Observation errors

Niels Bormann

NWP SAF Training Course

ECMWF

Outline

1. What are observation errors?
2. Estimating observation errors
3. Specification of observation errors in practice
4. Accounting for observation error correlations
5. Summary

Outline

Errors in observations

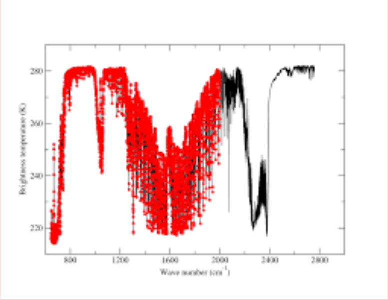
- **Every observation has an error vs the truth:**
  - **Systematic error**
    - Needs to be removed through bias correction (previous lecture)
  - **Random error**
    - Topic of this lecture!

Contributions to observation error

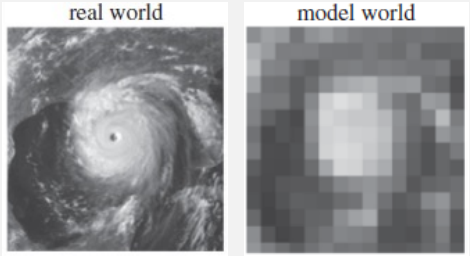
Measurement error
E.g., instrument noise for satellite radiances

Representation error
(e.g., Janjić et al 2017)

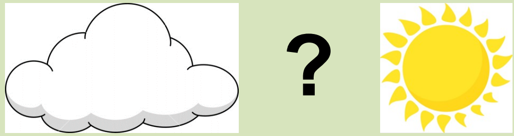
Forward model (observation operator) error
E.g., radiative transfer error



Representativeness error
E.g., point measurement vs model representation



Quality control/pre-processing error
E.g., error due to the cloud detection scheme missing some clouds in clear-sky radiance assimilation

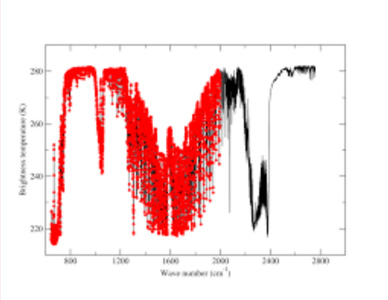


Contributions to observation error

Representation error
(e.g., Janjić et al 2017)

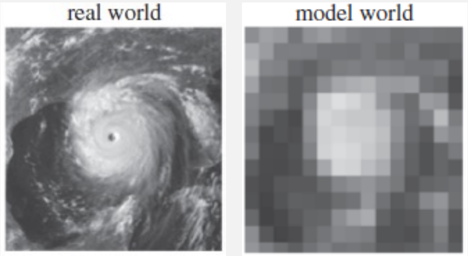
Measurement error
E.g., instrument noise for satellite radiances

Forward model (observation operator) error
E.g., radiative transfer error

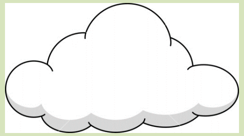


- Are the errors situation-dependent?
- Are the errors correlated (spatially, temporally, between channels)?
- Are the errors systematic (→bias correction)?

Representativeness error
E.g., point measurement vs model representation

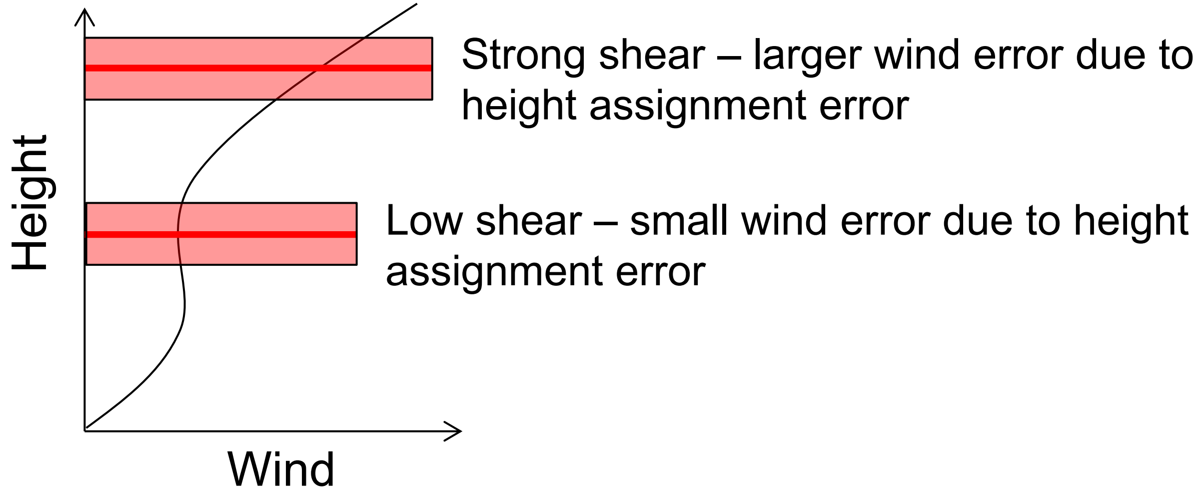


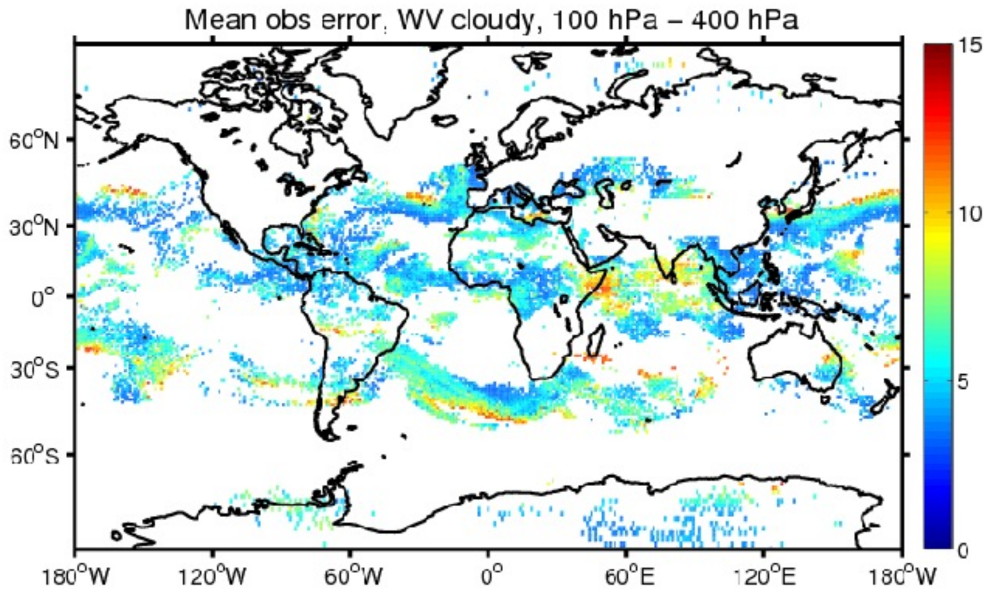
Quality control/pre-processing error
E.g., error due to the cloud detection scheme missing some clouds in clear-sky radiance assimilation


?

Examples of situation-dependence of representation error

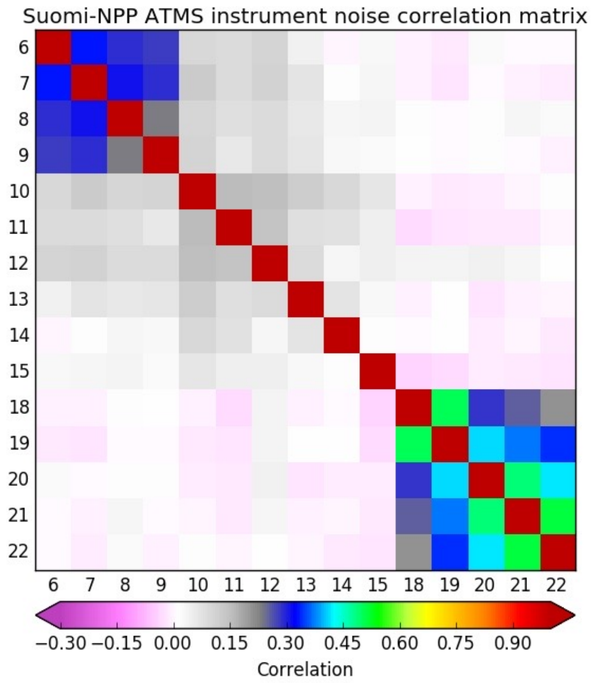
- Cloud/rain-affected radiances: Representativeness error is much larger in cloudy/rainy regions than in clear-sky regions
- Effect of height assignment error for Atmospheric Motion Vectors:





Examples of correlated observation error

- Different channels with similar radiative transfer error.
- Different channels with similar error in spatial representativeness.
- Different channels with similar cloud sensitivity in clear-sky assimilation.
- Even instrument noise can be correlated.



Observation error and the cost function

- In data assimilation, observation errors are commonly assumed Gaussian.
- Denoted by the observation error covariance matrix "**R**" in the observation cost function:

$$J(\mathbf{x}) = \frac{1}{2}(\mathbf{x}-\mathbf{x}_b)^T \mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}_b) + \frac{1}{2}(\mathbf{y}-\mathbf{H}[\mathbf{x}])^T \mathbf{R}^{-1}(\mathbf{y}-\mathbf{H}[\mathbf{x}])$$

- It is often specified through the square root of the diagonals ("σ_o") and a correlation matrix (which can be the identity matrix).

Role of observation error

- **R** and the background error **B** together determine the weight of an observation in the assimilation.
- In the linear case, the minimum of the cost function can be found at x_a:

$$\underbrace{(\mathbf{x}_a - \mathbf{x}_b)}_{\text{Increment}} = \mathbf{B}\mathbf{H}^T(\mathbf{H}\mathbf{B}\mathbf{H}^T + \mathbf{R})^{-1}\underbrace{(\mathbf{y} - \mathbf{H}\mathbf{x}_b)}_{\text{Departure, innovation, “o-b”}}$$

  – ***“Large” observation error*** → ***smaller increment***, analysis draws less closely to the observations

  – ***“Small” observation error*** → ***larger increment***, analysis draws more closely to the observations

Current observation error specification for satellite data in the ECMWF system

- Globally constant, diagonal:
  - Scatterometer data
- Globally constant fraction, dependent on impact parameter; diagonal:
  - GPS-RO
- Globally constant, inter-channel error correlations taken into account:
  - IASI, CrIS, AIRS, ATMS (with different values for different satellites)
- Situation dependent, diagonal:
  - All-sky treatment of radiances from passive microwave instruments: dependent on satellite, channel and cloud amount
  - AMVs: dependent on level and shear (and satellite, channel, height assignment method)
  - Aeolus: based on physically estimated error for each derived wind

Outline

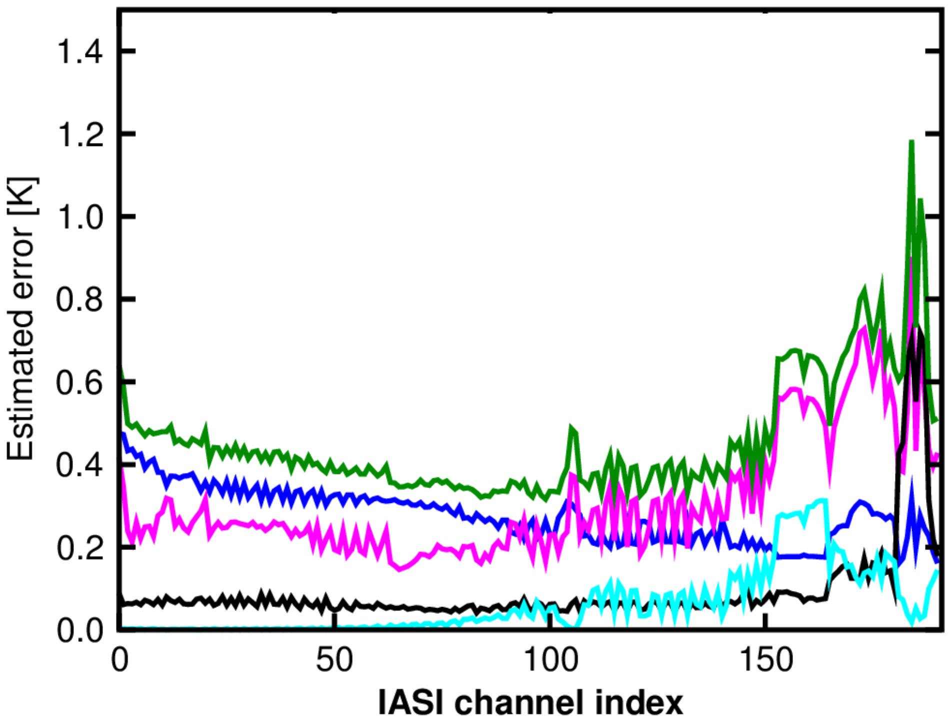
1. What are observation errors?
2. **Estimating observation errors**
3. Specification of observation errors in practice
4. Accounting for observation error correlations
5. Summary

How can we estimate observation errors?

