AN INNER/OUTER LOOP ENSEMBLE-VARIATIONAL DATA ASSIMILATION METHOD

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ABSTRACT

Data assimilation (DA) for the non-differentiable parameterized moist physical processes is a complicated and difficult problem, which may result in the discontinuity of the cost function (CF) and the emergence of multiple extreme values. To solve the problem, this paper proposes an inner/outer loop ensemble-variational algorithm (I/OLEnVar) to DA. It uses several continuous sequences of local linear quadratic functions with single extreme values to approximate the actual nonlinear CF so as to have extreme point sequences of these functions converge to the global minimum of the nonlinear CF. This algorithm requires no adjoint model and no modification of the original nonlinear numerical model, so it is convenient and easy to design in assimilating the observational data during the non-differentiable process. Numerical experimental results of DA for the non-differentiable problem in moist physical processes indicate that the I/OLEnVar algorithm is feasible and effective. It can increase the assimilation accuracy and thus obtain satisfactory results. This algorithm lays the foundation for the application of I/OLEnVar method to the precipitation observational data assimilation in the numerical weather prediction (NWP) model.

KEYWORDS

Ensemble-variational Data Assimilation, Non-differentiable, Inner/Outer Loop.

1. INTRODUCTION

NWP is an initial/boundary value problem. The more accurate initial condition is, the better the quality of prediction will be [1,2]. DA is a method by which initial values for NWP can be yielded from observation data and short-term numerical prediction results. Due to large uncertainty in convective and stratiform condensation processes relating to clouds and precipitation, great importance has been attached to parameterized methods. Generally, these parameterized moist physical processes of cloud and precipitation in the NWP mode often contain non-differentiable processes, thus causing the discontinuity of DA cost function and the appearance of multiple extreme values [3,4].

The conventional variational adjoint method (ADJ) to DA is based upon the differentiability of the system; therefore, how to tackle the non-differentiable parameterized moist physical processes becomes a significant and difficult problem in the study of DA. To solve it, many researchers have carried out a lot of meaningful work, including ADJ improvement [5] and the application of many other methods, such as the smoothing and regularization method [6], the

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generalized tangent and adjoint method [7,8], the cluster method [9,10], the non-linear perturbation equation [2,11-14], the particle fliter and the genetic algorithm [15,16], etc. Nevertheless, these methods are more or less unsatisfactory, unable to find the global optimal solution or requiring huge efforts to modify the original nonlinear model and the corresponding adjoint model or to reconstruct the generalized tangent and adjoint model. Meanwhile, the particle filter method needs lots of particles and the genetic algorithm has to deal with the setting of parameters and other proplems (e.g. the population size or the probability of crossover and mutation) and the selection of genetic operators[17]. Therefore, the non-differentiable prblem in parameterized cloud and precipitation physical processes brings much trouble to the assimilation of actual observational data.

In recent years, the ensemble-variational data assimilation (EnVar) that absorbs the merits of the variational filter and ensemble filter has become the focus of the field. Qiu et al. proposed the four dimensional variational (4D-Var) method based on ensembles, using the technology of singular value decomposition (SVD-En4Dvar) [18]. Liu et al. applied the background error covariance estimated from forecast ensembles to variational data assimilation (VDA) and formed the ensemble-based variational method (En4DVar) [19]. Zupanski et al. put forward the maximum likelihood ensemble filter [20]. Wu Zhuhui et al. suggested a method based on regional successive analysis scheme [21]. Numerical results illustrated that the EnVar data assimilation can generate better assimilating effects than the ensemble Kalman filter and the 4D-Var method. Such a method can realize the flow-dependent evolution of the background error covariance matrix and improve the analytical quality of the dramatic element field of temporal spatial variation without much energy to complete and maintain the adjoint model [22, 23].

However, when the EnVar is used to deal with the non-differentiable parameterized moist physical processes, the discontinuity of CF still happens and multiple extreme values keep showing up. Using inner/outer loop thought and iterative method for reference [24-27], this paper combines the EnVar algorithm with the inner/outer loop algorithm and uses multiple linear quadratic function values to fit the cost function value of the original non-differentiable process. This approach can avoid the possible CF discontinuity and multiple extreme values and enable the function to converge to the global minimum point. As a result, it is named inner/outer loop ensemble-variational algorithm (I/OLEnVar). Numerical experimental results of DA for the non-differentiable process in cloud and precipitation indicate that such an algorithm requires no modification for the original non-linear numerical model and can better tackle the above-mentioned DA problems in cloud and precipitation procedures.

