Variational Ensemble Kalman Smoothing

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Introduction

- Various forms of Kalman filtering, especially different types of Ensemble Kalman filters and hybrid variational/ensemble Kalman filters, have become popular in geophysical data assimilation.
- Kalman filters work well but they have a characteristic defect in that, unlike 4DVar, they leave behind discontinuous model trajectories that do not correspond to physically consistent and continuous model states.
- This is a problem in areas such as re-analysis of climate history. For that reason, a smoothing operation that is consistent with the corresponding Kalman filter algorithm is highly desirable.

Introduction

- We have implemented and compared the resulting model trajectories and corresponding model errors of two advanced Kalman smoothers,
- The Variational Kalman Smoother (VKS) and the
- Variational Ensemble Kalman Smoother (VEnKS) that are based on
- The Variational Kalman Filter (VKF) and
- The Variational Ensemble Kalman Filter (VEnKF), respectively.

Introduction

The main benefits of Variational Ensemble Kalman Filter and Smoother from high-performance computing point-of-view are the following:

1. Accuracy comparable to EKF or FIKS (Fixed Interval Kalman Smoother)
2. Serial computational complexity proportional to that of 4DVar
3. Ensemble members can be executed in parallel
4. Error covariance matrices stored in vector form, so that their memory requirement is a linear multiple of that of 4DVar

Introduction

- The comparison is done using the Lorenz95 model, so that the resulting similarities and differences in forecast skill and the quality of the ensuing model trajectories can be clearly understood and discerned in subsequent analysis.
- VEnKF has also been run on a satellite data data assimilation system for algal blooms from which a one month analysis is presented.

Variational Kalman Filter (VKF)

- We shall assume a dynamic model $\mathcal{M}$ and an observation operator $\mathcal{K}$, the forecast and observation mappings are given by

$$\boldsymbol{x}_{k+1} = \mathcal{M}_k(\boldsymbol{x}_k) + \varepsilon_k, \qquad \boldsymbol{y}_{k+1} = \mathcal{K}_{k+1}(\boldsymbol{x}_{k+1}) + \eta_{k+1},$$

- The noise terms are assumed normally distributed zero mean stochastic processes with $\mathbf{C}_{\varepsilon_k}$ and $\mathbf{C}_{\eta_{k+1}}$ as their assumed covariance matrices, respectively, and k is a time index.
- In VKF the nonlinear forward model $\mathcal{M}$ must also be linearized to its tangent linear model $\mathbf{M}$ and its adjoint $\mathbf{M}^T$.

Variational Kalman Filter (VKF)

The Variational Kalman Filter (VKF) was introduced in **Auvinen et al** (2009) and its algorithm reads as:

Step 0: Select an initial guess $\mathbf{x}^a(t_0)$ and a covariance $\mathbf{P}^a(t_0)$, and set $i = 1$.

Step 1: Compute model state and prior covariance estimates:

(i) Compute $\mathbf{x}^f(t_i) = \mathcal{M}(t_i, t_{i-1})(\mathbf{x}^a(t_{i-1}))$;

(ii) Minimize $(\mathbf{P}^f(t_i))^{-1} = (\mathbf{M}_i \mathbf{P}^a(t_{i-1}) \mathbf{M}_i^{\mathrm{T}} +_i)^{-1}$

by the LBFGS method;

Variational Kalman Filter (VKF)

Step 2: Compute the Variational Kalman Filter state estimate and the posterior covariance estimate:

(i) Minimize

$$\ell(\mathbf{x}^a(t_i)|\mathbf{y}_i^o) = (\mathbf{y}_i^o - \mathcal{K}_i\mathbf{x}^a(t_i))^{\mathrm{T}}(\mathbf{R}_i)^{-1}(\mathbf{y}_i^o - \mathcal{K}_i\mathbf{x}^a(t_i)) +$$

$$(\mathbf{x}^f(t_i) - \mathbf{x}^a(t_i))^{\mathrm{T}}(\mathbf{P}^f(t_i))^{-1}(\mathbf{x}^f(t_i) - \mathbf{x}^a(t_i))$$

by the LBFGS method;

Variational Kalman Filter (VKF)

(ii) Store the result of the minimization as a VKF estimate $\mathbf{x}^a(t_i)$;

(iii) Store the limited memory approximation to $\mathbf{P}^a(t_i)$;

Step 3: Update $i := i + 1$ and return to Step 1.

