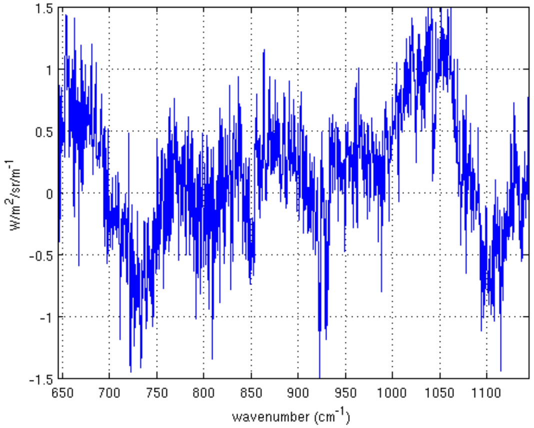
IASI PC compression – Searching for signal in the residuals

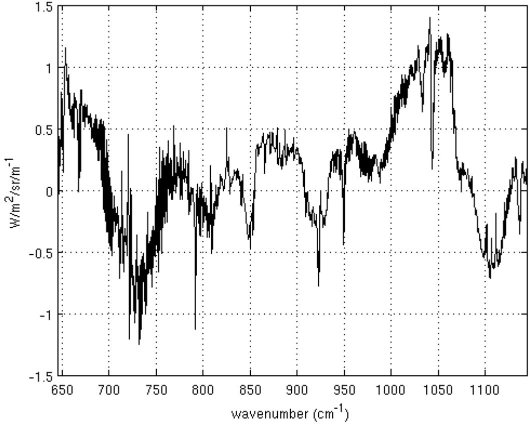
Tim.Hultberg@EUMETSAT.INT
Thomas August, Nigel Atkinson, Fiona Smith

Raw radiance
(minus background)



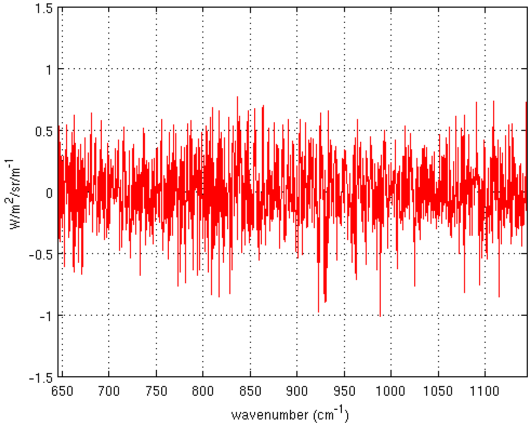
=

Reconstructed radiance
(minus background)



+

Residual



ECMWF / EUMETSAT NWP-SAF Workshop Efficient Representation of Hyper-spectral Infrared Satellite Observations
5-7 November 2013, ECMWF, Reading, UK

Lossless compression = Noise preserving compression

SIGNAL

spectral redundancy ➔ exploited in the current PC compression
spatial redundancy ➔ could be exploited to compress further

RANDOM NOISE

no spectral redundancy and no spatial redundancy
➔ no compression possible, except entropy encoding (like Huffman coding)

Noise constitutes the bulk of the "information" in the spectra

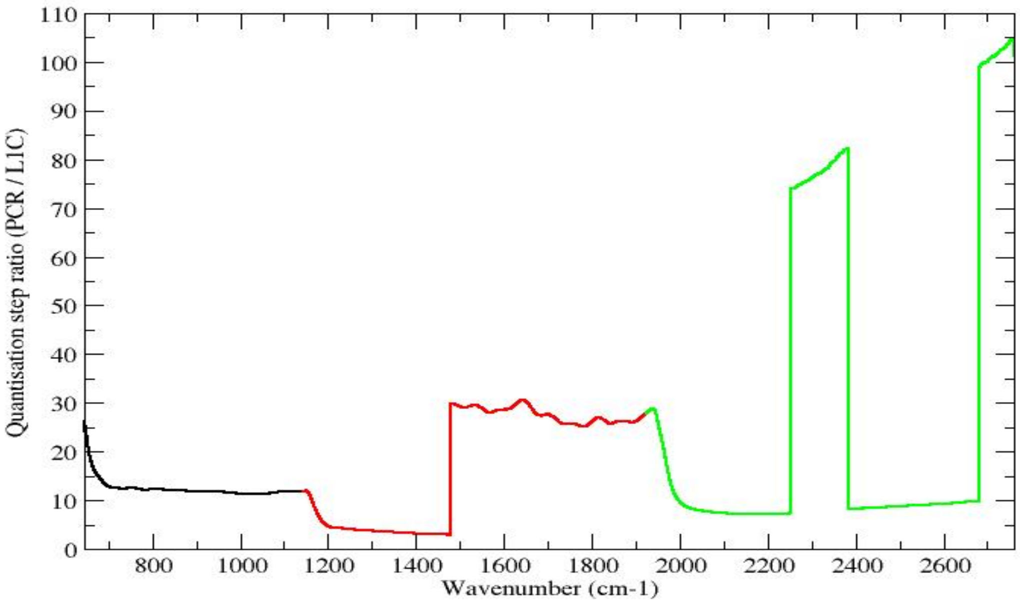
insisting on preserving instrument noise imposes strict limits to the obtainable compression factor - the limit depends on the chosen quantisation step

QUANTISATION STEP

A. As in L1C product (ad hoc, 16 bits and scale factor)
B. Half NEDR step size (Tony Lee)
   Compression factor 4.4

Half NEDR quantisation step size
➔round-off error
➔standard deviation of error increase by 1%
(this is what is currently used for the residuals (IASI_PCR product))

PCR quantisation compared to L1C quantisation



Essence of EUMETSATs IASI PC compression

A. Band separation
   - compression of Band 1 and 2 still possible when Band 3 is bad
   - inter band correlation not exploited ➔ need 40 PC scores extra

B. Diagonal noise normalisation matrix (N)
   - uniformises but doesn't decorrelate the noise

C. Eigenvectors built from training set of real measurements (Y)
   - outliers added to capture rare situations like fires and volcanic eruptions

D. Number of retained eigenvectors (90, 120, 90) based on spatial correlation of PC scores

➔ E a truncated set of eigenvectors of COV($N^{-1}Y$)

$p = E^T N^{-1}(y - \bar{y})$ PC scores

$\tilde{y} = NEp + \bar{y}$ Reconstructed radiances

$\tilde{y} = Ay + (I - A)\bar{y}$ where $A = NEE^T N^{-1}$

The transformation to reconstructed radiances is a projection!

The most important slide! (or how to split a spectrum into four parts)

Total		Signal		Noise	
y	$=$	y_0	$+$	ε	Raw radiance
$\tilde{y}$	$=$	$\boxed{\tilde{y}_0}$	$+$	$\boxed{A\varepsilon}$	Reconstructed radiance
$y - \tilde{y}$	$=$	$\boxed{y_0 - \tilde{y}_0}$	$+$	$\boxed{(I - A)\varepsilon}$	Residual

Atmospheric signal retained in reconstructed radiance

Instrument noise retained in reconstructed radiance

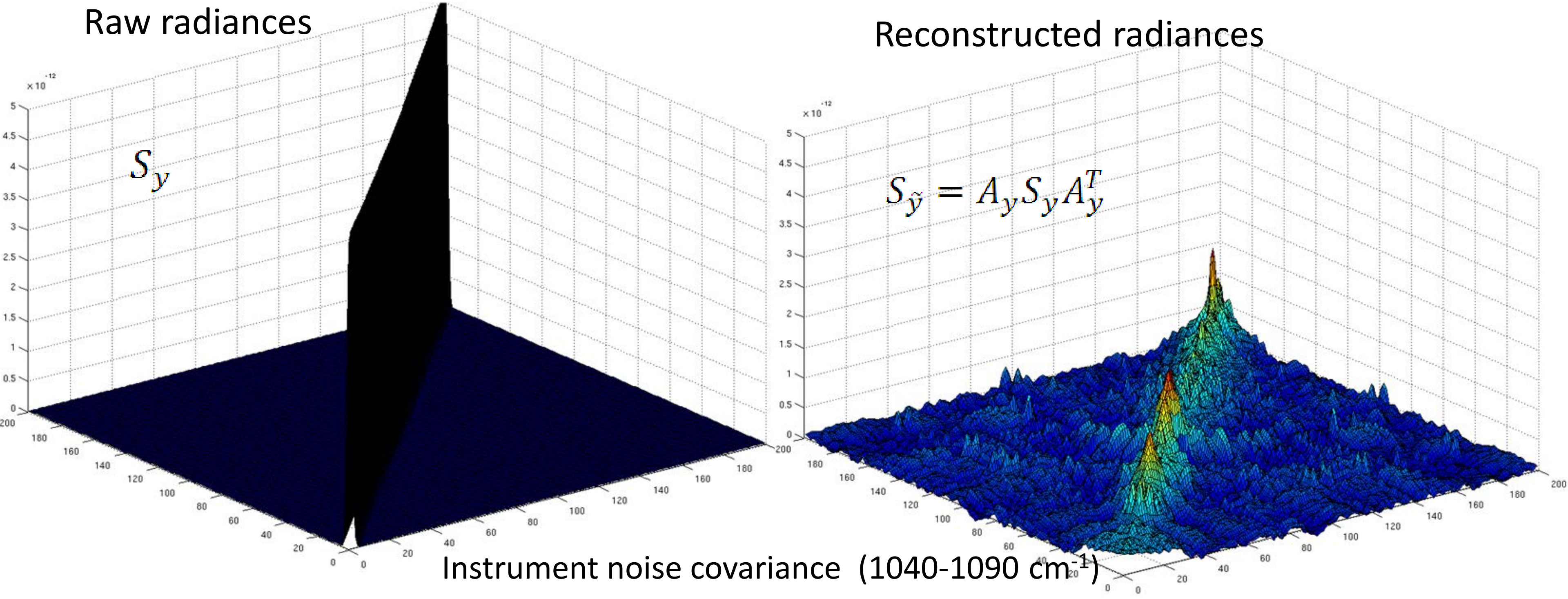
Atmospheric signal in residual (RECONSTRUCTION ERROR ☹)

Instrument noise in residual

the covariance of the residuals is the sum of
the noise in the residuals and the covariance of the reconstruction error

Raw and reconstructed noise covariance matrices:

$$\overset{\text{Raw noise}}{S_y} = \overset{\text{Reconstructed noise}}{A\, S_y A^T} + \overset{\text{Noise in residuals}}{(I - A) S_y (I - A)^T}$$



