Comparison between Four-Dimensional LETKF and Ensemble-Based Variational Data Assimilation with Observation Localization

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Abstract

In data assimilation for weather forecast, ensemble Kalman filter assumes linearity of the observation operator and Gaussianity of the probability distribution function (PDF) to explicitly solve the analysis. As a method avoiding errors based on these assumptions, we describe a four-dimensional ensemble-based variational method (4D-EnVAR) with observation localization. This formulation differs from that of the four-dimensional local ensemble transform Kalman filter (4D-LETKF) only in two points: (1) not assuming linearity of the observation operator and (2) calculating it globally. Using single-observation assimilation experiments and the observation system simulation experiments with a low-resolution atmospheric general circulation model, we demonstrate that 4D-EnVAR with observation localization has an advantage over 4D-LETKF because the observation operator is globally calculated in EnVAR.

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1. Introduction

In the four-dimensional data assimilation (temporal extension of the three-dimensional data assimilation), analyses are done with a flow-dependent forecast error covariance. In the four-dimensional variational method (4D-VAR), this error covariance is forecasted from a statistically estimated error covariance with the tangent linear model in a limited analysis window. In the ensemble Kalman filter (EnKF) method, on the other hand, the error covariance is derived from an ensemble forecast in which the forecast time is not limited; therefore, EnKF is generally preferable when the forecast error covariance is changeable. However, the analytical method in EnKF is simplified to explicitly solve the analysis variable (first guess) of ensemble transform Kalman filter (4D-LETKF, Hunt et al. 2007) method.

One unavoidable problem in developing an ensemble data assimilation system is the sampling error generated by limiting the number of ensemble members. To reduce this error, spatial localization should be used in EnVAR as well as in EnKF. In some EnVAR systems (e.g., Buehner 2005; Liu et al. 2009; Aonashi and Eito 2011), spatial localization has been applied to non-diagonal components of the forecast error covariance matrix (B localization). To improve the performance of parallel processing in making calculations, however, it is better to apply observation localization, the practice adopted in local ensemble transform Kalman filter (LETKF, Hunt et al. 2007) method.

In the present study, we designed a 4D-EnVAR system with observation localization and demonstrated that the result of 4D-EnVAR was closer to the true value than that of 4D-LETKF. Section 2 presents the formulation of our 4D-EnVAR system. In Section 3, we compare LETKF and EnVAR by means of single-observation assimilation experiments, and in Section 4, we compare them by means of observation system simulation experiments (OSSEs) using a low-resolution atmospheric general circulation model (AGCM). Section 5 presents discussions and summary.

2. Formulation of 4D-EnVAR with observation localization

The formulation of 4D-EnVAR in the present study is derived from the cost function J with the localized forecast error covariance matrix (B localization) defined as

\[ J = \frac{1}{2} \sum_{t=0}^{T} \left( x_t^f - \bar{x}_t^f \right)^T B_t \left( x_t^f - \bar{x}_t^f \right) + \frac{1}{2} \sum_{i=1}^{r} \left| H \left( x_{t,k}^f \right) \right|^2 R_k^{-1} \left| H \left( x_{t,k}^f \right) - y_t \right|^2, \]

(1)

where \( x_t^f \) is ensemble mean of vector \( \left( x_{t,1}^f, \ldots, x_{t,m}^f \right) \) and \( x_{t,i}^f \) is the analysis variable (first guess) of ensemble member \( j (1 \leq j \leq m) \) at point \( (1 \leq i \leq n) \) at time slot \( t (0 \leq t \leq T) \). \( y_t = \left( y_{t,1}, \ldots, y_{t,k} \right) \) and \( H \left( x_{t,k}^f \right) = \left[ H_t \left( x_{t,1}^f \right), \ldots, H_t \left( x_{t,k}^f \right) \right] \) are K-dimensional vectors at time slot \( t \). \( y_{t,k} \) is an observation at point \( k (1 \leq k \leq K) \) and \( H_t \left( x_{t,k}^f \right) \) is the observation operator to convert the value corresponding to observation \( y_{t,k} \) from analysis \( x_{t,k}^f \). \( R_k \) is \( K \times K \) observation error covariance matrix at time slot \( t \). In the present study, \( (k, k) \) component of \( R_k \) is defined as

\[ \left( R_k \right)_{kk} = \frac{R_{kk}}{m - 1} \left( k = k \right) \]

(2)

