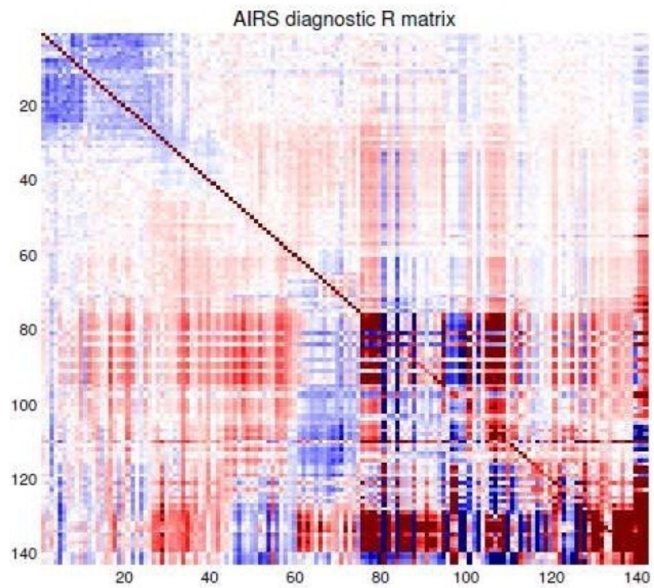
Diagnosis, Conditioning and Regularization of Error Covariances



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Optimal Bayesian Estimate

Minimize with respect to initial state $\mathbf{x}_0$:

$$J(\mathbf{x}_0) = \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}_0^b)^T \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}_0^b) + \frac{1}{2}(\mathcal{H}(\mathbf{x}_0) - \mathbf{y})^T \mathbf{R}^{-1}(\mathcal{H}(\mathbf{x}_0) - \mathbf{y})$$

- Background state $\mathbf{x}_0^b$
- Observations $\mathbf{y}$
- Observation operator $\mathcal{H}$
- Error covariance matrices $\mathbf{B}$, $\mathbf{R}$

The solution at the minimum, x^a , is the analysis.

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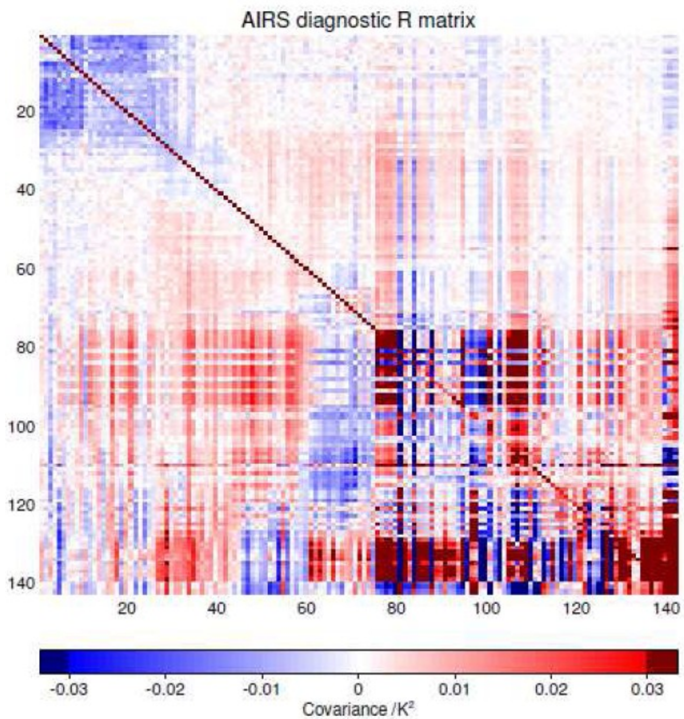
Outline

- Observation Errors
- Diagnosing Observation Error Covariances
- Incorporating Observation Errors in DA
- Sensitivity of the Analysis
- Regularization
- Conclusions

1. Observation Errors

Observation Errors



Observation Error Covariance Matrix

- Observation errors have been assumed to be uncorrelated in data assimilation.

- Observation errors in real data are found to be correlated. (*Stewart et al, 2009, 2013; Bormann et al, 2010; Waller et al, 2013, 2014a*.)

- Using observation error correlations in data assimilation is shown to improve the state estimate. (*Stewart et al, 2008, 2010, 2014; Weston, 2014*.)

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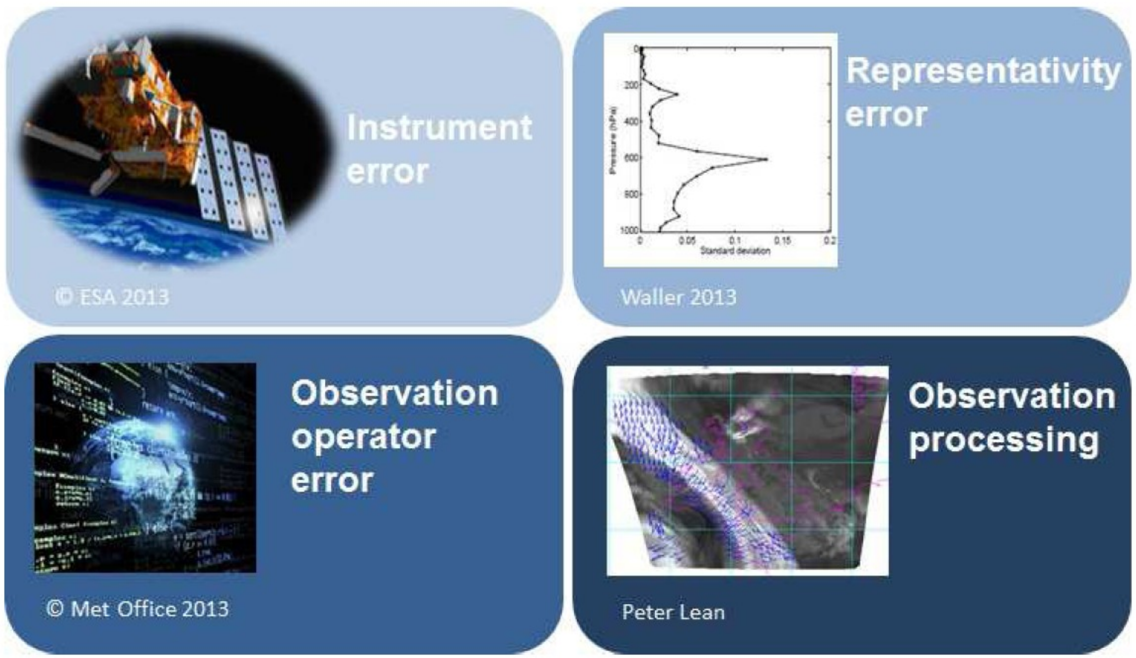
Observation Errors

Four main sources of observation errors, which are time and spatially varying:



