Data assimilation algorithms and key elements

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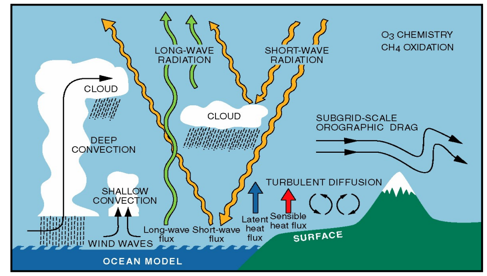
Acknowledgements: Materials/contents from many sources

What is Data Assimilation ?

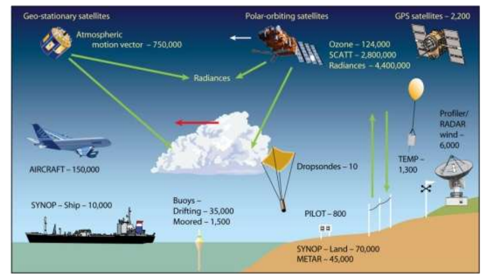
- Models give a complete description of the atmospheric, but **errors grow rapidly** in time
- Observations provide an **incomplete description** of the atmospheric state, but bring up to date information
- Data assimilation **combines** these two sources of information to produce an optimal (best) estimate of the atmospheric state
- This state (the *analysis*) is used as **initial conditions** for extended forecasts.

The assimilation system:

- Model



- Observations



- Assimilation algorithm

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

The forecast model

$\mathbf{X}_{t=0}$ → $\mathbf{X}_{t=t}$

Assimilation Algorithm Combining information

- At NCMRWF we employ **variational data assimilation** methods

- These are based upon the **maximum likelihood combination** of observations and background information

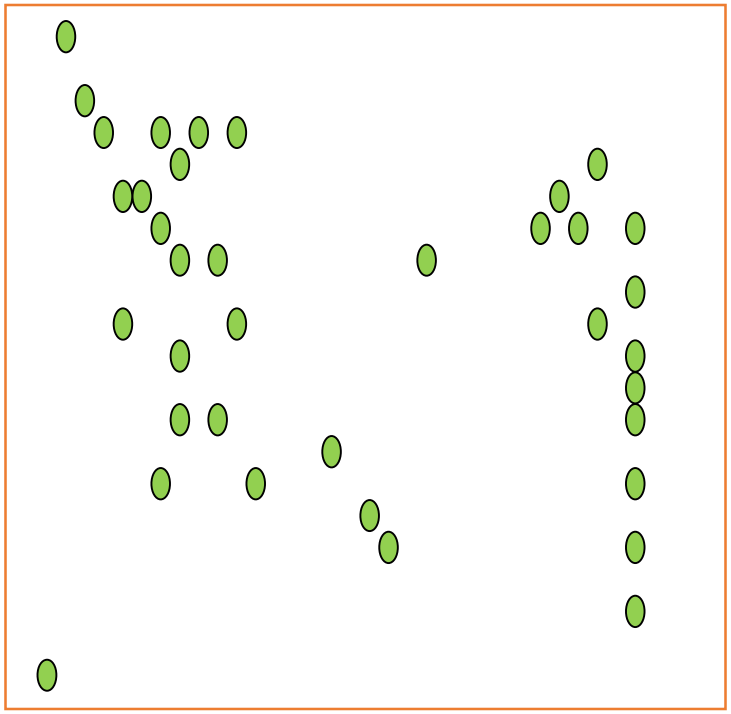
- It can be shown that the most probable state of the atmosphere given a background $\mathbf{X_b}$ and some observations **Y** is that which minimises a **cost or penalty function J**

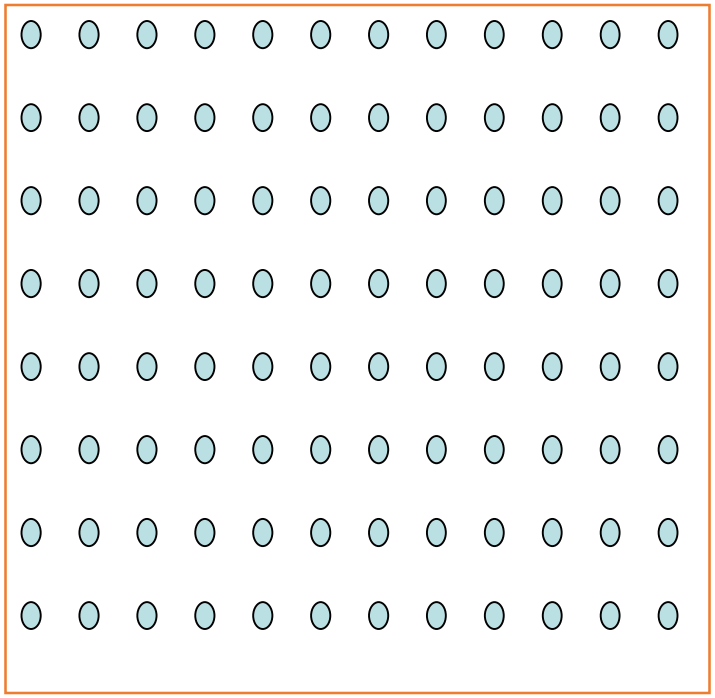
- The solution obtained is **optimal** in that it fits the prior (or background) information and measured radiances **respecting the uncertainty in both.**

Objective Analysis

Observations at irregular location

Regular Grid Point





Objective analysis

Polynomial expansion (Panofsky, 1949)

- **Coefficients determined by least squares fit**

Gilchrist and Cressman (1954)

- **Also polynomial expansion, but used a trial field (short-range forecast)**
- **fitting done locally rather than over full domain**

Bergthorsson and Doos (1955)

- **Analyzed differences between observations and a trial field**
- **First attempt at deriving optimal weights using statistics**

Optimal (statistical) interpolation (OI)

Rutherford 1972

Three-dimensional variational analysis

Spectral statistical interpolation (NMC, 1991)

ECMWF, 1996

4-Dimensional Variational Method (4D-Var)

Kalman Filter (KF, with approximation)

Ensemble Kalman Filter (EnKF)

Hybrid Method (4D-Var + EnKF)

Different popular techniques of objective analysis are :

- **Polynomial interpolation or surface fitting method**
- **Successive correction method (Cressman Analysis)**
- **Statistical Interpolation :OI (Optimum Interpolation)**
- **Variational Analysis**

Variational Assimilation
The cost function J (X)

background error covariance

model state

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

observations

observation error covariance

observation operator
(maps the model state to the observation space)

The cost function components (J_b)

$$J(x) = \boxed{(x - x_b)^T \mathbf{B}^{-1} (x - x_b)} + (y - \mathrm{H}[x])^T \mathbf{R}^{-1} (y - \mathrm{H}[x])$$

Fit of the solution to the background estimate of the atmospheric state weighted inversely by the background error covariance **B**

The cost function components (J_O)

$$J(x) = (x - x_b)^T \mathbf{B}^{-1} (x - x_b) +$$

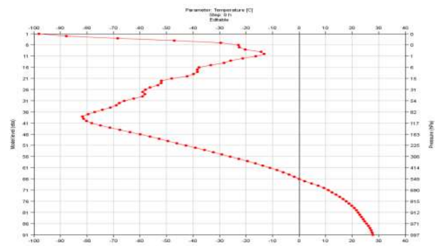
$$(y - \mathrm{H}[x])^T \mathbf{R}^{-1} (y - \mathrm{H}[x])$$

Fit of the solution to the observations weighted inversely by the measurement error covariance **R** (observation error + error in observation operator **H**)

Various implementations of the assimilation algorithm

- 1D-Var
- 3D-Var
- 4D-Var

One dimensional variational analysis (1D-Var)



