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# Simultaneous estimation of covariance inflation and observation errors within an ensemble Kalman filter

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**ABSTRACT:** Covariance inflation plays an important role within the ensemble Kalman filter (EnKF) in preventing filter divergence and handling model errors. However the inflation factor needs to be tuned and tuning a parameter in the EnKF is expensive. Previous studies have adaptively estimated the inflation factor from the innovation statistics. Although the results were satisfactory, this inflation factor estimation method relies on the accuracy of the specification of observation error statistics, which in practice is not perfectly known. In this study we propose to estimate the inflation factor and observational errors simultaneously within the EnKF. Our method is first investigated with a low-order model, the Lorenz-96 model. The results show that the simultaneous approach works very well in the perfect model scenario and in the presence of random model errors or a small systematic model bias. For an imperfect model with large model bias, our algorithm may require the application of an additional method to remove the bias. We then apply our approach to a more realistic high-dimension model, assimilating observations that have errors of different size and units. The SPEEDY model experiments show that the estimation of multiple observation error parameters is successful in retrieving the true error variance for different types of instruments separately. Copyright © 2009 Royal Meteorological Society

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## 1. Introduction

Data assimilation algorithms seek to find the optimal combination of model forecast ('background') and available observations to generate improved initial conditions ('analysis') for numerical weather predictions. Most assimilation schemes are based on linear estimation theory in which the background and the observations are given weights proportional to the inverse of their specified error covariances. As such, the accuracy of a data assimilation scheme relies highly on the accuracy of the specification of the error statistics of both the background and the observations. The observation error covariance is usually assumed to be diagonal and time invariant but the error variance can be incorrectly specified. The background error covariance is actually flow-dependent. Ensemble-based Kalman filter (EnKF) techniques estimate the background error covariance from an ensemble of forecasts allowing the inclusion of information on the flow-dependent errors of the day that change both in space and in time.

In the past ten years, EnKF methods have become more mature. These methods have been implemented in various models, from simple research models (e.g. Whitaker and Hamill, 2002) to sophisticated operational models (e.g. Houtekamer *et al.*, 2005), and from global-scale (e.g. Whitaker *et al.*, 2008; Szunyogh *et al.*, 2008) to regional-scale models (e.g. Snyder and Zhang, 2003; Zhang *et al.*, 2006; Torn *et al.*, 2006), due to their ease of implementation and the flow-dependent background error covariance. In practice, the flow-dependent background error covariance estimated from the ensemble perturbations in EnKF usually underestimates the true forecast error, partly due to the limited number of ensemble members and also due to the presence of significant model errors, making the filter eventually diverge. Multiplicative and additive covariance inflation schemes (Anderson and Anderson, 1999; Corazza *et al.*, 2002) are the easiest and prevailing techniques to deal with the covariance underestimation. However these inflation algorithms require considerable tuning in order to obtain good performance of the filter. Tuning the inflation parameter in EnKF is expensive, since it requires many forecast–analysis cycles, especially if the inflation factor is regionally and/or variable dependent. Wang and Bishop (2003) adopted the maximum likelihood parameter estimation theory of Dee (1995) to estimate online an inflation factor $\Delta$ from the innovation statistics

$$\mathbf{d}^{\mathrm{T}}\mathbf{d} = \mathrm{trace}(\Delta \mathbf{H}\mathbf{P}^{\mathrm{b}}\mathbf{H}^{\mathrm{T}} + \mathbf{R})$$

in their ensemble forecast scheme. (Symbols are defined below.) Miyoshi (2005) reported the use of a similar

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method to estimate the covariance inflation factor within the EnKF. Although both studies reported satisfactory results, these estimations of the inflation factor rely on the assumption that the observational error covariance, **R**, is known. This assumption is valid for simulated observations but not for real observations. Miyoshi and Yamane (2007) reported that the adaptive covariance inflation did not work when assimilating real data and using the observational error standard deviations as specified in the Japan Meteorological Agency operational system.

Additional information may be needed to obtain the correct statistics of observation error if we want to apply the inflation estimation scheme described above when assimilating real observations. Desroziers and Ivanov (2001) proposed an approach based on a consistency check of analysis to adaptively estimate either observation or both observation and background error statistics, assuming that the correlation lengths are very different for observation and background errors. Chapnik *et al.* (2006) applied this approach in an operational system to tune observation error variance. Building on these works, Desroziers *et al.* (2005, hereafter denoted DEA05) developed a set of diagnostics based on the combinations of *observation-minus-analysis, observation-minus-background* and *analysis-minus-background* to adaptively tune observation and background errors. All these studies have been done in a variational framework. Here we investigate whether these diagnostics can be adapted in an EnKF framework to tune the mis-specified observation error variance and simultaneously implement the adaptive estimation of inflation. All observation errors in this study are uncorrelated, normally distributed random noise while the background errors have correlations in physical space. Although observation errors can also be spatially correlated (section 7 in DEA05), this case is beyond the scope of this paper.

As will be discussed later, adaptive estimation of inflation requires accurate observation error statistics and, conversely, an accurate estimate of observation error relies on the use of an optimal inflation factor in an EnKF. In this study, we propose to estimate the inflation factor and observation errors simultaneously within the analysis cycle, for which we use the Local Ensemble Transform Kalman Filter (LETKF; Hunt *et al.*, 2007) as one efficient representative among many EnKF schemes. We will use the diagnostics of DEA05 to estimate the observation errors, and the Wang and Bishop (2003) method (or other diagnostics of DEA05) to estimate the inflation factor. We compute estimates of observation errors and inflation factor at every analysis cycle but allow the system to slowly evolve until it converges to the optimal value for observation error variance (or the optimal range for the inflation factor).

This paper is organized as follows. Section 2 describes the algorithms to adaptively estimate inflation and observation error variance separately and propose the simultaneous approach. Section 3 reviews the local ensemble transform Kalman filter. Our simultaneous approach is implemented on a low-order model in section 4 and a global atmospheric general circulation model in section 5. Conclusions are provided in section 6.