\( B_k \) is \( n \times n \) localized forecast error covariance matrix at time slot \( t \) and \( i, j \) component of \( B_k \) is

\[ \left( B_k \right)_{ij} = \frac{\alpha^2}{m - 1} \sum_{l=1}^{n} \delta x_{t,l}^f \delta x_{t,l}^f, \]

(3)

where \( \delta x_{t,l}^f = x_{t,l}^f - \bar{x}_{t,l}^f \) is ensemble perturbation of first guess \( \bar{x}_{t,l}^f \).
and $\alpha$ is the multiplicative inflation parameter to increase the underestimated forecast error perturbation (Anderson and Anderson 1999). $L_{ij}$ is the factor of the localization between points $i$ and $j$, defined as

$$L_{ij} = \begin{cases} \exp\left(-\frac{r_{ij}^2}{2\sigma^2}\right), & (r_{ij}^2 \leq \frac{10}{3}\sigma^2) \\ 0, & (r_{ij}^2 > \frac{10}{3}\sigma^2) \end{cases}$$

(4)

where $r_{ij}$ is the distance between points $i$ and $j$, and $\sigma$ is the constant called “localization length” (cf. Miyoshi et al. 2007).

Using Eqs. (2) and (3) and variable transformation from $x_i^t$ to $\tilde{w}_i$ by

$$\bar{x}_i^t = x_i^t + \sum_{j=1}^n L_{ij}^2 \delta x_j^t, \tilde{w}_i,$$

(5)

where $L_{ij} = \sum_{l=1}^\alpha L_{ij}^2 L_{il}^2 L_{lj}^2$, Eqs. (1) is rearranged to

$$\dot{\bar{y}} = \frac{m-1}{\alpha} \bar{w}_i + \sum_{j=1}^n \frac{1}{R_{ij}} H_i(x_i^t) \left[ H_i(x_i^t) - y_{ki} \right] = 0$$

(7)

To minimize $\dot{\bar{y}}$ as a function of $\tilde{w}_i$, is required, where

$$H_i(x_i^t) = \sum_{j=1}^n \frac{\partial H_i(x_i^t)}{\partial \bar{y}_i} = \sum_{j=1}^n \frac{\partial H_i(x_i^t)}{\partial x_j^t}$$

(8)

When $H_i(x_i^t)$ is linear and calculated only at observation point $k$, the right hand side of Eq. (8) is equal to $L_{ij}^2 \delta H_{ij}$, where $\delta H_{ij} = H_i(x_i^t + \delta x_j^t) - H_i(x_i^t)$. Therefore, from Eqs. (7), (8), and $L_i = \sum_{j=1}^n L_{ij}^2 L_{ij}^2$, is obtained. When $w_i$ is defined as $w_i = \sum_{j=1}^n L_{ij}^2 \tilde{w}_j$, Eqs. (5) and (9) are rearranged to

$$\bar{x}_i^t = x_i^t + \sum_{j=1}^n \delta x_j^t, w_j$$

(10)

respectively, where the left hand side of Eq. (11) is defined as $\partial \tilde{y}/\partial \tilde{w}_i$.

Eqs. (5) and (7) are approximately equal to Eqs. (10) and (11); in other words, the cost function $J$ is minimized by solving Eq. (11). Because $x_i^t$ can be calculated independently for each analysis point through Eq. (10), solving $w_i$ in Eq. (11) is easier than solving $\tilde{w}_i$ in Eq. (7) with parallel computing. For that reason, Eq. (11) was used in this system instead of Eq. (7).

The analysis ensemble perturbation in this 4D-EnVAR system

$$\delta x_{g,i}^t = x_{g,i}^t - \bar{x}_i^t$$

is calculated with the following equations:

$$\delta x_{g,i}^t = \sum_{j=1}^n \delta x_j^t, T_{ji},$$

(12)

$$T_{ji} = \sqrt{m-1} \sum_{n=1}^m U_{jn}^{\mathbf{w}},$$

(13)

where $T_{ji}$ is $(j, i)$ component of $m \times m$ transformation matrix from ensemble perturbation of first guess at point $i$, and $\lambda_j$ and $(U_{jn}^{\mathbf{w}}, \ldots, U_{mn}^{\mathbf{w}})$ are the $j$th eigenvalue and eigenvector of the Hessian $\nabla_i^2 J$. $\nabla_i^2 J$ is an $m \times m$ matrix and its $(j, j)$ component, derived from the left hand side of Eq. (11), is shown as

$$\nabla_i^2 J_{ji} = \frac{\partial^2 J}{\partial w_i \partial w_j} = \frac{m-1}{\alpha^2} \delta_{ij} + \sum_{k=1}^n L_{kj}^2 \delta H_{ik} \delta H_{jk}$$

