Ensemble clustering in deterministic ensemble Kalman filters*

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Outline

1. Ensemble Kalman filtering
    1. The ETKF family
2. Ensemble Clustering
3. A comprehensive study on Ensemble Clustering
4. Experiments
    1. Lorenz 1963 model
    2. More complicated models (with inflation, localization, etc.)
5. Summary

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1. (Ensemble) Kalman filtering

Dynamical **model**

$$\mathbf{x}_t = f(\mathbf{x}_{t-1}) + \mathbf{w}_t$$

$$\mathbf{x} \in \Re^N$$

Observations

$$\mathbf{y}_t = h(\mathbf{x}_t) + \mathbf{v}_t$$

$$\mathbf{y} \in \Re^L$$

Model error

$$E(\mathbf{v}_t) = \mathbf{0}$$

$$Cov(\mathbf{v}_t) = \mathbf{Q}$$

Observation error

$$E(\mathbf{w}_t) = \mathbf{0}$$

$$Cov(\mathbf{w}_t) = \mathbf{R}$$

KF is **optimal** when:

- The **forecast** and **observation** operators are **linear**.
- The **errors** are **Gaussian**.

The **validity of these conditions** depends upon:

- **Length** of the **forecast window / frequency** of **observations**.
- **Magnitude** of **observational error**.
- **Nonlinearity** in the **model dynamics**.

1. Ensemble Kalman filtering

Updating the ensemble **mean** and **covariance** is **straightforward**, **updating** the perturbations **is not**.

$$\mathbf{X}^b \rightarrow \mathbf{X}^a$$

Deterministic EnSRF

- A **direct transformation** from background to analysis (not unique), can use **observations serially or all-at-once**.
- The KF **covariance equation** is **satisfied exactly**.
- Any **distortions** of the **ensemble** are prone to **persist**.

Stochastic EnKF

- Ensemble members are updated individually using **perturbed observations**.
- The **KF covariance equation** is **fulfilled** only **statistically**.
- The **ensemble** is constantly ‘**refreshed**’.

1. Ensemble Transform Kalman Filter family

Within the EnSRFs, the **ETKF** family relies on a **post-multiplication** to update perturbations **all-at-once**.

$$\mathbf{X}^a = \mathbf{X}^b\mathbf{W}^a, \mathbf{W}^a \in \Re^{M\times M} \qquad \mathbf{C}\boldsymbol{\Gamma}\mathbf{C}^{\mathrm{T}} = \left({\mathbf{Y}^b}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{Y}^b\right)/(\boldsymbol{M}-\mathbf{1})$$

- **One-sided** ETKF (Bishop et al., 2001) $\mathbf{W}^a = \mathbf{C}(\mathbf{I}+\boldsymbol{\Gamma})^{-\frac{1}{2}}$
- **Symmetric** ETKF (Wang et al., 2004; Hunt et al., 2007) $\mathbf{W}^a = \mathbf{C}(\mathbf{I}+\boldsymbol{\Gamma})^{-\frac{1}{2}}\mathbf{C}^{\mathrm{T}}$
- **No-symmetric** solutions (e.g. Sakov and Oke, 2008) $\mathbf{W}^a = \mathbf{C}(\mathbf{I}+\boldsymbol{\Gamma})^{-\frac{1}{2}}\mathbf{S}^{\mathrm{T}}$

The **one-sided ETKF is biased**, the **symmetric ETKF is unbiased**, for the **not symmetric ETKFs it depends upon the particular** (possibly random) **matrix S** (Livings et. al, 2008).

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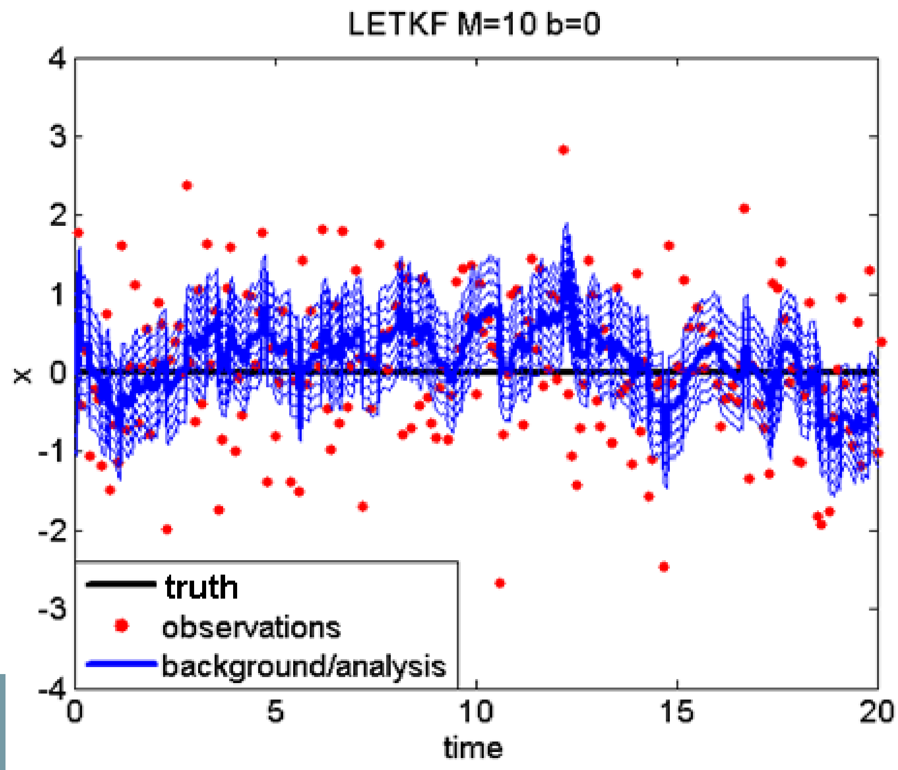
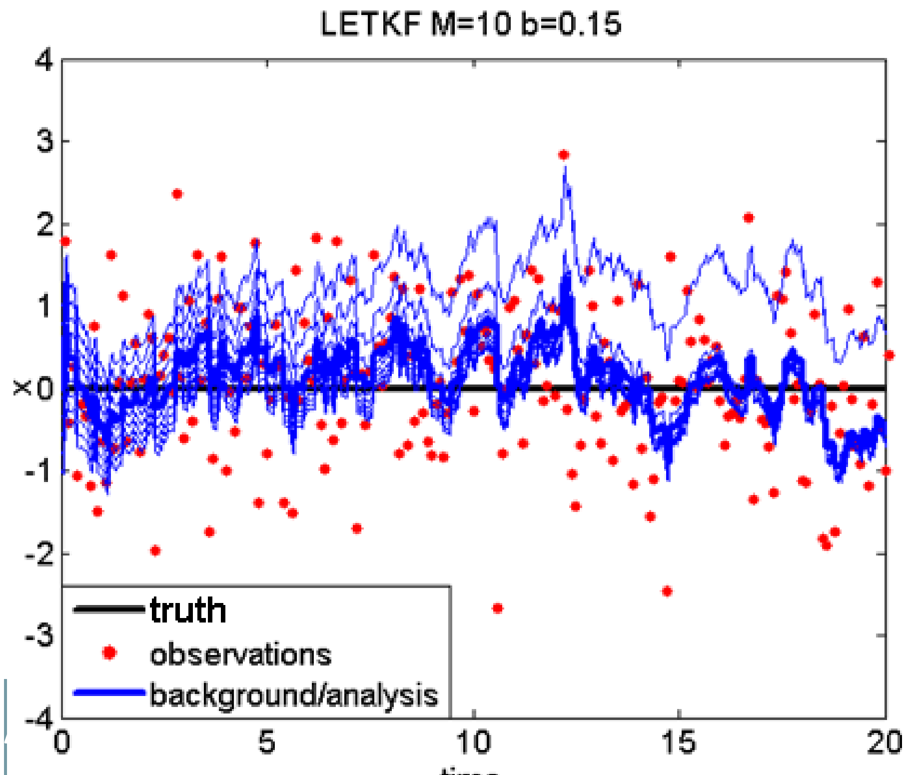
2. Ensemble clustering

Consider the **univariate quadratic model** (Anderson, 2010):

$$x_{t+1} = x_t + 0.05\left(x_t + \underline{b}\,|x_t|\,x_t\right)$$

It has an **unstable fixed point**; we use it as truth $x^t = 0$. The model is integrated with $\Delta t = 0.01$ and we observe ($\mathbf{H} = \mathbf{I}$) every 2 steps. We use S-ETKF for a **linear** $(b = 0)$ and a **nonlinear** $(b = 0.15)$ case, $M = 10$.



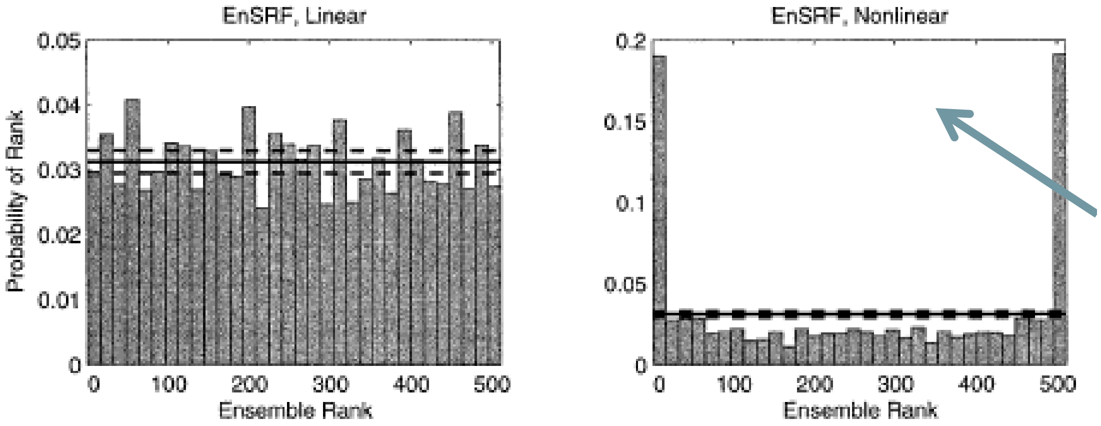


2. Ensemble clustering

As soon as nonlinearity strikes EC appears in EnSRFs. It **does not happen in the stochastic EnKF.** It results from the **disparity of nonlinear forecast and linear analysis** (Anderson, 2010).

