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

Hong Li[1, 2*], Eugenia Kalnay[1], and Takemasa Miyoshi[3]

[1] University of Maryland, College Park, Maryland, USA

[2] Shanghai Typhoon Institute, Shanghai, CHINA

[3]Numerical Prediction Division, Japan Meteorological Agency

Submitted to QJRMS – December 2007

ABSTRACT

Covariance inflation plays an important role within 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 EnKF is expensive. Wang and Bishop (2003), followed by Miyoshi (2005), adaptively estimated the inflation factor from the innovation statistics. Although the results were satisfactory it is clear that this inflation factor estimation method relies on the accuracy of the estimated observation error covariance, 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 results for the Lorenz-96 model show that without accurate observation error statistics, a scheme for adaptively estimating inflation alone does not work appropriately. By contrast, the simultaneous approach works very well in the perfect model scenario and in the presence of random model errors or 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.

KEYWORDS: Ensemble data assimilation, Parameter estimation, Simultaneous approach

* *Corresponding author address:* Hong Li, 166 Puxi Road, Shanghai Typhoon Institute, Shanghai 200030. Email: lih@mail.typhoon.gov.cn

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 the linear estimation theory in which the background and the observation 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 estimation of the error statistics of both the background and the observations. It is a common experience that Observing System Simulation Experiments (OSSEs) give better forecasts than real observation experiments. This is generally attributed to the fact that in OSSEs the model errors are neglected, but another important difference between OSSEs and real observation experiments is that the observation error statistics are perfectly known in the OSSEs but not in real forecast experiments.

In the past decade, ensemble based Kalman filters (EnKF) 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.*, 2007) to regional-scale models (e.g., Snyder and Zhang, 2003; Zhang *et al.*, 2006), due to their ease of implementation and their ability to estimate the flow-dependent background and analysis error covariances. 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 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 the amplitude of these inflation algorithms requires considerable tuning in order to obtain good performance of the filter. Tuning a parameter in EnKF is expensive, since it requires many forecast-analysis cycles. Even worse, it becomes infeasible 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 the inflation factor from the innovation statistics $\mathbf{d}^T\mathbf{d} = trace[(1+\Delta)\mathbf{HP}^b\mathbf{H}^T + \mathbf{R}]$ in their ensemble forecast scheme. Miyoshi (2005) reported the use of a similar method to estimate the covariance inflation factor within the EnKF data assimilation scheme. Although both studies reported satisfactory results, it is obvious that these estimations of the inflation factor rely on the assumption that the observational error covariance $\mathbf{R}$ is known. This assumption is valid for simulated observations but not for real observations. When assimilating real data, additional methods may be needed to obtain the correct statistics of observation errors if we want to apply the inflation estimation scheme above. In fact, Miyoshi and Yamane (2007) reported the adaptive inflation did not work when assimilating the real data by using the observational error standard deviations as in JMA operational system.

Recent diagnostic work (e.g., Desroziers and Ivanov, 2001; Talagrand, 1999; Cardinali *et al.*, 2004; Chapnik *et al.*, 2006) suggests that the innovation (observations minus background) and other analysis cycle statistics can be used to diagnose both observation and background errors. A formulation on the cost function of such diagnostics has been proposed and tested in a variational framework. Building on these works, Desroziers *et al*. (2005) (DEA05 hereafter) developed a set of diagnostics based on the combinations of *observation-minus-analysis*, *observation-minus-background* and *background-minus-analysis* statistics to adaptively tune observation and background errors. Here we adapt one of these diagnostics for estimating observation error variance into the EnKF.

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 method (or other diagnostics of DEA05) to estimate the inflation factor. We compute the 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 and 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. In section 4, our simultaneous approach is implemented on a low-order model and the results are shown in the perfect model scenario and in the presence of model errors. A summary and discussion are provided in section 5.

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 of the observational errors $\mathbf{R}$, assuming these errors are uncorrelated, the well-known relationship

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

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 $h(x^b)$, where h is the non-linear observation operator projecting the background $\mathbf{x}^b$ to the observation space and $\mathbf{H}$ is the linear tangent matrix of h operator. The brackets represent an average over many cases or statistical expectation. This classical innovation statistics shown in equation (1) provides a global check on the specification of $\mathbf{P}^b$ and $\mathbf{R}$.