- Observation errors are ***departures from the truth*** – which we don't know.
- We can only ***estimate*** observation errors. Several methods exist to do this, broadly categorised as:
  - **Error inventory:**
    - Based on considering all contributions to the error/uncertainty
  - **Diagnostics with collocated observations, e.g.:**
    - Hollingsworth/Lönnberg on collocated observations
    - Triple-collocations/3-cornered hat
  - **Diagnostics based on output from DA systems, e.g.:**
    - O-b statistics
    - Hollingsworth/Lönnberg
    - Desroziers et al 2005
    - Methods that rely on an explicit estimate of B
  - **Adjoint-based methods**

Error inventory

- Estimate the error from ***physical estimates of <u>all</u> uncertainty*** contributions.
- Example: error inventory for IASI



Instrument noise (information from data providers)

Radiative transfer error (difficult…)

Spatial representativeness error (e.g, through high vs low-resolution simulations)

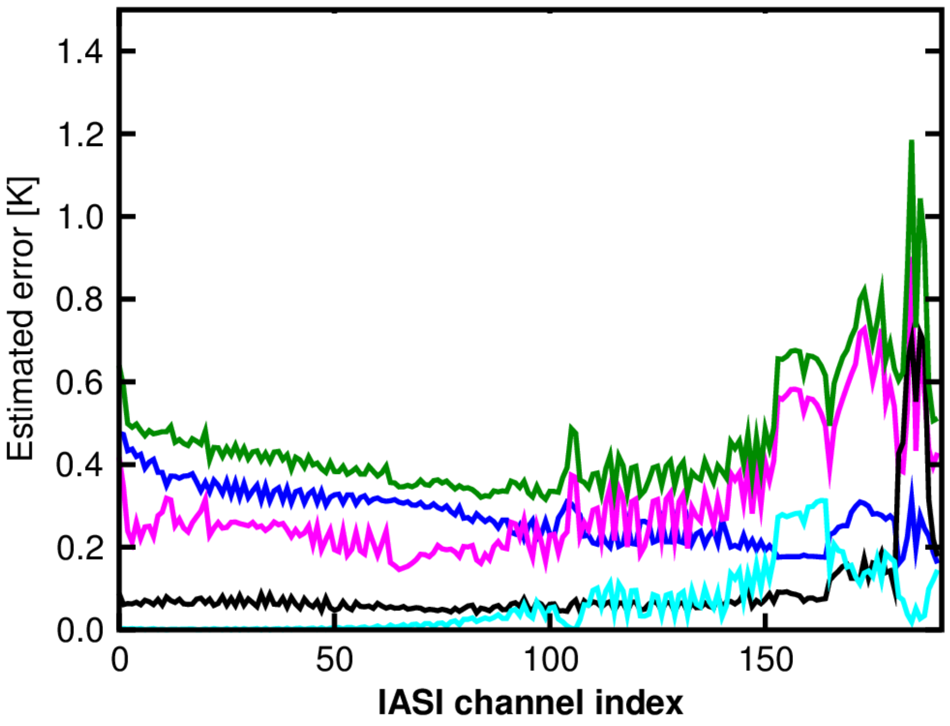
Cloud detection error (e.g., using simulations of cloudy radiances)

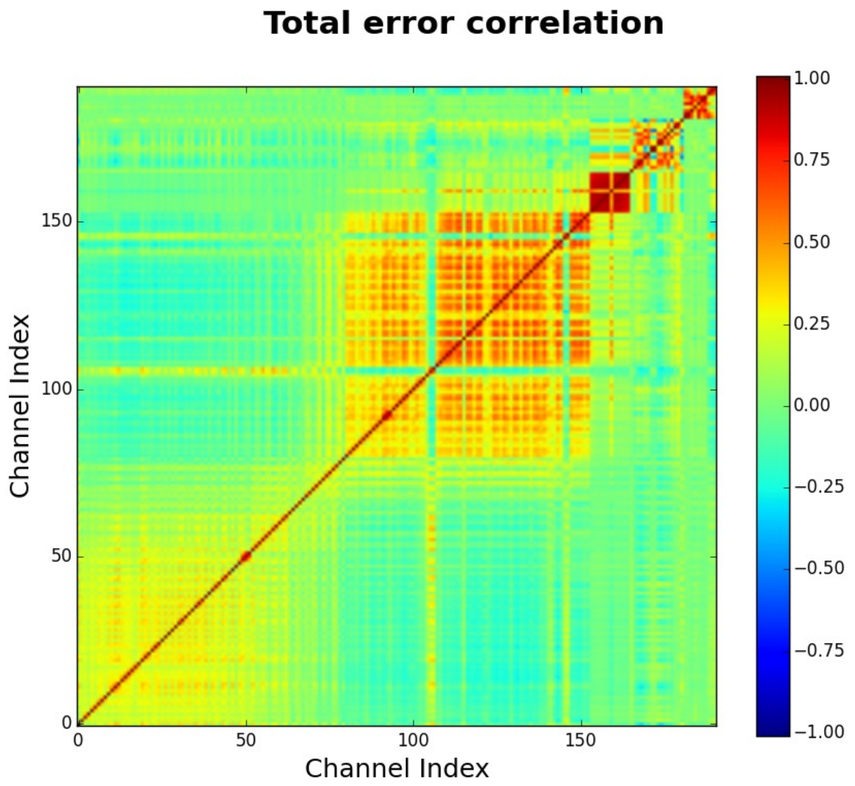
Total error

(Courtesy Hyoung-Wook Chun, Reima Eresmaa)

Error inventory

- Estimate the error from ***physical estimates of <u>all</u> uncertainty*** contributions.
- Example: error inventory for IASI



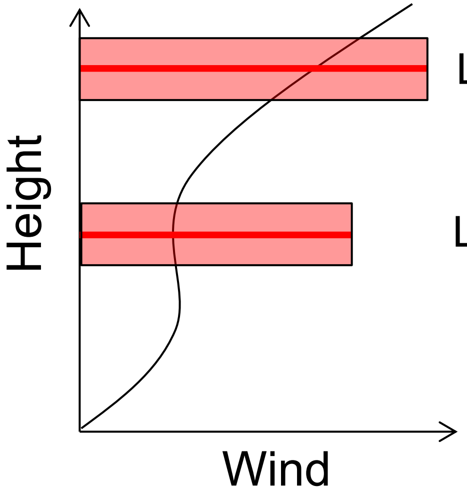


- Very useful to ***understand*** error contributions.
- ***How realistic*** is each estimate?

Error inventory and physical observation error models

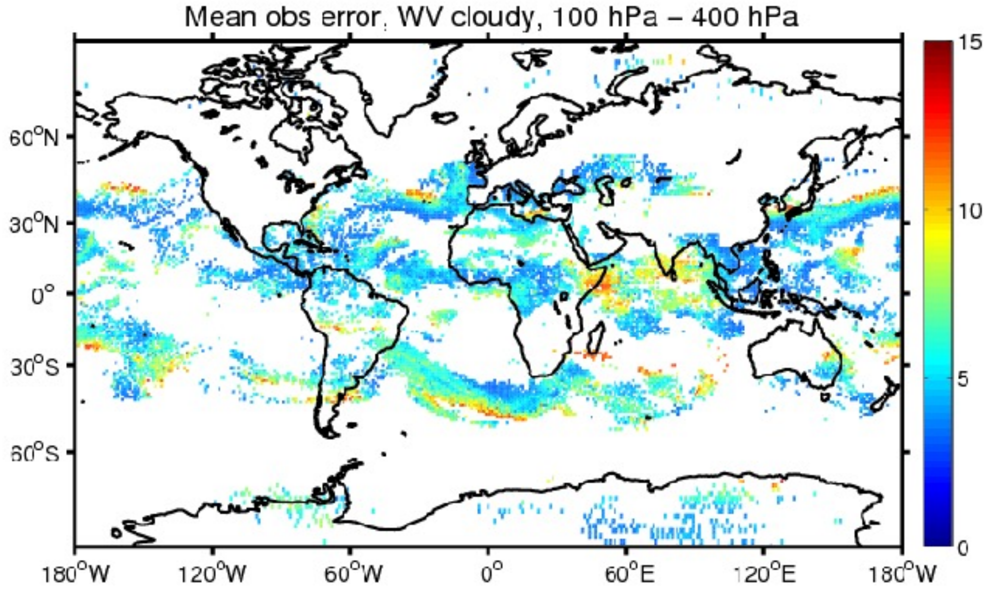
- Other applications of an inventory approach:
  - Physical error models: propagate parameter uncertainty through observation operator/retrieval
  - Useful for identifying leading contributors of observational uncertainty
  - Basis for “observation error models” to capture situation-dependence of observation errors

Example: Atmospheric Motion Vectors and the error due to height assignment:



Large **shear** – larger error due to **height assignment error**

Low **shear** – smaller error due to **height assignment error**



An observation error model for the height assignment uncertainty could be: $\sigma_{HA} \approx \sigma_p \frac{dv}{dp}$

How can we estimate observation errors?

- Observation errors are ***departures from the truth*** – which we don't know.
- We can only ***estimate*** observation errors. Several methods exist to do this, broadly categorised as:
  - **Error inventory:**
    - Based on considering all contributions to the error/uncertainty
  - **Diagnostics with collocated observations, e.g.:**
    - Hollingsworth/Lönnberg on collocated observations
    - Triple-collocations
  - **Diagnostics based on output from DA systems, e.g.:**
    - O-b statistics
    - Hollingsworth/Lönnberg
    - Desroziers et al 2005
    - Methods that rely on an explicit estimate of B
  - **Adjoint-based methods**

Departure-based diagnostics

- Several methods have been developed that are based on departures from data assimilation systems (ie o-b, o-a).
- If observation errors and background errors are ***uncorrelated*** then:

$$Cov[(\mathbf{y} - \mathbf{H}[\mathbf{x}_b]), (\mathbf{y} - \mathbf{H}[\mathbf{x}_b])] \quad = \quad \mathbf{HB}_{true}\mathbf{H}^T + \mathbf{R}_{true}$$

- In this case, stdev(o-b) is an ***upper bound for σ_o***.

- Statistics of background departures give information on ***observation and background error combined***. To separate the two, we need to ***make assumptions*** (which may or may not be true).

Departure-based observation error diagnostics: Methods that rely on an estimate of the background error

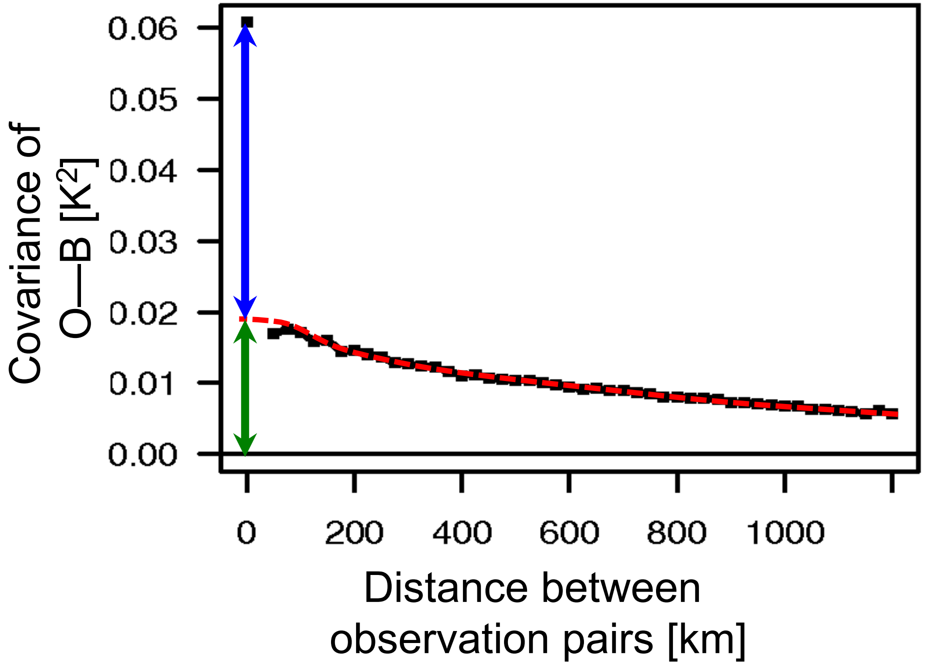
- **Basic assumptions:**
  - Background and observation error are ***uncorrelated***.
  - We have a ***reliable estimate of the background error***, for instance:
    - Background error is small: $\mathbf{R} = Cov[(\mathbf{y} - \mathbf{H}[\mathbf{x}_b]), (\mathbf{y} - \mathbf{H}[\mathbf{x}_b])] \quad - \quad \cancel{\mathbf{HBH}^T}$
    - Or: we "know" $\mathbf{H}\,\mathbf{B}_{true}\,\mathbf{H}^T$ from the assimilation system:

$$\mathbf{R} = Cov[(\mathbf{y} - \mathbf{H}[\mathbf{x}_b]), (\mathbf{y} - \mathbf{H}[\mathbf{x}_b])] \quad - \quad \mathbf{HBH}^T$$

Departure-based observation error diagnostics: Hollingsworth/Loennberg method

- **Basic assumption:**
  - Background errors are spatially correlated, whereas observation errors are not.
  - This allows to separate the two contributions to the variances of background departures.