Waller et al, 2014a; Stewart, 2014; Hodyss & Nichols, 2014

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Observation Errors

It is important to be able to account for observation error correlations:

- Avoids thinning (high resolution forecasting)
- More information content
- Better analysis accuracy
- Improved forecast skill scores

Stewart et al, 2008, 2009, 2010, 2013, 2014; Bormann et al, 2010; Waller et al, 2013, 2014a; Weston, 2014

2. Diagnosing Observation Error Covariances

DBCP Diagnostic (Desroziers et al, 2005)

Let

$$\mathbf{d}_b^o = \mathbf{y} - \mathcal{H}(\mathbf{x}^b),$$
$$\mathbf{d}_a^o = \mathbf{y} - \mathcal{H}(\mathbf{x}^a).$$

DBCP Diagnostic (Desroziers et al, 2005)

Let

$$\begin{aligned} \mathbf{d}_b^o &= \mathbf{y} - \mathcal{H}(\mathbf{x}^b), \\ \mathbf{d}_a^o &= \mathbf{y} - \mathcal{H}(\mathbf{x}^a). \end{aligned}$$

Then

$$E[\mathbf{d}_a^o \mathbf{d}_b^{o\,T}] = \widetilde{\mathbf{R}}(\mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^{\mathbf{T}} + \widetilde{\mathbf{R}})^{-1}(\mathbf{H}\mathbf{B}\mathbf{H}^T + \mathbf{R}) = \mathbf{R}^e,$$

where

$\mathbf{B}$ and $\mathbf{R}$ are the exact background and observation covariance matrices.

$\widetilde{\mathbf{R}}$ and $\widetilde{\mathbf{B}}$ are the assumed observation and background error statistics used in the assimilation.

DBCP Diagnostic (Desroziers et al, 2005)

Let

$$
\begin{aligned}
\mathbf{d}_b^o &= \mathbf{y} - \mathcal{H}(\mathbf{x}^b), \\
\mathbf{d}_a^o &= \mathbf{y} - \mathcal{H}(\mathbf{x}^a).
\end{aligned}
$$

Then

$$E[\mathbf{d}_a^o \mathbf{d}_b^{o\,T}] = \widetilde{\mathbf{R}}(\mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^{\mathbf{T}} + \widetilde{\mathbf{R}})^{-1}(\mathbf{H}\mathbf{B}\mathbf{H}^T + \mathbf{R}) = \mathbf{R}^e,$$

If the observation and forecast errors used in the assimilation are exact, $\widetilde{\mathbf{R}} = \mathbf{R}$ and $\widetilde{\mathbf{B}} = \mathbf{B}$, then

$$E[\mathbf{d}_a^o \mathbf{d}_b^{o\,T}] = \mathbf{R}$$

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DBCP Diagnostic in Spectral Space

Analysis of the diagnostic in spectral space, under some simplifying assumptions, shows that if the observation errors are correlated, then assuming in the assimilation that the correlation matrix is diagonal results in an estimate $\mathbf{R}^e$ with: :

- underestimated observation error variances;
- underestimated observation error correlation length scales;

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- underestimated observation error variances;
- underestimated observation error correlation length scales.

But a better estimate of the observation error covariance matrix than an uncorrelated diagonal matrix.

Waller et al, 2016a

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Summary: DBCP Diagnostic

The DBCP diagnostic has been successfully applied in operational systems to determine the observation error covariances for a variety of different observation types: including:

- Doppler radar wind data;
- atmospheric motion vectors;
- remotely sensed satellite data –
  eg SEVIRI, IASI, AIRES, CRis and others

Stewart et al, 2014; Waller et al, 2016b, 2016c; Cordoba et al, 2016.

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3. Incorporating Correlated Observation Errors in Ensemble DA

ETKF Filter

Step 1 Use the full non-linear model to forecast each ensemble member from $\mathbf{x}^a_{n-1}$ to $\mathbf{x}^f_n$.

Step 2 Calculate the ensemble mean $\bar{\mathbf{x}}^f_n$ and approximate covariance matrix $\mathbf{B}_n$.

Step 3 Using the ensemble mean at time t_n , calculate the innovation $\mathbf{d}^o_{b\,n}$.

Step 4 The ensemble mean is updated using

$$\bar{\mathbf{x}}^a_n = \bar{\mathbf{x}}^f_n + \mathbf{K}_n \mathbf{d}^o_{b\,n}$$

where the gain $\mathbf{K}_n = \mathbf{Z}_n \mathbf{H}_n^T \mathbf{R}_n^{-1} \approx \mathbf{B}_n \mathbf{H}_n^T (\mathbf{H}_n \mathbf{B}_n \mathbf{H}_n^T + \mathbf{R}_n)^{-1}$

Livings et al, 2008

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Ensemble Filter with Diagnostic

Procedure:

- Select initial **R**
- Run ETKF and store samples of $\mathbf{d}^b$ and $\mathbf{d}^a$
- Compute $E[\mathbf{d}^a\, \mathbf{d}^{bT}]$
- Symmetrize (and regularize) to obtain new estimate for **R**
- Repeat steps of ETKF using samples from rolling window of length N_s to update **R**

Waller et al, 2014a

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Example:

Use high resolution Kuromoto-Sivashinsky model

Add errors to observations from normal distribution with known SOAR covariance $\mathbf{R}_t$.

- Assume incorrect $\mathbf{R}_\mathrm{I}$ = diagonal at $t = 0$. Recover fixed true covariance.
- Allow length scale in true covariance to vary slowly. Recover time-varying true covariance.

Results – Static R_t :

