Towards the estimation of optimal covariance matrices in multi-ensemble data assimilation

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AVENUE Project Workshop 2017

Outline

- Motivation
- A framework for maximum likelihood estimation
- Maximum likelihood estimation with multi-ensembles
- Application to ensemble-based Kalman filters
- Numerical experiments

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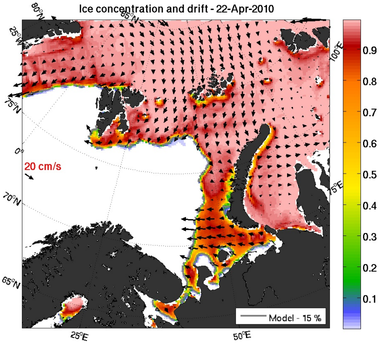
Data assimilation combines in an optimal way the heterogeneous and uncertain information provided by model and observations in order to estimate the state of a system.



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Linear Gaussian framework

$$\begin{array}{lll} \text{Advance in time:} & \mathbf{x}_k = \mathbf{M}_k \mathbf{x}_{k-1} + \mathbf{v}_k, & \mathbf{v}_k \sim \mathcal{N}(0, \mathbf{Q}_k) \\ \text{Observation:} & \mathbf{z}_k = \mathbf{H}_k \mathbf{x}_k + \mathbf{w}_k, & \mathbf{w}_k \sim \mathcal{N}(0, \mathbf{R}_k) \end{array}$$

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Kalman filter

Forecast

$$
\begin{aligned}
\mathbf{x}_k^f &= \mathbf{M}_k \mathbf{x}_{k-1}^a \\
\mathbf{P}_k^f &= \mathbf{M}_k \mathbf{P}_{k-1}^a \mathbf{M}_k^T + \mathbf{Q}_k
\end{aligned}
$$

Analysis

$$
\begin{aligned}
\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{x}_k^a &= \mathbf{x}_k^f + \mathbf{K}_k (\mathbf{z}_k - \mathbf{H}_k \mathbf{x}_k^f) \\
\mathbf{P}_k^a &= (\mathbf{I} - \mathbf{K}_k \mathbf{H}_k) \mathbf{P}_k^f
\end{aligned}
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Kalman filter

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$$\mathbf{x}_k^f = \mathbf{M}_k \mathbf{x}_{k-1}^a$$
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Challenges

- storage of covariance matrices
- non-linearity
- non-Gaussian noise

Ensemble Kalman filter

- To avoid updating the error covariance matrix explicitly, the Kalman equations are applied to an ensemble of state vectors (with $i = 1, \dots, n$).

$$\begin{aligned} \text{Forecast:} \quad & \mathbf{x}_k^{f,i} = \mathcal{M}_k(\mathbf{x}_{k-1}^{a,i}) + \mathbf{v}_k, & \mathbf{v}_k \sim \mathcal{N}(0, \mathbf{Q}_k) \\ \text{Analysis:} \quad & \mathbf{x}_k^{a,i} = \mathbf{x}_k^{f,i} + \mathbf{K}_k(\mathbf{z}_k - \mathbf{H}_k \mathbf{x}_k^{f,i} + \mathbf{w}_k), & \mathbf{w}_k \sim \mathcal{N}(0, \mathbf{R}_k) \end{aligned}$$

with $\mathbf{K}_k = \mathbf{P}_k^f \mathbf{H}_k^T (\mathbf{H}_k \mathbf{P}_k^f \mathbf{H}_k^T + \mathbf{R}_k)^{-1}$ the Kalman gain matrix.