The rest of the paper is organised as follows. In Section 2, the I/OLEnVar Algorithm to DA is proposed and the algorithm process is described in detail. In Section 3, we present two numerical experiments (referred to as OSSEs) to gauge the performance of our I/OLEnVar approach. Finally, the paper is concluded with a summary and a few concluding remarks given in Section 4.

2. The I/OLEnVar Algorithm to DA

Based on the four dimensional sequenced ensemble-variational algorithm to DA, the CF is defined as:

$$J(\boldsymbol{x}) = \frac{1}{2}(\boldsymbol{x}-\boldsymbol{x}_b)^{\mathrm{T}} \boldsymbol{B}^{-1}(\boldsymbol{x}-\boldsymbol{x}_b) + \frac{1}{2}\sum_{k=1}^{K}\left(\boldsymbol{y}^k - H_k\left(\boldsymbol{x}^k\right)\right)^{\mathrm{T}} \boldsymbol{O}_k^{-1}\left(\boldsymbol{y}^k - H_k\left(\boldsymbol{x}^k\right)\right), \tag{1}$$

in this equation, $\boldsymbol{x}_b$ is the ambient field, $\boldsymbol{B}$ is the background error covariance matrix, $\boldsymbol{y}^k$ is the observational data at the moment k, H_k is the observational operator at the moment k, $\boldsymbol{O}_k$ is the observational error covariance matrix, the superscript T indicates the vector transition, K is the observation frequency in the assimilation window and $\boldsymbol{x}^k = M_k\left(\boldsymbol{x}\right)$ is the variable value of model predication at the moment k. The purpose of DA is to search for the analytical value $\boldsymbol{x}$ that coordinates with the numerical model so that the CF (1) can reach its minimum point.

With incremental representation [28, 29], the analytical result of Eq. (1) with EnVar method can be presented as:

$$\boldsymbol{x} = \boldsymbol{x}_b + \delta\boldsymbol{x}\ , \quad \delta\boldsymbol{x} = \boldsymbol{X}_b'\boldsymbol{w}\ , \tag{2}$$

where $\boldsymbol{X}_b' = \left(\boldsymbol{x}_1'\ , \boldsymbol{x}_2'\ , \ldots\ , \boldsymbol{x}_N'\right)$ is N initial ensemble perturbations, which satisfies $\boldsymbol{B} \approx \dfrac{\boldsymbol{X}_b'\left(\boldsymbol{X}_b'\right)^{\mathrm{T}}}{N}$. N represents the number of ensemble prediction members and $\boldsymbol{w} = \left(w_1, w_2, \ldots\ , w_N\right)^{\mathrm{T}}$ accounts for the weighting factor. To have the CF reach its minimum by using the quasi-Newton method, conjugate gradient method or other optimal iterative algorithms, a method similar to previous literature [19, 30] is adopted to form a CF when the control variable in the 4D ensemble-variational method is $\boldsymbol{w}$ and generate the gradient equation for its control variables. They are as follows:

$$J\left(\boldsymbol{w}\right) = \frac{1}{2}N\boldsymbol{w}^{\mathrm{T}}\boldsymbol{w} + \frac{1}{2}\sum_{k=1}^{K}\left(\boldsymbol{I}^k - \boldsymbol{H}_k\boldsymbol{M}_k\boldsymbol{X}_b'\boldsymbol{w}\right)^{\mathrm{T}}\boldsymbol{O}_k^{-1}\left(\boldsymbol{I}^k - \boldsymbol{H}_k\boldsymbol{M}_k\boldsymbol{X}_b'\boldsymbol{w}\right),$$

$$\nabla_{\boldsymbol{w}}J = N\boldsymbol{w} + \sum_{k=1}^{K}\left(\boldsymbol{H}_k\boldsymbol{M}_k\boldsymbol{X}_b'\right)^{\mathrm{T}}\boldsymbol{O}_k^{-1}\left(\boldsymbol{H}_k\boldsymbol{M}_k\boldsymbol{X}_b'\boldsymbol{w} - \boldsymbol{I}^k\right),$$