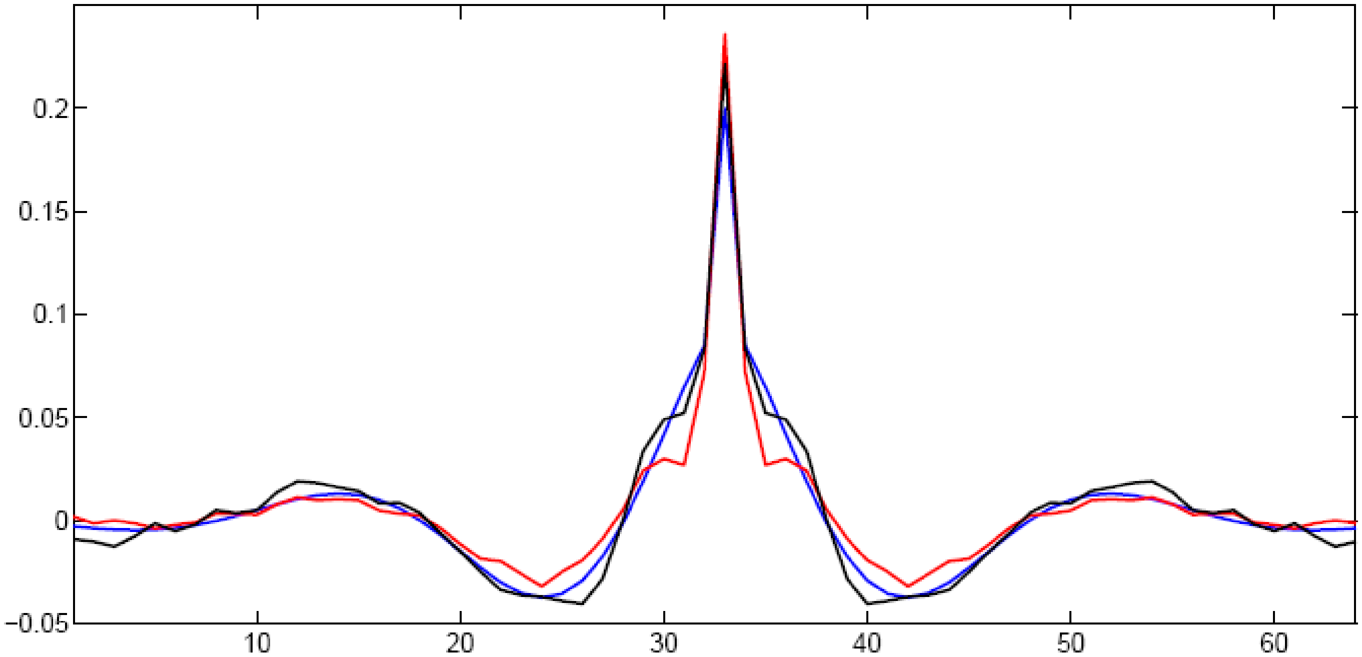
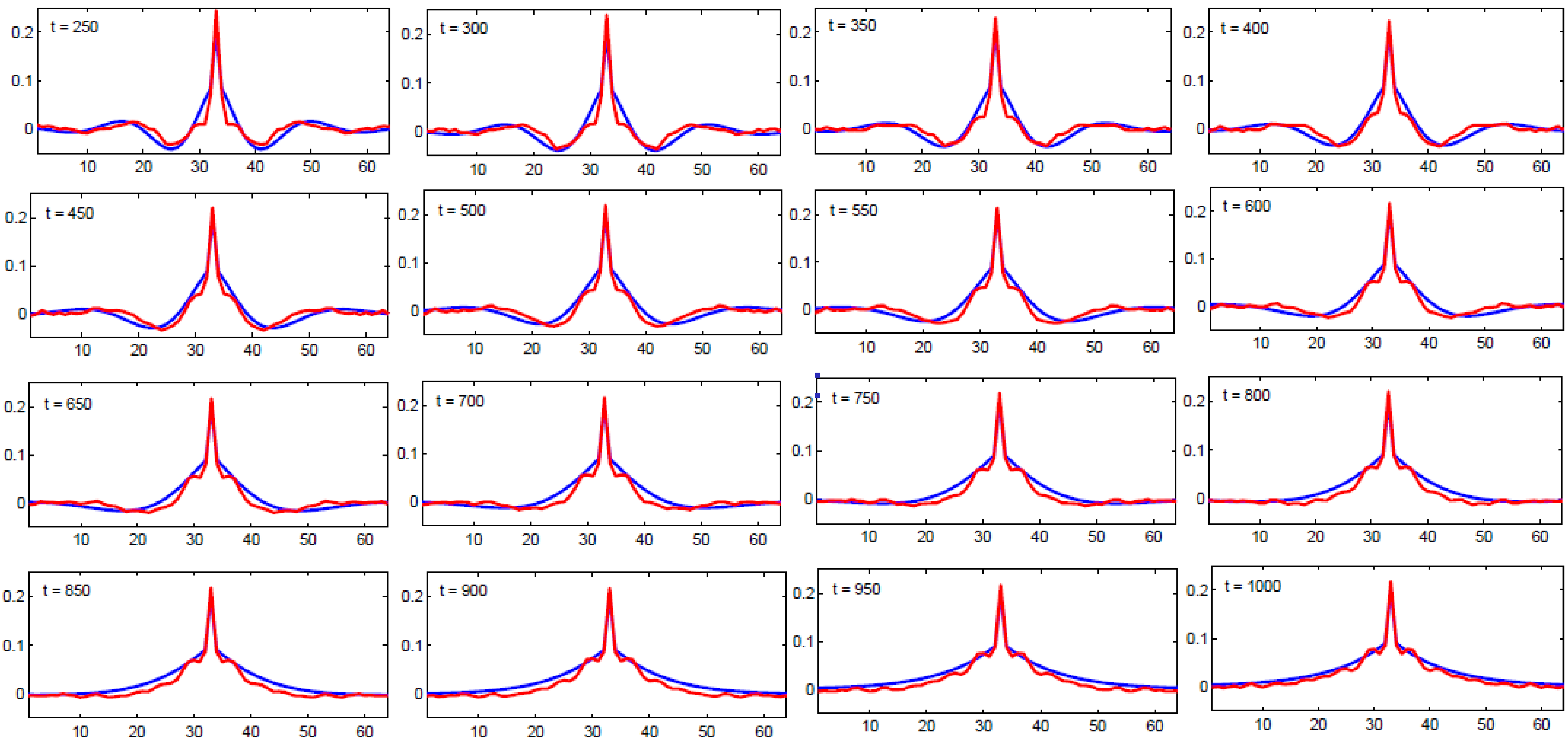


Figure : Rows of the true (blue) and estimated (red, initial estimation, black final estimation)correlation matrices for Experiment 4

Results – Time Varying R_t :



Rows of the true and estimated correlation matrices

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Results – Analysis Errors:

Time averaged RMSE analysis errors:

Static True $\mathbf{R}_t$

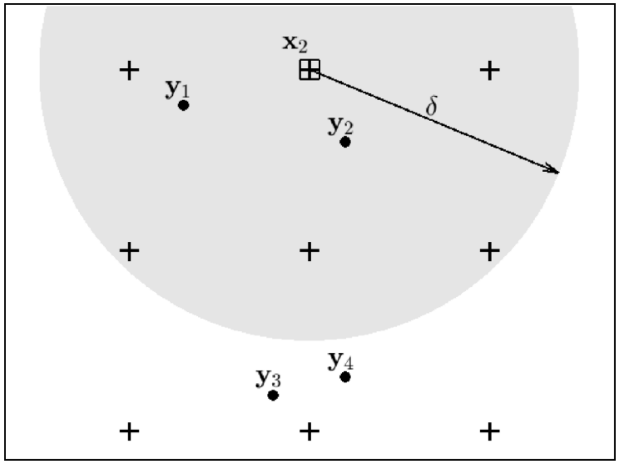
- Experiment: Exact $\mathbf{R}_t$ 0.246
- Experiment: $\mathbf{R} = \mathbf{R}_I$ fixed 0.275
- Experiment: $\mathbf{R}$ updated 0.251

Time Varying True $\mathbf{R}_t$ 0.255

Conclude: the analysis is improved by incorporating the estimated observation error covariance in the DA

Localization and DBCP Diagnostic

Regularization of the matrix **$\mathbf{R}^e$** is needed to ensure stability of the filter. With domain localization, states are only updated using observations within a localization radius.