(14)

To summarize the above formulation of 4D-EnVAR, the analysis $\bar{x}_i^t$ is calculated by Eqs. (10) and (11), and the analysis ensemble perturbation $\delta x_{g,i}^t$ is calculated by Eqs. (12)–(14). The resulting values of $\bar{x}_i^t$, and $\delta x_{g,i}^t$ become the initial values for the ensemble forecasts of the next cycle. Tangent-linear or adjoint versions of the observation operator and forecast model are not required in this method.

If the observation operator $H_i(x)$ is a linear function, then

$$\delta H_{g,i} = H_i(x_i^t + \delta x_{g,i}^t) - H_i(x_i^t)$$

(15)

Moreover, if $H_i(x_i^t)$ in Eq. (11) is linear and can be calculated from $x_i^t$ alone, then

$$H_i(x_i^t) = H_i(x_i^t) + \sum_{j=1}^n \delta H_{g,j}w_j.$$  

(16)

If these equations can be established, then $\partial \bar{y}/\partial \tilde{w}_i$ in Eq. (11) is a linear function of $\tilde{w}_i$ and $\nabla_i^2 J$ in Eq. (14) is independent of $\tilde{w}_i$; these Eqs. (11) and (14) then mean that exp($-J$), which is assumed to be the PDF in the variational method, is Gaussian.

When Eqs. (15) and (16) are established, $w_i$ is explicitly solved with Eqs. (11) and $T_{ji}$ is solved independently of $w_i$ from Tom Eq. (13). In this case, the equations to solve $w_i$ and $T_{ji}$ are independent for every analysis point $i$ and identical to the equations of LETKF with observation localization by the physical distance between analysis points $i$ and observation points $k$ (Hunt et al. 2007; Miyoshi et al. 2007). Therefore, the analysis and its perturbation of EnVAR are the same as those of LETKF when $H_i(x)$ is linear and analysis point $i$ is located at observation point $k$. In other words, the analysis and its perturbation of LETKF are obtained from Eqs. (10)–(14) if $H_i(x)$ is linear and $J$ is locally defined.

If the non-Gaussianity of the PDF is weak, then $\exp(-J)$ is a good approximation of the PDF (Tsyukui 2014). Therefore, the result from EnVAR, which minimizes globally defined $J$ without assuming linearity of $H_i(x)$, should be closer to the true value than that of LETKF when $H_i(x)$ is non-linear or when observations globally affect physically distant analysis points.

3. Single-observation assimilation experiments

To clarify the difference between LETKF and EnVAR arising from the use of Eqs. (15) and (16), we performed single-observation assimilation experiments, in which 20-member ensemble forecasts with the “simplified parameterizations, primitive-equation dynamics” (SPEEDY) model (Molteni 2003) were used for the first guess. The SPEEDY model is an AGCM with a T30L7 resolution (represented by 96 × 48 × 7 grid points), and the model variables are zonal and meridional winds (u, v), temperature $T$, specific humidity $q$, and surface pressure $p$. In the present study, these variables are also used as control variables in assimilation with LETKF and EnVAR.
Figure 1 shows the first guess made by the SPEEDY model, which included a zonal wind of $-9.8$ m s$^{-1}$ and relative humidity of 53.2%, at 180$^\circ$E, 20$^\circ$N, and 0.835$\sigma$ (sigma coordinate). We assimilated the single observation from that point to this first guess with LETKF and with EnVAR, where the horizontal and vertical localization lengths were 1000 km and 0.1$\sigma$, respectively.

For the first experiment, we assimilated a single observation of zonal wind $u = 5.0$ m s$^{-1}$ at 180$^\circ$E, 20$^\circ$N, and 0.835$\sigma$. In both LETKF and EnVAR, the analysis increments (differences between the analysis and the first guess) of horizontal wind were westerly near the observation point and on its south side, and easterly on the north side of the observation point (arrows in Figs. 2a, b). Analysis increments of relative humidity were positive to the north of the observation point and negative to the south (color in Figs. 2a, b). These results suggest that the distribution of relative humidity (Fig. 1) shifted to the direction of the incremental wind, which means that the flow-dependent error covariance was adopted properly in both LETKF and EnVAR.