where $\boldsymbol{I}^k = \boldsymbol{y}^k - H_k\left[M_k\left(\boldsymbol{x}_b\right)\right]$; $\boldsymbol{H}_k$ and $\boldsymbol{M}_k$ are tangent operators of the observational operator H_k and the model operator M_k respectively; and

$$\boldsymbol{H}_k\boldsymbol{M}_k\boldsymbol{X}_b' = \left(\boldsymbol{H}_k\boldsymbol{M}_k\boldsymbol{x}_1', \boldsymbol{H}_k\boldsymbol{M}_k\boldsymbol{x}_2', \ldots\ , \boldsymbol{H}_k\boldsymbol{M}_k\boldsymbol{x}_N'\right).$$

When the ensemble membership value of the results of the numerical computation is projected onto the observational space, it can be obtained that

$$\boldsymbol{H}_k\boldsymbol{M}_k\boldsymbol{x}_i' \approx H_k\left[M_k\left(\boldsymbol{x}_b + \boldsymbol{x}_i'\right)\right] - H_k\left[M_k\left(\boldsymbol{x}_b\right)\right], \left(i = 1, 2, \ldots\ , N\right).$$

By doing so, the use of tangent operators $\boldsymbol{H}_k$ and $\boldsymbol{M}_k$ is avoided and $\nabla_{\boldsymbol{w}}J$ is computed.

The I/OLEnVar algorithm to DA (see Figure 1) adopts the computation of the above-given CF for the gradient of the control variable. The inner loop needn't consider the non-linear effect of the observational and model operators. In process of inner loop, the $\boldsymbol{H}_k$ and $\boldsymbol{M}_k$ are considered to be constant and variable perturbations are presented in a linear development, and then nonlinear CF is replaced by a local quadratic function. As a result, the inner loop needs no numerical integration to get $J(\boldsymbol{w})$ and $\nabla_w J$, so a lot of computation can be saved. On the other hand, the outer loop contains the non-linear influence of the observational and model operators, and the $\boldsymbol{H}_k$ and $\boldsymbol{M}_k$ operators used in inner loop process are calculated. By outer loop and inner loop procedures' iteration and interaction, the analytical DA results obtained from the iterative algorithm can converge and approximate to the minimum value of the nonlinear CF.

During the DA for the non-differentiable process in moist physical processes, the non-differentiable, nonlinear process will lead to the discontinuity of the CF and the appearance of multiple extreme values (see Figure 2). The conventional variational adjoint gradient algorithm will cause the divergence of the assimilation or limited convergence to the local minimum. By adopting the I/OLEnVar algorithm (see Figure 2), we use several favorable (with continuous and single extreme values) sequences of local linear quadratic functions $J^1, J^2, \mathrm{L}, J^*$ to approximate to the actual nonlinear CF. Since function (1) possesses the nature of a linear quadratic function near the global minimum, extreme points of these sequences $\boldsymbol{x}^0, \boldsymbol{x}^1, \boldsymbol{x}^2 \mathrm{L}$ will approximate to the global minimum $\boldsymbol{x}^*$ of the nonlinear CF. Since the local quadratic function is a linear function in the inner loop of this algorithm, we can use optimal iterative algorithms to find the minimum of the quadratic function instead of numerical integration, which saves a lot of computation.