Caveat: Computing the DBCP diagnostic using samples from an ensemble filter with domain localization does not give the correct values of all the observation error covariances, even if all theoretical assumptions hold.

Waller, Dance & Nichols, 2017

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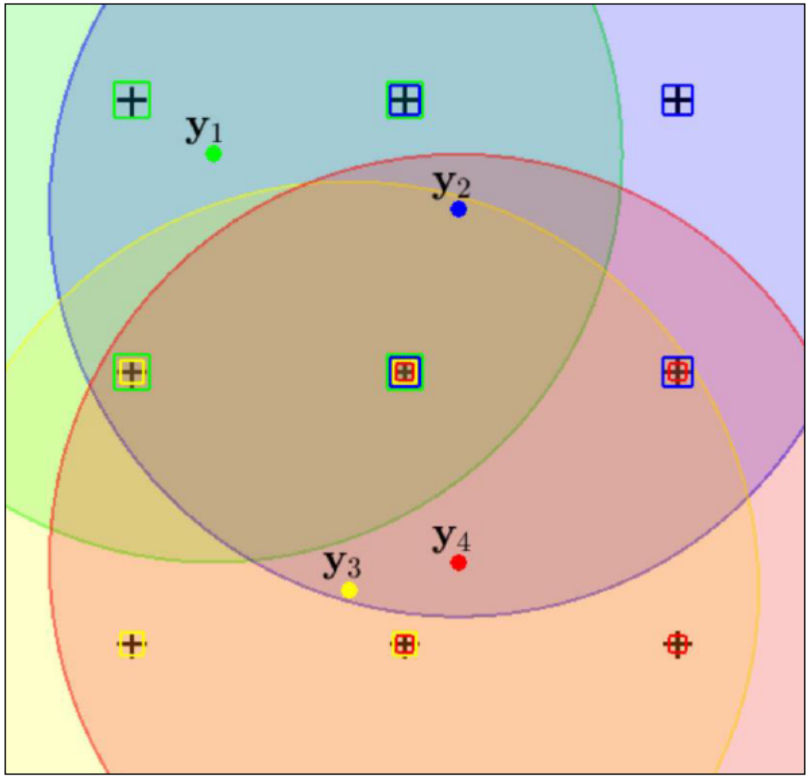
Definitions:

- The **domain of dependence** of an observation $\boldsymbol{y}_i$ is the set of elements of the model state that are used to calculate the model equivalent of $\boldsymbol{y}_i$.

- The **region of influence** of an observation is the set of analysis states that are updated in the assimilation using the observation $\boldsymbol{y}_i$.



Definitions:

The DD region is determined by **H** . The RI region is determined by **F** and depends on the radius of localization.

$$\mathbf{H} = \begin{bmatrix} \checkmark & \checkmark & \times & \checkmark & \checkmark & \times & \times & \times & \times \\ \times & \checkmark & \checkmark & \times & \checkmark & \checkmark & \times & \times & \times \\ \times & \times & \times & \checkmark & \checkmark & \times & \checkmark & \checkmark & \times \\ \times & \times & \times & \times & \checkmark & \checkmark & \times & \checkmark & \checkmark \end{bmatrix}$$

$$\mathbf{F} = \begin{bmatrix} \checkmark & \checkmark & \times & \times \\ \checkmark & \checkmark & \times & \times \\ \times & \checkmark & \times & \times \\ \checkmark & \checkmark & \checkmark & \checkmark \\ \checkmark & \checkmark & \checkmark & \checkmark \\ \times & \checkmark & \checkmark & \checkmark \\ \times & \times & \checkmark & \checkmark \\ \times & \times & \checkmark & \checkmark \\ \times & \times & \checkmark & \checkmark \end{bmatrix}$$

Theorem:

The correlation $\mathbf{R}_{ij}$ between observations y_i and y_j is determined correctly by the DBCP diagnostic only if the domain of dependence of y_i lies within the region of influence of observation y_j .

That is: the (i, j) element of $\mathbf{H}(\mathbf{F} - \mathbf{B}\mathbf{H}^T) = 0$.

Waller, Dance & Nichols, 2017

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Summary : DBCP Diagnostic in Ensemble DA

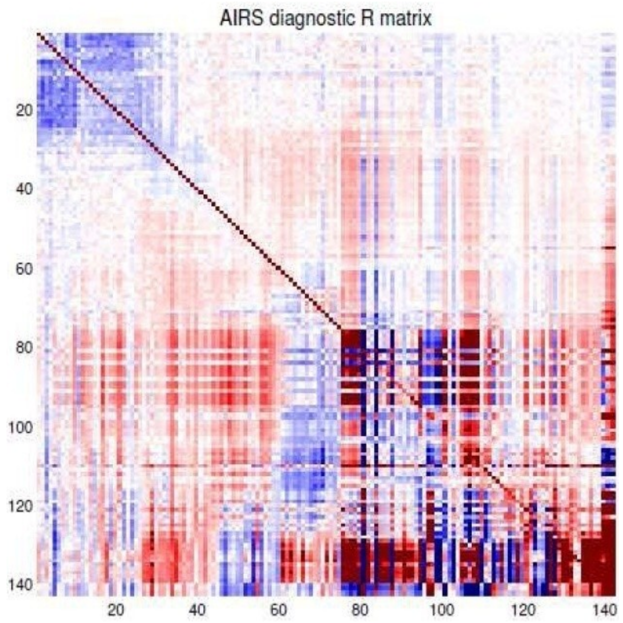
The DBCP diagnostic can be used with care to estimate the observation error correlation matrix **R** in ensemble DA.

In practice the diagnosed matrix **R** may be ill-conditioned and may need to be reconditioned.

Accounting for the correlated errors in practice is a computational challenge, now being tackled.

