# Constraining overestimation of error covariances in ensemble Kalman filters

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Toulouse, November 13th, 2012

#### Observational Data

Forecast Model

## Data Assimilation

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Forecast Model

## Data Assimilation

Climatological Information

## Using climatology on sparse observational grids

#### What is the effect of the sparsity of observations?

- The obvious: We don't have much information
- Overestimation of error covariances (exacerbated by finite ensemble sizes) (*Whitaker et al. 2009*)

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- sparse observational networks
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#### Further applications are

- re-analysis of climate
- when direct observations are not available (mesosphere)
- general slow-fast systems

#### Our particular perspective here:

Proper (noisy) observations are available for some variables (observables) but not for other unresolved variables, for which only their statistical climatic behaviour such as their variance and their mean is available (pseudo-observables).

#### Question:

How can the statistical information available for some data which are otherwise not observable, be effectively incorporated into data assimilation to control overestimation? Assume an N-dimensional dynamical system whose dynamics is given by  $\dot{\mathbf{z}} = f(\mathbf{z})$  with the state variable  $\mathbf{z} \in \mathbb{R}^N$  (no model error for now).

#### observables

Observations  $\mathbf{x}_{\mathrm{obs}}$  at observation times  $t_n = n \Delta t_{\mathrm{obs}}$ 

- observation operator  $\mathbf{H}: \mathbb{R}^N \to \mathbb{R}^n$
- $\mathbf{x}_{obs}(t_i) = \mathbf{H}\mathbf{z}(t_i) + \mathbf{r}_{obs}(t_i)$  with observational noise  $\mathbf{r}_{obs}$
- $\mathbf{r}_{obs} \sim \mathcal{N}(0, \mathbf{R}_{obs})$  with error covariance matrix  $\mathbf{R}_{obs}$

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#### pseudo-observables

Assume climatic knowledge about the pseudo-observables  ${\bf y}$  (mean  ${\bf a}_{target}$  and variance  ${\bf A}_{target}$ )

- pseudo-observation operator  $\mathbf{h}: \mathbb{R}^N \to \mathbb{R}^m$
- $\mathbf{R}_{w}$  is the unknown error covariance matrix associated with the pseudo-observables

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#### Question:

#### How do we choose/find the error covariance matrix $\mathbf{R}_{w}$ ?

An ensemble (Evensen, 1996) with k members  $\mathbf{z}_k$ 

$$\mathbf{Z} = [\mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_k] \in \mathbb{R}^{N imes k}$$

is propagated by the full nonlinear dynamics

$$\dot{\mathbf{Z}} = F(\mathbf{Z}), \qquad \mathbf{Z}(0) = \mathbf{Z}_b \;.$$

The ensemble is split into its mean  $\bar{z}$  and its ensemble deviation matrix  $Z^\prime$ 

Step 1: Forecast step

$$\mathbf{Z}_f = F(\mathbf{Z}_b)$$
$$\mathbf{P}_f = \frac{1}{k-1} \mathbf{Z}'_f(t) [\mathbf{Z}'_f(t)]^T$$

Remark:  $\mathbf{P}_f(t)$  is rank-deficient for k < N ( $N \sim 10^9$  and  $k \sim 100$ )

#### Step 2: Analysis step

$$J(\mathbf{z}) = \frac{1}{2} (\mathbf{z} - \mathbf{z}_f)^T \mathbf{P}_f^{-1} (\mathbf{z} - \mathbf{z}_f) + \frac{1}{2} (\mathcal{H}\mathbf{z} - \mathcal{Y})^T \mathcal{R}^{-1} (\mathcal{H}\mathbf{z} - \mathcal{Y})$$
$$\mathcal{Y} = \begin{pmatrix} \mathbf{x}_{\text{obs}} \\ \mathbf{a}_{\text{target}} \end{pmatrix}, \mathcal{H} = \begin{pmatrix} \mathbf{H} \\ \mathbf{h} \end{pmatrix}, \mathcal{R}^{-1} = \begin{pmatrix} \mathbf{R}_{\text{obs}}^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{R}_{\text{w}}^{-1} \end{pmatrix}$$