This has been studied in the Ikeda model (Lawson and Hansen, 2004), the Lorenz 1963 and 1996 models (Anderson, 2010) with **infrequent observations** and large **observational errors**.

It **does not affect the ensemble covariance**, but it does affect higher order moments.



The **truth is not statistically indistinguishable from the ensemble members** (from Lawson and Hansen, 2004).

2. Questions about EC

a) Is there a **simple way** to **diagnose** it?

b) Is it an **irreversible** phenomenon of EnSRFs?

c) How much does it **affect** the **accuracy** of EnSRFs? Does it **handicap** them?

d) Alternatives can be used to avoid it (e.g. **Non Symmetric ETKFs**, Anderson's Rank Histogram Filter). Are they **advantageous**?

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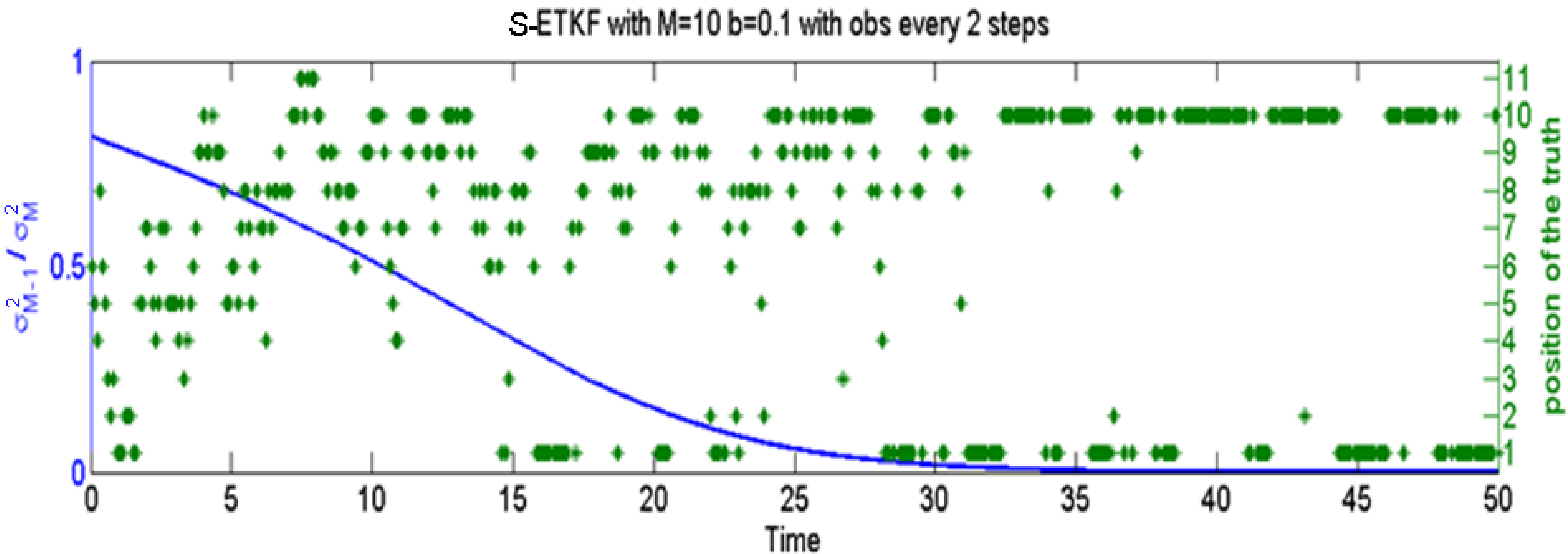
3. Measuring EC

We use the following **metric**, which we denominate '**clustering degree**'.

$$CD = \frac{\sigma^2_{M-1}}{\sigma^2_M} \qquad CD = \frac{Trace(P_{M-1})}{Trace(P_M)}$$

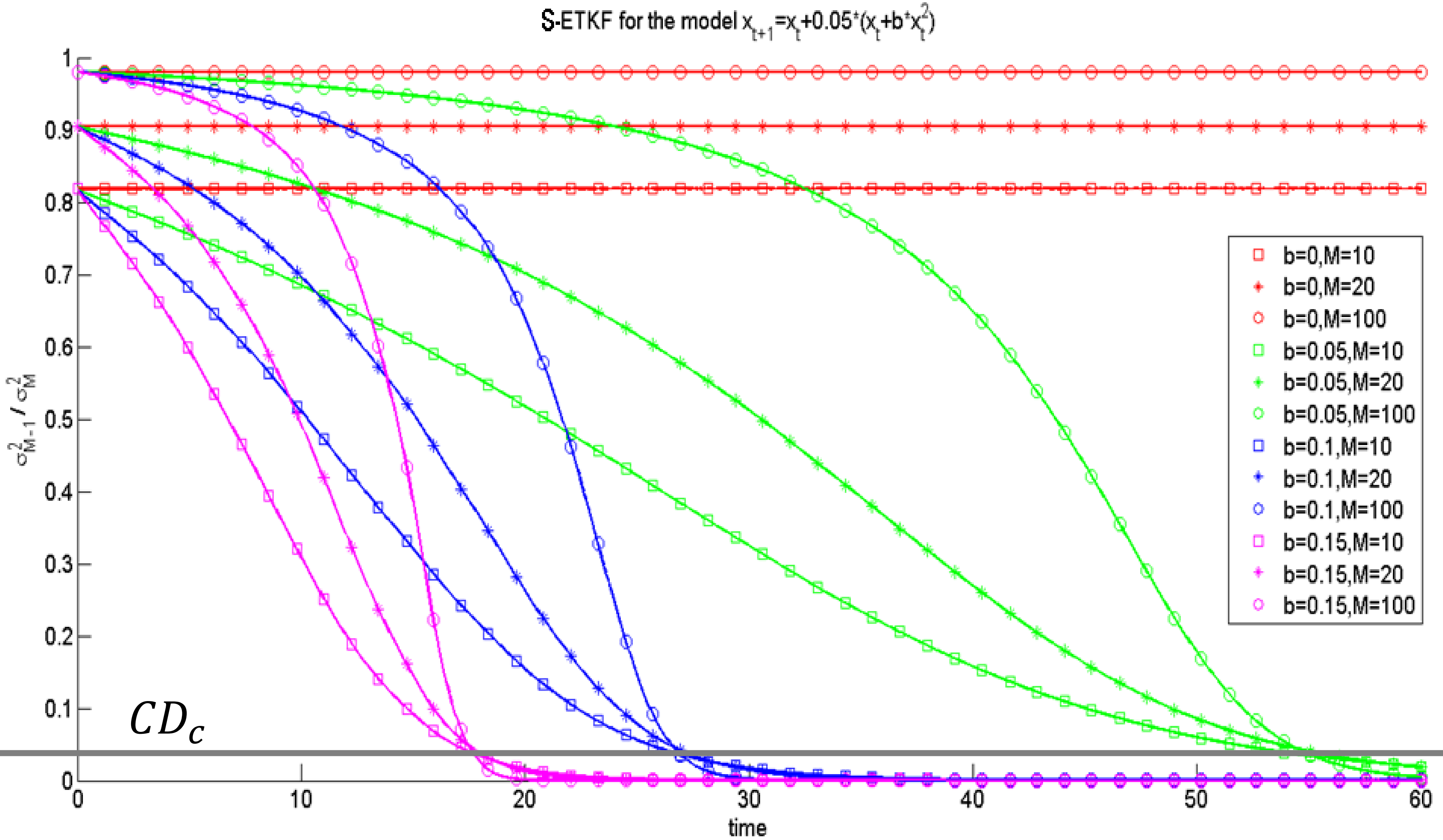
$$N = 1 \qquad N > 1$$

Considering again the model: $x_{t+1} = x_t + 0.05(x_t + b|x_t|x_t)$



3. Measuring EC

Varying the **ensemble size** and the **strength of the nonlinearity**:

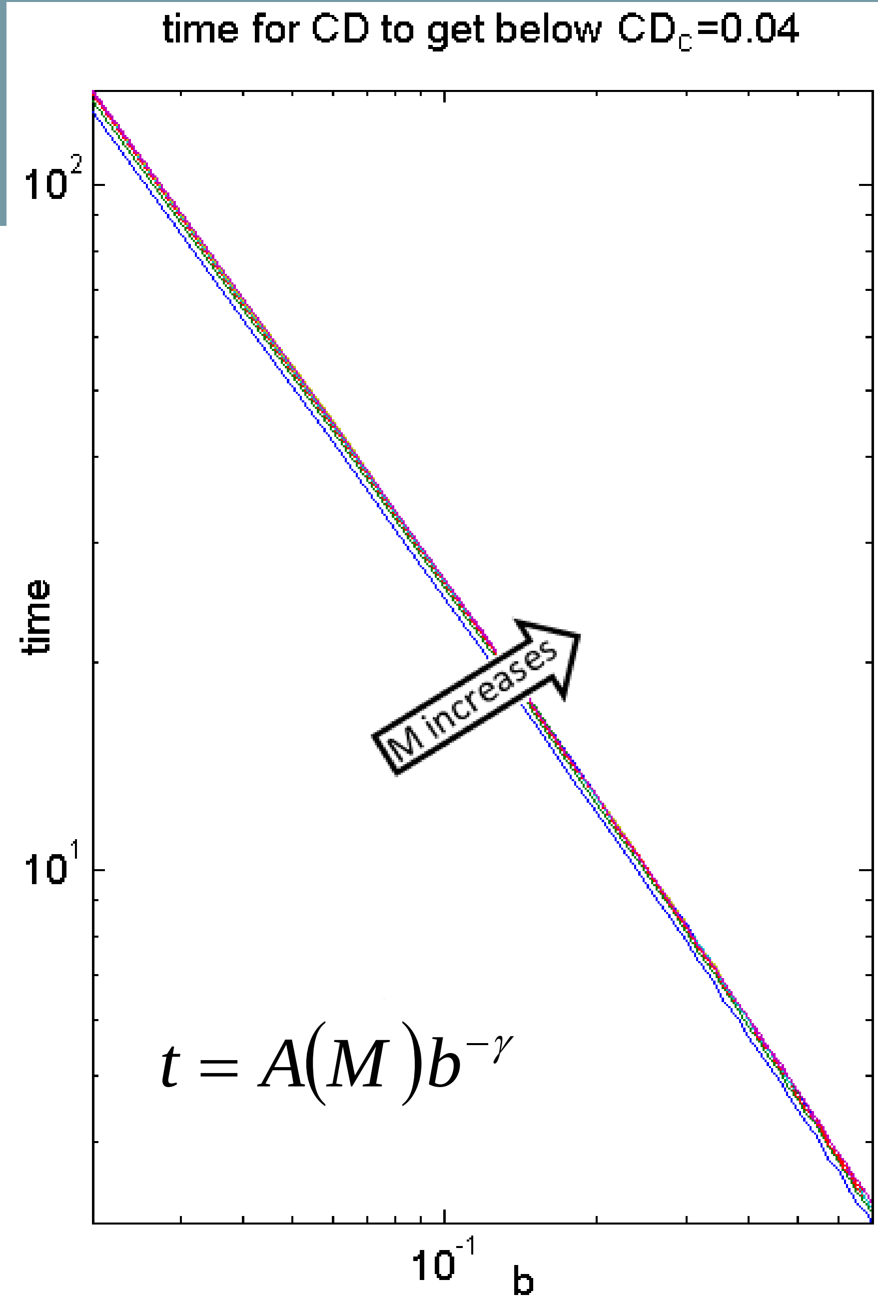


Outline

How **fast** does EC occur?