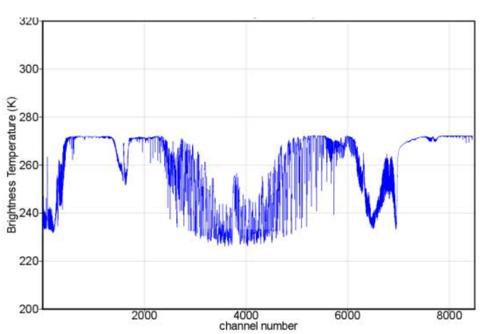
1D model state profile

$$J(x) = (x - x_b)^T \mathbf{B}^{-1} (x - x_b) +$$

$$(y - \mathrm{H}[x])^T \mathbf{R}^{-1} (y - \mathrm{H}[x])$$

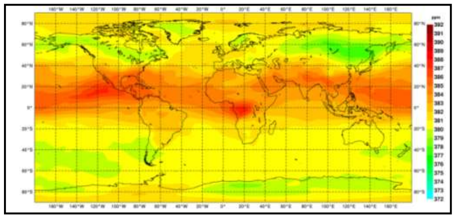
vector of measured radiances at one location

observation Operator = radiative transfer model



$$L(\nu) = \int_0^{\infty} B(\nu, T(z)) \left[\frac{d\tau(\nu)}{dz} \right] dz$$

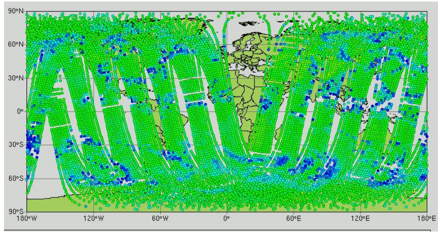
Three dimensional variational analysis (3D-Var)



3D model state

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

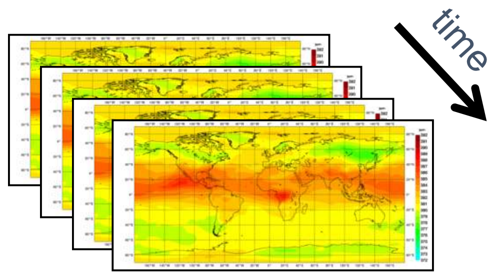
global vector of
measured radiances



observation operator
= spatial interpolation +
radiative transfer model

$$L(\nu) = \int_0^\infty B(\nu, T(z)) \left[\frac{d\tau(\nu)}{dz} \right] dz$$

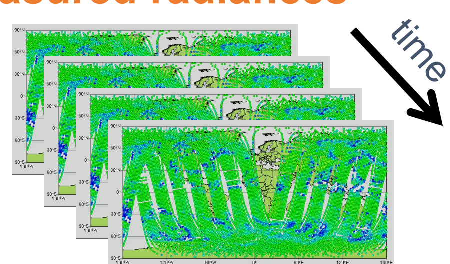
Four dimensional variational analysis (4D-Var)



4D model state

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

global time windows of
measured radiances



observation operator
= spatial interpolation + forecast model
+ radiative transfer model

$$L(\nu) = \int_0^\infty B(\nu, T(z)) \left[\frac{d\tau(\nu)}{dz} \right] dz$$

$\mathbf{X}_{t=0}$ → $\mathbf{X}_{t=t}$

The key elements of a satellite data assimilation system

Key elements of a data assimilation system

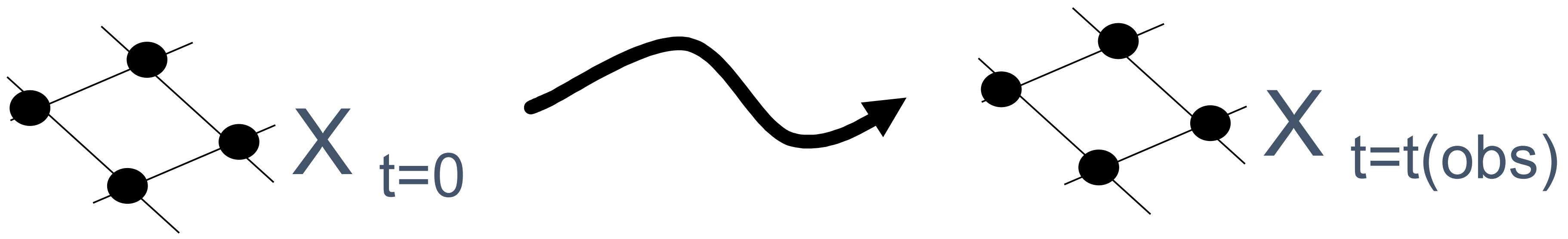
- observation operator
- background errors
- observation errors
- bias correction
- data selection and quality control

Observation operator

- The observation operator must map the model state at beginning of the assimilation window (t=0) to the observation time and location.
- In the **direct assimilation of radiance observations**, the observation operator must incorporate an additional step to compute radiances from the model state variables.
- This means that radiance observations are significantly more computationally expensive than conventional observations

