



Bayesian approach to the data assimilation problem based on the use of ensembles of forecasts and observations

Ekaterina Klimova ICT SB RAS

Introduction

•The task of data assimilation is usually understood as the time-sequential estimation of an unknown quantity from observational data.

• The purpose of data assimilation - both the preparation of initial fields for subsequent forecasting and the more general one - the description of the behavior of the studied fields over time, the study of climate, the estimation of parameters, etc.

Bayesian approach to the data assimilation problem

The time change of the estimated quantity:

$$\mathbf{x}^{k+1} = f_{k+1,k}(\mathbf{x}^k) + \mathbf{\eta}^k$$

The observations:

$$\mathbf{y}^k = h_k(\mathbf{x}^k) + \boldsymbol{\varepsilon}^k$$

 $\mathbf{\eta}^k$, $\mathbf{\epsilon}^k$ - random errors of forecast and observations

The Bayesian approach consists of applying the Bayes theorem to obtain an optimal estimate from observational data and a forecast:

$$p(\mathbf{x} | \mathbf{y}) = \frac{p(\mathbf{y} | \mathbf{x}) p(\mathbf{x})}{p(\mathbf{y})}$$

Bayesian approach to the data assimilation problem

There are various options for assessing the state of data and forecast:

 $p(\mathbf{x}_{l} | \mathbf{y}_{k,1}), k > l$ - forecast,

 $p(\mathbf{x}_k \mid \mathbf{y}_{k,1})$ - filtration,

 $p(\mathbf{x}_{k,0} | \mathbf{y}_{k,1})$ - smoothing,

where $\mathbf{x}_{k,0} = \{\mathbf{x}_k, \mathbf{x}_{k-1}, \dots, \mathbf{x}_0\}, \ \mathbf{y}_{k,1} = \{\mathbf{y}_k, \dots, \mathbf{y}_1\}.$

Bayesian approach to the data assimilation problem: the ensemble Kalman filter

Consider a nonlinear dynamic system $\mathbf{x}_{k}^{t} = f(\mathbf{x}_{k-1}^{t}) + \mathbf{\eta}_{k-1}^{t}$ An observation equation $\mathbf{y}_{k} = h(\mathbf{x}_{k}^{t}) + \mathbf{\varepsilon}_{k}^{t}$

 $\mathbf{\epsilon}_{k}^{t}$ and $\mathbf{\eta}_{k-1}^{t}$ are Gaussian random variables: $E(\mathbf{\epsilon}_{k}^{t}) = 0, E(\mathbf{\eta}_{k-1}^{t}) = 0$ $E[\mathbf{\epsilon}_{k}^{t}(\mathbf{\epsilon}_{k}^{t})^{T}] = \mathbf{R}_{k}^{t}, E[\mathbf{\eta}_{k-1}^{t}(\mathbf{\eta}_{k-1}^{t})^{T}] = \mathbf{Q}_{k-1}^{t}$

The ensemble Kalman filter consists of an ensemble of forecasts $\{\mathbf{x}_{k}^{f,n}, n=1,\dots,N\}$

$$\mathbf{x}_{k}^{f,n} = f(\mathbf{x}_{k-1}^{a,n}) + \mathbf{\eta}_{k-1}^{n}$$

and an ensemble of analyses $\{\mathbf{x}_{k}^{a,n}, n=1,\dots,N\} \mathbf{x}_{k}^{a,n} = \mathbf{x}_{k}^{f,n} + \mathbf{K}_{k}(\mathbf{y}_{k}^{n} + \mathbf{\varepsilon}_{k}^{n} - h(\mathbf{x}_{k}^{f,n}))$