In this simple model it seems to follow a **power law** independent from *b* and weakly dependent on *M*.

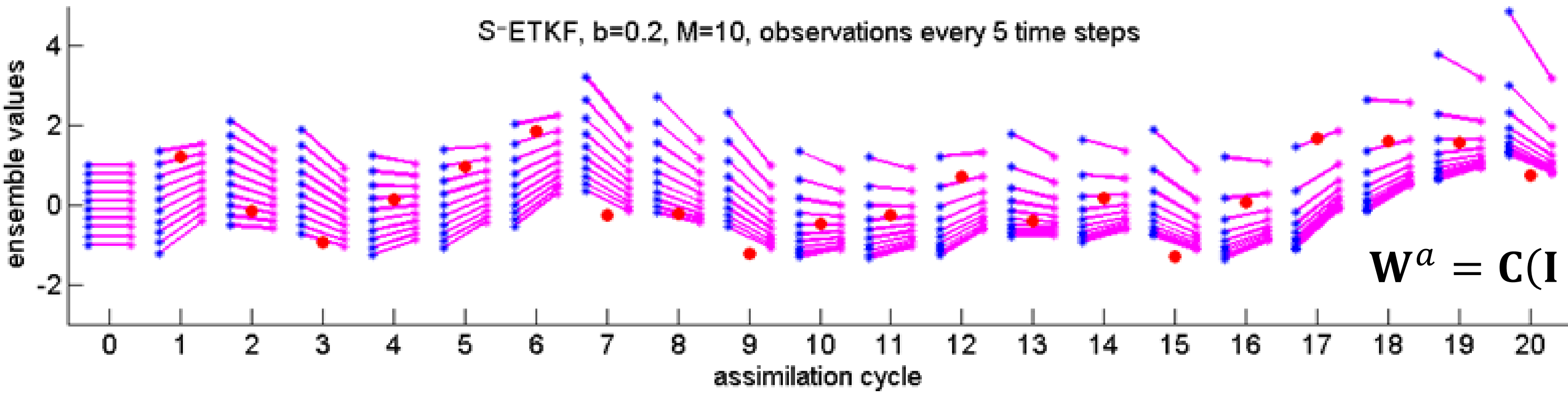
In **this case, clustering is inevitable.** Is this **always the case?**



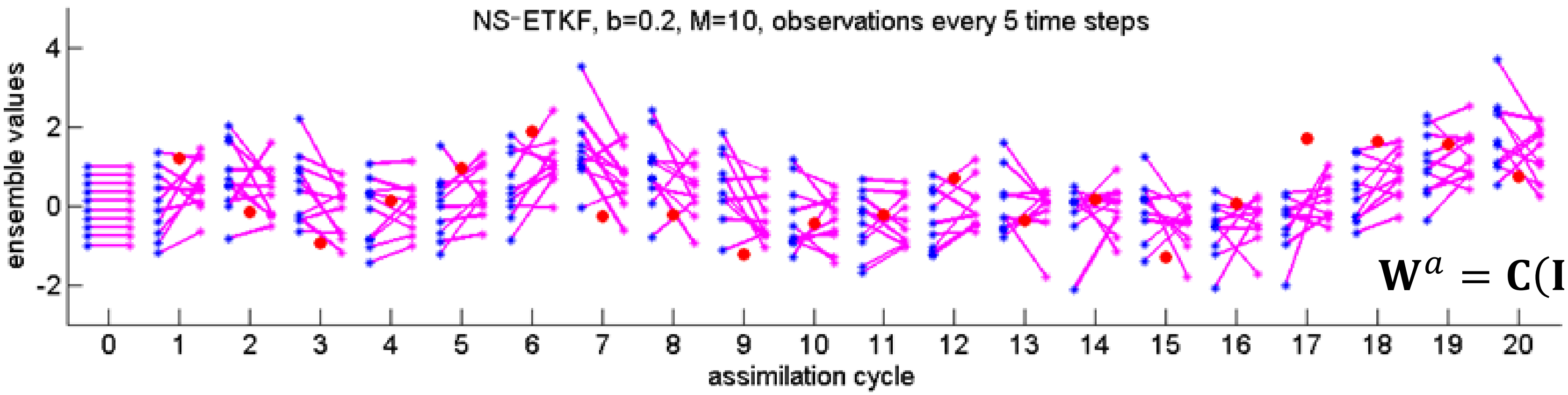
$$t = A(M)b^{-\gamma}$$

3. Avoiding EC: NS-ETKFs

(Unbiased) **randomly-rotated EnSRFs** **avoid clustering**.



$$\mathbf{W}^a = \mathbf{C}(\mathbf{I}+\boldsymbol{\Gamma})^{-\frac{1}{2}}\mathbf{C}^{\mathrm{T}}$$

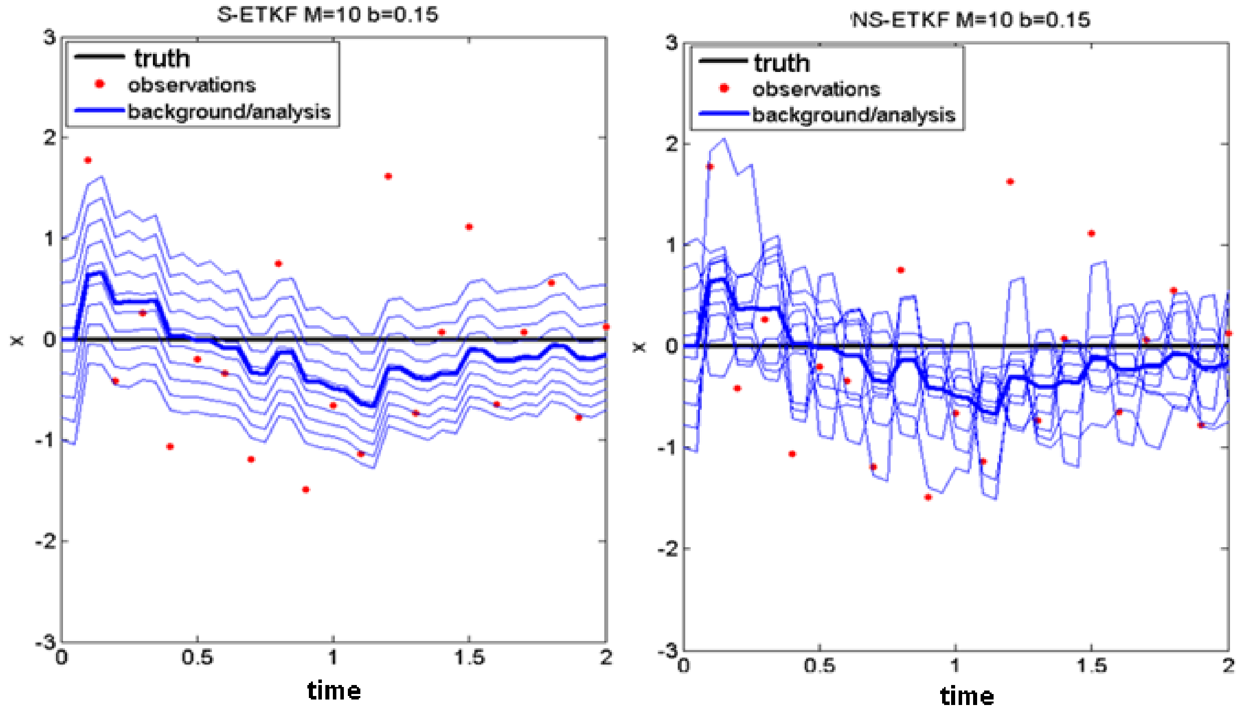


$$\mathbf{W}^a = \mathbf{C}(\mathbf{I}+\boldsymbol{\Gamma})^{-\frac{1}{2}}\mathbf{S}^{\mathrm{T}}$$

The **constant ‘scrambling’ of the ensemble** prevents the outlier from being persistent and eventually ‘escaping’.

3. Avoiding EC: NS-ETKFs

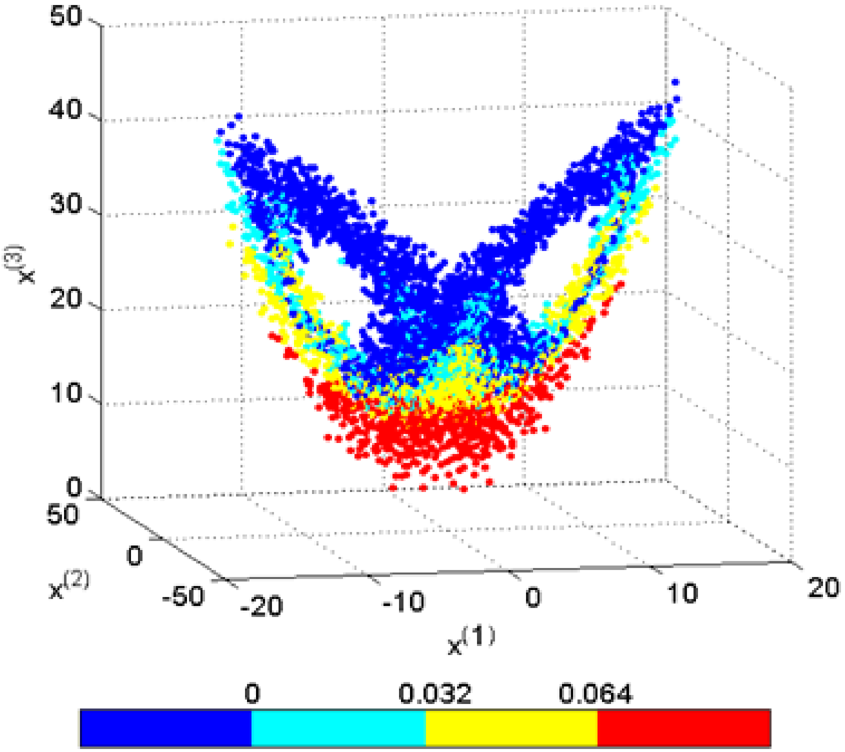
However, this **constrained resampling** of the ensemble **erases** the memory from **individual trajectories**, the effect of the '**errors of the day**' is modified. It is like "**rebooting**" at each analysis instant.



