameter is independent of the location, and thus can be correlated with state variables at any location. Different approaches to consider localization in the parameter estimation problem can be found in the literature. Aksoy et al. 2006, Hu et al. 2010, and Fertig et al. 2009

Table 1.   True, initial and imperfect-model parameter values used in the experiments. The selected
parameters are: the inverse of the convective adjustment time scale (TRCNV), the boundary layer
relative humidity threshold for convection initiation (RHBL), and the maximum lateral entrainment
rate (ENTMAX).

Parameter	True value	Initial value	Imperfect-model value
TRCNV $[hr^{-1}]$	0.16	0.50	0.50
RHBL $[\%]$	0.90	0.80	0.80
ENTMAX $[unitless]$	0.50	0.30	0.30

applied a spatial localization scheme for global parameters in the same way as for state variables. In this approach, the global parameters are transformed to a uniform two-dimensional horizontal field prior to the assimilation step. Spatial localization is applied to estimate the parameters at each location during the assimilation step. Finally, the estimated local parameters are averaged horizontally, and the global values are used in the forecast step. Alternatively, Koyama and Watanabe 2010 estimated global parameters without applying spatial localization. They showed that spatial localization is not necessary for the estimation of global parameters. It should be pointed out that localization is necessary in the case of the estimation of local parameters (i.e., parameter values changing from one grid point to another), as in the case of bias estimation (Baek et al. 2006) or CO_2 surface fluxes (Kang 2009).

Another important issue of parameter estimation is how to represent uncertainty in the optimal parameters, which is usually a priori unknown. This issue is discussed in Ruiz et al. 2013.

Finally, the estimated parameter values for each individual ensemble member should remain within a realistic physical range. This restriction is similar to the case of some state variables, for example, specific humidity that cannot be less than 0 and not much greater than 100. Hu et al. 2010 used a transformation for the parameters that avoids this issue. In their work, a hyperbolic tangent was used to map the parameter range to the interval $[-\infty; \infty]$. A logarithmic transformation has also been used by Annan et al. 2005 for positive definite parameters. These approaches guarantee that the estimated parameters will always be within the physical meaningful limits. However, these types of transformations may introduce additional nonlinearities in the parameter estimation problem.

3.1   Experimental setting

Twin experiments were performed in this study to illustrate how parameters can be estimated using the LETKF approach. In the twin experiments, a nature run (or true evolution) was generated by running the model for a relatively long period of time, and synthetic observations were produced by introducing a random observational Gaussian error of covariance $\boldsymbol{R}$ around the nature states.

The SPEEDY model (Molteni 2003) was used in the experiments. The SPEEDY model is an atmospheric GCM with a T30 spectral resolution transformed to a Gaussian grid with 96 points in the west–east direction and 48 points in the south–north direction. It has seven vertical sigma levels and a set of simplified physical parametrizations. Although the SPEEDY model has simpler physical schemes compared to the state-of-the-art models, it has all major components of a GCM. The SPEEDY model has been used in several previous studies for testing data assimilation schemes (Miyoshi 2005, Kang 2009, Kang et al. 2011, Harlim and Hunt 2007, Fertig et al. 2009, Miyoshi 2011).

First, two nature runs were generated using the SPEEDY model with certain sets of parameters that will be referred to as true model parameters. One nature run was generated using parameters that are constant in time, and the other used temporally varying parameters. The true parameter values used in the constant parameter nature run are summarized in Table 1. These values are chosen to be the standard settings of the SPEEDY model. Both nature runs were from January 1st to May 30th of the same year.

The parameter values in the nature run with time-varying parameters are specified as follows:

$$\boldsymbol{x}_p(t) = \boldsymbol{a}\cos(\Omega t) + \boldsymbol{x}_p(0) \tag{7}$$

where $\boldsymbol{a}$ is the amplitude of the parameter oscillations, which is unique to each parameter, t is time, Ω is the frequency of parameter oscillations, which is the same for each parameter, and $x_p(o)$ is a reference parameter set, which in these experiments is equal to the set of parameters used in the constant parameter nature run (Table 1). $\Omega = \frac{2\pi}{80}\ day^{-1}$ is used in the experiments. Time-varying true parameters are introduced because in practice, the value of certain parameters can be a function of time of the year or the weather regime.

Therefore, the ability of the parameter estimation methods to capture the temporal variations needs to be assessed. This can also be an improvement of current forecasting systems in which parameters remain constant. In this case, even when the true parameters are time-varying, the parameter estimation problem assumes that the parameters remains constant within each assimilation window (i.e., the parameter remains constant during the forecast with the model).