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$$ar{\mathbf{z}}_a = ar{\mathbf{z}}_f - \mathcal{K} \left[ \mathcal{H} \mathbf{z}_f - \mathcal{Y} 
ight]$$

where 
$$\mathcal{K} = \mathbf{P}_f \mathcal{H}^T (\mathcal{H} \mathbf{P}_f \mathcal{H}^T + \mathcal{R})^{-1}$$

with the covariance of the analysis

$$\mathbf{P}_a = \left[\mathbf{I} - \mathcal{K}\mathcal{H}\right]\mathbf{P}_f$$

#### Step 2: Analysis step

Constraining the variance of the pseudo-observable  $\mathbf{h}\mathbf{z}$  is done by requiring

 $\mathbf{h}\mathbf{P}_{a}\mathbf{h}^{T} = \mathbf{A}_{\text{target}}$ 

Introducing  $\mathcal{P}_{\mathbf{a}}^{-1} = \mathbf{P}_{f}^{-1} + \mathbf{H}^{T}\mathbf{R}_{obs}^{-1}\mathbf{H}$ , we obtain

$$\mathbf{R}_{w}^{-1} = \mathbf{A}_{\text{target}}^{-1} - \left(\mathbf{h}\mathcal{P}_{\mathbf{a}}\mathbf{h}^{T}\right)^{-1}$$

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For sufficiently small background error covariance P<sub>f</sub>, the error covariance R<sub>w</sub> is not positive definite ("switch"):
 Update only *overestimating* eigendirections with |hP<sub>a</sub>h<sup>T</sup>| > |A<sub>target</sub>|

#### Step 3: Update of the ensemble

The ensemble needs to be consistent with

$$\mathbf{P}_{a} = \frac{1}{k-1} \mathbf{Z}_{a}^{\prime} \left[ \mathbf{Z}_{a}^{\prime} \right]^{T}$$

Method of ensemble square root filters:

- Ensemble transform Kalman filter (EnTKF) (*Tippett et al 2003*):  $\mathbf{Z}'_{a} = \mathbf{Z}'_{f} S_{w}$  with  $S_{w} \in \mathbb{R}^{k \times k}$
- Ensemble adjustment Kalman filter (EnAKF) (Anderson 2001):  $\mathbf{Z}'_a = \mathbf{A}\mathbf{Z}'_f$  with  $\mathbf{A} \in \mathbb{R}^{N \times N}$

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#### Step 4: Update of the forecast

Set  $\mathbf{Z}_b = \mathbf{Z}_a$  to propagate the ensemble forward again with the full dynamics to the next observation time

## Summary of VLKF

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$$\mathbf{P}_f = \frac{1}{k-1} \mathbf{Z}'_f(t) [\mathbf{Z}'_f(t)]^T$$

Step 2: Analysis step

$$\begin{split} \bar{\mathbf{z}}_{a} &= \bar{\mathbf{z}}_{f} - \mathbf{K}_{\text{obs}} (\mathbf{H} \bar{\mathbf{z}}_{f} - \mathbf{x}_{\text{obs}}) - \mathbf{K}_{\text{w}} (\mathbf{h} \bar{\mathbf{z}}_{f} - \mathbf{a}_{\text{target}}) \\ \mathbf{K}_{\text{obs}} &= \mathbf{P}_{f} \mathbf{H}^{T} (\mathbf{H} \mathbf{P}_{f} \mathbf{H} + \mathbf{R}_{\text{obs}})^{-1} , \quad \mathbf{K}_{\text{w}} = \mathbf{P}_{f} \mathbf{h}^{T} (\mathbf{h} \mathbf{P}_{f} \mathbf{h} + \mathbf{R}_{\text{w}})^{-1} \\ \mathbf{R}_{\text{w}}^{-1} &= \mathbf{A}_{\text{target}}^{-1} - (\mathbf{h} \mathcal{P}_{\mathbf{a}} \mathbf{h}^{T})^{-1} \end{split}$$