- **Recipe:**
  - Take a large database of pairs of departures and bin by distance between the observations.
  - Calculate covariance of departures for each bin.



Spatially uncorrelated variance → Observation error

Spatially correlated variance → Background error

- **Drawback:**
  - Not reliable when observation errors are spatially correlated.

Departure-based observation error diagnostics: Desroziers diagnostic (I)

- **Basic assumptions:**
  - Assimilation process can be adequately described through linear estimation theory.
  - Weights used in the assimilation system are consistent with true observation and background errors.
- Then the following relationship can be derived:

$$\mathbf{R} = Cov[\mathbf{d}_a, \mathbf{d}_b]$$

with $\mathbf{d}_a = (\mathbf{y} - \mathbf{H}[\mathbf{x}_a])$ (analysis departure)

$\mathbf{d}_b = (\mathbf{y} - \mathbf{H}[\mathbf{x}_b])$ (background departure)

(see Desroziers et al. 2005, QJRMS)

- ***Consistency diagnostic*** for the specification of **R**. Increasingly used to estimate **R**.

Some points on departure-based diagnostics

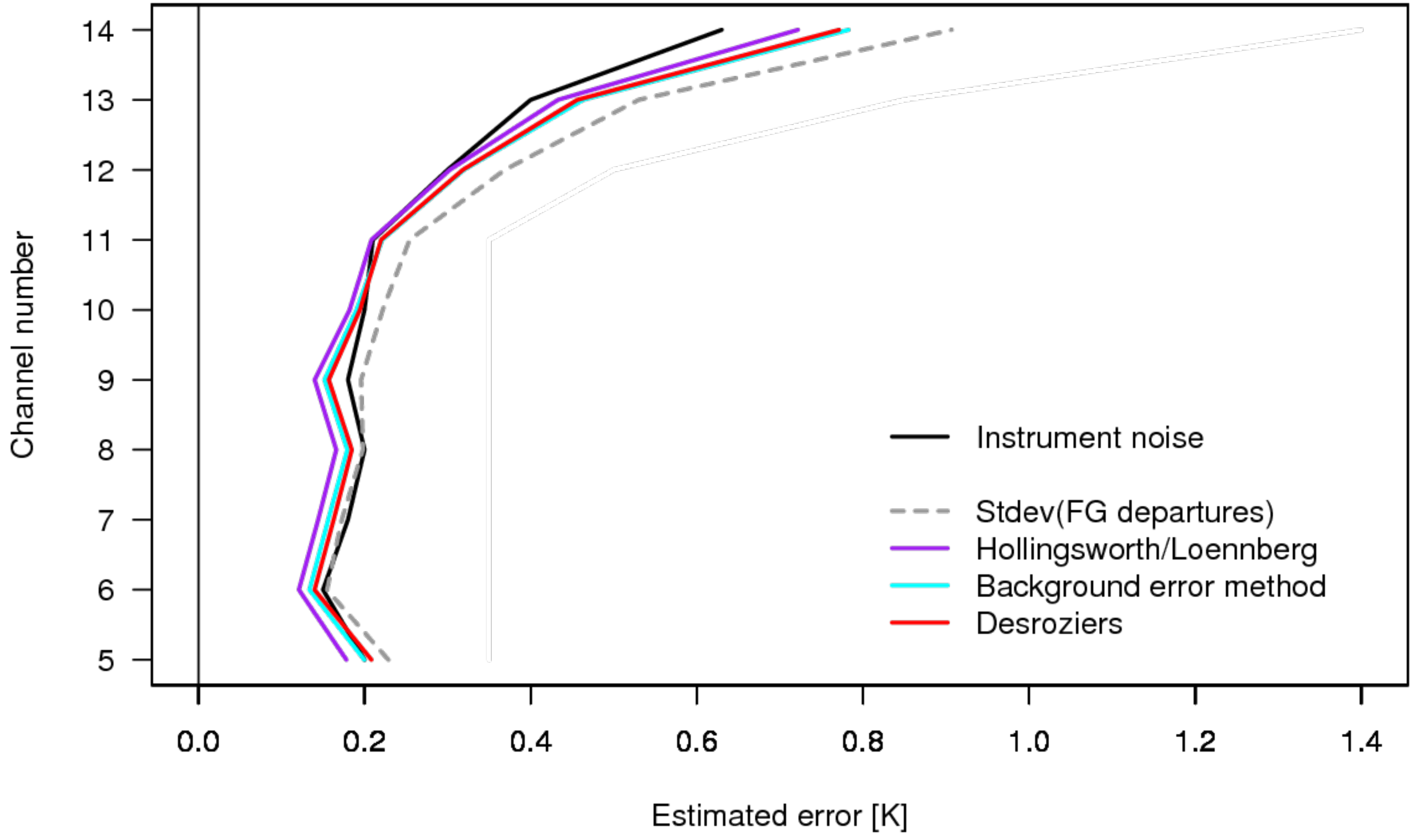
- All departure-based diagnostics rely on assumptions (which may or may not be true):
  - Assume we ***know the background error*** characteristics → remove B
  - Assume a ***certain structure of the errors*** → Hollingsworth/Lönnberg
  - Assume ***weights*** used in the assimilation system are ***accurate*** → Desroziers diagnostic
- All diagnostics additionally assume that the ***error in the observations and background are uncorrelated.***

- ***Before applying any diagnostic, think about whether the assumptions are likely to be true.***

- It is best to ***use several diagnostics*** to avoid misleading estimates due to violated assumptions.
- Diagnostics do not tell you where the error comes from.
  - ***Additional physical understanding*** of the error sources will be beneficial → ***error inventory***.
  - Diagnostics can be used together with physical error models.

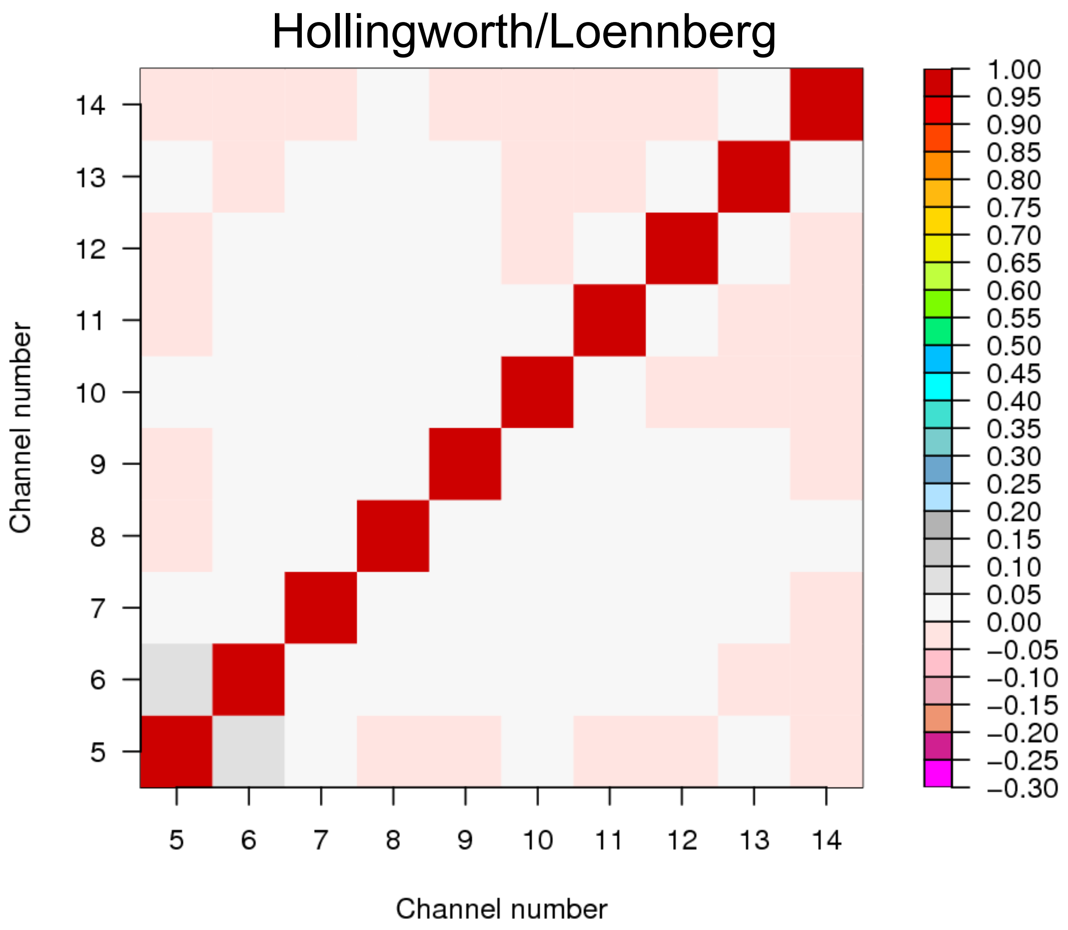
Examples of applying observation error diagnostics: AMSU-A