Bayesian approach to the data assimilation problem: the ensemble Kalman filter

$$\mathbf{K}_{k} \text{ is a matrix of the form } \mathbf{K}_{k} = \mathbf{P}_{k}^{f} \mathbf{H}_{k}^{T} (\mathbf{H}_{k} \mathbf{P}_{k}^{f} \mathbf{H}_{k}^{T} + \mathbf{R}_{k})^{-1}$$

$$\mathbf{P}_{k}^{f} \triangleq \frac{1}{N-1} \sum_{n=1}^{N} \mathbf{d} \mathbf{x}_{k}^{f,n} (\mathbf{d} \mathbf{x}_{k}^{f,n})^{T}, \mathbf{R}_{k} \triangleq \frac{1}{N-1} \sum_{n=1}^{N} \boldsymbol{\varepsilon}_{k}^{n} (\boldsymbol{\varepsilon}_{k}^{n})^{T}$$

$$\overline{\mathbf{x}}_{k}^{f,n} \cong \frac{1}{N} \sum_{n=1}^{N} \mathbf{x}_{k}^{f,n} \quad \{\mathbf{d} \mathbf{x}_{k}^{f,n} = \mathbf{x}_{k}^{f,n} - \overline{\mathbf{x}_{k}^{f,n}}, n = 1, \cdots, N\} \quad \text{- an ensemble of forecast errors}$$

$$\{\mathbf{\varepsilon}_{k}^{n}, n = 1, \cdots, N\} \quad \text{- an ensemble of observation errors}$$

$$\{\mathbf{\eta}_{k-1}^{n}, n = 1, \cdots, N\} \quad E[\mathbf{\eta}_{k-1}^{n} (\mathbf{\eta}_{k-1}^{n})^{T}] = \mathbf{Q}_{k-1} \text{- an ensemble of model noise}$$

$$\mathbf{H}_{k} \text{ is the linearized operator } h(\mathbf{x}_{k}) \cong h(\overline{\mathbf{x}_{k}^{f,n}}) + \mathbf{H}_{k} \mathbf{\varepsilon}_{k}^{f}$$

The analysis error covariance matrix

$$\mathbf{P}_{k}^{a} \triangleq \frac{1}{N-1} \sum_{n=1}^{N} \mathbf{d} \mathbf{x}_{k}^{a,n} \left(\mathbf{d} \mathbf{x}_{k}^{a,n} \right)^{T}$$
$$\{\mathbf{d} \mathbf{x}_{k}^{a,n} = \mathbf{x}_{k}^{a,n} - \overline{\mathbf{x}_{k}^{a,n}}, n = 1, \cdots, N\}$$
$$\overline{\mathbf{x}_{k}^{a,n}} \cong \frac{1}{N} \sum_{n=1}^{N} \mathbf{x}_{k}^{a,n}$$

λ/

Bayesian approach to the data assimilation problem

- 1. Given a large sample of realizations for each of the prior *pdfs*, the joint *pdfs* can be evaluated by integration of each individual realization forward in time using stochastic model equation.
- 2. The prior *pdfs* do not need to be Gaussian distributed.
- 3. The analysis step of EnKF consists of the updates performed on each of the model state ensemble members.
- 4. For the case with a linear dynamical model a Gaussian prior *pdfs* the variance minimizing analysis equals the maximum likelihood estimate.
- 5. For a nonlinear dynamical model the *pdfs* for the model evolution will become non-Gaussian. In this case analysis will provide only an approximate solution.

Approaches to the implementation of ensemble Kalman filter

$$(Stochastic filter) = f_{k}(x_{k}^{t}) + \eta_{k}^{t}$$

$$(EnKF) = Ensemble of forecasts$$

$$x_{k+1}^{f(i)} = f_{k}(x_{k}^{a(i)}) + \eta_{k}^{(i)}$$

$$Ensemble of analysis$$

$$x_{k}^{a(i)} = x_{k}^{f(i)} + K_{k}(y_{k}^{0(i)} - H_{k}x_{k}^{f(i)})$$

$$\delta^{a} = \{x^{t} - \overline{x^{a(i)}}\}, \delta^{f} = \{x^{t} - \overline{x^{f(i)}}\}$$