4. Sensitivity of the Analysis

Problems for DA:



Diagnosed correlation matrices:

- Non-symmetric
- Variances too small
- Not positive-definite
- Very ill-conditioned

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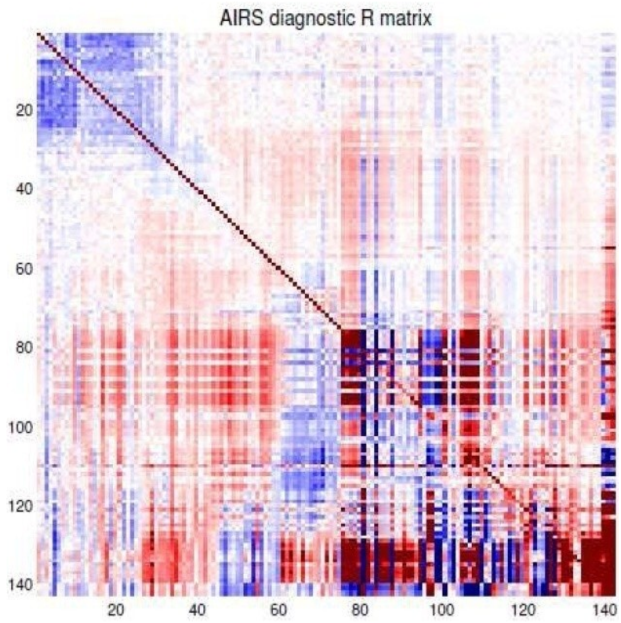

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- Non-symmetric
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Aim: to examine the sensitivity of the analysis to the conditioning of the estimated observation error covariances.

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Sensitivity of the Analysis

Sensitivity of the analysis, is bounded in terms of the condition number of:

$$\mathbf{S} = \mathbf{B}^{-1} + (\mathbf{H})^{T}\mathbf{R}^{-1}\mathbf{H}$$

where $\mathbf{B}$ and $\mathbf{R}$ are covariance matrices with structures that depend on the variances and correlation length scales of the background and observation errors, respectively.

Sensitivity

We can establish the following theorem:

Let $\mathbf{B} \in \mathbb{R}^{N \times N}$ *and* $\mathbf{R} \in \mathbb{R}^{p \times p}$*, with* $p < N$*, be the background and observation error covariance matrices respectively. Additionally, let* $\mathbf{H} \in \mathbb{R}^{p \times N}$ *be the observation operator. Then the following bounds are satisfied by the condition number of the Hessian,* $\mathbf{S} = \mathbf{B}^{-1} + \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H}$*,*

$$\frac{\kappa(\mathbf{B})}{\left(1 + \frac{\lambda_{max}(\mathbf{B})}{\lambda_{min}(\mathbf{R})} \lambda_{max}(\mathbf{H}\mathbf{H}^T)\right)} \leq \kappa(\mathbf{S}) \leq \left(1 + \frac{\lambda_{min}(\mathbf{B})}{\lambda_{min}(\mathbf{R})} \lambda_{max}(\mathbf{H}\mathbf{H}^T)\right) \kappa(\mathbf{B}).$$

Haben et al, 2011; Haben 2011; Tabeart, 2016; Tabeart et al, 2018

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$$\frac{\kappa(\mathbf{B})}{\left(1 + \frac{\lambda_{max}(\mathbf{B})}{\lambda_{min}(\mathbf{R})}\lambda_{max}(\mathbf{H}\mathbf{H}^T)\right)} \leq \kappa(\mathbf{S}) \leq \left(1 + \frac{\lambda_{min}(\mathbf{B})}{\lambda_{min}(\mathbf{R})}\lambda_{max}(\mathbf{H}\mathbf{H}^T)\right)\kappa(\mathbf{B}).$$

Note: the upper bound grows as $\frac{1}{\lambda_{min}(\mathbf{R})}$ grows and depends also on the observation operator.

Haben et al, 2011; Haben 2011; Tabeart, 2016; Tabeart et al, 2018

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Sensitivity

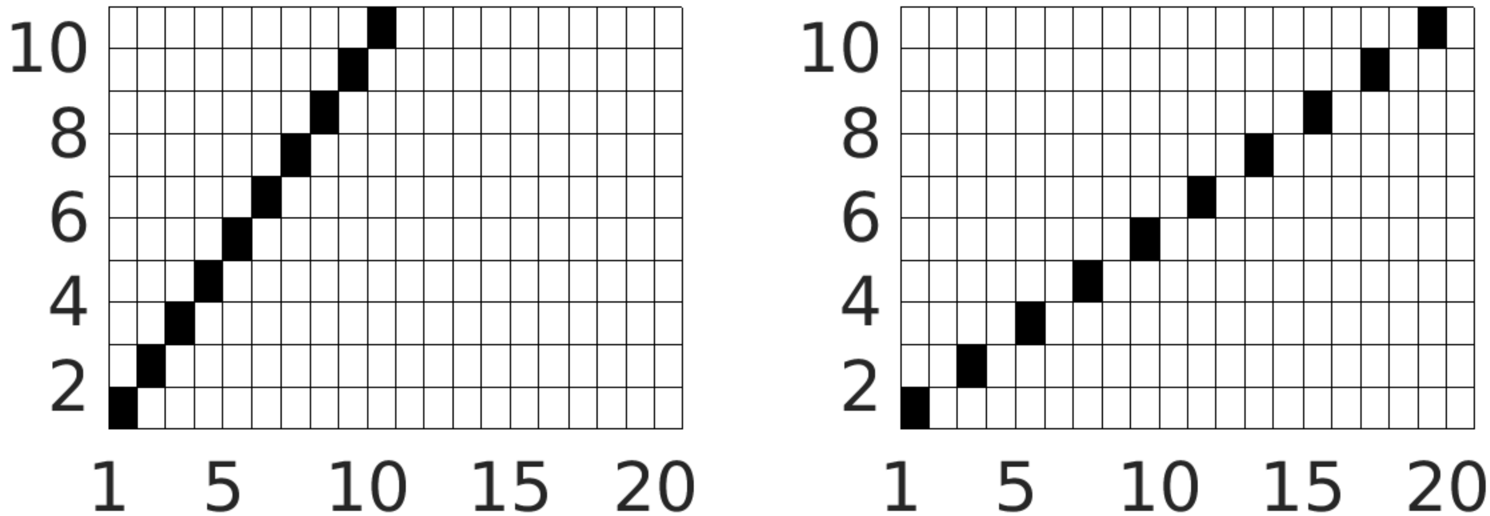
Key questions:

- What happens when we change the length scales of **R** and **B** - separately? together?
- What affect does the choice of observation operator have?
- How does changing the minimum eigenvalue of **R** affect the conditioning of **S** ? Operationally?

Example:

We examine how the choice of operator and the length scales in **R** and **B** affect the sensitivity of the analysis.