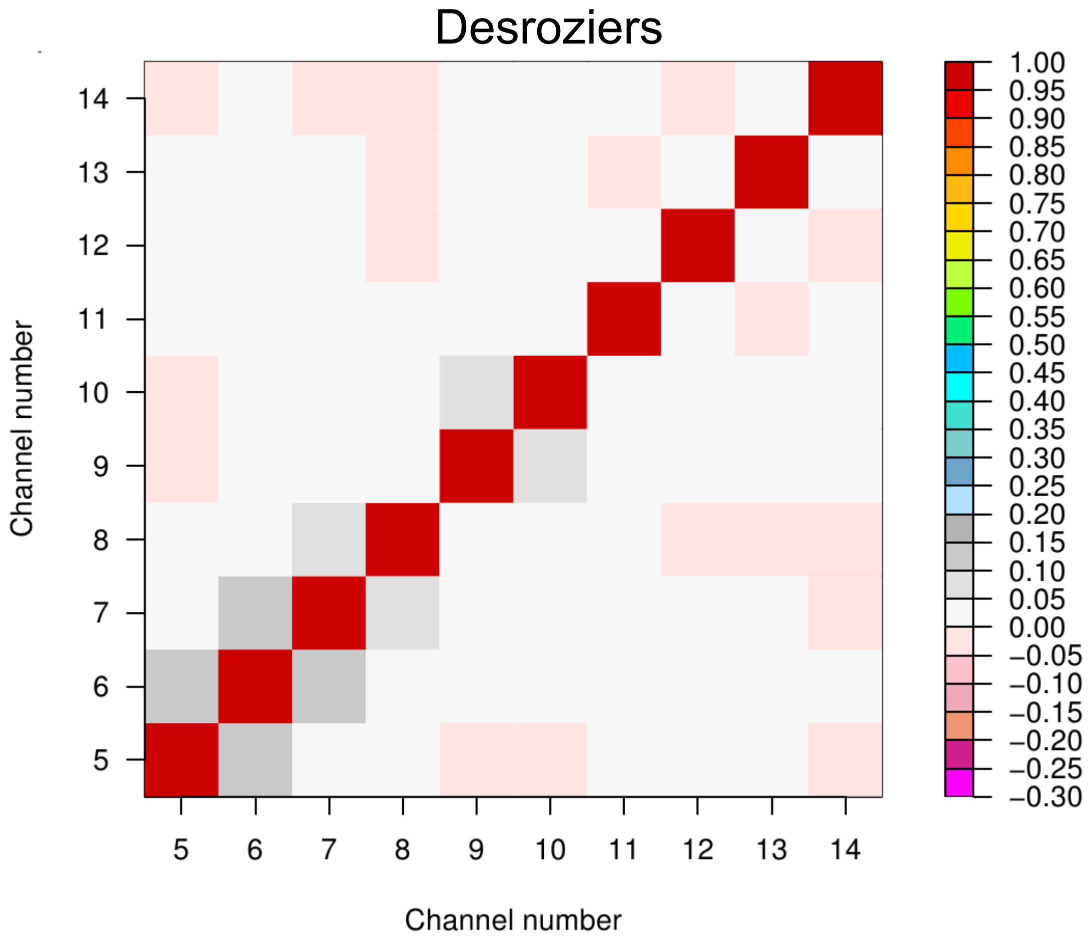
Diagnostics for σ_o



Examples of applying observation error diagnostics: AMSU-A

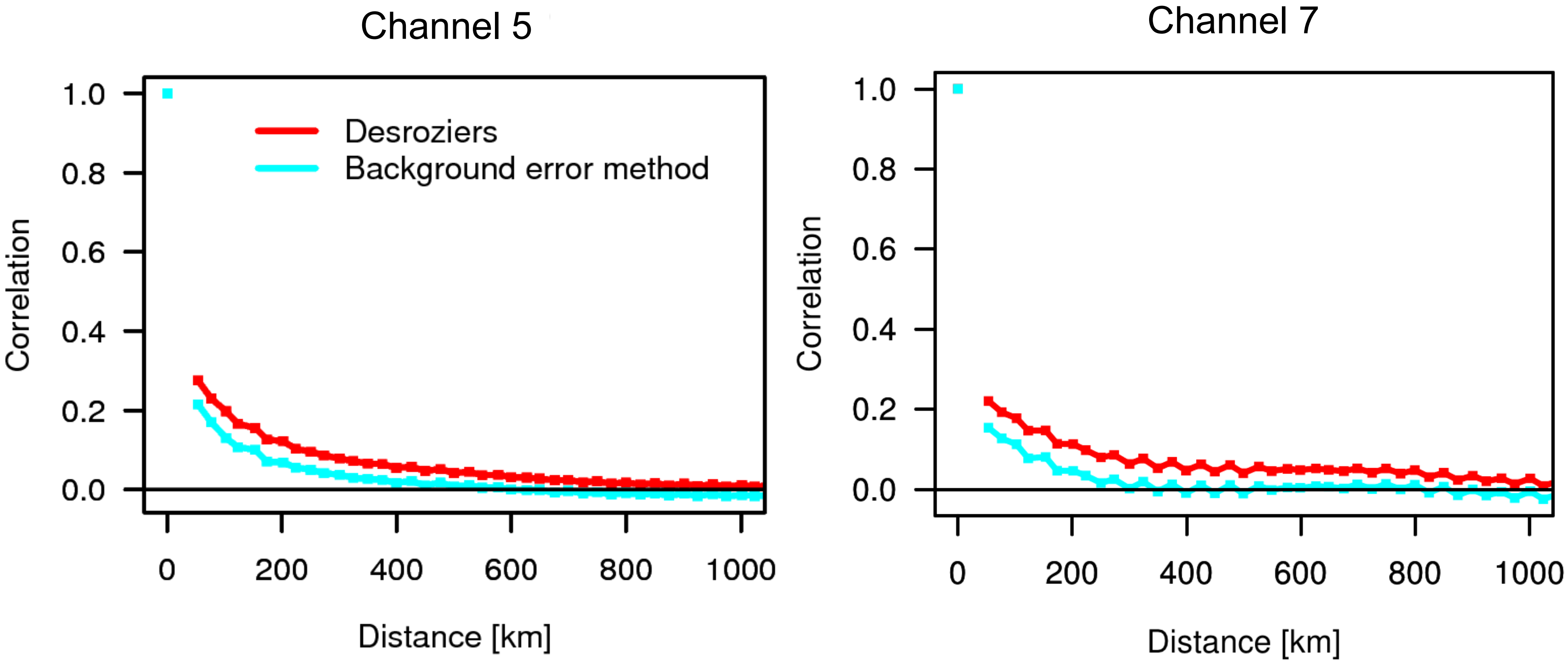
Inter-channel error correlations:





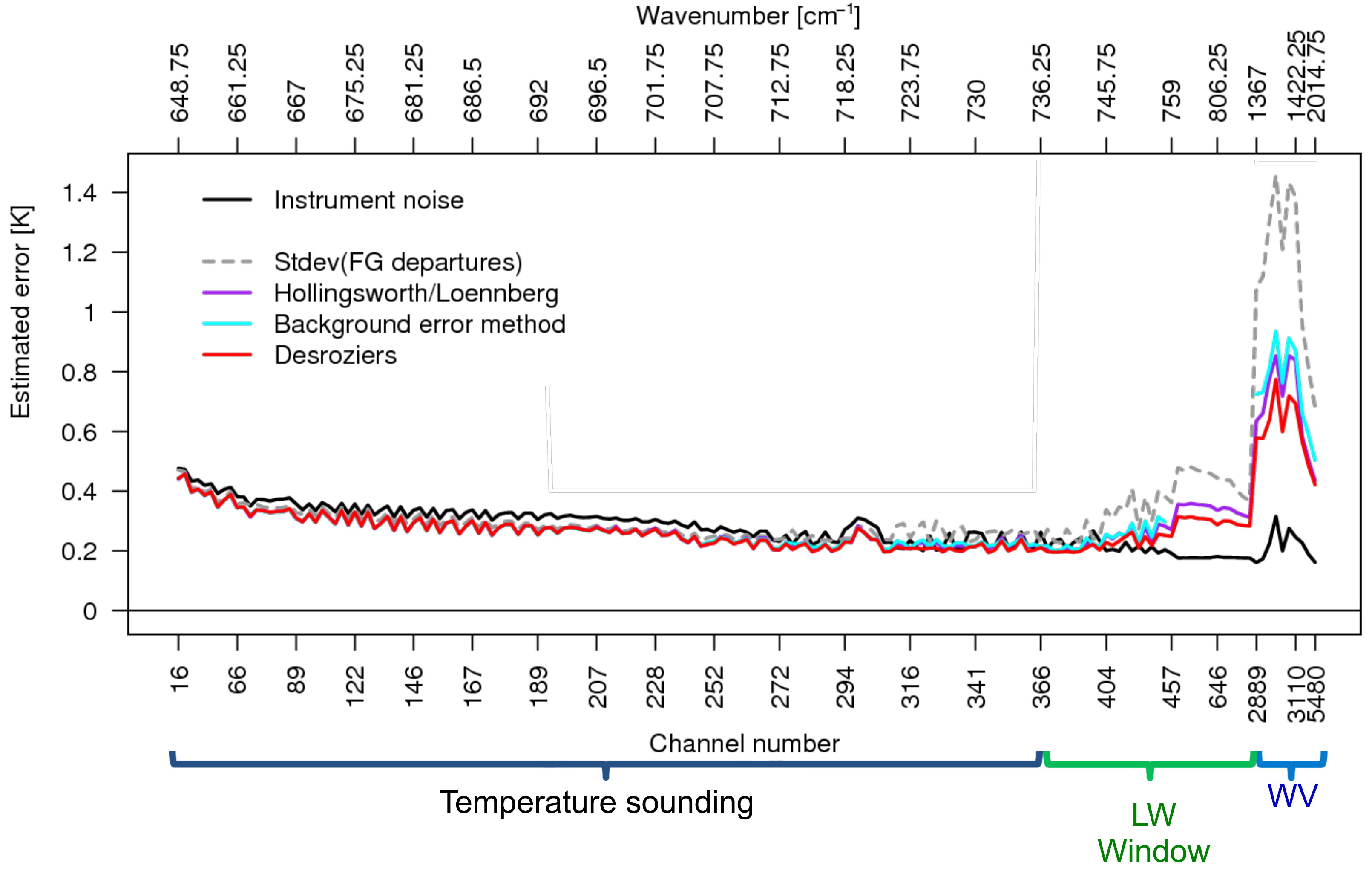
Examples of applying observation error diagnostics: AMSU-A

Spatial error correlations:



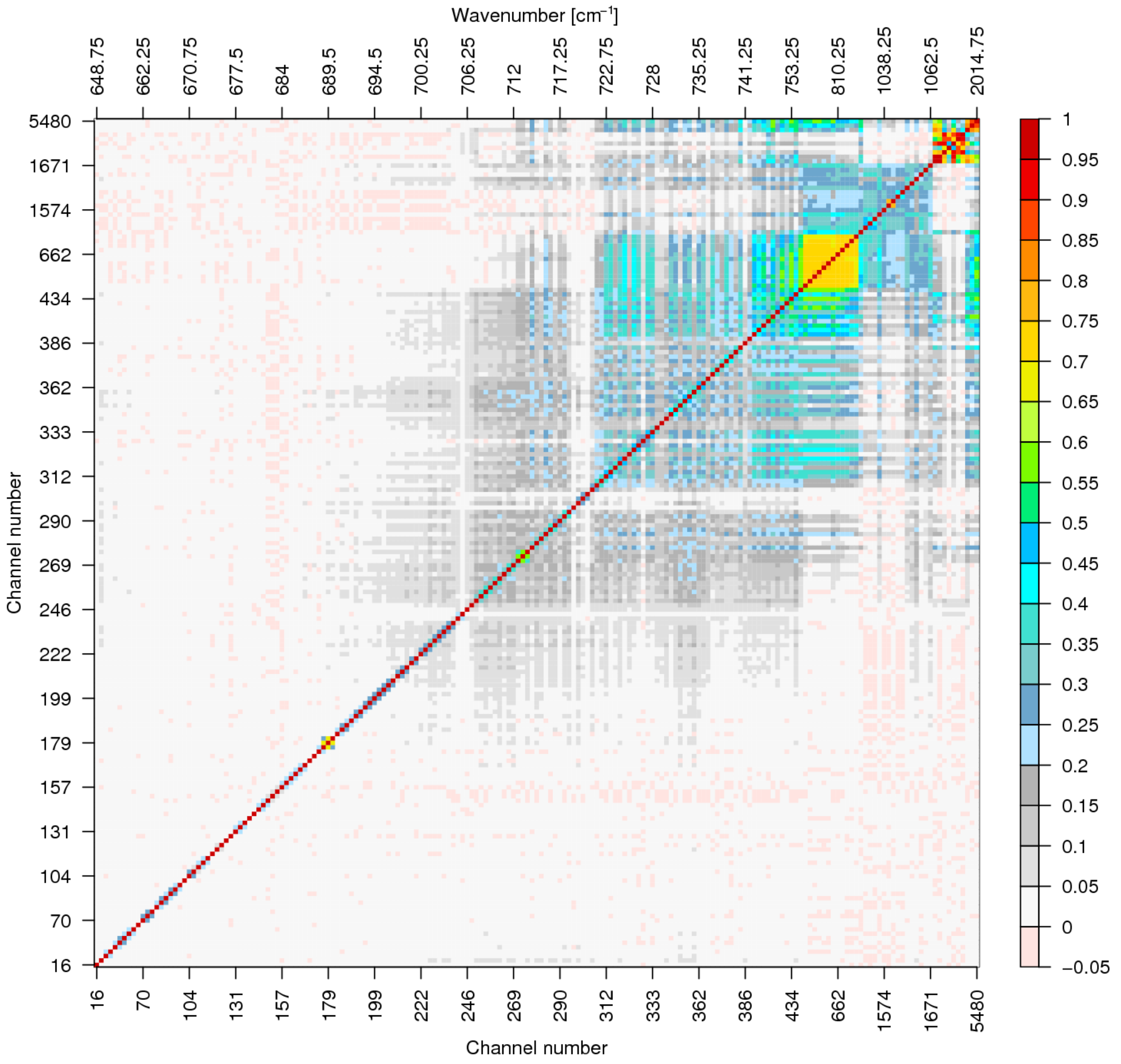
Examples of applying observation error diagnostics: IASI

Diagnostics for σ_O



Examples of applying observation error diagnostics: IASI

Inter-channel error correlations

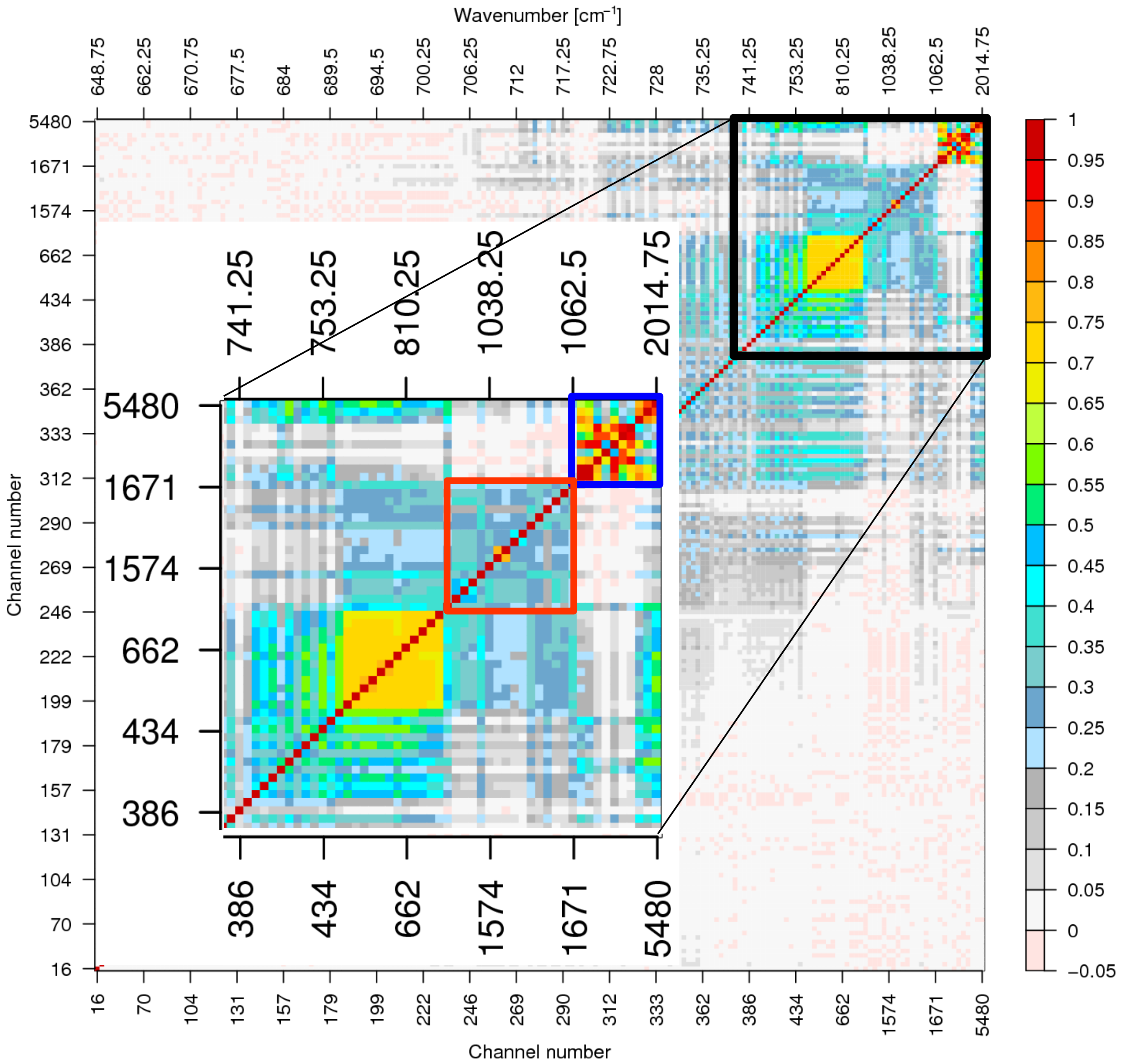


Examples of applying observation error diagnostics: IASI

Inter-channel error correlations

Humidity

Ozone



Outline

1. What are observation errors?
2. Estimating observation errors
3. **Specification of observation errors in practice**
4. Accounting for observation error correlations
5. Summary

How do I specify observation errors in practice?