DEA05 proposed another diagnostic to check the specified background error covariance $\mathbf{P}^b$ in variational data assimilation scheme,

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

where $\mathbf{d}_{a-b}$ is the difference between the analysis and the background (analysis increment) in observation space, i.e., $\mathbf{d}_{a-b} = H(\mathbf{x}^a) - H(\mathbf{x}^b)$

Unlike 3DVAR or 4DVAR, in which the background error covariance $\mathbf{P}^b$ is assumed to be constant, 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 and 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 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,

$$\mathbf{P}^b \leftarrow (1+\Delta)\mathbf{P}^b \tag{3}$$

Here Δ is referred to as a covariance inflation factor that needs to be tuned for a good performance of the ensemble filter. However, *tuning* the inflation parameter is expensive, and furthermore, there is no reason why the inflation should be assumed to be constant. Wang and Bishop (2003) proposed adapting equation (1) to estimate the inflation factor in ensemble forecasting. Plugging (3) into equation (1) and considering only the diagonal term, they estimated the inflation factor Δ online by

$$\widetilde{\Delta} = \frac{\mathbf{d}_{o-b}^T \mathbf{d}_{o-b} - Tr(\mathbf{R})}{Tr(\mathbf{H}\mathbf{P}^b\mathbf{H})} - 1 \tag{4}$$

where Tr denotes the trace of a matrix.

Similarly, by plugging (3) into equation (2), we obtain another equation to estimate the inflation factor:

$$\widetilde{\Delta} = \frac{\mathbf{d}_{a-b}^T \mathbf{d}_{o-b}}{Tr(\mathbf{H}\mathbf{P}^b\mathbf{H})} - 1 \tag{5}$$

We denote equation (4) and (5) as *OMB²* and *AMB*OMB* methods, respectively. An accurate estimate of Δ from these two methods requires a correct observation error covariance **R**. This is obvious for equation (4) but is also implicitly true for (5), since $\mathbf{d}_{a-b}$ itself is based on the use of the (generally incorrect) specified **R**. In order to estimate online the inflation factor using either *OMB²* or *AMB*OMB* method, an additional method is necessary to estimate **R** if it is not known accurately.

2.2 Adaptive estimation of observation errors

DEA05 showed that the relationship:

$$< \mathbf{d}_{o-a}\mathbf{d}_{o-b}^T >= \mathbf{R} \tag{6}$$

is valid if the matrices specified in $\mathbf{HK} = \mathbf{HP}^b\mathbf{H}^T(\mathbf{HP}^b\mathbf{H}^T + \mathbf{R})^{-1}$ are the true covariances for background and observation error, where **K** is the Kalman gain, and $\mathbf{d}_{o-a}$ ($\mathbf{d}_{o-b}$) 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 on-line (within the cycle). For any subset of observations i with p_i observations, it is possible to compute the variance

$$(\tilde{\sigma}_o^2)_i = (\mathbf{d}_{o-a})^T{}_i(\mathbf{d}_{o-b})_i / p_i = \sum_{j=1}^{p_i}(y_j^o - y_j^a)(y_j^o - y_j^b)/p_i \quad (7)$$

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

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

2.3 Simultaneous estimation

As we have shown, adaptive estimation of inflation requires knowing the observation error variance σ_o^2 while an accurate estimate of σ_o^2 relies on using an optimal inflation factor. When neither the optimal inflation factor nor the true σ_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 the optimal value (or range of values) for the observation error variance and the inflation factor.

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 α^o (of either $\tilde{\Delta}^o$ or $\tilde{\sigma}_o^2$) 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 best combine α^o and α^f, the value derived by persistence from the previous time step, to get a new estimate denoted as the analysis α^a:

$$\alpha^a = \frac{v^o \alpha^f + v^f \alpha^o}{v^o + v^f} \tag{8}$$

where v^f / v^o denotes the forecast/observational error variance weights for the adaptive regression. The error variance of α^a is given by

$$v^a = (1 - \frac{v^f}{v^f + v^o}) v^f \tag{9}$$

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:

$$\alpha^f{}_{t+1} = \alpha^a{}_t \tag{10}$$

$$v^f{}_{t+1} = \kappa v^a{}_t \tag{11}$$

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

3. LETKF DATA ASSIMILATION SCHEME

The LETKF belongs to the family of ensemble square-root filter 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. Specifically, in the LETKF, the analysis mean is given by

$$\overline{\mathbf{x}}^a = \overline{\mathbf{x}}^b + \mathbf{X}^b \widetilde{\mathbf{P}}^a (\mathbf{H}\mathbf{X}^b)^T \mathbf{R}^{-1} [\mathbf{y}^o - h(\overline{\mathbf{x}}^b)] \tag{12}$$

where $\overline{\mathbf{x}}^a$, $\overline{\mathbf{x}}^b$ are the ensemble mean of analysis and background respectively, and $\mathbf{X}^a, \mathbf{X}^b$ 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:

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

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

$$\tilde{\mathbf{P}}^a = \left[(K-1)I + (\mathbf{HX}^b)^T \mathbf{R}^{-1} (\mathbf{HX}^b)\right]^{-1} \tag{14}$$

of dimension $K \times K$, 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*. (2007).

4. IMPLEMENTATION ON THE LORENZ-96 MODEL

We test our approach in the Lorenz 96 model (Lorenz, 1996; Lorenz and Emanuel, 1998) which has been widely used to test data assimilation methods:

$$\frac{dx_i}{dt} = x_{i-1}(x_{i+1} - x_{i-2}) - x_i + F \tag{15}$$

where, $i = 1, \cdots N$, and the boundary is cyclic. As in Lorenz (1996), we choose N=40 and F=8.0 in which case this model behaves chaotically. Equation (15) is solved with a 4th-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 analysis steps. Normally distributed random noise with variance σ_o^2=1 is then added to the 'truth' to generate the observations. Each state variable is observed so that 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 cutoff-based localization with a local patch l=6 which covers 13 model grids. Since the normally distributed noise is uncorrelated with each other and the error variance is 1, the true observation error matrix is diagonal, i.e., $\mathbf{R}_t = \sigma_{o(t)}^2 \mathbf{I} = \mathbf{I}$.

The LETKF is used to assimilate observations at each analysis step and for a total of 2000 steps, but results are only reported for the last 1000 steps.

a. Correctly specified observation variance

We first assume that the observation error variance is perfectly known, i.e., the specified value is $\sigma^2_{o(s)}=\sigma^2_{o(t)}=1$. In this case we do not estimate the observation error variance, but attempt to estimate on-line the inflation parameter using this correctly specified observation error variance. We found that the "observed" inflation $\tilde{\Delta}^o$ directly obtained from either *OMB*^{2} or *AMB*OMB* has large oscillations at each analysis step due to sampling insufficient number of observations and 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 extremely unrealistic values of $\tilde{\Delta}^o$ 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 estimation, we impose reasonably wide upper and lower limits in the "observed" inflation $\tilde{\Delta}^o$, e.g., $-0.1 \le \tilde{\Delta}^o \le 0.2$ 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 large number of available observations, Wang and Bishop (2003) have shown the "observed" inflation $\tilde{\Delta}^o$ calculated directly from *OMB*^{2} remained within a reasonable range. In that situation, 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, we only apply the temporal-smoothing strategy since no large oscillations were found in the "observed" σ^2_o presumably because there is no division by a potentially small number in equation (7).

Table 1 shows that *OMB*^{2} and *AMB*OMB* methods produce similar results with estimated Δ around 0.04 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 1 will serve as a benchmark for the latter experiments where σ^2_o is not perfectly specified.

Δ method	$\sigma^2_{o(s)}$	Δ	RMSE
OMB^2	1	0.044	0.202
*AMB*OMB*	1	0.042	0.202
(tuned) constant	1	0.046	0.201

Table 1**:** Time mean of adaptive inflation Δ 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 ($\sigma^2_{o(s)}$=1). For comparison, the value of best-tuned constant inflation and its resulting analysis error are also shown.