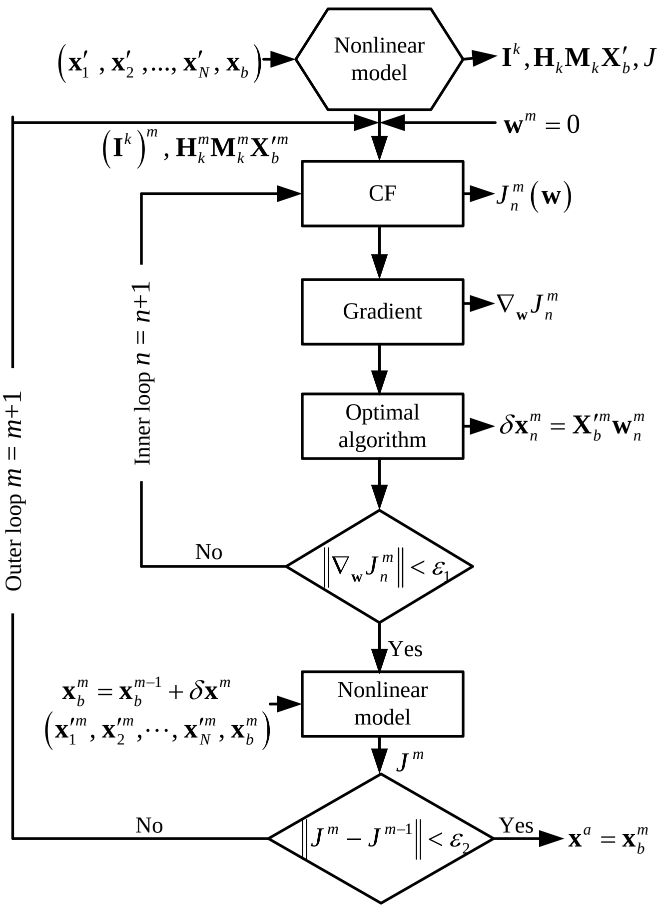

Figure 1. Flowchart of the I/OLEnVar algorithm

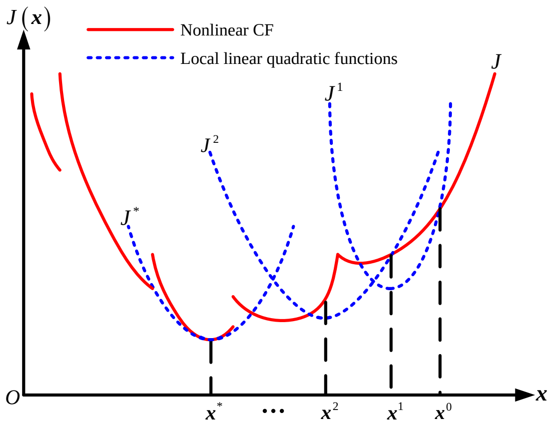

Figure 2. Illustration of the I/OLEnVar algorithm when the CF for the non-differentiable process is discontinuous and with multiple extreme values

The chosen optimal iterative algorithm in this paper is the conjugate gradient algorithm [31]. The following are the steps:

Step 1. Select an initial value $\boldsymbol{x}^0 = \boldsymbol{x}_b \Leftrightarrow \boldsymbol{w}_0 = 0$ and define $\boldsymbol{d}_0 = -(\nabla_w J)_0 = -\nabla_w J(\boldsymbol{w}_0)$.

Step 2. Compute $(\nabla_w J)_{i+1} = \nabla_w J(\boldsymbol{w}_{i+1})$.

Step 3. Let $\boldsymbol{d}_{i+1} = -(\nabla_w J)_{i+1} + \beta_i \boldsymbol{d}_i$, in which $\beta_i = \dfrac{(\nabla_w J)_{i+1}^{\mathrm{T}} (\nabla_w J)_{i+1}}{(\nabla_w J)_i^{\mathrm{T}} (\nabla_w J)_i}$ (the Fletcher-Reeve scheme) or $\beta_i = \dfrac{\left[(\nabla_w J)_{i+1} - (\nabla_w J)_i\right]^{\mathrm{T}} (\nabla_w J)_{i+1}}{(\nabla_w J)_i^{\mathrm{T}} (\nabla_w J)_i}$ (the Polak-Ribiere scheme).

Step 4. $\boldsymbol{w}_{i+1} = \boldsymbol{w}_i + \alpha_i \boldsymbol{d}_i$ and α_i satisfies the conditions that $J(\boldsymbol{w}_i + \alpha_i \boldsymbol{d}_i)$ is the minimum and $\boldsymbol{x}^{i+1} = \boldsymbol{x}_b + \boldsymbol{X}_b' \boldsymbol{w}^{i+1}$.

Step 5. Return to Step 2 and loop; if $\|\nabla_w J\| < \varepsilon$, stop the iteration.

