Observation quality control: methodology and applications

Pierre Gauthier
Department of Earth and Atmospheric Sciences
Université du Québec à Montréal (CANADA)

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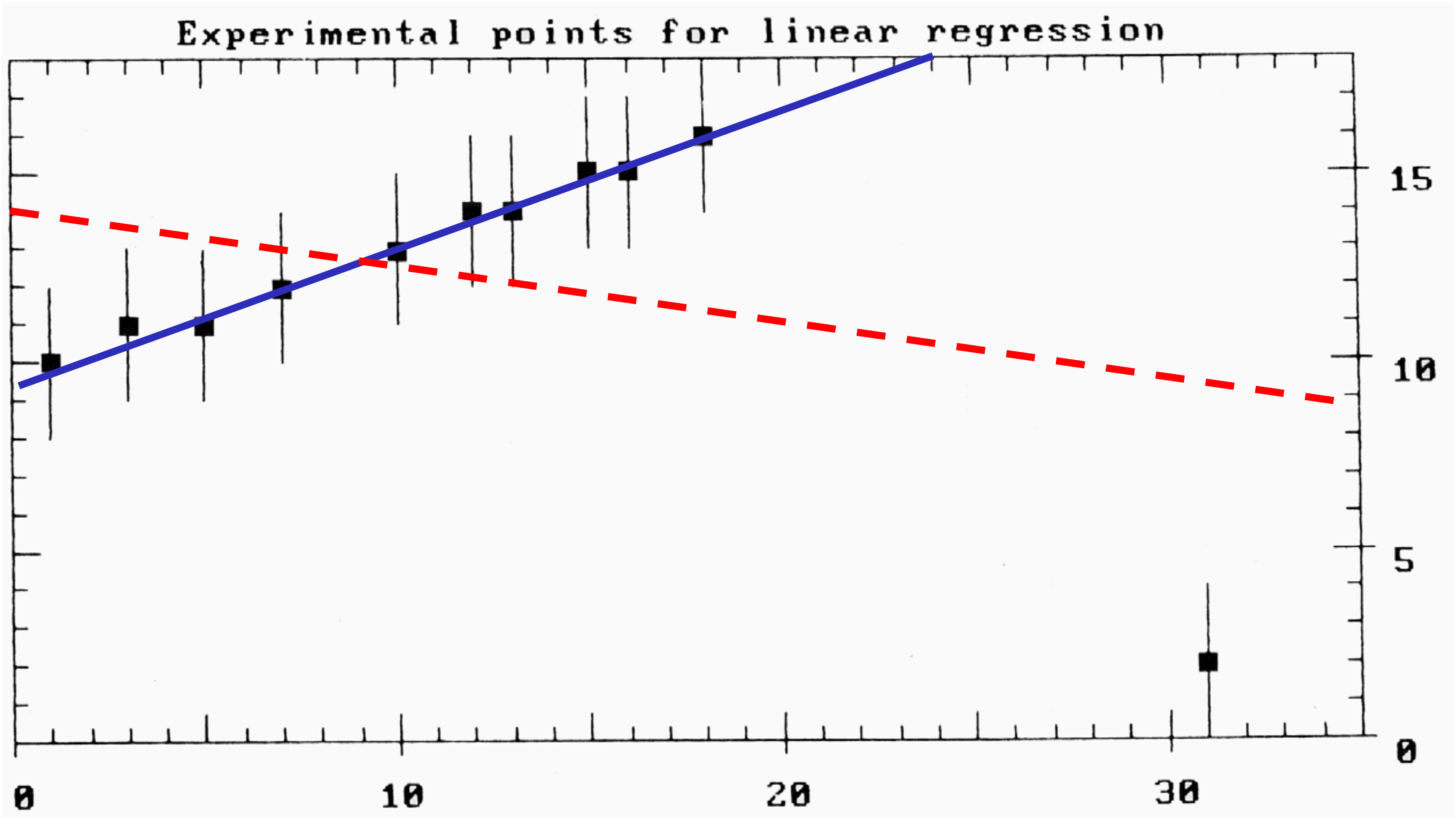
Introduction

- **Nature of data received and used at operational centres**
  * Wide variety of data that come from numerous sources
  * Many possible problems can corrupt the data
- **Incorrect data can have a significant impact on the assimilation**
- **Data acquisition and quality control**
  * Reception of the data
  * Check the quality of the data and reject data that have a high probabibility of being erroneous

Example: least-square fit involving an erroneous datum (from Tarantola, 2005)

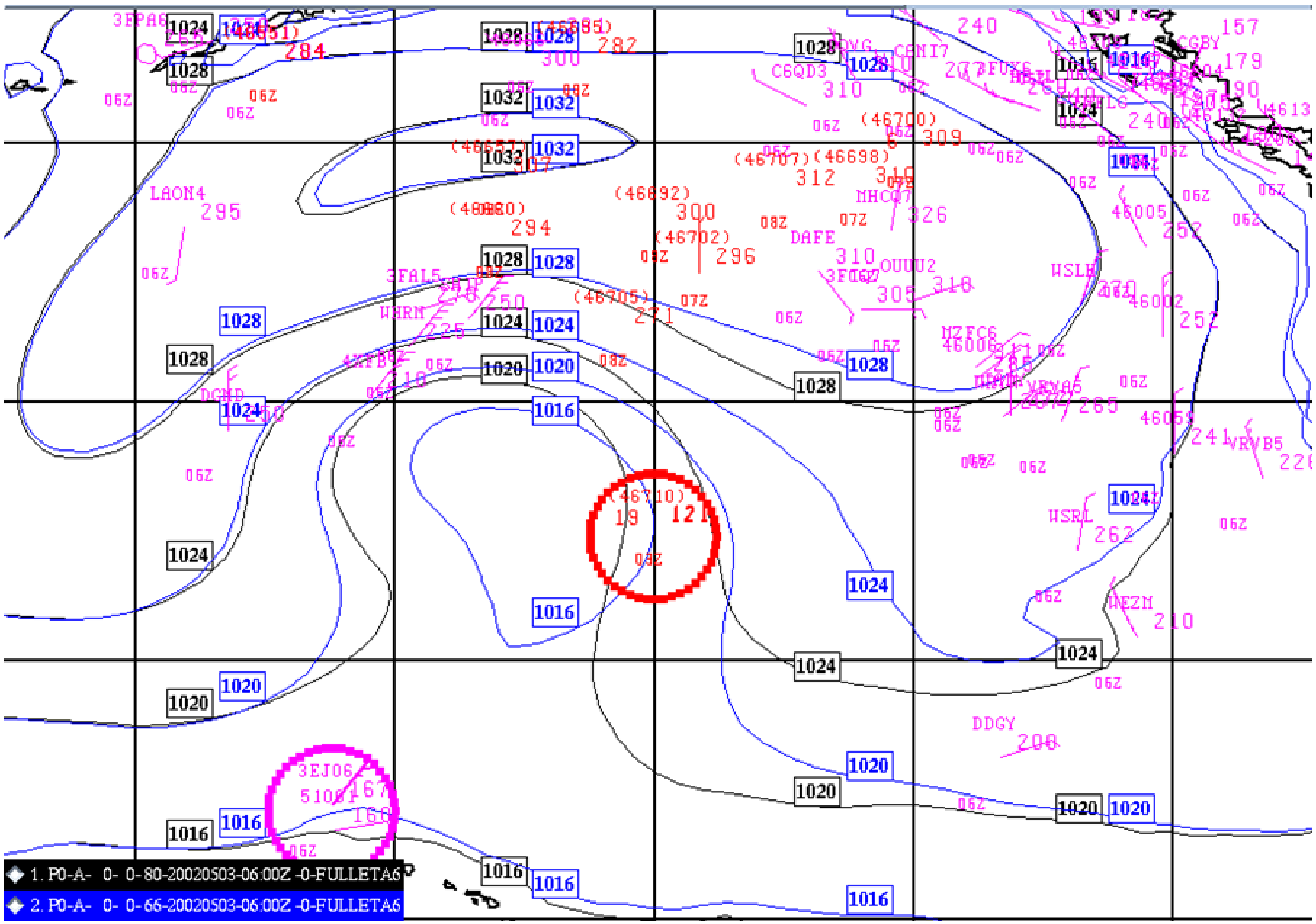
- **Least-square fit of data: y = ax + b**



Impact of an erroneous datum on the analysis

<u>Report from a drifting buoy</u>:p = 1012.1 hPa (10 hPa too low)

Analysis with QC in black **Analysis without QC in blue**



Quality Control

- **Sources of errors :**
  - * measurement errors inherent in the instruments
  - * error of representativeness
  - * improperly calibrated instruments
  - * incorrect registration of observations
  - * data coding errors
  - * data transmission errors

- **Goals :**
  - * reject all errors other than measurement errors
  - * associate predefined flags with each observation throughout its assimilation

Quality Control

- **Preliminary checks for individual reports :**
  - * at decoding stage, verification of observation source and location
  - * hydrostatic checks for temperatures and geopotential heights from upper air soundings
  - * check for limiting wind shear in wind profiles from upper air soundings
  - * verification of deviation from climatological values

Quality Control

Limit values for surface temperature								
	Winter				Summer			
Area	Min2	Min1	Max1	Max2	Min2	Min1	Max1	Max2
45°S - 45°N	-40°C	-30°C	+50°C	+55°C	-30°C	-20°C	+50°C	+60°C
45°N - 90°N 45°S - 90°S	-90°C	-80°C	+35°C	+40°C	-40°C	-30°C	+40°C	+50°C

Limit values for surface dew-point temperature								
	Winter				Summer			
Area	Min2	Min1	Max1	Max2	Min2	Min1	Max1	Max2
45°S - 45°N	-45°C	-35°C	+35°C	+40°C	-35°C	-25°C	+35°C	+40°C
45°N - 90°N 45°S - 90°S	-99°C	-85°C	+30°C	+35°C	-45°C	-35°C	+35°C	+40°C

Notations

Model state

$\mathbf{x}$:	model state comprising 3D and surface atmospheric fields (N= NV3D x NLEVELS x NI x NJ ~ 10^8)
$\mathbf{x}_b$:	background state (*a priori* estimate of the state of the atmosphere)
$\mathbf{x}_t$:	true (unknown state) of the atmosphere
$\varepsilon_b = \mathbf{x}_b - \mathbf{x}_t$:	background error

Observations

$\mathbf{y}$:	observation vector ($M \sim 10^6$)
$\mathbf{y}_t$:	true observations
$\varepsilon_o = \mathbf{y} - \mathbf{y}_t$:	observation error

Notations

Observation operator

H: observation operator producing a model equivalent of all observations ($R^N \rightarrow R^M$)

H = ($\partial H/\partial \mathbf{x}$) : Jacobian of the observation operator (linear operator associated with an (MxN) matrix)

Error statistics

R: observation error covariance matrix (MxM)
(diag **R** = σ_o^2 observation error variances)

B: background error covariances

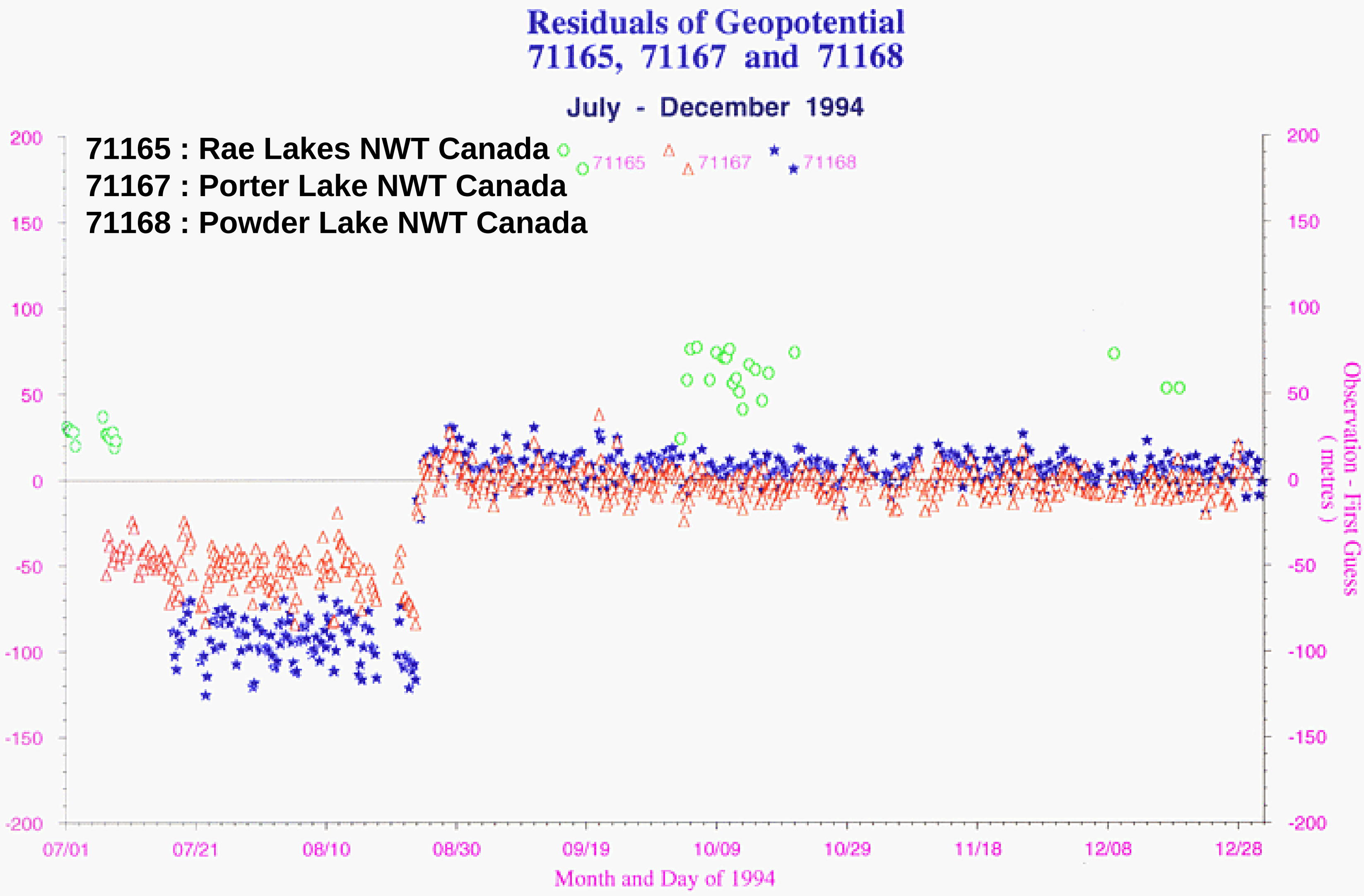
(diag **B** = σ_b^2 background error variances)