$$\frac{True value''}{x_{k+1}^{t}} = f_{k}(x_{k}^{t}) + \eta_{k}^{t}$$

$$\frac{x^{a(i)} = \overline{x}^{a} + dx^{a(i)}}{dx^{a(i)}dx^{a(i)T}} = P^{a}$$

$$\frac{True value''}{x_{k+1}^{t}} = f_{k}(x_{k}^{t}) + \eta_{k}^{t}$$

$$\frac{x^{a(i)} = \overline{x}^{a} + dx^{a(i)}}{dx^{a(i)}dx^{a(i)T}} = P^{a}$$

$$\frac{True value''}{x_{k+1}^{t}} = f_{k}(x_{k}^{t}) + \eta_{k}^{t}$$

$$\frac{x^{a(i)} = \overline{x}^{a} + dx^{a(i)}}{dx^{a(i)}dx^{a(i)T}} = P^{a}$$

$$\frac{True value''}{x_{k}^{t}} = \{x^{t} - \overline{x^{a(i)}}\}, \delta^{f} = \{x^{t} - \overline{x^{f(i)}}\}$$

$$\frac{True value''}{(ESRF, ETKF, LETKF)}$$

Practical implementation of ensemble algorithms

- 1. Algorithms with the transformation of forecast ensembles.
- 2. Local algorithms.
- 3. Methods to increase ensemble spread.

Local Ensemble Transform Kalman Filter- LETKF (Hunt et al, 2007)

$$X^{a} = \{x^{a(i)} - \overline{x^{a(i)}}\}$$
$$X^{f} = \{x^{f(i)} - \overline{x^{f(i)}}\}$$

- the ensembles of analysis and forecasts

LETKF:

 ρ - "inflation factor".

1)
$$\tilde{P}^{a} = \left[(k-1)I / \rho + (Y^{f})^{T} R^{-1} Y^{f} \right]^{-1}, Y^{f} = HX^{f}$$

2) $W^{a} = \left[(k-1)\tilde{P}^{a} \right]^{1/2}$
3) $\bar{w}^{a} = \tilde{P}^{a}C(y_{o} - H\bar{x}^{f}), C = (Y^{f})^{T} R^{-1}$
4) $x^{a(i)} = \bar{x}^{f} + X^{f} w^{a(i)}, w^{a(i)} - i - th row of W$
5) $\bar{x}^{a} = \bar{x}^{f} + X^{f} \bar{w}^{a}$ 6) $P^{a} = X^{f} \tilde{P}^{a} \left(X^{f} \right)^{T}$

Ensemble π -algorithm

The ensemble π -algorithm is a stochastic filter in which the analysis step is performed only for the ensemble mean.

The ensemble of analysis errors **D** is a matrix the columns of which are vectors

$$\{\mathbf{dx}_k^n, n=1,\ldots,N\}$$

 $\mathbf{D}^{\mathrm{T}} = (\mathbf{I} + \mathbf{\Pi}^{\mathrm{T}})^{-1}\mathbf{B}^{\mathrm{T}}, \quad \mathbf{\Pi}^{\mathrm{T}} = (\mathbf{C} + 0, 25\mathbf{I})^{\frac{1}{2}} - 0, 5\mathbf{I}, \mathbf{C} = \frac{1}{N-1}\mathbf{F}^{\mathrm{T}}\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}(\mathbf{H}\mathbf{B} + \mathbf{E}) = \mathbf{C}_{1} + \mathbf{C}_{2}.$

B is a matrix with columns $\{\mathbf{b}_k^n, n = 1, ..., N\}$ $\mathbf{b}_k^n = \mathbf{x}_k^{f,n} - \overline{\mathbf{x}_k^{f,n}}$

E is a matrix with columns $\boldsymbol{\varepsilon}_k^n$ - the ensemble of observation errors

Klimova E. A suboptimal data assimilation algorithm based on the ensemble Kalman filter. Quarterly Journal of the Royal Meteorological Society. 2012. DOI: 10.1002/qj.1941. Klimova E.G. The Kalman stochastic ensemble filter with transformation of perturbation ensemble. Siberian. J. Nun, Math. /Sib. Branch of Russ. Acad. of Sci. – Novosibirsk, 2019. Vol. 22 N 1. P.27-40.

Classical particle filter

Ensemble $x^{(l)}$ of states representing the prior probability distribution p_k^b at time t_k .