Because the observation operator is the identity transformation (linear) in this case, Eqs. (15) and (16) are established in the EnVAR analysis at the observation point; therefore, the EnVAR and LETKF analyses of zonal wind at 180$^\circ$E, 20$^\circ$N, and 0.835$\sigma$ ($u = -0.9$ m s$^{-1}$) are identical (Figs. 2a, b). However, except for the zonal wind at the observation point, the analysis increment in EnVAR (Fig. 2b) was smaller than that in LETKF (Fig. 2a). This increment was smaller because the observation localization in EnVAR, which was shown to be almost the same as the $B$ localization in the previous section, was stronger (i.e., it ignored observation information more quickly with distance) than the observation localization in LETKF (Greybush et al. 2011).

We also assimilated a single observation of relative humidity (30.0%) at the same location. The resulting analysis increments in both LETKF and EnVAR (Figs. 2c, d) had the character of assimilation with the flow-dependent error covariance. In this case, the observation operator was the non-linear function of $T$, $q$, and $p$ at the observation point. Therefore, even at the observation point, the EnVAR analysis produced 39.6% relative humidity (Fig. 2d) as contrasted with 44.2% in the LETKF analysis (Fig. 2c).
4. Observation system simulation experiments

We also performed OSSEs with the SPEEDY model that compared 20-member ensemble forecasts from 4D-LETKF and 4D-EnVAR. In the OSSEs, the true value was defined as the forecast with the SPEEDY model. We used 20 forecasts from the initial true value, in which forecast times ranged from 744 to 972 hours at 12-hour intervals, for the initial values of the 20-member ensemble forecasts. A 6-hour assimilation window was used, extending 3 hours before and after the analysis time. Assimilated observations were created by adding random errors to the true values at 2-hour intervals at the points shown in Fig. 3, which were $u$, $v$, $T$, $p_s$, and the relative humidity as calculated from $T$, $q$, and $p_s$. The amplitudes of these random errors were 1 m s$^{-1}$ for $u$ and $v$, 1 K for $T$, 100 hPa for $p_s$, and 10% for relative humidity. The horizontal and vertical localization lengths were same as in the single-observation assimilation experiments (1000 km and 0.1 s, respectively). The multiplicative inflation parameter $\alpha$ (Anderson and Anderson 1999) was 1.1. The analysis-forecast cycle was repeated 160 times (40 days).

Differences from true values of the ensemble means of every-6-hour ensemble forecasts from the LETKF and EnVAR analyses are shown in Fig. 4. The root mean square errors (RMSEs) from EnVAR were generally smaller than those from LETKF (Figs. 4b, d). The biases of variables in EnVAR and LETKF were almost the same (e.g., Fig. 4a) except that the bias of specific humidity was smaller from EnVAR than from LETKF (Fig. 4c).

Figure 5 shows histograms of differences of observations assimilated in EnVAR from ensemble means of their forecasts (O – F) at all analysis times. Five of these histograms (Figs. 5a, b, c, d, e) were close to Gaussian. However, the histogram for specific humidity (which was not assimilated directly) was far from Gaussian (Fig. 5f), which is consistent with the result of ensemble experiments with 10,240 members (Miyoshi et al. 2014).

Locally calculating the observation operator is a major reason why the LETKF analysis in this OSSE was worse than the EnVAR analysis. In fact, even when all observation operators were linear (including direct assimilation of specific humidity rather than relative humidity), the RMSEs and the bias of specific humidity from EnVAR were smaller than those from LETKF (not shown). Moreover, when only non-linear $H_k(x)$ was treated like EnVAR but analyses were solved independently for every analysis point $i$ as in LETKF (an assimilation method called EnVAR-PNT hereafter), RMSEs and biases almost equaled those from LETKF (blue lines in Fig. 4) because the observation operator was locally calculated in EnVAR-PNT, as was the case in LETKF.

5. Summary and discussion

We developed an EnVAR system with observation localization, and examined the differences of this system from LETKF using single-observation assimilation experiments and OSSEs with the SPEEDY model. The single-observation assimilation experiments with the linear observation operator (Figs. 2a, b) showed that the observation localization in EnVAR, which is almost the same as the B localization, has stronger effects than the observation localization in LETKF (Greybush et al. 2011). In addition, we confirmed that with a non-linear observation operator (Figs. 2c, d), the EnVAR analysis at the observation point differs from the LETKF analysis although results from the two systems are the same with a linear operator.