In this study, we aim to optimize the parameters of convective parameterizations. The diabatic heating associated with convection produces strong and remote effects on atmospheric circulation. Convection itself is intermittent in space and time and is more frequent in tropical regions, introducing additional challenges to the estimation of optimal parameters. It is also associated with strong and fast instabilities (1−3 h). The convective scheme is also associated with the skill of quantitative precipitation forecast, which is one of the most unreliable variables derived from numerical weather and climate predictions.

Three parameters associated with the convective parameterizations are evaluated. The convective parameterization of the SPEEDY model is a mass flux scheme; for further details, see Molteni 2003. The selected parameters are as follows: the inverse of the convective adjustment time scale (TRCNV), the boundary layer relative humidity threshold for convection initiation (RHBL), and the maximum lateral entrainment rate (ENTMAX). There are two other tunable parameters in the convective scheme associated with the representation of shallow convection (SMF and RHIL), but early experiments showed that changes in these parameters resulted in weak sensitivity to the model state (i.e., they are not identifiable and thus they cannot be accurately estimated).

The simulated observing network has a regular spatial distribution with observations located at every other grid point and at every vertical level of the model grid, which approximately corresponds to a 7.5 degrees horizontal resolution and a vertical resolution of 150 hPa. Observations are available every 6 h, which is equal to the time between two assimilations. Independent Gaussian random errors are added to the nature states at the observed grid points. The standard deviation of the observational errors are chosen to be 1.0 ms^{-1} for wind components, 1.0 K for temperature, 1.0 gkg^{-1} for specific humidity, and 1.0 hPa for surface pressure.

Using the observations generated from the nature runs, data assimilation and parameter estimation

cycles are performed using an assimilation window of 6 h. The model used to obtain the first guess starts the cycle using the set of parameters shown in Table 1 as initial values. Apart from the values of the parameters being estimated, the model is exactly the same as the one used in the nature runs. This implies that though the model used in the data assimilation system is imperfect, the imperfection is purely due to the differences in the three parameters. The initial conditions to start the data assimilation cycles are chosen randomly from the nature runs, so that only climatological information is considered at the beginning of the cycles. The same initial ensemble is used in all the experiments.

The LETKF algorithm is used for the simultaneous estimation of the model state and parameters. The algorithm is thoroughly described by Hunt et al. 2007. The implementation is similar to that presented in Miyoshi et al. 2007. This implementation has been applied to several numerical weather prediction models, including the Japan Meteorological Agency (JMA) regional and global models (Miyoshi and Aranami 2006, Miyoshi et al. 2010), the atmospheric GCM for the Earth Simulator, (Miyoshi and Yamame 2007), and most recently, the Weather Research and Forecasting (WRF) model (Miyoshi and Kunii 2012). This algorithm has also been employed for the estimation of model parameters by Kang 2009 and Ruiz et al. 2013. The additional computational cost associated with the estimation of global parameters is $O(k^2 l)$, because the analysis update is computed in the subspace spanned by the ensemble members.

In the experiments presented in this paper, a time-independent multiplicative inflation factor is applied to all state variables. Only global parameters are estimated so that no spatial localization is used. Namely, a Kalman gain is computed for the parameters using the nonlocalized forecast error covariance matrix. This Kalman gain is used only to update the values of the parameters and not to update the state variables.

3.2 Model sensitivity to the parameters

The sensitivity of the model to the parameters is examined following Crook 1996 and Tong and Xue 2008b. The sensitivity is explored individually for each parameter with the other parameters fixed at their true values. The model is integrated for 6 h using 40 different parameter values within their meaningful physical range ($p^{(1)}, \cdots, p^{(j)}, \cdots, p^{(40)}$). The same initial condition is used for all the model simulations. Then, a cost function similar to the one used by Tong and Xue
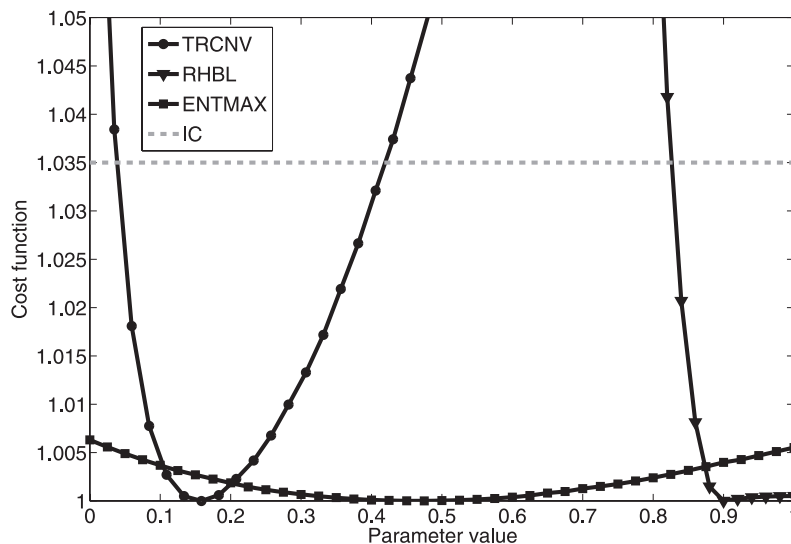
Fig. 1.   Time-averaged normalized cost function for the three parameters associated with the convective scheme in the SPEEDY model as a function of the parameter value: TRCNV (circles), ENTMAX (squares), and RHBL (triangles). Time-averaged sensitivity to initial condition perturbations is also included for reference (grey dashed line).