## 2. Simultaneous estimation of covariance inflation and observation errors

### 2.1. Adaptive estimation of covariance inflation

For a system with correctly specified covariance of background errors $\mathbf{P}^b$ and observational errors $\mathbf{R}$, where these errors are assumed to be uncorrelated, the well-known relationship

$$< \mathbf{d}_{o-b}\mathbf{d}_{o-b}{}^{T} >= \mathbf{HP}^b\mathbf{H}^T + \mathbf{R} \tag{1}$$

is satisfied (e.g. Houtekamer *et al.*, 2005). Here the innovation vector $\mathbf{d}_{o-b}$ is the difference between observations $\mathbf{y}^o$ and their corresponding background $h(\mathbf{x}^b)$, where $h$ is the nonlinear observation operator projecting the background $\mathbf{x}^b$ to the observation space and $\mathbf{H}$ is the linear tangent matrix of the $h$ operator. The $< >$ brackets represent an average over many cases or statistical expectation. The classical innovation statistics shown in Equation (1) provides a global check on the specification of $\mathbf{P}^b$ and $\mathbf{R}$.

Another diagnostic on background errors can be obtained by the combination of innovation $\mathbf{d}_{o-b}$ and *analysis-minus-background* $\mathbf{d}_{a-b}$. DEA05 proved that the relationship

$$< \mathbf{d}_{a-b}(\mathbf{d}_{o-b})^T >= \mathbf{HP}^b\mathbf{H}^T \tag{2}$$

is valid when the analysis is optimal and pointed out that (2) can be used to check the optimality of an assimilation scheme and provides a separate consistency diagnostic on the background error covariance in observation space.

In the ensemble filter, $\mathbf{P}^b$ is updated from the background ensemble every analysis cycle as

$$\mathbf{P}^b = \frac{1}{K-1}\sum_{k=1}^{K}(\mathbf{x}_k^b - \overline{\mathbf{x}}^b)(\mathbf{x}_k^b - \overline{\mathbf{x}}^b)^T,$$

where $k$ indexes the ensemble member, $K$ is the ensemble size, and the overbar is the ensemble mean. However, this background error covariance tends to underestimate the true background error covariance, partly due to sampling errors associated with the use of a small ensemble size, as well as due to the presence of model errors, and as a result the filter gives too much credence to the background. This can compound the underestimation in the next cycle, and as a result may lead to filter divergence. Multiplicative covariance inflation (Anderson and Anderson, 1999) is a simple and widely used method to address this problem by 'inflating' the prior ensemble: the background error covariance is increased by a factor greater than one.

$$\mathbf{P}^b \longleftarrow \Delta \times \mathbf{P}^b. \tag{3}$$

Here $\Delta$ is referred to as a covariance inflation factor that needs to be tuned in order to obtain a good performance of the ensemble filter. However, tuning



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the inflation parameter is expensive and, furthermore, there is no reason why the inflation should be assumed to be constant in space or time. Wang and Bishop (2003) proposed adapting Equation (1) to estimate the inflation factor in ensemble forecasting. Substituting the background error covariance in (3) into Equation (1) and considering only the diagonal term, they estimated the inflation factor $\Delta$ online by

$$\tilde{\Delta} = \frac{\mathbf{d}_{\mathrm{o-b}}^{\mathrm{T}}\mathbf{d}_{\mathrm{o-b}} - \mathrm{Tr}(\mathbf{R})}{\mathrm{Tr}(\mathbf{HP}^{\mathrm{b}}\mathbf{H})}, \quad (4)$$

where Tr denotes the trace of a matrix.

Similarly, from Equations (2) and (3), we obtain another equation to estimate the inflation factor:

$$\tilde{\Delta} = \frac{\mathbf{d}_{\mathrm{a-b}}^{\mathrm{T}}\mathbf{d}_{\mathrm{o-b}}}{\mathrm{Tr}(\mathbf{HP}^{\mathrm{b}}\mathbf{H})}. \quad (5)$$

We denote Equations (4) and (5) as $OMB^2$ and $AMB \times OMB$ estimation methods, respectively. An accurate estimate of $\Delta$ from these two methods requires a correct observation error covariance $\mathbf{R}$. This is obvious for Equation (4) but is also implicitly true for (5), since $\mathbf{d}_{\mathrm{a-b}}$ itself is based on the use of the (generally incorrectly) specified $\mathbf{R}$. In order to estimate online the inflation factor using either the $OMB^2$ or $AMB \times OMB$ method, an additional method is necessary to estimate $\mathbf{R}$ if it is not known accurately.

### 2.2. Adaptive estimation of observation errors

DEA05 showed that the relationship

$$< \mathbf{d}_{\mathrm{o-a}}\mathbf{d}_{\mathrm{o-b}}^{\mathrm{T}} >= \mathbf{R} \quad (6)$$

is valid if the matrices specified in

$$\mathbf{HK} = \mathbf{HP}^{\mathrm{b}}\mathbf{H}^{\mathrm{T}}(\mathbf{HP}^{\mathrm{b}}\mathbf{H}^{\mathrm{T}} + \mathbf{R})^{-1}$$

are the true covariances for background and observation error. Here $\mathbf{K}$ is the Kalman gain, and $\mathbf{d}_{\mathrm{o-a}}(\mathbf{d}_{\mathrm{o-b}})$ are the difference between the observation and analysis (background) in observation space. This is a diagnostic providing a consistency check on observation error covariance, but it also depends implicitly on the background error covariance. One application of this relationship is to diagnose observation error variance offline (after the analysis cycle has been completed) or to estimate it online (within the cycle). For any subset of observations $i$ with $p_i$ observations, it is possible to compute an estimate of the error variance

$$\begin{aligned} (\tilde{\sigma}_{\mathrm{o}}^2)_i &= \frac{(\mathbf{d}_{\mathrm{o-a}})^{\mathrm{T}}{}_i(\mathbf{d}_{\mathrm{o-b}})_i}{p_i} \\ &= \sum_{j=1}^{p_i} \frac{(y_j^{\mathrm{o}} - y_j^{\mathrm{a}})(y_j^{\mathrm{o}} - y_j^{\mathrm{b}})}{p_i}, \end{aligned} \quad (7)$$

where $y_j^{\mathrm{o}}$ is the value of observation $j$ and $y_j^{\mathrm{a}}$, $y_j^{\mathrm{b}}$ are their analysis and background counterparts.

We denote Equation (7) as the $OMA \times OMB$ method. The accuracy of this method relies on $\mathbf{d}_{\mathrm{o-a}}$ and $\mathbf{d}_{\mathrm{o-b}}$ which in turn depend on the observation and background error covariances, and therefore on the inflation factor in EnKF.