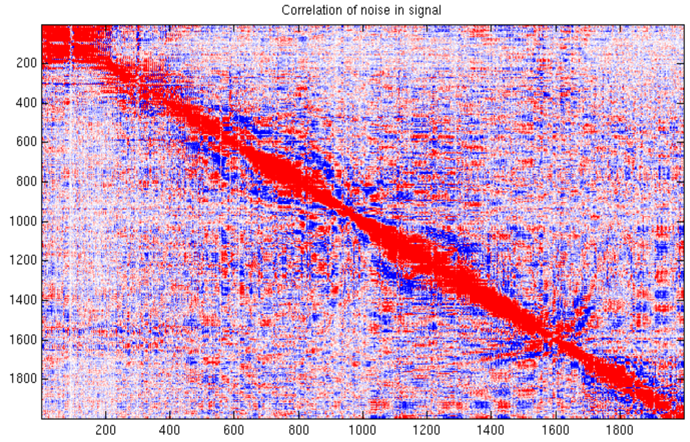
Raw radiances

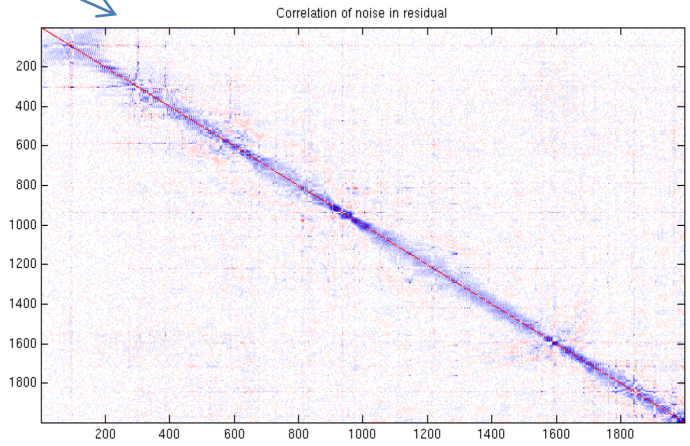
Reconstructed radiances

Instrument noise covariance (1040-1090 cm^{-1})

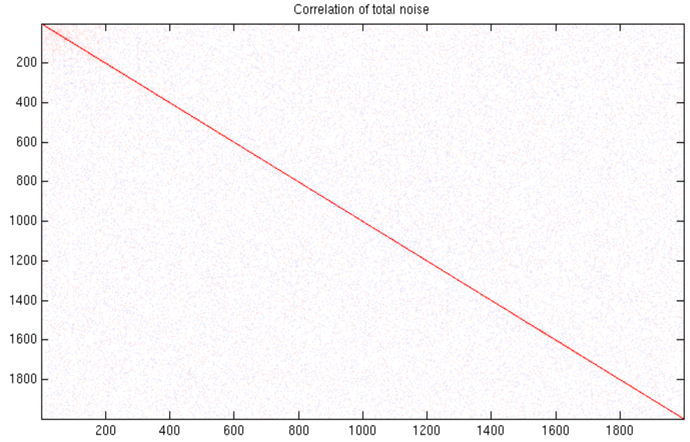
Estimation of full noise covariance matrix

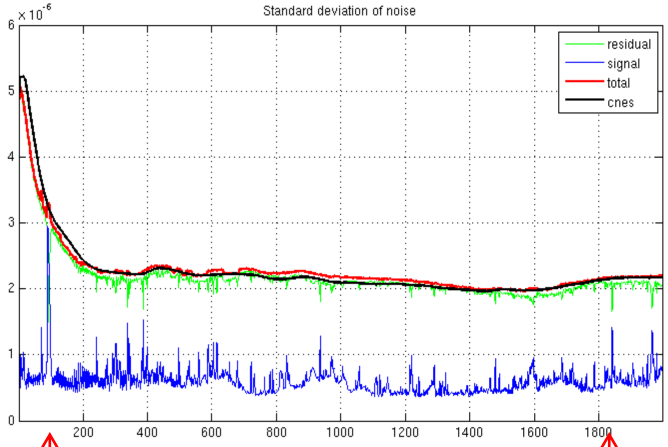
Total noise = Noise in signal + Noise in residual $[S_y = AS_yA^T + \mathrm{cov}(y-\tilde{y})]$





Band 1



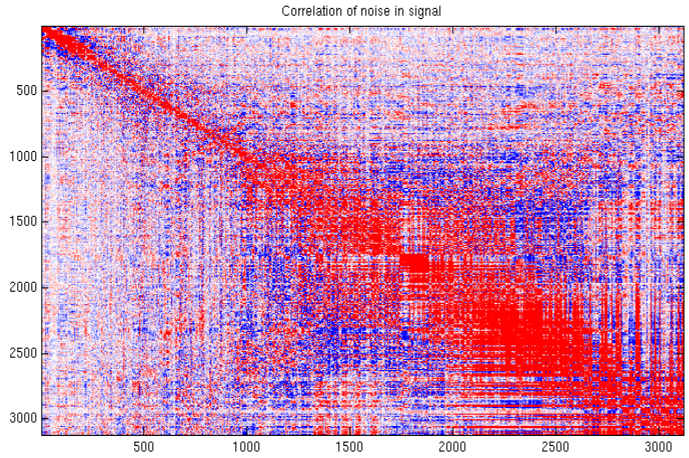


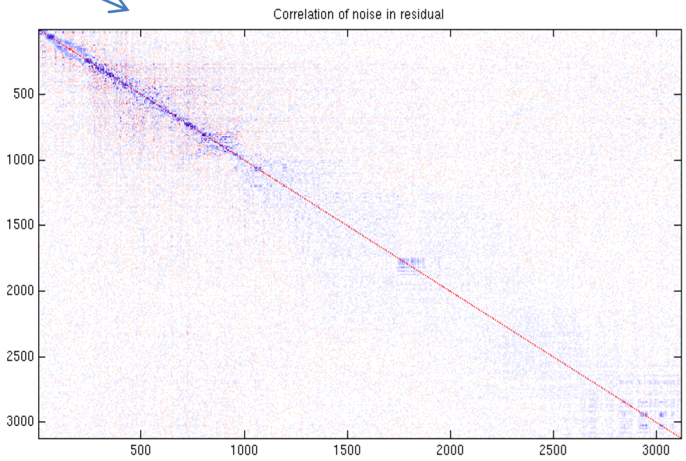
Spikes correspond to spectrally narrow features, where reconstructed radiances are closer to raw radiances.

Estimation of full noise covariance matrix

Additional noise correlation caused by spectral calibration difficulties in the band overlap regions.

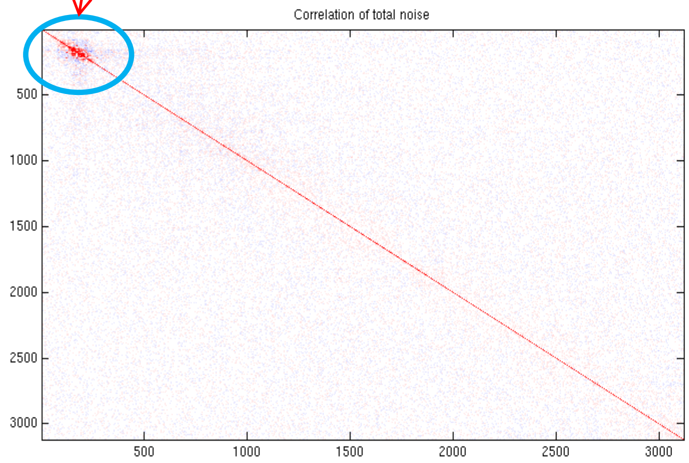
Total noise = Noise in signal + Noise in residual

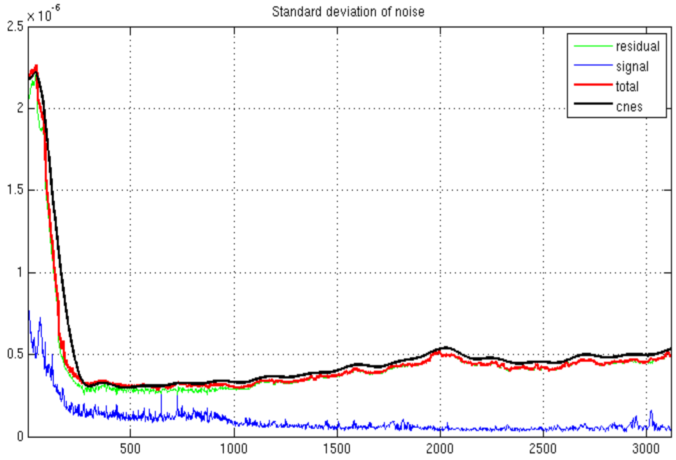




Correlated noise in band overlap region!