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- The mean and error covariance are approximated by the ensemble mean and covariance:

$$\bar{\mathbf{x}}_k^f = \frac{1}{n} \sum_{i=1}^{n} \mathbf{x}_k^{f,i}, \quad \mathbf{P}_k^f = \frac{1}{n-1} \mathbf{A}^f (\mathbf{A}^f)^T \;\; \text{with} \;\; \mathbf{A}^f = \left[\mathbf{x}_k^{f,1} - \bar{\mathbf{x}}_k^f, \ldots, \mathbf{x}_k^{f,n} - \bar{\mathbf{x}}_k^f \right]$$

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- Feasible for large applications with ~ 100 ensemble members with moderation techniques (inflation, localization).

Motivation for multi-ensembles

- Large-scale geophysical applications may involve
  - ▷ several numerical models
  - ▷ different grid sizes
  - ▷ significant i/o costs for storage of model output

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- Can we apply ensemble-based Kalman filters with ensembles of different accuracies?
  - ▷ How do we take into account the differences in accuracy between ensembles?
  - ▷ How can we estimate the error covariance matrix given ensembles of different accuracies?

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Setting (I)

- Random variable:

$$\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \text{ with } \boldsymbol{\mu} \in \mathbb{R}^m \text{ and } \boldsymbol{\Sigma} \in \mathbb{R}^{m \times m} \text{ unknown.}$$

- Samples available:

$$\mathbf{X} = [\mathbf{x}_1, \ldots, \mathbf{x}_n] \in \mathbb{R}^{m \times n}$$

- Goal: Compute estimates $\hat{\mu} \approx \boldsymbol{\mu}$ and $\widehat{\boldsymbol{\Sigma}} \approx \boldsymbol{\Sigma}$

Maximum likelihood estimation

- Maximize the likelihood function of the normal distribution:

$$\mathcal{L}(\hat{\mu}, \widehat{\mathbf{\Sigma}}|\mathbf{X}) \propto \prod_{i=1}^{n} \det(\widehat{\mathbf{\Sigma}})^{-1/2} \exp\left(-\frac{1}{2}(\mathbf{x_i} - \hat{\mu})^T \widehat{\mathbf{\Sigma}}^{-1}(\mathbf{x_i} - \hat{\mu})\right)$$

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- Minimize the negative log-likelihood:

$$g(\hat{\mu}, \widehat{\mathbf{\Sigma}}) = \frac{n}{2} \log\det(\widehat{\mathbf{\Sigma}}) + \frac{1}{2}\mathrm{trace}(\widehat{\mathbf{\Sigma}}^{-1} \mathbf{A}\mathbf{A}^T)$$

where **A** is the matrix of anomalies:

$$\mathbf{A} = [\mathbf{x}_1 - \hat{\mu}, \ldots, \mathbf{x}_n - \hat{\mu}]$$

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- Differentiate with respect to $\hat{\boldsymbol{\mu}}$:

$$\sum_{i=1}^{n} (\mathbf{x}_i - \hat{\boldsymbol{\mu}})^T \widehat{\boldsymbol{\Sigma}}^{-1} \{\mathrm{d}\hat{\boldsymbol{\mu}}\} = 0 \quad \Rightarrow \quad \hat{\boldsymbol{\mu}} = \bar{\mathbf{x}} = \frac{1}{n} \sum_{i=1}^{n} \mathbf{x}_i$$

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provided $n > m$

Setting (II)

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- Very few samples available:

$$\mathbf{X} = [\mathbf{x}_1, \ldots, \mathbf{x}_n] \in \mathbb{R}^{m \times n} \quad \text{with } n < m$$

- Goal: Compute estimates $\hat{\boldsymbol{\mu}} \approx \boldsymbol{\mu}$ and $\widehat{\boldsymbol{\Sigma}} \approx \boldsymbol{\Sigma}$

Maximum likelihood estimation when $n < m$

- Pick a subspace of dimension $p \ll m$:

$$\mathbf{Q} \in \mathbb{R}^{m \times p}, \quad \mathbf{Q}^T\mathbf{Q} = \mathbf{I}$$

- Search for an estimate of the covariance matrix of the form

$$\widehat{\boldsymbol{\Sigma}} = \mathbf{QMQ}^T = \mathbf{QLL}^T\mathbf{Q}^T$$

where $\mathbf{M} \in \mathbb{R}^{p \times p}$ is symmetric positive definite and $\mathbf{M} = \mathbf{LL}^T$ is either a Cholesky or symmetric square root factorization.