3. NUMERICAL EXPERIMENTS AND RESULTS

3.1. Numerical Experiments of One-Dimensional Non-Differentiable Processes

During the non-differentiable changing of the moist physical processes, the equation describing the evolution of specific humidity at one grid point can be simplified as:

$$\begin{cases} \dfrac{dq}{dt} = F + \beta H(q - q_c), \\ q|_{t=0} = q_0. \end{cases} \tag{3}$$

This model [7, 9, 14, 16] is a typical model used to test the DA algorithm for the non-differentiable process. Where q represents the specific humidity, a scalar greater than 0. β is a constant and the source item caused by parameterization. F is the source item caused by other physical processes. $H(\cdot)$ is the Heaviside function, which is defined as:

$$H(q-q_c)=\begin{cases}0, & q<q_c,\\ 1, & q\ge q_c,\end{cases} \tag{4}$$

Where q_c denotes the saturation specific humidity (a threshold of precipitation). It can be known the Heaviside function that at the threshold q_c it is non-differentiable. Eq. (4) mimics the change of specific humidity q before and after the precipitation.

To discretize Eq. (4), q_k is recorded as the numerical solution of the discretization model when $t_k = k\Delta t\ (k=0,1,\ldots,N)$. When the initial value is q_0, the discrete form is

$$\begin{aligned} &q_0 = q_0, \\ &q_k = q_{k-1} + F\Delta t, && q_{k-1} < q_c, \\ &q_k = q_{k-1} + (F+\beta)\Delta t, && q_{k-1} \ge q_c, \end{aligned} \tag{5}$$

The time step is 0.05 and the integral step number N is 20. CF (1) can be simplified as

$$J(q_0)=\frac{1}{2}\sum_{k=0}^{N-1}\left(q_k-q_k^{obs}\right)^2\Delta t, \tag{6}$$

Where q_k^{obs} is the numerical solution when $q_0^{obs}=0.25$ and $t=k\Delta t$ and the observation data are supposed to be error-free. For other parameters, $F=2.0$, $\beta=-1.5$ and $q_c=0.46$. The CF is shown in Figure 3. We can see that it is discontinuous and has multiple extreme points. Since the conventional ADJ can only accurately compute the gradient of control variables when the CF is continuous, if this gradient is used in the iterative solution for the minimum value of the cost function, different initial values will lead to problems like non-convergent DA results or limited convergence to the local minimum.

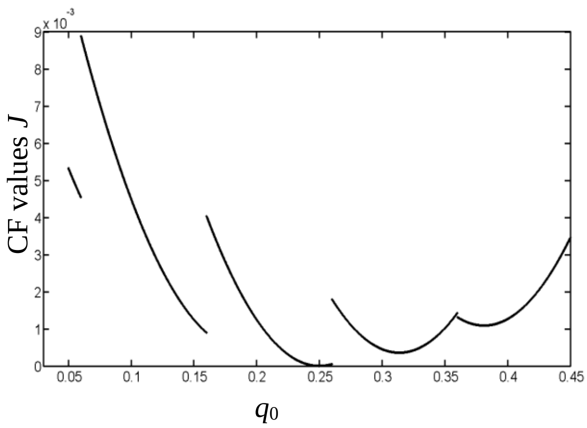

Figure 3. CF values under the influence of one-dimensional non-differentiable process in the precipitation

To test the effect of the I/OLEnVar to DA during the non-differentiable parameterized moist physical processes, a numerical experiment is conducted when 0.07, 0.16, 0.34 and 0.43 are selected as initial values. The number of ensemble members for the initial perturbation is 20, the variance is 2×10^{-3} and DA finally converges to a minimum value of 0.25. When the initial value is 0.43 and 0.07, the change of the normalized CF along with the increase of iteration number is given in Figure 4. In this numerical experiment, to get satisfactory results, the outer loop only needs 3 or 4 iterations while the inner loop 10 or 20 iterations. The experimental results preliminarily illustrate that the I/OLEnVar algorithm proposed by this paper is a feasible and effective solution to DA in the non-differentiable parameterized moist physical processes of cloud and precipitation. However, the experiment here targets a relatively simple and low-dimensional issue. In the following section, a more complicated and authentic model is adopted to further test the effectiveness of the I/OLEnVar algorithm.