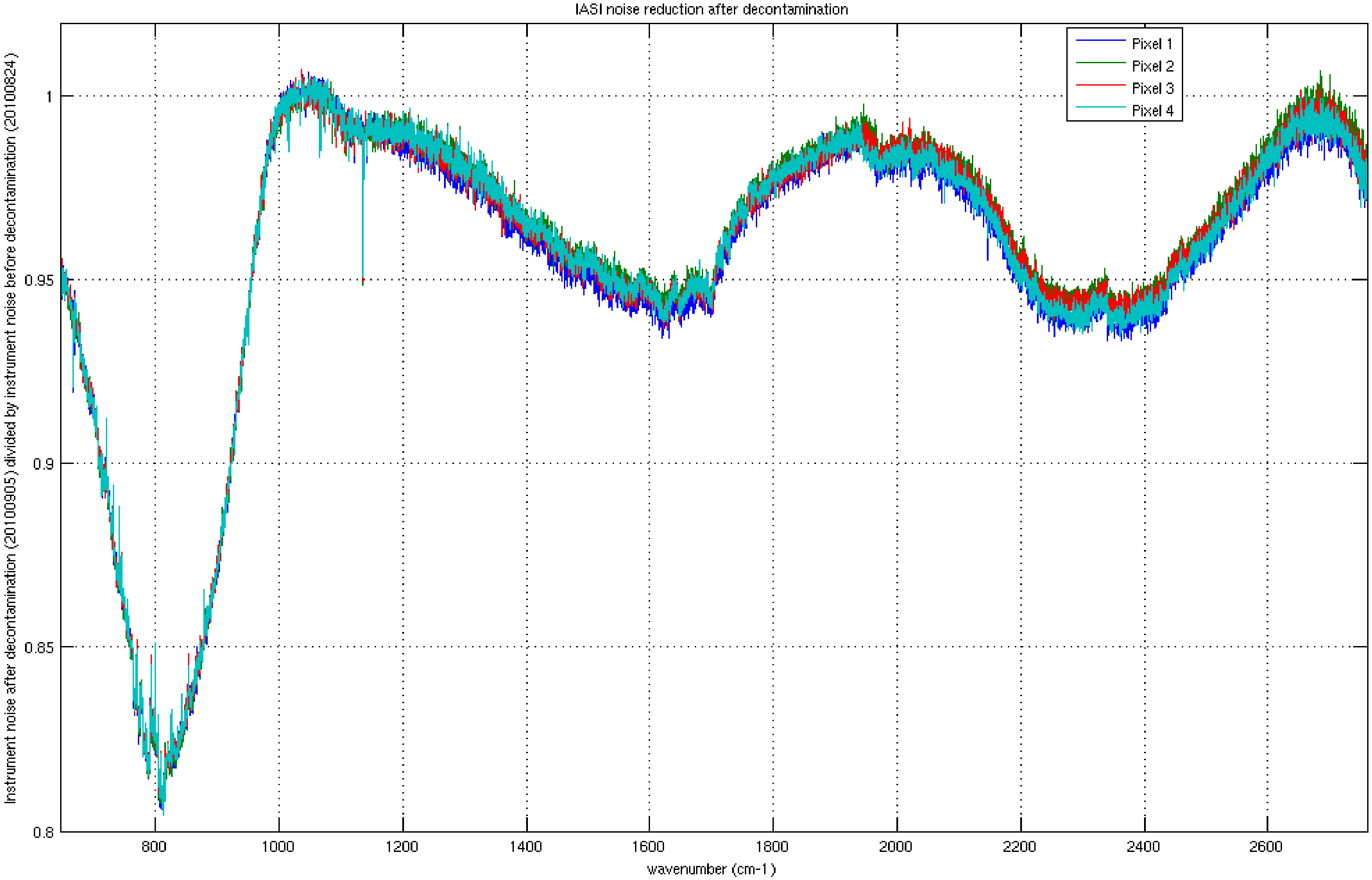
Band 2

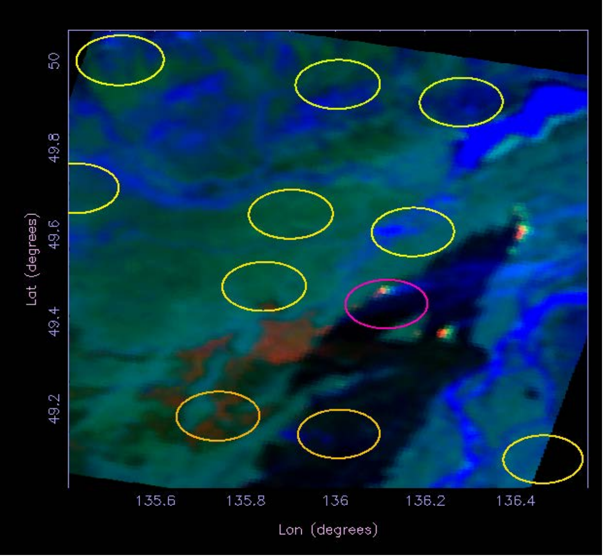




Monitoring of noise evolution

Decontamination, September 2010.
Noise reduction of 0 -20% in each channel.
Agrees well with black body based estimates of the noise reduction

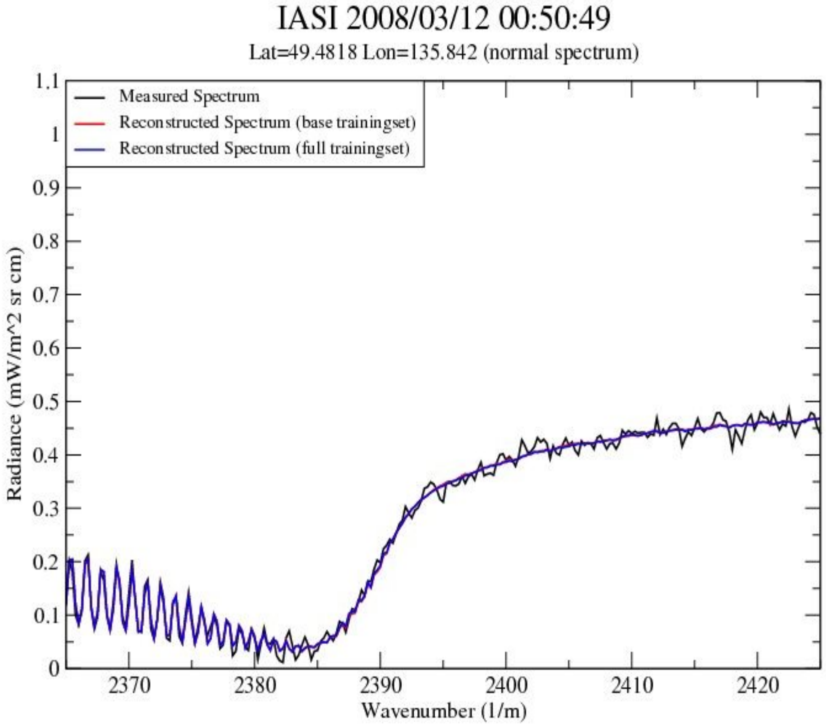


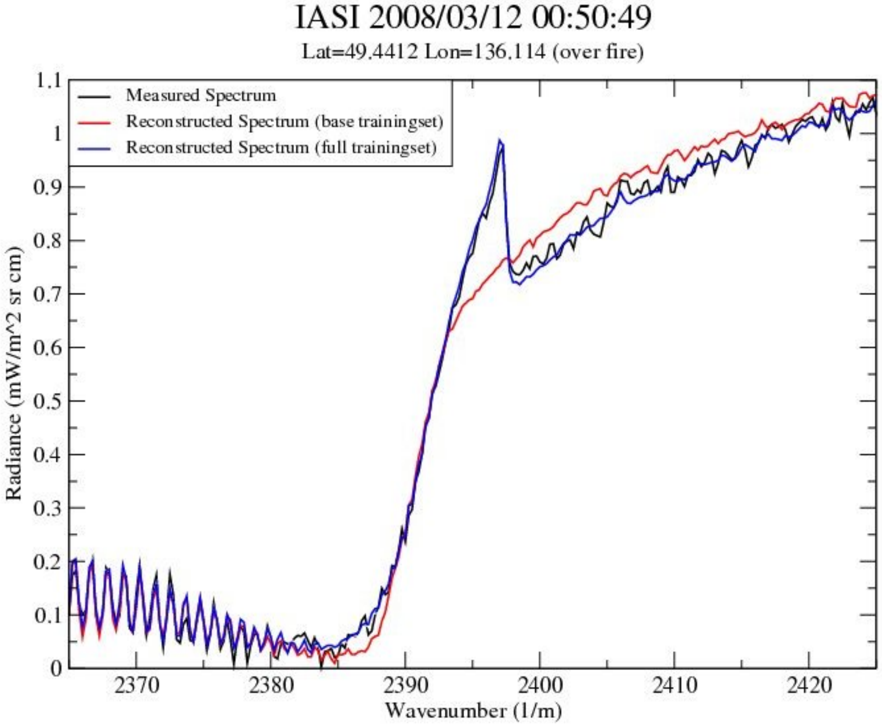


Outliers

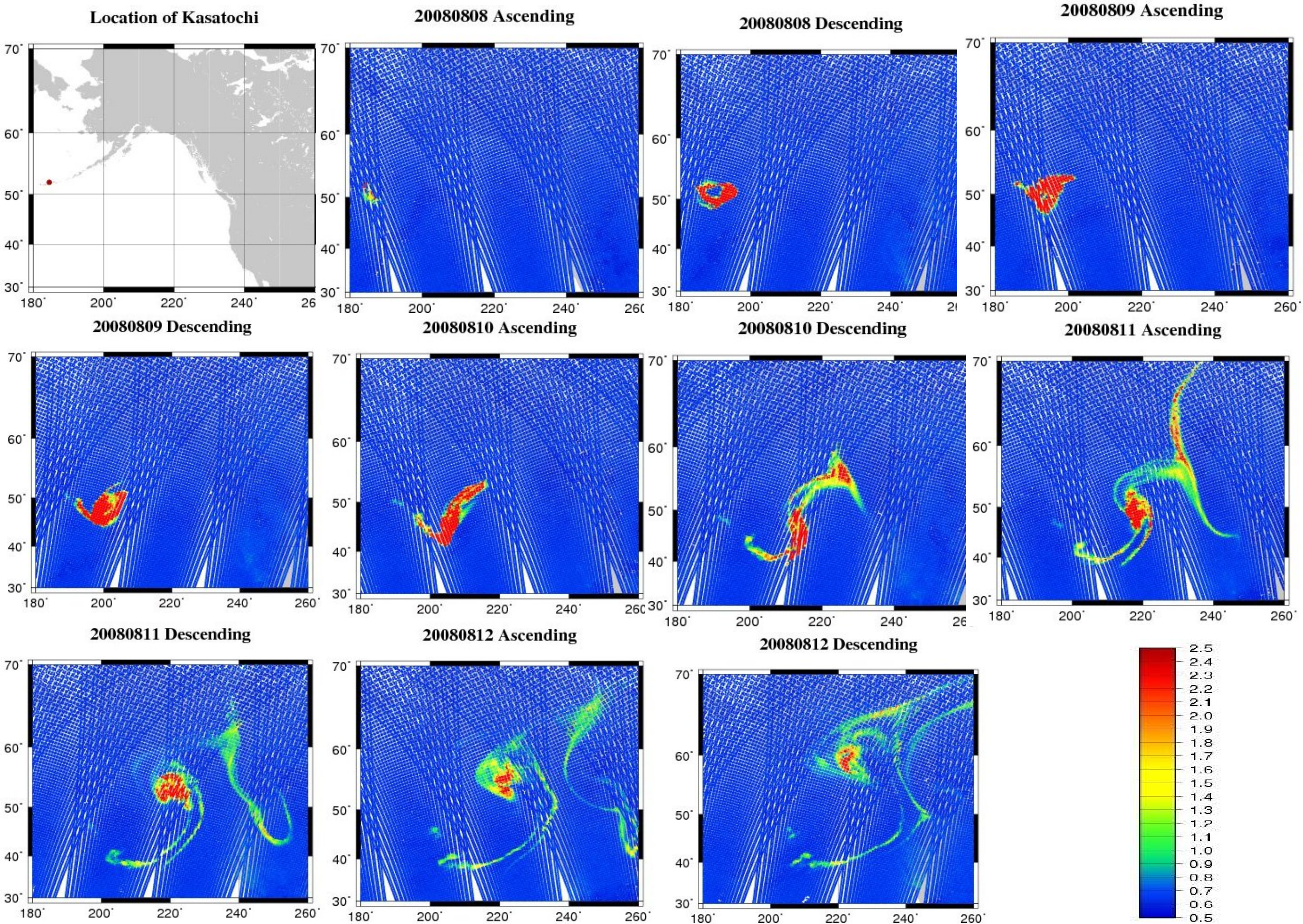
spectra which don’t reconstruct well

RMS of noise normalised residual (reconstruction score)
- one for each IASI band
- disseminated with the IASI PC score product





Kasatochi eruption (Band 2 Residual RMS)