2008b is defined:

$$J(p^{(j)}) = (y^o - y^{(j)})^T R^{-1}(y^o - y^{(j)}) \qquad (8)$$

where $J(p^{(j)})$ is the cost function at a given time for the $p^{(j)}$ parameter value. The vector $y^{(j)}$ is the forecast in the observational space, i.e., $y^{(j)} = H(x^{(j)})$, where $x^{(j)}$ is the model state obtained using that parameter value.

The relative cost function (J_r) is defined as the cost function for each parameter value divided by the cost function for the optimal parameters. The initial condition that we use is the analysis ensemble mean from a data assimilation cycle performed with the true parameters. Because of the errors in the initial conditions and observations, the cost function associated with the true parameters is not equal to 0. Using J_r, the relative magnitude of the errors associated with model parameters can be compared to the errors associated with the uncertainty in the initial conditions and observations.

Figure 1 shows the time-mean relative cost function as a function of the parameter values. The time average is performed over 15 days (60 forecasts). The parameters that are highly sensitive are RHBL and TRCNV, while ENTMAX shows much weaker sensitivity (on the order of 1 % of the total forecast error). RHBL and TRCNV show a nonlinear response (most evident for RHBL), while ENTMAX shows a quadratic cost function; therefore, the model response to the parameter is linear.

The sensitivity is not the same for all variables and locations. The strongest sensitivity for wind speed is found at upper and lower levels (with a relative minimum at mid levels) and in the latitudinal range 40 S to 40 N. The temperature shows strongest sensitivity at mid levels but is confined within the range 20 S to 20 N. The specific humidity shows stronger sensitivity at low levels as expected and the surface pressure also shows strong sensitivity to the parameters within the same latitude range. This variable dependence and spatial distribution of the stronger sensitivity is consistent with the response of the atmospheric circulation to changes in the intensity or frequency of the convective activity, which is more frequent in the tropics. The spatial and vertical distribution of the model sensitivity to the parameters is important to design an error covariance matrix localization for the parameter. In this case, for instance, observations from higher latitudes seem to have a weak covariance with the parameters. This means that observations at those latitudes do not have a significant amount of information about the optimal value of the parameter, and hence they can be neglected. This can also be used to design a variable localization approach as in Kang et al. 2011.

The time-mean sensitivity to the initial condition perturbations is also shown in Fig. 1. This sensitivity is measured as the relative cost function of one of the ensemble runs with perturbed initial conditions and
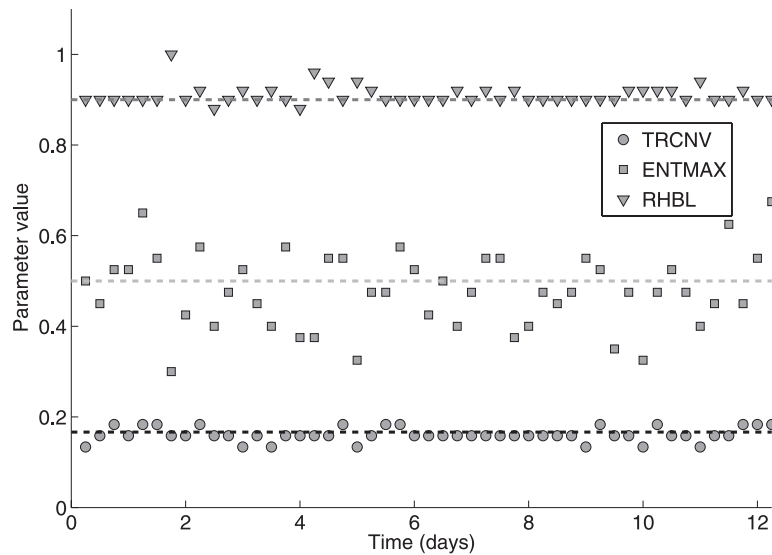
Fig. 2.   Parameter value that produces the minimum cost function as a function of time for the three parameters: TRCNV (circles), ENTMAX (squares), and RHBL (triangles). The true value of the parameters is also indicated: TRCNV (black dashed line), ENTMAX (light grey dashed line), and RHBL (dark grey dashed line).

true parameters and is computed in the same way as the sensitivity to the parameters. As the sensitivity is examined globally, the relative cost function for some parameter values exceeds that associated with the initial conditions perturbations. This is the case for the TRCNV and RHBL but not for ENTMAX.