Following individual trajectories was one of the advantages of EnSRFs (Anderson, 2001). **Is it worth losing this ability**?

3. 'Local' nonlinearities

The **growth/decay perturbations is not constant** (neither linearly nor nonlinearly) **in an attractor**.



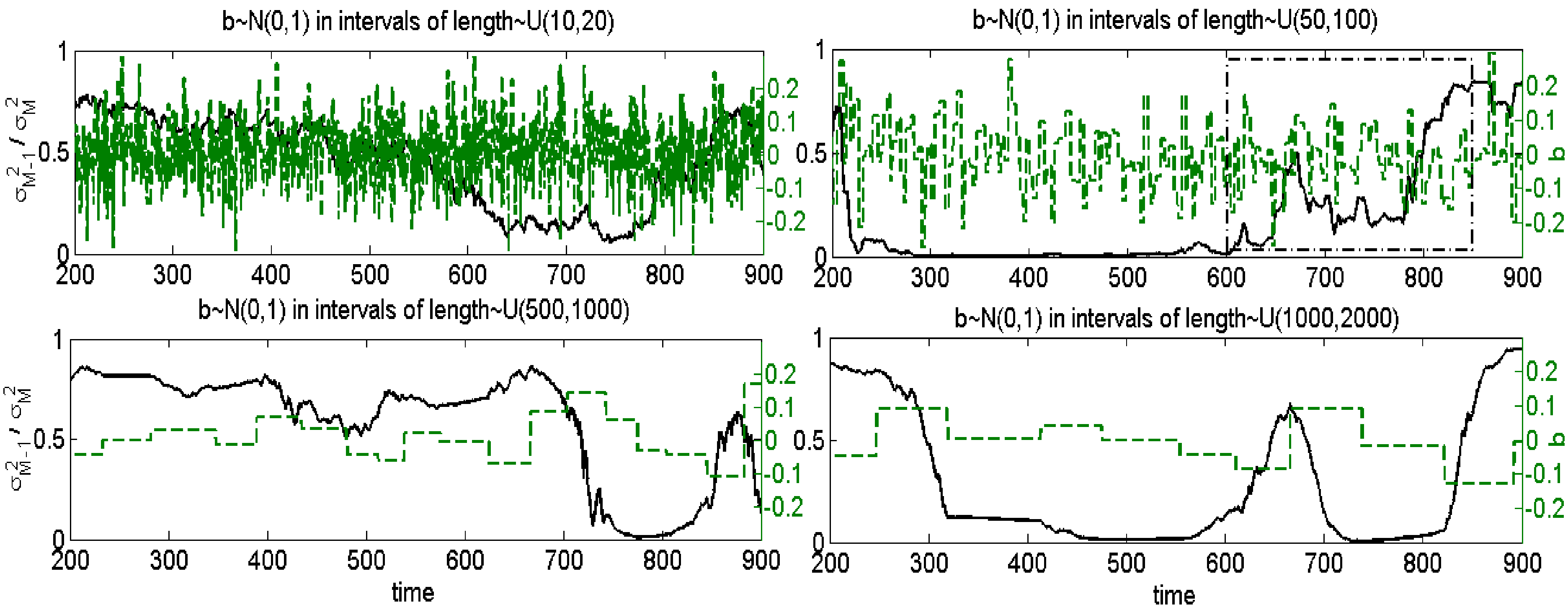
Reproduced from Evans *et al.*, 2004.

Bred vector growth in the Lorenz 1963 model showing the **growth rate for perturbations**. For different regions, there can be **decay** or growth (**slow**, **moderate**, **fast**).

3. ‘Local’ nonlinearities

$$x_{t+1} = x_t + 0.05\left(x_t + b|x_t|x_t\right)$$

Let’s draw **a new** $b \sim N(0,1)$ **every** $L \sim Unif\left(L_0, 2L_0\right)$ **steps**, perform DA in this model, and measure the clustering degree.



3. 'Local' nonlinearities

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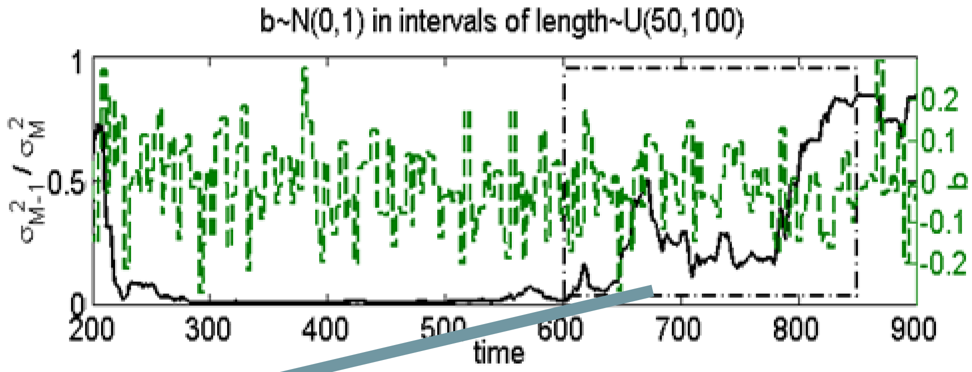

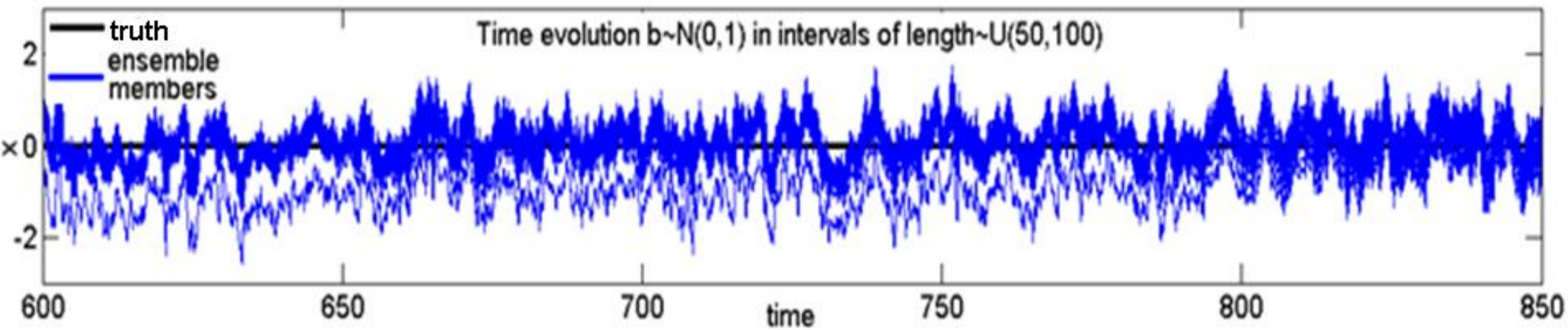

Clustering can be **reverted** by the **alternation of nonlinear growth and decay**. It is an **intermittent phenomenon**.

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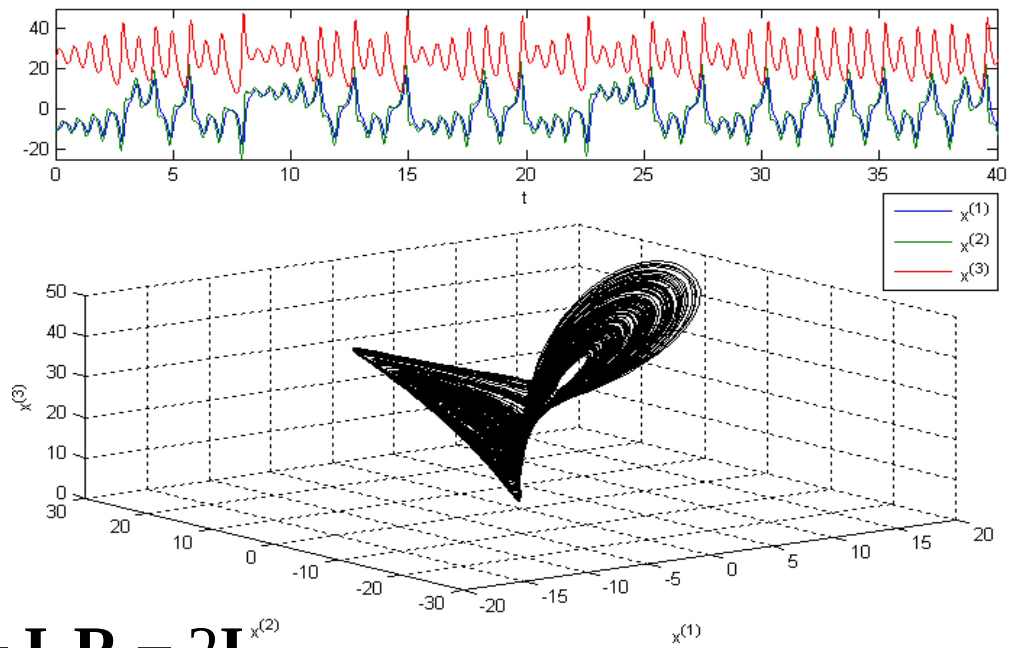
4. EC in the Lorenz 1963 (L63) model