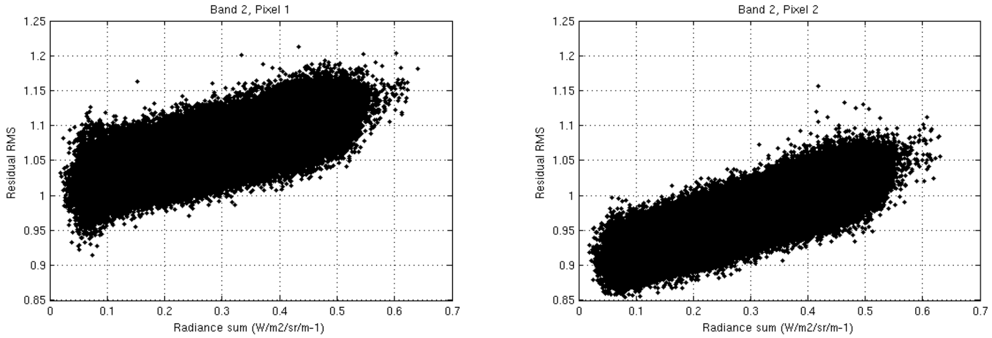


Photonic noise - increases with the signal

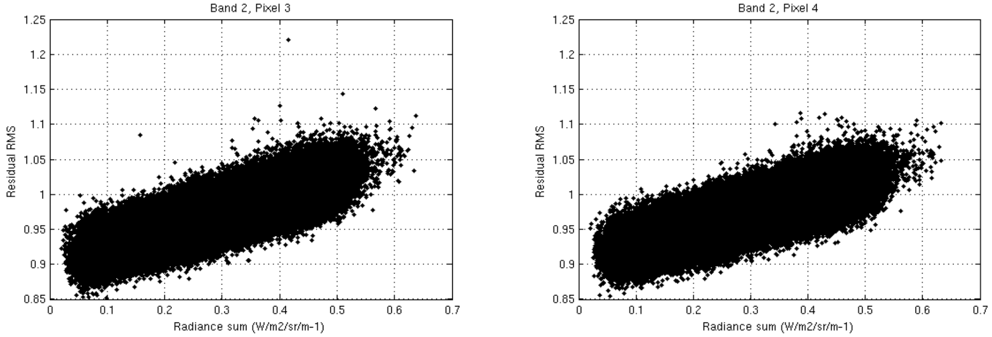
The noise and therefore the expected value of the residual RMS depends on the radiance sum and the detector ➔

This must be taken into account to get a sensitive detections of outliers.

Detector 1 Detector 2



Detector 3 Detector 4

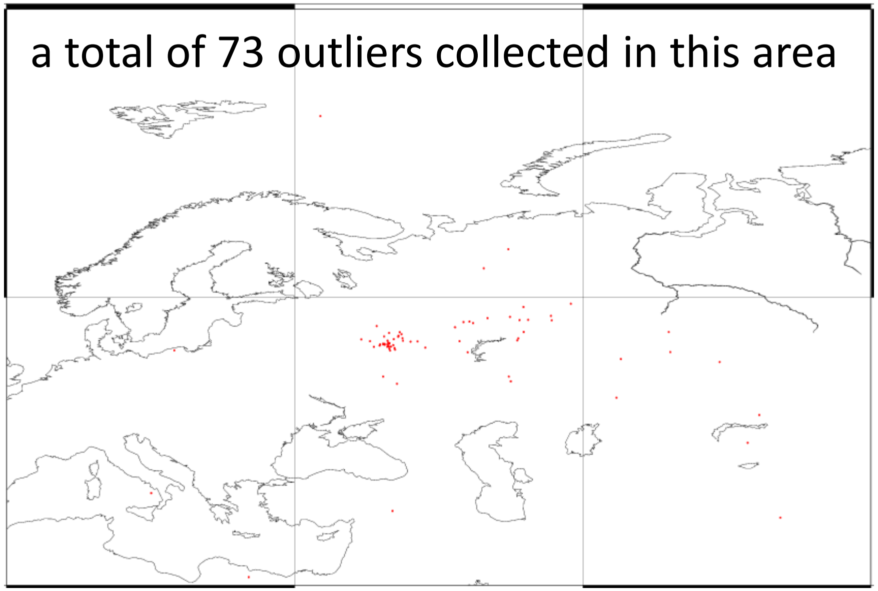


Scatter plots of residual RMS vs. radiance sum (Band 2)

Residual_RMS – slope*Radiance_Sum > Threshold(detector)

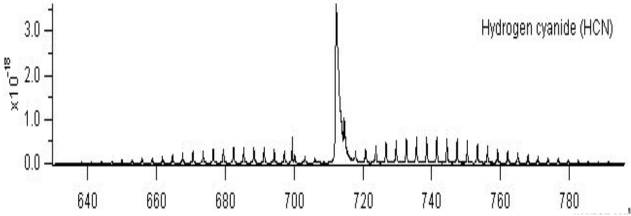
- outlier spectra gathered in an auxiliary product (IASI_IPO)

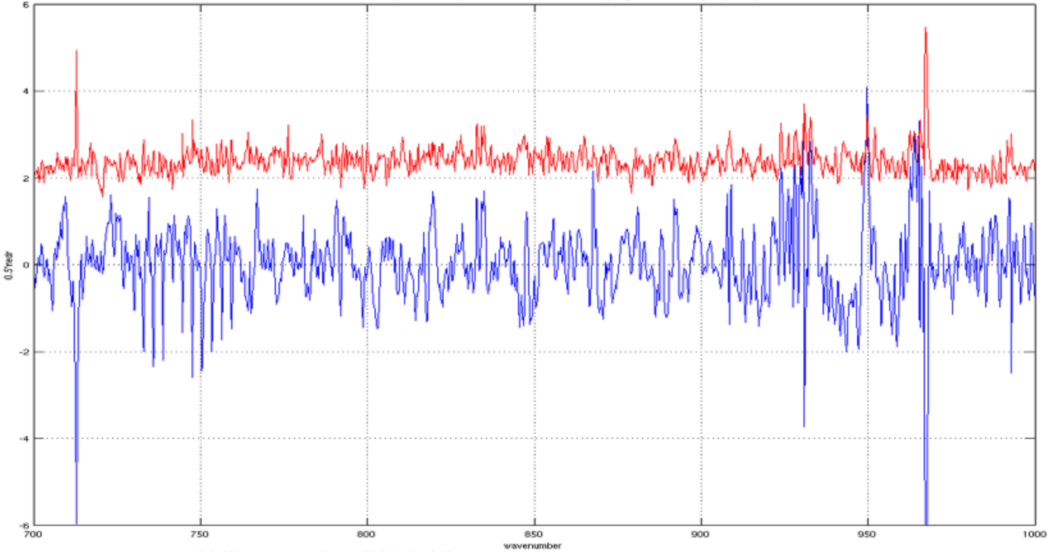
Russian fires, August 3. to 12. 2010



a total of 73 outliers collected in this area

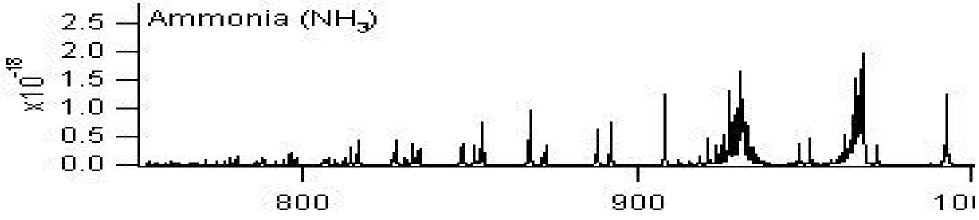
Hydrogen cyanide (HCN)