b. Incorrectly specified observation error variance

In reality we do not exactly know the true value of the observation error variance, and the specified value used in the analysis is only an estimate. In our second experiment with the Lorenz-96 model we use an erroneously specified $\sigma^2_{o(s)}$ which is either one quarter or 4 times the size of the true $\sigma^2_{o(t)}$, equivalent to one-half or twice the true observational error standard deviation. With a large $\sigma^2_{o(s)}$=4.0, the estimated Δ is smaller than its optimal value (Table 7), therefore 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 $\sigma^2_{o(s)}=0.25\sigma^2_{o(t)}$ we noticed that the estimated Δ is the upper-limit 0.2 of the prescribed possible range, $-0.1 \le \tilde{\Delta}^o \le 0.2$ (Table 7). This happened because the "observed" inflation $\tilde{\Delta}^o$ at each single analysis time step was always larger than 0.2, and was then forced to be 0.2. As a result it did not represent the value estimated from equation *OMB²* or *AMB*OMB*. Our experience indicates that $-0.1 \le \tilde{\Delta}^o \le 0.2$ is a reasonable range of Δ when σ^2_o is correctly specified, but there is no reason to assume that the inflation should remain within this normal range in an abnormal experiment. Removing this constraint we obtained a value for Δ of 7.70 (6.81) with the estimation method *OMB²* (*AMB*OMB*) and the resulting analysis RMS error of 0.80 (0.79) much worse than the optimal value of 0.2.

Δ method	$\sigma^2_{o(s)}$	Δ	RMSE
OMB²	0.25	0.2	0.265
*AMB*OMB*		0.2	0.262
OMB²	4.0	0.021	1.635
*AMB*OMB*		0.033	1.523

Table 2: Time mean of adaptive inflation parameter Δ 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 $\sigma^2_{o(s)}$ is either 1/4 or 4 times the true $\sigma^2_{o(t)}$ but without attempting to estimate and correct it. The inflation factor is constrained to be within an interval $-0.1 \le \widetilde{\Delta}^o \le 0.2$. See text for the results when this constrained is removed.

c. Simultaneous estimation of the inflation and the observation error variance

We have seen that neither *OMB*^{2} nor *AMB*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*OMB* and *OMB*^{2} (or *AMB*OMB*) followed by the simple KF method.

We start our experiment with an initial miss-specification of the observation error variance. Table 8 shows that even if the initial specification of the observation error variance $\sigma^2_{o(ini)}$ is poor (one-quarter or four times the true σ^2_o), the *OMA*OMB* method has the ability to correct it. The time mean of estimated σ^2_o over the last 1000 analysis step is essentially the same as the true σ^2_o. With the corrected **R** matrix, we obtain a reasonable adaptive inflation Δ of about 0.04 for all the cases in Table 8. The resulting analysis RMS errors are also similar to that of the benchmark. The results are not sensitive to the initial incorrect value of $\sigma^2_{o(ini)}$, since σ^2_o 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 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*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 0.04. If we fix it and under-specify it to be 0.01, we get an estimated σ^2_o =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.

R method	Δ method	$\sigma^2_{o(ini)}$	σ^2_o	Δ	RMSE
*OMA*OMB*	*OMB²*	0.25	1.002	0.046	0.208
	*AMB*OMB*		1.003	0.043	0.205
	OMB²	4.0	1.000	0.046	0.202
	*AMB*OMB*		1.000	0.043	0.203

Table 3: Time mean of adaptive inflation parameter Δ, the estimated observation error variance σ_o^2 and the resulting analysis RMS error, averaged over the last 1000 steps of a 2000 step assimilation in a perfect model scenario, with simultaneous estimation of both the inflation and the observation error variance which is initially miss-specified.

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 the assumption that the estimated 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 section is to test whether our on-line estimation algorithm will still work well in a more realistic situation with model errors.

a. 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:

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

where $\varepsilon_i \sim N(0,1)$ and a 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 9 shows the estimated values of observation error, adaptive inflation and their resulting analysis errors for different amplitudes a of the random model error. As benchmarks, we manually tuned the system to find the optimal time-constant inflation (case A), and estimated on-line 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 temporal-smoothing for all the cases with different α values, and set the lower limit of "observed" σ_o^2 to 0 when a =100 (corresponding to very large random errors). We have seen in the perfect model experiments that our method is not sensitive to the initial specification of the observational error variance or to the method used to calculate the "observed" inflation parameter, so that we only test our method with $\sigma_{o\,(ini)}^2$ =0.25 and use the OMB^2 method to estimate the inflation parameter.