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- Similar to regularization/shrinkage techniques (Ledoit and Wolf 2004, Ueno et. al. 2009, 2010, 2014, Johns and Mandel 2010, etc.)

Maximum likelihood estimation when $n < m$

- Maximize the likelihood function with respect to the degenerate normal distribution:

$$\mathcal{L}(\widehat{\boldsymbol{\Sigma}}|\mathbf{X}) \propto \prod_{i=1}^{n} \det{}^*(\widehat{\boldsymbol{\Sigma}})^{-1/2} \exp\left(-\frac{1}{2}(\mathbf{x_i} - \bar{\mathbf{x}})^T \widehat{\boldsymbol{\Sigma}}^{\dagger} (\mathbf{x_i} - \bar{\mathbf{x}})\right)$$

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where

▷ $\det^*(\widehat{\mathbf{\Sigma}})$ is the pseudo-determinant

$$\det{}^*(\widehat{\mathbf{\Sigma}}) = \det{}^*(\mathbf{QLL}^T\mathbf{Q}^T) = \mathbf{Q}\det(\mathbf{LL}^T)\mathbf{Q}^T$$

▷ $\widehat{\mathbf{\Sigma}}^{\dagger}$ is the More-Penrose generalized inverse

$$\widehat{\mathbf{\Sigma}}^{\dagger} = (\mathbf{QLL}^T\mathbf{Q}^T)^{\dagger} = \mathbf{Q}(\mathbf{LL}^T)^{-1}\mathbf{Q}^T$$

Maximum likelihood estimation when $n < m$

- Minimize the negative log-likelihood:

$$g(\mathbf{L}) = n \log \det(\mathbf{L}) + \frac{1}{2}\mathrm{trace}\big((\mathbf{L}\mathbf{L}^T)^{-1}\mathbf{Q}^T\mathbf{A}\mathbf{A}^T\mathbf{Q}\big)$$

where $\mathbf{A}$ is the matrix of anomalies.

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- First order optimality conditions:

$$\mathbf{L}\mathbf{L}^T = \frac{1}{n}\mathbf{Q}^T\mathbf{A}\mathbf{A}^T\mathbf{Q}$$

$$\widehat{\mathbf{\Sigma}} = \mathbf{Q}\mathbf{L}\mathbf{L}^T\mathbf{Q}^T = \frac{1}{n}\mathbf{Q}\mathbf{Q}^T\mathbf{A}\mathbf{A}^T\mathbf{Q}\mathbf{Q}^T$$

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Remarks:

- ▷ For $\mathbf{L}$ to be nonsingular: $p \le n - 1$.
- ▷ $\widehat{\mathbf{\Sigma}}$ is a projection of the sample covariance matrix.
- ▷ If $\text{range}(\mathbf{Q}) = \text{range}(\mathbf{A})$ then $\widehat{\mathbf{\Sigma}}$ is the sample covariance matrix.

Numerical optimization

- To compute the entries of the optimal **L** numerically, we use the one-to-one correspondence between

$$\mathbf{L} = \begin{bmatrix} \ell_{1,1} & & & \\ \ell_{2,1} & \ell_{2,2} & & \\ \vdots & & \ddots & \\ \ell_{p,1} & \dots & \dots & \ell_{p,p} \end{bmatrix} \qquad \longleftrightarrow \qquad \boldsymbol{\ell} = \begin{bmatrix} \ell_{1,1} \\ \vdots \\ \ell_{p,1} \\ \ell_{2,2} \\ \vdots \\ \ell_{p,p} \end{bmatrix}$$