The analysis step at time t_k : calculation of new weights

$$w_{(k,l)} = p_k^a(x^{(l)}) = cp(y_k | x^{(l)}) p_k^b(x^{(l)})$$

Gaussian particle filter

The Gaussian particle filter treats each particle as a Gaussian probability distribution

$$p(x_k | Y_{k-1}) = \sum_{l=1}^{L} N(x^{(b,l)}, B_{k-1})$$

$$p(x_k | Y_k) = \sum_{l=1}^{L} N(x^{(a,l)}, B_k)$$

The analysis ensembles $x^{(a,l)}$ are calculated by treating each particle as an individual Gaussian distribution:

$$x^{(a,l)} = x^{(b,l)} + K_k (y_k - H_k x^{(b,l)})$$
$$K_k = B_{k-1} H_k (H_k B_{k-1} H_k^T + R)$$
$$B_k = (I - K_k H_k) B_{k-1}$$

Nonlinear ensemble filter (T.Bengtsson, C.Snyder, D.Nychka J. of Geoph. Res. V. 108 No D24 2003)

Suppose that

$$p(x_{k} | Y_{k-1}) = \sum_{l=1}^{L} \pi_{k,l}^{f} N(x_{k,l}^{f}, P_{k,l}^{f})$$

$$p(x_{k} | Y_{k}) = \sum_{l=1}^{L} \pi_{k,l}^{a} N(x_{k,l}^{a}, P_{k,l}^{a})$$

$$x_{k,l}^{a} = x_{k,l}^{f} + K_{k,l}(y_{k} - H_{k}x_{k,l}^{f})$$

$$K_{k} = P_{k,l}^{f} H_{k}(H_{k}P_{k,l}^{f}H_{k}^{T} + R)$$

$$P_{k,l}^{a} = (I - K_{k}H_{k})P_{k,l}^{f}$$

$$\pi_{k,l}^{a} = \frac{\pi_{k,l} w_{l}}{\sum_{j=1}^{L} \pi_{k,j}^{f} w_{j}}$$
$$w_{l} = \left| (H_{k} P_{k,l}^{f} H_{k}^{T} + R) \right|^{-1/2} \exp[-1/2(y_{k} - H_{k} x_{k,l}^{f})^{T} (H_{k} P_{k,l}^{f} H_{k}^{T} + R)^{-1} (y_{k} - H_{k} x_{k,l}^{f})]$$

Ensemble of analysis $x_{k,j}^a = x_{k,j}^f + K_{k,j}(y_k + \varepsilon_j - H_k x_{k,j}^f)$

Sampling according to $p(x_k | Y_k)$

The behavior of ensemble spread in the ensemble Kalman filter (stochastic filter)

The stochastic ensemble Kalman filter can be written in the following form:

$$\mathbf{x}_{k}^{n} = (\mathbf{I} - \mathbf{K}_{k}\mathbf{H}_{k})\left[f(\mathbf{x}_{k-1}^{n}) + \mathbf{\eta}_{k-1}^{n}\right] + \mathbf{K}_{k}(\mathbf{y}_{k}^{n} + \mathbf{\varepsilon}_{k}^{n})$$

The optimal estimate in the ensemble Kalman filter is the ensemble mean value \mathbf{x}_{k}^{n}

Deviation from the mean (spread) simulates the estimate error $\mathbf{d}\mathbf{x}_k^n = \mathbf{x}_k^n - \mathbf{x}_k^n$

$$\mathbf{d}\mathbf{x}_{k}^{n} = (\mathbf{I} - \mathbf{K}_{k}\mathbf{H}_{k})(f(\mathbf{x}_{k-1}^{n}) - f(\mathbf{x}_{k-1}^{n}) + \mathbf{\eta}_{k-1}^{n}) + \mathbf{K}_{k}\mathbf{\varepsilon}_{k}^{n}$$