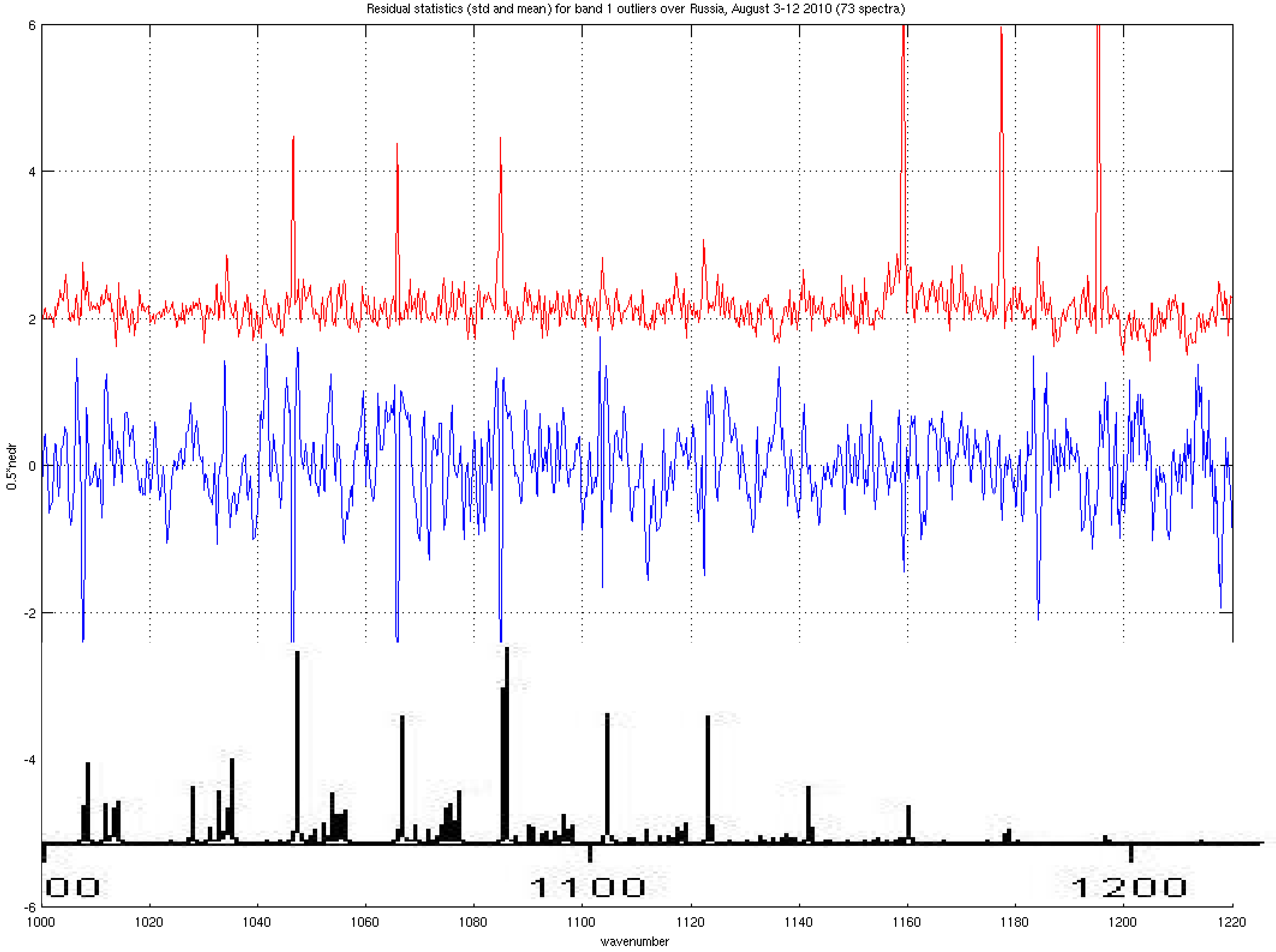


Residual standard deviation

Residual mean

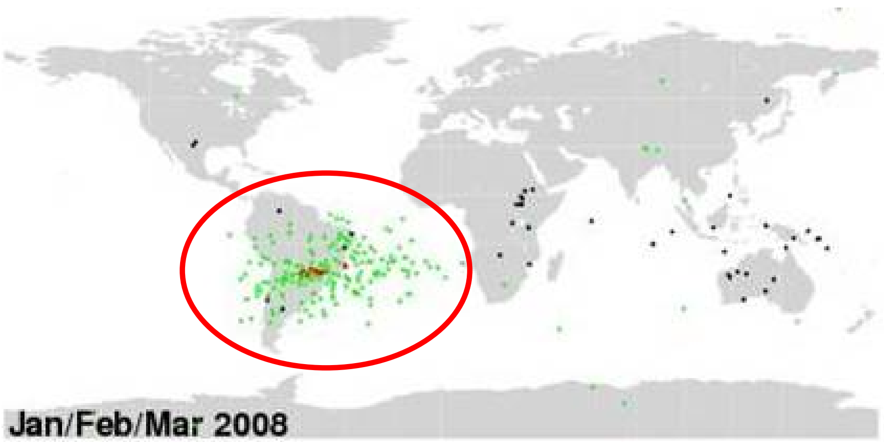


Ammonia (NH)

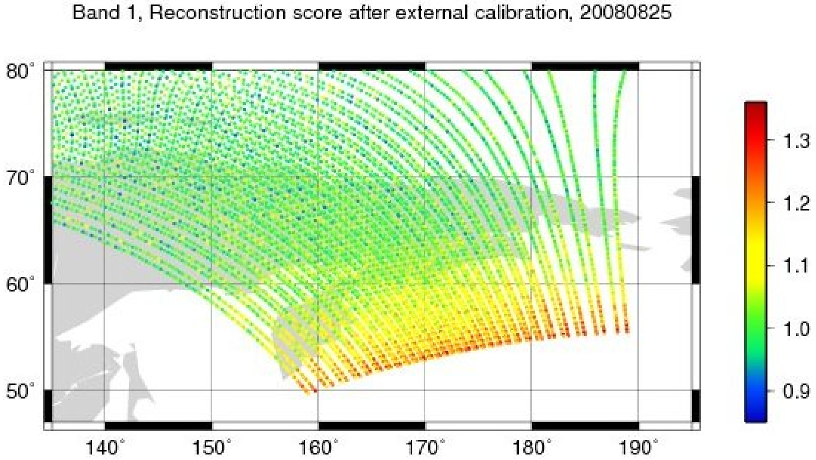

Residual statistics (std and mean) for band 1 outliers over Russia, August 3-12 2010 (73 spectra)
0.5*nedr
6
4
2
0
-2
-4
-6
1000
1020
1040
1060
1080
1100
1120
1140
1160
1180
1200
1220
wavenumber
00
1100
1200

What causes the remaining outliers?

Undetected "spikes":
High-frequency disturbance of the interferogram, most often observed in the South Atlantic Anomaly. (Band 2 outliers)



Back to normal operation after external calibration mode:
No history available for deriving filtered calibration coefficients.

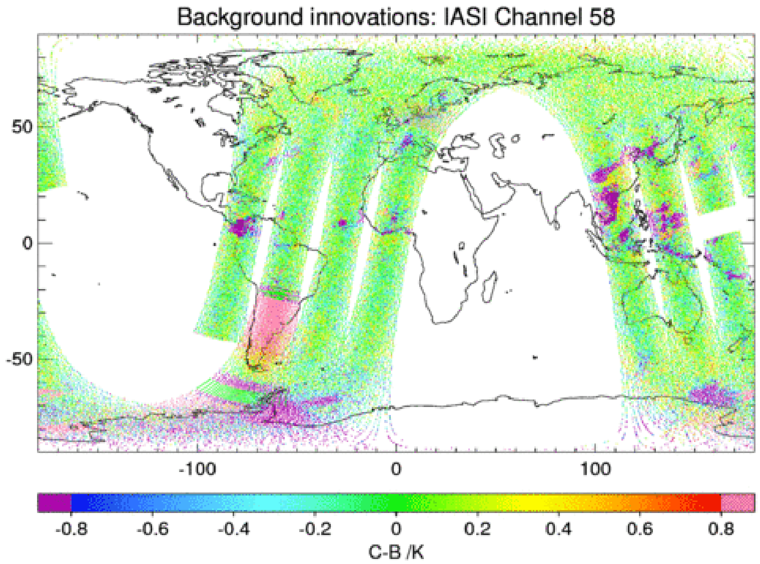


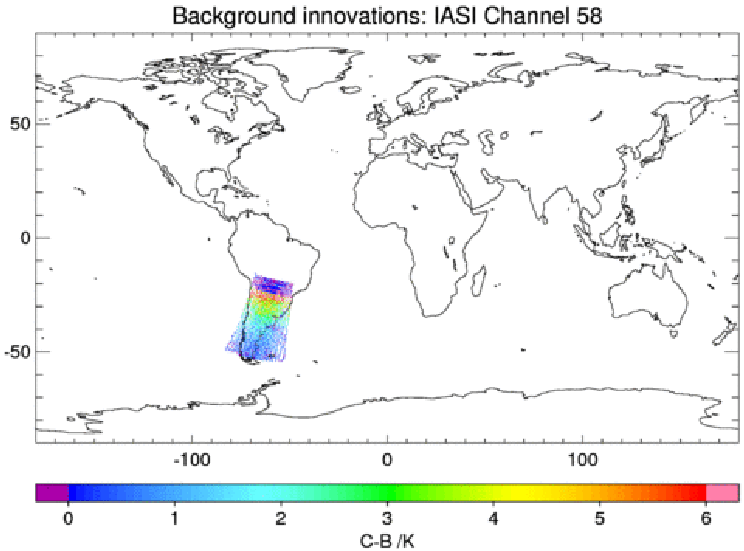
Residual RMS detects some bad quality spectra not flagged in L1C

What causes the remaining outliers?

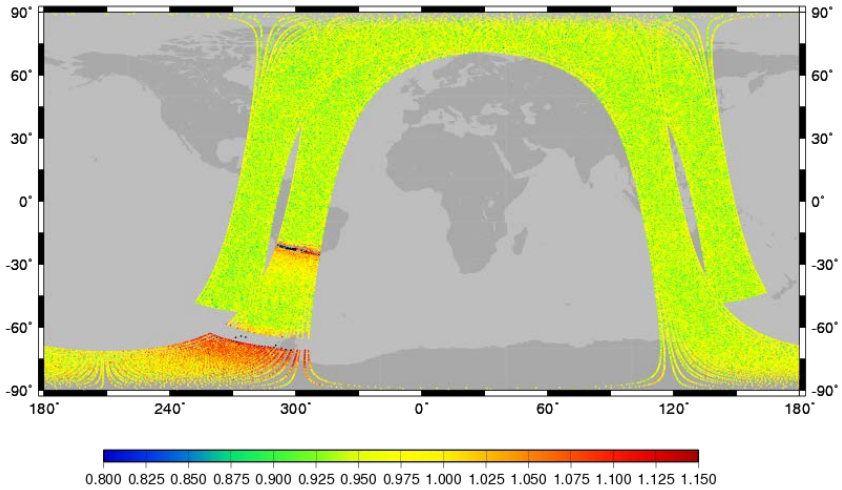
Anomaly related to Metop-B manoeuvre on 20130807:

Met-office noticed a sudden increase in bias over Brazil when the manoeuvre occurred (plots from Nigel Atkinson)


Background innovations: IASI Channel 58


Background innovations: IASI Channel 58

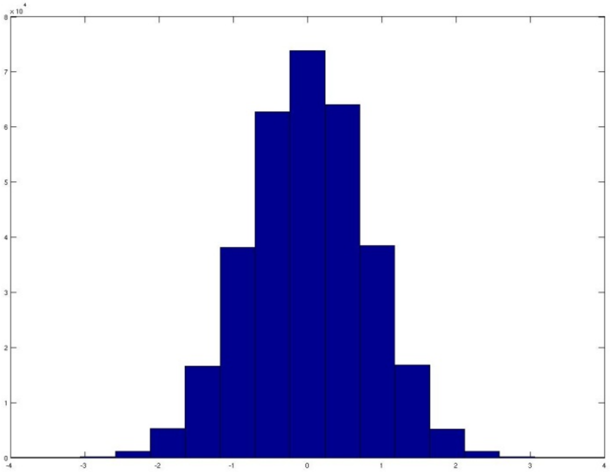
Anomaly clearly observed in the residual RMS ➔