HBH^T: image in observation space of the background error covariances

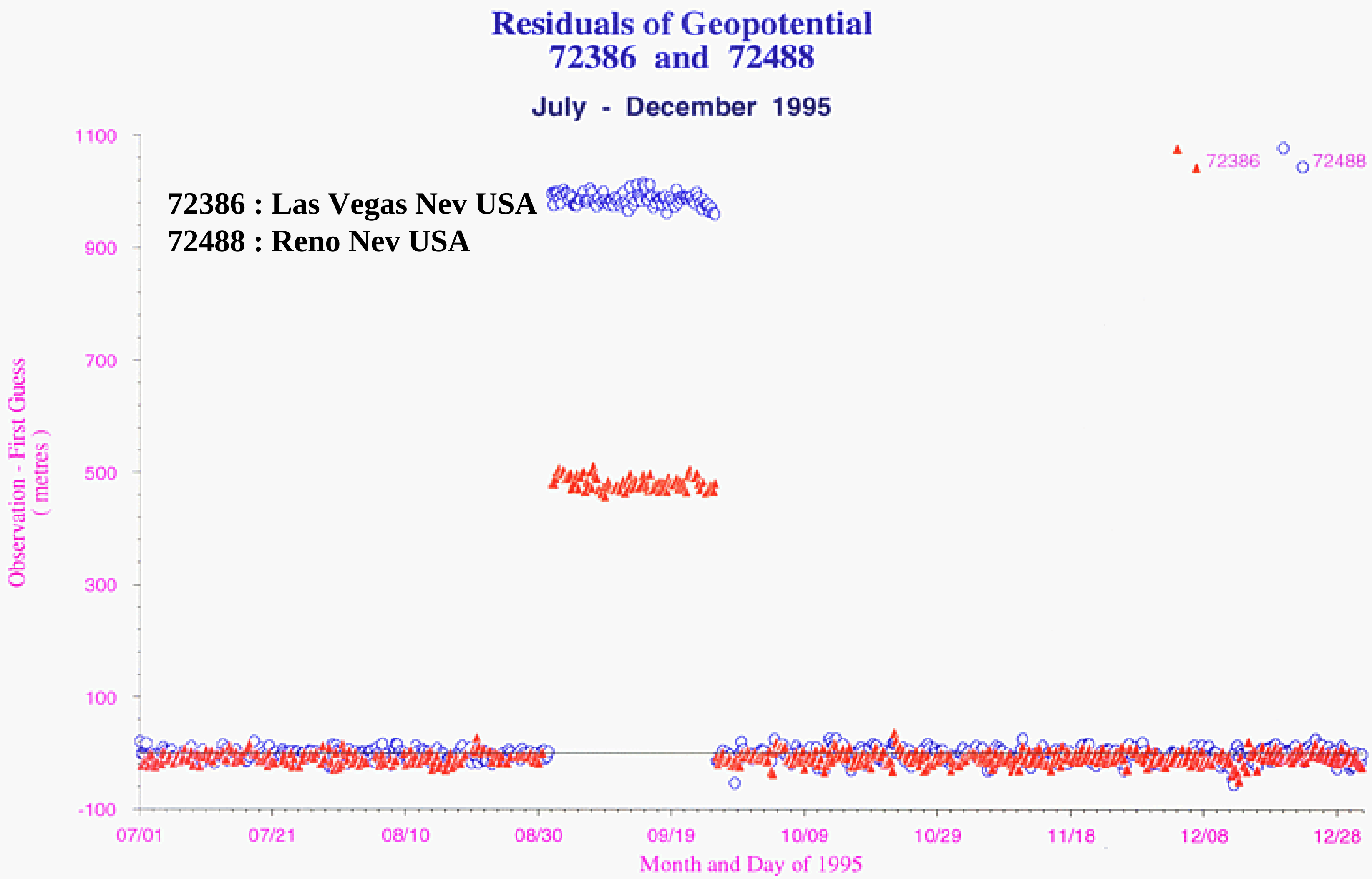
Information contained in innovations

- **Innovation vector:** $\mathbf{d} = \mathbf{y} - H\left(\mathbf{x}_b\right)$
  - short-term forecast (background) contains information gained from past observations
  - Comparison of observations against the background which is our *a priori* knowledge of the state of the atmosphere
  - Offers a common ground against which it is possible to compare all observations

- **Monitoring of observations**
  - innovations are represented by observation types and averaged over a large number of data, binned according to different categories
  - Allows to detect systematic problems with observations



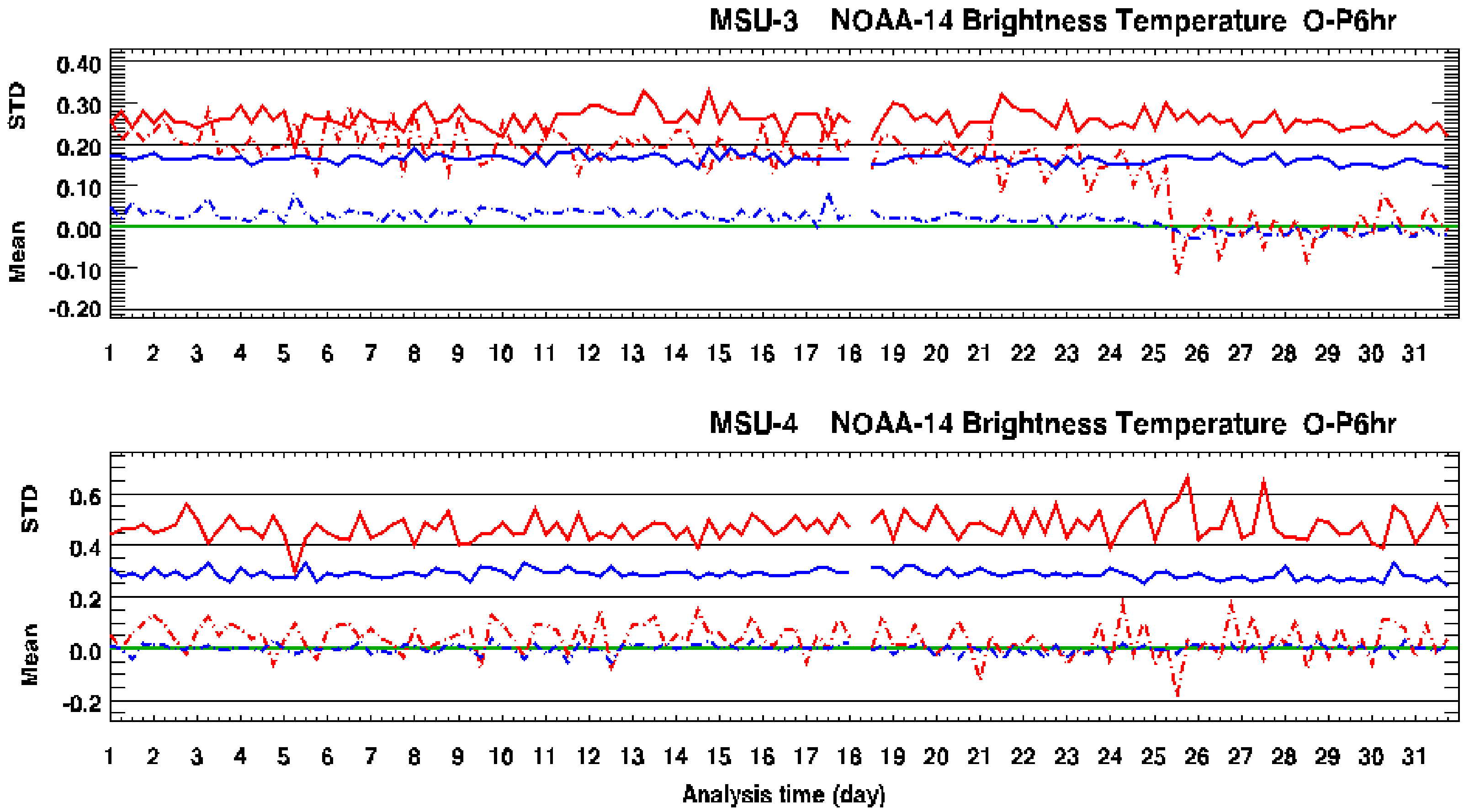
wrongly assigned station elevation



wrongly assigned station pressure

Monitoring and quality control

Statistics based on innovations ($y - HX_b$): example from TOVS radiances



Monitoring Web Site of the Canadian Meteorological Centre (CMC)

http://collaboration.cmc.ec.gc.ca/cmc/data_monitoring/

User:	**monitoring**
Password:	**CMC**
	with CMC in *uppercase.*

Verification against the background state

- **Observation departure from $\mathbf{x}_b$:** $\mathbf{d} = \mathbf{y} - \mathbf{H}(\mathbf{x}_b)$

$$\mathbf{y} - \mathbf{H}(\mathbf{x}_b) = \mathbf{y}_t + \varepsilon_o - H(\mathbf{x}_t + \varepsilon_b) \cong (\mathbf{y}_t - H(\mathbf{x}_t)) + \varepsilon_o - \mathbf{H}'\varepsilon_b$$

$$= \varepsilon_o - \mathbf{H}'\varepsilon_b$$

$$\left\langle (\varepsilon_o - \mathbf{H}'\varepsilon_b)(\varepsilon_o - \mathbf{H}'\varepsilon_b)^T \right\rangle = \mathbf{R} + \mathbf{H}'\mathbf{B}\mathbf{H}'^T$$

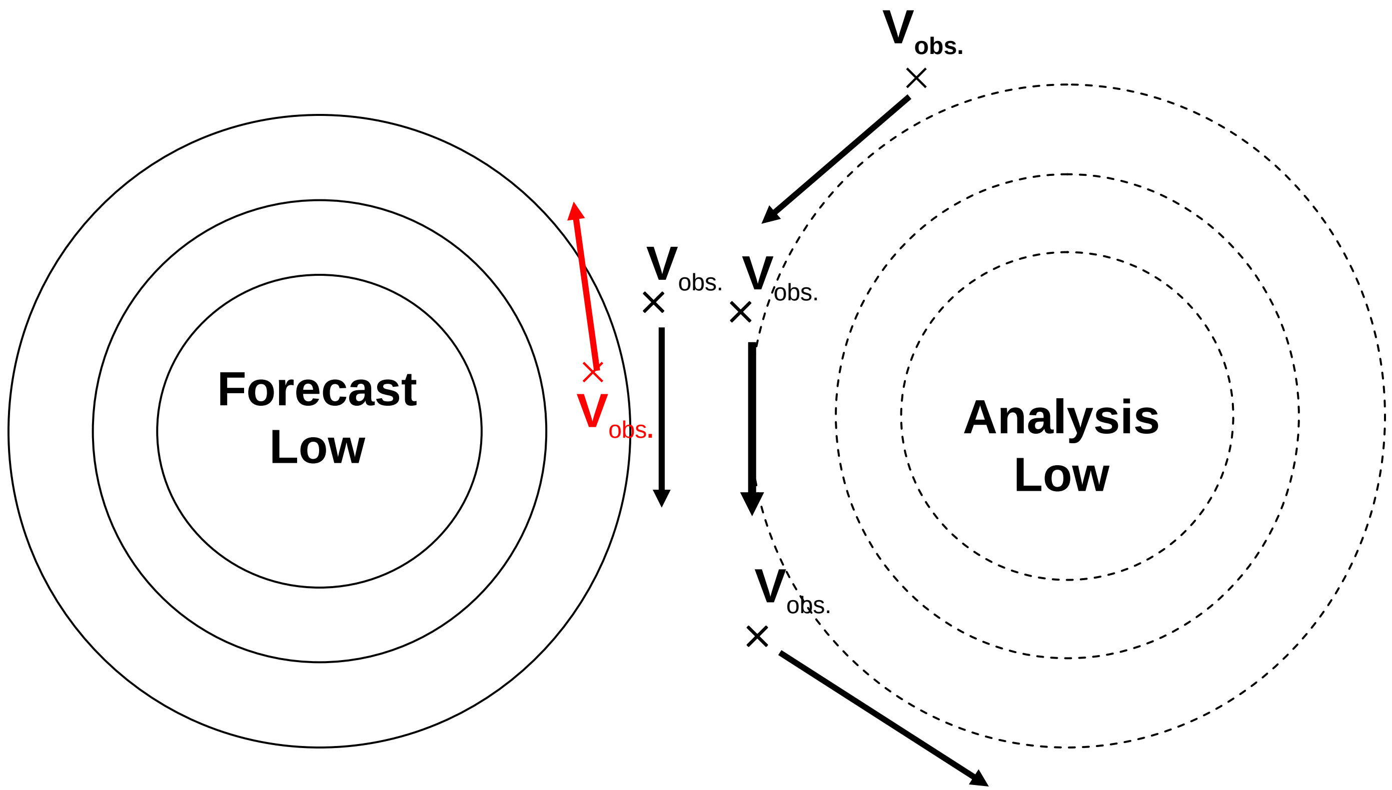
- For a single observation: $(y - H(\mathbf{X}_b))^2 \cong \sigma_o^2 + \sigma_b^2$
- Need to compute $\mathbf{H}'\mathbf{B}\mathbf{H}'^T$ which can be done by a randomization method

- Observation is rejected if

$$\hat{y} = y - H\mathbf{x}_b \geq \lambda(\sigma_o^2 + \sigma_b^2)^{1/2}$$

with λ being large enough.