### 2.3. Simultaneous approach

As indicated above, adaptive estimation of inflation requires knowing the observation error variance $\sigma_{\mathrm{o}}^2$, while an accurate estimate of $\sigma_{\mathrm{o}}^2$ relies on using an optimal inflation factor. When neither the optimal inflation factor nor the true $\sigma_{\mathrm{o}}^2$ are known, and both of them need to be estimated, this becomes a nonlinear problem. In this study, we propose to estimate the inflation and observation error variance simultaneously within the EnKF at each analysis step and allow the system itself to gradually converge to a consistent value (or range of values) for the observation error variance and the inflation factor consistent with (1), (2) and (6).

### 2.4. Temporal smoothing

We estimate the observation error variance and inflation parameter adaptively at each analysis time step. However, in the numerical examples shown in section 4 with a low-order model, the number of samples available at each step is relatively small, introducing large sampling error. To reduce this problem, we use adaptive regression based on a simple scalar Kalman Filter (KF) approach usually used to postprocess model output (e.g. Kalnay, 2003, Appendix C) to accumulate past information and make observation error variance and inflation gradually converge to the optimal value while still allowing for time variations. This approach can be considered as a temporal smoother and was used by Miyoshi (2005) in estimating the inflation. We regard the estimated values directly obtained from Equation (7) or (4) or (5) as an 'observed' estimate $\alpha^{\mathrm{o}}$ (of either $\tilde{\Delta}^{\mathrm{o}}$ or $\tilde{\sigma}_{\mathrm{o}}^2$) for the current time step. Instead of directly using it as the final estimate for that time step, we use the simple scalar KF approach to optimally combine $\alpha^{\mathrm{o}}$ and $\alpha^{\mathrm{f}}$, the value derived by persistence from the previous time step, to get a new estimate denoted as the analysis $\alpha^{\mathrm{a}}$:

$$\alpha^{\mathrm{a}} = \frac{v^{\mathrm{o}}\alpha^{\mathrm{f}} + v^{\mathrm{f}}\alpha^{\mathrm{o}}}{v^{\mathrm{o}} + v^{\mathrm{f}}}, \quad (8)$$

where $v^{\mathrm{f}}(v^{\mathrm{o}})$ denotes the forecast (observational) error variance weights for the adaptive regression. The error variance of $\alpha^{\mathrm{a}}$ is given by

$$v^{\mathrm{a}} = \left(1 - \frac{v^{\mathrm{f}}}{v^{\mathrm{f}} + v^{\mathrm{o}}}\right) v^{\mathrm{f}}. \quad (9)$$

Assuming persistence as the forecast model for the estimated variable, and allowing for some error in the 'persistence forecast' (Kalnay, 2003, Appendix C), we have

$$\begin{aligned} \alpha^{\mathrm{f}}{}_{t+1} &= \alpha^{\mathrm{a}}{}_t, & (10) \\ v^{\mathrm{f}}{}_{t+1} &= \kappa v^{\mathrm{a}}{}_t. & (11) \end{aligned}$$



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where $\kappa > 1.0$ is a 'forgetting' parameter which allows for a slow increase of the forecast error. Although two additional control parameters, the observation error variance $\nu^{\mathrm{o}}$ and error growth parameter $\kappa$ have been introduced here, Miyoshi (2005) showed the final estimate is not sensitive to their values. Following Miyoshi (2005), we use $\nu^{\mathrm{o}} = 1.0$ and $\kappa = 1.03$ in this study.

## 3. LETKF data assimilation scheme

The LETKF (Hunt *et al.*, 2007) belongs to the family of ensemble square-root filters in which the observations are assimilated to update only the ensemble mean and the ensemble perturbations are updated by transforming the background perturbations through a transform matrix. The most important difference between LETKF and other square-root filters (Tippett *et al.*, 2003) is that LETKF updates the model variables at each grid point simultaneously assimilating all observations in a predefined local region centred at that point, rather than assimilating observations sequentially.

Specifically, in the LETKF, the analysis mean is given by

$$\bar{\mathbf{x}}^{\mathrm{a}} = \bar{\mathbf{x}}^{\mathrm{b}} + \mathbf{X}^{\mathrm{b}}\tilde{\mathbf{P}}^{\mathrm{a}}(\mathbf{H}\mathbf{X}^{\mathrm{b}})^{\mathrm{T}}\mathbf{R}^{-1}[\mathbf{y}^{\mathrm{o}} - h(\bar{\mathbf{x}}^{\mathrm{b}})], \qquad (12)$$

where $\bar{\mathbf{x}}^{\mathrm{a}}$, $\bar{\mathbf{x}}^{\mathrm{b}}$ are the ensemble mean of analysis and background respectively, and $\mathbf{X}^{\mathrm{a}}$, $\mathbf{X}^{\mathrm{b}}$ the analysis and background ensemble perturbations (matrices whose columns are the difference between the ensemble members and the ensemble mean). The analysis ensemble perturbations are updated by

$$\mathbf{X}^{\mathrm{a}} = \mathbf{X}^{\mathrm{b}}[(K-1)\tilde{\mathbf{P}}^{\mathrm{a}}]^{1/2} \qquad (13)$$

using the symmetric square root, and where $\tilde{\mathbf{P}}^{\mathrm{a}}$, the analysis error covariance in ensemble space, is given by

$$\tilde{\mathbf{P}}^{\mathrm{a}} = [(K-1)I + (\mathbf{H}\mathbf{X}^{\mathrm{b}})^{\mathrm{T}}\mathbf{R}^{-1}(\mathbf{H}\mathbf{X}^{\mathrm{b}})]^{-1} \qquad (14)$$

of rank $K-1$, usually much smaller than the dimension of both the model and the number of observations. As a result, the LETKF performs the analysis in the space spanned by the forecast ensemble members, which greatly reduces the computational cost. More details about the LETKF are available in Hunt *et al.* (2007) and Szunyogh *et al.* (2008).

## 4. Implementation in the Lorenz-96 model

We first test our approach in the Lorenz-96 model (Lorenz and Emanuel, 1998) which has been widely used to test data assimilation methods:

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = x_{i-1}(x_{i+1} - x_{i-2}) - x_i + F, \qquad (15)$$

where, $i = 1, \cdots N$, and the boundary is cyclic. As in Lorenz and Emanuel (1998), we choose $N = 40$ and $F = 8.0$, in which case this model behaves chaotically. Equation (15) is solved with a fourth-order Runge–Kutta scheme using a time step of 0.05 non-dimensional units that corresponds to about 6 hours in the atmosphere, as shown by Lorenz and Emanuel (1998).