The system:

$$\dot{x}^{(1)} = \sigma\left(x^{(2)} - x^{(1)}\right) \qquad \sigma = 10$$

$$\dot{x}^{(2)} = x^{(1)}\left(r - x^{(3)}\right) - x^{(2)} \qquad r = 8/3$$

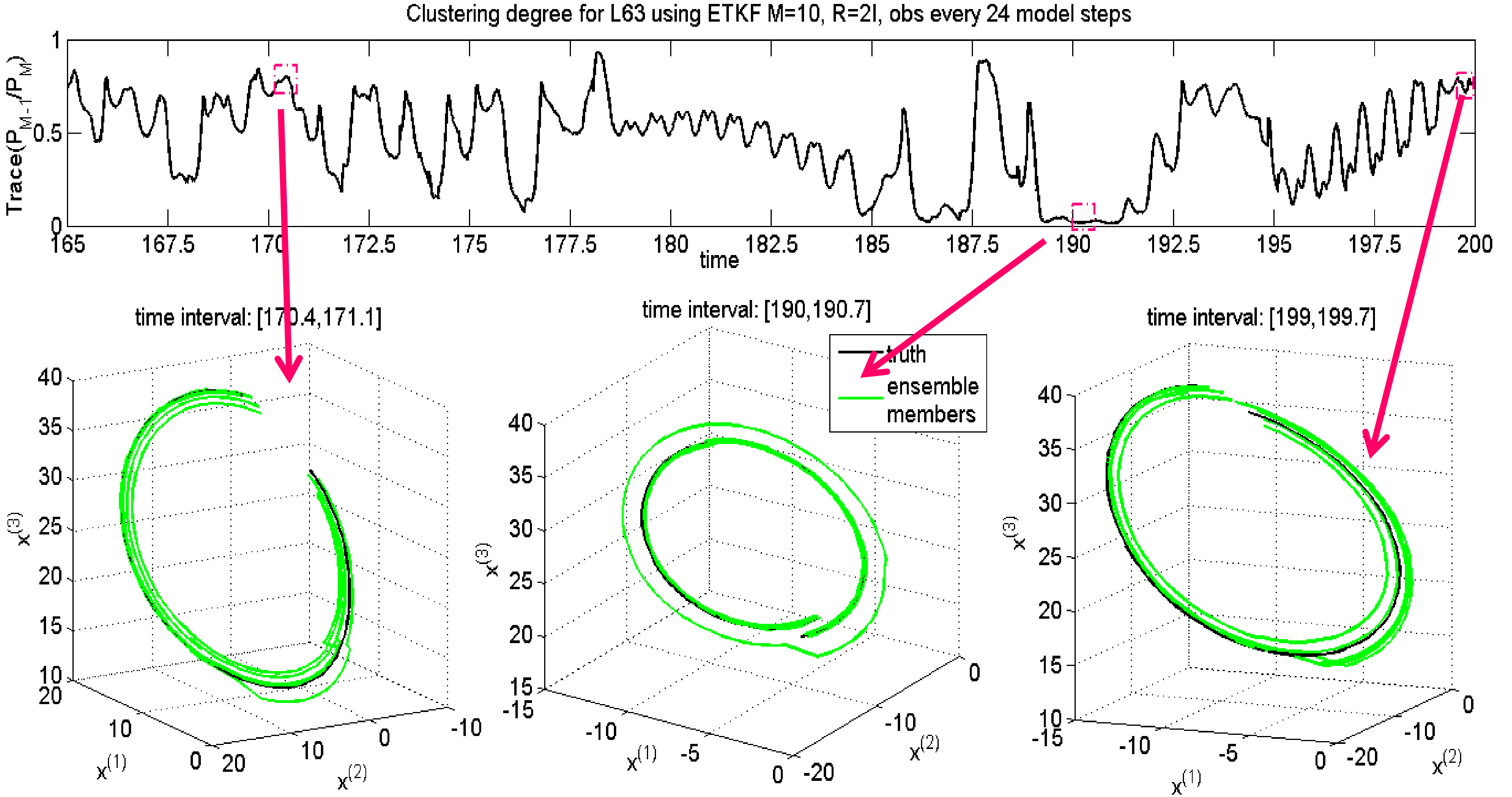
$$\dot{x}^{(3)} = x^{(1)}x^{(2)} - bx^{(3)} \qquad b = 28$$



Settings (Miller et al., 1997; Kalnay et al., 2007): $\Delta t = 0.01, \mathbf{H} = \mathbf{I}, \mathbf{R} = 2\mathbf{I}$

- "**Frequent**" **observations**: every **8 steps**, **linear** regime.
- "**Infrequent**" **observations**: every **24 steps**, **nonlinear** regime.

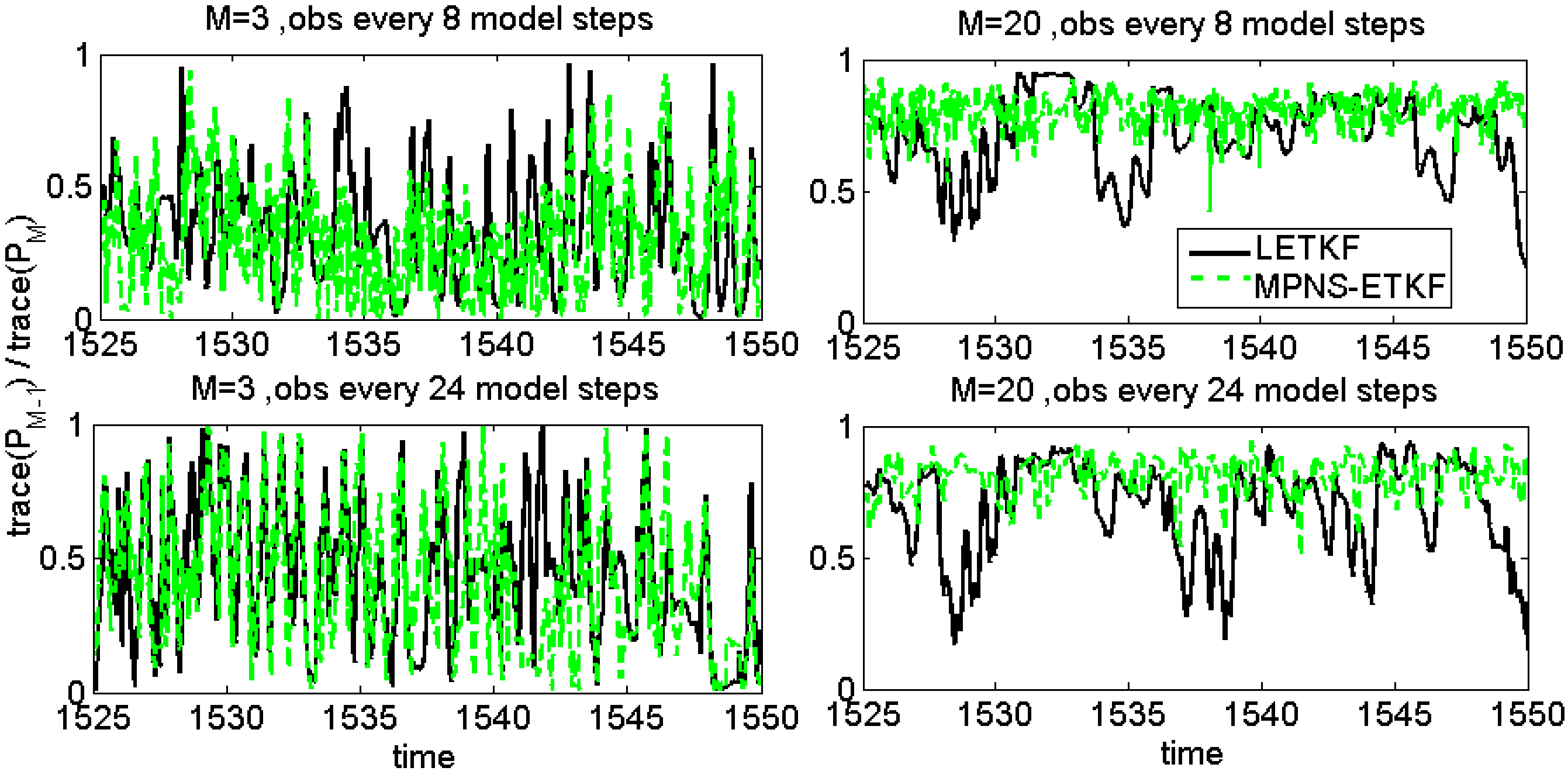
4. EC in L63



Clustering is intermittent.

4. EC in L63

As usual, **the Non-Symmetric ETKF does not present clustering**.



4. EC in L63

Clustering is **intermittent**, and **less persistent than in the univariate quadratic model**. Why?

In the **univariate model**, only the **magnitude of *b* could vary**. Plus, this model didn't present mixing.