Difficulties that arise with the background-check procedure



Quality control based on local analyses

- **Consider a set of *k* observations y_1, ..., y_k**

- **Probability of $y_1 = y_t$ assuming that all the other observations are true**

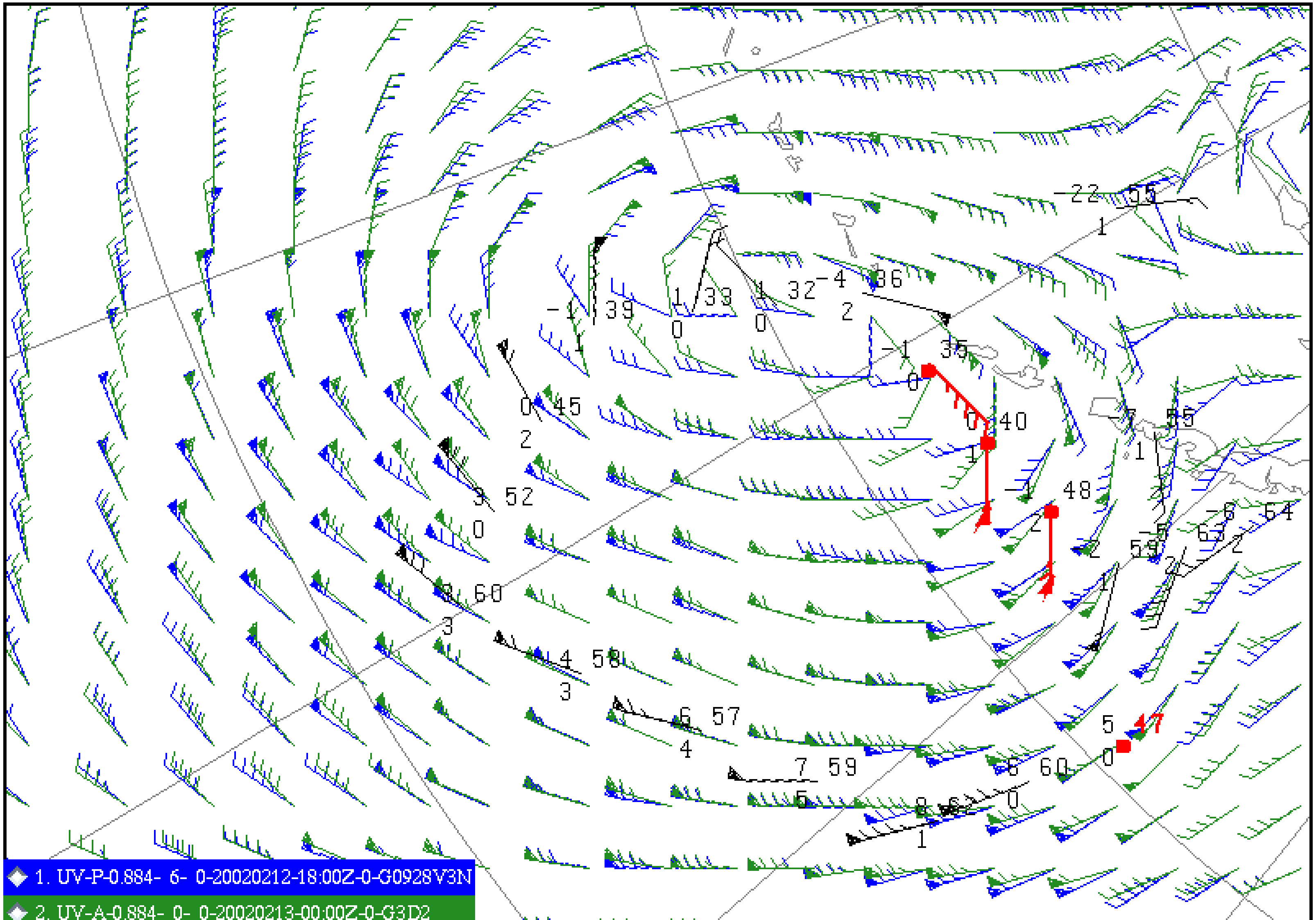
- **Analysis is made using all observations but y_1 and then comparing y_1 against the resulting analysis**

$$\left(y - H(\mathbf{x}_a^{(k-1)})\right)^2 = \sigma_o^2 + \sigma_a^2$$

$$\hat{y} = y - H\mathbf{x}_a^{(k-1)} \geq \lambda(\sigma_o^2 + \sigma_a^2)^{1/2}$$

- **To avoid contamination by erroneous data, the procedure is repeated until no more data are being rejected**

Dropsonde data rejected by Bgnd Check



Bayesian approach to inverse problems

Joint probability distribution function (pdf): p(**x**,**y**)

– Associated marginal probability densities

$$P(\mathbf{x}) = \int p(\mathbf{x},\mathbf{y})d\mathbf{y}, \quad P(\mathbf{y}) = \int p(\mathbf{x},\mathbf{y})d\mathbf{x}$$

* *A priori* pdf P(**x**): probability of $\mathbf{x}=\mathbf{x}_t$

* Example: the Gaussian case in which we know the error covariance and we have $\mathbf{x}_b$ as the only realization of **x**.

$$P(\mathbf{x}) = \frac{1}{C}\exp\left\{-\tfrac{1}{2}(\mathbf{x}-\mathbf{x}_b)^T\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}_b)\right\}$$

x in normally distributed with mean $\mathbf{x}_b$ and covariance **B**

In absence of any other information, $\mathbf{x} = \mathbf{x}_b$ is the most probable state

Similarly, for P(y), if y_o stands for the actual observation,

P(**y**) : probability of **y** = $\mathbf{y}_t$

Estimate of the mean : **y** = $\mathbf{y}_o$

Gaussian case :

$$P(\mathbf{y}) = \frac{1}{C_2} \exp\left\{-\tfrac{1}{2}(\mathbf{y}-\mathbf{y}_o)^T \mathbf{R}^{-1}(\mathbf{y}-\mathbf{y}_o)\right\}$$

* Normally distributed with mean $\mathbf{y}_o$ and covariance **R**

Bayes' Theorem

Conditional probability distribution

Probability of having **y** given that **x** = $\mathbf{x}_t$

$$p(\mathbf{y} \mid \mathbf{x} = \mathbf{x}_t) = \frac{p(\mathbf{x}_t, \mathbf{y})}{\int p(\mathbf{x}_t, y) d\mathbf{y}} \equiv \frac{p(\mathbf{x}_t, \mathbf{y})}{P(\mathbf{x}_t)}$$

Probability of having **x** given that **y** = $\mathbf{y}_o$

$$p(\mathbf{x} \mid \mathbf{y} = \mathbf{y}_o) = \frac{p(\mathbf{x}, \mathbf{y}_o)}{\int p(\mathbf{x}, \mathbf{y}_o) d\mathbf{x}} \equiv \frac{p(\mathbf{x}, \mathbf{y}_o)}{P(\mathbf{y}_o)}$$

Thus, $p(\mathbf{x}_t, \mathbf{y}_0) = p(\mathbf{x}_t \mid \mathbf{y}_0) P(\mathbf{y}_0) = p(\mathbf{y}_0 \mid \mathbf{x}_t) P(\mathbf{x}_t)$

Bayes' Theorem: $p(\mathbf{x} \mid \mathbf{y} = \mathbf{y}_o) = \dfrac{p(\mathbf{y} \mid \mathbf{x} = \mathbf{x}_t) P(\mathbf{x} = \mathbf{x}_t)}{P(\mathbf{y} = \mathbf{y}_o)}$

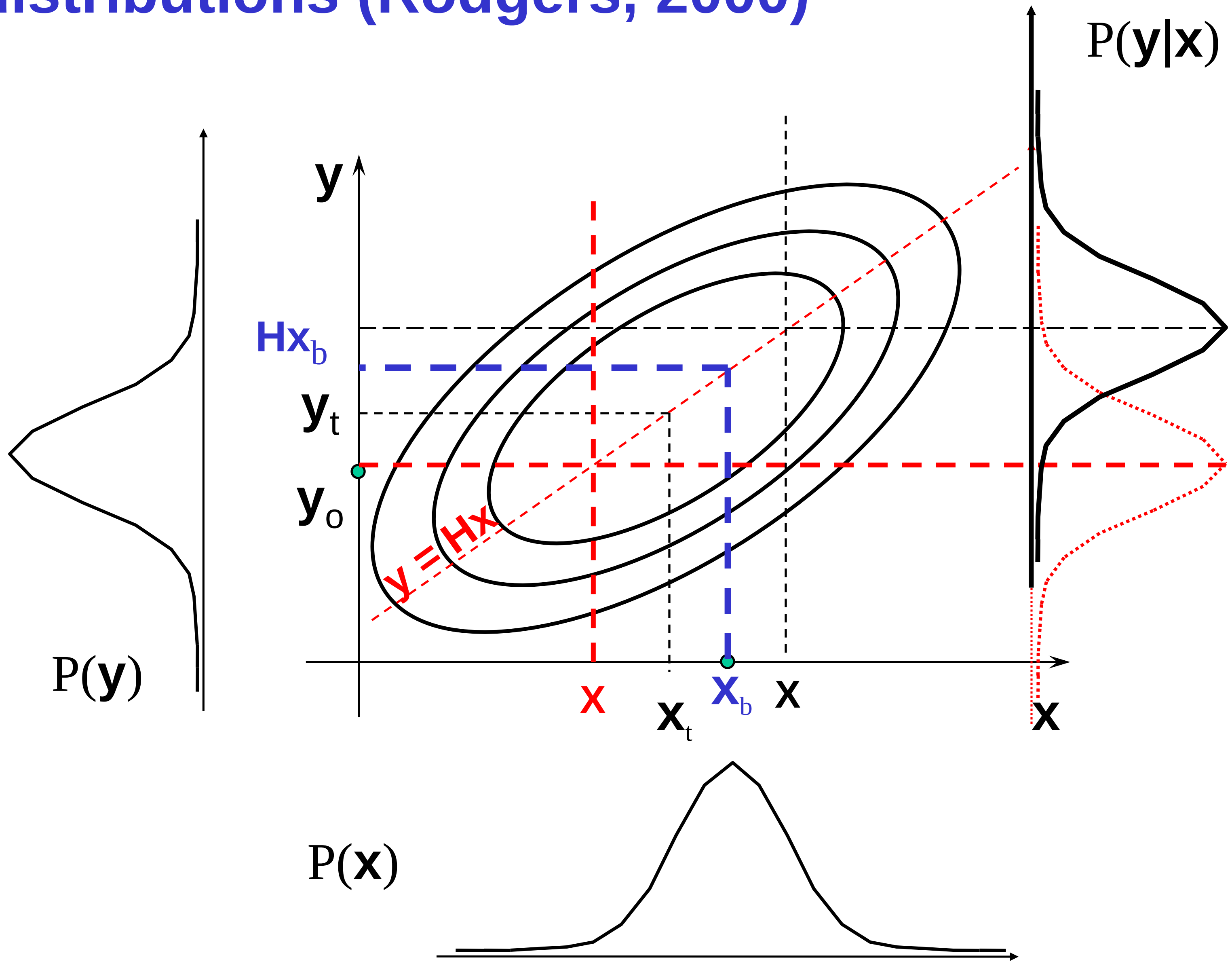
Conditional probability

- **p(x|y): probability that x= x_t given that y = y_o has been observed**
  - A posteriori probability distribution associated with that of the analysis error
- **p(y|x=x_t): probability of y given that x is the true value**
  - **Hx**: estimate of the mean value of **y**.

    $\rightarrow$ If $\mathbf{x} = \mathbf{x}_t$, then $\mathbf{Hx}_t = \mathbf{y}_t$.
  - ($\mathbf{y}$ - $\mathbf{Hx}$) = $\mathbf{y}_t + \varepsilon_o - \mathbf{Hx}_t = \varepsilon_o$
  - (**y** - **Hx**) is normally distributed with zero mean and covariance **R**

$$p(\mathbf{y}|\mathbf{x}) = \frac{1}{C_3}\exp\left\{-\frac{1}{2}(\mathbf{y}-\mathbf{Hx})^T\mathbf{R}^{-1}(\mathbf{y}-\mathbf{Hx})\right\}$$

Representation of the associated probability distributions (Rodgers, 2000)



Mode: $$\frac{d}{dx}\left(-\ln p\right) = -\frac{1}{p}\frac{dp}{dx} = 0 \quad \Rightarrow \quad \frac{dp}{dx} = 0$$

From Bayes' theorem:

$$p(x \mid y) = C\,\frac{\exp\left\{-\tfrac{1}{2}\left(\mathbf{y}-\mathbf{Hx}\right)^T\mathbf{R}^{-1}\left(\mathbf{y}-\mathbf{Hx}\right)\right\}\exp\left\{-\tfrac{1}{2}(\mathbf{x}-\mathbf{x}_b)^T\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}_b)\right\}}{\exp\left\{-\tfrac{1}{2}\left(\mathbf{y}-\mathbf{y}_o\right)^T\mathbf{R}^{-1}\left(\mathbf{y}-\mathbf{y}_o\right)\right\}}$$

$$-\ln p(\mathbf{x}|\mathbf{y}) = J(\mathbf{x})$$

$$= \frac{1}{2}\left(\mathbf{x}-\mathbf{x}_b\right)^T\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}_b)^T + \frac{1}{2}(\mathbf{Hx}-\mathbf{y})^T\mathbf{R}^{-1}(\mathbf{Hx}-\mathbf{y}) + C$$

- **In the case of Gaussian error statistics, the maximum likelihood and the minimum variance estimate coincide.**

- **Formulation includes the case where H(x) is nonlinear.**

References

Rodgers, R.D., 2000: *Inverse Methods for Atmospheric Sounding: theory and practice*. World Scientific Series On Atmospheric and Planetary Physics, vol.2, 238 pages.