As shown in Table 4, 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 tuning a constant inflation. With wrongly specified initial observation error information (case C), we estimate it on-line together with the estimation of inflation, and the 'true' $\sigma_o^2 = 1$ is also well 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. Manually searching for the optimal time-constant inflation factor (case A) requires a considerable number of iterations for each value of a .

Error amplitude (random)	A: true σ_o^2=1.0 (tuned) constant Δ		B: true σ_o^2=1.0 adaptive Δ		C: adaptive σ_o^2 adaptive Δ		
a	Δ	RMSE	Δ	RMSE	Δ	RMSE	σ_o^2
4	0.25	0.36	0.27	0.36	0.39	0.38	0.93
20	0.45	0.47	0.41	0.47	0.38	0.48	1.02
100	1.00	0.64	0.87	0.64	0.80	0.64	1.05

Table 4: Case A: best-tuned constant inflation using true observation variance and the resulting analysis RMSE; Case B: time mean of adaptive inflation using true observation variance and the resulting analysis RMSE; Case C: time mean of simultaneous adaptive inflation and observation error, and the resulting analysis RMSE. Each case is tested for a wide range of a , the amplitude of random model errors. Results are averaged over the last 1000 analysis steps.

b. Systematic model bias

For our final experiment, we introduce a systematic model bias. In the linear estimation theory, basis of most data assimilation schemes, both background and observation errors are assumed to be unbiased. However in reality the background is usually biased due to the use of an imperfect model, and ideally the model bias should be estimated and subtracted from the biased forecast. Here we violate the assumption that background is unbiased in order to check the behavior 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.

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

where $\beta_i = 1.6\sin(2\pi \frac{i-1}{N})$ describes the spatial structure of the model bias and α determines its size. In Baek et al. (2006) α =1, corresponding to a model bias of

$b_i = 1.6\sin(2\pi\frac{i-1}{N})\Delta t = 1.6\sin(2\pi\frac{i-1}{N})\times 0.05 = 0.08\sin(2\pi\frac{i-1}{N})$. This is a relatively small bias compared with the observation noise (1.0 in our experiments). Here we examine a wider range of model bias by applying different coefficients α. As in Baek *et al.* (2006) and in our experiments with random model errors we also test our method with 20 ensemble members.

Table 5 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" σ_o^2 is set to 0 when α =4 and α =7 for cases B and C. In general, the three cases give similar analysis accuracy for small and medium size of model bias. When the bias amplitude increases to α =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.

Error amplitude (bias)	A: true σ_o^2=1.0 (tuned) constant Δ		B: true σ_o^2=1.0 adaptive Δ		C: adaptive σ_o^2 adaptive Δ		
α	Δ	RMSE	Δ	RMSE	Δ	RMSE	σ_o^2
1	0.35	0.40	0.31	0.42	0.35	0.41	0.96
4	1.00	0.59	0.78	0.61	0.77	0.61	1.01
7	1.50	0.68	1.11	0.71	0.81	0.80	1.36

Table 5: As Table 9, but in the presence of a constant model bias with different amplitudes α.

To further explore the less successful results with large model bias, we compare the forecast ensemble spread (after inflation) with the 'true' forecast error (ensemble mean minus 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 case A and B.

	A: true σ_o^2=1.0 (tuned) constant Δ	B: true σ_o^2=1.0 adaptive Δ	C: adaptive σ_o^2 adaptive Δ
σ_o^2	1.00	1.00	1.36
Δ	1.50	1.11	0.81
Error	0.94	0.99	1.11
Spread	1.16	0.98	0.95

Table 6: Time mean of observation error variance (σ_o^2), adaptive inflation (Δ), the ensemble forecast mean rms error (*note that we show forecast error rather than analysis error as in Table 5*) and the ensemble forecast spread, for the case 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 σ_o^2 and Δ.