Choice of observation operator:



$\mathbf{H}_1$ $\mathbf{H}_2$

Example - $\mathbf{H}_1$:

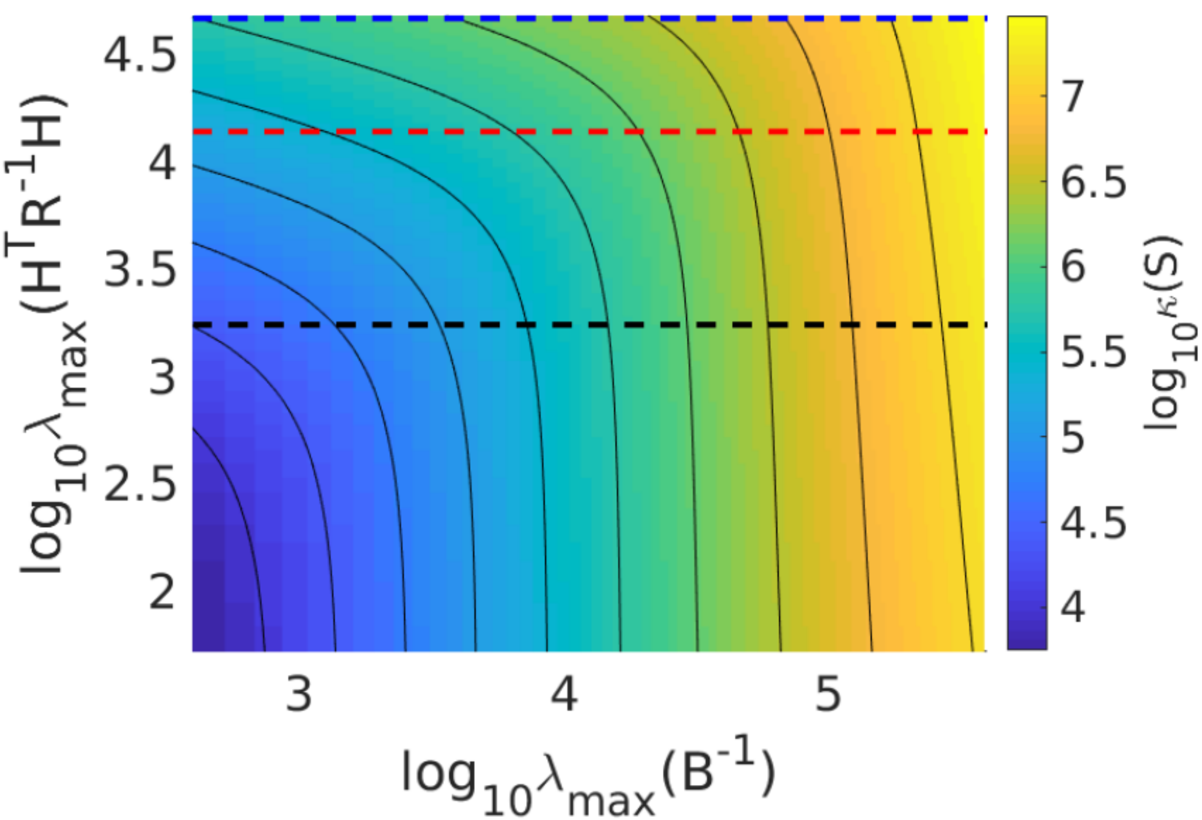


Figure: Plot of changing $\lambda_{max}(\mathbf{B}^{-1})$ against $\lambda_{max}(\mathbf{H}^T \mathbf{R}^{-1} \mathbf{H})$with colour denoting the condition number of $\mathbf{S}$ when first 100 state variables observed.

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Example - $\mathbf{H}_2$:

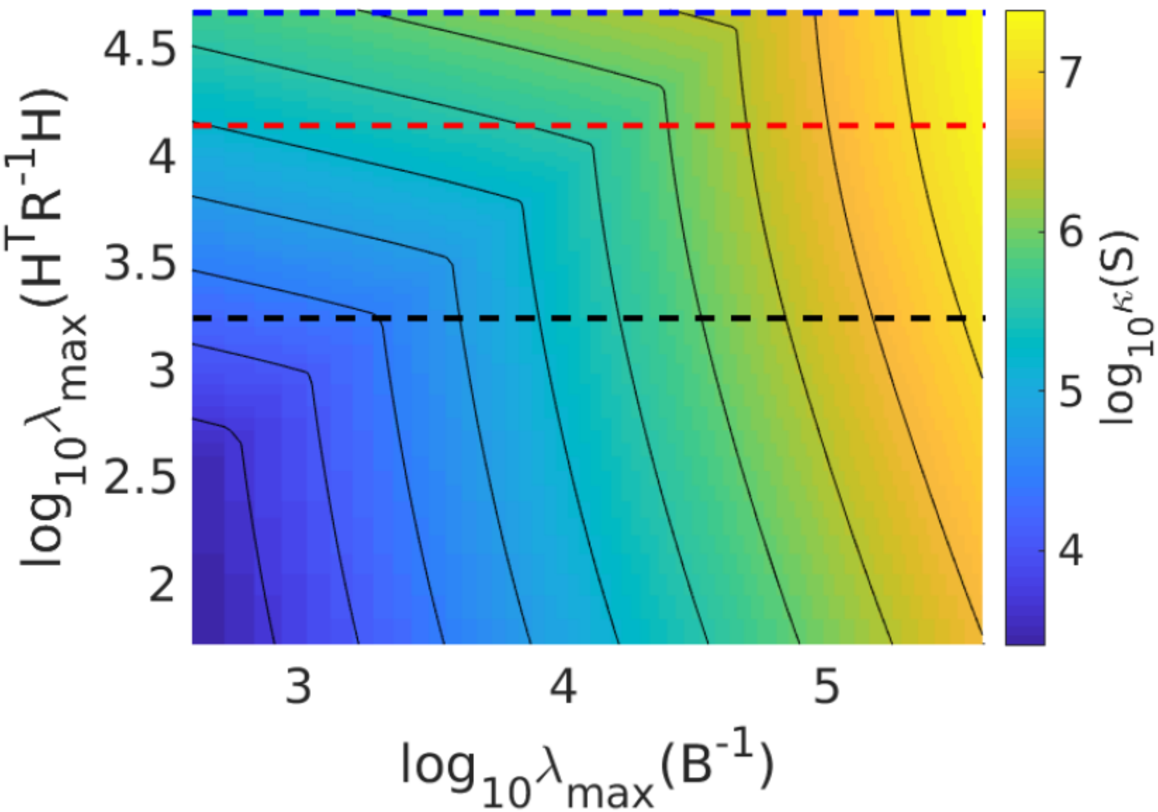

Figure: Plot of changing $\lambda_{max}(\mathbf{B}^{-1})$ against $\lambda_{max}(\mathbf{H}^T \mathbf{R}^{-1} \mathbf{H})$with colour denoting the condition number of $\mathbf{S}$ when alternate state variables observed

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Summary: Conditioning of the Problem

We find that the condition number of $\mathbf{S}$ increases as:

- the observations become more accurate
- the observation length scales increase
- the prior (background) becomes less accurate
- the prior error correlation length scales increase
- the observation error covariance becomes ill-conditioned - ie when $\frac{1}{\lambda_{min}(\mathbf{R})}$ becomes large

Haben et al, 2011; Haben 2011; Tabeart, 2016; Tabeart et al, 2018

5. Regularization

Reconditioning **R**

To improve the conditioning of **R** (and **S**) we alter the eigenstructure of **R** so as to obtain a specified condition number for the modified covariance matrix by:

- Ridge regression (RR): add constant to all diagonal elements to achieve given condition number.
- Eigenvalue modification (ME): increase the smallest eigenvalues of **R** to a threshold value to achieve the given condition number, keeping the rest unchanged.

