Review of the development of ocean data assimilation

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Abstract

Data assimilation compensates for the deficiency of a numerical model and minimizes the short-term forecasting error by combining observation data and numerical results. Data assimilation has become a popular research topic all over the world in recent years. The development of ocean data assimilation is introduced in this paper. 4D variational and Kalman filter methods are considered the best means of data assimilation. Thus, these two methods are described in detail. Several novel research methods of assimilation, including assimilation with a constraint condition and dimensionality reduction, are discussed.

Keywords: data assimilation, 4D variational, Kalman filter

1 Introduction

Data assimilation originated from early meteorological methods. Assimilation methods integrate different space–time observations into a numerical model through physical and temporal constraints. During the development of ocean observation technology, the observations spread in a larger space–time range and promote assimilation methods. Data assimilation methods have been applied in many ocean operational numerical models. Using observations from various sources, assimilation methods improve the initial background accuracy and forecast capability. In this study, we review the development process of data assimilation, introduce the characteristics of these methods, and make a simple comparison of these methods. Furthermore, 4D variational and Kalman filter methods are discussed in detail.

2 Development of data assimilation

2.1 INTERPOLATION METHOD

Early methods are simple. They maximize the interpolation (such as linear or polynomial interpolation), and the information at the observation position is interpolated in the background grid. Interpolation methods ignore the error between observations and numerical results and do not consider the relationship among multi variables. Therefore, interpolation methods are less theoretical. Nudging, an interpolation method, was proposed by Gilchrist [1] in 1954. The nudging factor is introduced into the model equation. The observations affect the numerical values in the grid points within the radius of influence, and the nudging factor is inversely proportional to the distance from the observation position. The difference between model simulation and analysis of observations is reduced by revising the numerical values during the model process. An appropriate nudging factor should be determined. If a large factor is selected, model simulation will converge to the observations very fast, and the time steps become insufficient for dynamic adjustment. By contrast, a small factor increases the model error before the nudging adjustment is implemented.

2.2 OPTIMAL INTERPOLATION METHOD

Statistical theory was incorporated into assimilation methods until Gandin proposed the optimal interpolation (OI) method in 1963 [2]. OI considers the observation and model errors and determines the maximum joint probability in the law of maximum likelihood estimation. Several assumptions exist in OI method. Examples of such assumptions include the background and observation errors are unbiased, error distributions have a Gauss function, and the observation operator is linear. The amount of computation is small, and implementing the method in a time-invariant model is easy. Since 1970, OI method has been utilized widely in many operational numerical forecast systems. The analysis field is derived from observation increment multiplied by the optimal weight matrix and added to the background field. The optimal weight matrix is equal to the background field error covariance matrix in observation space multiplied by the inverse of the total error covariance matrix (background error covariance matrix plus observation error covariance matrix) in model space. White [3] assimilated Geosat altimetry sea level observations into a realistic wind-driven numerical synoptic ocean model of the California current in 1990. Mellor and Ezer [4] and Ezer and Mellor [5] proposed a continuous OI assimilation scheme with a primitive equation and multilayer numerical model and projected the surface observation information into a deep ocean. Tacker et al. [6] implemented the OI method and assimilated expendable bathythermographic

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(XBT) data for 1972 to 1991 into a hybrid coordinate ocean model (HYCOM) for the Atlantic Ocean. Bluelink [7] is Australia's contribution to the Global Ocean Data Assimilation Experiment (GODAE). BODAS is an ensemble optimal interpolation system that estimates background error covariance.

2.3 3D VARIATIONAL METHOD

Variational methods are utilized to determine the maximum value of the objective function to measure the distance between the model and observation fields through the Lagrange function. 3D variational method is essentially equivalent to OI method. Owing to the difference in the solutions of the two methods, the analysis fields are not exactly equal. Fu [8] discussed the similarities and differences between 3DVAR and Ensemble Optimal Interpolation. Dobricic et al. [9] described the development and evaluation of an oceanographic 3D variational (3D-VAR) data assimilation scheme based on a novel specification of the background error covariance. The new 3D-VAR scheme allows for regional variability of the background error covariance matrix, complex coastal boundary conditions, and variable bottom topography.