Variational Kalman Smoother (VKS)

- The Variational Kalman Smoother iterates VKF over the entire assimilation window but instead of observations it uses the analysis from the previous iteration cycle as the observations.
- The VKF method provides an estimate $\mathbf{x}^a(t_i)$ and a corresponding limited memory approximation to the covariance matrix $\mathbf{P}^a(t_i)$ after each observation time step t_i.
- In nonlinear VKS, we use these results from the previous k_0 time steps, where the parameter k_0 determines the length of the time lag used.

Variational Kalman Smoother (VKS)

- We couple these results together by using the following cost function:

$$J(\mathbf{x}(t_{i-k_0})) = \sum_{\tau=i-k_0}^{i} (\mathcal{M}(t_\tau, t_{i-k_0})(\mathbf{x}(t_{i-k_0})) - \mathbf{x}^a(t_\tau))^{\mathrm{T}} \times$$

$$(\mathbf{P}^a(t_\tau))^{-1}(\mathcal{M}(t_\tau, t_{i-k_0})(\mathbf{x}(t_{i-k_0})) - \mathbf{x}^a(t_\tau)),$$

- The minimization of the cost function is done using the 4D-Var method, once again employing LBFGS as the minimization method.

Variational Ensemble Kalman Filter (VEnKF)

- The Variational Ensemble Kalman Filter (VEnKF) introduced first in **Solonen** (2012) is a hybrid method that uses a cost function similar to that of 3D-Var, with the innovation of estimating background covariance using an ensemble.
- The cost function is numerically minimized using a quasi-Newton method (e.g LBFGS).
- In this way VEnKF solves the memory issue that troubles many Kalman Filter methods, and it also addresses the difficulty of making tangent linear and adjoint codes, as they are not required in VEnKF.

Variational Ensemble Kalman Filter (VEnKF)

After setting the initial guesses for the state and covariance to $\boldsymbol{x}_0^{est}$ and $\mathbf{C}_0^{est}$, defining the initial ensemble $s_{0,i}$ and letting $k = 0$, the **VEnKF algorithm** is as follows:

1. Propagate both the model forecast and ensemble forecast forward in time
2. Define a matrix $\mathbf{X}_k$ as $\mathbf{X}_k = \left(\left(\boldsymbol{s}_{k,1} - \boldsymbol{x}_k^p\right), \ldots, \left(\boldsymbol{s}_{k,S} - \boldsymbol{x}_k^p\right)\right) / \sqrt{n}$ where n is the ensemble cardinality.
3. Calculate the prior covariance by Sherman Morrison Woodbury (SMW) matrix inversion $\mathbf{C}_{k+1}^p = \mathbf{X}_k {\mathbf{X}_k}^T + \mathbf{C}_{\varepsilon_k}$ to get $[\mathbf{C}_{k+1}^p]^{-1}$.

Variational Ensemble Kalman Filter (VEnKF)

4. Apply LBFGS to minimize the cost function (4) below. The minimizer is the filter estimate and the inverse Hessian of (4) equals $\mathbf{C}_{k+1}^{est}$

$$\mathrm{J}(\boldsymbol{x}|\boldsymbol{y}_{k+1}) = \frac{1}{2}\left(\boldsymbol{x} - \boldsymbol{x}_{k+1}^{p}\right)^{T}\left(\mathbf{C}_{k+1}^{p}\right)^{-1}\left(\boldsymbol{x} - \boldsymbol{x}_{k+1}^{p}\right) +$$

$$+ \frac{1}{2}\left(\boldsymbol{y}_{k+1} - \mathcal{K}_{k+1}\boldsymbol{x}\right)^{T}\left(\mathbf{C}_{\eta_{k+1}}\right)^{-1}\left(\boldsymbol{y}_{k+1} - \mathcal{K}_{k+1}\boldsymbol{x}\right)$$

5. Generate a new ensemble $\boldsymbol{s}_{k+1,i} \sim \mathcal{N}\left(\boldsymbol{x}_{k+1}^{\mathrm{est}}, \mathbf{C}_{k+1}^{\mathrm{est}}\right)$. Go to 1.

Variational Ensemble Kalman Filter (VEnKF)

An important characteristic of VEnKF is therefore very frequent regeneration of new ensembles. Its analysis does not guarantee continuity of either the state or the error covariance matrix.