Theoretical Results:

- Both methods reduce the condition number of **R**.
- Both methods increase all the standard deviations, but ridge regression creates a larger increase than does the eigenvalue modification method.
- Ridge regression decreases the moduli of all the cross-correlations.
- The eigenvalue modification method is equivalent to minimizing the KyFan 1-p (trace) norm of the distance to the nearest covariance matrix with condition number less or equal to a given value κ_{max} .

Tabeart et al, 2018

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Example:

Given a covariance matrix, constructed by sampling a SOAR correlation function, with condition number 81121 and fixing the variances to be constant. Recondition using RR and ME.

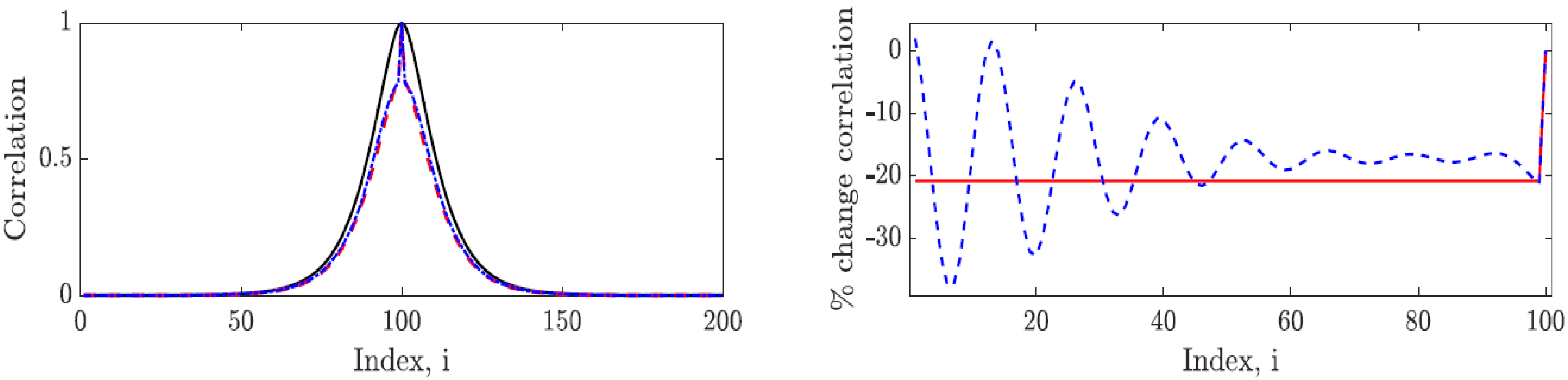
Table 1: Change to standard deviations of the SOAR matrix.

κ_{max}	σ	σ_{RR}	% change RR	σ_{ME}	% change ME
1000	2.23606	2.26471	+1.28%	2.25439	+0.82%
500	2.23606	2.29340	+2.56%	2.27599	+1.79%
100	2.23606	2.51306	+12.39%	2.45737	+9.90%

Example:

Given a covariance matrix, constructed by sampling a SOAR correlation function, with condition number 81121 and fixing the variances to be constant. Recondition using RR and ME.

Figure 1: Changes to correlations for $\kappa_{max} = 100$.



RR = red solid, ME= blue dashed, Original = black solid

Operational Tests - Met Office

Experiments using the Met Office 1D satellite retrieval system

- Aim to test qualitative conclusions in an operational system.
- Focus on observations from IASI (Infrared Atmospheric Sounding Interferometer) instrument (on MetOp-A satellite). Note the observation operator is non-linear in this case.
- Investigate how changing the minimum eigenvalue of **R** affects the condition number of **S** - we only show results using the ridge regression method.

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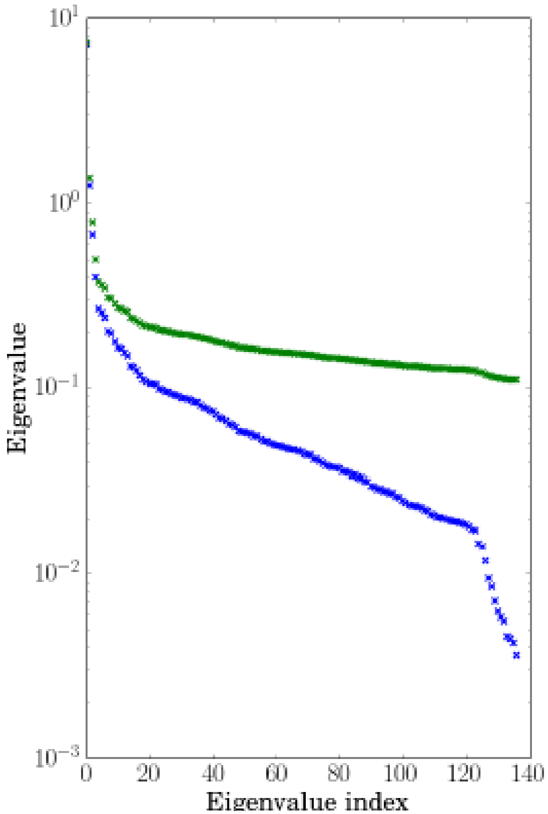
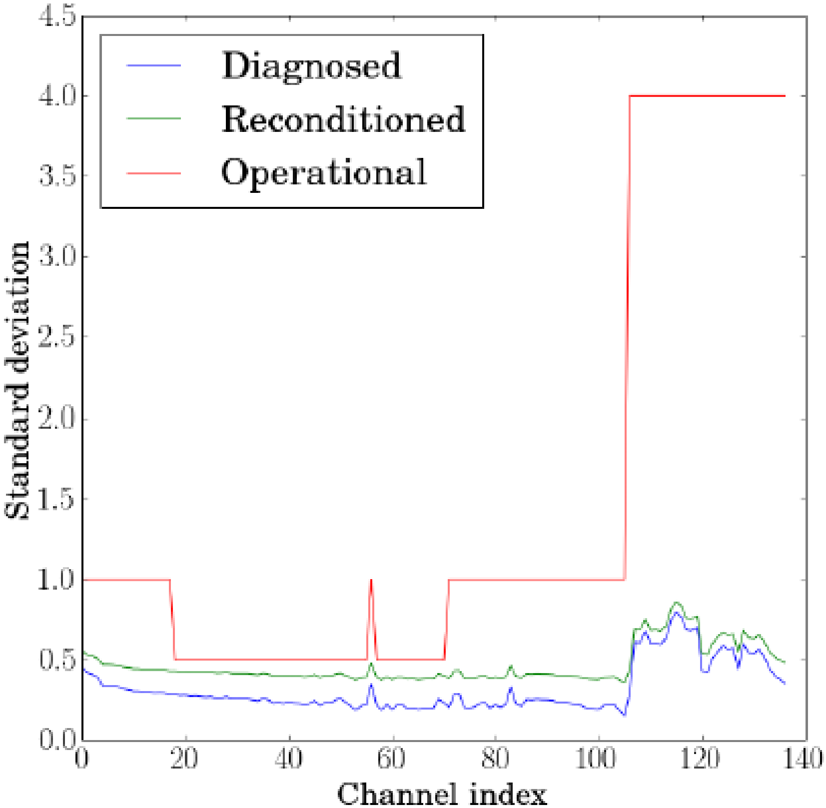
Results - 1:



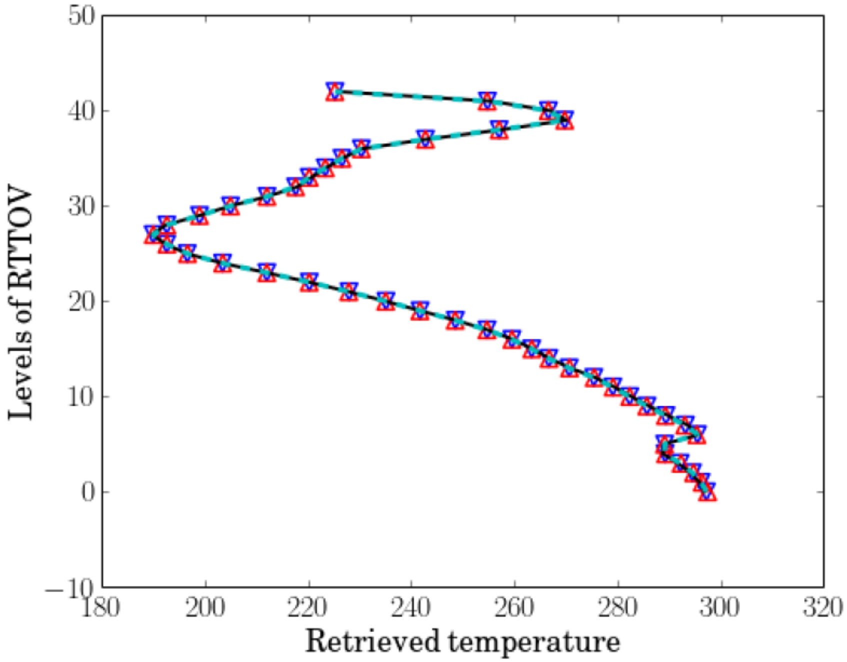
(a) Change in eigenvalues of $\mathbf{R}^{137}$

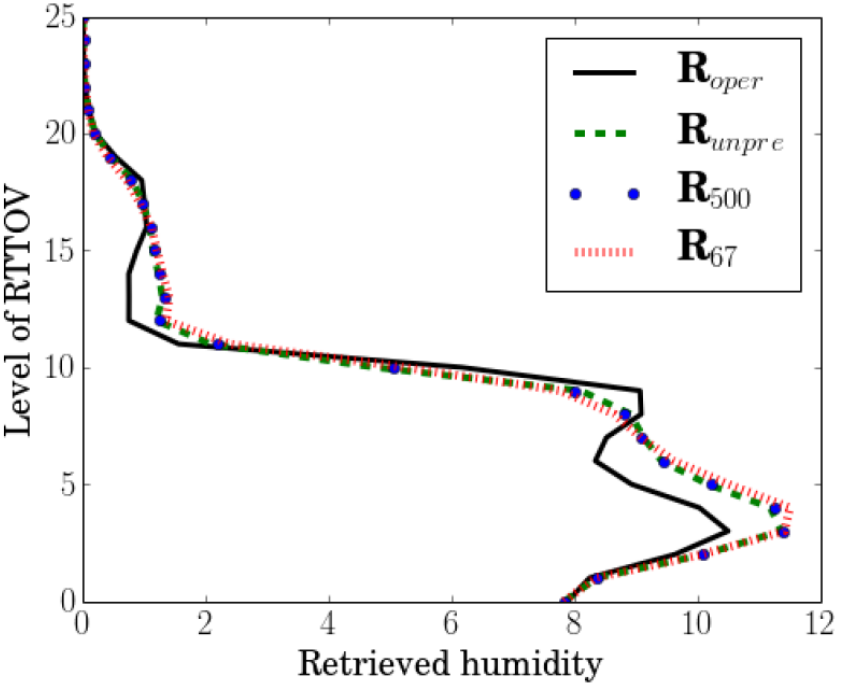


(b) Standard deviations for different $\mathbf{R}^{137}$

The method of reconditioning is that described in Algorithm 1. Figure (a) depicts how the ridge regression method changes the eigenvalues of the covariance matrix $\mathbf{R}^{137}$. Eigenvalues of the raw Desroziers $\mathbf{R}^{137}_{unpre}$ are shown in blue, and those of $\mathbf{R}^{137}_{RC}$ reconditioned so that $\kappa(\mathbf{R}_{RC}) = 67$ are shown in green. Figure (b) compares the standard deviations of $\mathbf{R}^{137}_{old}$ (red), $\mathbf{R}^{137}_{unpre}$ (blue), and $\mathbf{R}^{137}_{67}$ (green).

Results - 2





Shown are the retrieved temperature and humidity profiles for 4 different choices of R: R_{oper}, R_{unpre}, R_{500} and R_{67}.

Summary: Regularization

- Developed theory on reconditioning of the matrix **R**.
- Theory tested in a twin experiment – showing effect of ridge regression and eigenvalue modfication on standard deviations and correlations of the modified covariance matrices.
- Operationally standard deviations of the diagnosed matrices are increased by the reconditioning . The impact on temperature retrievals was minimal, but the impact on humidity retrievals much larger.

Tabeart, 2016; Tabeart et al, 2018b

6. Conclusions

Conclusions

Ensemble DA allows the statistical estimation of the background and observation covariance matrices from sampled states.

In practice the diagnosed matrices are commonly singular or very ill-conditioned. Regularization is required to ensure the stability of the filter.

A variety of techniques are available, including localization and reconditioning. A combination of these two approaches have been applied to an 4DEnVar simplified system and shown to be of benefit.

Smith et al, 2017

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Many more challenges left!

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