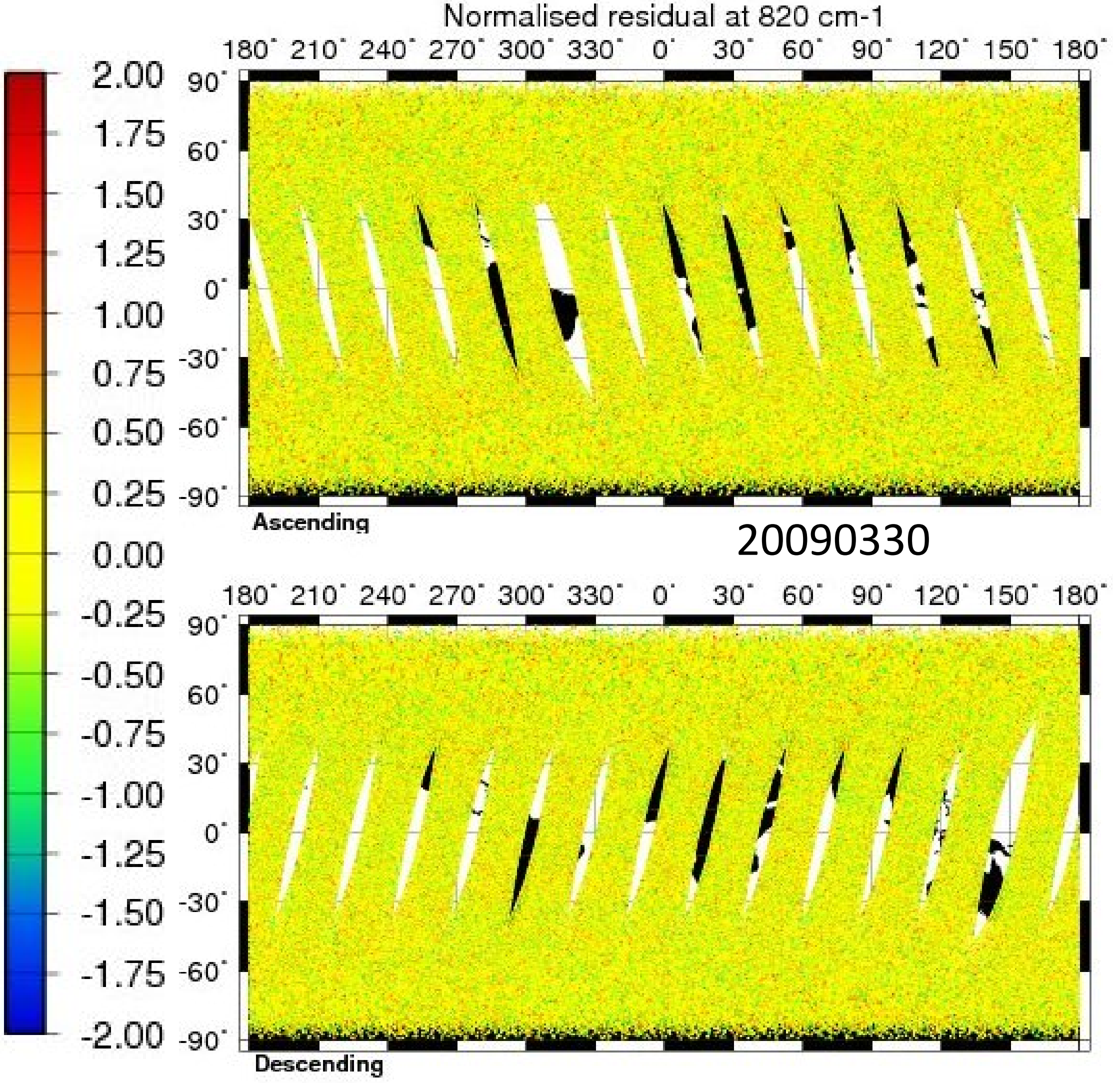


Searching for signal in the residuals.

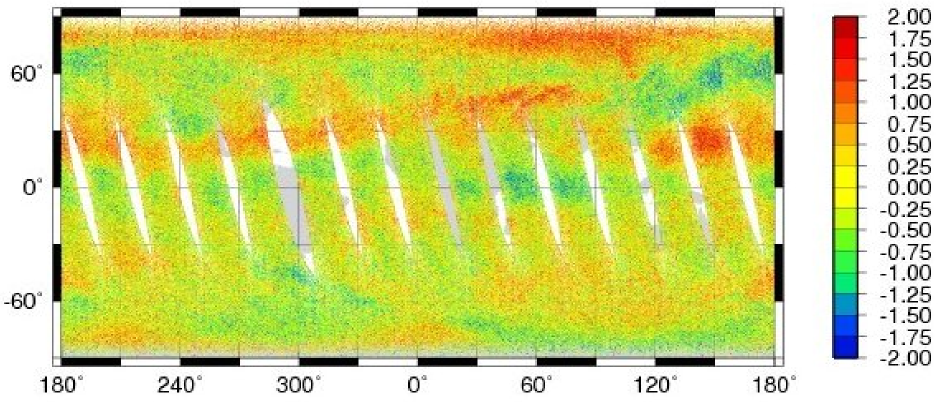
Good luck!

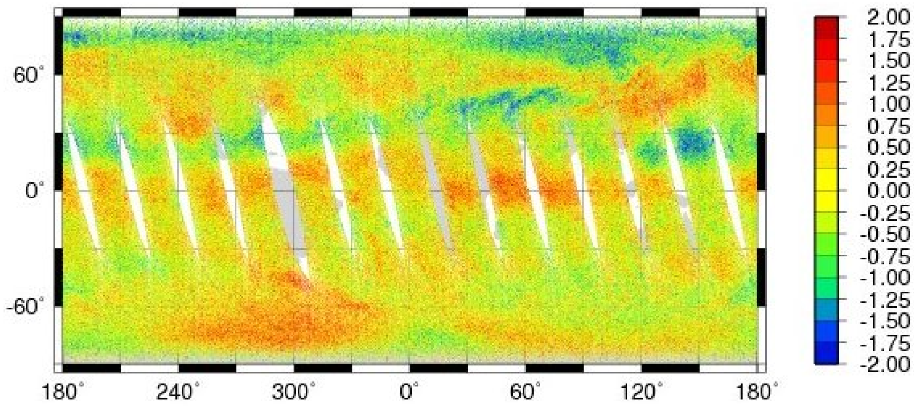
Histogram of normalised residual at 820 cm-1



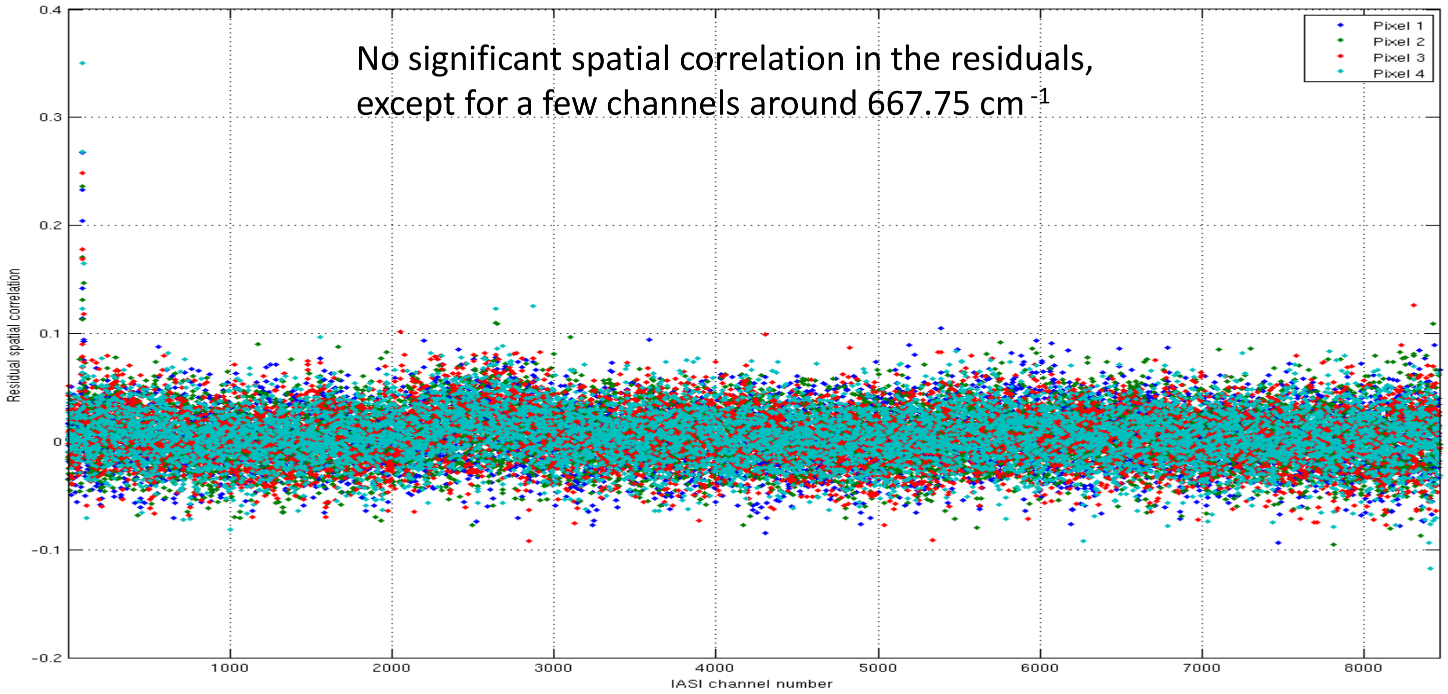

Normalised residual at 820 cm-1

20090330

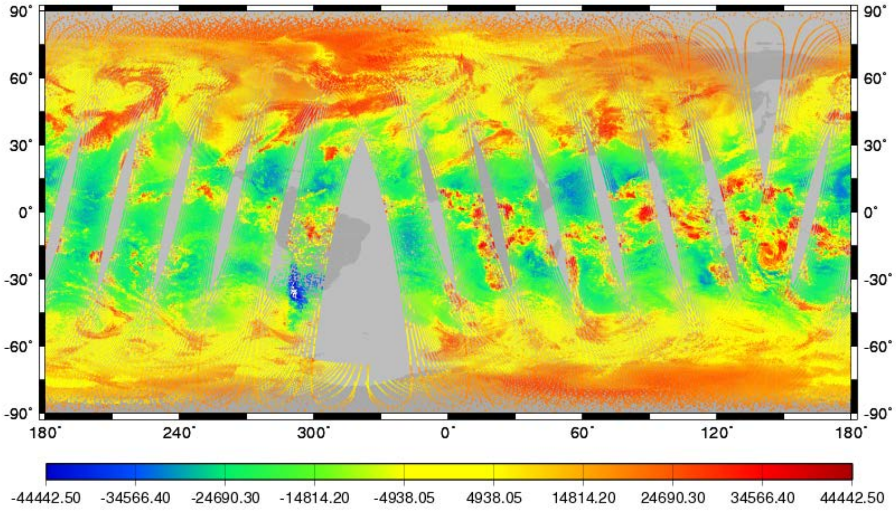

Normalised residual at 668 cm-1, 20091181 Asc. (spatial correlation 0.26)


Normalised residual at 667.5 cm-1, 20091181 Asc. (spatial correlation 0.35)

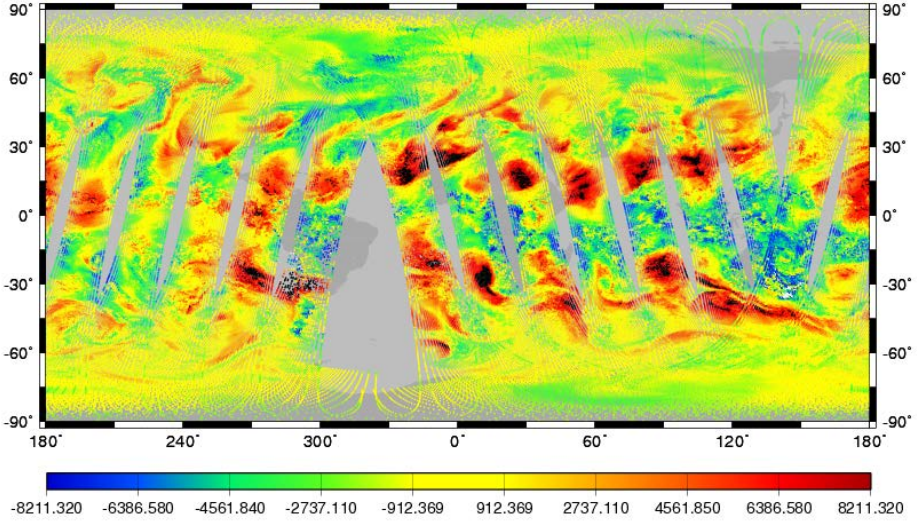
Residual spatial correlation (20110202)