- Observation error diagnostics or error inventories can provide guidance for observation error specification in DA, including on:
  - ***Relative size*** of observation and background errors
  - Presence of observation ***error correlations***
  - ***Situation-dependence*** of observation errors

- **But:**
  - Estimates might have short-comings (violated assumptions).
  - Observation errors specified in assimilation systems often need to be ***simplified***:
    - Observation error covariance is often ***assumed to be diagonal or globally constant***.

→ ***Assumed*** observation errors may need ***adjustments*** compared to estimated ones.

Too large assumed observation errors tend to be safer than too small ones. Why?

Consider a linear combination of two estimates x_b and y:

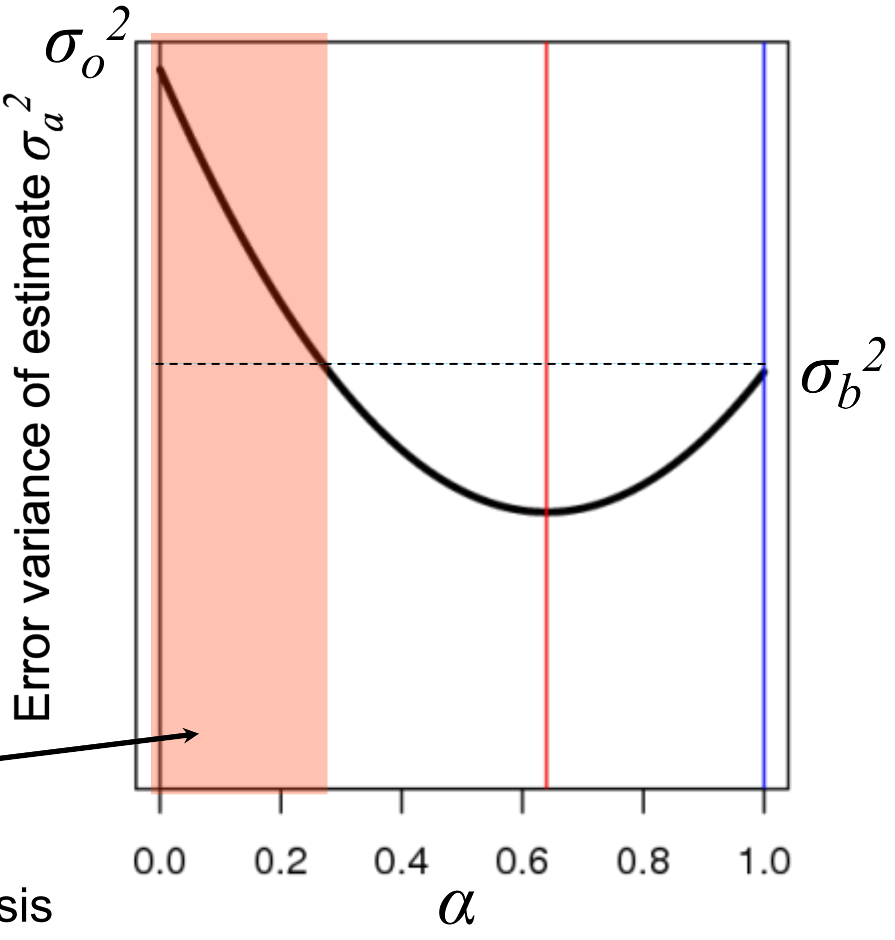
$$x_a = \alpha x_b + (1-\alpha) y$$

The error variance of the linear combination is:

$$\sigma_a^2 = \alpha^2 \sigma_b^2 + (1-\alpha)^2 \sigma_o^2$$

The optimal weighting (ie minimum σ_a) is:

$$\alpha = \frac{\sigma_o^2}{\sigma_b^2 + \sigma_o^2}$$



Danger zone: Too small *assumed* σ_o will lead to an analysis worse than the background when the (true) $\sigma_o > \sigma_b$.

Assuming an inflated σ_o will never result in deterioration.

What to do when there are error correlations?
Option 1: Thinning

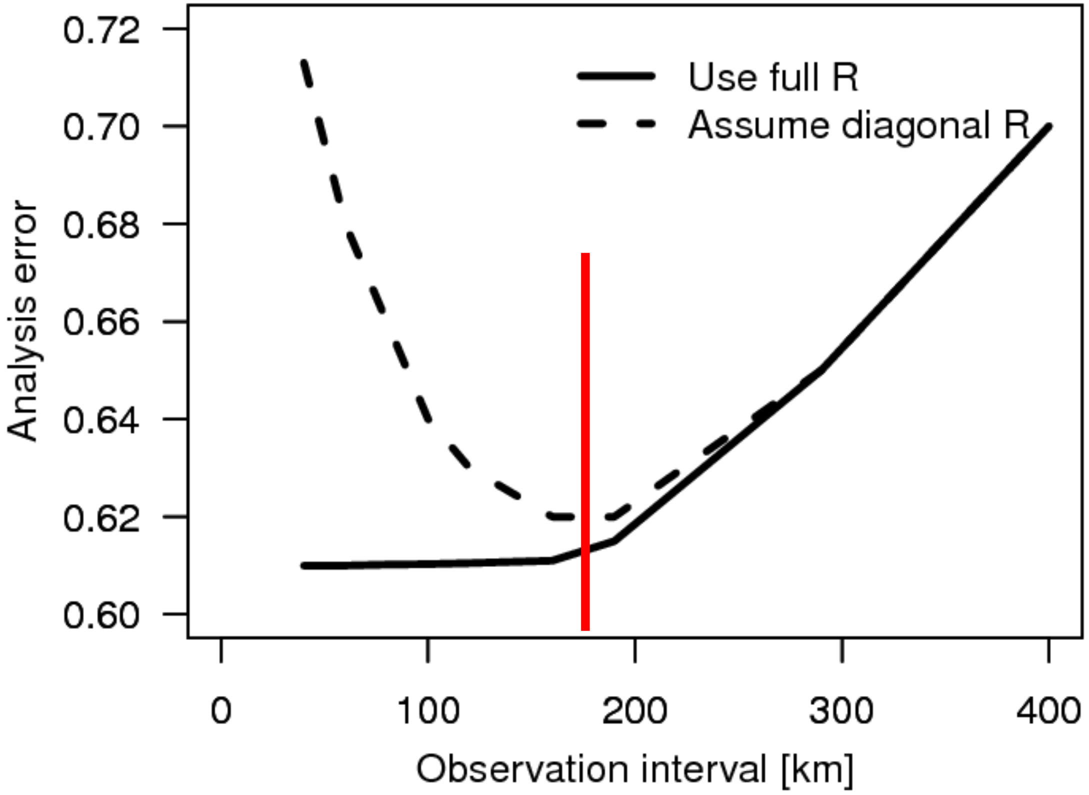
- If the observations have ***spatial error correlations, but these are neglected*** in the assimilation system, assimilating these observations too densely can have a ***negative effect***.

- ***Pragmatic solution 1:*** Select one observation within a “thinning box”.

- See Liu and Rabier (2003), QJRMS: “Optimal” thinning when r ≈ 0.15-0.2

- Using ***fewer*** observations gives ***better*** results!

- (But we lose out on information on smaller scales.)



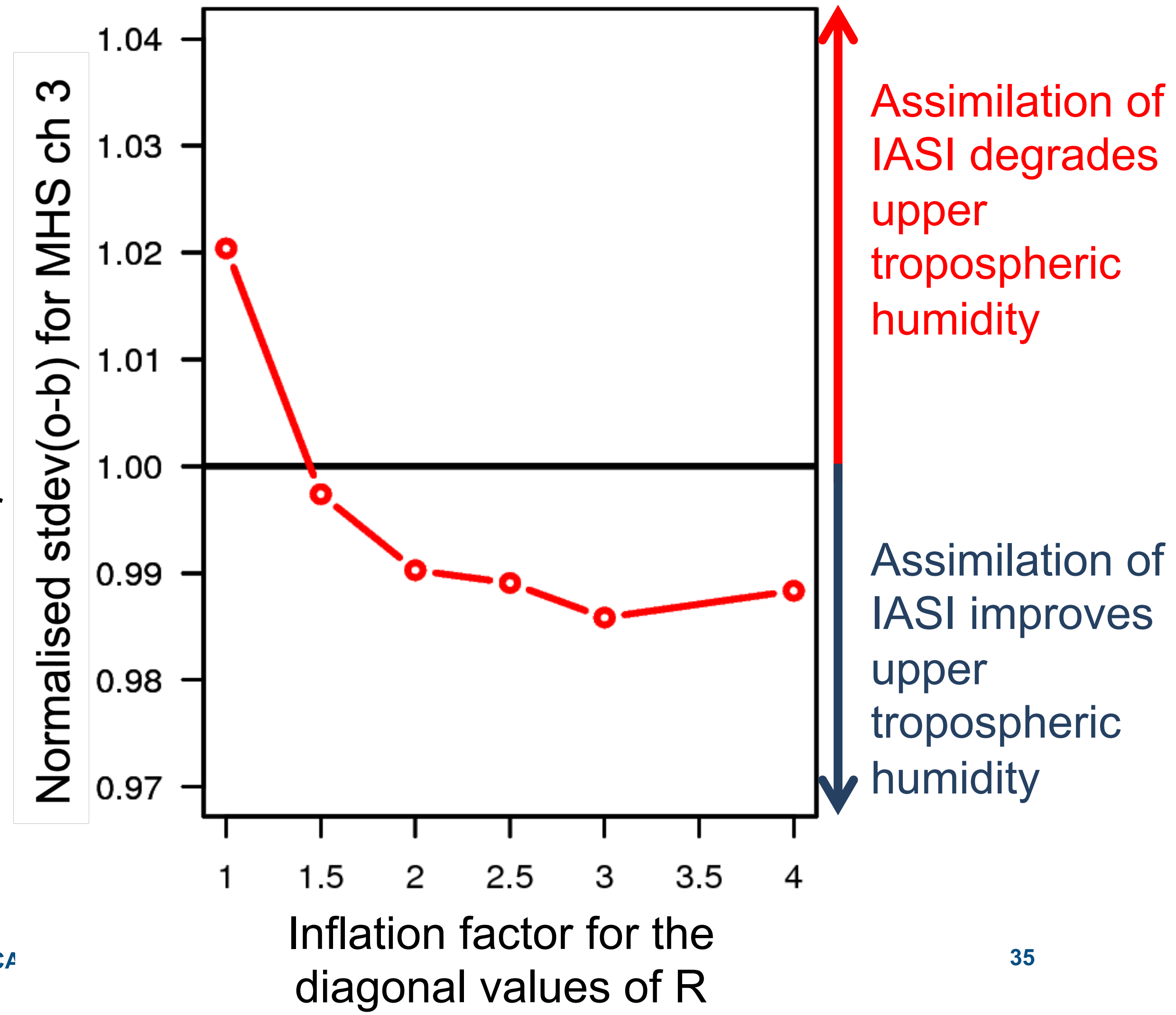
What to do when there are error correlations? Option 2: Inflation

- If the observations have ***error correlations, but these are neglected*** in the assimilation system, assimilating them can have a ***negative effect***.