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$$\mathbf{P}_{a} = \left[\mathbf{I} - \mathbf{K}_{ ext{obs}}\mathbf{H} - \mathbf{K}_{ ext{w}}\mathbf{h}
ight] \mathbf{P}_{f} = rac{1}{k-1}\mathbf{Z}_{a}^{\prime}\left[\mathbf{Z}_{a}^{\prime}
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## I. Lorenz-96 model: $\dot{z}_i = z_{i-1} (z_{i+1} - z_{i-2}) - z_i + F$

The pseudo-observables contain the prior climatic knowledge:  $\mathbf{a}_{\text{target}} = \mu_{\text{clim}}$  and  $\mathbf{A}_{\text{target}} = \sigma_{\text{clim}}^2 \mathbf{I}$  with  $\mu_{\text{clim}} = 2.34$  and  $\sigma_{\text{clim}} = 3.6$ measured from a long time trajectory  $N_{\text{obs}} = 5$ ,  $\Delta t_{\text{obs}} = 4$  hours,  $\mathbf{R}_{\text{obs}} = (0.25\sigma_{\text{clim}})^2 \mathbf{I}$ 



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## I. Lorenz-96 model

• Nobs

Quantify the skill improvement by the r.m.s error

$$\mathcal{E} = \sqrt{\langle \frac{1}{LD} \sum_{l=1}^{L} \| \bar{\mathbf{z}}_{a}(l\Delta t_{obs}) - \mathbf{z}_{truth}(l\Delta t_{obs}) \|^{2} \rangle}$$
Skill:  $S = \frac{\mathcal{E}^{E}}{\mathcal{E}^{\nabla}}$ 
Best performance of VLKF over ETKF for:  
• small  $\Delta t_{obs}$   
•  $N_{obs} = 4$ 

$$\mathcal{L}$$

$$\mathcal{L}$$

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VLKF produces significant skill in sparse observational grids for

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## The overestimation of error covariances in sparse networks is a finite ensemble size effect

## II. Filter divergence and blow-up with sparse observations

(traditional) filter divergence: Underestimation of error covariance leads to filter trusting its own forecast for sufficiently large  $\mathbf{R}_{obs}$  (cf. *Ng et al (2011)*)

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(traditional) filter divergence: Underestimation of error covariance leads to filter trusting its own forecast for sufficiently large  $\mathbf{R}_{obs}$  (cf. *Ng et al (2011)*) catastrophic filter divergence: Filter develops machine-infinity blow-up for sufficiently small  $\mathbf{R}_{obs}$  (*Harlim & Majda (2010); GAG, Mitchell, Reich (2011)*)

#### **ETKF**

			$\Delta \tau_{obs}$									
		3 h	6 h	9 h	12 h	15 h	18 h	21 h	24 h	27 h	30 h	
		1	0	0	0	0	0	0	0	0	0	0
		2	0	0	0	0	0	0.01	0	0.01	0.05	0.15
	Nobs	3	0	0	0	0.03	0.04	0.11	0.15	0.44	0.58	0.67
	NT	4	0	0.04	0.22	0.29	0.49	0.64	0.77	0.83	0.89	0.82
		5	0.02	0.40	0.67	0.73	0.84	0.89	0.94	0.82	0.49	0.19
		6	0.14	x	x	0.98	0.96	0.76	0.32	0.05	0.02	0.01

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			3 h	6 h	9 h	12 h	15 h	18 h	21 h	24 h	27 h	30 h
		1	0	0	0	0	0	0	0	0	0	0
-	$N_{obs}$	2	0	0	0	0	0	0	0	0	0	0.01
		3	0	0	0	0.02	0	0.01	0.01	0.01	0	0
		4	0	0.03	0.22	0.12	0.06	0.02	0	0	0	0
		5	0	0.24	0.36	0.10	0.01	0	0	0	0	0
		0	0.01	0.42	0.11	0.01	0	0	0	0	0	0

#### VLKF

We study the 5D Lorenz-96 model  $\dot{z}_i = z_{i-1}(z_{i+1} - z_{i-2}) - z_i + F$   $i = 1, \cdots, 5$ with negative forcing F = -16Lyapunov exponents:  $\lambda = (2.72, 0.09, -0.09, -1.83, -5.89)$ Attractor dimension:  $D_{\text{attr}} = 4.15$ 