The optimal parameters, i.e., those that give the minimum of the cost function, are close to the true parameter values. Figure 2 shows the value of the parameters corresponding to the minimum of the cost function at each time instant and for each parameter as a function of time. Errors in the initial conditions and observations produce significant deviations from the true parameter values. The uncertainty in the determination of the optimal parameters is, as expected, larger for ENTMAX, which shows weaker sensitivity. RHBL also shows a behavior consistent with the shape of its cost function. The error in the position of the minimum is usually found at higher values with respect to the true parameter, because for higher values, the model shows weaker sensitivity to this parameter. In some cases, the cost function computed for a particular time instant exhibits multiple local minima (in this case only, the global minimum has been considered for the plot shown in Fig. 2). These multiple local minima may arise from nonlinearities in the model response to changes in the parameter.

3.3   Estimation of parameters with LETKF

In this section, some experiments of parameter estimation using the LETKF method are described.

Figure 3a shows the estimated parameter evolution for temporally fixed true parameters. The parameter ensemble spread evolves with time owing to the implementation of the online estimation of the parameter ensemble spread (See Ruiz et al. 2013 for further discussion on this issue). The estimated parameter values converge to the true parameter values in less than 20 days; after that, the estimated parameters oscillate around the true value. This oscillation is mostly associated with the uncertainty originating from errors in the state and in observations as well as sampling errors in the computation of the covariances between the observed variables and parameters.

Figure 3b shows the estimated parameter evolution for time-varying parameters. The method can adequately capture the evolution of the parameters. However, even when the frequency of the parameter oscillation is low, there is a temporal lag between the estimated parameters and their true evolution. When the frequency of the true parameter increases, the temporal lag usually grows. For a time frequency that is six times larger than the one presented in this experiment, filter divergence occurs for the parameters. These issues are partly because persistence is assumed for the parameter evolution during the
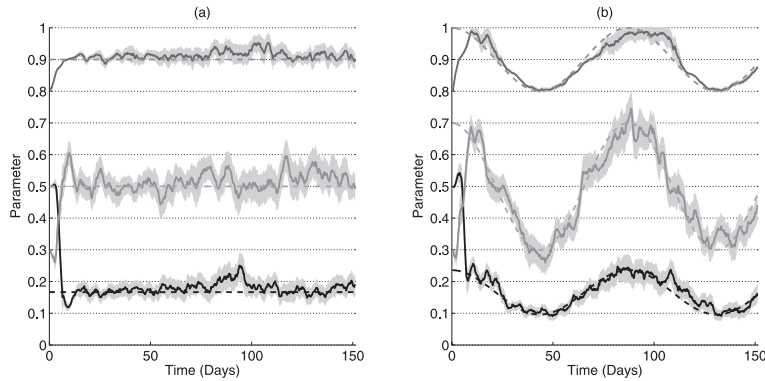
Fig. 3. (a) Time evolution for the constant true parameter experiment of the three estimated parameters: TRCNV (black solid line), ENTMAX (light grey solid line), and RHBL (dark grey solid line). The shade around the estimated parameters indicates the ensemble spread (one parameter ensemble perturbation spread). The true parameter values evolution are also indicated: TRCNV (black dashed line), ENTMAX (light grey dashed line), and RHBL (dark grey dashed line). (b) Time evolution of the estimated parameters for the time-dependent true parameter experiment.

forecast step. If the true parameter changes rapidly with time, the corresponding forecast model for the parameter needs to be considered. The problem is that, in general, the dynamics of the parameter evolution are ignored simply because they are unknown most of the time.

The effect of parameter estimation on the error in the state variables is also analyzed. The analysis error for the state variables is computed using an RMSE normalized by the typical error magnitude of each variable:

$$RMSE = \sqrt{\frac{1}{N}(\overline{x}^a - \overline{x}^t)^T A^{-1}(\overline{x}^a - \overline{x}^t)}. \tag{9}$$

where A is a diagonal matrix of size $N \times N$ that contains the typical error magnitudes of each state variable. The typical error magnitudes are chosen to be equal to the observational errors of each variable. This definition considers the relative order of the magnitude of the different variables involved. Only the model state variables are considered for the computation of the analysis RMSE.