The OSSEs showed advantages of our EnVAR system as compared to LETKF. Namely, the RMSEs of all model variables...
and the bias of specific humidity were generally smaller in 4D-EnVAR than in 4D-LETKF (Fig. 4). The smaller RMSEs in 4D-EnVAR are explained by how to calculate the observation operator: non-linear operator is globally calculated in EnVAR and linear operator is locally calculated in LETKF. The smaller bias of specific humidity in 4D-EnVAR results is because the PDF of specific humidity is especially far from Gaussian (Fig. 5f). Specific humidity is close to zero at more grid points than relative humidity, especially in the upper layer, which causes the difference from forecasts (O – F) to be far from Gaussian. If the PDF is weak non-Gaussian, the EnVAR analysis is better than LETKF one because EnVAR minimizes globally defined (more accurate) cost function.  

Optimal localization scales may be different between LETKF and EnVAR. However, RMSEs from EnVAR with this horizontal localization radius (1000 km) is smaller than those from any LETKFs with various horizontal localization scales (Fig. 6). This suggests that the EnVAR analysis in the present study is essentially better than LETKF one.

This advantage of the EnVAR analysis is mainly because the observation operator is globally calculated. The results of the EnVAR-PNT system show that the effect of non-linearity of the observation operator is relatively small, which means that the improvement resulting from globally calculating the observation operator is particularly important for accurate analyses in EnVAR.  

The computational cost for the analysis in the OSSE with 4D-EnVAR was several times greater than with LETKF. The main reason was that repeated identical calculations of the observation localization factor were needed to keep memory usage at the same level as LETKF. If the computational cost of the LETKF analysis is 10–20% of the cost of ensemble forecasts and the other processes in the forecast-analysis cycle as in semi-operational implementations (Hamrud et al. 2015; Bonavita et al. 2015) and these costs are proportional to the number of ensemble members, the cost of the EnVAR cycle is almost same as the LETKF one with 1.5–2.5 times number of members. In the OSSE framework of this study, EnVAR was still better than LETKF with twice the number of members (Fig. 6). However, we need to clarify whether EnVAR is practical even in operational implementations.

Fig. 5. Histograms of observation minus forecast for all analysis times in EnVAR: (a) zonal winds (m s$^{-1}$), (b) meridional winds (m s$^{-1}$), (c) temperature (K), (d) surface pressure (hPa), (e) relative humidity (%), and (f) specific humidity (g kg$^{-1}$). Note that specific humidity was not assimilated in the experiments shown in Fig. 4.

Fig. 6. Same as (a) Fig. 4b and (b) Fig. 4d but 6-hour forecasts from 20-member LETKF analyses with various horizontal localization (dotted light blue: 500 km, solid light blue: 800 km, solid black: 1000 km, solid green: 1200 km, dotted green: 1500 km), 40-member LETKF analysis with 1000-km horizontal localization (dotted black), and 20-member EnVAR analyses with 1000-km horizontal localization (red).
The 4D-EnVAR system with observation localization in the present study considers only accurately calculating the non-linear observation operator. The non-linearity of the forecast model also should be considered in efforts to gain more accuracy; however, repeated calculations of a non-linear model to minimize the cost function would require the much larger computational cost.

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Appendix

A pseudo-code description of the EnVAR algorithm proposed in the present study is shown below. Loops of the point $i$ are parallelized as in LETKF.

\[
w_i \leftarrow 0 \text{ for all } i \text{ and } j
\]
Repeat
- Compute $\overline{x_i}$ with Eq. (10) for each $i$
- Compute $H_{x_i}$ for each $k$
- Compute $\delta H_{x_i}$ for each $k$ and $j$
  For each $i$
  - Compute $L_x$ with Eq. (4) for each $k$
  - Compute $\partial J/\partial x_i$ for each $j$
  Update $w_i$ based on Eq. (11) for each $i$ and $j$
Until convergence
For each $i$
- Compute $L_x$ with Eq. (4) for each $k$
- Compute $\partial J/\partial x_i$ with Eq. (14) for each $i$, $j$, and $k$
- Eigenvalue decomposition of $\nabla^2 J$
- Compute $\delta x_i$ with Eqs. (12) and (13) for each $j$

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