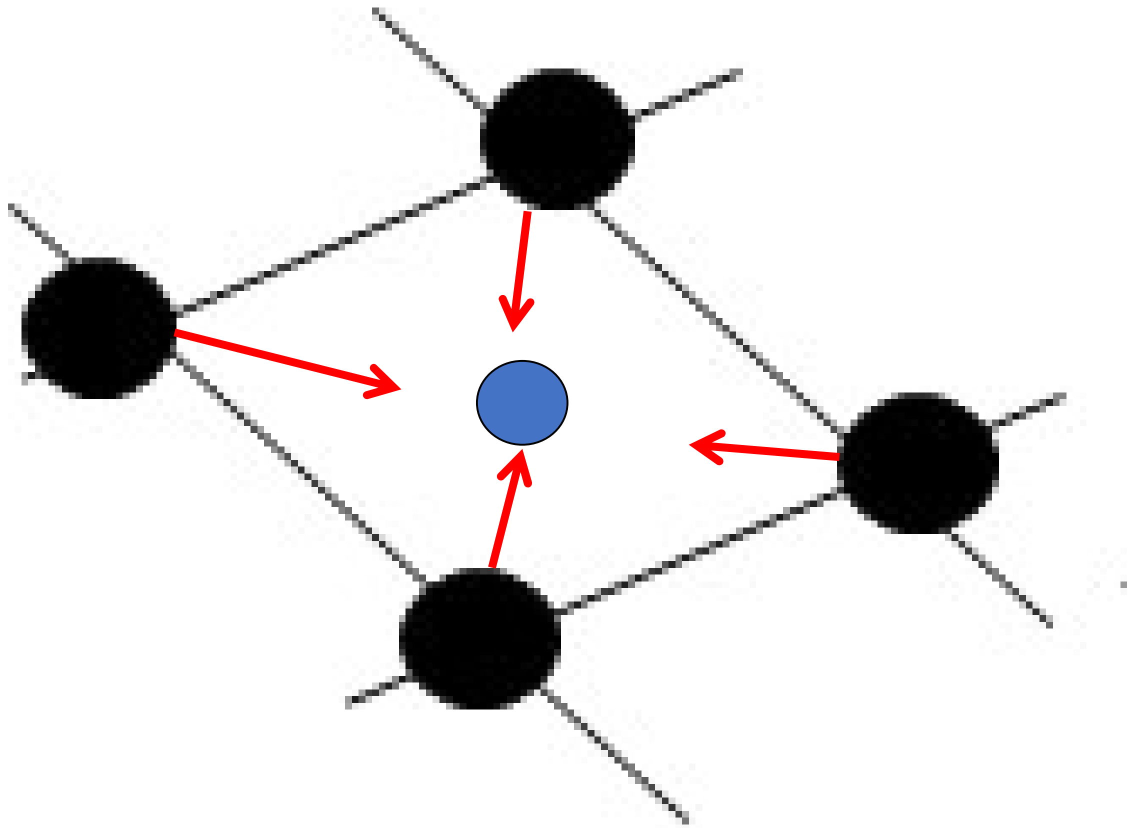
Observation operator

1) Time evolution of forecast model field to OBS time



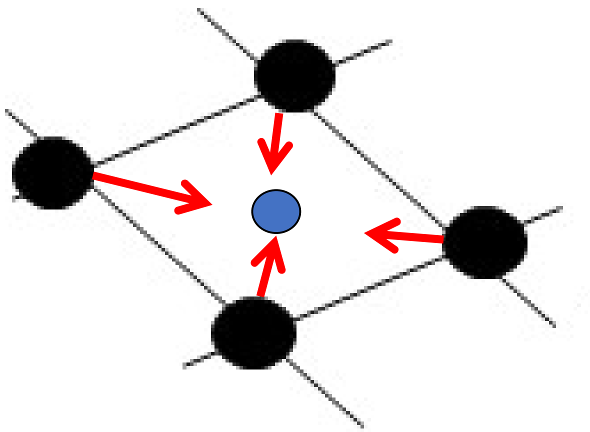
Observation operator

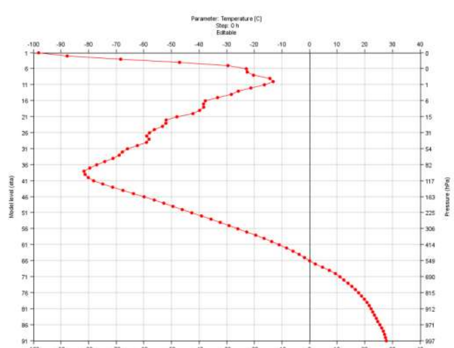
2) Spatial interpolation of model grid to OBS location



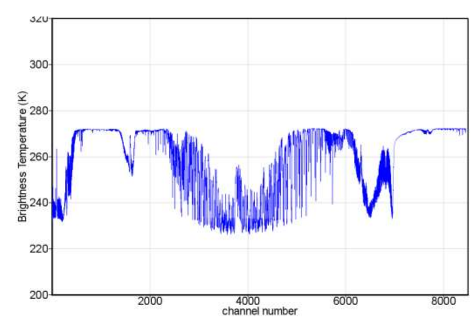
Observation operator

3) Radiative transfer calculation from model state at that location to radiances at that location





RT Model



Observation operator (RT component)

- The RT model should produce an accurate simulation of the satellite radiance from the model state, based upon the best knowledge of the instrument characteristics and up to date spectroscopic information.

- However, the model must be fast enough to process huge quantities of data in near real time

- In addition, the adjoint and tangent linear versions of the RT model are required by the algorithm that minimises the cost function

- Ideally the same RT model should be used for all satellite sensors being assimilated

Background errors (and vertical resolution)

- The matrix B must accurately describe errors in the background estimate of the atmospheric state. It determines the weight given to the background information.

- A very important aspect for the assimilation of near-nadir viewing satellite radiances are the **vertical correlations** that describe how background errors are distributed in the vertical (sometimes called structure functions)

- These are important because satellite radiances have very **limited vertical resolution**

How do we determine background errors?

• Innovation departure statistics – i.e. comparison of X_b with **radiosondes** (best estimate of truth but limited coverage)

•comparison of forecasts differences e.g. 48hr and 24hr (so called ***NMC method***)

•comparison of **ensembles** of analyses made using perturbed observations

None of these approaches are perfect!

What do we want our background errors to do ?

- Describe our confidence in the background estimate of the atmosphere X_b
- Describe how background errors are correlated with each other:
  - vertically (between different model levels)
  - spatially (between different grid points)
  - between variables (T / Q / O3 / wind)
  - impose balance (e.g. geostrophic)

- **They should be data and flow dependent!**

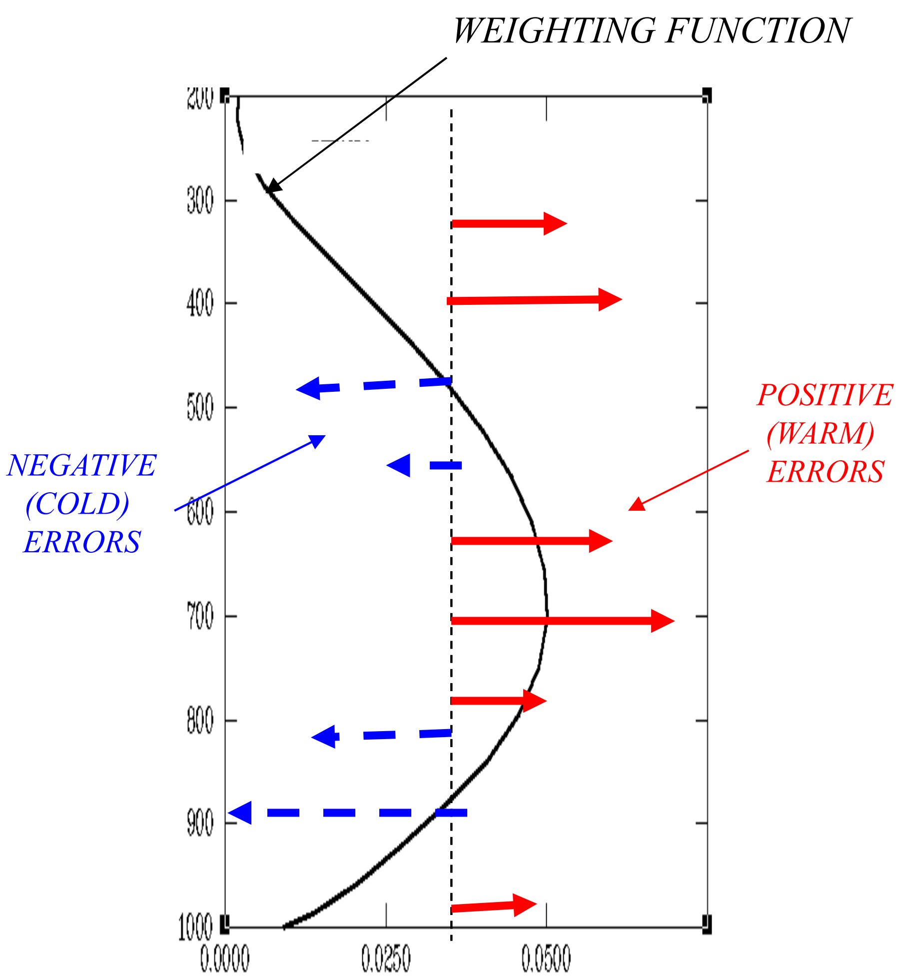
Background errors and radiance assimilation

- The physics of radiative transfer mean that radiances measured by downward looking satellite sounders have very **poor vertical resolution** (they are broad vertical averages)

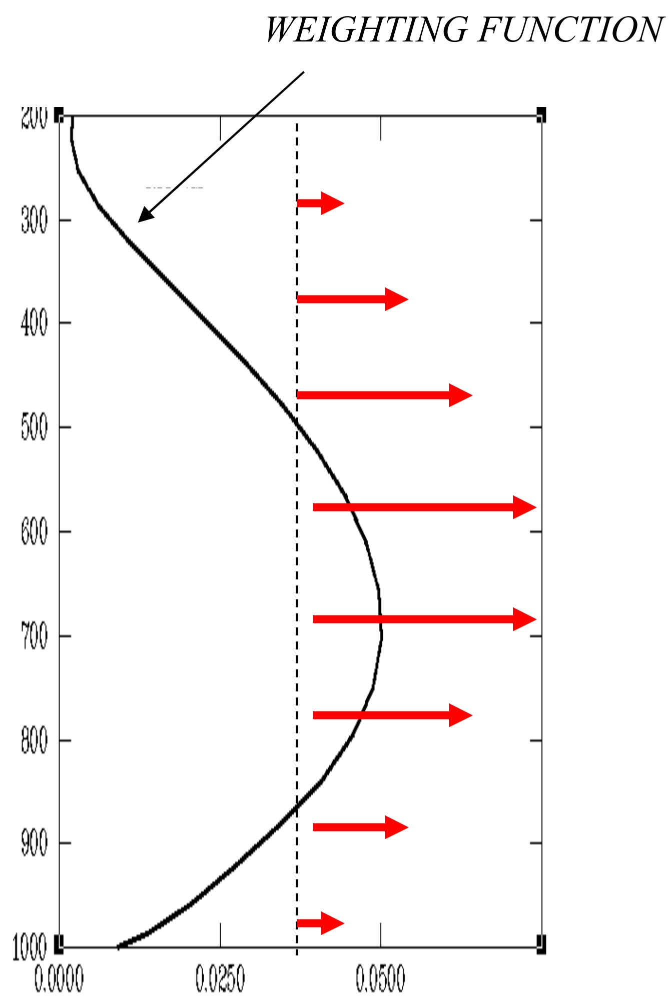
- If we wish to **correct errors in the background** with radiance observations (in DA) the vertical structure of these errors is very important.