No significant spatial correlation in the residuals, except for a few channels around 667.75 cm^{-1}

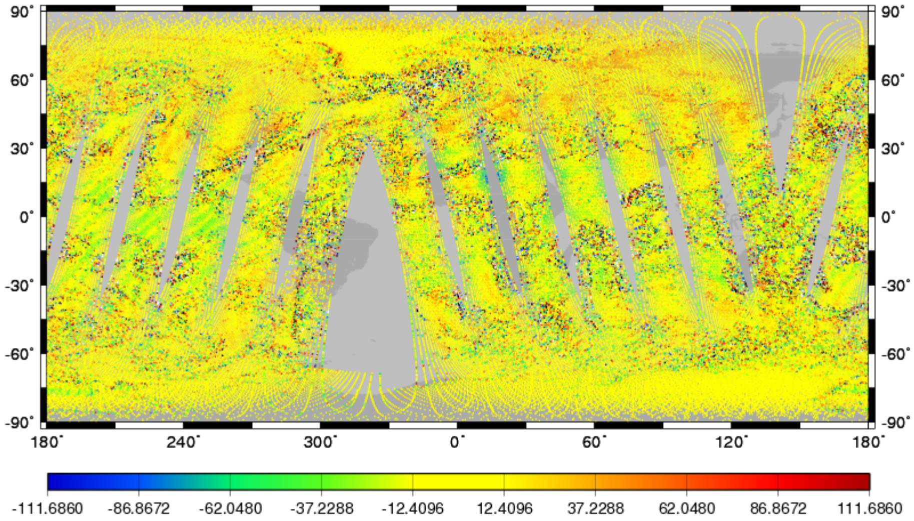
Lets look at some PC scores and guess what we see



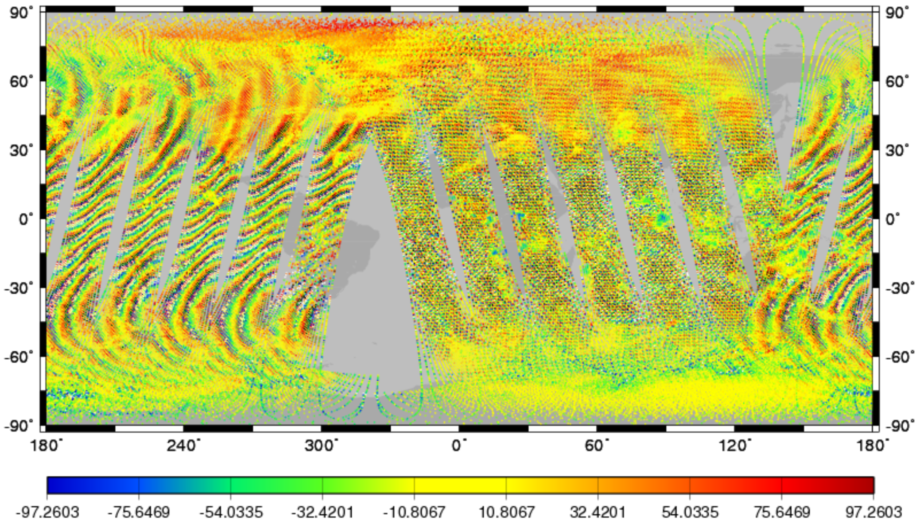
Band 2, PC score 1, Pixel 1 (20110202 12-24)



Band 2, PC score 2, Pixel 1 (20110202 12-24)



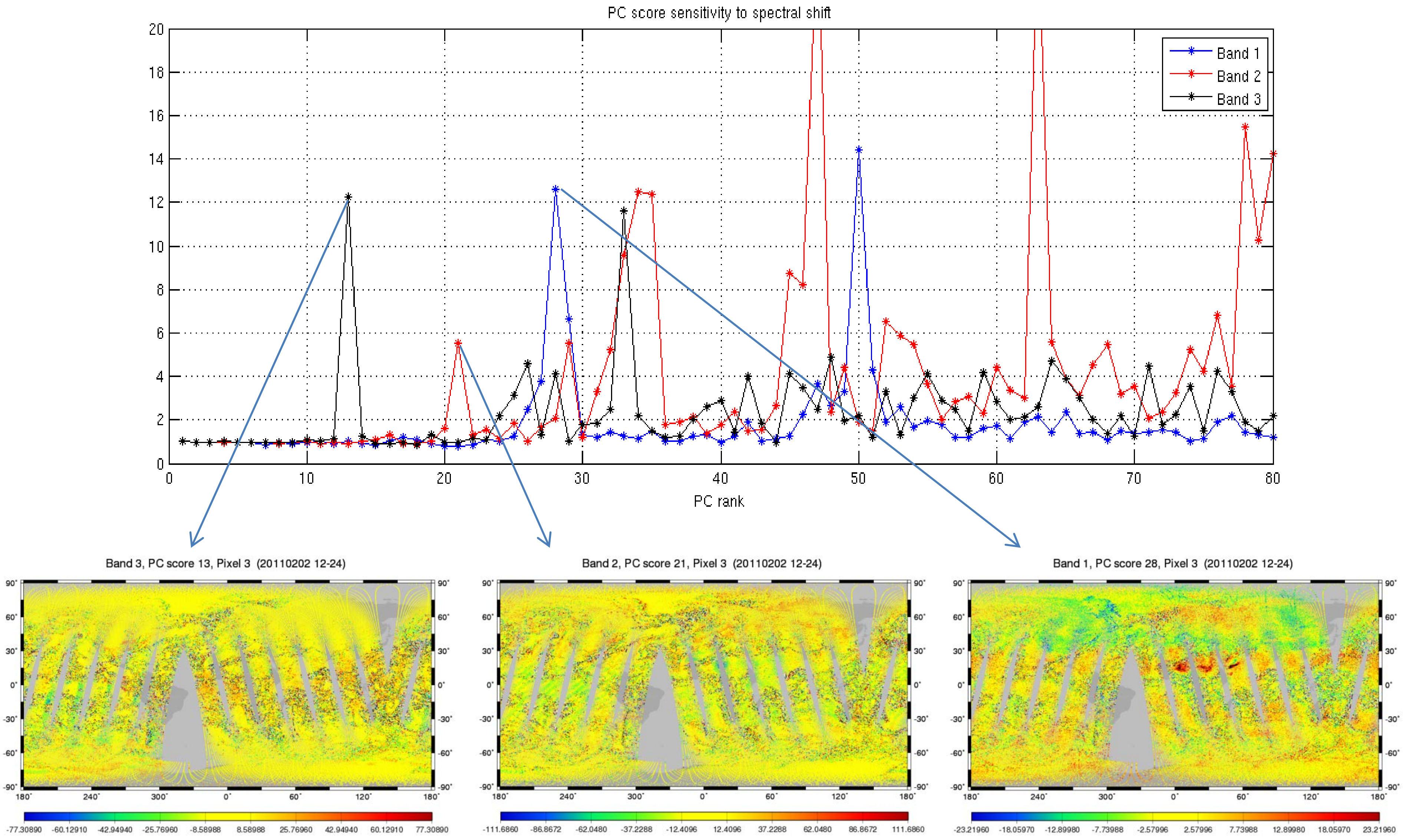
Band 2, PC score 21, Pixel 3 (20110202 12-24)



Band 2, PC score 24, Pixel 1 (20110202 12-24)

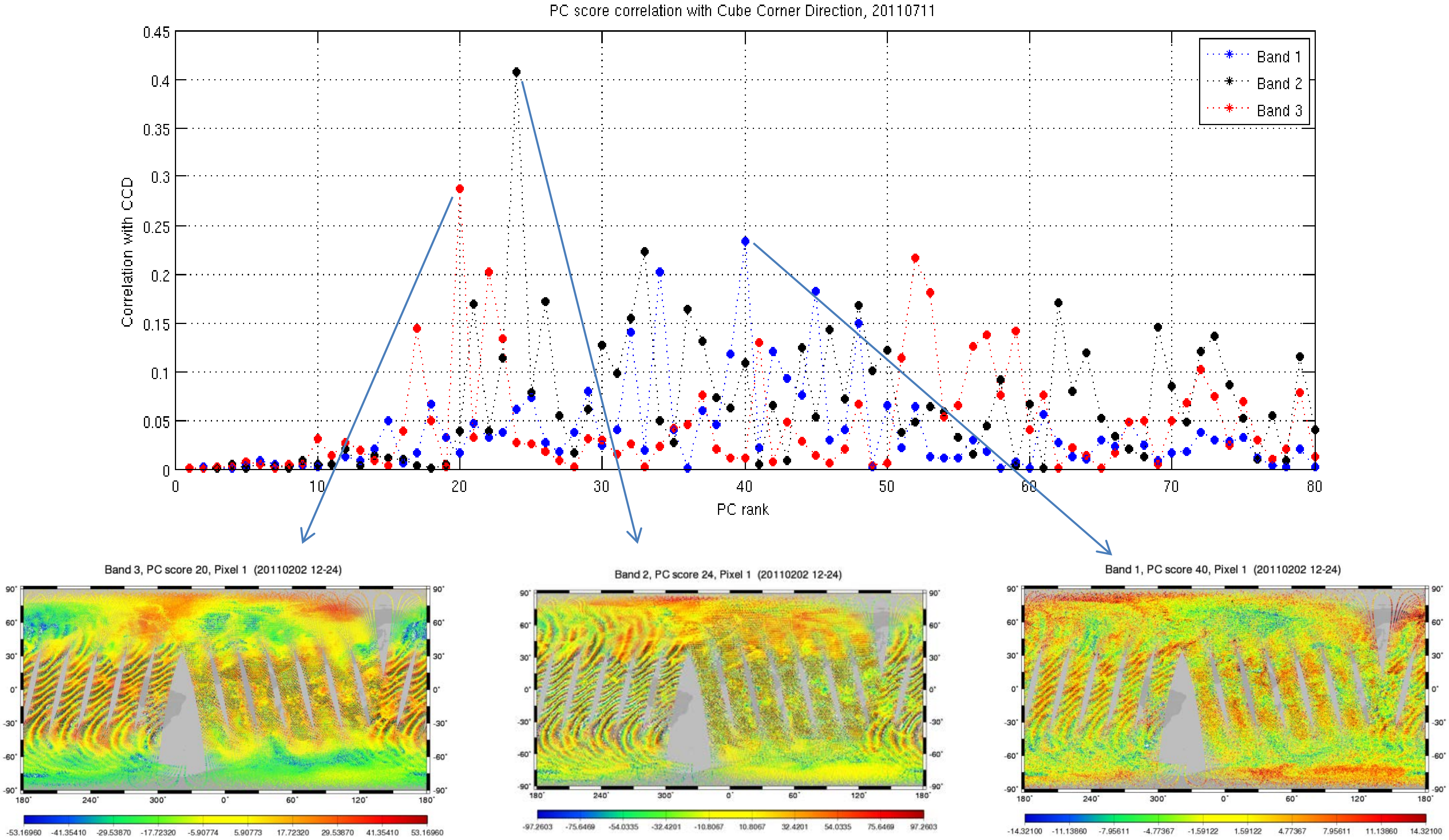
Some PC scores are very sensitive to spectral shift.