### 4.1. Perfect model experiments

First we test our approach in the perfect model scenario in which the multiplicative inflation is used to prevent filter divergence due to small ensemble size. We generate the 'true' state by integrating the Lorenz-96 model for 2000 steps. Normally distributed random noise with variance $\sigma_{\mathrm{o}}^2 = 1$ is then added to the 'truth' to generate the observations. Each state variable is observed so that the observation number is $p = 40$ and no interpolation is needed. We assimilate these observations every analysis cycle using the LETKF with $K = 10$ ensemble members. Following Ott *et al.* (2004), we use a cut-off-based localization with a local patch $l = 6$ which covers 13 model grid points. The background error covariance $\mathbf{P}^{\mathrm{b}}$ is updated every analysis cycle from the background ensemble spread. Since the normally distributed errors are uncorrelated with each other and the error variance is 1, the true observation error matrix is diagonal, i.e. $\mathbf{R}_t = \sigma_{\mathrm{o(t)}}^2\mathbf{I} = \mathbf{I}$.

The LETKF is used to assimilate observations at each analysis step and for a total of 2000 steps. Following Whitaker and Hamill (2002), we ignore the first 1000 steps to allow for any spin-up and report the results only for the last 1000 steps.

#### *4.1.1. Correctly specified observation variance*

We first assume that the observation error variance is perfectly known, i.e. the specified value is $\sigma_{\mathrm{o(s)}}^2 = \sigma_{\mathrm{o(t)}}^2 = 1$. In this case we do not estimate the observation error variance, but attempt to estimate online the inflation parameter using this correctly specified observation error variance. We found that the 'observed' inflation $\tilde{\Delta}^{\mathrm{o}}$ directly obtained from either $OMB^2$ or $AMB \times OMB$ has large oscillations at each analysis step due to (i) sampling an insufficient number of observations and (ii) the relative small background error variance in these perfect model experiments, so that the results are very sensitive to the denominator in Equation (4) or (5). Some very unrealistic values of $\tilde{\Delta}^{\mathrm{o}}$ might occur, making the temporal-smoothing strategy itself not sufficient to handle the sampling error problem. To avoid the possibility of such unrealistic estimation of $\tilde{\Delta}$ that could ruin the assimilation, we impose wide upper and lower limits in the 'observed' inflation $\tilde{\Delta}^{\mathrm{o}}$, e.g. $0.9 \leqslant \tilde{\Delta}^{\mathrm{o}} \leqslant 1.2$ before applying the simple scalar KF smoothing procedure. The final estimation of $\tilde{\Delta}$ after smoothing is then used to inflate the background ensemble spread. In a more realistic data assimilation system with a much larger number of available observations and relatively big background error, Wang and Bishop (2003) have shown the 'observed' inflation $\tilde{\Delta}^{\mathrm{o}}$ calculated directly from $OMB^2$ remained within a reasonable range. In that situation,



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as in the results presented in section 5, there is no need to prescribe a range for $\tilde{\Delta}^o$ but time smoothing of the estimates might still be desirable. As for the estimation of observational error variance in the latter experiments, we only apply the temporal-smoothing strategy since no large oscillations were found in the 'observed' $\sigma_o^2$ presumably because there is no division by a potentially small number in Equation (7) as there is in (4) or (5).

Table I shows that $OMB^2$ and $AMB \times OMB$ methods produce similar results with an estimated inflation factor $\Delta$ of about 1.04 and an analysis error of about 0.20. These results are very similar to the best-tuned constant inflation obtained from many tuning trials. The experiments in Table I will serve as a benchmark for the latter experiments where $\sigma_o^2$ is not perfectly specified.

#### 4.1.2. *Incorrectly specified observation error variance*

In reality we do not know exactly the true value of the observation error variance, and the specified value in the analysis is only an estimate. In our second experiment with the Lorenz-96 model, we use an erroneously specified $\sigma_{o(s)}^2$ which is either one quarter or four times the size of the true $\sigma_{o(t)}^2$, equivalent to one-half or twice the true observational error standard deviation. With a large $\sigma_{o(s)}^2 = 4.0$, the estimated $\Delta$ is smaller than its optimal value (Table II), so that the LETKF gives too much weight to the background and not enough to the observations, resulting in a very degraded analysis.

In the case of $\sigma_{o(s)}^2 = 0.25\sigma_{o(t)}^2$ we noticed that the estimated $\Delta$ is the upper limit 1.2 of the prescribed possible range, $0.9 \leqslant \tilde{\Delta}^o \leqslant 1.2$ (Table II). This happened because the 'observed' inflation $\tilde{\Delta}^o$ at each single analysis time step was always larger than 1.2, and was then forced to be 1.2. As a result it did not represent the value estimated from equation $OMB^2$ or $AMB \times OMB$. Removing this constraint, we obtained a value for $\Delta$ of 8.70 (7.81) with the estimation method $OMB^2$ ($AMB \times OMB$) respectively and the resulting analysis RMS error of 0.80 (0.79) – much worse than the optimal value of 0.2.

Table I. Time mean of adaptive inflation factor $\Delta$ and the corresponding analysis RMS error, averaged over the last 1000 steps of a 2000-step assimilation in a perfect model scenario and in the case when the observational error variance is perfectly specified ($\sigma_{o(s)}^2 = 1$). For comparison, the value of best-tuned constant inflation and its resulting analysis error are also shown.

| $\Delta$ method | $\sigma_{o(s)}^2$ | $\Delta$ | RMSE |
|---|---|---|---|
| $OMB^2$ | 1 | 1.044 | 0.202 |
| $AMB \times OMB$ | 1 | 1.042 | 0.202 |
| (Tuned) constant | 1 | 1.046 | 0.201 |

Table II. Time mean of adaptive inflation factor $\Delta$ and the resulting analysis RMS error, averaged over the last 1000 steps of a 2000-step assimilation in a perfect model scenario and in the case when the specified observation variance $\sigma_{o(s)}^2$ is either a quarter of or four times the true $\sigma_{o(t)}^2$ but without attempting to estimate and correct it. The inflation factor is constrained to be within an interval $0.9 \leqslant \tilde{\Delta}^o \leqslant 1.2$. See text for the results when this constraint is removed.

| $\Delta$ method | $\sigma_{o(s)}^2$ | $\Delta$ | RMSE |
|---|---|---|---|
| $OMB^2$ | 0.25 | 1.2 | 0.265 |
| $AMB \times OMB$ | 0.25 | 1.2 | 0.262 |
| $OMB^2$ | 4.0 | 1.021 | 1.635 |
| $AMB \times OMB$ | 4.0 | 1.033 | 1.523 |

#### 4.1.3. *Simultaneous estimation of the inflation and the observation error variance*

We have seen that neither $OMB^2$ nor $AMB \times OMB$ work appropriately when estimating the inflation parameter if the specified observation error variance is substantially wrong. In the third experiment, we estimate the observation error variance and inflation simultaneously by using $OMA \times OMB$ and $OMB^2$ (or $AMB \times OMB$) followed by the simple KF method.