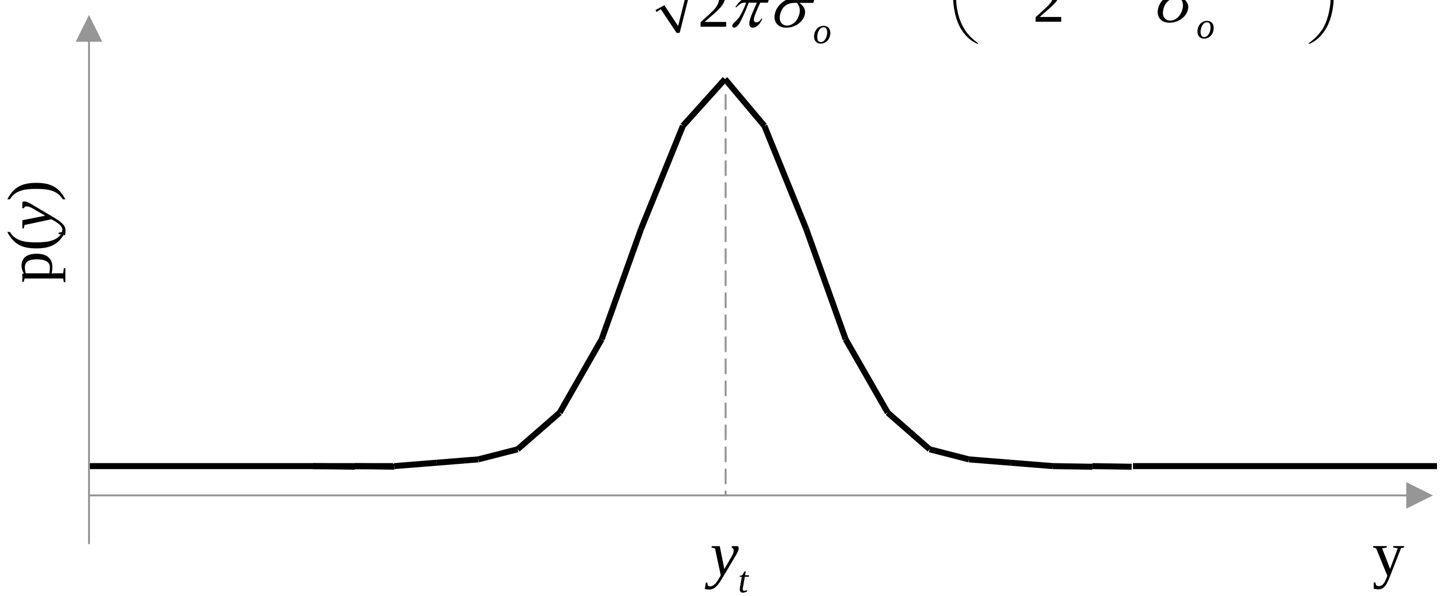
Tarantola, A., 2005: *Inverse problem theory and methods for model parameter.* SIAM, Philadelphia, USA, 342 pages.

Variational Quality Control (QC-Var)

- **Dharssi *et al.* (1992), Ingleby and Lorenc (1993), Andersson and Järvinen (1999)**
- **Probability of having a gross error**

* consider that $y_t - D/2 \le y \le y_t + D/2$

$$p(y) = P/D + \frac{(1-P)}{\sqrt{2\pi}\sigma_o} \exp\left(-\frac{1}{2} \frac{(y-y_t)^2}{\sigma_o^2} \right)$$



QC-Var

Definition of the cost function

$$J_o^{QC}(\mathbf{x}) \equiv J_o^{QC}(\hat{y}(\mathbf{x})) = -\ln p(y_o \mid H(\mathbf{x}))$$

where

$$= -\ln\left(P/D + C\exp\left(-J^N(\hat{y})\right)\right)$$

$$J^N(\hat{y}(\mathbf{x})) = \frac{1}{2}\hat{y}^T\mathbf{R}^{-1}\hat{y} \equiv \frac{1}{2}\frac{(H(\mathbf{x}) - y_o)^2}{\sigma_o^2}$$

Gradient of the QC-Var cost function

$$\nabla_{\hat{y}} J_o(\mathbf{x}) = \frac{\exp(-J^N)}{\gamma + \exp(-J^N)} \nabla_{\hat{y}} J^N(\hat{y}) \equiv W_{QC} \nabla_{\hat{y}} J_o^N(\hat{y})$$

$$= W_{QC} \frac{(H(\mathbf{x}) - y_o)}{\sigma_o^2}$$

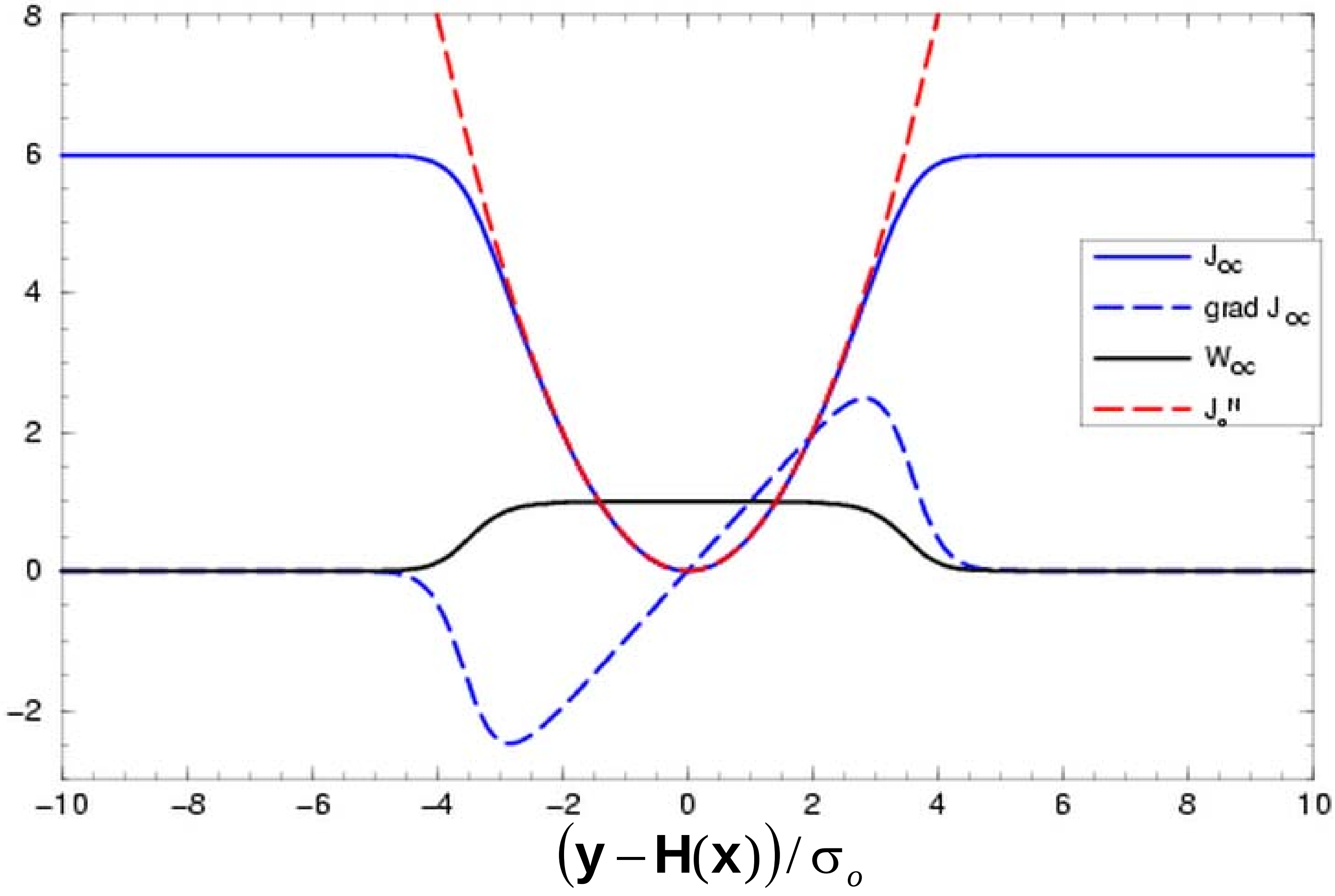
$$\nabla_{\mathbf{x}} J_o(\mathbf{x}) = \left[\frac{\partial H}{\partial \mathbf{x}}(\mathbf{x}) \right]^* W_{QC} \frac{(H(\mathbf{x}) - y_o)}{\sigma_o^2}$$

where $\gamma = (P\sigma_o \sqrt{2\pi}) / (1 - P) D$

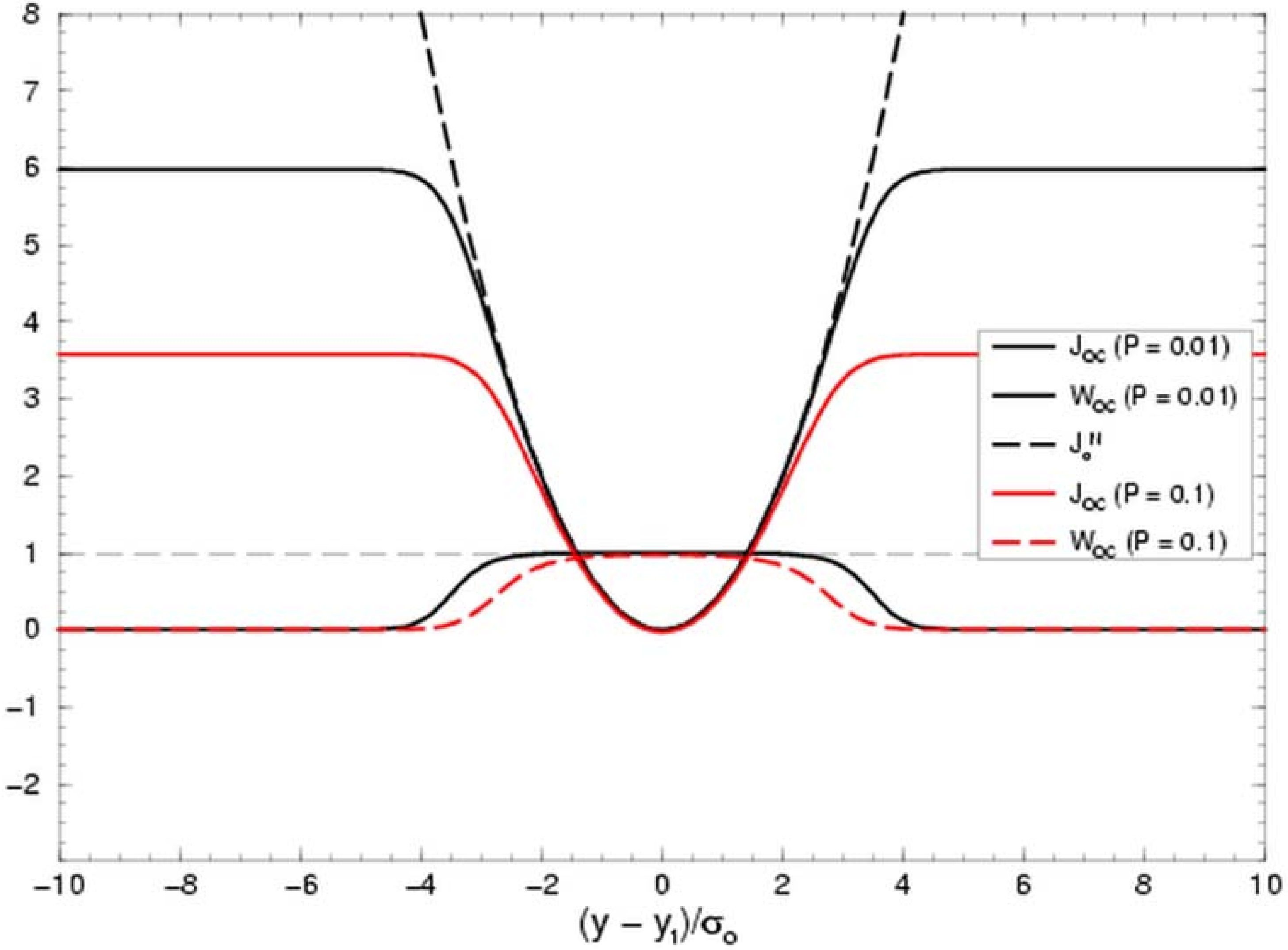
W_{QC} **depends on the current estimate of the state.**

- ***A posteriori weights*** **are then based on the departure from the analysis**

Representation of the QC-Var cost function (P = 0.01)



QC-Var cost function with different probabilities of gross errors (P = 0.01 and 0.1)



Observation - Forecast $(y - H(x_b))$

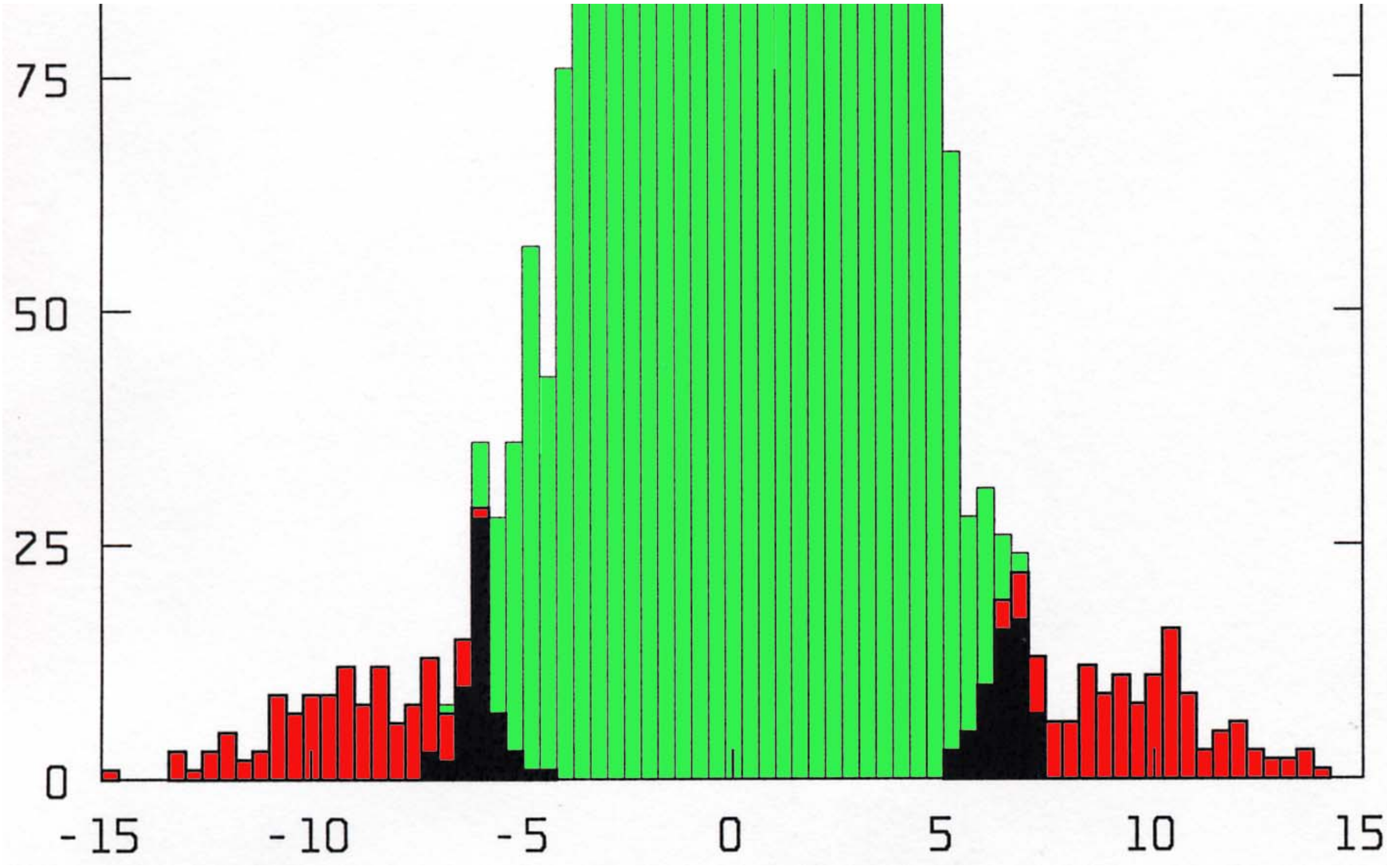
AIREP temperatures Period: March-April 2002