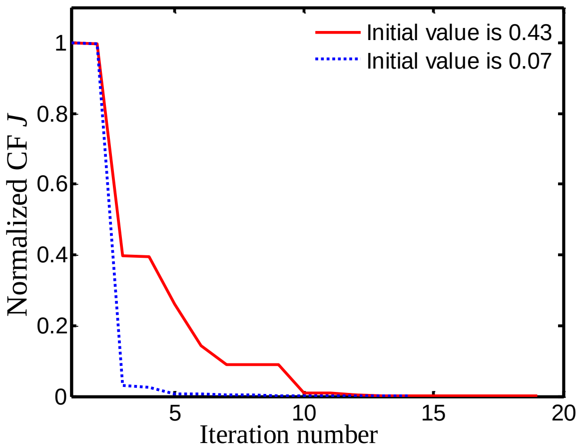

Figure 4. Change of the normalized CF along with the increase of iteration number in the one-dimensional non-differentiable numerical experiments

3.2. Numerical Experiments of High-Dimensional Non-Differentiable Processes

For the high-dimensional model of parameterized moist physical processes of cloud and precipitation, the equation that describes the evolution of specific humidity at grid point can been defined as follows [16]:

$$\begin{cases} \dfrac{\partial q}{\partial t}+\zeta\dfrac{\partial q}{\partial l}=F-\beta H\left(q-q_c\right), \\ 0\le l\le L, 0\le t\le T; \\ q\left(t,l\right)\big|_{t=0}=q_0\left(l\right), \\ 0\le l\le L; \\ \left.\dfrac{\partial q\left(t,l\right)}{\partial l}\right|_{t=0}=0, \\ 0\le t\le T. \end{cases} \tag{7}$$

Here $q(t,l)$ refers to the specific humidity, q_c denotes the saturation specific humidity, and l represents the horizontal variables x, y or the vertical variable z; $\zeta(t,l)$, the velocity in l direction, is a given function with first order continuous partial derivations; H, F and β have the same meanings as above.

Model (7) can be discretized in upwind scheme as follows:

$$q_0^i = q_0(l_i),\ i = 0,1,\ldots,I\ ;$$

when $i = 0$,

$$q_k^i = q_{k-1}^i + \left[F - gH\left(q_{k-1}^i - q_c\right)\right]\Delta t\ ;$$

when $1 \le i \le I$,

$$q_k^i = q_{k-1}^i - \frac{\Delta t}{\Delta l}\zeta\left(t_{k-1}, l_i\right)\left(q_{k-1}^i - q_{k-1}^{i-1}\right) + \left[F - gH\left(q_{k-1}^i - q_c\right)\right]\Delta t.$$

where Δt denotes the time step, $t_k = k\Delta t$, k is the time level, $1 \le k \le N$ and $N = T/\Delta t$, the total time levels in integration; Δl is the space step, $l_i = i\Delta l$, i is the space grid point and $I = L/\Delta l$, denoting the total number of space discrete levels.

In the numerical experiment, parameters $F = 8$, $g = 7$ and $q_c = 0.58$; $L = 1$, $\Delta l = 0.05$ and $I = 20$; $T = 1$, $\Delta t = 0.01$ and $N = 100$; $\zeta(t,l) = (1+t)(1-l)$ is the velocity along l direction. For this model, CF (1) can be simplified as:

$$J(q_0) = \frac{1}{2}\sum_{k=0}^{N-1}\sum_{i=0}^{I-1}\left[q_k^i - \left(q^{obs}\right)_k^i\right]^2 \Delta l \Delta t. \tag{8}$$

If the observation generates no errors, $\left(q^{obs}\right)_k^i$ is obtained through nonlinear numerical integration under the circumstance that the initial observation $\left(q^{obs}\right)_0^i = 0.28 - 0.26\sin\left(\pi i\Delta l/2\right), \left(i = 0,1,\ldots,I\right)$. To intuitively display the change of the CF with initial conditions, we fix $I-2$ components of the initial condition q_0^{obs} and change values of components q_0^5 and q_0^{15} at one grid point. The 3D contours of the corresponding CF are given in Figure 5. It can be seen that when the non-differentiable process occurs, the CF becomes discontinuous and has multiple extreme values.