We start our experiment with the same initial misspecification of the observation error variance. Table III shows that, even if the initial specification of the observation error variance $\sigma_{o(ini)}^2$ is poor (one quarter of or four times the true $\sigma_o^2$), the $OMA \times OMB$ method has the ability to correct it. The time mean of estimated $\sigma_o^2$ over the last 1000 analysis steps is essentially the same as the true $\sigma_o^2$. With the corrected $\mathbf{R}$ matrix, we obtain a reasonable adaptive inflation $\Delta$ of about 1.04 for all the cases in Table III. The resulting analysis RMS errors are also similar to that of the benchmark. The results are not sensitive to the initial incorrect value of $\sigma_{o(ini)}^2$, since $\sigma_o^2$ is gradually corrected and reaches its 'true' value after an initial transition period no matter what initial value is specified.

We have shown that the estimation of adaptive inflation alone does not work with an incorrectly specified observation error variance. By estimating the inflation and observation errors simultaneously, our method has the ability to retrieve both their 'true' values. We now check whether $OMA \times OMB$ can retrieve a correct observation error variance if the inflation is wrongly specified. From the previous experiments, we know the optimal inflation factor is about 1.04. If we fix it and underspecify it to be 1.01, we get an estimated $\sigma_o^2 = 10.33$, confirming that the estimations of inflation factor and observation errors depend on each other. Unless one of them is accurately known, both of them need to be simultaneously estimated.

### 4.2. Imperfect model experiments

We have tested our approach in the LETKF with the simulated observations and shown its ability to retrieve both the true observation error variance and the optimal inflation parameter in a perfect model scenario. In this section we focus on a more realistic situation by introducing model errors. Recall that our method is based on



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Table III. Time mean of adaptive inflation factor $\Delta$, the estimated observation error variance $\sigma_o^2$ and the resulting analysis RMS error, averaged over the last 1000 steps of a 2000 step assimilation in a perfect model scenario and in the case of simultaneous estimation of both the inflation and the observation error variance which is initially mis-specified.

| R method | $\Delta$ method | $\sigma^2_{o(ini)}$ | $\sigma_o^2$ | $\Delta$ | RMSE |
|---|---|---|---|---|---|
| $OMA \times OMB$ | $OMB^2$ | 0.25 | 1.002 | 1.046 | 0.208 |
| | $AMB \times OMB$ | 0.25 | 1.003 | 1.043 | 0.205 |
| | $OMB^2$ | 4.0 | 1.000 | 1.046 | 0.202 |
| | $AMB \times OMB$ | 4.0 | 1.000 | 1.043 | 0.203 |

the assumption that the specified matrices $\mathbf{P}^b$ and $\mathbf{R}$ in

$$\mathbf{HK} = \mathbf{HP}^b\mathbf{H}^T(\mathbf{HP}^b\mathbf{H}^T + \mathbf{R})^{-1}$$

agree with the true covariances for background and observation. In the perfect model scenario, the required inflation is small and the inflated background error covariance with a reasonable number of ensemble members can usually approximate well the true background error covariance, but this is not the case for an imperfect model in the absence of additional methods to correct model error, when only the covariance inflation algorithm is used to account for the effect of model errors. In this case the inflated background error covariance may not be good enough to represent the true background error covariance. Our goal in this subsection is to test whether our online estimation algorithm will still work in a more realistic situation with model errors.

#### *4.2.1. Random model errors*

First, we study our scheme in the presence of random model errors in which the real atmosphere is assumed to behave like a noisy version of the numerical forecast model. The evolution of the 'true' atmosphere is simulated by adding the zero-mean random noise to the Lorenz-96 model at each model time step:

$$\frac{dx_i}{dt} = x_{i-1}(x_{i+1} - x_{i-2}) - x_i + F + \alpha \times \varepsilon_i, \qquad (16)$$

where $\varepsilon_i \sim N(0, 1)$ and $\alpha$ is a constant factor. Our forecast model is the standard Lorenz-96 model shown in (12), so that we now have (unbiased) random model errors. Since more uncertainties are involved in the imperfect model experiments, we increase the ensemble size from 10 to 20.

Table IV shows the estimated values of observation error, adaptive inflation and their resulting analysis errors for different amplitudes $\alpha$ of the random model error. As in benchmark, we manually tuned the system to find the optimal time-constant inflation (case A), and estimated online the inflation using the 'true' observation error variance (case B). For case C, we simultaneously estimated the values of observation error and adaptive inflation. To handle sampling errors in cases B and C, we did the temporal smoothing for all the situations of different $\alpha$ and set the lower limit of 'observed' $\tilde{\Delta}^o$ to 1.0 when $\alpha = 100$ (corresponding to very large random errors). In the perfect model experiments, we have seen our method is not sensitive to the initial specification of the observational error variance and the method to calculate the 'observed' inflation parameter, so that we only test our method with $\sigma^2_{o(ini)} = 0.25$ and use the $OMB^2$ method to estimate the inflation parameter. As shown in Table IV, all three cases give similar results, with the required inflation and the resulting analysis error increasing with the amplitude of the model random errors. When the observation error is perfectly known (case B), adaptive inflation reaches an analysis error similar to that obtained by tuning a constant inflation. With wrong initial observation error information (case C), we estimate it online together with the estimation of inflation, and the 'true' $\sigma_o^2$ is also approximated. The resulting analyses are as good as those from the best-tuned inflation. These results indicate that the adaptive algorithm simultaneously estimating inflation and observation errors is able to produce successful assimilations over a wide range of random model errors. By contrast, manually searching for the optimal time-constant inflation factor (case A) requires a considerable number of iterations for each value of $\alpha$.