As shown in Table 6, even though the spread agrees quite well with the forecast error in case B compared to that in case A, the analysis error (Table 5) and forecast error (Table 6) in case B are bigger than those with best tuned inflation (case A). This apparent contradiction can be attributed to the fact that inflating the background error with a uniform inflation factor is not good enough to parameterize large model bias. Recall that multiplicative inflation assumes that the model error is in proportional to the forecast spread, which implies that the model errors and the forecast errors have the same error structures, but for large biases this is not a good assumption. A systematic bias with a sine-function in space, as in our experiments, cannot be well represented by the dynamical growing error. The adaptive inflation estimation scheme OMB^2 does not know about the spatial structure of model error since it only uses information about the trace of covariance rather than its structure. Thus $\widetilde{\Delta} = \frac{\mathbf{d}_{o-b}^T \mathbf{d}_{o-b} - Tr(\mathbf{R})}{Tr(\mathbf{H}\mathbf{P}^b\mathbf{H})} - 1$ produces a single value of inflation optimal when spatially averaged but not for individual grid points. Thus, although the spatially-averaged spread in Table 6 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 modeling bias structure by over-inflating the ensemble covariance to give more weights to the observations.

As a result, the best-tuned inflation is always larger than the adaptive inflation. The bigger the model bias, the bigger the over-estimation (Table 5). These results are consistent with those of Anderson (2007) where an adaptive inflation from a hierarchical Bayesian method was compared to the best tuned time-constant inflation. With the suboptimal inflation from OMB^2 (actually under-estimating the best tuned inflation) it is not surprising that the results in case C are even worse when the observational error are also estimated because the suboptimal inflation could affect the accuracy of the estimated σ_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 σ_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 *et al.* (2005), Danforth *et al*. (2007), and Li (2007) for several successful methods to estimate the bias.

5. SUMMARY AND DISCUSSION

The accuracy of an analysis system depends on the use of appropriate statistics of observation and background errors. For ensemble-based Kalman filter, tuning the covariance inflation parameter is expensive, especially if this parameter depends on space and on the type of variables. The online estimation method can objectively estimate the covariance inflation parameter but requires accurate information on observational errors. In this study, we estimate observational errors and the inflation coefficient for the background error simultaneously within LETKF. The results with Lorenz-96 model 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 on-line, our approach works impeccably in a perfect model scenario, as well as with random model errors and a small bias. The estimated observation error variances are very close to their true value, 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 with a globally constant inflation factor tends to underestimate the observation error variance and results a sub-optimal analysis. This is not surprising, since the covariance inflation has a very different structure than the model bias and cannot represent it well.

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 observation is non-uniformly distributed. With a spatially dependent inflation, we may be able to better deal with irregularly observing network. Tuning the spatial-dependent inflation is not feasible in practice, whereas the adaptive inflation, if successful, could be easily implemented.

Although here we only presented the results of our approach in a low-order model where only one type of observations is available, an additional series of experiments using a more realistic global primitive equations model known as SPEEDY (Molteni, 2003; Miyoshi 2005) has shown that the approach is also able to retrieve the true observation error variances for different types of instruments when assimilating wind, temperature and pressure observations with errors of different size and units (Li, 2007).

We also note that in this study we have focused on multiplicative covariance inflation, but that our simultaneous approach is equally applicable to adaptively estimate the scale of the additive noise in additive inflation schemes (Corazza *et al,* 2002, Whitaker *et al*., 2007).

We have addressed the issue of observation error variance but the presence of observational error correlations is another potential problem, especially when dealing with satellite observations. We plan to extend our approach to estimate off-diagonal terms in the observation error covariance and investigate whether this approach will be able to adaptively estimate the observation error correlations as well as their variances.

6. ACKNOWLEDGEMENTS

This research was partially supported by NASA grant NNG04G29G.

7. REFERENCES

Anderson, J. L. and S.L. Anderson, 1999: A Monte Carlo implementation of the nonlinear filtering problem to produce ensemble assimilations and forecasts. *Mon. Wea. Rev.* **127,** 2741–2758.

Anderson, J. L., 2007: An adaptive covariance inflation error correction algorithm for ensemble filters. *Tellus*, **59A**, 210-224.

Baek, S.J., B. R., Hunt, E. Kalnay, E. Ott, and I. Szunyogh 2006: Local ensemble Kalman filtering in the presence of model bias, *Tellus*, **58A**, 293-306.

Cardinali, C, S. Pezzuli, and E. Andersson, 2004: Influence matrix diagnostic of a data assimilation system. *Q. J. R. Meteo. Soc*, **130**, 2767-2786.