- ***Pragmatic solution 2:*** Use larger σ_o than expected ("***Error inflation***").

- ***Neglecting error correlation with no inflation*** can result in an analysis that is ***worse*** than the background!

- Note: Background departure statistics for other observations are a useful indicator to tune observation errors.



Outline

Accounting for error correlations

- Accounting for observation error correlations is an area of active research.

- Efficient methods exist if the error correlations are restricted to small groups of observations (e.g., ***inter-channel error correlations***).

  – E.g., calculate R^{-1} (y – H(x)) without explicit inversion of R, by using Cholesky decomposition (algorithm for solving equations of the form Az = b).

  – Used operationally for IASI, CrIS, AIRS and ATMS at ECMWF and many other centres

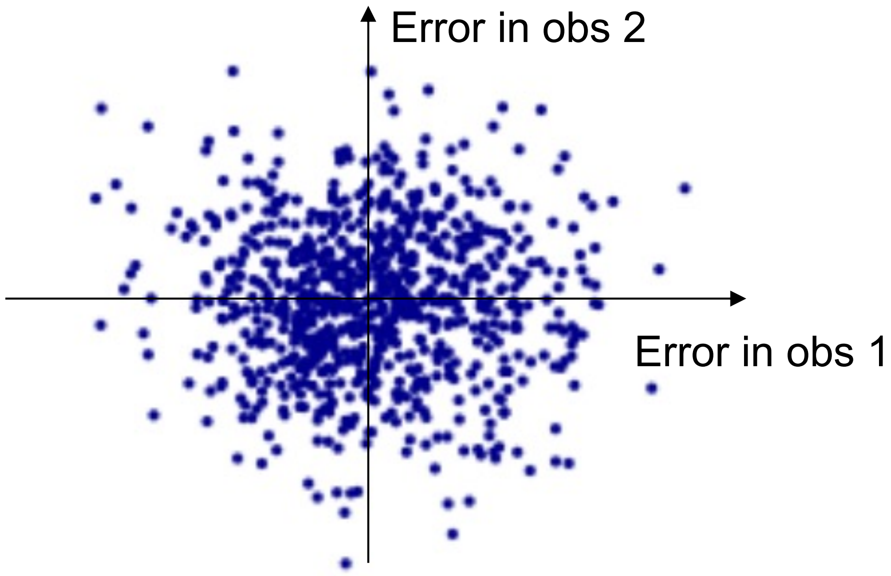
- Accounting for ***spatial error correlations*** is technically more difficult in variational algorithms, though methods are being developed.

  – Met Office is taking spatial error correlations into account in the operational assimilation of Doppler radar data in their limited area model (Simonin et al 2019)

What is the effect of error correlations?

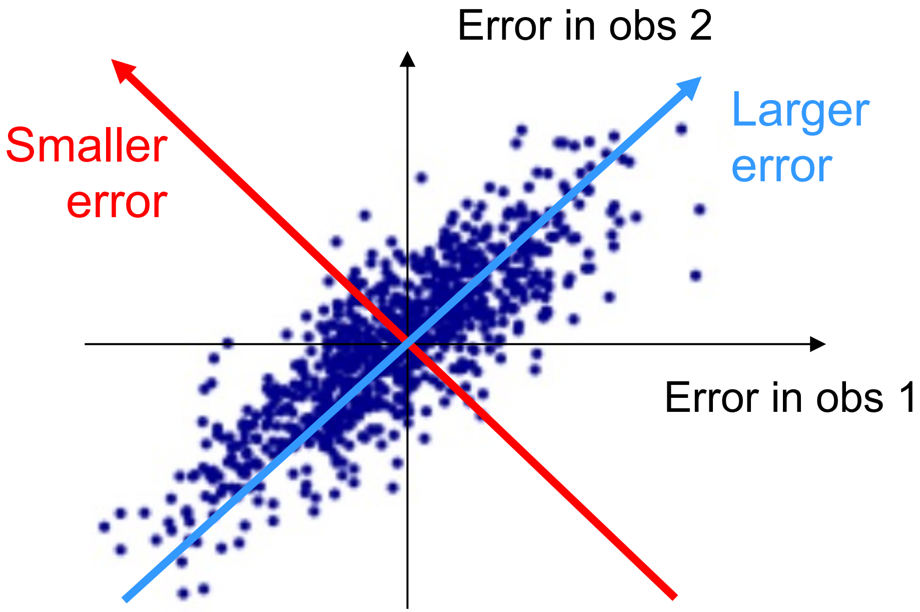
Uncorrelated error

$$\mathbf{R} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$



Correlated error

$$\mathbf{R} = \begin{pmatrix} 1 & 0.8 \\ 0.8 & 1 \end{pmatrix}$$



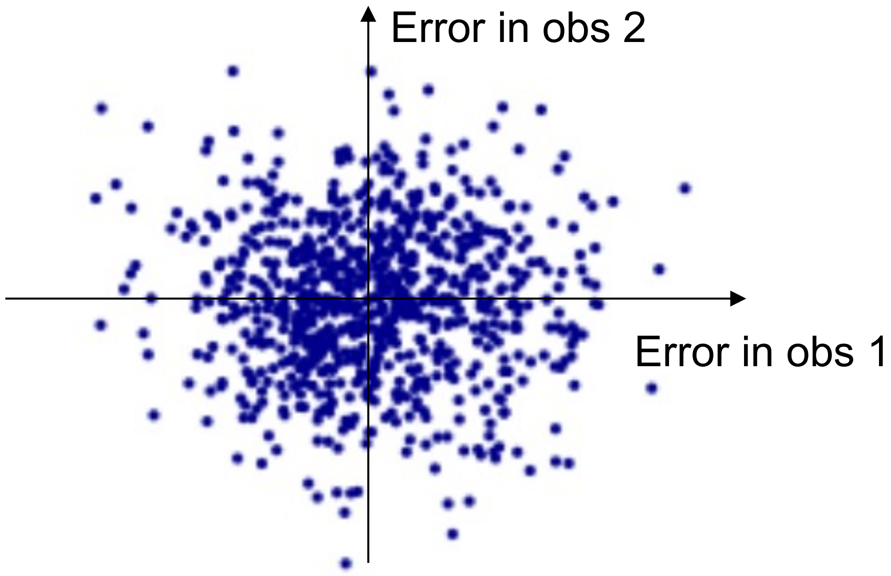
If errors ***are correlated*** and we ***assume no error correlations***, we assign…

- … an error that is ***too small*** for features along the blue direction (mean-like features), leading to over-weighting of the observations. Hence inflation helps.
- … an error that is ***too large*** for features along the red direction (gradient-type features).

What is the effect of error correlations?

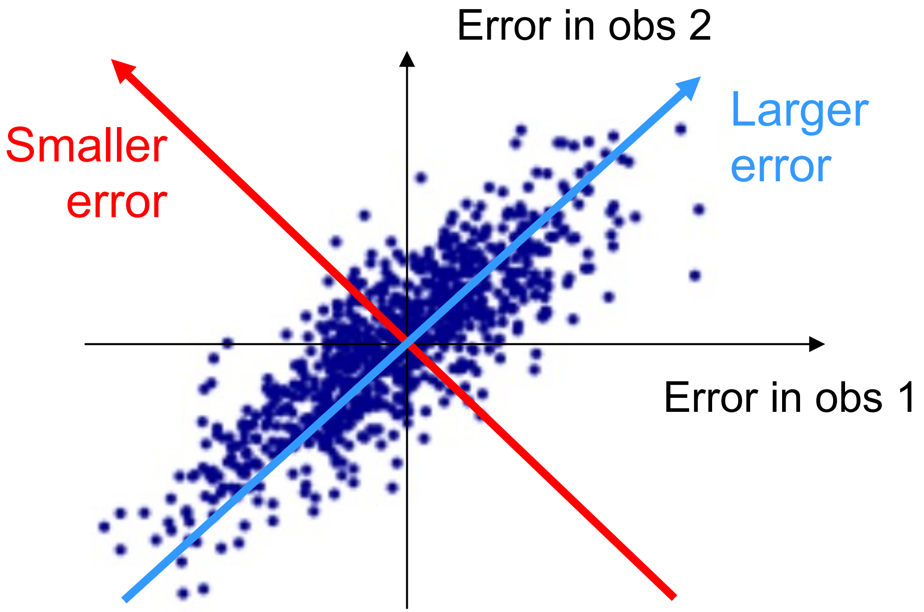
Uncorrelated error

$$\mathbf{R} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$



Correlated error

$$\mathbf{R} = \begin{pmatrix} 1 & 0.8 \\ 0.8 & 1 \end{pmatrix}$$



Similarly, when we ***account for observation error correlations*** we tell the assimilation system that…

… ***departures*** that are ***similar*** for different observations are ***more likely*** due to errors in the observations.

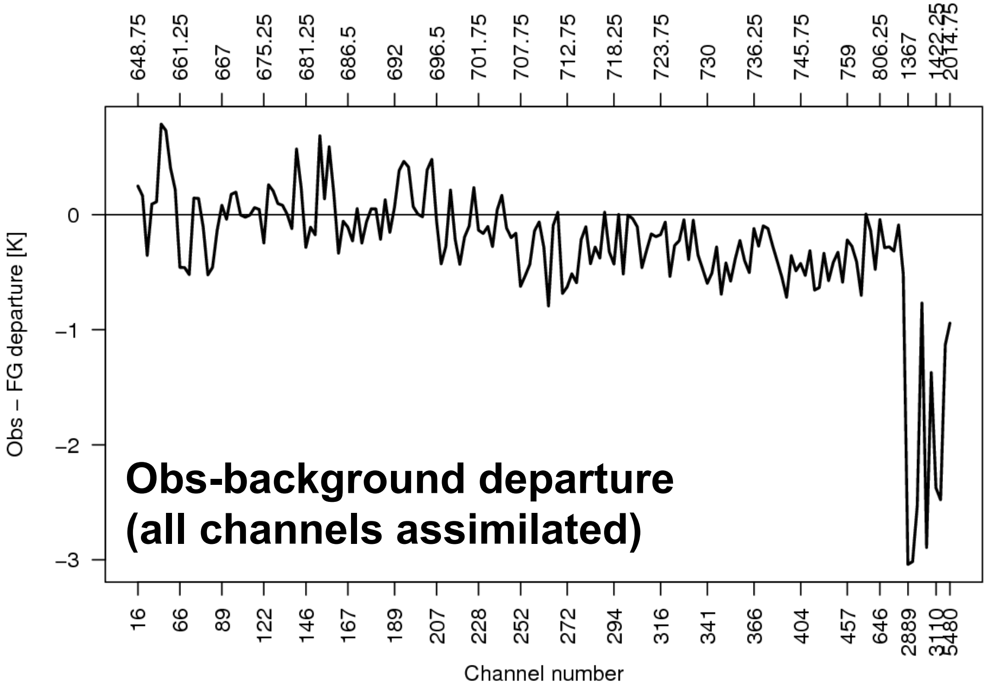
… ***departures*** that are ***different*** for different observations are ***less likely*** due to errors in the observations.

Example: Assimilation of a IASI spectrum (I)

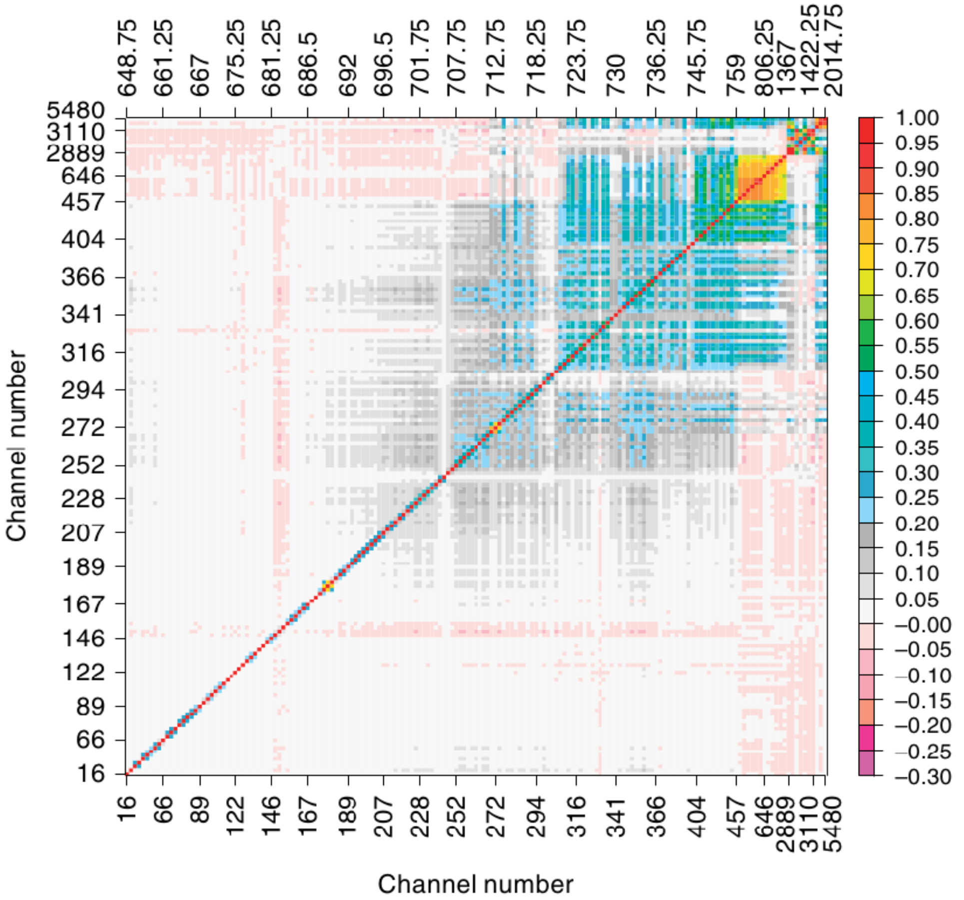
Assimilate a single IASI spectrum,

- assuming **no error correlations**,
- assuming diagnosed error correlations

(σ_o unchanged in both cases).