#### *4.2.2. Systematic model bias*

For our final experiment with the Lorenz-96 model, we introduce a systematic model bias. In the linear estimation theory, the basis of most data assimilation schemes, both background and observation error vectors are assumed to be unbiased. However in reality the background is usually biased due to the imperfect model, and ideally the model bias should be estimated and subtracted from the biased forecast. Here we violate the assumption that the background is unbiased in order to check the behaviour of our method in a more realistic situation with model bias.

We generate the model bias as in Baek *et al.* (2006) by adding a constant sine function to the forcing term in the Lorenz-96 model.

$$\frac{dx_i}{dt} = x_{i-1}(x_{i+1} - x_{i-2}) - x_i + F + \alpha \times \beta_i, \qquad (17)$$

where $\beta_i = 1.6\sin\{2\pi(i-1)/N\}$ describes the spatial structure of the model bias and $\alpha$ determines its size. In Baek *et al.* (2006), $\alpha = 1$, corresponding to a model bias of $b_i = 1.6\sin\{2\pi(i-1)/N\} \times 0.05 = 0.08\sin\{2\pi(i-1)/N\}$. This is a relatively small bias compared with the observation noise (1.0 in our experiments). Here we

 

Table IV. Results in the presence of random model errors. Case A – value of best-tuned constant inflation using true observation variance and the resulting analysis RMSE; Case B – time mean value of adaptive inflation using true observation variance and the resulting analysis RMSE; Case C – time mean values of simultaneous adaptive inflation and observation error, and the resulting analysis RMSE. Each case is tested for a wide range of $\alpha$, amplitude of random model errors. Results are averaged over the last 1000 analysis steps.

| | A: true $\sigma_o^2 = 1.0$, (tuned) constant $\Delta$ | | B: true $\sigma_o^2 = 1.0$, adaptive $\Delta$ | | C: adaptive $\sigma_o^2$, adaptive $\Delta$ | | |
|---|---|---|---|---|---|---|---|
| Error amplitude, $\alpha$ | $\Delta$ | RMSE | $\Delta$ | RMSE | $\Delta$ | RMSE | $\sigma_o^2$ |
| 4 | 1.25 | 0.35 | 1.27 | 0.36 | 1.39 | 0.38 | 0.93 |
| 20 | 1.45 | 0.47 | 1.41 | 0.47 | 1.38 | 0.48 | 1.02 |
| 100 | 2.00 | 0.64 | 1.87 | 0.64 | 1.80 | 0.64 | 1.05 |

Table V. As Table IV, but in the presence of a constant model bias with different amplitudes, $\alpha$.

| | A: true $\sigma_o^2 = 1.0$, (tuned) constant $\Delta$ | | B: true $\sigma_o^2 = 1.0$, adaptive $\Delta$ | | C: adaptive $\sigma_o^2$, adaptive $\Delta$ | | |
|---|---|---|---|---|---|---|---|
| Error amplitude, $\alpha$ | $\Delta$ | RMSE | $\Delta$ | RMSE | $\Delta$ | RMSE | $\sigma_o^2$ |
| 1 | 1.35 | 0.40 | 1.31 | 0.42 | 1.35 | 0.41 | 0.96 |
| 4 | 2.00 | 0.59 | 1.78 | 0.61 | 1.77 | 0.61 | 1.01 |
| 7 | 2.50 | 0.68 | 2.11 | 0.71 | 1.81 | 0.80 | 1.36 |

examine a wider range of model bias by applying different coefficients $\alpha$. As in Baek *et al.* (2006) and in our experiments with random model errors, we also test our method with 20 ensemble members.

Table V shows the analysis results obtained from the best-tuned inflation (case A), adaptive inflation using the 'true' observation error variance (case B), adaptive inflation and adaptive observation error variance (case C), in the presence of model bias. A lower limit of 'observed' $\tilde{\Delta}^o$ is set to 1.0 when $\alpha = 4$ and $\alpha = 7$ for cases B and C. In general, the three cases give similar analysis accuracy for small- and medium-sized model bias. When the bias amplitude increases to $\alpha = 7$, the simultaneous approach does not work well, giving a relatively large estimate of observational error variance and analysis error. The best-tuned inflation yields the best results. The mean values of adaptive inflation in case B are always smaller than the best-tuned inflation (case A), presumably because the ensemble does not 'know' about model errors.

To further explore the results with large model bias, we compare the forecast ensemble spread (after inflation is applied) with the forecast RMS error with respect to the 'true' state *averaged* over all 40 variables for all three cases when the model bias is large, $\alpha = 7$. Let us first focus on cases A and B. As shown in Table VI, though the spread agrees quite well with the forecast error in case B compared to that in case A, the analysis error (Table V) and forecast error (Table VI) themselves in case B are bigger than those with best-tuned inflation. This apparent contradiction can be attributed to the fact that inflating the background error with a uniform inflation factor is not good enough to parametrize large model error. The multiplicative covariance inflation assumes that the structure of model errors is the same as that of background ensemble spread, but in general this is not true. A systematic bias with a sine function in space as in our experiments cannot be represented by the dynamical growing error. The adaptive inflation estimation scheme $OMB^2$ ignores the spatial structure of model error since it is only concerned about the trace of covariance rather than the structure. Thus Equation (4) produces a single value of inflation, which is optimal in the sense of spatial average but not for individual observations. Thus, although the spatially averaged spread in Table VI for case B is consistent with the forecast error, it is not optimal for the analysis. The tuned inflation result is expected to be the best because the inflation factor is repeatedly tuned in terms of the resulting analysis error. The best-tuned result overcomes the errors in modelling bias structure by overinflating the ensemble covariance to give more weights to the observations.