Rejected by background check (303)

Rejected by QC-Var (103)

Accepted (31,926)

Total Number of data **32239**



Estimation of the probability of gross error

Distribution of innovations

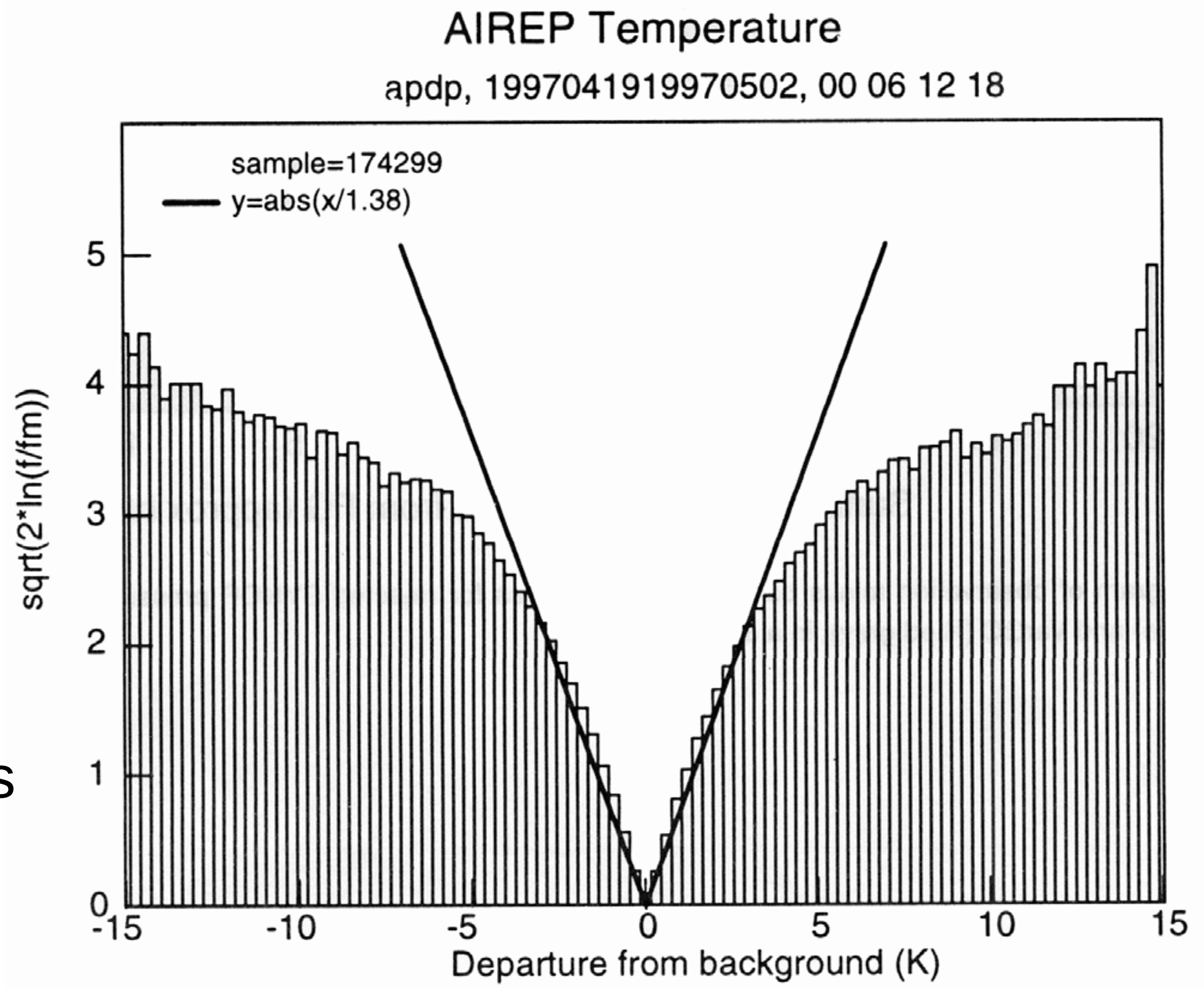
Gaussian:

$$-\ln p(\hat{y}) = \frac{\hat{y}^2}{2\sigma_o^2} + C$$

$$\sqrt{-2\ln p(\hat{y})} = \frac{\hat{y}}{\sigma_o}$$

Probability of gross error is obtained in the limit where

$$|\hat{y}| >> \sigma_o$$



(from Järvinen and Andersson, 1999)

Comparison of the two QC procedures

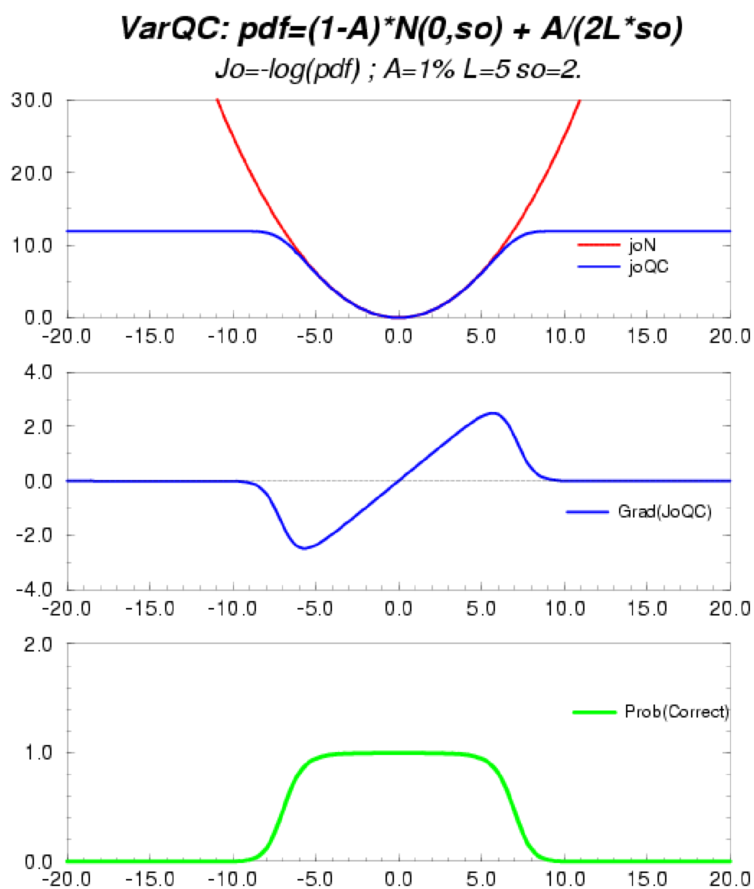
Obs. Type	Obs. Quantity	Rejection Ratio (%)		Approximate Rejection Limits	
		VarQC	OIQC	VarQC	OIQC
SYNOP	Pressure (height)	2.7	1.9	3.6 hPa	n/a
	$(T-T_d)$	0.3	0.0	8.5 K	22 K
	Temperature	2.2	1.2	6.6 K	16.6 K
SHIP	Wind	7.6	0.5	8 m/s	19 m/s
	Pressure (height)	2.3	3.5	8.5 hPa	n/a
	$(T-T_d)$	0.3	0.0	9.5 K	26 K
	Temperature	1.5	0.9	5.7 K	11.7 K
DRIBU	Pressure (height)	2.8	3.1	6.6 hPa	n/a
	Temperature	3.1	2.4	5.8 K	6.2 K
TEMP	Wind	2.7	0.4	8 - 14 m/s	11 - 20 m/s
	$(T-T_d)$	1.8	0.0	5 - 16 K	14 - 22 K
	Temperature	3.0	1.3	2.1 - 6.6 K	3.4 - 9.4 K

Obs. Type	Obs. Quantity	Rejection Ratio (%)		Approximate Rejection Limits	
		VarQC	OIQC	VarQC	OIQC
AMDAR	Wind Temperature	1.0 0.7	0.4 0.5	11 m/s 4.0 K	15 m/s 5.0 K
SATOB	Wind	1.3	0.2	13 - 27 m/s	16 - 36 m/s
AIREP	Wind	5.2	1.0	13 m/s	29 m/s
	Temperature	1.7	0.8	5.7 K	9.2 K
ACARS	Wind	2.3	1.0	10 m/s	14 m/s
	Temperature	1.6	2.1	4.0 K	5.0 K

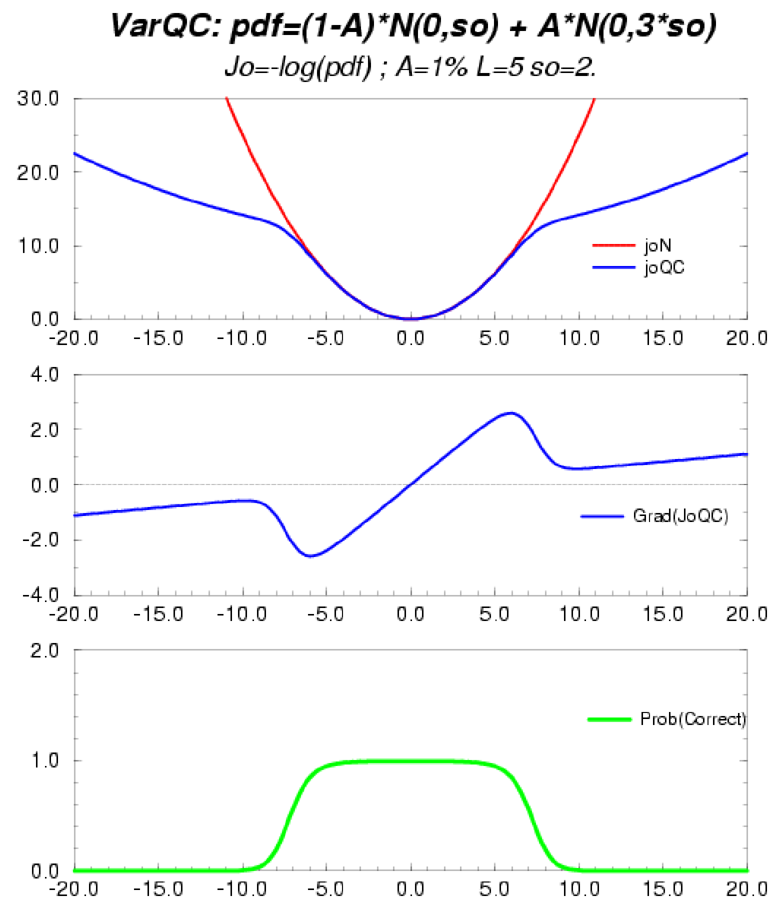
Comments

- **When observation error is uncorrelated:**
  - QC-Var is easy to implement and computationally inexpensive
  - A number of iterations need to be done *without* the W_{QC} to correct main deficiencies that may exist in the background state (assuming the bulk of the observations to be good ones)
- **Procedure aims at detecting punctual observations that may be in error**
- **Complexities arise when observation errors are correlated but they can be addressed (Järvinen *et al.*,1999)**

Gaussian + flat PDF



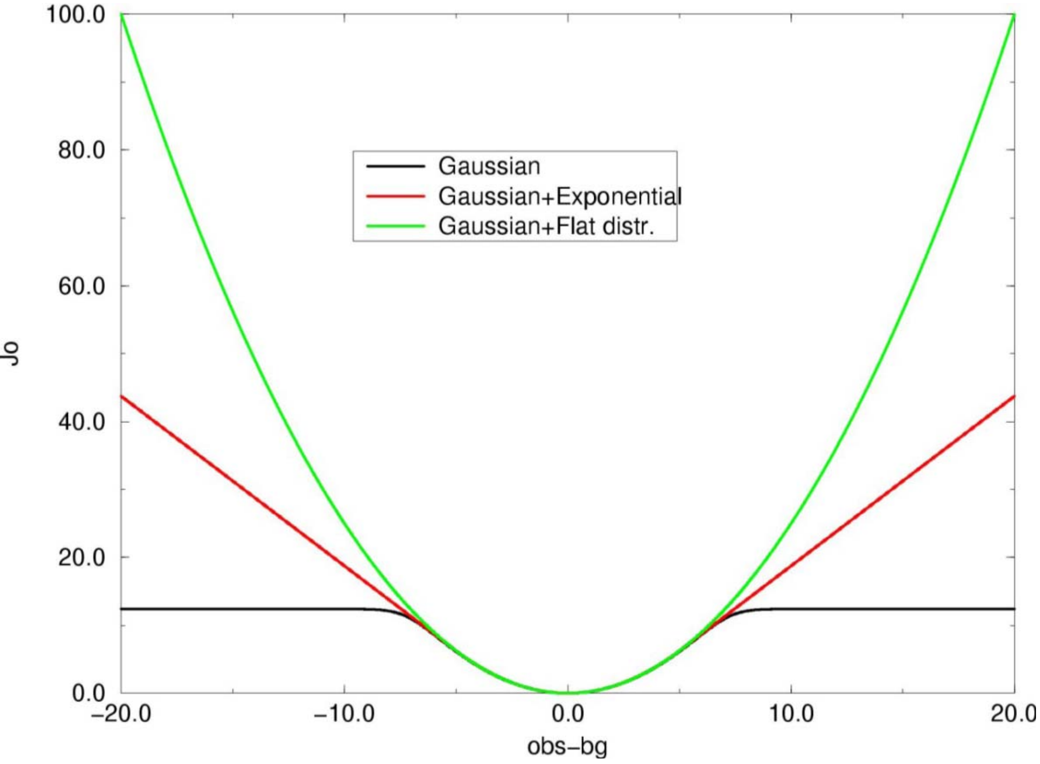
Sum of 2 Gaussians



(Isaksen, 2010 ECMWF)

Recent developments in variational quality control

(Isaksen, L., 2010: presentation at the ECMWF training course)



Huber norm

- * Adds some weight on observations with large departures
- * A set of observations with consistent large departures will influence the analysis

(Isaksen, 2010 ECMWF)