Decay rate of the autocorrelation:  $\tau_{\rm corr} \approx 0.14$ 

## II. Genesis of blow-up



#### RMS error

- stable until  $t_1 \approx 10$
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Finite size effects: Ensemble dimension (Patil et al (2001))

$$D_{\text{ens}} = \frac{\left(\sum_{i=1}^{k} \sqrt{\mu_i}\right)^2}{\sum_{i=1}^{k} \mu_i} \in (1, \min(k, D))$$

where  $\mu_i$  are eigenvalues of the  $k \times k$  covariance matrix  $C = X_f^T X_f$ 

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Filter pushes analysis off the attractor

$$\bar{\mathbf{z}}_{a,i} = \bar{\mathbf{z}}_{f,i} - \frac{\mathbf{P}_{f\,i1}}{\mathbf{P}_{f\,11} + \mathbf{R}_{\text{obs}}} \left[ \bar{\mathbf{z}}_{f,i} - \mathbf{x}_{\text{obs}} \right]$$

Lyapunov exponents  $\lambda = (2.72, 0.09, -0.09, -1.83, -5.89)$ 

## II. Filter divergence and blow-up with sparse observations

Blow-up is caused by the forecast scheme (numerical instability):



#### Take home message:

Catastrophic blow up may be caused by the combination of finite size ensembles and fast attraction towards the attractor when

- there are sparse but accurate observations
- the underlying system has high variance

Modified Lorenz-96 system (Bergemann & Reich (2010))

$$\dot{x}_{j} = (1 - \eta) \left( x_{j-1} (x_{j+1} - x_{j-2}) \right) - x_{j} + F$$
$$+ \eta \left( x_{j-1} h_{j+1} - x_{j-2} h_{j-1} \right)$$
$$\varepsilon^{2} \ddot{h}_{j} = -h_{j} + \alpha^{2} \left( h_{j-1} - 2h_{j} + h_{j+1} \right) + x_{j}$$

- fast part is purely dispersive
- nonlinear terms conserve energy  $H = \frac{\eta}{2} \sum_{j=1}^{D} \left( \frac{\eta - 1}{\eta} x_j^2 + \epsilon^2 \dot{h}_j^2 + h_j^2 + \alpha^2 (h_{j+1} - h_{j-1})^2 - 2x_j h_j \right)$ • approximate slow manifold given by  $\mathcal{B}_j(x_j, h_j) = x_j - \left( h_j - \alpha^2 \left( h_{j-1} - 2h_j + h_{j+1} \right) \right) = 0$

Initially balanced fields with

$$\mathcal{B}_{j}(x_{j}, h_{j}) = x_{j} - \left(h_{j} - \alpha^{2} \left(h_{j-1} - 2h_{j} + h_{j+1}\right)\right) = 0$$

do not develop unbalanced motion on very long times: The amount of unbalance (fast energy) can be measured by

$$\bar{\mathcal{B}}(t) = \sqrt{\frac{1}{D} \sum_{j=1}^{D} (x_j - h_j + \alpha^2 (h_{j-1} - 2h_j + h_{j+1}))^2}$$



The filtering procedure can severely disturb balance (cf. Lorenc (2003), Kepert (2009), Greybush et al (2011)) - this is the case with and without localization in sparse observational networks Here only x is observed with  $N_{obs} = 2$  with  $\mathbf{h} = \mathcal{B}$  and  $\mathbf{a}_{target} = 0$ 



Red: ETKF Blue: DEnKF with localisation

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Red: ETKF Blue: DEnKF with localisation Magenta: VLKF

A major problem of ensemble filters is underdispersiveness (*Buizza et al 2005*).

This can be linked to

- *dynamical model error*: misrepresentation of unresolved subgrid scale processes (*Palmer 2001*)
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  - unrealistic drainage of energy out of the system (Shutts 2005)
  - frontogenesis (Blumen 1990)
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Main question: Can one get away with underdamped forecast models, yet still control the resulting covariance overestimation within the data assimilation procedure?

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Main question: Can one get away with underdamped forecast models, yet still control the resulting covariance overestimation within the data assimilation procedure?