A perfect model experiment, i.e., a data assimilation cycle using the true parameter values, and an imperfect model experiment were also performed. For the constant parameter case, the imperfect model experiment consists of a data assimilation cycle using the model with an incorrect set of parameters, as shown in Table 1. In the case of the time-varying parameters, the imperfect model consists of a data assimilation cycle that uses the time average of the true time-varying parameters. In this case, the imperfect model does not

consider the time variability of the true parameters; however, the selected value for the parameters is one of the most reasonable choices that can be implemented.

In Figure 4a, the analysis error in the imperfect model experiment is significantly larger than in the perfect model experiment after the spin up of the filter. In the parameter estimation experiment, the analysis error is almost as low as in the perfect model case. This indicates that parameter estimation can find the optimal values for the parameters and effectively removes model errors associated with the uncertain parameters. The fluctuations observed in the estimated parameters do not significantly affect the quality of the analysis.

Figure 4b shows the time evolution of the analysis RMSE in the experiment with time-dependent parameters. In this case, the analysis error in the imperfect model experiment shows time fluctuations that coincide with the frequency of the oscillation of the true parameters. These oscillations are not present in the parameter estimation experiment because the temporal dependence of the parameters is adequately captured by the method. This shows that even if a reasonable value for the parameters is used (i.e., the time average of the true parameter), the analysis error can be relatively large. However, the impact of including the temporal dependence of the parameters will depend on the amplitude of the oscillations of the optimal parameters and the model sensitivity to the parameters. In these experiments, the temporal lag between the estimated parameters and the true
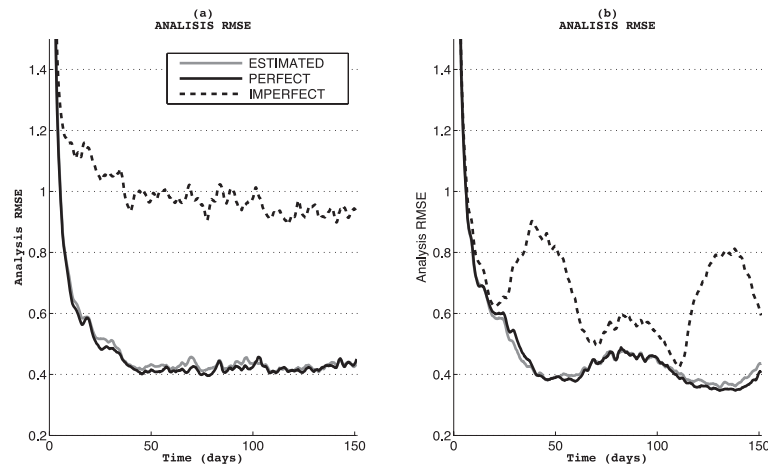
Fig. 4.   Total analysis RMSE as a function of time for the perfect model experiment (black solid line), imperfect model experiment (black dashed line), and parameter estimation experiment (grey solid line). (a) For the constant true parameters case and (b) for the time dependent true parameters case.

parameters does not seem to significantly degrade the analysis. This may be because the temporal frequency of the true parameters is relatively low compared to the typical frequency associated with changes in the state variables and also low compared to the observing frequency.

These simple experiments illustrate some results that have been previously discussed in the literature and highlight the importance of parameter estimation as a method to estimate and partially correct model errors. It should be noted that these experiments are over optimistic in the sense that uncertainty in the optimal value of the estimated parameters is the only source of model errors.

3.4   Parameter estimation impact on ensemble forecast skill

In this section, the effect of parameter estimation on forecast skill is quantified following the framework of the simple twin experiments presented so far. Several experiments were performed using the SPEEDY model to generate 15-day ensemble forecasts with 20 members. The forecast experiments started on February 1st and ended on March 31th of the same year. Temporally fixed true parameters were used in these experiments. Here, four different experiments using different initial conditions and parameters will be presented:

- Perfect model (PM): Perfect parameter values are used for the forecasts. The initial conditions are obtained from the data assimilation experiment that uses the perfect parameter values.

- Imperfect model (IM): The imperfect parameter values shown in Table 1 are used for the forecasts. The initial conditions are obtained from the data assimilation experiment that uses the imperfect parameter values without parameter estimation.

- Imperfect initial conditions with perfect model in the forecasts (IICPM): The analyses resulting from imperfect parameter values (same as IM) are used as the initial conditions. The forecasts are produced with the perfect model.

- Estimated parameter (EP): The initial conditions are obtained with a data assimilation experiment that includes an augmented state so that both the state and parameters are estimated. Each forecast ensemble member uses parameter values taken from the corresponding estimated parameter ensemble. In this way, the ensemble represents the uncertainty in the initial conditions as well as the uncertainty in the optimal value for the parameters.