A 'theoretical' estimation error (skill) $\mathbf{d}\mathbf{x}_k^t = \mathbf{x}_k^t - \mathbf{x}_k^n$

$$\mathbf{d}\mathbf{x}_{k}^{t} = (\mathbf{I} - \mathbf{K}_{k}\mathbf{H}_{k})(f(\mathbf{x}_{k-1}^{t}) - f(\mathbf{x}_{k-1}^{n}) + \mathbf{\eta}_{k-1}^{t}) + \mathbf{K}_{k}\mathbf{\varepsilon}_{k}^{t}$$

The behavior of ensemble spread in the ensemble Kalman filter (deterministic filter)

The deterministic ensemble Kalman filter (analysis step) consists of the equation for the mean

$$\mathbf{x}_{k}^{a,n} = \mathbf{x}_{k}^{f,n} + \mathbf{K}_{k}(\mathbf{y}_{k}^{n} - h(\mathbf{x}_{k}^{f,n}))$$

and an estimate of the ensemble of analysis errors such that the corresponding covariance matrix satisfies the Kalman filter equation

$$\mathbf{P}_k^a = (\mathbf{I} - \mathbf{K}_k \mathbf{H}_k) \mathbf{P}_k^f$$

The transformation of an ensemble of forecast errors into analysis errors in a deterministic filter can be represented in the form of left multiplication

$$\mathbf{d}\mathbf{x}_{k}^{a,n} = \mathbf{A}_{k}\mathbf{d}\mathbf{x}_{k}^{f,n}$$
 where $\mathbf{A}_{k}\mathbf{P}_{k}^{f}\mathbf{A}_{k}^{T} = \mathbf{P}_{k}^{a}$

The ensemble of analyses of the deterministic filter:

$$\mathbf{x}_{k}^{a,n} = \mathbf{x}_{k}^{a,n} + \mathbf{A}_{k} (\mathbf{x}_{k}^{f,n} - \mathbf{x}_{k}^{f,n})$$

The equation for ensemble spread in the ensemble Kalman filter (stochastic filter)

The equation for ensemble spread in the stochastic Kalman filter

$$\mathbf{dx}_{k}^{n} = (\mathbf{I} - \mathbf{K}_{k}\mathbf{H}_{k})(\mathbf{F}_{k}\mathbf{dx}_{k-1}^{n} + \mathbf{\eta}_{k-1}^{n}) + \mathbf{K}_{k}\mathbf{\varepsilon}_{k}^{n}$$

Instead of the nonlinear model operator f we take the linearized operator \mathbf{F}_k

$$\mathbf{d}\mathbf{x}_{k}^{n} = \mathbf{\Psi}(k,0)\mathbf{d}\mathbf{x}_{0}^{n} + \sum_{i=1}^{k}\mathbf{\Psi}(k,i)\mathbf{K}_{i}\mathbf{\varepsilon}_{i}^{n} + \sum_{i=1}^{k}\mathbf{\Psi}(k,i)(\mathbf{I} - \mathbf{K}_{i}\mathbf{H}_{i})\mathbf{\eta}_{i-1}^{n}$$
$$\mathbf{\Psi}(k,i) = \prod_{j=i+1}^{k}(\mathbf{I} - \mathbf{K}_{j}\mathbf{H}_{j})\mathbf{F}_{j} \quad k > i$$

 $\Psi(k,k) = \mathbf{I}$

The estimation error

The estimation error (the deviation of the mean from the 'true' value)

$$\mathbf{d}\mathbf{x}_{k}^{t} = (\mathbf{I} - \mathbf{K}_{k}\mathbf{H}_{k})(\mathbf{F}_{k}\mathbf{d}\mathbf{x}_{k-1}^{t} + \mathbf{\eta}_{k-1}^{t}) + \mathbf{K}_{k}\mathbf{\varepsilon}_{k}^{t}$$

The simulated estimation error tends to the theoretical error if the random vectors of observational errors and model noise being simulated have the same covariance matrices as the true ones.