Variational Ensemble Kalman Smoother (VEnKS)

- The Variational Ensemble Kalman Smoother is inspired by the relationship between VKF and VKS. But because VEnKF does not use a tangent linear or adjoint model, VEnKS cannot accomplish its task of taking into account observations from the future as well as from the past by repeated application of VEnKF.
- However, it can ensure continuity of both the state and the error covariance by imposing increasing length upon its ensembles.
- Like VKS, it does replace original observations by analysis results from the previous iteration, but in this case these include both the state and the ensemble that forms the low-memory approximation to the error covariance.

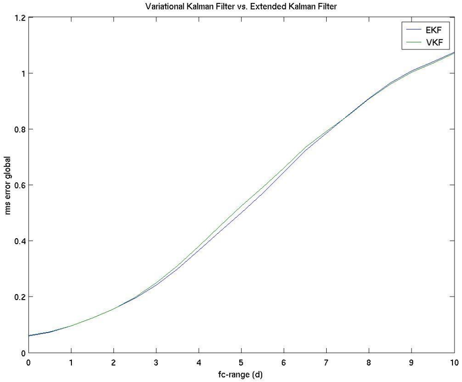
Variational Ensemble Kalman Smoother (VEnKS)

- At every iteration the length of each ensemble is doubled and halved successively, analogously with multigrid methods in space
- Each ensemble overlaps with one subsequent sampling interval from the previous iteration and creates two half intervals of its own, until a single ensemble and its corresponding error covariance matrix span the entire assimilation window.

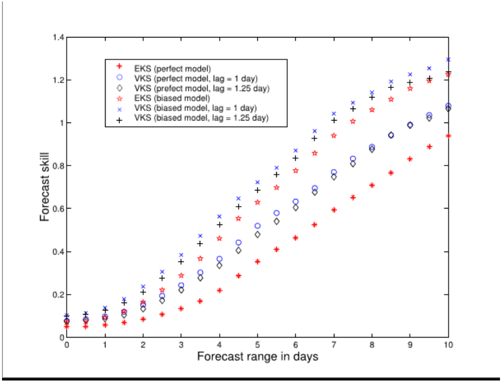
One-dimensional results

Results with a Lorenz95 model.

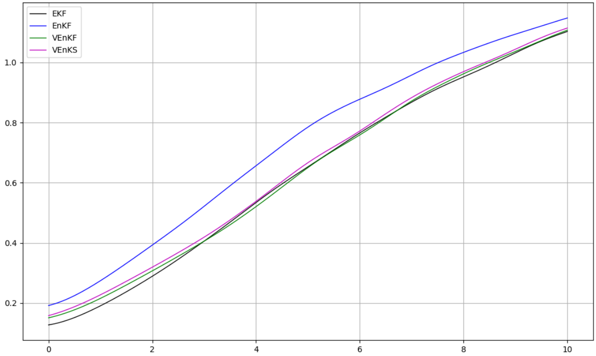
Forecast skill of VKF vs. EKF



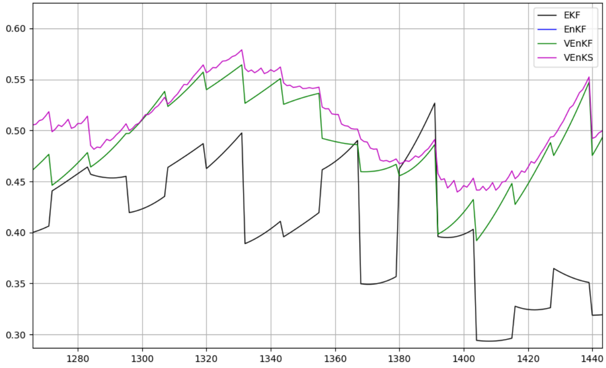
Forecast skill comparison of EKF, VKF, FIKS and VKS, respectively, with an unbiased and a biased model



Forecast skill of a 20 member ensemble with EKF, EnKF, VEnKF and VEnKS, respectively



Forecast close-up of RMSE of a 15 member ensemble with EKF, EnKF, VEnKF and VEnKS



Two-dimensional results

- VEnKF-filtered algal bloom data from MERIS imagery with a random walk model.
- 600×1000 grid cells, 60 m resolution