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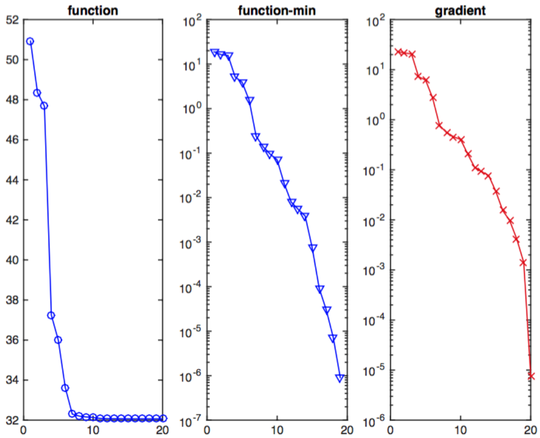
- We use BFGS to minimize the negative log-likelihood $g(\boldsymbol{\ell})$.
  - ▷ Find a search direction $\mathbf{p}_k$ by solving $\mathbf{B}_k \mathbf{p}_k = -\nabla g(\boldsymbol{\ell}_k)$.
  - ▷ Perform a linesearch to find an acceptable step-size α_k.
  - ▷ Take a step: $\boldsymbol{\ell}_{k+1} = \boldsymbol{\ell}_k + \alpha_k \mathbf{p}_k$.
  - ▷ Use a low-rank update to obtain $\mathbf{B}_{k+1}$ from $\mathbf{B}_k$.



Example from a L40 simulation

$m = 40,\ n = 5,\ p = 4$

Q chosen to be the left singular vectors of **A**

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Setting (III)

- Random variables:

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$$\mathbf{y} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma} + \mathbf{C}) \text{ with } \mathbf{C} \in \mathbb{R}^{m \times m} \text{ known.}$$

- Very few samples available:

$$\mathbf{X} = [\mathbf{x}_1, \ldots, \mathbf{x}_{n_x}] \in \mathbb{R}^{m \times n_x}$$
$$\mathbf{Y} = [\mathbf{y}_1, \ldots, \mathbf{y}_{n_y}] \in \mathbb{R}^{m \times n_y}$$

with $n_x + n_y < m$.

- Goal: Compute estimates $\hat{\boldsymbol{\mu}} \approx \boldsymbol{\mu}$ and $\widehat{\boldsymbol{\Sigma}} \approx \boldsymbol{\Sigma}$

Maximum likelihood estimation with multi-ensembles

- Given samples "high-fidelity" samples $\mathbf{X}$ and "noisy" samples $\mathbf{Y}$, the likelihood function with respect to the degenerate normal distribution is

$$\begin{aligned}&\mathcal{L}(\widehat{\boldsymbol{\Sigma}}|\mathbf{X},\mathbf{Y})\\ &\propto \prod_{i=1}^{n_x} \det{}^*(\widehat{\boldsymbol{\Sigma}})^{-1/2} \exp\left(-\tfrac{1}{2}(\mathbf{x_i}-\bar{\mathbf{x}})^T \widehat{\boldsymbol{\Sigma}}^{\dagger}(\mathbf{x_i}-\bar{\mathbf{x}})\right)\\ &\qquad \times \prod_{j=1}^{n_y} \det{}^*(\widehat{\boldsymbol{\Sigma}}+\mathbf{C})^{-1/2} \exp\left(-\tfrac{1}{2}(\mathbf{y_j}-\bar{\mathbf{x}})^T (\widehat{\boldsymbol{\Sigma}}+\mathbf{C})^{\dagger}(\mathbf{y_j}-\bar{\mathbf{x}})\right)\end{aligned}$$

where $\det^*(\cdot)$ is the pseudo-determinant and $(\cdot)^\dagger$ denotes the More-Penrose generalized inverse.