Chapnik B., G. Desroziers, F. Rabier and O. Talagrand, 2006: Diagnosis and tuning observational error in a quasi-operational data assimilation setting. *Q. J. R. Meteo. Soc*, **132**, 543-565.

Corazza, M., E. Kalnay, D. J. Patil, S.-C. Yang, R. Morss, M. Cai, I. Szunyogh, B. R. Hunt, and J. A. Yorke, 2002: Use of the breeding technique to estimate the structure of the analysis "error of the day". *Nonlinear Processes in Geophysics*, **10**, 233-243.

Danforth, C., E. Kalnay, and T. Miyoshi, 2007: Estimating and correcting global weather model error. *Mon. Wea. Rev.*, **135**, 281-299.

Dee, D. P., 1995: On-line estimation of error covariance parameters for atmospheric data assimilation. *Mon. Wea. Rev*., **123**, 1128-1196.

Dee, D. P. and A. M. Da Silva, 1998: Data assimilation in the presence of forecast bias. *Quart. J. Roy. Meteor. Soc.*, **124**, 269-295.

Desroziers G. and S. Ivanov, 2001: Diagnosis and adaptive tuning of osservation-error parameters in a variational assimilation. *Q. J. R. Meteor. Soc*, **127,** 1433-1452.

Desroziers G., L. Berre, B.Chapnik, and P.Poli, 2005: Diagnosis of observation, background and analysis error statistics in observation space. *Q. J. R. Meteor. Soc*, **131**, 3385-3396.

Houtekamer, P. L., H. L. Mitchell, G. Pellerin, M. Buehner, M. Charron, L. Spacek, and B. Hansen, 2005: Atmospheric data assimilation with an ensemble Kalman filter: Results with real observations. *Mon. Wea. Rev.*, **133**, 604-620.

Hunt, B. R., E. Kostelich, I. Szunyogh, 2007: Efficient data assimilation for spatiotemporal chaos: a local ensemble transform Kalman filter. *Physica D*, **230**, 112-126.

Kalnay, E., 2003: Atmospheric modeling, data assimilation and predictability. Cambridge University Press, 341 pp.

Li, H. 2007: Local ensemble transform Kalman filter with realistic observations, PhD Thesis at the University of Maryland.

Lorenz E. N., and K. A. Emanuel, 1998: Optimal sites for supplementary weather observations: Simulation with a small model. *J. Atmos. Sci.*, **55**, 399–414.

Molteni, F., 2003: Atmospheric simulations using a GCM with simplified physical parametrizations. I: Model climatology and variability in multi-decadal experiments. *Climate Dyn.*, **20**, 175-191.

Miyoshi, T., 2005: Ensemble Kalman filter experiments with a primitive-equation global model, PhD Thesis at the University of Maryland.

Miyoshi, T., S. Yamane, 2007: Local ensemble transform Kalman filtering with an AGCM at a T159/L48 resolution. *Mon. Wea. Rev.*, **135,** 3841-1677.

Ott, E., B. R. Hunt, I. Szunyogh, A. V. Zimin, E. J. Kostelich, M. Corazza, E. Kalnay, D. J. Patil, and J. A. Yorke, 2004: A local ensemble Kalman filter for atmospheric data assimilation. *Tellus*, **56A**, 415-428.

Snyder, C., and F. Zhang, 2003: Assimilation of simulated Doppler rador observations with an ensemble Kalman filter. *Mon. Wea. Rev.*, **131,** 1663-1677.

Szunyogh, I., E. J. Kostelich, G. Gyarmati, E. Kalnay, B. R. Hunt, E. Ott, E. Scatterfield and J. A. Yorke, 2007: A local ensemble transform Kalman filter data assimilation system for the NCEP global model. *Tellus*, accepted.

Talagrand, O., 1999: a posteriori verification of analysis and assimilation algorithms. Proceeding of workshop on *Diagnosis of Data Assimilation Syst*em, November 1998, Reading, United Kingdom: ECMWF, 17-28

Wang, X., and C. H. Bishop, 2003: A comparison of breeding and ensemble transform Kalman filter ensemble forecast schemes. *J. Atmos. Sci.*, **60**, 1140-1158.