#### We will use climatological information of the mean and variance

$$\frac{dz_i}{dt} = z_{i-1}(z_{i+1} - z_{i-2}) - \gamma z_i + F$$
Truth:  $\gamma = 1$ 
Forecast model:  $\gamma < 1$ 

Perfect model case:  $S \approx 1$  for  $\Delta t_{\rm obs} \gg 1$ Now we will be interested in the case of  $\Delta t_{\rm obs} \gg 1$ 



 $\Delta t_{\rm obs} = 24 \ {\rm hours}$  Reproducing the truth

 $\Delta t_{\rm obs} = 48 \ {\rm hours}$  Reproducing the statistics

(Truth VLKF ETKF)

#### Reproducing the statistics



(ETKF VLKF truth)

We consider performance over standard ETKF

$$S = \frac{\mathcal{E}^{\mathrm{E}}}{\mathcal{E}^{\mathrm{V}}}$$
,

and over using the "poor man's" analysis of observations and climatology



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and over using the "poor man's" analysis of observations and climatology



 $\Delta t_{\rm obs} = 24 {\rm hrs} \quad \Delta t_{\rm obs} = 36 {\rm hrs} \quad \Delta t_{\rm obs} = 48 {\rm hrs}$ Trade-off: The smaller  $\gamma$ , the better skill over ETKF, but the less skill compared with "poor man's" analysis

## Summary

#### We have here

- derived a variance limiting Kalman filter (VLKF) which adaptively damps unrealistic excitation of ensemble spread in underresolved regions
- applied this filter to a sparse observational grid
  - ▶ has better skill than ETKF for small ( $\leq 6h$ ) observation times
  - has better skill for observables and pseudo-observables
- proposed a mechanism for blow-up filter divergence
- applied this filter to control balance
  - has better skill than DEnKF and controls unbalance
- applied this filter to model error (underdamping)
  - ▶ has better skill than ETKF for large observation intervals ( $\geq 36h$ )
  - trade-off between superior skill over ETKF and being better than observations/climatology

(GAG, Mitchell & Reich, MWR 2011; Mitchell & GAG, QJRMS 2012, in press)

## Lorenz-96 model

How is the skill distributed over



#### Lorenz-96 model

Dependency on observational noise level  $\mathbf{R}_{obs} = (\eta \, \sigma_{clim})^2 \, \mathbf{I}, \, N_{obs} = 4$ 0.8 0.8 0.8 0.6 0.6 0.6 Е E Е 0.4 0.4 0.4 0.2 0.2 0.05 0.1 0.15 0.2 0.25 0.05 0.1 0.15 0.2 0.25 0.05 0.1 0.15 0.2 0.25  $\Delta t_{\rm obs} = 0.025$  $\Delta t_{\rm obs} = 0.05$  $\Delta t_{\rm obs} = 0.25$ (1 hour) (2 hours) (5 hours) Red: Observations Green: ETKF Blue: VI KF

Constraining the covariances produces more reliable ensembles – even in the case when there is no skill improvement with  $\mathcal{S}=1$ 

#### Ranked probability histograms for the observables

- sort the forecast ensemble  $\mathbf{X}_f = [x_{f,1}, x_{f,2}, ..., x_{f,k}]$  and create bins  $(-\infty, x_{f,1}]$ ,  $(x_{f,1}, x_{f,2}]$ , ...,  $(x_{f,k}, \infty)$  at each forecast step
- increment whichever bin the actual truth falls into at each forecast step

Convex histogram: underestimating ensemble Concave histogram: overestimating ensemble Flat histogram: reliable ensemble for which each ensemble member has equal probability of being nearest to the truth



$$\gamma = 0.5$$
 and  $\Delta t_{
m obs} = 48$ hrs

#### Lorenz-96 model

There is an order of magnitude difference between the RMS errors for the observables and the pseudo-observables for large  $N_{\rm obs}$ . This suggests that the information of the observed variables does not travel too far away from the observational sites.



Remark:The advective time scale of the Lorenz-96 system is much smaller than  $\Delta t_{\rm obs}$  which explains why the skill is not equally distributed over the sites, and why, especially for large values of  $N_{\rm obs}$  we observe a big difference between the site-averaged skills of the observed and unobserved variables.