The time-mean RMSE is used as a measure of the forecast skill. The evolution of the RMSE as a function of forecast lead time for the different experiments is shown in Fig. 5a. As expected, the best results are achieved by the PM experiment and the worst results
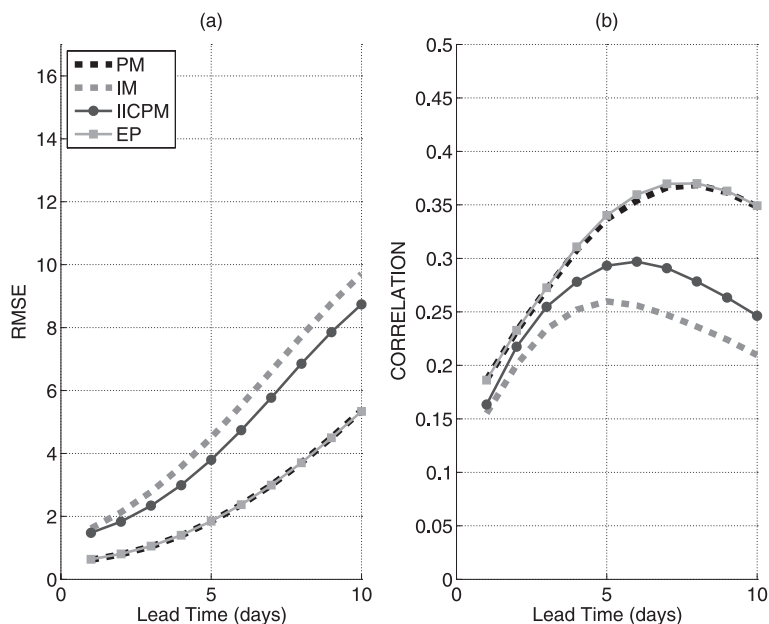
Fig. 5. (a) Globally and temporally averaged ensemble mean RMSE as a function of the forecast lead time for the perfect model (black dashed line), imperfect model (grey dashed line), imperfect initial conditions with perfect model (dark grey solid line with circles), and estimated parameter (light grey solid line with squares) experiments (see the text for details). (b) As in (a) but for the globally and temporally averaged correlation between the ensemble mean error and ensemble spread.

by the IM experiment. The reduction in the error growth rate at the end of the 15-day period in the IM experiment suggests nonlinear saturation of errors. The EP experiment shows excellent results with RMSE values very close to those for the PM experiment, indicating an effective reduction of model errors associated with the optimization of the parameters values. The differences between IICPM and IM are smaller than those between PM and IICPM, suggesting that the parameter errors in the forecast model are less important in this case. Instead, model imperfections introduce errors in the initial conditions, and the impact of the initial condition errors is more important than the impact of model errors during the forecast. The impact of model errors on initial conditions depends on the kind and number of observations available; therefore, this particular result might be sensitive to the number and distribution of the available observations.

Another important aspect of ensemble forecasting, which is strongly related to model errors, is the relationship between the ensemble spread and forecast error. Ideally, for a perfect ensemble system, there should be a relationship between the ensemble spread and ensemble mean error (Kalnay 2003). If the

ensemble spread is large, the ensemble mean is expected to be far from the true state. When perturbations in the initial conditions are used to generate the ensemble, only the initial condition uncertainty is considered. However, as model error is also present, the growth of the perturbations during the forecasts may fail to capture the magnitude of the forecast error. In other words, model errors reduce the ability of an initial condition ensemble to estimate forecast uncertainty.