Maximum likelihood estimation with multi-ensembles

- Search for an estimate of the covariance matrix of the form

$$\widehat{\mathbf{\Sigma}} = \mathbf{QMQ}^T = \mathbf{QLL}^T\mathbf{Q}^T, \quad \text{where} \quad \mathbf{Q} \in \mathbb{R}^{m \times p}, \; \mathbf{Q}^T\mathbf{Q} = \mathbf{I}.$$

- As in the single-ensemble case:

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- We approximate $\widehat{\mathbf{\Sigma}} + \mathbf{C}$ by projection:

$$\widehat{\mathbf{\Sigma}} + \mathbf{C} = \mathbf{QLL}^T\mathbf{Q}^T + \mathbf{C} \approx \mathbf{Q}(\mathbf{LL}^T + \mathbf{Q}^T\mathbf{CQ})\mathbf{Q}^T$$

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- Then

$$\det{}^*(\widehat{\mathbf{\Sigma}} + \mathbf{C}) \approx \mathbf{Q}\det(\mathbf{LL}^T + \mathbf{Q}^T\mathbf{CQ})\mathbf{Q}^T$$

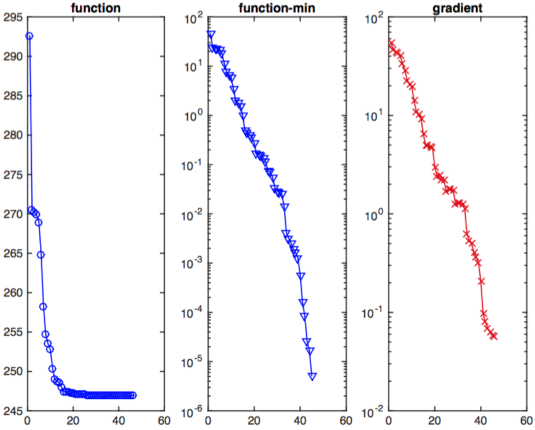
$$(\widehat{\mathbf{\Sigma}} + \mathbf{C})^\dagger \approx \mathbf{Q}(\mathbf{LL}^T + \mathbf{Q}^T\mathbf{CQ})^{-1}\mathbf{Q}^T$$

Maximum likelihood estimation with multi-ensembles

- Minimize the negative log-likelihood:

$$g(\mathbf{L}) = n_x \log\det(\mathbf{L}) + \frac{n_y}{2} \log\det(\mathbf{L}\mathbf{L}^T + \mathbf{Q}^T\mathbf{C}\mathbf{Q})$$
$$+ \operatorname{trace}\big((\mathbf{L}\mathbf{L}^T)^{-1}\mathbf{Q}^T\mathbf{A}_x\mathbf{A}_x^T\mathbf{Q}\big)$$
$$+ \operatorname{trace}\big((\mathbf{L}\mathbf{L}^T + \mathbf{Q}^T\mathbf{C}\mathbf{Q})^{-1}\mathbf{Q}^T\mathbf{A}_y\mathbf{A}_y^T\mathbf{Q}\big)$$

with $\mathbf{A}_x$ and $\mathbf{A}_y$ the anomalies of samples $\mathbf{X}$ and $\mathbf{Y}$, respectively.



Example from a L40 simulation

$m = 40,\ n_x = 5,\ n_y = 15,\ p = 19$

noise: truncation of the vector components to 10^{-6}, $\mathbf{C} = 10^{-12}\mathbf{I}$

$\mathbf{Q}$ chosen to be the left singular vectors of matrix of anomalies

convergence of $\hat{\boldsymbol{\Sigma}} = \mathbf{Q}\mathbf{L}\mathbf{L}^T\mathbf{Q}^T$ close to the sample covariance $\sim$ variance of the noise

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Anomalies-based formulation (Sakov et. al., 2010)