As a result, the best-tuned inflation is always larger than the adaptive inflation, and the bigger the model bias, the bigger the overestimation (Table V). These results are consistent with those of Anderson (2007), where an adaptive inflation from a hierarchical Bayesian was compared to the best-tuned time-constant inflation. With the suboptimal inflation from $OMB^2$ (actually underestimating the best-tuned inflation), it is not surprising that the results in case C are even worse when the observational errors are also estimated because the suboptimal inflation could affect the accuracy of the estimated $\sigma_o^2$ which further gives a poor feedback to the adaptive inflation. This failure happens when model bias is large. In order to get the best estimation of both $\sigma_o^2$ and the inflation factor, an additional method is required to remove the model bias. The reader is referred to Dee and da Silva (1998), Baek



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Table VI. Time mean of observation error variance $\sigma_o^2$, adaptive inflation $\Delta$, the forecast ensemble mean RMS error in the presence of bias (N.B. forecast error rather than analysis error as in Table V) and the forecast ensemble spread, with a model bias of $\alpha = 7$. Case A: best-tuned constant inflation; B: adaptive inflation estimated with true observation error variance; C: simultaneous estimation of both $\sigma_o^2$ and $\Delta$. Results are reported as an average over the last 1000 steps of a 2000-step assimilation.

| | A: true $\sigma_o^2$ (= 1.0), (tuned) constant $\Delta$ | B: true $\sigma_o^2$ (= 1.0), adaptive $\Delta$ | C: adaptive $\sigma_o^2$, adaptive $\Delta$ |
|---|---|---|---|
| $\sigma_o^2$ | 1.00 | 1.00 | 1.36 |
| $\Delta$ | 2.50 | 2.11 | 1.81 |
| Error | 0.94 | 0.99 | 1.11 |
| Spread | 1.16 | 0.98 | 0.95 |

*et al.* (2006), Danforth *et al.* (2007), and Li (2007) for several successful methods to estimate the bias.

## 5. SPEEDY model results

In the previous section we have tested our algorithm in a low-order model where we have only one set of observations with one 'true' observation error variance. In this section we apply our approach to a more realistic model, assimilating several types of observations. The size and unit for the different sets of observations are different. The SPEEDY (Simplified Parametrization, primitivE-Equation DYnamics; Molteni, 2003) atmospheric general circulation model, is used for this purpose. It solves the primitive equation for prognostic variables of zonal wind, $u$, meridional wind, $v$, temperature, $T$, specific humidity, $q$, and surface pressure, $p_s$, at the truncation of wavenumber 30, corresponding to $96 \times 48$ grid points and 7 sigma levels.

We perform an Observing System Simulation Experiment (OSSE) in which the 'true' observation error is known and can be used to verify the results. The observations are obtained by adding zero mean, normally distributed noise to the 'true state', defined as the two-month integration of the SPEEDY model from 1 January to 28 February 1982. The observations are available on the model grid at every other grid point for $u$, $v$, $T$, $q$, $p_s$ in both zonal and meridional directions, i.e. at 25% of the number of model grid points at every level. The standard deviations of the observation errors are 1 m s$^{-1}$ for $u$, $v$ wind, 1 K for $T$, $10^{-4}$ kg kg$^{-1}$ for $q$ and 1 hPa for $p_s$. Whereas with the small Lorenz-96 model the 'observed value' of $\tilde{\Delta}^o$ obtained from Equations (4) or (5) showed large oscillations, in the SPEEDY model, which has a much larger number of available observations ($p_i = 1152 \times 7$ for each variable), the oscillations due to sampling in the 'observed' inflation $\tilde{\Delta}^o$ were much reduced (as was the case in Wang and Bishop, 2003), so that we only set its lower limit to be 1.0.

We started the experiment by running 20 initial ensembles at 0000 UTC on 1 January 1982. The 20 initial ensembles are created by adding the random noise to the 'true state' at 0600 UTC on 1 January 1982. In this way, the initial ensemble mean is 6 hours apart from the truth. We doubled the true observational errors to get our first guess of the observational errors. Within the LETKF, we estimate and correct these initially incorrect observation errors every analysis time step (6 hours). Since the value and unit for different observed variables are all different, we estimate the observational error variance for each observed variable separately.

From the experiments of Lorenz-96 model, we have seen that, as long as the observational error is recovered, we can get similar results whether we use $OMB^2$ or $AMB \times OMB$ to estimate the inflation parameter. Therefore we only tested here the more widely used $OMB^2$ method.

Figure 1 shows the online estimated observational errors for each observed variable. The experiment starts from incorrectly specified observational errors with 2 m s$^{-1}$ for $u$ and $v$, 2 K for $T$, $2 \times 10^{-4}$ kg kg$^{-1}$ for $q$ and 2 hPa for $p_s$. After only one week (30 analysis steps), the estimated observational errors are all very close to their corresponding true values. Of all the observation errors, the estimated temperature error converges fastest (in only 2 days), presumably due to the dynamical constraints imposed by geostrophic adjustment on long baroclinic waves (e.g. Kalnay, 2003, pp. 186–190), with winds and humidity taking longer to converge. This rate of convergence is slower than that reported in DEA05, where it takes about 5 cycles to get a close estimate to the true error variance. Desroziers *et al.* (2005) tuned error statistics iteratively within a variational data assimilation cycle, which is time consuming but makes convergence faster than our approach here. Another reason is that, unlike an operational set-up, the initial background error covariance in this cold-started experiment is unphysical, since it is created from random fields added to the mean state. The SPEEDY–LETKF system takes time to adjust the structure of background error covariance from the initial randomly perturbations towards the 'errors of the day' during the spin-up, in addition to tuning the observation error variance and inflation factor. An iterative procedure recently proposed by Kalnay and Yang (2009) to accelerate the spin-up of the LETKF using a no-cost smoother (Kalnay *et al.*, 2007) could be adapted for the problem addressed in this paper. Since the estimation of the inflation factor by $OMB^2$ depends on the accuracy of the specified observation error covariance $\mathbf{R}$, there is a delay in the time needed for the inflation factor to reach a stable optimal value

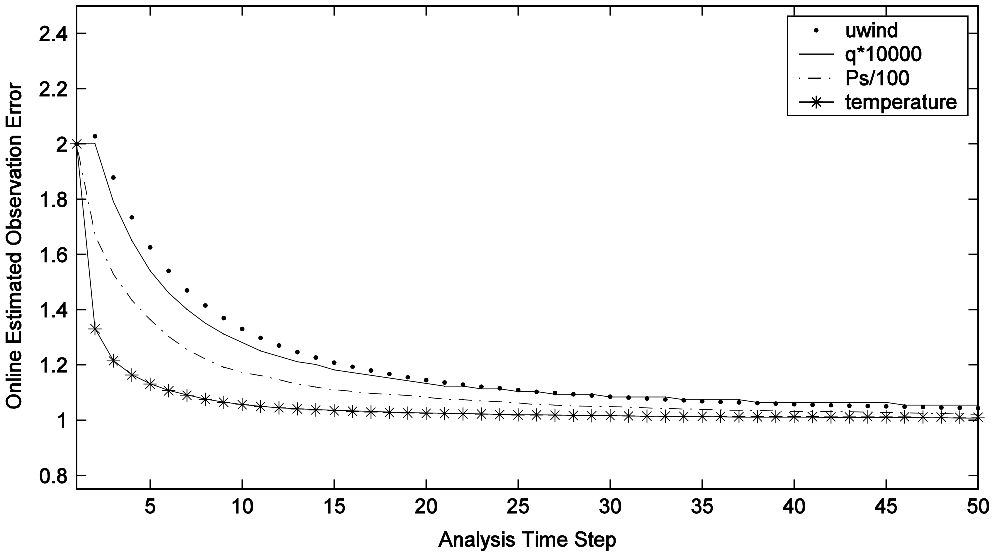


Figure 1. Time series of online estimated observation errors of $u$, $q$, $p_s$, and $T$, for the first 50 analysis time steps (corresponding to 00 UTC on 1 January to 06 UTC on 13 January 1982)