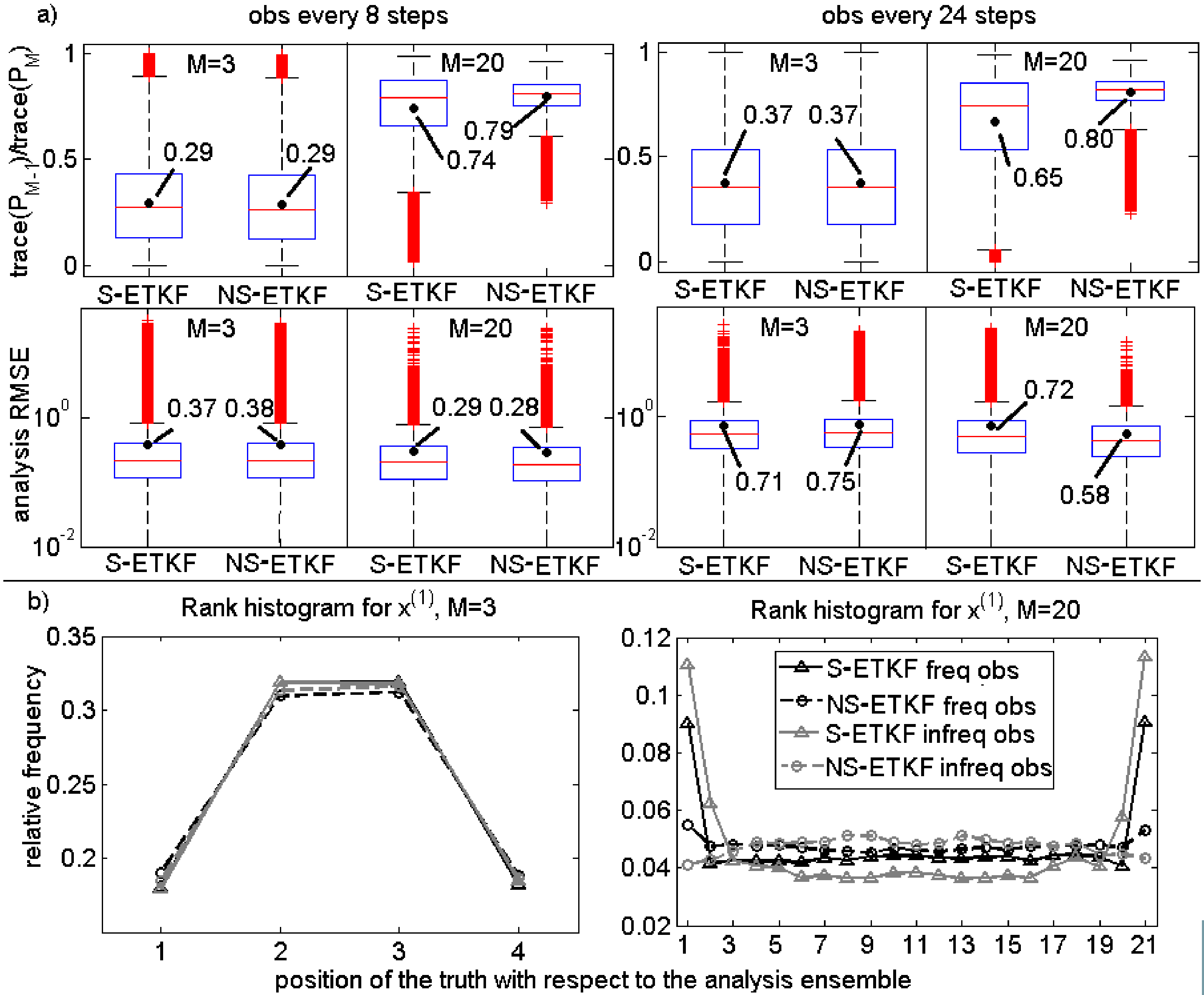
In the **Lorenz 1963 model**, both the **direction and magnitude of the nonlinear growth can vary**. Besides, this model presents mixing.

4. EC in L63

A **statistical summary** with 2 ensemble sizes (*M=3,10*).

Clustering affects the performance of S-ETKF (in terms of RMSE) **for large size ensembles**.

Random rotations **improve** the **rank histograms**, but **not when inflation is used** (*M=3*).



4. Larger models: localization

Larger models require **localization**. A natural choice for the **ETKF family** is **grid-point R localization**.

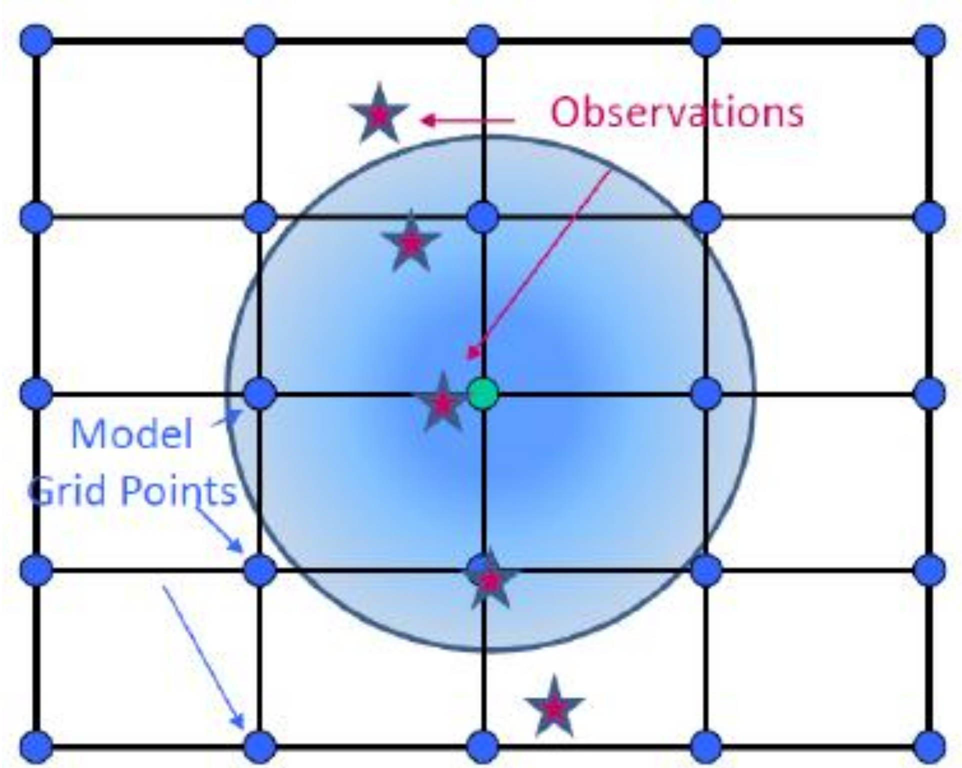


*Figure courtesy of Steven Greybush.

An **independent analysis** is carried out for **each grid-point** considering the neighboring observations.

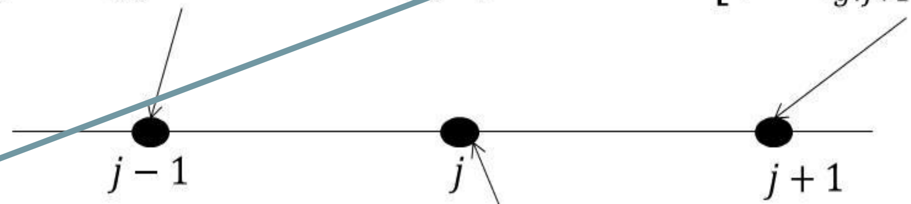
The **analysis ensemble** is constructed by **sets of rows**.

R-localization allows for **spatially varying adaptive inflation** (Miyoshi, 2011).

4. Larger models: localization

$$\mathbf{W}_{g:j-1}=\begin{bmatrix}(w_{1,1})_{g:j-1} & \cdots & (w_{1,M})_{g:j-1}\\ \vdots & \ddots & \vdots\\ (w_{M,1})_{g:j-1} & \cdots & (w_{M,M})_{g:j-1}\end{bmatrix}$$

$$\mathbf{W}_{g:j+1}=\begin{bmatrix}(w_{1,1})_{g:j+1} & \cdots & (w_{1,M})_{g:j+1}\\ \vdots & \ddots & \vdots\\ (w_{M,1})_{g:j+1} & \cdots & (w_{M,M})_{g:j+1}\end{bmatrix}$$



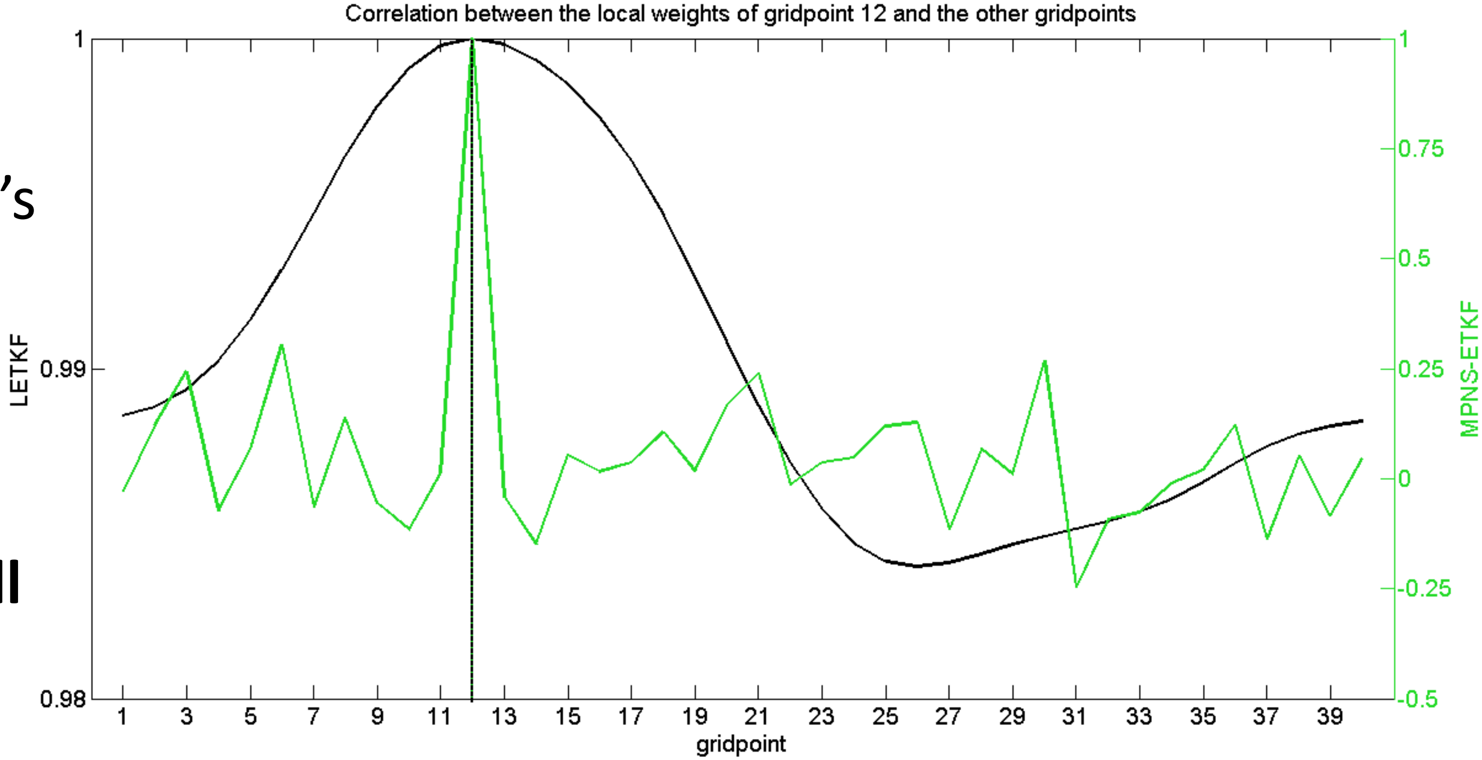
$$\mathbf{W}_{g:j-1}=\begin{bmatrix}(w_{1,1})_{g:j} & \cdots & (w_{1,M})_{g:j}\\ \vdots & \ddots & \vdots\\ (w_{M,1})_{g:j} & \cdots & (w_{M,M})_{g:j}\end{bmatrix}$$

The **transition between these matrices must be as smooth as possible** from one point *j* to the neighbors *j-1, j+1*

This was one of the reasons why the **symmetric square root was used in LETKF** (Hunt et al., 2007).