- This structure is described by the **vertical correlations in the background error covariance**

Background errors (and vertical resolution)



"Difficult" to correct



"Easy" to correct

Can we quantify the impact of vertical background error correlations on analysis accuracy ?

…a helpful linear analogue …

model state

background error covariance

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

observations

observation error covariance

observation operator
(maps the model state to the observation space)

…when we minimise J(x) …

...we correct background errors

It can be shown that the state that minimizes the cost function is equivalent to a linear **correction** of the background using the observations:

$$x_a = x_b + [\mathbf{HB}]^T [\mathbf{HBH}^T + \mathbf{R}]^{-1} (y - \mathbf{H}x_b)$$

…where the **correction** is the **Kalman Gain Matrix** multiplied by the **innovation vector** (observation minus radiances simulated from the background)

correction term = $\mathbf{HB}]^T [\mathbf{HBH}^T + \mathbf{R}]^{-1} (y - \mathbf{H}x_b)$

Kalman gain **x** **innovation**

…and reduce the error …

Furthermore when we apply this **correction** we produce a state (the analysis) that is more accurate than the background. We can compute the improvement as an **error reduction** of the analysis error (**A**) compared to the error in the background (**B**) …

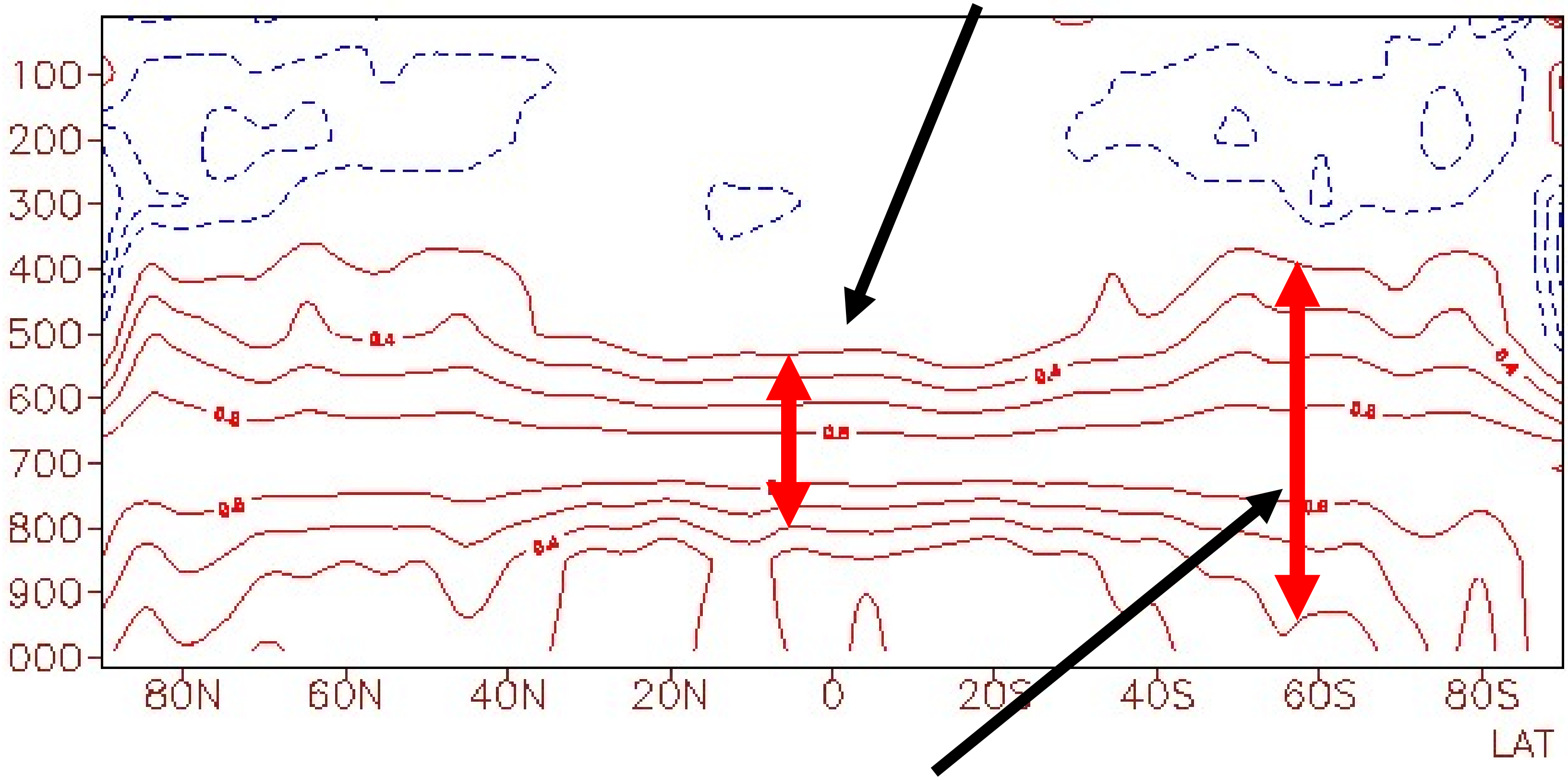
$$\mathbf{A} = \mathbf{B} - \underbrace{[\mathbf{HB}]^T[\mathbf{HBH}^T + \mathbf{R}]^{-1}\,\mathbf{HB}}_{\text{error reduction}}$$

So we can look at how **A** performs for two different types of vertical correlation present in **B**

Sharp and broad vertical correlation

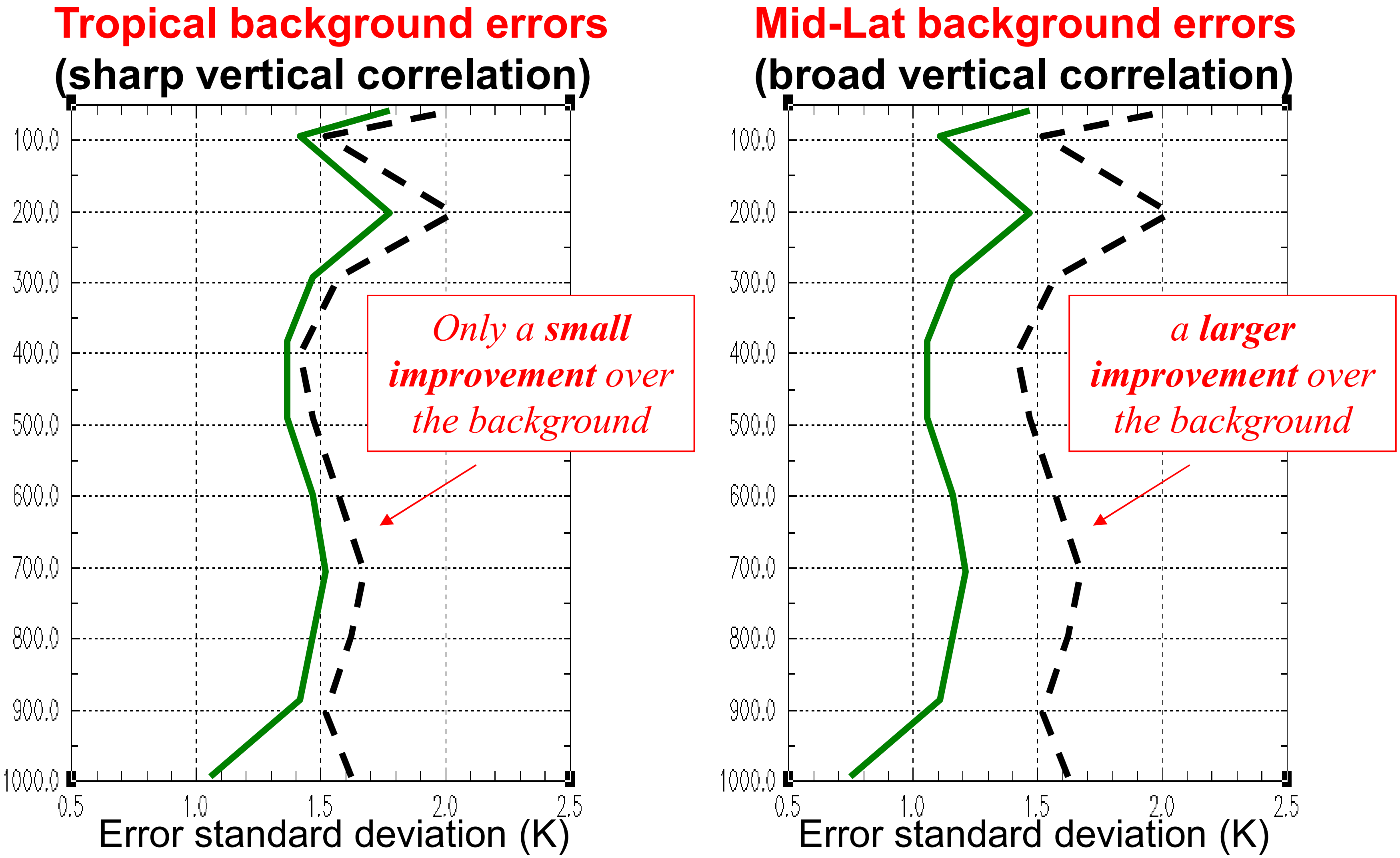
Sharper error correlations in the Tropics