Definition of the pdf associated with the Huber norm

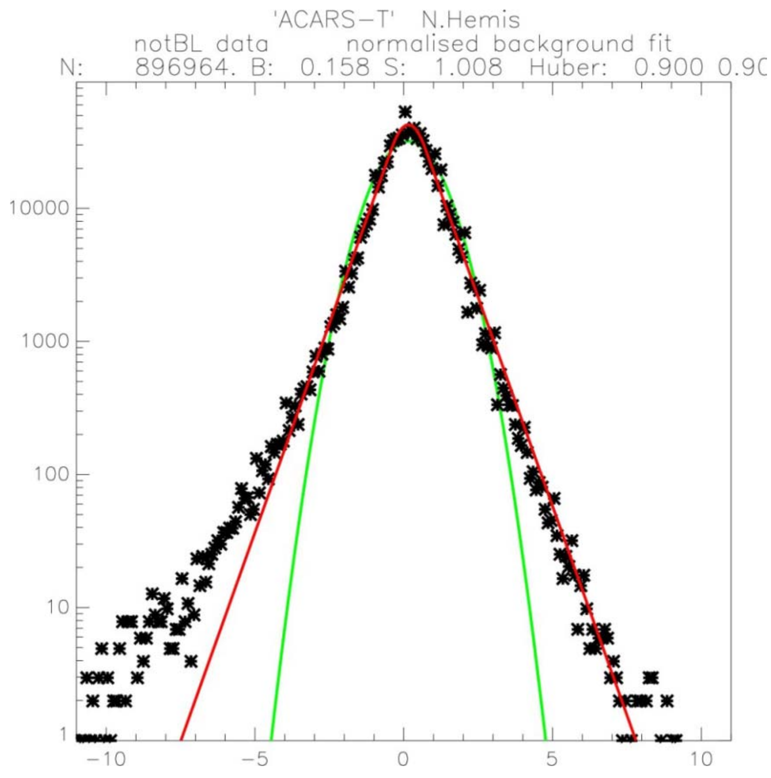
$$p(y\,|\,x)=\begin{cases}\dfrac{1}{\sigma_o\sqrt{2\pi}}\exp\left(\dfrac{a^2}{2}-|\,ad\,|\right) & if\ a<d\\[2ex] \dfrac{1}{\sigma_o\sqrt{2\pi}}\exp\left(-\dfrac{1}{2}d^2\right) & if\ a\le d\le b\\[2ex] \dfrac{1}{\sigma_o\sqrt{2\pi}}\exp\left(\dfrac{b^2}{2}-|\,bd\,|\right) & if\ d>b\end{cases}$$

with

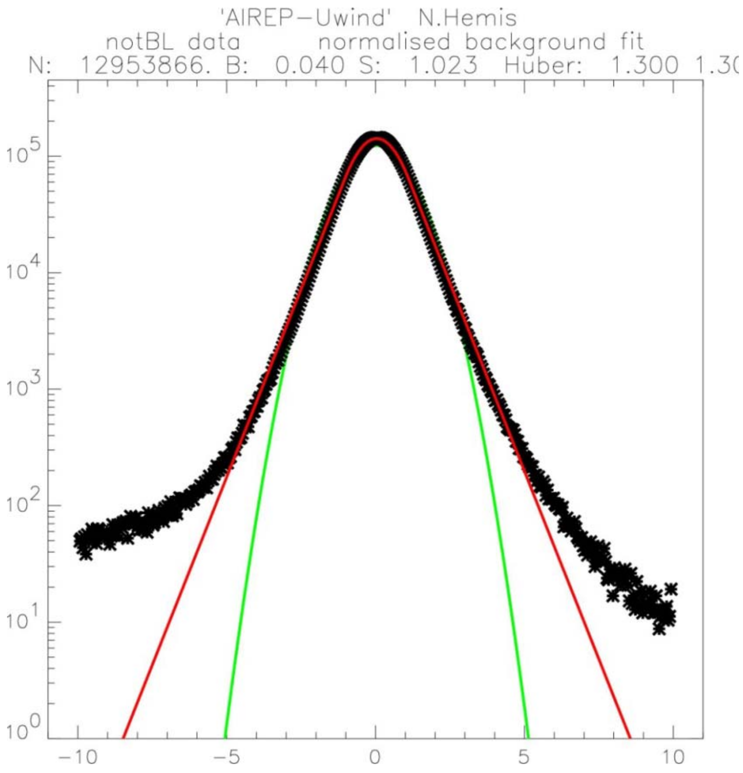
$$d=\frac{y-H(\mathbf{x})}{\sigma_o}$$

Aircraft temperature and winds Northern Hemisphere

Huber norm distributed with some deviation for cold departures



Normalized departures



Normalized departures

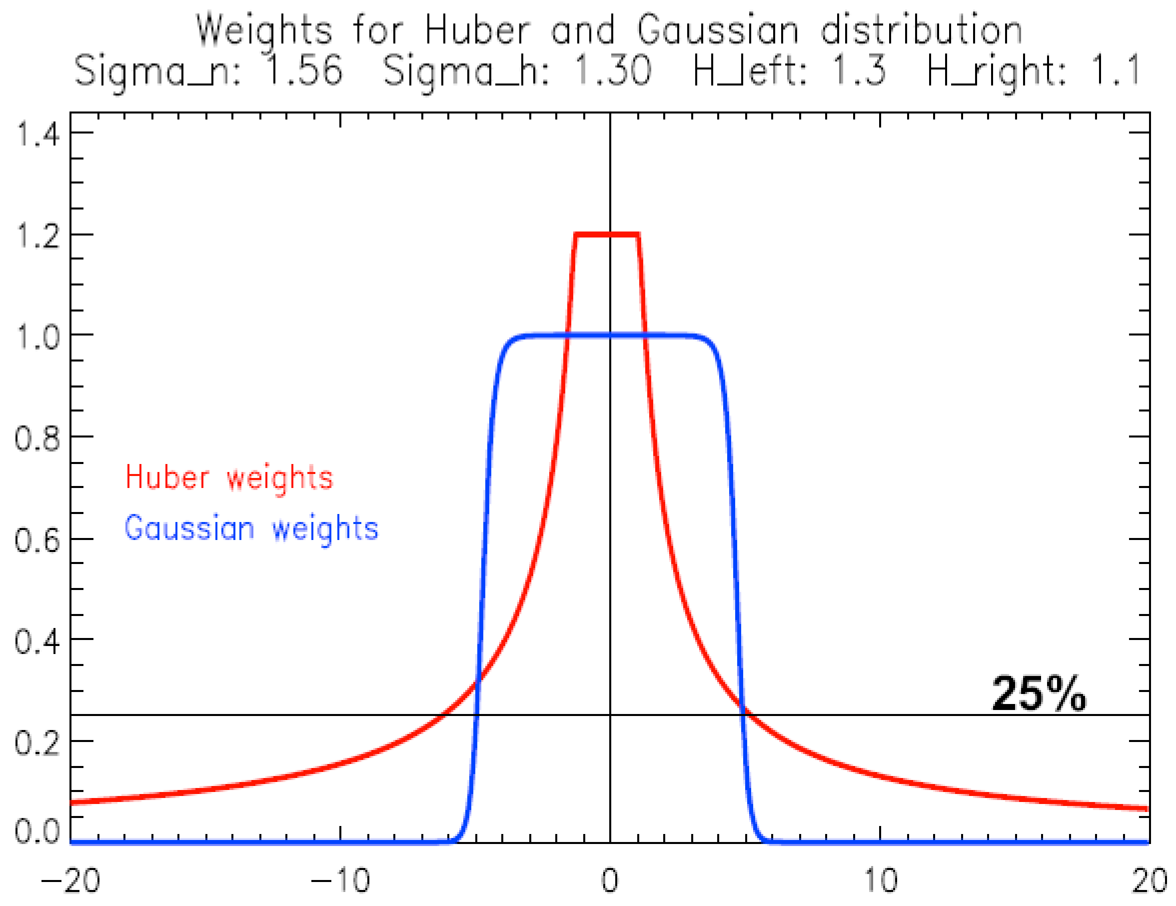
(Isaksen, 2010 ECMWF)

Comparing observation weights:

Huber-norm (red) versus Gaussian+flat (blue)

- **More weight in the middle of the distribution**
- **More weight on the edges of the distribution**
- **More influence of data with large departures**

Weights: 0 – 25%



(Isaksen, 2010 ECMWF)

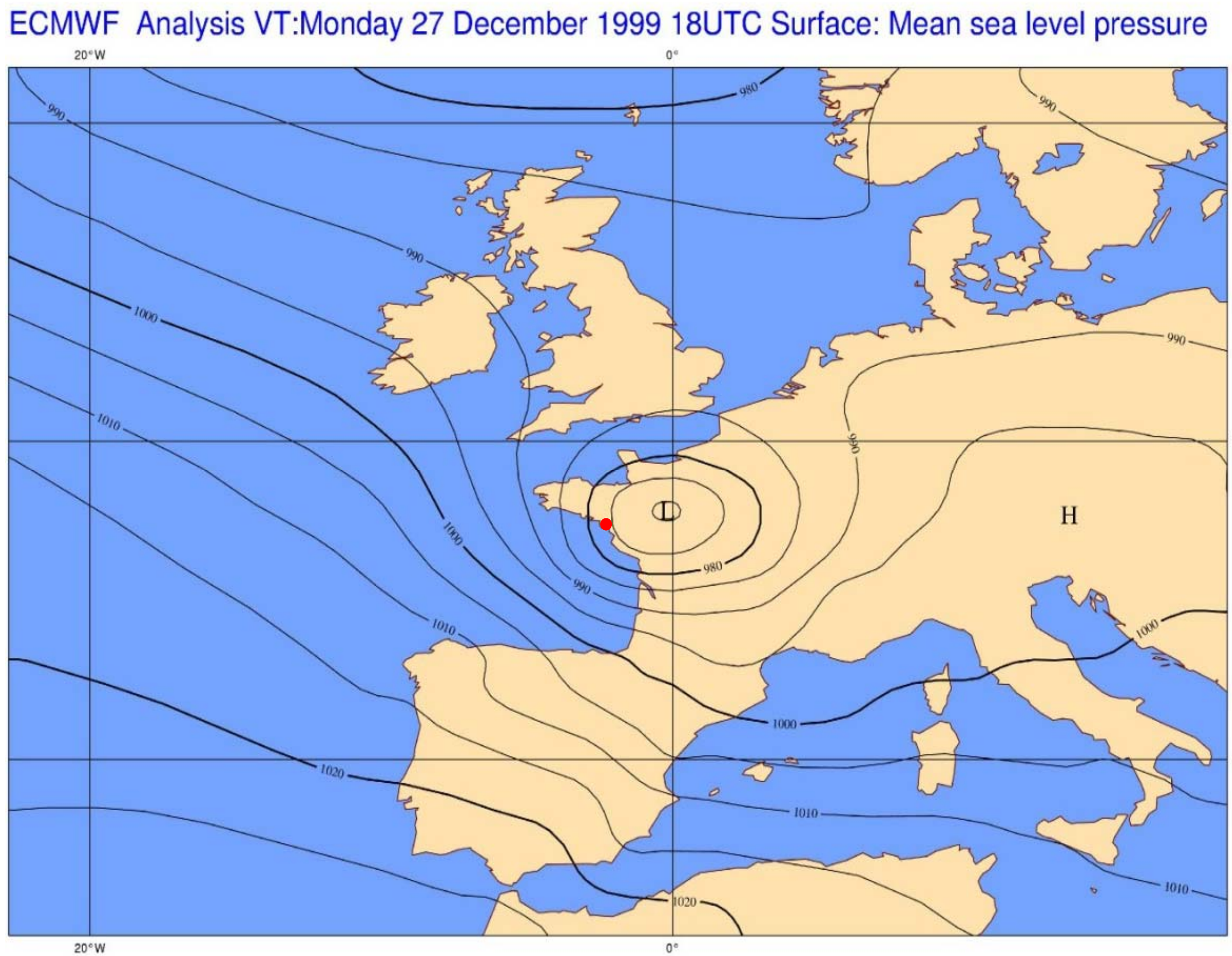
27 Dec 1999 –French storm 18UTC (Example from Isaksen, 2010 ECMWF)

- **Era interim analysis produced a low with min 970 hPa**
- **Lowest pressure observation (SYNOP: red circle)**

–963.5 hPa (supported by neighbouring stations)

–At this station the analysis shows 977 hPa

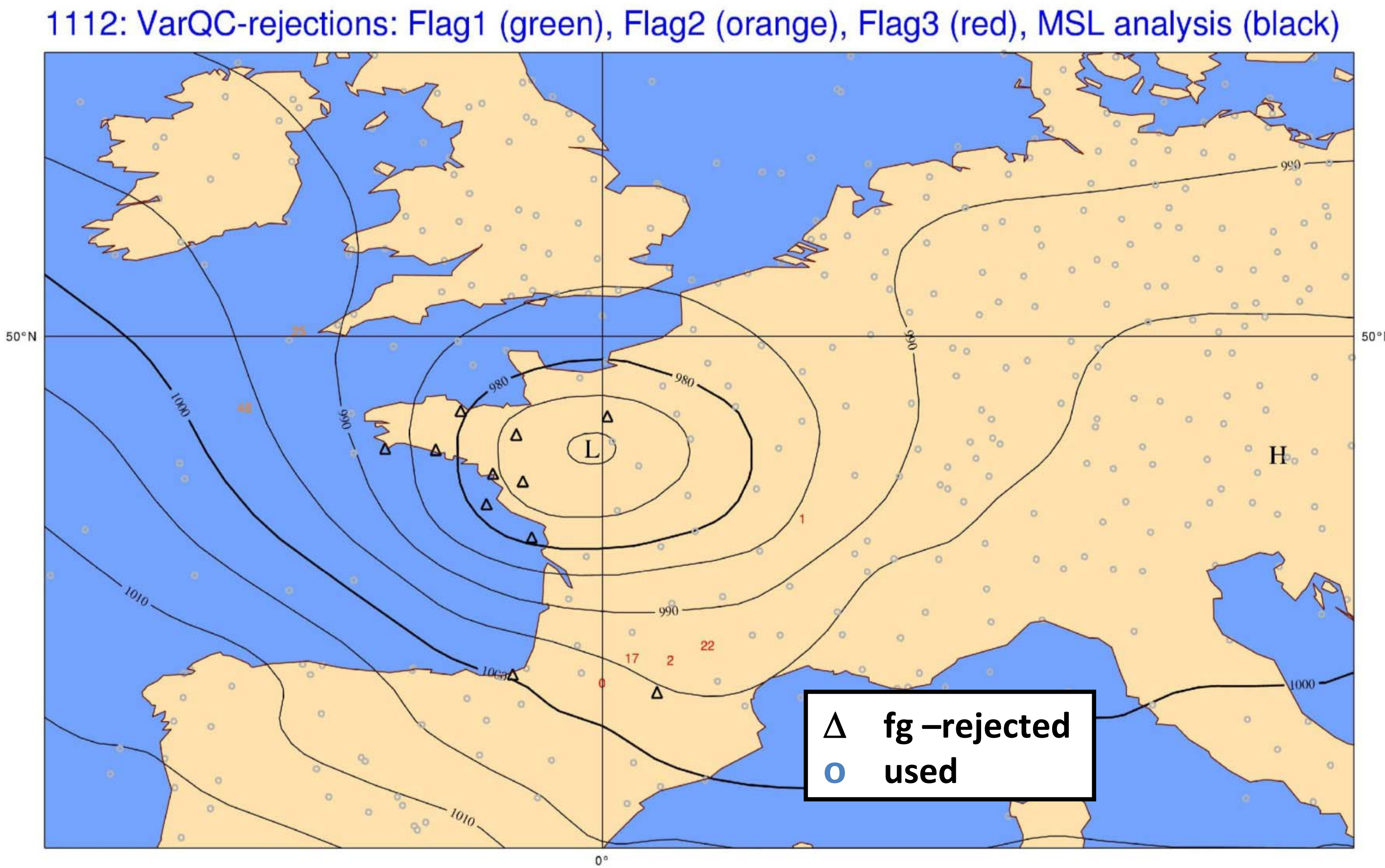
–Analysis wrong by 16.5 hPa!