Error correlation matrix

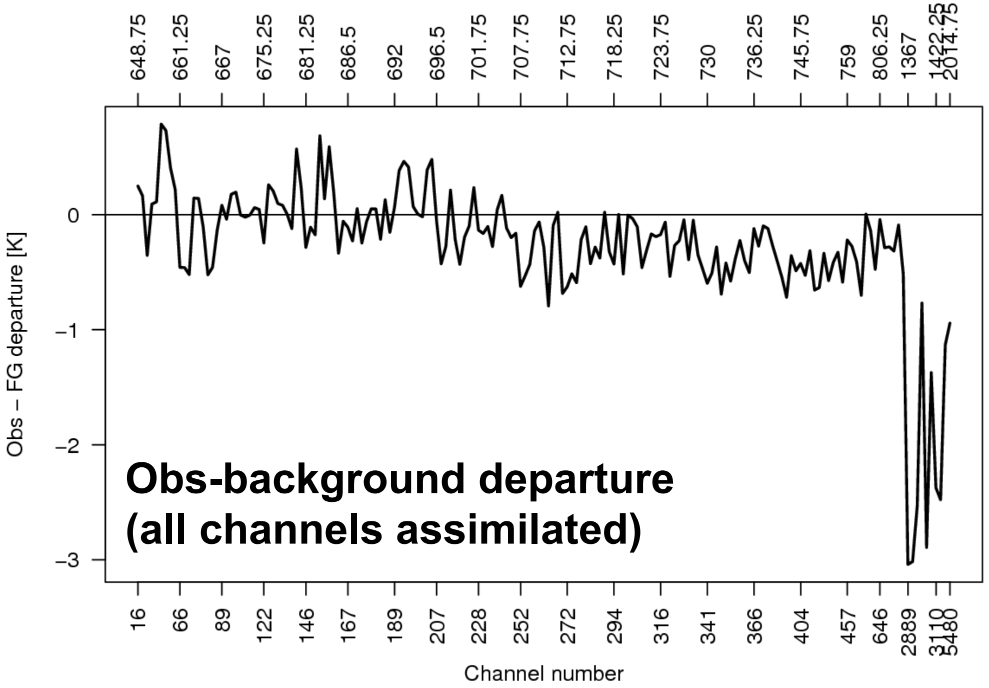


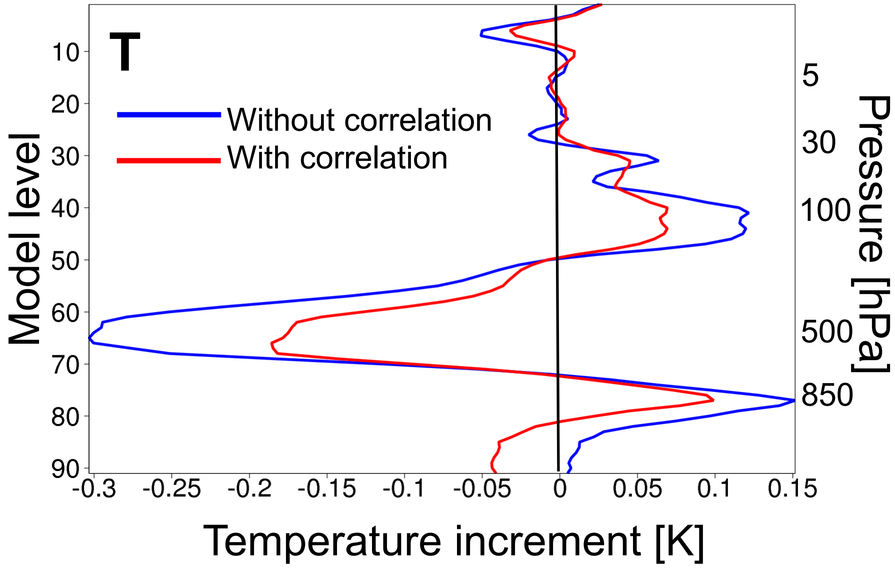
Example: Assimilation of a IASI spectrum (I)

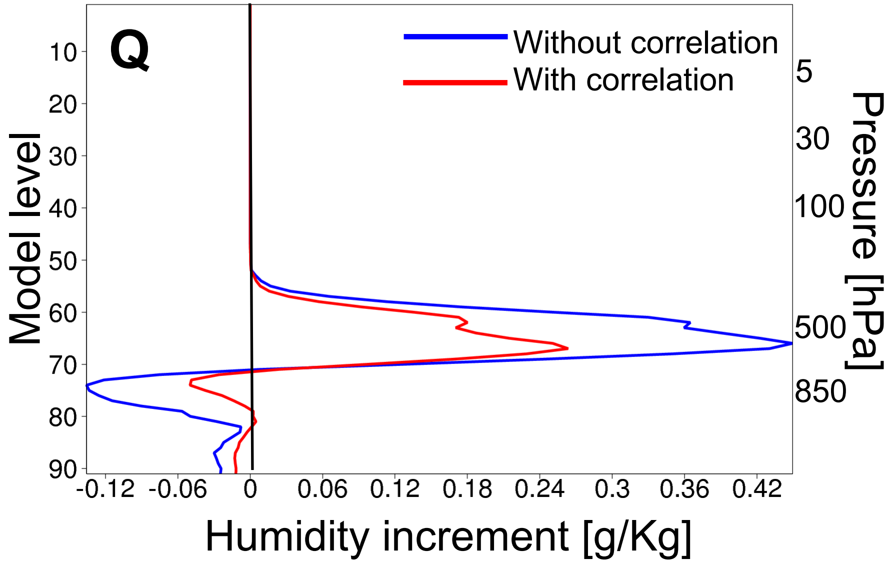
Similar departures → increments reduced with error correlations taken into account

Assimilate a single IASI spectrum,
- assuming **no error correlations**,
- assuming diagnosed error correlations

(σ_o unchanged in both cases).





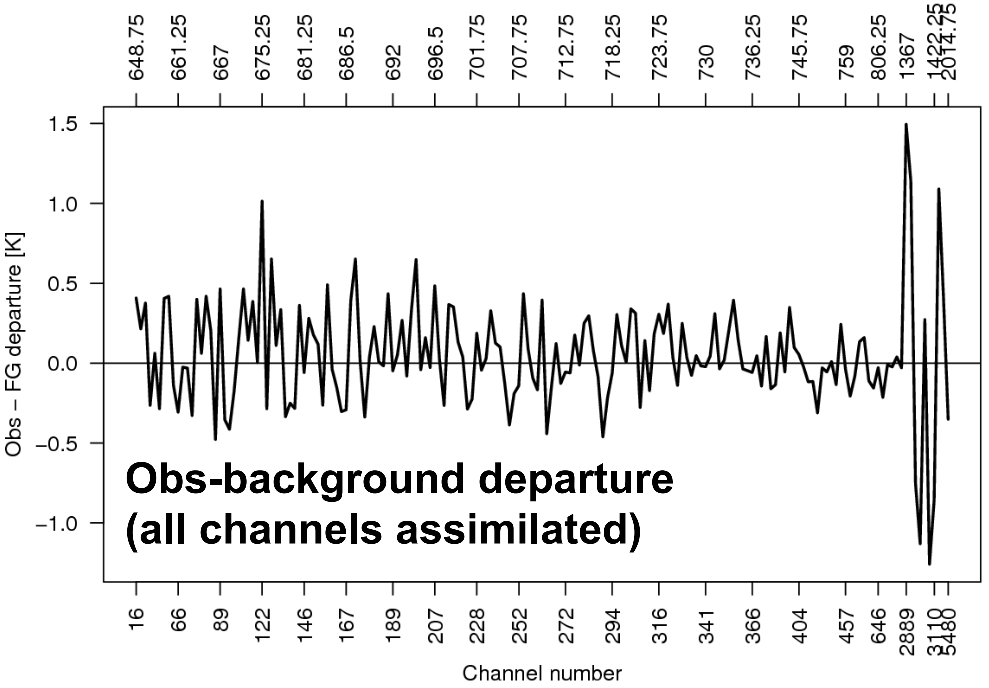


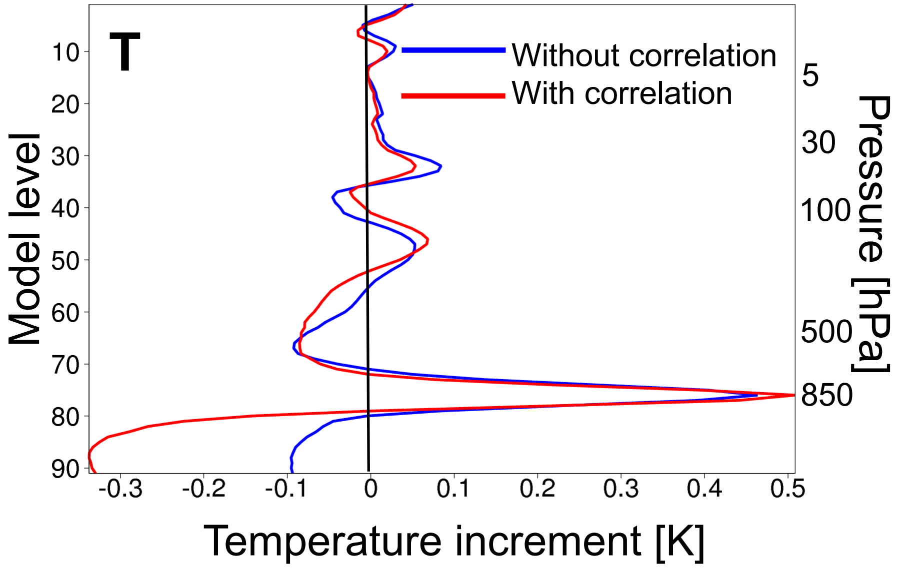
Example: Assimilation of a IASI spectrum (II)

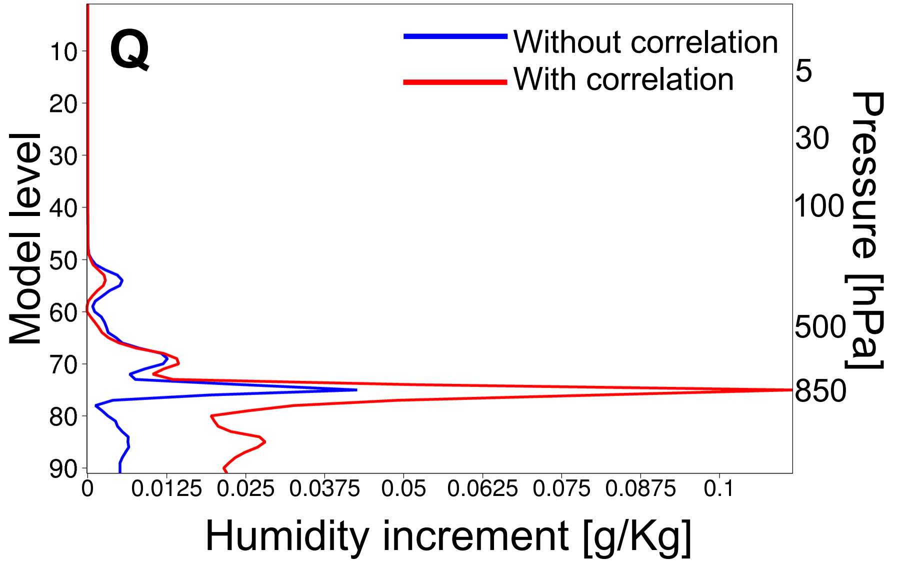
Different departures → increments *increased* with error correlations taken into account

Assimilate a single IASI spectrum,
- assuming **no error correlations**,
- assuming diagnosed error correlations

(σ_o unchanged in both cases).