2.4 PHYSICAL SPACE STATISTICAL ANALYSIS

Another 3D assimilation method called physical space statistical analysis system (PSAS) was proposed by Cohn in 1998 [10]. The amount of computation in PSAS is less than that in 3D variational or OI method. The reduction in computation is due to two aspects. First, the objective function is based on observation space rather than model space. Generally, the dimensions of observation space are far less than those of model space. Second, solving the inverse background covariance matrix is avoided in the resolution process of PSAS [11].

2.5 4D VARIATIONAL METHOD

The methods described above are time invariant. 3D variational method is expanded to 4D method when the time dimension is involved in the objective function. Among variational approaches, 4D variational method provides the best estimate of the initial condition, which leads to an accurate fitting forecast during the assimilation of time windows. Powell et al. [12] applied the 4D variational method in the Intra-Americas Sea. Smith and Ngodock [13] also applied this method to the base of the Navy Coastal Model.

2.6 KALMAN FILTER

Kalman filter is another 4D method. The amount of computation in the extended Kalman filter is considerably large, and the method cannot be applied in operational forecasting systems. Thus, many simplified versions of the Kalman filter have been proposed; Ensemble Kalman filter [14] is one of them. Ensemble Kalman filter (EnKF) method with an ensemble size of K allows for K number of model integrations (such as OI or 3D variational) computation. However, the computation cost is less than that in the extended Kalman filter method. Simplified methods include reduced-order extended Kalman filter (ROEK) [15, 16], singular evolutive extended Kalman filter (SEEK) [17], ensemble Kalman smoother (EnKS), error subspace statistical estimation (ESSE) [18], singular evolutive interpolated Kalman filter (SEIK) [19], and reduced-order information filter (FOIF) [20].

The final analysis field of 4D variational method is similar to that of extended Kalman filter. The covariance matrix is implicit in the 4D variational computation process, and the implicit covariance matrix in the final state is inaccessible. However, Kalman method can explicitly generate the error covariance matrix in model space.

2.7 SUMMARY OF THE DEVELOPMENT PROCESS

Data assimilation methods developed from simple interpolation methods, such as nudging, to advanced assimilation methods with mathematical and physical theories. 4D variational and Kalman methods are popular topics in international research on data assimilation methods. For most countries and regions with forecast centers, the computation involved in the two methods is overwhelming because of the large amount of calculation. OI method is widely utilized in most operational forecast systems. The operational 4D variational system was applied in the European Centre for Medium-Range Weather Forecasts in 1997 and in France in 2000. However, Kalman method is rarely employed in operational forecasting.

3 Introduction of 4D variational method

4D variational method minimizes the objective function. The deviation between model results and observation data is minimized via adjustment of the control variable. In 4D variational method, observations at different times and locations can be employed in the same manner to obtain an accurate estimate of the initial condition. Satellite and radar observations are difficult to use in OI but easy to use in 4D variational method. 4D method is an extension of 3D method. Thus, the processing of observations, background error, and optimal algorithm are similar in the two methods. Nonlinear, tangent, and adjoint models are introduced in the assimilation method because the observations and the model field at different times are considered in the 4D method. In mathematics, the objective function of 4D method can be expressed as:

$$J(X_0)=\frac{1}{2}[X_0\text{-}X_0^b]^T B_0^{-1}[X_0\text{-}X_0^b]+ \frac{1}{2}\sum_{i=0}^{p}\left[H(X_i)\text{-}y_i^o\right]^T R^{-1}\left[H(X_i)\text{-}y_i^o\right], \tag{1}$$

where X_0 is the initial state of the forecast model, $X_0^{\ b}$ is the background field at initial time, y_i^o is the *i* observation, H is the observation operator, and X_i is the model result with the same time as y_i^o and originates from initial state X_0 through the nonlinear model, $x_i = M_{t_0,t_i}(x_0)$. The formula presents the process of the model from time t_0 to t_i.

This objective function is related to initial state X_0, and the model results during the assimilation window originate from initial state X_0. Thus, the objective function is composed of two factors, namely, J_b and J_o. J_b is the deviation between the background and analysis fields in the initial state. J_o is the deviation between the observations and analysis field during the assimilation of the window.