The behavior of ensemble spread in the ensemble Kalman filter (deterministic filter)

Writing the formula for the analysis perturbations in terms of 'left multiplication', we obtain the following equation for ensemble spread in the deterministic Kalman filter:

$$\mathbf{dx}_{k}^{n} = \mathbf{A}_{k} (\mathbf{F}_{k} \mathbf{dx}_{k-1}^{n} + \mathbf{\eta}_{k-1}^{n})$$

$$\mathbf{dx}_{k}^{n} = \mathbf{\Psi}_{det}(k, 0) \mathbf{dx}_{0}^{n} + \sum_{i=1}^{k} \mathbf{\Psi}_{det}(k, i) \mathbf{A}_{i} \mathbf{\eta}_{i-1}^{n}$$

$$\mathbf{\Psi}_{det}(k, i) \triangleq \prod_{i=i+1}^{k} \mathbf{A}_{j} \mathbf{F}_{j}$$

The formula for the deterministic filter lacks the term with $\mathbf{K}_i \mathbf{\epsilon}_i^n$

which simulates ensemble spread as a function of observational data distribution and observational error covariances.

Equation for estimation error (particle filter)

Given N independent samples x^1, \dots, x^N from a density p, an estimator of p can be obtained as a mixture of N Gaussian densities. In that case

$$\hat{x}^{a} = \sum_{j=1}^{N} \pi_{j}^{a} x_{j}^{a}$$
$$\varepsilon_{j}^{a} = (I - KH)\varepsilon_{j}^{f} + K\varepsilon^{o}$$
$$\varepsilon_{t} = (I - KH)\sum_{j=1}^{L} \pi_{j}^{a}\varepsilon_{j}^{f} + K\varepsilon^{o}$$

Methods of improving convergence in the ensemble Kalman filter

Some of the most frequently used methods of improving convergence of the ensemble Kalman filter are multiplicative inflation and additive inflation.

Let us consider the ensemble spread modification in general form. In the case of analysis step it has the form

$$\mathbf{dx}_{k}^{n} = \alpha_{k}\mathbf{dx}_{k}^{n} + \boldsymbol{\beta}_{k}^{n}$$

 $\boldsymbol{\beta}_k^n$ is a random vector with a specified covariance matrix

in the case of forecast step, the form

$$\mathbf{dx}_{k}^{n} = (\mathbf{I} - \mathbf{K}_{k}\mathbf{H}_{k})(\boldsymbol{\alpha}_{k}\mathbf{F}_{k-1}\mathbf{dx}_{k}^{n} + \boldsymbol{\alpha}_{k}\boldsymbol{\eta}_{k-1}^{n} + \boldsymbol{\beta}_{k}^{n}) + \mathbf{K}_{k}\boldsymbol{\varepsilon}_{k}^{n}$$

Methods of improving convergence in the ensemble Kalman filter

In the case of analysis step the formula for a stochastic filter

$$\mathbf{dx}_{k}^{n} = \tilde{\mathbf{\Psi}}(k,0)\mathbf{dx}_{0}^{n} + \sum_{i=1}^{k}\tilde{\mathbf{\Psi}}(k,i)\alpha_{i}\tilde{\mathbf{K}}_{i}\varepsilon_{i}^{n} + \sum_{i=1}^{k}\tilde{\mathbf{\Psi}}(k,i)\alpha_{i}(\mathbf{I}-\tilde{\mathbf{K}}_{i}\mathbf{H}_{i})\eta_{i-1}^{n} + \sum_{i=1}^{k}\tilde{\mathbf{\Psi}}(k,i)\beta_{i-1}^{n}$$

in the case of forecast step

$$\mathbf{dx}_{k}^{n} = \tilde{\mathbf{\Psi}}(k,0)\mathbf{dx}_{0}^{n} + \sum_{i=1}^{k}\tilde{\mathbf{\Psi}}(k,i)\tilde{\mathbf{K}}_{i}\boldsymbol{\varepsilon}_{i}^{n} + \sum_{i=1}^{k}\tilde{\mathbf{\Psi}}(k,i)(\mathbf{I}-\tilde{\mathbf{K}}_{i}\mathbf{H}_{i})\boldsymbol{\alpha}_{i}\boldsymbol{\eta}_{i-1}^{n} + \sum_{i=1}^{k}\tilde{\mathbf{\Psi}}(k,i)(\mathbf{I}-\tilde{\mathbf{K}}_{i}\mathbf{H}_{i})\boldsymbol{\beta}_{i-1}^{n}$$

$$\tilde{\boldsymbol{\Psi}}(k,i) \triangleq \prod_{j=i+1}^{k} \alpha_{j} (\mathbf{I} - \tilde{\mathbf{K}}_{j} \mathbf{H}_{j}) \mathbf{F}_{j}$$