(Isaksen, 2010 ECMWF)

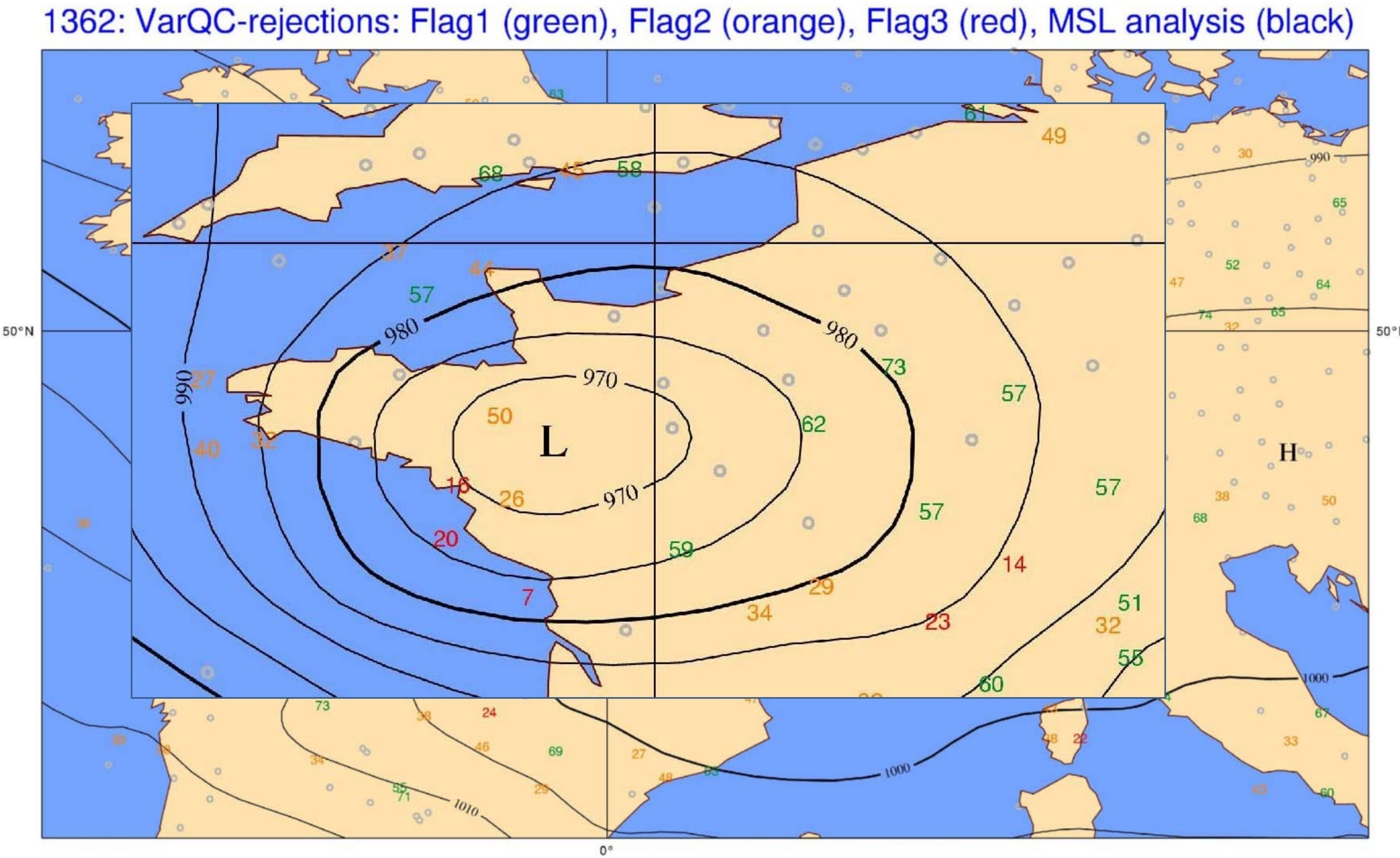
Data rejection and VarQC weights

(Isaksen 2010)



Data rejection and VarQC weights

with Huber norm formulation (Isaksen, 2010)



Conclusion

- **Quality control is a crucial component of any data assimilation system**
- **Acceptance of bad data and rejection of good data happens**
    - * to avoid this as much as possible, the error characteristics need to be regularly reestimated (e.g., probability of gross error, existence of biases, background and observational error covariances).
- **In 4D-Var, small changes to the analysis can lead to substantial differences in the forecast**
    - * Impact of accepting bad data or rejecting good ones can be significant
- **Management of a huge database of information associated with the observations is technically challenging**

Bias correction

(from Auligné. McNally and Dee, QJ 2007)

A quick introduction to bias correction

- **Systematic errors in the analysis can be attributed to observation and/or background error**
- **Biases can be observed in innovations for a particular instrument**
  - * If no bias is observed for other instruments, then it is likely the observations that is biased
- **Principle in bias correction schemes**
  - * Find a way to detect biases (e.g., monitoring) and relate it to likely causes of the source of systematic error and correct it
  - * Example: systematic error associated with the scan angle of a satellite instruments.

Static bias correction

- Consider innovations $\mathbf{d} = \mathbf{y} - H(\mathbf{x}_b)$ over a period of time (order of a month)

- Modify the observation operator as

$$\tilde{H}(\mathbf{x}, \beta) = H(\mathbf{x}) + \sum_{i=0}^{N} \beta_i P_i(\mathbf{x})$$

- Find the coefficients β by minimising

$$J(\beta) = \frac{1}{2}\left(\mathbf{y} - \tilde{H}(\mathbf{x}_b, \beta)\right)^T \left(\mathbf{y} - \tilde{H}(\mathbf{x}_b, \beta)\right)$$

- The quantities $P_i(\mathbf{x})$ are the predictors which relate to the measurements

Predictors used for different satellite instruments

Instrument		Predictors		
AIRS	1000-300	200-50	10-1	50-5
ATOVS	1000-300	200-50	10-1	50-5
GEOS	1000-300	200-50	TCWV	
SSMI	V_s	T_s	TCWV	

- Geopotential thicknesses for the layers comprised between the pressures (in hPa)
- TCWV: total content in water vaport
- V_s: surface wind speed T_s: skin temperature

Limitations of the static scheme

- **Bias is assumed to be constant over the period**
  - * Inappropriate to detect instrument problems
- **Based on the assumption that the background error itself is unbiased**
  - * Background error is constrained by *all* observations
    - → Justified where unbiased observations are available (e.g., radiosondes)

$$\langle \mathbf{y} - H(\mathbf{x}_b) \rangle = \langle \varepsilon_o - \mathbf{H}\varepsilon_b \rangle = \langle \varepsilon_o \rangle + \langle \mathbf{H}\varepsilon_b \rangle \approx \langle \varepsilon_o \rangle$$

Adaptive offline scheme

- **Bias correction is recalibrated before every analysis**

$$J(\beta)=\frac{1}{2}\left(\mathbf{y}-\tilde{H}\left(\mathbf{x}_b,\beta\right)\right)^T\mathbf{R}^{-1}\left(\mathbf{y}-\tilde{H}\left(\mathbf{x}_b,\beta\right)\right)+\frac{1}{2}\left(\beta-\beta_b\right)^T\mathbf{B}_\beta^{-1}\left(\beta-\beta_b\right)$$

- **Second term acts as a "memory" of past evaluations**
  - * Could be interpreted as a static scheme applied with a running mean.

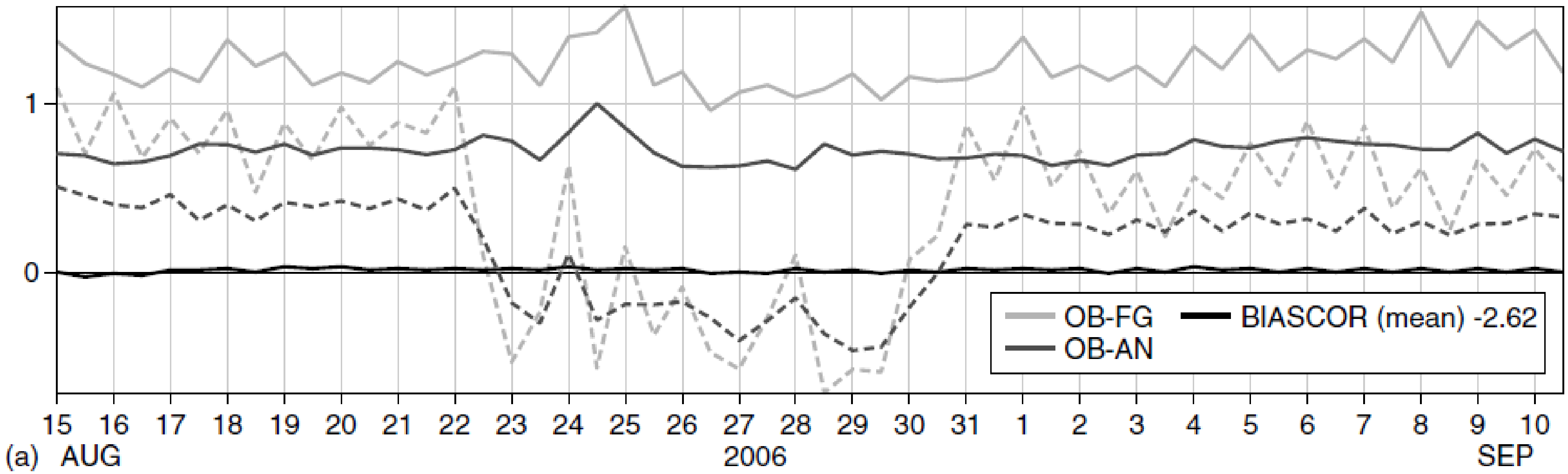
Adaptive online scheme: Var-BC

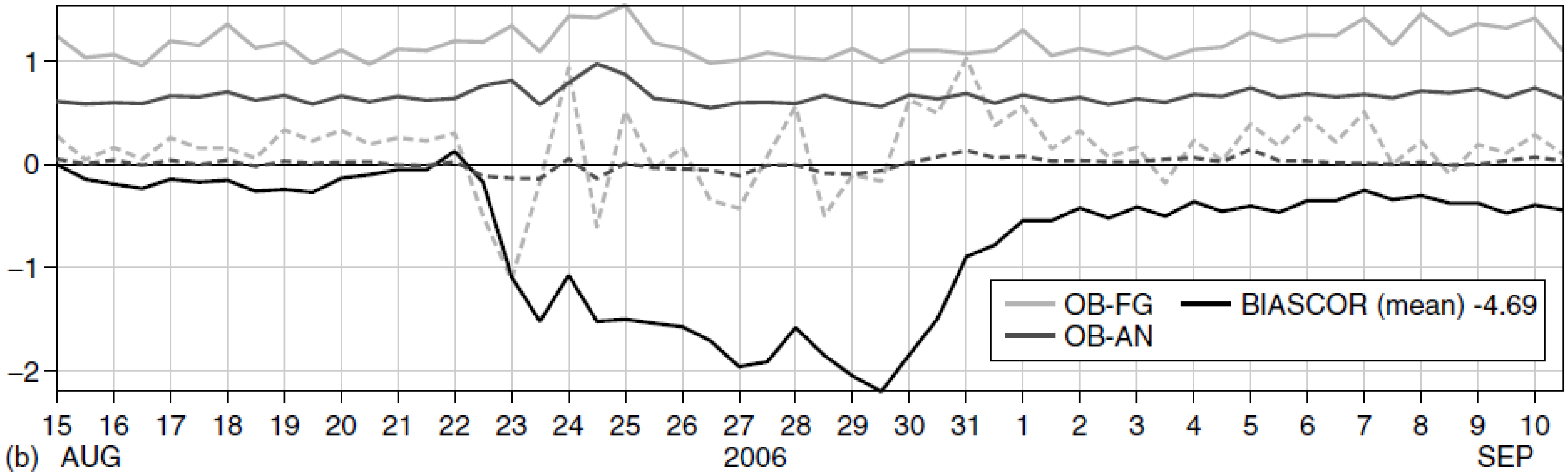
- **Bias correction is incorporated within the assimilation scheme itself**

$$J(\beta)=\frac{1}{2}\left(\mathbf{y}-\tilde{H}(\mathbf{x}_b,\beta)\right)^T\mathbf{R}^{-1}\left(\mathbf{y}-\tilde{H}(\mathbf{x}_b,\beta)\right)$$
$$+\frac{1}{2}(\beta-\beta_b)^T\mathbf{B}_\beta^{-1}(\beta-\beta_b)$$
$$+\frac{1}{2}(\mathbf{x}-\mathbf{x}_b)^T\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}_b)$$