The relationship between day-to-day changes in the ensemble mean error and ensemble spread is not strictly linear or even deterministic because a larger spread means that the probability of having a large error is larger but not that the error will actually be large. However, the linear correlation coefficient has been extensively used to measure the strength of this relationship. In this work, the linear correlation coefficient between the ensemble mean error and ensemble spread was used to measure the impact of including parameter estimation in the data assimilation cycle. Linear correlations between the time series of spread and error were computed at each grid point for the entire forecast period and then averaged over the globe and over the different model variables. Figure
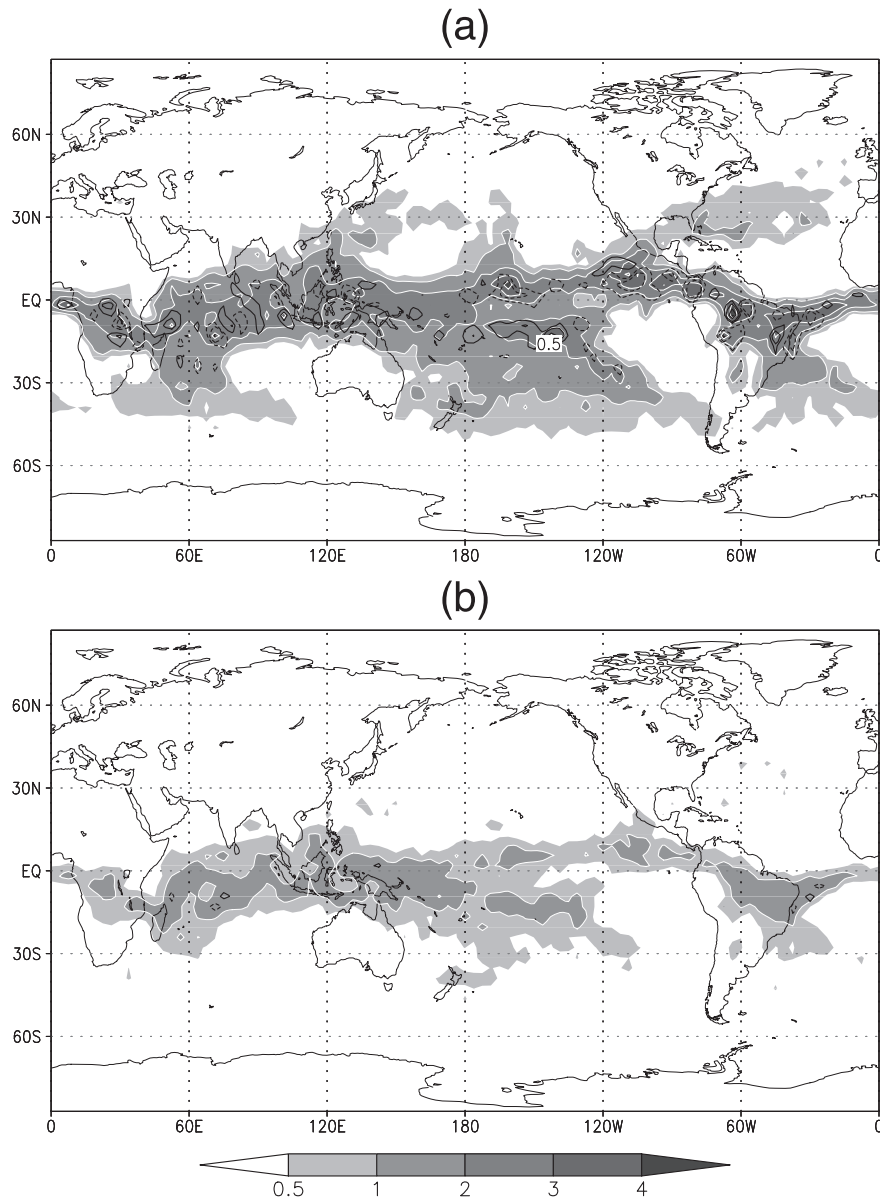
(a)

(b)

Fig. 6.   24 h forecast of accumulated precipitation, RMSE (shaded) and bias (contours) (*mm6hr*$^{-1}$). Bias contours are -3, -2, -1, -0.5, 0.5, 1, 2, and 3. Positive values are shown with solid lines and negative values with dashed lines. (a) Imperfect model experiment and (b) Estimated parameters experiment.

5b shows the linear coefficient between the ensemble mean error and spread as a function of the forecast lead time. The strongest relationship is achieved between 6 and 10 days, which is in close agreement to the results obtained by Grimit and Mass 2007. The PM and EP experiments show the strongest correlation coefficient as expected, indicating a good relationship between the ensemble spread and forecast uncertainty. It is worth

mentioning that the inclusion of parameter perturbations among the ensemble members in the EP experiments does not produce significantly better results than when the parameter ensemble mean is used in all the members (not shown). This suggests that considering optimal parameter uncertainty in the ensemble forecast does not produce an improvement of the error-spread relationship in this particular case.

This might be because only three parameters associated with the convective scheme are being perturbed.

Figure 5b also shows that the error-spread relationship in the IM case is significantly weaker than in the case of estimated parameters, indicating that model errors have an important impact on the error-spread relationship. The major part of this degradation comes from errors in the forecasts initial conditions.