 $\tilde{\mathbf{K}}_{i}$ is calculated using the modified covariance matrices

Methods of improving convergence in the ensemble Kalman filter

For a deterministic filter in the case of analysis step

$$\mathbf{dx}_{k}^{n} = \tilde{\mathbf{\Psi}}_{det}(k,0)\mathbf{dx}_{0}^{n} + \sum_{i=1}^{k}\tilde{\mathbf{\Psi}}_{det}(k,i)\alpha_{i}\mathbf{A}_{i}\mathbf{\eta}_{i-1}^{n} + \sum_{i=1}^{k}\tilde{\mathbf{\Psi}}_{det}(k,i)\boldsymbol{\beta}_{i}^{n}$$

in the case of forecast step

$$\mathbf{dx}_{k}^{n} = \tilde{\mathbf{\Psi}}_{det}(k,0)\mathbf{dx}_{0}^{n} + \sum_{i=1}^{k}\tilde{\mathbf{\Psi}}_{det}(k,i)\alpha_{i}\mathbf{A}_{i}\mathbf{\eta}_{i-1}^{n} + \sum_{i=1}^{k}\tilde{\mathbf{\Psi}}_{det}(k,i)\mathbf{A}_{i}\mathbf{\beta}_{i}^{n}$$
$$\tilde{\mathbf{\Psi}}_{det}(k,i) = \prod_{i=i+1}^{k}\alpha_{j}\mathbf{A}_{j}\mathbf{F}_{j}$$

The equation for the error when modifying the ensemble spread:

i=i+1

$$\mathbf{d}\mathbf{x}_{k}^{t} = \tilde{\mathbf{\Psi}}_{t}(k,0)\mathbf{\Delta}_{0}^{n} + \sum_{i=1}^{k}\tilde{\mathbf{\Psi}}_{t}(k,i)\tilde{\mathbf{K}}_{i}\mathbf{\varepsilon}_{i}^{t} + \sum_{i=1}^{k}\tilde{\mathbf{\Psi}}_{t}(k,i)(\mathbf{I}-\tilde{\mathbf{K}}_{i}\mathbf{H}_{i})\mathbf{\eta}_{i-1}^{t}$$
$$\tilde{\mathbf{\Psi}}_{t}(k,i) \triangleq \prod_{i=1}^{k}(\mathbf{I}-\tilde{\mathbf{K}}_{j}\mathbf{H}_{j})\mathbf{F}_{j}$$

Methods of improving convergence in the ensemble Kalman filter

- 1. The perturbation ensembles of deterministic and stochastic filters with the thus modified ensemble spread do not correspond to the error ensemble.
- 2. For $\beta_k^n = 0$ we obtain a version of multiplicative inflation.
- 3. For $\alpha_k = 1$ we obtain a version of additive inflation. In this case, additive inflation can be specified so that the covariance matrix coincides with the matrix obtained when using multiplicative inflation:

$$\boldsymbol{\beta}_{k}^{n} = \boldsymbol{\delta} \mathbf{Q}_{k} \boldsymbol{\xi}^{n}$$
$$\boldsymbol{\delta} \mathbf{Q}_{k} = (\boldsymbol{\alpha}_{k}^{2} - 1) \mathbf{P}_{k}$$

Numerical experiments. Lorenz-96 model

The equations of the model

$$\frac{\mathrm{d}x_j}{\mathrm{d}t} = (x_{j+1} - x_{j-2})x_{j-1} - x_j + F_0, \ j = 1, \cdots, J$$
$$x_{-1} = x_{J-1}, \ x_{J+1} = x_1,$$

★ x₁,...,x_J (J=40) are the variables being forecasted;
★ a fourth-order finite-difference Runge-Kutta scheme;
★ Δt = 0.05 corresponds to 6 hours (t=1 is taken for five days);
★ F₀ =8. To simulate 'true values' in the numerical data assimilation experiments, **x**^t₀ ≅ N(F₀/4;F₀/2)

and $N_t = 1000$ time steps are made.