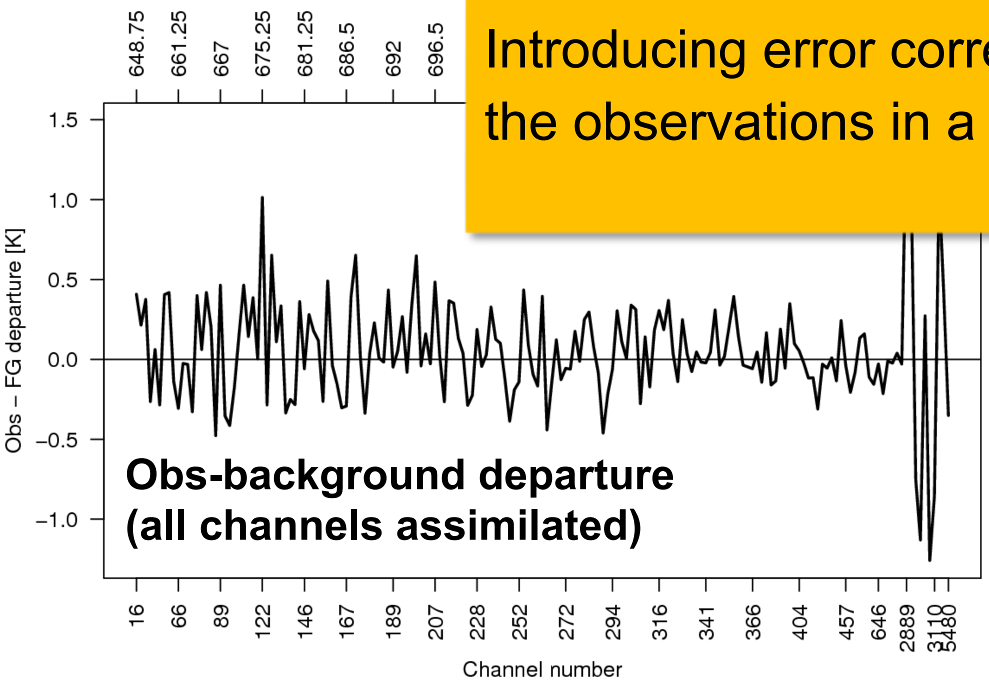
Example: Assimilation of a IASI spectrum (II)

Different departures → increments ***increased*** with error correlations taken into account

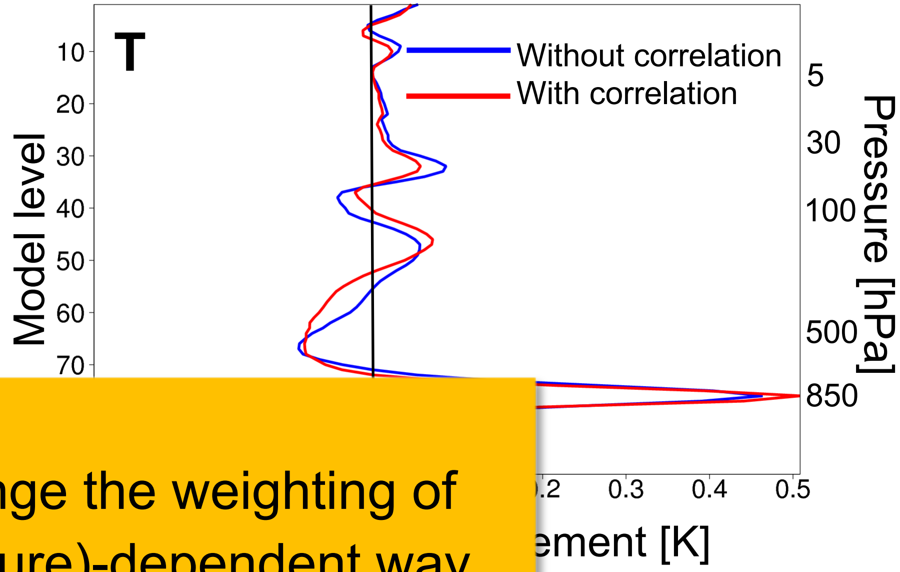
Assimilate a single IASI spectrum,

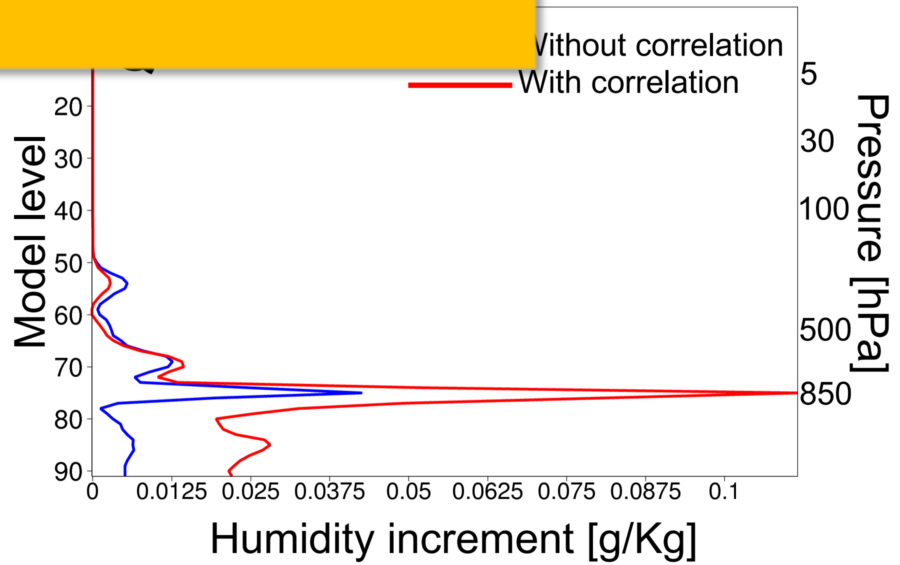
- assuming **no error correlations**,
- assuming diagnosed error correlations

(σ_o unchanged in both cases).

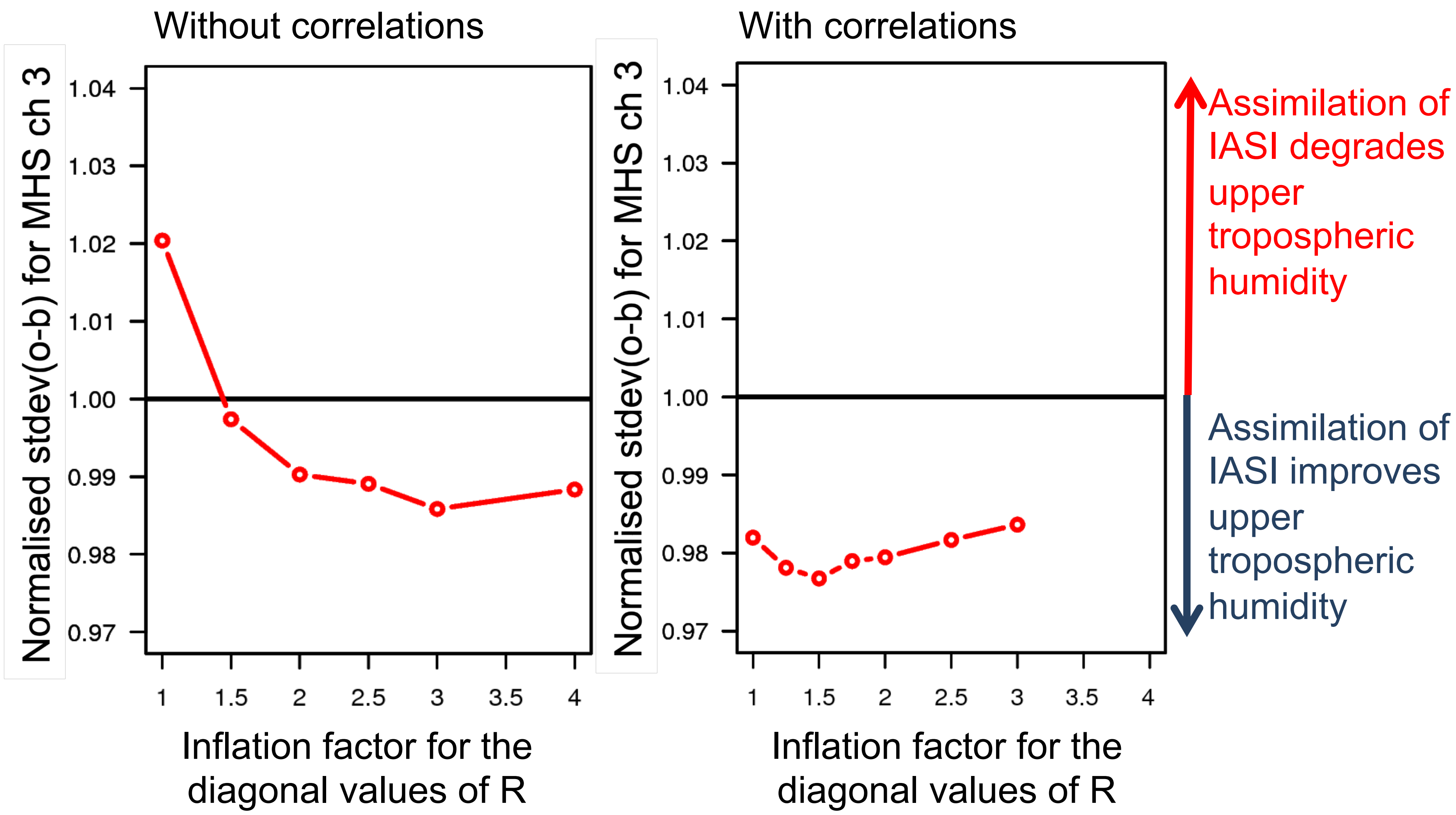


Introducing error correlations will change the weighting of the observations in a situation(/departure)-dependent way.





Effect of accounting for error correlations in the assimilation of IASI



Most centres now take inter-channel error correlations into account for the assimilation of hyperspectral IR data.

Some points on accounting for observation error correlations

- Accounting for observation error correlations is an ***active area of research***.
- ***Benefits*** have been ***demonstrated*** at many centres for accounting for inter-channel error correlation; used widely operationally.

- Note:
  - Assuming error correlations puts ***more weight on differences between observations.*** Are these differences reliable? How reliable are ***inter-channel calibration/bias correction***?
  - Are the ***estimates of error correlations reliable***?
  - Accounting for observation error correlations can affect the ***conditioning*** of the assimilation and lead to slower convergence.
  - Error correlation matrices ***may need adjustments*** ("re-conditioning", inflation).
- How important it is to account for error correlations may additionally depend on the structure of the background error.

Outline

1. What are observation errors?
2. Estimating observation errors
3. Specification of observation errors in practice
4. Accounting for observation error correlations
5. **Summary**

Summary

- Assigned observation and background errors determine how much ***weight*** an observation receives in the assimilation.
- For satellite data, "true" ***observation errors are often correlated*** (spatially, in time, between channels, etc) and ***situation-dependent***.
- Careful use of ***departure-based diagnostics*** can provide ***guidance*** on the setting of observation errors.
- Diagonal observation errors are still widely assumed for many observations, and ***thinning and error inflation*** are used to counter-act the effects of error correlations.
- Areas of active research:
  - Development of "***observation error models***" to account for situation-dependence of observation errors.
  - ***Accounting for observation error correlations*** (inter-channel, spatial).
  - ***Estimation of observation errors.***

Further reading

- Bédard, Beaulne, Buehner and Beaudoin (2019): Increased density of assimilated satellite radiances in global 4D-EnVar: The link between observation thinning and error variance inflation. Presentation at ITSC-22, http://cimss.ssec.wisc.edu/itwg/itsc/itsc22/presentations/5%20Nov/13.05.bedard.pdf
- Bormann and Bauer (2010): Estimates of spatial and inter-channel observation error characteristics for current sounder radiances for NWP, part I: Methods and application to ATOVS data. QJRMS, 136, 1036-1050.
- Bormann et al. (2010): Estimates of spatial and inter-channel observation error characteristics for current sounder radiances for NWP, part II: Application to AIRS and IASI. QJRMS, 136, 1051-1063.
- Bormann et al (2016): Enhancing the impact of IASI observations through an updated observation-error covariance matrix. QJRMS, 142: 1767–1780.
- Desroziers et al. (2005): Diagnosis of observation, background and analysis error statistics in observation space. QJRMS, 131, 3385-3396.
- Hollingworth and Loennberg (1986): The statistical structure of short-range forecast errors as determined from radiosonde data. Part I: The wind field. Tellus, 38A, 111-136.
- Janjić, T. , Bormann, N. , Bocquet, M. , Carton, J. A., Cohn, S. E., Dance, S. L., Losa, S. N., Nichols, N. K., Potthast, R. , Waller, J. A. and Weston, P. (2017), On the representation error in data assimilation. QJRMS, doi:10.1002/qj.3130
- Liu and Rabier (2003): The potential of high-density observations for numerical weather prediction: A study with simulated observations. QJRMS, 129, 3013-3035.
- Simonin et al (2019): A pragmatic strategy for implementing spatially correlated observation errors in an operational system: An application to Doppler radial winds. Q J R Meteorol Soc. 2019; 145: 2772– 2790.
- Weston et al (2014): Accounting for correlated error in the assimilation of high-resolution sounder data. Q.J.R. Meteorol. Soc., 140: 2420–2429. doi: 10.1002/qj.2306