It is also interesting to show how the precipitation forecast is affected by the estimation of the parameters, given that the estimated parameters are from the convective parameterization in the model. Figure 6 shows the RMSE and bias of the 24 h forecast of the total precipitation. The total precipitation is obtained as the sum of precipitation produced by the convective scheme and also from the parameterization of large-scale condensation. In this figure, parameter estimation has a positive impact on the short-range precipitation forecast. The bias in the precipitation forecast produced by the imperfect parameter values is almost completely removed and the RMSE of the precipitation forecast is also reduced. The RMSE values obtained in the parameter estimation experiment are close to the ones obtained in the perfect model experiment (not shown). Note that RMSE is usually not a good measure for assessing the forecasted precipitation skill. Other measures of skill were evaluated in the experiments, including scores for the probabilistic quantitative precipitation forecast, and in all cases, we obtained the same conclusions.

4. Conclusions

Various methods for parameter estimation have been reviewed, with particular focus on the ones based on data assimilation. Data assimilation methods are promising since they provide an efficient and objective way to constrain the values of different model parameters on the basis of the available observations. Parameter estimation can be implemented using many kinds of data assimilation methods that include the time evolution of the forecast error covariance matrix, e.g., 4D-Var schemes and Kalman filter- and particle filter-based methods. Parameter estimation can be more easily implemented in ensemble-based methods since they do not need an adjoint model. Some of the methods for parameter estimation can be implemented at very low additional computational cost, making them appealing for their operational implementation.

Experiments using a method for parameter estimation based on the LETKF in a simple GCM were presented. Three parameters associated with the convective scheme of the GCM were estimated simultaneously with the state variables. Although the response of the model to perturbations in these parameters showed some nonlinearities, the LETKF could estimate the true value of the parameters in the absence of other model error sources. More experiments should be performed to investigate the performance of Kalman filter-based methods under stronger nonlinear responses to changes in the parameters and also their relative skill compared with other methods such as particle filter-based methods that are designed to account for nonlinearities.

One important issue regarding parameter estimation using ensemble-based data assimilation is how to represent the uncertainty in the optimal parameters, which is not known a priori. In this paper, the uncertainty in the optimal parameters, was assumed to be constant in time. This particular issue is further discussed in Ruiz et al. 2013, in which a new approach is proposed for the estimation of optimal parameter uncertainty.

The experiments presented in this work as well as several experiments discussed in the literature show the potential of the parameter estimation techniques to obtain the temporal and spatial distribution of the optimal model parameters. This is particularly important in the context of short-to medium-range weather forecasting because it would allow for a flexible and computationally efficient model optimization (Wu et al. 2012).

The experiments show that estimating parameters in a data assimilation system has the potential to improve the short-to medium-range forecasts. The greatest improvement is found in association with the improvement of the initial conditions. The results show that a small improvement is associated with the reduction of model errors during the forecasts. Parameter estimation efficiently reduces model errors associated the value of the convective parameterization parameters, leading to an improvement of the spread-error relationship. In the experiments, the inclusion of parameter perturbations in the forecast ensemble does not lead to a significant improvement of the forecast, i.e., neither a reduction of RMSE nor an increase in the error-spread correlation. This could be because model errors are only associated with the optimal values of the convective scheme parameters in this case and the parameter estimation process successfully removes them by an accurate estimation of these values. Thus, the incidence of including this source of uncertainty in the forecast is small.

Parameter estimation also has the potential to

improve model climatology. This can be of great importance for climate and climate change studies. Model parameters can be trained during relatively short periods (i.e., a couple of years) using a data assimilation cycle, and then the estimated parameters can be used for climate simulations.

Although parameter estimation techniques are very promising, there are still some issues that need more attention before this method can be used operationally for tuning complex numerical models. One of the main problems would be the effect on the estimated parameters of other sources of model errors not directly related with the parameters being estimated. In the experiments presented in this work, the model imperfections were directly related to the value of the convective scheme parameters. In real world applications, the sources of model errors are diverse, such as different parameterizations and limited resolution. The presence of other sources of model errors can contaminate the estimated parameters because other sources of errors can project onto directions defined by the model sensitivity to the parameters. This is one of the main issues that need to be further explored as well as the impact of errors related to the formulation of the observation operator (Youngsun et al. 2010). In the presence of model errors, the optimum parameters from the viewpoint of global model errors can be different from those parameters that produce an optimal representation of a particular subgrid scale phenomenon (e.g., convection or boundary layer turbulence). This can lead to suboptimal or even nonphysical representation of subgrid scale phenomena. In this sense, parameter estimation based on data assimilation is a very efficient tool that has an enormous potential but has to be used with caution in order to avoid getting the right answer based on the wrong reasons. Moreover, the knowledge of tuning experts and model developers will still be crucial for the success of the parameter estimation in order to determine the key parameters to be estimated, identify the appropriate bounds for these parameters, and verify that the result is physically meaningful and it is not just an attempt of the method to correct other sources of errors that are not related to the parameters.

Acknowledgements

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