700hPa T error



Broader vertical correlations in the mid-latitudes

Sharp and broad vertical correlation

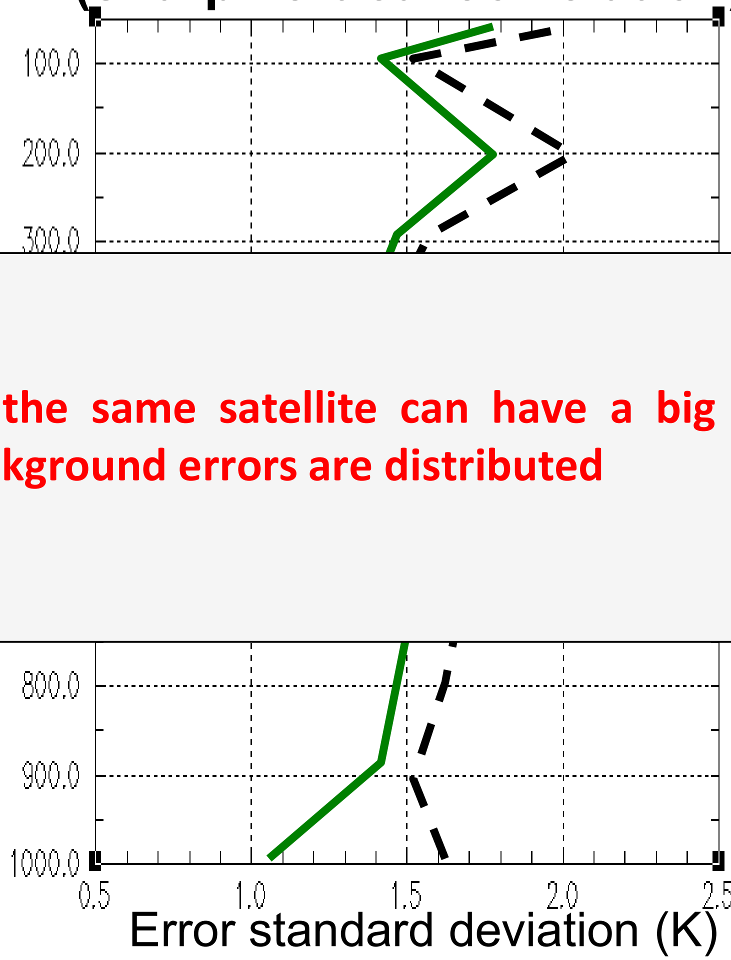


background error ---- Analysis error ——

Sharp and broad vertical correlation

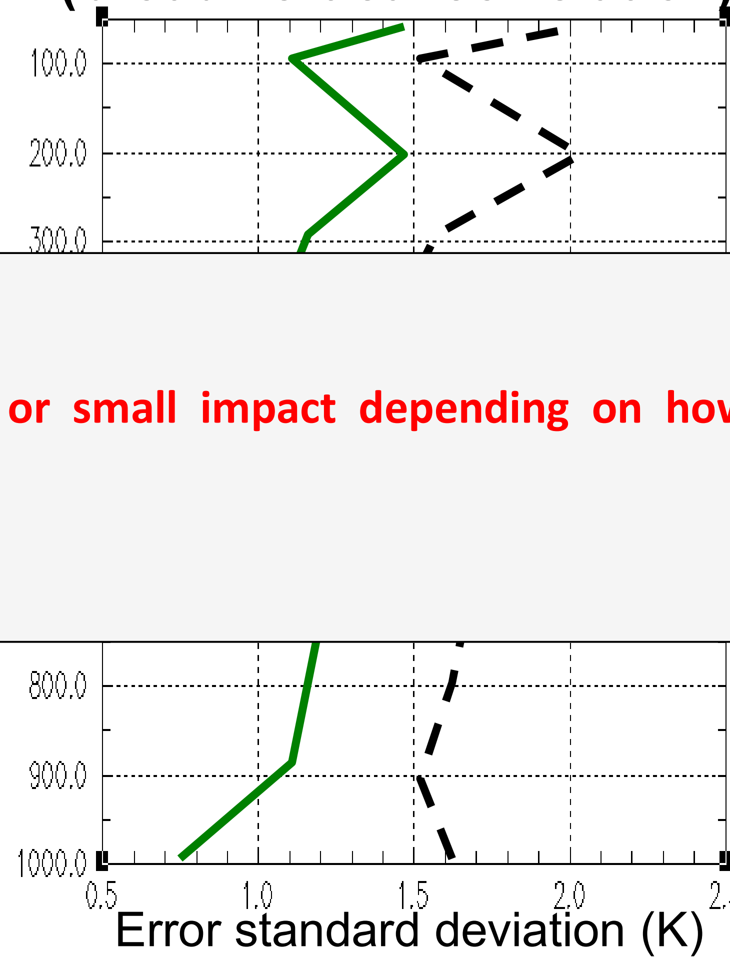
Tropical background errors

(sharp vertical correlation)



Mid-Lat background errors

(broad vertical correlation)



So the same satellite can have a big impact or small impact depending on how the background errors are distributed

background error ---- Analysis error ——

Observation errors:

- These determine the weight we give to the radiance observations. The observation error must account for random uncertainties in the observation operator (e.g. RT model), errors in data screening (e.g. residual clouds) and errors of representativeness (e.g. scale mismatch).