4. Larger models: localization

Using the **40-variable Lorenz 1996 model**, let's compute the **correlation among the weights of 1 gridpoint and all others.**

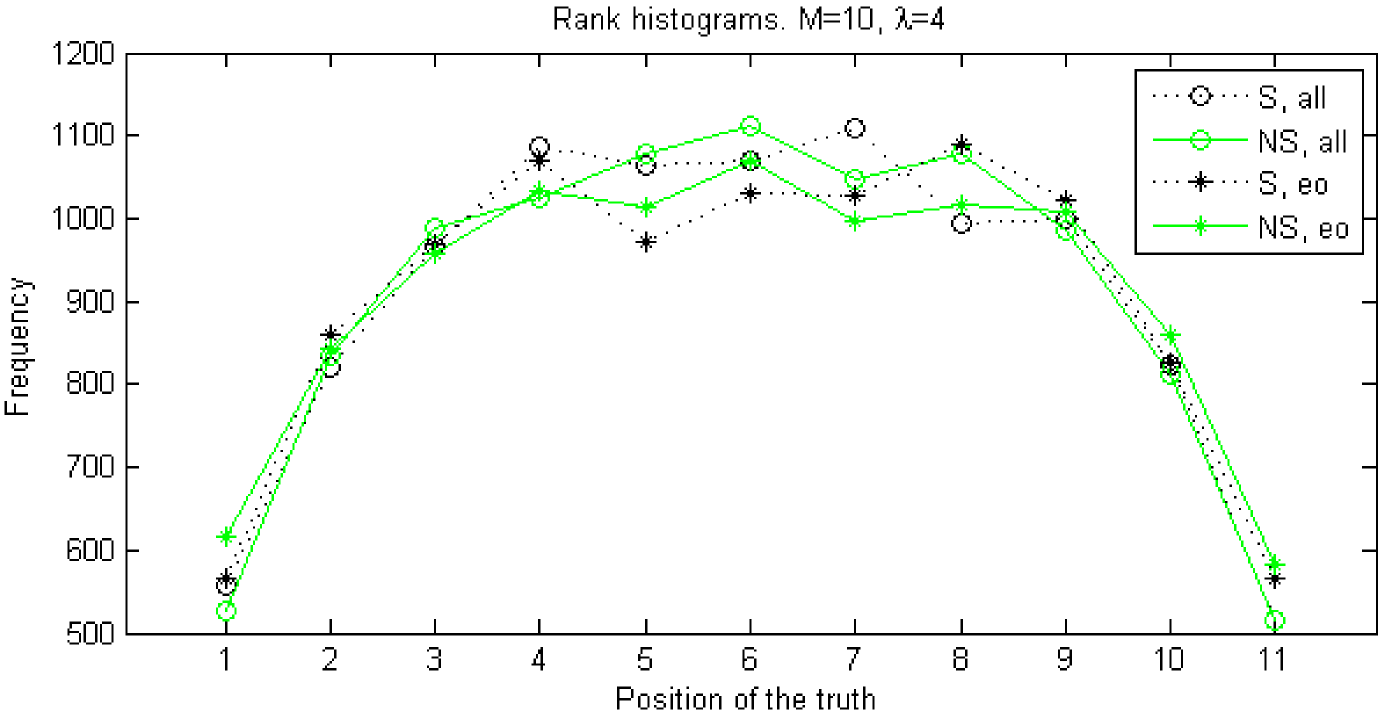


The randomly rotated ETKF **cannot be applied directly**, since a smooth transition among weight matrices (**W**) of neighboring gridpoints is not guaranteed.

4. Larger models: localization/inflation

Using **L96**, we perform experiments **observing** (a) **all variables** and (b) every **other variable** using **R-localization and adaptive inflation**. The observations are taken every 2 model steps ($\mathbf{R} = \mathbf{I}$).

No **perceivable difference in analysis RMSE** is noted. What happens with the **rank verification of truth**?

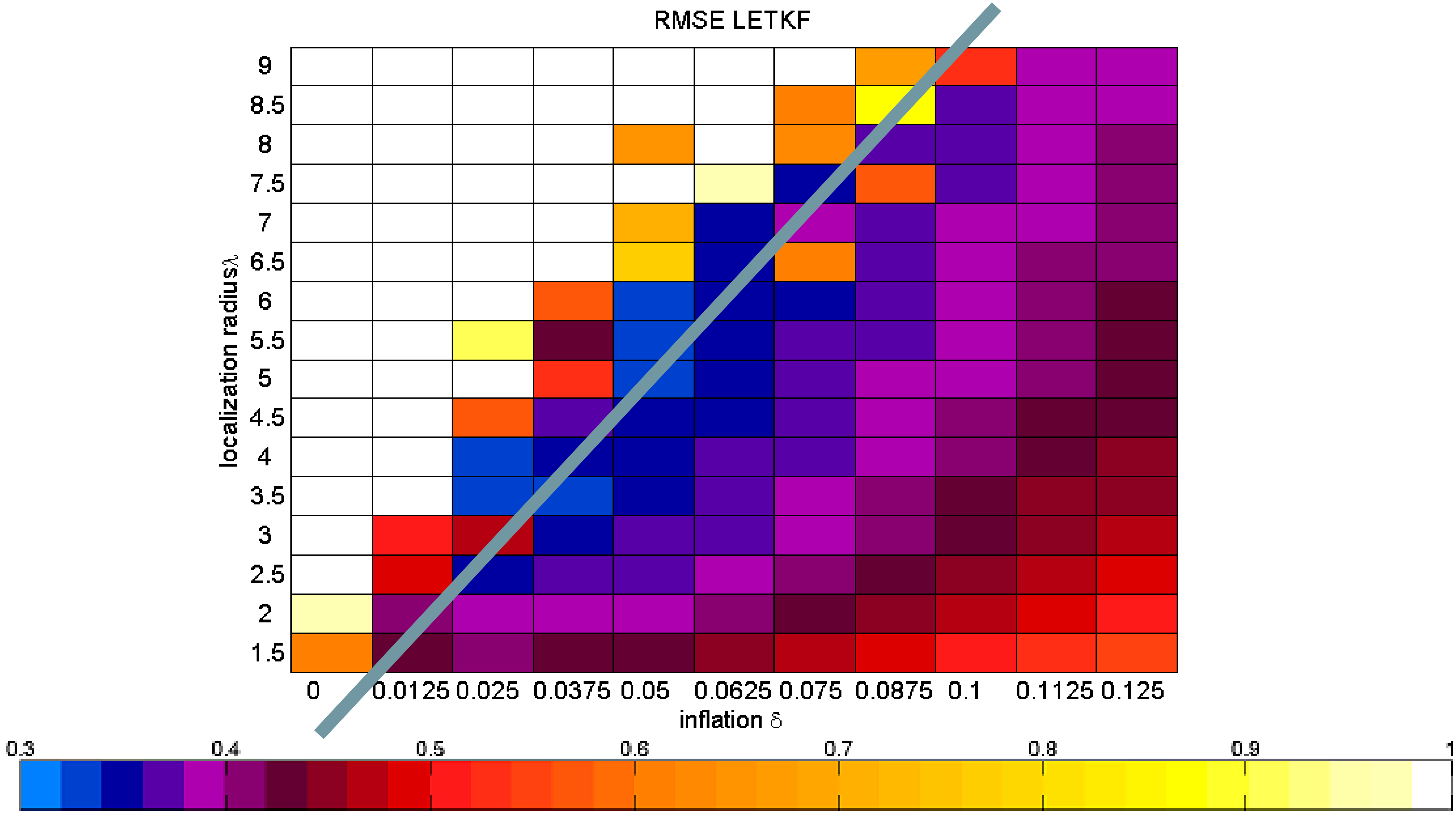


Inflation can lead to **over-dispersive ensembles** in all cases for these settings.

4. Larger models: localization/inflation

The **inflation is adaptive**. Why are the **ensembles overdispersive**?

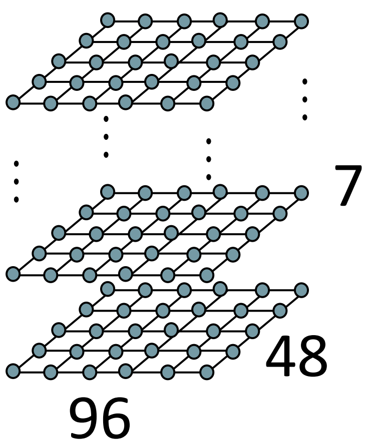
It is tough to find the **optimal inflation**, it **is close to filter divergence**.