#### Application: Model error and forecast bias



#### Application: Model error and forecast bias



 $\gamma = 1$   $\gamma = 0.9$   $\gamma = 0.8$  ( $\Delta t_{\rm obs} = 48$ hrs) continuous: ETKF dashed: VLKF • increased sparsity and model error lead to overestimation • covariances of observables are also limited for VLKF





#### pseudo-observables

- VLKF outperforms ETKF with increasing model error  $\gamma$  and increasing sparsity  $N_{\rm obs}$
- VLKF becomes less effective compared to poor man's analysis with increasing model error γ and increasing sparsity N<sub>obs</sub>
- issue of overestimation



#### pseudo-observables

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#### observables

- ETKF outperforms VLKF for decreasing model error and decreasing sparsity
- ETKF performs worse than poor man's analysis for small model error
- convergence of ETKF andVLKF to  $\mathcal{E}_o^{\star} < \sqrt{\mathbf{R}_{\mathrm{obs}}}$  for sufficiently large model error
- issue of underestimation

## Dependency of skill on observation noise $\mathbf{R}_{\mathrm{obs}} = (\eta \sigma_{\mathrm{clim}})^2 \mathbf{I}$



- VLKF outperforms ETKF and the poor man's analysis for sufficiently large observational noise since large noise gives more preference to the pseudo-observables which are controlled by the VLKF
- trade-off between skill over ETKF and efficacy over poor man's analysis with increasing model error

Toulouse, November 13th 2012

## Application: Model error and forecast bias

How is the RMS error distributed over the observables and the pseudo-observables ( $\Delta t_{\rm obs} = 48 \rm hrs$ )?



## Model Error

Dependency of skill on sparsity  $N_{\rm obs}$ 





Dependence of climatic mean (left) and variance (right) on damping parameter  $\gamma$ . As well as the climatic variance (black, circles, solid) we show the average variance calculated over forecast intervals  $\Delta t_{\rm obs} = 12$  hours (red, squares, dotted),  $\Delta t_{\rm obs} = 24$  hours (green, triangles, dash-dotted) and  $\Delta t_{\rm obs} = 48$  hours (blue, crosses, dashed).

## Overestimation of forecast error covariance

Finite size ensemble sizes can lead to

- ullet underestimation of diagonal elements of the forecast error covariance  $\mathbf{P}_f$
- ullet overestimation of off-diagonal elements of the forecast error covariance  $\mathbf{P}_f$

To control off-diagonal terms one uses *localization* (*Houtekamer and Mitchell (1998)*), for example

$$\mathbf{P}_f \to C_{\mathrm{loc}} \circ \mathbf{P}_f$$

Can VLKF act as a form of localization?

### Overestimation of forecast error covariance

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Can VLKF act as a form of localization? 2-d example z = (x, y) where only x is observed:

$$\kappa_{loc} = \frac{1}{P_{f_{11}} + R} \left( \begin{array}{c} P_{f_{11}} \\ C_{loc\,21} P_{f_{21}} \end{array} \right)$$

$$\begin{split} & \boldsymbol{\mathcal{K}}_{VLKF} = \boldsymbol{\mathcal{K}}_{VLKF}(R_{\rm w}): \\ & \bullet \quad R_{\rm w} \to \infty: \ \boldsymbol{\mathcal{K}}_{VLKF} \to \frac{1}{P_{f_{11}} + R} \left( \begin{array}{cc} P_{f_{11}} & 0 \\ P_{f_{21}} & 0 \end{array} \right) \\ & \bullet \quad R_{\rm w} \to \varepsilon R_{\rm w}, \ R \to \frac{1}{\varepsilon} R: \ \boldsymbol{\mathcal{K}}_{VLKF} \to \left( \begin{array}{cc} \varepsilon \frac{\vartheta}{P_{f_{22}}R} & \frac{P_{f_{12}}}{P_{f_{22}}} \\ \varepsilon^2 \frac{P_{f_{12}}R_{\rm w}}{P_{f_{22}}R} & 1 \end{array} \right) \\ & \text{ with } \ \vartheta = \det(\mathbf{P}_f) \end{split}$$