4D method requires an iterative solution of nonlinear, tangent, and adjoint model. Hence, the computation is extensive and related to the resolution of X_0. Ideally, the resolution of X_0 is similar to the model's. The cost of minimizing the objective function in high resolution is tremendous. Courtier's [21] research indicates that minimizing the incremental analysis of X_0 instead of X_0 itself significantly reduces the computational cost. The objective function is transformed into an incremental form, and the incremental analysis is minimized in low resolution. The low resolution incremental analysis result is transformed back to high resolution, and the final analysis result comprises the high resolution incremental analysis and initial state X_0. Thus, the computational cost is reduced with a low resolution.

Furthermore, the preconditioning process is necessary because it enhances the iterative efficiency. Preconditioning transforms the coordinator of initial state X_0 [22], decreases the Hessian matrix (the second derivative of the objective function) condition number, and accelerates the convergence rate of the iterative algorithm. Andrew 2011 [23] utilized preconditioning technology to reduce the computation time.

3.1 INCREMENTAL FORM OF 4D METHOD

Standard variational methods, such as steepest descent and conjugate gradient methods, result in large amounts of computation. Incremental method generates a Taylor series expansion at approximate solutions and approaches the more accurate approximation solution iteratively.

In the beginning of incremental method, the background field is the iterative initial value, $x_0^0 - x_b$. For the *n*-th iterator, the analysis value is $x_0^n = x_0^{n-1} + \delta x_0^n$. Thus, the incremental objective function is:

$$J\left(\delta x_0^n\right)+\frac{1}{2}\left[\delta x_0^n+\left(x_0^{n-1}-x_b\right)\right]^T B^{-1}\left[\delta x_0^n+\left(x_0^{n-1}-x_b\right)\right]+ \frac{1}{2}\sum_{i=0}^{p}\left\{H_i\left[M_{t_0,t_i}\left(x_0^{n-1}-\delta x_0^n\right)\right]-y_i^o\right\}^T R^{-1}\left\{H_i\left[M_{t_0,t_i}\left(x_0^{n-1}-\delta x_0^n\right)\right]-y_i^o\right\} ,\tag{2}$$

For the nonlinear model M_{t_0,t_i}, the Taylor series at x_0^{n-1} that ignores the second-order term is:

$$M_{t_0,t_i}\left(x_0^{n-1}-\delta x_0^n\right)=M_{t_0,t_i}\left(x_0^{n-1}\right)+L_{t_0,t_i}\left(\delta x_0^n\right).$$

Based on the hypothesis of the linear observation operator, H_i is:

$$H_i\left[M_{t_0,t_i}\left(x_0^{n-1}-\delta x_0^n\right)\right]\approx H_i\left[M_{t_0,t_i}\left(x_0^{n-1}\right)\right]+H_iL_{t_0,t_i}\left(\delta x_0^n\right). \tag{3}$$

Thus, the final incremental form is:

$$J\left(\delta x_0^n\right)+\frac{1}{2}\left[\delta x_0^n+\left(x_0^{n-1}-x_b\right)\right]^T B^{-1}\left[\delta x_0^n+\left(x_0^{n-1}-x_b\right)\right]+ \frac{1}{2}\sum_{i=0}^{p}\left\{H_i\left[L_{t_0,t_i}\left(\delta x_0^n\right)\right]-d_i^{n-1}\right\}^T R^{-1}\left\{H_i\left[L_{t_0,t_i}\left(\delta x_0^n\right)\right]-d_i^{n-1}\right\}, \tag{4}$$

d_i^{n-1} is the deviation between the model result and observation y_i^o, is expressed as:

$$d_i^{n-1}H_i\left[M_{t_0,t_i}\left(x_0^{n-1}\right)\right]-y_i^0=H_i\left[x_i^{n-1}\right]-y_i^0, \tag{5}$$

L_{t_0,t_i} is the tangent model to calculate disturbance quantity δx_i^n at time t_i.

The partial derivative of objective function is:

$$\frac{\partial J}{\partial \delta x_0^n}=B^{-1}[\delta x_0^n-(\delta x_0^{n-1}-x_b)]+ \sum_{i=0}^{p}L_{t_i,t_0}{}^T H_i^T R^{-1}\left(H_i\left[L_{t_0,t_i}\left(\delta x_0^n\right)\right]-d_i^{n-1}\right), \tag{6}$$

where $L_{t_i,t_0}{}^T$ is the adjoint model for resolving the initial disturbance from the final state reversely.