- Notation:
  - ▷ ensemble $\mathbf{E} = [\mathbf{X}, \mathbf{Y}] \in \mathbb{R}^{m \times n}$
  - ▷ ensemble mean $\mathbf{x} = \frac{1}{n}\mathbf{E}\mathbf{e} \in \mathbb{R}^m$, where $\mathbf{e} = [1, \ldots, 1]^T$
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- The analysis step updates the mean and the anomalies instead of the ensemble members.
- To recover the analysis ensemble: $\mathbf{E} = \mathbf{x}\mathbf{e}^T + \mathbf{A}$

Anomalies-based formulation (Sakov et. al., 2010)

- Update of the **ensemble mean**:

$$\mathbf{x}^a = \mathbf{x}^f + \mathbf{A}^f \mathbf{G} \mathbf{R}^{-\frac{1}{2}} (\mathbf{z} - \mathbf{H}\mathbf{x}^f)/\sqrt{n-1}$$

with

$$\mathbf{G} = \mathbf{S}^T (\mathbf{I} + \mathbf{S}\mathbf{S}^T)^{-1}, \qquad \mathbf{S} = \mathbf{R}^{-\frac{1}{2}} \mathbf{H} \mathbf{A}^f / \sqrt{n-1}.$$

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- Update of the **ensemble anomalies**: $\mathbf{A}^a = \mathbf{A}^f + \mathbf{A}^f\mathbf{T}$
  - ▷ **EnKF**: $\mathbf{T} = \mathbf{G}(\mathbf{D} - \mathbf{S})$ where the columns of $\mathbf{D}$ are Gaussian samples
  - ▷ **ETKF**: $\mathbf{T} = (\mathbf{I}_n + \mathbf{S}^T\mathbf{S})^{-\frac{1}{2}} - \mathbf{I}_n$
  - ▷ **DEnKF**: $\mathbf{T} = -\frac{1}{2}\mathbf{G}\mathbf{S}$

QL-based formulation

- Deriving the filters using **QL** instead of the anomalies $\mathbf{A}^f$:

$$\mathbf{P}^f = \left(\frac{\mathbf{A}^f}{\sqrt{n-1}}\right)\left(\frac{\mathbf{A}^f}{\sqrt{n-1}}\right)^T \quad \longrightarrow \quad \mathbf{P}^f = \mathbf{QL}(\mathbf{QL})^T$$

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- **QL** not similar to an anomalies matrix:
  - ▷ $\mathbf{QL} \in \mathbb{R}^{m\times p}$, with $p \leq n-1$ and $\mathbf{A} \in \mathbb{R}^{m\times n}$ of rank $n-1$.
  - ▷ $\mathbf{QLe} \neq 0$.

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- To interpret **QL** as an anomalies matrix:

$$\mathbf{P}^f = \mathbf{QL}(\mathbf{QL})^T = \mathbf{QLV}^T(\mathbf{QLV}^T)^T$$

where $\mathbf{V} \in \mathbb{R}^{n\times p}$, $\mathbf{V}^T\mathbf{V} = \mathbf{I}$, $\mathbf{Ve} = 0$, e.g.,
  - ▷ right singular vectors from the SVD of $\mathbf{A}^f$
  - ▷ random orthogonal matrices with columns orthogonal to **e** (SEIK filter; Hoteit et. al., 2002).

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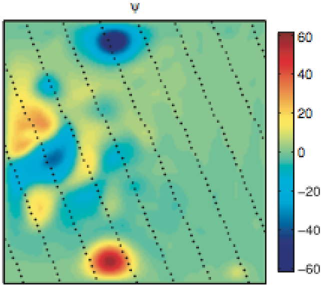
A quasi-geostrophic model

- Model
  - ▷ a 1.5-layer reduced-gravity QG model with double-gyre wind forcing and biharmonic friction
  - ▷ nonlinear, 129×129 grid points
  - ▷ dimension $m = 1.6 \times 10^4$
  - ▷ EnKF-Matlab toolbox (Sakov, 2013).
- Ensembles
  - ▷ "Accurate" ensemble $\mathbf{X}$: $n_x = 5$ members.
  - ▷ "Noisy" ensemble $\mathbf{Y}$: $n_y = 20$ members, truncation to 1 digit before the analysis.
  - ▷ Noise covariance matrix $\mathbf{C}$: diagonal (variance estimated from a large sample).