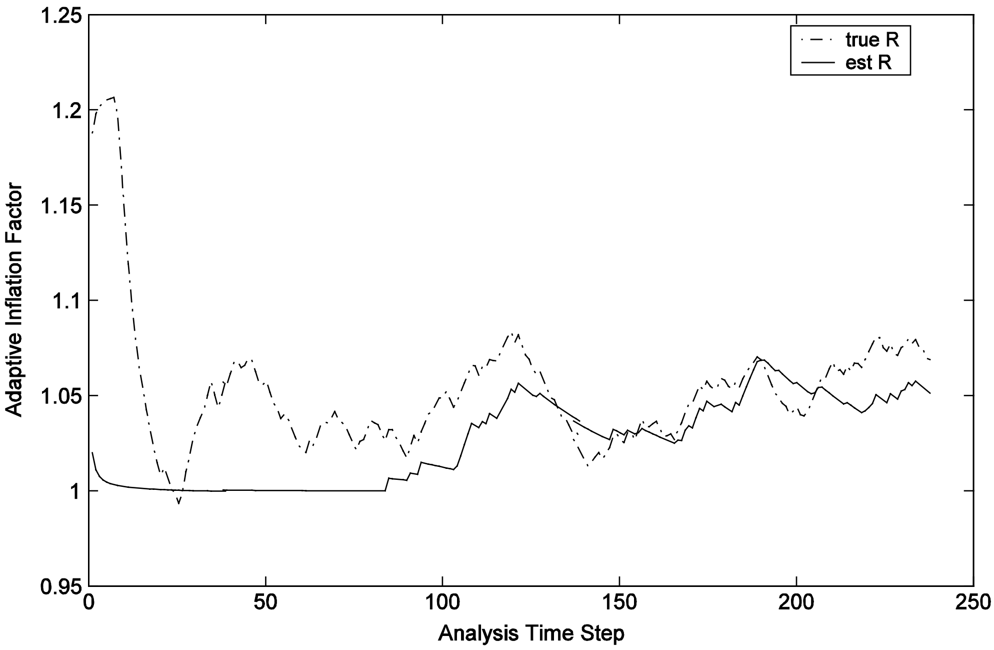


Figure 2. Time series of estimated inflation factor for 236 analysis time steps (corresponding to 00 UTC on 1 January to 18 UTC on 28 February 1982) when using a perfectly specified observation error variance (dashed-dotted line) and an initially erroneous observation error variance but estimating it adaptively (solid line)

(about one month, solid curve in Figure 2) compared to the case in which **R** is specified correctly (dashed-dotted curve in Figure 2). This dashed-dotted curve can be considered as the optimal choice of the adaptive inflation at each time step, and after the spin-up, the solid curve follows the dashed-dotted curve very well. This indicates that no matter how poorly the observation error statistics are specified initially, as long as we estimate and correct this information we can obtain an accurate adaptive inflation factor. As a result, the obtained analysis is about as good as the one obtained from the experiment in which **R** is perfectly known (e.g. the one-month averaged analysis error after the first month spin-up period for 500 hPa height is 2.9 m and 2.7 m for the estimated and the true **R** cases, respectively).

## 6. Conclusion

The accuracy of an analysis system depends on the use of appropriate statistics of observation and background errors. For an ensemble-based Kalman filter, tuning the covariance inflation factor is expensive, especially if it depends on space and on the type of variables. The online estimation method can objectively estimate the covariance inflation factor but requires accurate information on observational errors. In this study, we apply the observation error estimation method in DEA05 into an EnKF system and estimate observational errors and the inflation coefficient simultaneously. First we examine our approach in the Lorenz-96 model, a low-order model where only one type of observation is available. The results show that the estimation of inflation alone does not work appropriately without accurate observation error statistics, and vice versa. By simultaneously estimating both inflation and observation error variance online, our approach works well in a perfect model scenario, as well as with random model errors or small bias. The estimated observation error variances are very close to their true values, and the resulting analyses are as good as those obtained from the best tuned inflation value. When the forecast model has a large systematic bias, our simultaneous estimation algorithm tends to overestimate the observation error variance and results in a sub-optimal analysis, indicating that a separate algorithm is required to handle model bias (e.g. Dee and da Silva, 1998; Baek *et al.*, 2006; Danforth *et al.*, 2007; Li, 2007).

We then applied our approach to a more realistic high-dimension model, assimilating several types of observation that have errors of different sizes and units. The SPEEDY model experiments show that the approach is able to retrieve the true observation error variance for different types of instruments separately. Because the number of observations was much larger, we found that the 'observed' inflation factor was much more stable in the SPEEDY model than in the Lorenz-96 model.

In the experiments in this study, we have used a globally uniform inflation factor, which is clearly not a good assumption in reality where the observations are non-uniformly distributed. With a spatially dependent inflation, we may be able to better deal with an irregularly observing network. Offline tuning the spatially dependent inflation is practically infeasible whereas adaptive inflation can be explored for this purpose, as long as there are enough observations in each subdomain.

We also note that in this study we have focused on multiplicative covariance inflation, but that our simultaneous approach is equally applicable to adaptively estimating the scale of the additive noise in additive inflation schemes (Corazza *et al.*, 2002; Whitaker *et al.*, 2008).

So far we have addressed the issue of observation error variance but the presence of observational error correlations is another concern, especially for satellite observations. Though it would not work when the observation error carries the same correlation structure as the background error, the method of DEA05 is at least able to recover the interchannel error cross-correlations (section 6 in DEA05), a usual case for satellite observations. In the next step, we plan to investigate if this statement is still valid in the EnKF application.

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