3.2 PRECONDITIONING

In the iteration process, preconditioning technology was adopted to accelerate the convergence. The inverse matrix of background error covariance matrix B^{-1} was utilized to determine the pre-conditioner as follows [24, 25]:

$$\delta x^n = Uv^n. \tag{7}$$

Transformational matrix U is the Cholesky decomposition of background error covariance matrix *B*.

Thus, $B = UU^T$. The new variable v^n is introduced as a control variable, so the new objective function is:

$$J\left(v^n\right) + \frac{1}{2}\left[\sum_{i=1}^{n} v^i\right]^T \sum_{i=1}^{n} v^i + \frac{1}{2}\sum_{i=0}^{p}\left\{H_i L_{t_0,t_i} U v^n + d_i^{n-1}\right\}^T R^{-1}\left\{H_i L_{t_0,t_i} U v^n + d_i^{n-1}\right\}. \tag{8}$$

After preconditioning, the condition number of the Hessian matrix is reduced and thus accelerates the convergence of the algorithm.

4 Kalman filter

The process of the Kalman filter is composed of forecast and analysis stages.

4.1 EXTENDED KALMAN FILTER

The extended Kalman filter can be expressed as follows:

1) Forecast stage:

$$x_i^b = M x_{i-1}^a, \tag{9}$$

$$P_i^b = L_{i-1} P_{i-1}^a L_{i-1}^T + Q. \tag{10}$$

2) Analysis stage:

$$K_i = P_i^b H^T [H P_i^b H^T + R]^{-1}, \tag{11}$$

$$x_i^a = x_i^b + K_i\left(y_i^o - H x_i^f\right), \tag{12}$$

$$P_i^a = \left[I - K_i H\right] P_i^b = \left[\left(P_i^b\right)^{-1} + H^T R^{-1} H\right]^{-1}, \tag{13}$$

M is the linear model, *P* is the error covariance matrix, *Q* is dynamic noise, *K* is the gain matrix, *y* is observation, and *H* is the observation operator. In the forecast stage, the forecast result and error covariance matrix were obtained. In the analysis stage, the gain matrix was obtained from the error covariance matrix. The analysis result and error covariance matrix are thus renewed.

Resolution of the error covariance matrix is computationally intensive in the extended Kalman filter. The dimension of *P* and *L* matrix is $n \times n$. In a typical operational forecast system, the number of is 10^7. Thus, the ensemble Kalman filter is utilized to reduce the computation.

4.2 EnKF

Extended Kalman filter is inapplicable because the operational ocean forecast system is a high-dimension nonlinear model, and the computation of the background error covariance matrix is extensive. EnKF is proposed to estimate the background error covariance matrix with an ensemble scheme. Monte Carlo short-term ensemble forecast is utilized to estimate the background error covariance matrix. At the initial moment, K initial model fields are generated from random disturbance. The optimal estimation model predictions are averaged by corresponding forecasts and expressed by the equation:

$$P_i^b \approx \frac{1}{K-1}\sum_{k=1}^{K}\left(x_k^f - \overline{x^f}\right)\left(x_k^f - \overline{x^f}\right)^T = \frac{1}{K-1} X^b X^{bT}. \tag{14}$$

Since Evensen [14] introduced EnKF into the ocean model in 1994, an increasing number of models adopted this method [26]. Miyazawa et al. [27] adopted the local ensemble transformation Kalman filter algorithm based on 20 members' ensemble simulations of the parallelized Princeton Ocean Model (Stony Brook Parallel Ocean Model) with a horizontal resolution of 1/36°. Deng [28] assumed that the statistical properties of the background errors do not change significantly at neighbouring analysis steps within a short time window and thus allow the ensembles generated in the previous steps to be used in the current steps. As such, a joint ensemble matrix that combines the ensembles of previous and present steps can be constructed to form a larger ensemble for estimating the background error covariance.