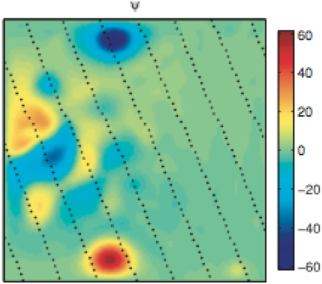


Water height, observations.

Sakov and Oke (2008)

A quasi-geostrophic model

- Observations
  - ▷ Normal distributed additive noise: $\mathcal{N}(0, \sigma_o^2 \mathbf{I})$.
  - ▷ $\mathbf{R} = \sigma_o^2 \mathbf{I}$.
  - ▷ $\sigma_0^2 = 4$, equidistant tracks, every fourth time step.
- Moderation
  - ▷ Inflation: 1.0 : 0.01 : 1.1.
  - ▷ Local analysis: localization radius $= 10$.
- Anomalies-like ensemble-based Kalman filters.
- Configuration similar to Sakov and Oke (2008).



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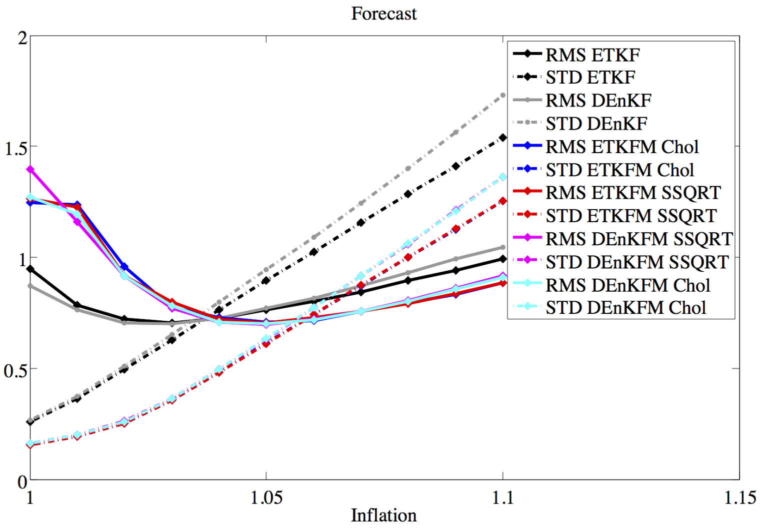
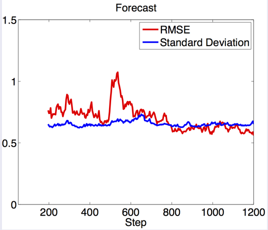


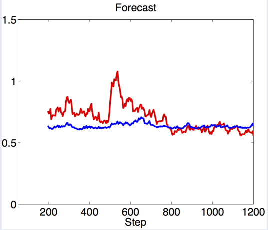
	ETKF	ETKFM (C)	ETKFM (S)	DEnKF	DEnKFM (C)	DEnKFM (S)
RMS	0.7044	0.7067	0.7043	0.7025	0.6999	0.6991
STD	0.6293	0.6138	0.6121	0.6534	0.6343	0.6323

Temporal evolution: errors

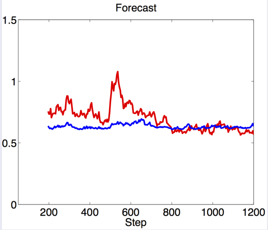
DEnKF



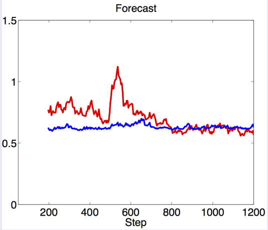
DEnKFM (Chol)