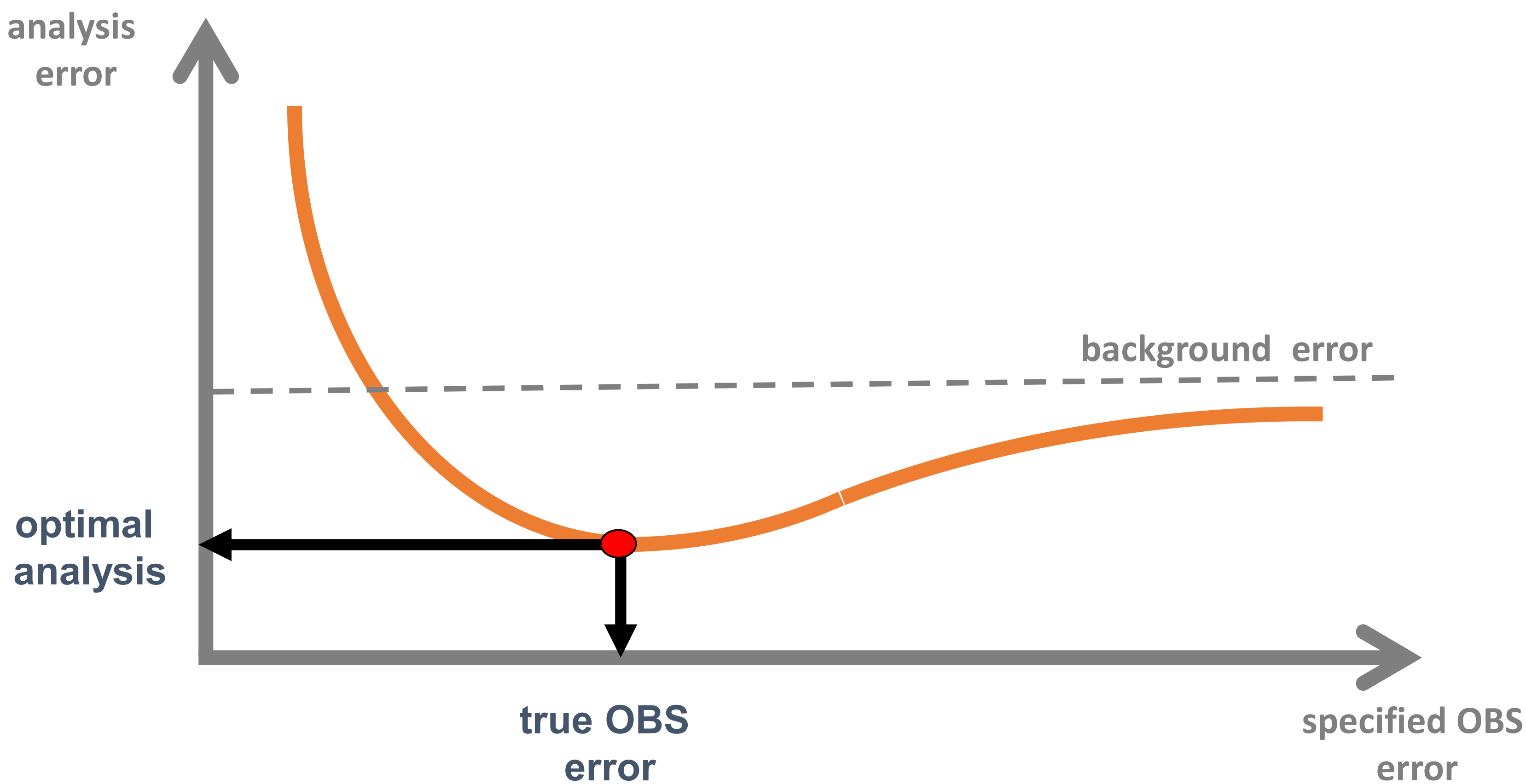
- R is a matrix, often specified through the square root of the diagonals (“σ_O”) and a correlation matrix (which can be the identity matrix).

- It is important to model both the magnitude of errors (diagonals of R) and any inter-channel correlations

- Wrongly specified observation errors can lead to an analysis with **larger errors than the background**!

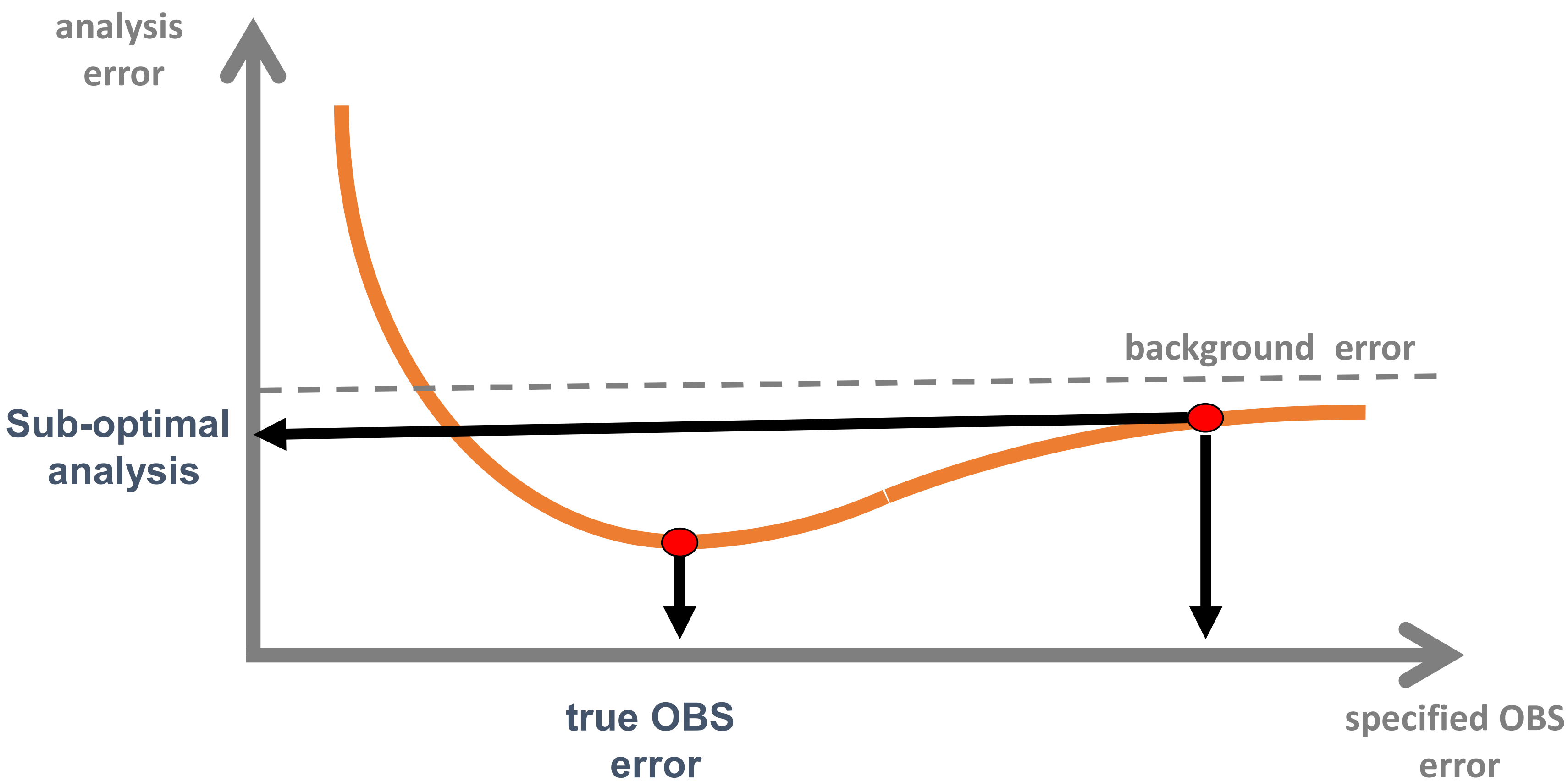
Observation errors:

- Specifying the correct observation error produces an optimal analysis with minimum error.