5 Frontier of ocean data assimilation

Current data assimilation research mainly focuses on two aspects: data assimilation with several constraints and reducing the computational complexity of assimilation.

5.1 DATA ASSIMILATION WITH CONSTRAINTS

In many cases, the value range of the control variable is limited by certain constraints. For example, salinity is distributed in a certain range and sea surface temperature is higher than the freezing point. These constraints contain useful information to improve the calculation precision. However, linear estimation methods (such as Kalman filter) cannot take advantage of this information on constraints. Recently, several methods were proposed to introduce constraints into data assimilation.

1) Adjustment operator method. Multivariate satellite observations [29] are assimilated into an isopycnic coordinate ocean model (Miami Isopycnic Coordinate Ocean Model). If a cold core ring of the Gulf Stream is absent from a model forecast and has to be introduced by the analysis, several layers must be corrected to outcrop at the bottom of the mixed layer. In this case, linear analysis would certainly introduce a number of negative layer thickness values that would need to be reset to zero. Simon [30] and Thacker [31] adopted similar methods.

2) Introduction of non-second-order terms to the objective function. The variational methods described above are based on the hypothesis of a quadratic objective function. The new algorithm should be proposed to minimize the non-quadratic objective function. Fujii [32] adopted two types of constraints in 3D oceanic variational analysis for the equatorial Pacific. One is the constraint for the variational quality control procedure, and the other is

employed to avoid density and temperature inversions.

3) Non-linear transformation for constrained variables. Bertino [33] reported that several positive variables are incorrectly described by the Gaussian model and can be addressed through the assimilation of their log transform. However, this approach may result in an asymmetric probability distribution.

4) Non-Gaussian error probability distribution function. Generally, assimilation methods with an error distribution assume that error probability distributions are Gaussian. The non-Gaussian distribution approach adopts an assimilation method with certain implicit constraints by modifying the probability distribution function. Lauvernet [34] showed that an optimal filter dealing with inequality constraints can be formulated under the assumption that the probability distributions are truncated Gaussian distributions. The statistical tools required to implement this truncated Gaussian filter were described. This method was then applied to a 3D hybrid coordinate ocean model (HYCOM) of the Bay of Biscay (at 1/15° resolution). The results revealed that the algorithm can deal with the hydrostatic stability condition in isopycnic and z coordinates.

A comparison of these four methods with constraints indicates that adjustment operator method lacks theoretical support because the process does not introduce the constraints and adjusts the model result forcibly to satisfy the constraints. A non-second-order objective function introduces the constraints via non-second-order terms, but the minimizing algorithm should be modified correspondingly. Non-linear transformation method may result in an asymmetric probability distribution. The non-Gaussian method has sufficient theoretical basis and allows for assimilation with certain implicit constraints by modifying the probability distribution function.

5.2 DIMENSIONALITY REDUCTION METHODS

To reduce the computation cost of assimilation, the objective function can be minimized in a subspace. By reducing the dimensions, the required memory and CPU can be reduced considerably. Generally, the control variables are projected onto a set of feature vectors, and most of the energy in the original space is reversed. Cai [35] employed bred vectors as feature vectors and found that minimizing the projection of the bred vectors on the observation-minus-analysis field may be a beneficial factor to achieving an operational forecast system.

Many dimensionality reduction methods for the Kalman filter have been developed. Cane [36] presented an approach to the Kalman filter that employs reduced state space representation for the required error covariance matrices. Kaplan [37-39] and Canizares [40] conducted similar dimensionality reduction research for meteorological and oceanographic historical datasets.

Blayo [41] and Durbiano [42] employed a low-dimensional space based on the first few EOFs or empirical orthogonal functions, which can be computed from a sampling of the model trajectory. Hoteit [43] and Robert [44] suggested reduced-order reduction method to improve the convergence rate of optimization by projecting the control vector onto a limited number and reducing the size of the control vector.

6 Summary

The development of data assimilation techniques was outlined in this paper. Two assimilation schemes, namely, 4D variational and Kalman filter, were introduced. In addition, several frontier ocean data assimilation methods, such as assimilation with a constraint condition and dimensionality reduction, were discussed.

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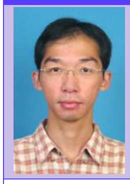

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