Whitaker, J. S., and T. M. Hamill, 2002: Ensemble data assimilation without perturbed observations. *Mon. Wea. Rev.*, **130,** 1913-1924.

Whitaker, J. S., T. M. Hamill, X. Wei, Yucheng Song and Z. Toth, 2007: Ensemble data assimilation with the NCEP global forecasting system. *Mon. Wea. Rev.,* to appear.

Zhang, F., Z. Meng and Aksoy, 2006: Test of an ensemble Kalman filter for mesoscale and regional-scale data assimilation. *Mon. Wea. Rev.,* **134,** 722-736.

Table 6**:** Time mean of adaptive inflation Δ 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 ($\sigma^2_{o(s)}$=1). For comparison, the value of best tuned constant inflation and its resulting analysis error are also shown.

Δ method	$\sigma^2_{o(s)}$	Δ	RMSE
OMB^2	1	0.044	0.202
*AMB*OMB*	1	0.042	0.202
(tuned) constant	1	0.046	0.201

Table 7: Time mean of adaptive inflation parameter Δ 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 $\sigma^2_{o(s)}$ is either 1/4 or 4 times the true $\sigma^2_{o(t)}$ but without attempting to estimate and correct it. The inflation factor is constrained to be within an interval $-0.1 \le \tilde{\Delta}^o \le 0.2$. See text for the results when this constrained is removed.

Δ method	$\sigma^2_{o(s)}$	Δ	RMSE
OMB^2	0.25	0.2	0.265
*AMB*OMB*		0.2	0.262
OMB^2	4.0	0.021	1.635
*AMB*OMB*		0.033	1.523

Table 8: Time mean of adaptive inflation parameter Δ, the estimated observation error variance σ_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 miss-specified.

R method	Δ method	$\sigma_{o(ini)}^2$	σ_o^2	Δ	RMSE
*OMA*OMB*	*OMB²*	0.25	1.002	0.046	0.208
	*AMB*OMB*		1.003	0.043	0.205
	OMB²	4.0	1.000	0.046	0.202
	*AMB*OMB*		1.000	0.043	0.203

Table 9: Case A: best tuned constant inflation using true observation variance and the resulting analysis RMSE; Case B: time mean of adaptive inflation using true observation variance and the resulting analysis RMSE; Case C: time mean of simultaneous adaptive inflation and observation error, and the resulting analysis RMSE. Each case is tested for a wide range of α, amplitude of random model errors. Results are averaged over the last 1000 analysis steps.

Error amplitude (random)	A: true σ_o^2=1.0 (tuned) constant Δ		B: true σ_o^2=1.0 adaptive Δ		C: adaptive σ_o^2 adaptive Δ		
α	Δ	RMSE	Δ	RMSE	Δ	RMSE	σ_o^2
4	0.25	0.36	0.27	0.36	0.39	0.38	0.93
20	0.45	0.47	0.41	0.47	0.38	0.48	1.02
100	1.00	0.64	0.87	0.64	0.80	0.64	1.05

Table 10: As in Table 9, but in the presence of a constant model bias with different amplitudes (α).

Error amplitude (bias)	A: true σ_o^2=1.0 (tuned) constant Δ		B: true σ_o^2=1.0 adaptive Δ		C: adaptive σ_o^2 adaptive Δ		
α	Δ	RMSE	Δ	RMSE	Δ	RMSE	σ_o^2
1	0.35	0.40	0.31	0.42	0.35	0.41	0.96
4	1.00	0.59	0.78	0.61	0.77	0.61	1.01
7	1.50	0.68	1.11	0.71	0.81	0.80	1.36

Table 6: Time mean of observation error variance (σ_o^2), adaptive inflation (Δ), the ensemble forecast mean rms error (*note: here we show forecast error rather than analysis error in Table 5*) and the ensemble forecast 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 σ_o^2 and Δ. Results are reported as an average over the last 1000 steps of a 2000-step assimilation.

	A: true σ_o^2=1.0 (tuned) constant Δ	B: true σ_o^2=1.0 adaptive Δ	C: adaptive σ_o^2 adaptive Δ
σ_o^2	1.00	1.00	1.36
Δ	1.50	1.11	0.81
Error	0.94	0.99	1.11
Spread	1.16	0.98	0.95