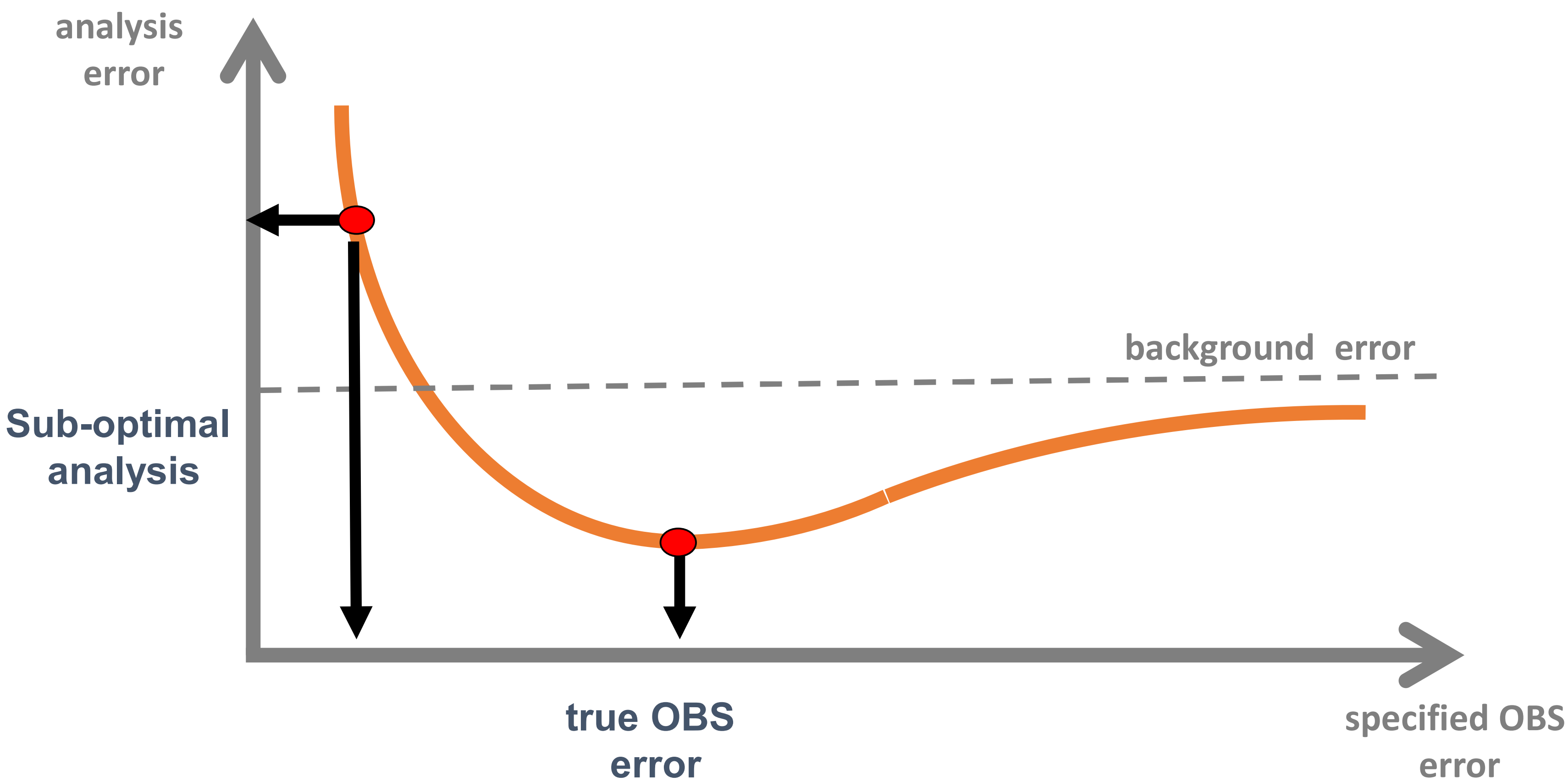
Observation errors:

- Over-estimating the OBS error degrades the analysis, but the result will not be worse than the background.



Observation errors:

- Under-estimating the OBS error degrades the analysis, and the result can be worse than the background!



What to do when there are error correlations?

- Thinning
  - reduce observation density so that error correlations are not relevant.

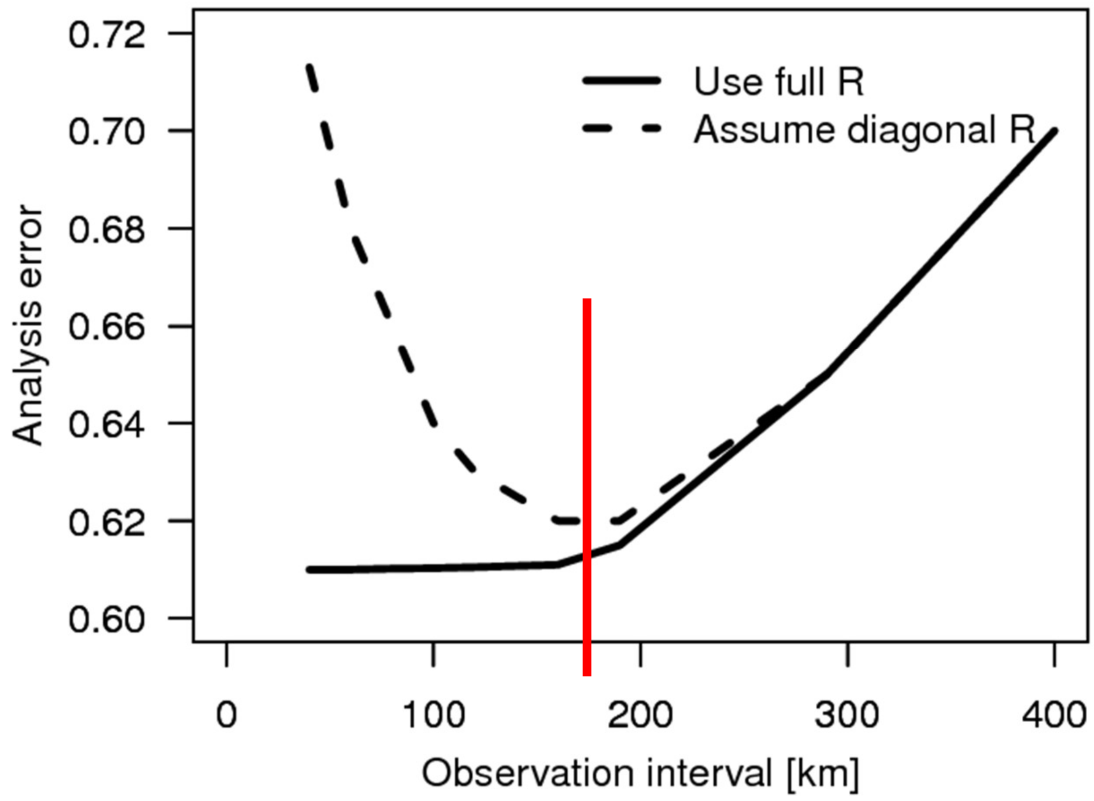
- Error inflation
  - use diagonal R with larger σ_O than diagnostics suggest.

- Take error correlations into account in the assimilation

Spatial error correlations and 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.

- **Practical solution: <u>Thinning,</u> ie select one observation within a "thinning box".**
- **Using fewer observations gives better results!**



Bias correction:

Systematic errors must be removed otherwise biases will propagate in to the analysis (causing **global damage** in the case of satellites!). A bias in the radiances is defined as:

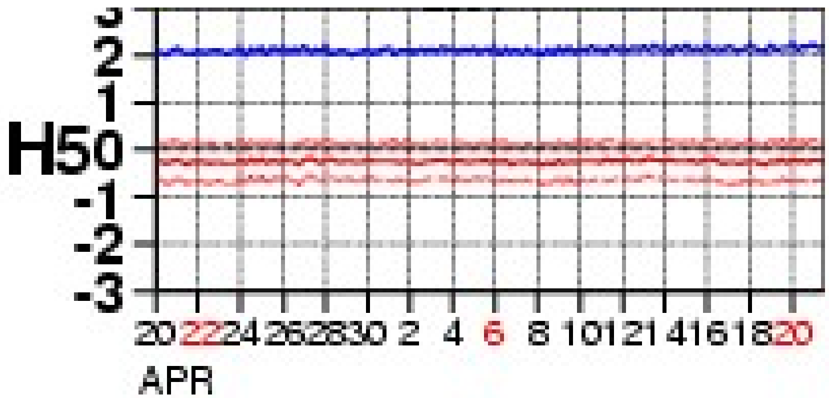
$$\textit{bias} = \textit{mean}\ [\ Y_{obs} - H(X_{true})\ ]$$

Sources of systematic error in radiance assimilation include:

- instrument error (scanning or calibration)
- radiative transfer error (spectroscopy or RT model)
- cloud / rain / aerosol screening errors