Initial data for forecasting: $\mathbf{x}_{d}(0) = \mathbf{x}_{t}(0) + \boldsymbol{\delta} , \boldsymbol{\delta} \sim N(0, s_{0})$

The following parameters are specified for the numerical experiments:

an ensemble of initial fields: $\mathbf{x}^{n}(0) = \mathbf{x}_{d}(0) + \boldsymbol{\delta}^{n}, \, \boldsymbol{\delta}^{n} \sim N(0, s_{0}), \, n = 1, \dots, N$ X observations: $\mathbf{y}_0 = \mathbf{x}_1(0) + \mathbf{\delta}_0, \ \mathbf{\delta}_0 \sim N(0, \varepsilon_0)$ * an ensemble of observations X with perturbations: $\mathbf{y}_0^n = \mathbf{y}_0 + \mathbf{\delta}_0^n, \, \mathbf{\delta}_0^n \sim N(0, \varepsilon_0), \, n = 1, \cdots, N$ model noise: $\mathbf{\eta}^n = 0$ $\eta^{t} = 0.01$ in simulating the 'truth': $s_0 = \varepsilon_0 = 1$ in all experiments: N=20 $\mathbf{R} = \varepsilon_0^2 \mathbf{I}$

The observations are available at each of the J=40 model grid points.

The experimental period has a length 3000 time steps, with assimilation being done at each time step or at every four time steps.

The numerical experiments are performed for ten versions of the 'truth', and all estimates were calculated as average values over these ten versions.

The following estimates were considered:

$$rms = \frac{1}{K} \sum_{k=1}^{K} \left\{ \frac{1}{L} \sum_{i=1}^{L} (\overline{x_{k,i}} - x_{k,i}^{t})^{2} \right\}^{\frac{1}{2}}$$

- the root-mean-square error averaged over *K*=10 versions of calculations (*k* is the number of a version and *i* is the number of a grid node)

$$sp = \frac{1}{K} \sum_{k=1}^{K} \left\{ \frac{1}{L(N-1)} \sum_{i=1}^{L} \sum_{n=1}^{N} (\overline{x_{k,i}^{n}} - x_{k,i}^{n})^{2} \right\}^{\frac{1}{2}}$$

- the mean value of the covariance matrix trace calculated over *K*=10 versions of calculations (*n* is the number of an ensemble member).

Two series of experiments were performed. In the first series, observational data were simulated at one time step intervals, and in the second series, at four time step intervals. The following experiments were performed in each of the series:

Experiment 1. In this experiment, multiplicative inflation α was used. $\alpha = 1.1$ in the first series and $\alpha = 1.2$ in the second series).

Experiment 2. In this experiment, additive inflation was used so that the change in the covariance matrix coincided with the change made in experiment 1.



The results of the first series of experiments for the ensemble π -algorithm



The results of the first series of experiments for the LETKF algorithm



The results of the second series of experiments for the ensemble π -algorithm



The results of the second series of experiments for the LETKF algorithm.

Conclusion

- In the ensemble approach, at the analysis step it is important to specify the ensembles corresponding to the density of the analysis error distribution. It is necessary to take into account the ensemble of errors of observation.
- To regulate the convergence of ensemble algorithms, it is preferable to use additive inflation.
- The results of the investigations show that ensemble spread in stochastic filters rather than in deterministic filters is closer to the theoretical estimation error.
- Multiplicative inflation and additive inflation change the general formula for ensemble spread.
- The formula for ensemble spread in a stochastic filter with additive inflation rather than with multiplicative inflation is closer to that for the estimation error.

Thanks for attention!