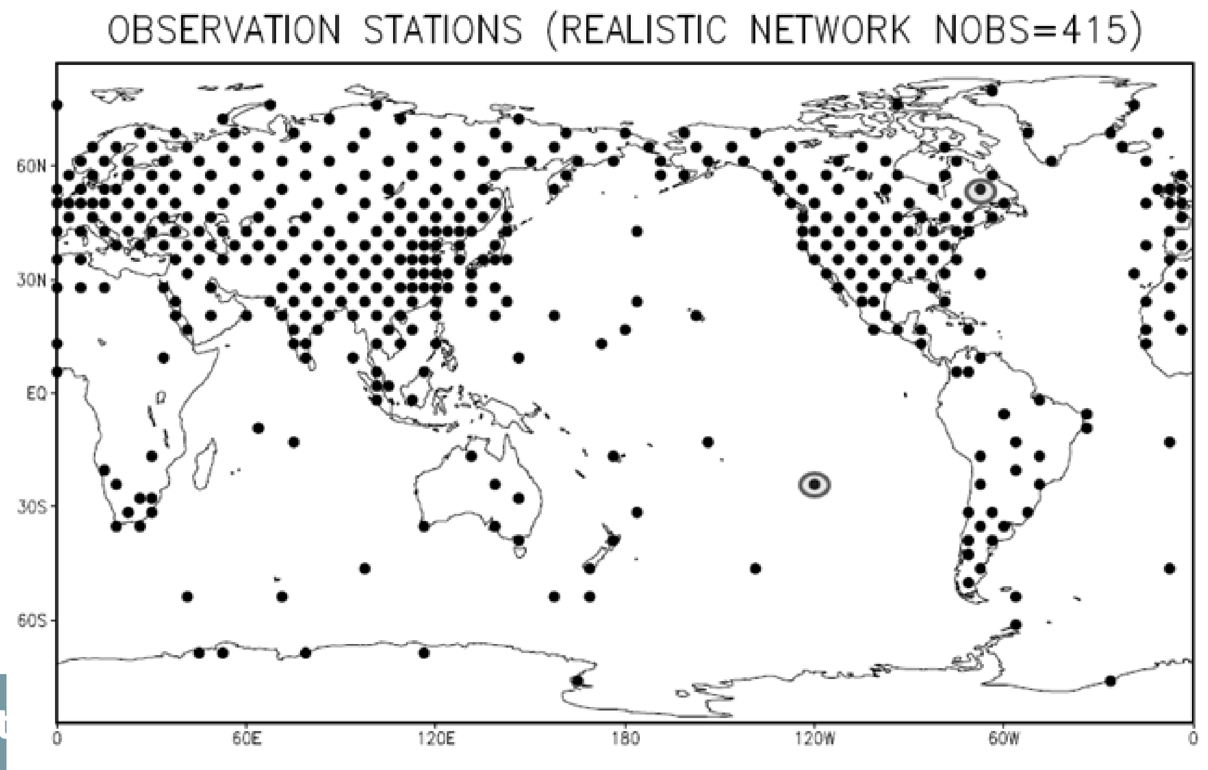


3. Larger models: a simplified AGCM

SPEEDY (Simplified Parameterizations, primitivE-Equations Dynamics, Molteni 2003)

- Time step is 40 minutes.
- Model variables: *u, v, T, q, ps*
- Spectral model with T30L7 resolution using σ-coordinates.

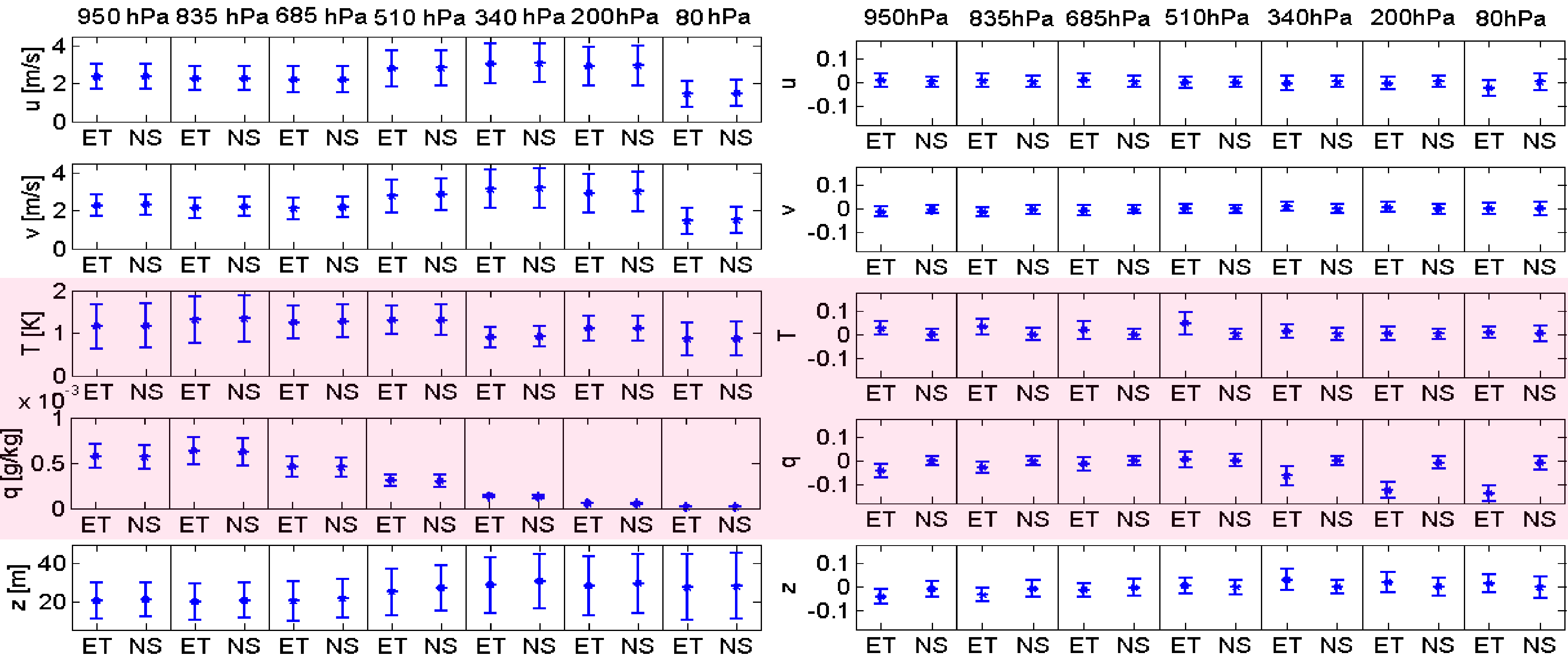




3. Larger models: a simplified AGCM

Computing **analysis RMSE and sample skewness** for all variables.

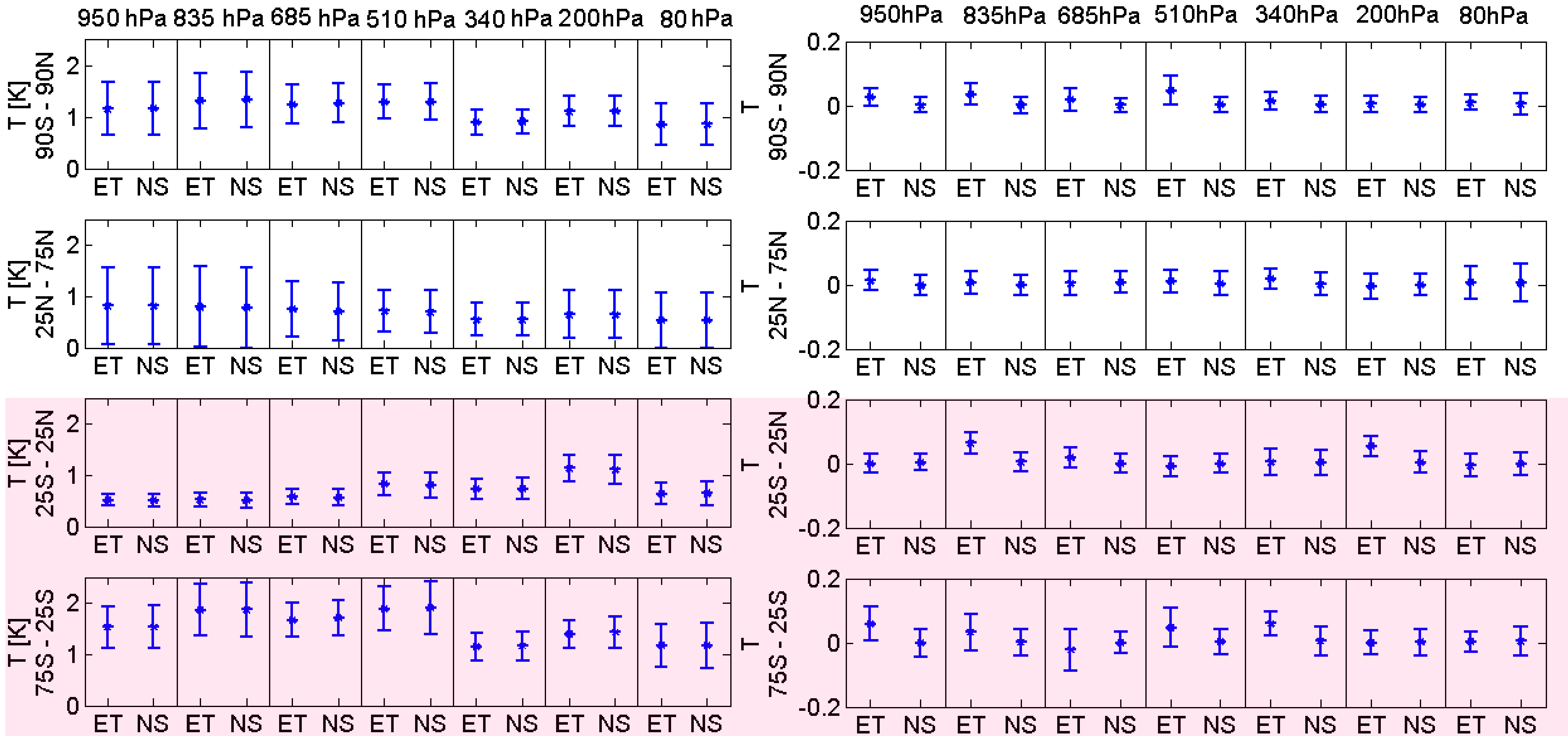
2 months of experiments, *M=20*, R-localization and adaptive inflation.



For some variables (***T* and *q***) we get **asymmetric ensembles**.

3. Larger models: a simplified AGCM

SPEEDY: **What happens with *T*?**



Asymmetric ensembles mainly in the **tropics** and in the **SH**. This **does not seem to affect RMSE**.

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- **Clustering** is **not** an **irreversible** phenomenon of (deterministic) EnSRFs. It is **intermittent**.

- The **local** (in time and space) **nonlinear** **expansion/contraction** of the **ensemble** **triggers/reverses** **clustering**.

- As the **model** **grows**, the **persistence** **of clustering is** **shorter**.

- We only found **EC affecting** the performance (in terms of **RMSE**) of data assimilation when the **ensemble size is much larger than the state dimension** (***M>>N***).

5. Summary

- **Non-symmetric** solutions of the **ETKF** **do not present clustering**. Nonetheless, they **lose track** **of individual trajectories**.

- For **R-localization**, it is indispensable to have a **symmetric solution** (for **smoothness**). One can apply **rotations** as an **extra step**.

- When **localization and inflation** are used, their **effects** tend to **dominate** and **clustering** is more **difficult to find**.

- In a **simplified AGCM** we find evidence of **asymmetric ensembles** for **some variables**, but this **does not affect the RMSE**. **No episodes of clustering were observed**.