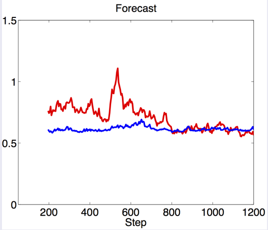
DEnKFM (SSQRT)



ETKF



ETKFM (Chol)



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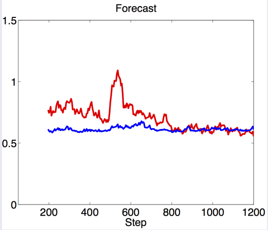
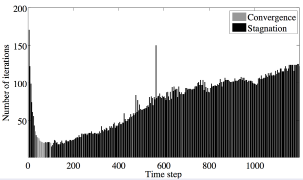


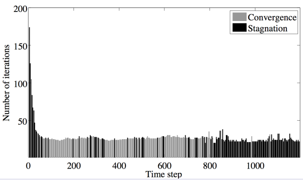
Temporal evolution: BFGS iterations [DEnKFM (SSQRT)]

$infl = 1.00$



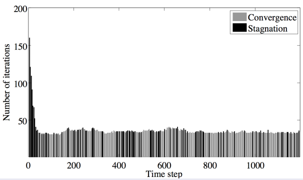
$Mean = 73.7, \; Conv = 4.3\%$

$infl = 1.03$



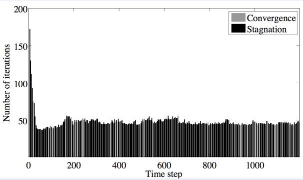
$Mean = 28.1, \; Conv = 51.7\%$

$infl = 1.05$



$Mean = 36.6, \; Conv = 67\%$

$infl = 1.08$



$Mean = 48.5, \; Conv = 12.3\%$

Summary

- A strategy for estimating mean and covariance matrix of multi-ensembles has been suggested.
  - ▷ Normally distributed random vectors: same mean, covariance matrices of the additional "noise" known.
  - ▷ Estimation in a subspace of smaller dimension.
  - ▷ Local minima can be computed numerically.
- Application to ensemble-based Kalman filters.
  - ▷ Derivation of a **QL**-based EnKF.
  - ▷ Adapted to specific variants of EnKF.
  - ▷ Anomalies-like **QL**-based formulation
- Preliminary results
  - ▷ Similar performances compared to anomalies-based filters, with a shift in the inflation.
  - ▷ Issues to be worked out: convergence of BFGS, choice of subspace, modelling of noise, choice of parameters.

Perspectives

- Ongoing work and perspectives.
  - ▷ Longer experiments (more analysis cycles), sensitivity to the dimension of the problem, the noise,...
  - ▷ Different strategies for building anomalies-like **QL**-based filters.
  - ▷ Nonlinear observation operators.
  - ▷ Numerical optimization on manifolds: fixed-rank symmetric positive semidefinite matrices.
  - ▷ Biased estimator?
- Towards multigrid strategies in ensemble-based Kalman filters.

References

- Gratton S., Simon E., Titley-Peloquin D.: Covariance matrix estimation with noisy samples. In preparation.
- Hoteit I., Pham D.-T., Blum J.: A simplified reduced order Kalman filtering and application to altimetric data assimilation in tropical Pacific, *Journal of Marine Systems*, 36, 101-127, 2002.
- Sakov P., Evensen G., Bertino L.: Asynchronous data assimilation with the EnKF, *Tellus*, 62A, 24-29, 2010.
- Sakov P., Oke P. R.: A deterministic formulation of the ensemble Kalman filter: an alternative to ensemble square root filters, *Tellus*, 60A, 361-371, 2008.
- Sakov P.: EnKF-Matlab toolbox.

Thank you for your attention!