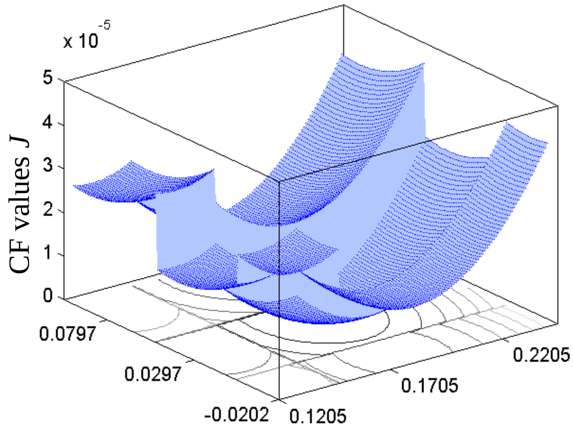

Figure 5. CF values under the influence of the non-differentiable process in cloud and precipitation

When the initial conditions are $q_0^i = 0.28 - 0.26\sin\left(\pi i \Delta l / 2\right) + 0.06$ (the experiment is referred to as plus 0.06) , $q_0^i = 0.28 - 0.26\sin\left(\pi i \Delta l / 2\right) - 0.06$ (the experiment is referred to as minus 0.06), and $\left(i = 0,1,\ldots,I\right)$, we carry out a comparative numerical experiment using the conventional EnVar algorithm and the I/OLEnVar algorithm. The experiment does not consider the influence of the observational errors. The ensemble member number of the initial perturbation is 40, and the variance is 2.25×10^{-4} . The change of the normalized CF with the increase of iteration number is displayed in Figure 6. It can be found that via the I/OLEnVar algorithm it only takes 9 or 10 iterations to decrease the CF to the lowest point in these two experiments. In contrast, when the conventional algorithm is applied, values of the CF oscillate as the iteration number increases and any effective decline cannot be easily realized.

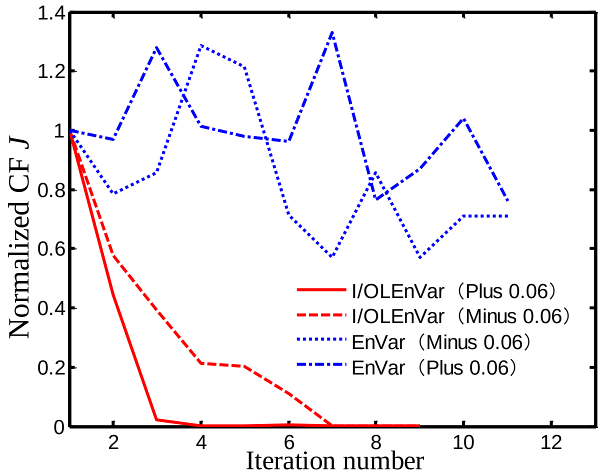

Figure 6. Change of normalized CF with the increase of iterations in the high-dimensional non-differentiable numerical experiments

4. CONCLUSIONS

In summary, the non-differentiable parameterized moist physical processes of cloud and precipitation can lead to the discontinuity of CF and the appearance of multiple extreme values for data assimilation. The conventional variational adjoint gradient algorithm may cause the divergence of assimilation or limited convergence to the local minimum. To solve these problems, we propose the I/OLEnVar algorithm based on the ensemble-variational method. This algorithm uses several favorable (with continuous and single extreme values) sequences of local linear quadratic functions to approximate to the actual nonlinear CF so as to let extreme point sequences of these local quadratic functions converge to the global minimum of the nonlinear CF. Apart from its simplicity and convenience, such an algorithm requires no adjoint model or modification of the original nonlinear numerical model, so DA can be easier. In addition, the nonlinear effects are considered at the outer-loop and the CF during the inner loop of the algorithm is a linear quadratic function, so the minimum point of the quadratic function can be computed by the optimal iterative algorithm instead of nonlinear numerical integration, which saves the computation cost. Numerical experimental results of DA for the non-differentiable process in cloud and precipitation indicate that the I/OLEnVar algorithm is feasible and effective. It can increase the assimilation accuracy and thus lead to satisfactory results.

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