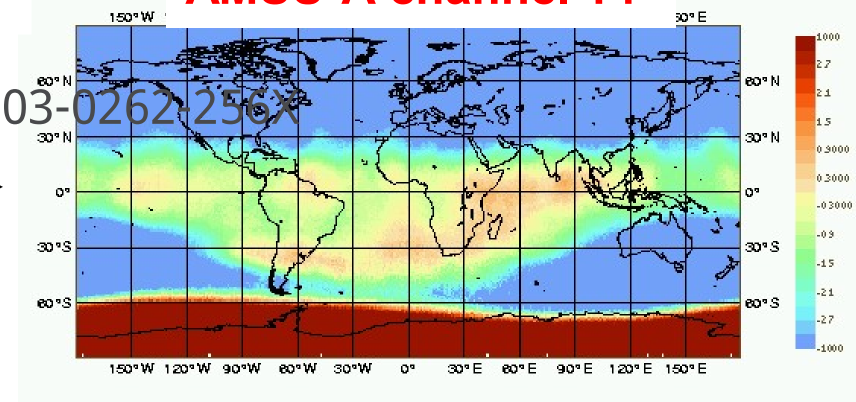
Bias correction:

HIRS channel 5



simple flat offset biases that are constant in time

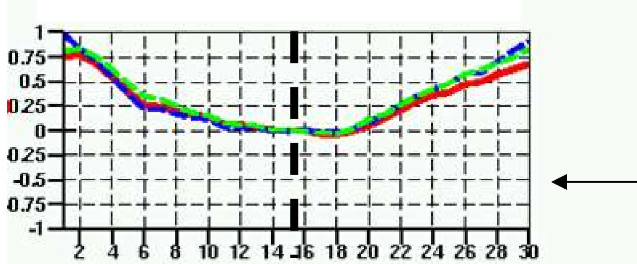
AMSU-A channel 14



https://orcid.org/0000-0003-0262-256X

biases that vary depending on location or air-mass

AMSU-A channel 7



limb

nadir

limb

biases that vary depending on the Scan position of the satellite instrument

Bias correction:

But sometimes **NWP systematic errors** can make it difficult to diagnose and correct observation biases

What we would like to quantify is:

$$\mathit{Bias} = \mathit{mean}\ [\ Y_{obs} - H(X_{true})\ ]$$

But in practice all we can monitor is :

$$\mathit{Bias} = \mathit{mean}\ [\ Y_{obs} - H(X_{b/a})\ ]$$

Data selection and quality control (QC):

The primary purpose of this is to ensure that the observations entering the analysis are consistent with the assumptions in the observations error covariance (**R**) and the observation operator (**H**).

Primary examples include the following:

- Rejecting bad data with **gross error** (not described by **R**)
- Rejecting data affected by **clouds** if **H** is a clear sky RT
- Thinning data if no **correlation** is assumed (in **R**)
- Always **blacklisting** data where we do not trust our QC!

Data selection and quality control (QC):

Often checks are performed using the forecast background as a reference. That is an observations is rejected if the departure from the background exceeds a threshold T_{QC}:

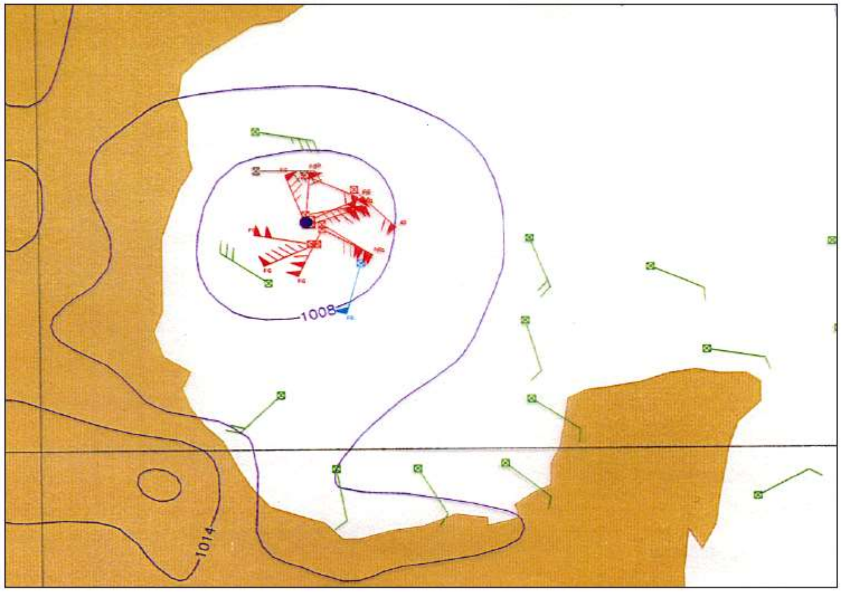
$$Y_{obs} - H(X_{true}) > T_{QC}$$

But sometimes large errors in the background can lead to:

- False rejection of a good observation
- Missed rejection of a bad observation

Data selection and quality control:

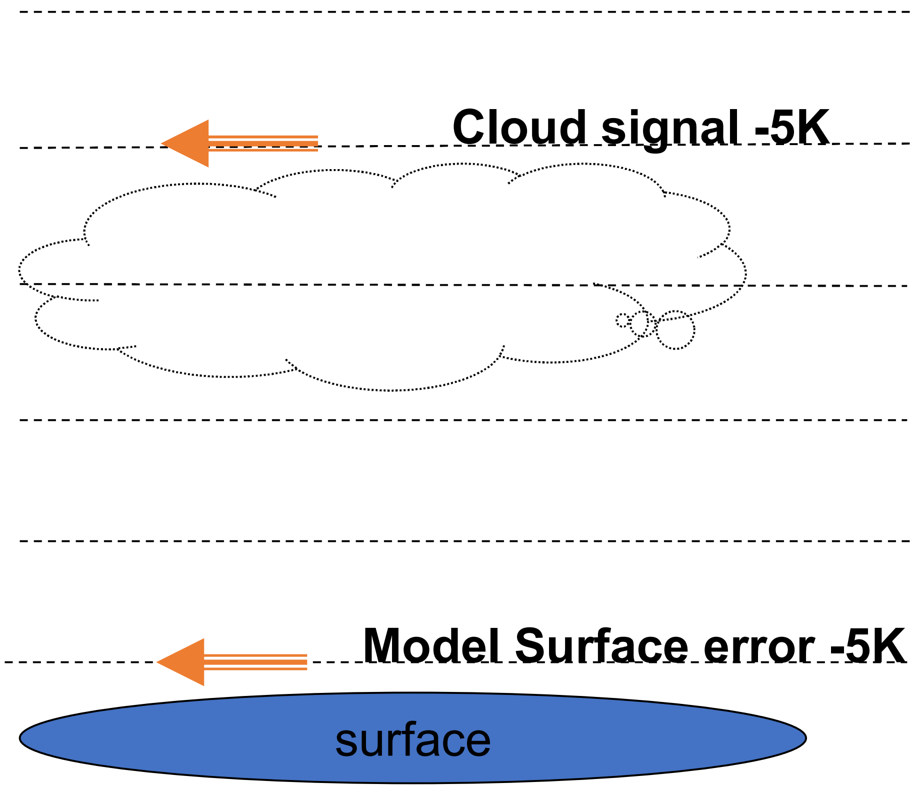
- False rejection of a **good** observation



The **numerous** failing observations are good, but a bad background is causing them to be rejected. We **need** these observations to improve the analysis !

Data selection and quality control:

- Missed rejection of a **bad** observation



The radiance are contaminated by cloud (**cold 5K**) compared to the clear sky value.

But our computation of the clear sky value from the background is also **cold by 5K** due to an error in the surface skin temperature.

Thus our checking (against the background) sees no reason to reject the observation and it is **passed**!

Summary

- observation operator

  (complex and expensive for radiances)
- background errors

  (important due to vertical resolution)
- observation errors

  (must be specified correctly)
- bias correction

  (global impact of small bias)
- data selection and quality control

  (false alarms and missed rejections)

Thanks