- **More apt to distinguish between model bias and observation biases.**

Auligné *et al.* (2007): comparaison between VarBC and static bias correction

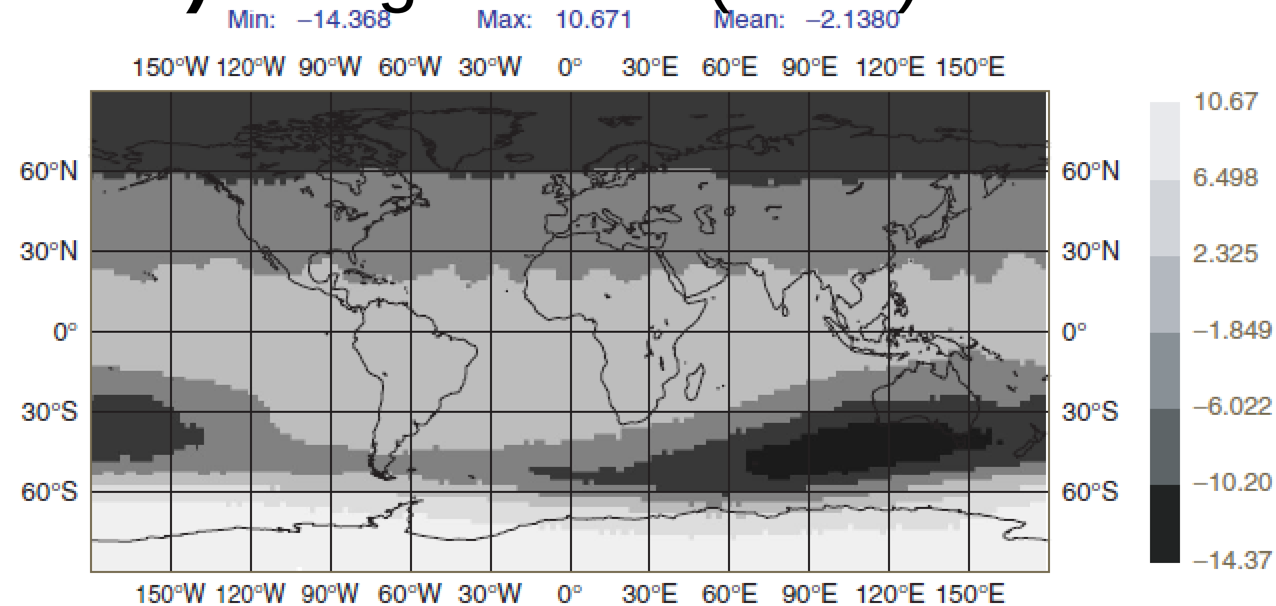




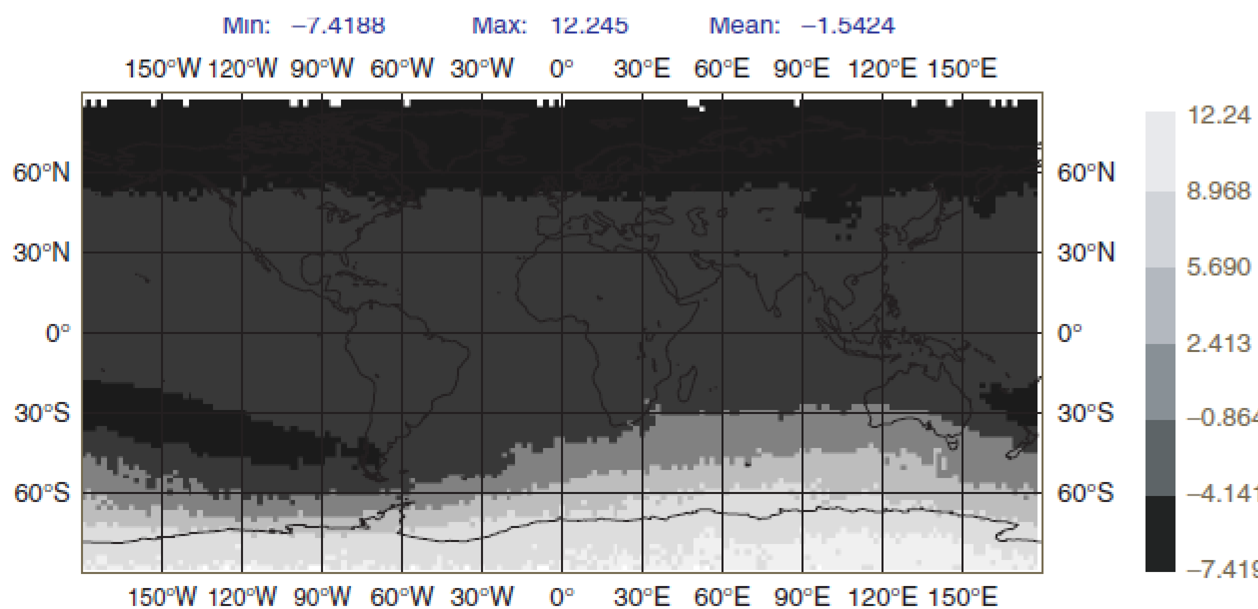
Results for AMSU-a channel 14 (peak at 1hPa) (average over 3 weeks) Auligné et al. (2007)

No assimilation of satellite data

$$\left\langle \mathbf{y} - H\left(\mathbf{x}_a\right) \right\rangle$$

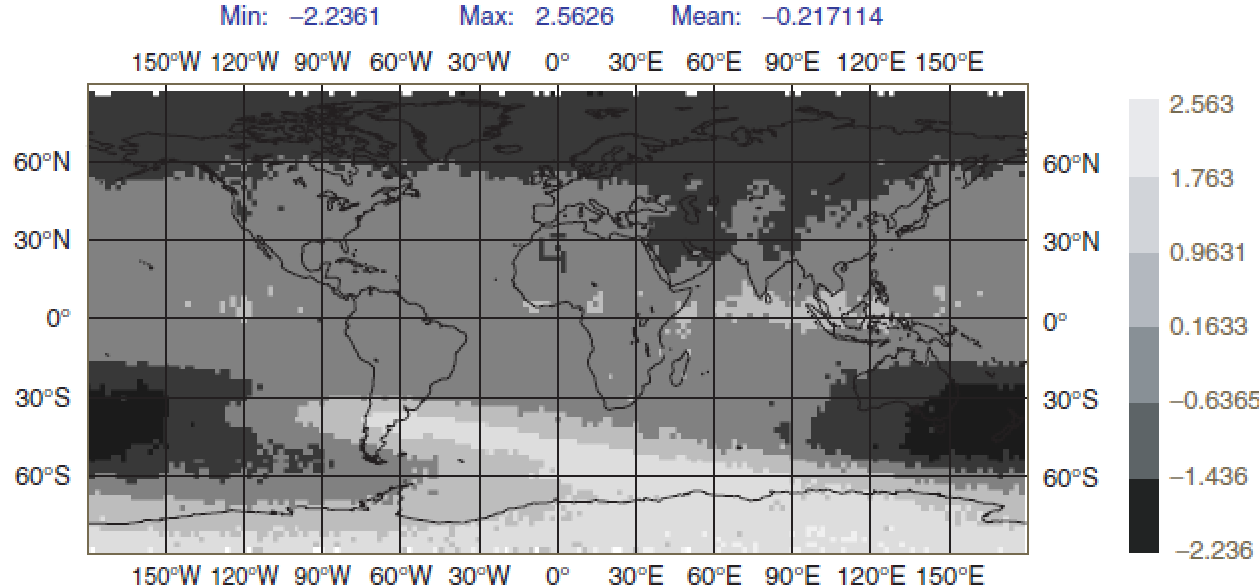


Offline bias correction

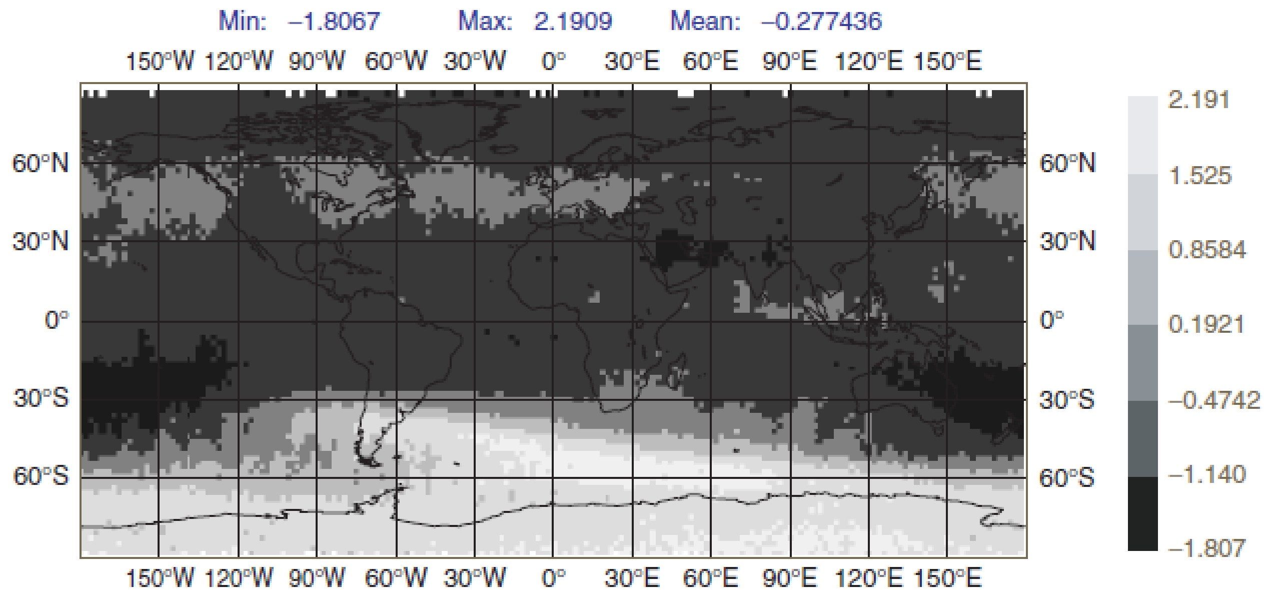


Results for AMSU-a channel 14 (average over 3 weeks) Auligné et al. (2007)

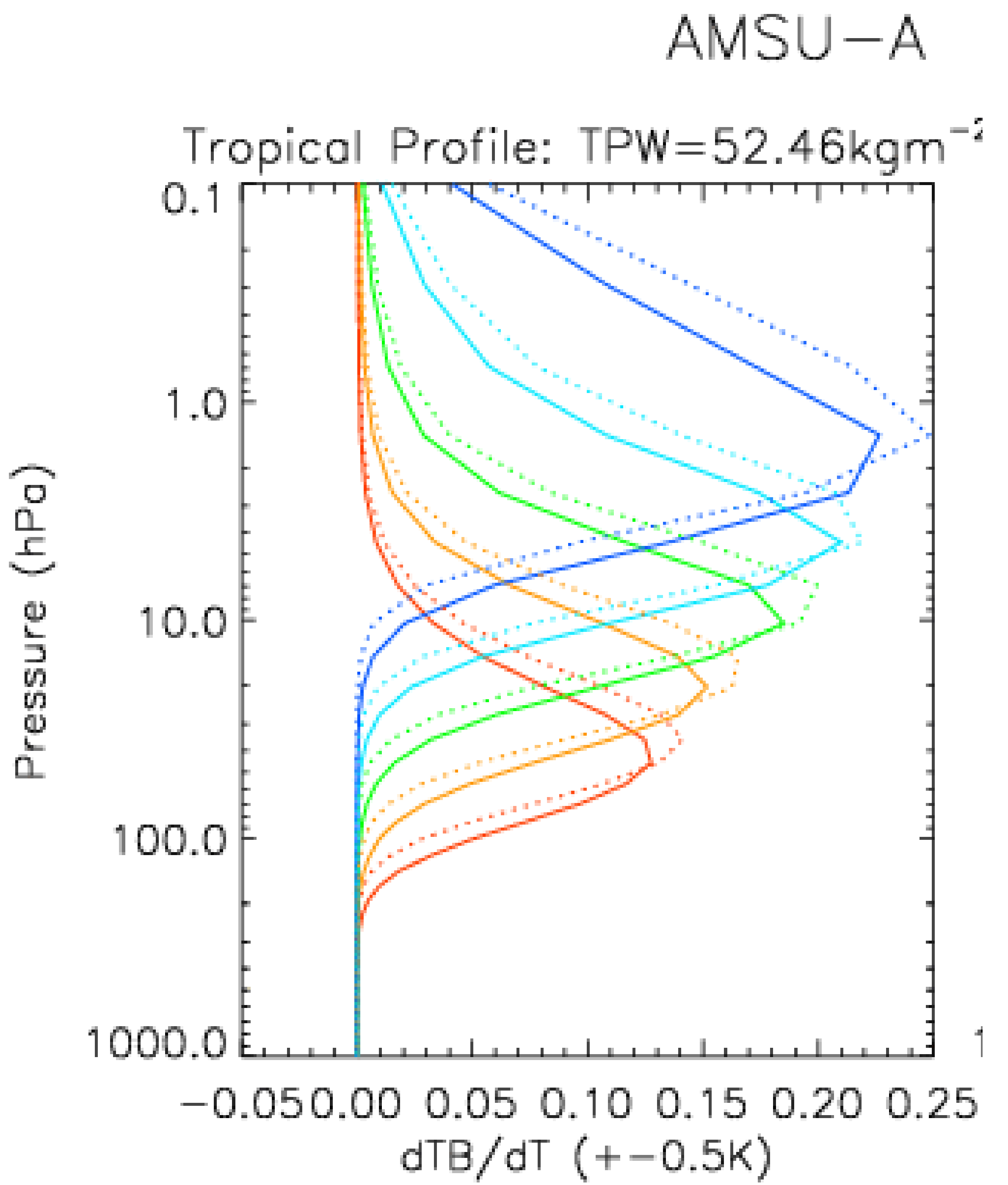
Var-BC bias correction



Var-BC bias correction using a mask



Sensitivity to temperature for different channels of AMSU-a



Conclusions

- **Distinguishing between model and observation biases remains delicate**
- **VarBc automates the bias corrections and has shown some skill to in distinguishing between the two**
- **Choice of the predictors is being revisited regularly to reflect the nature of the instrument**
- **Long term drift may result due to the interaction between QC-Var and Var-BC (Auligné and McNally, 2007)**
  - Important for reanalyses as biases in the analyses may be wrongly interpreted as a climate drift.