(measured by the variance of the PC score computed from spectrally shifted spectra divided by the original variance)



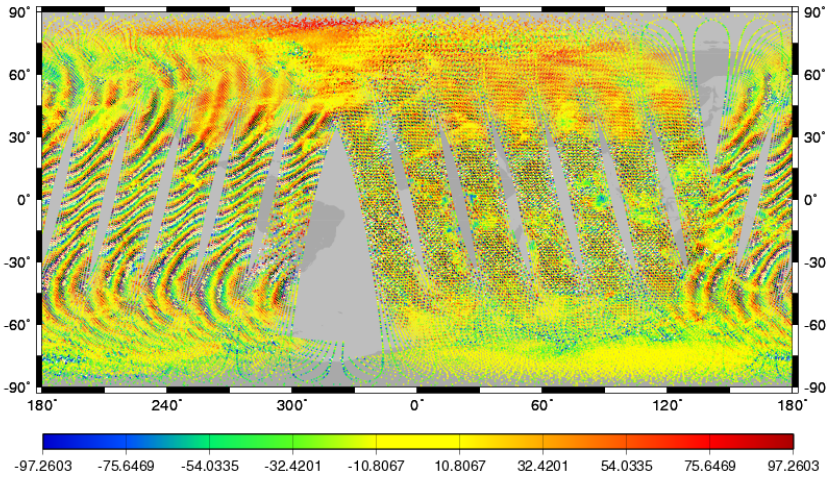
Black dots correspond to inhomogeneous fields of view ➔ non-uniform scene ILS effects

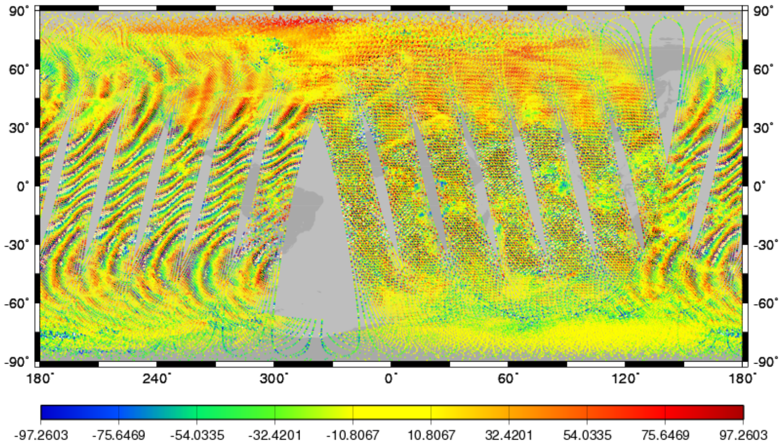
Do you think the upwelling radiance is correlated with IASI’s cube corner direction?

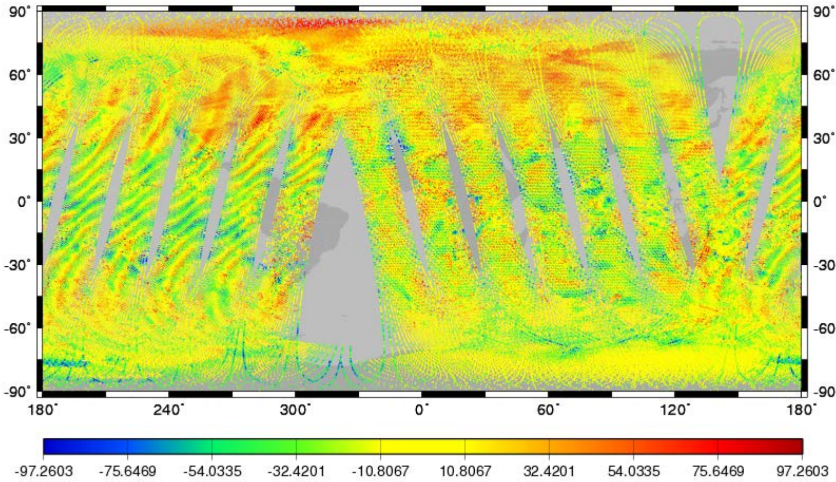


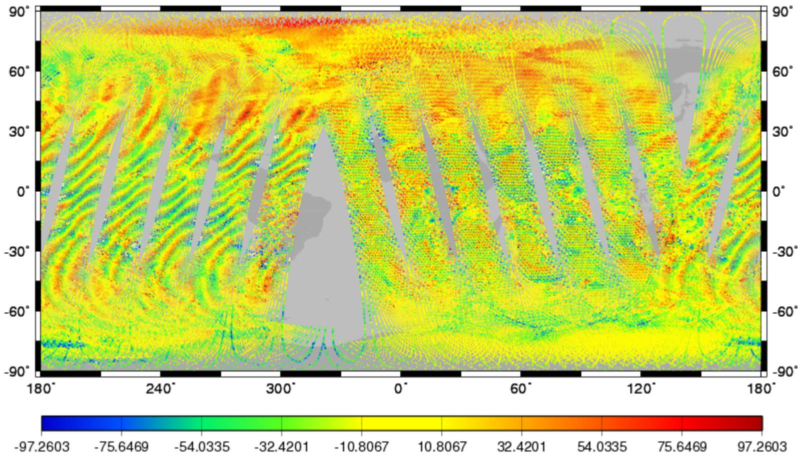
Probably not, but several directions of the measurements are!

Same PC score, 4 different detectors


Band 2, PC score 24, Pixel 1 (20110202 12-24)

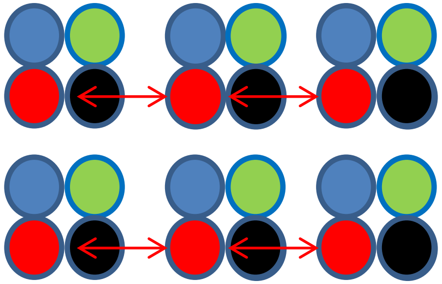

Band 2, PC score 24, Pixel 2 (20110202 12-24)

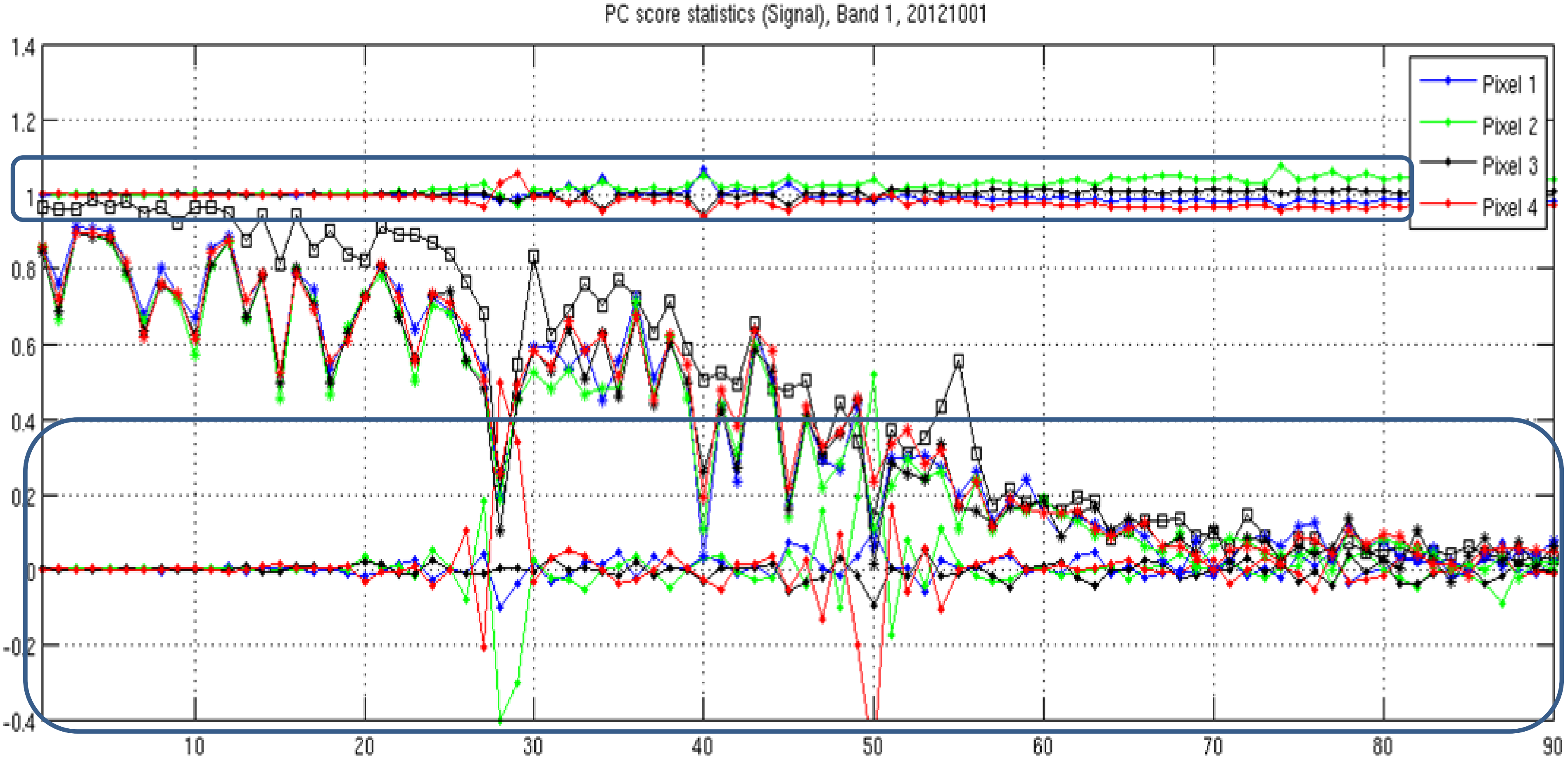

Band 2, PC score 24, Pixel 3 (20110202 12-24)

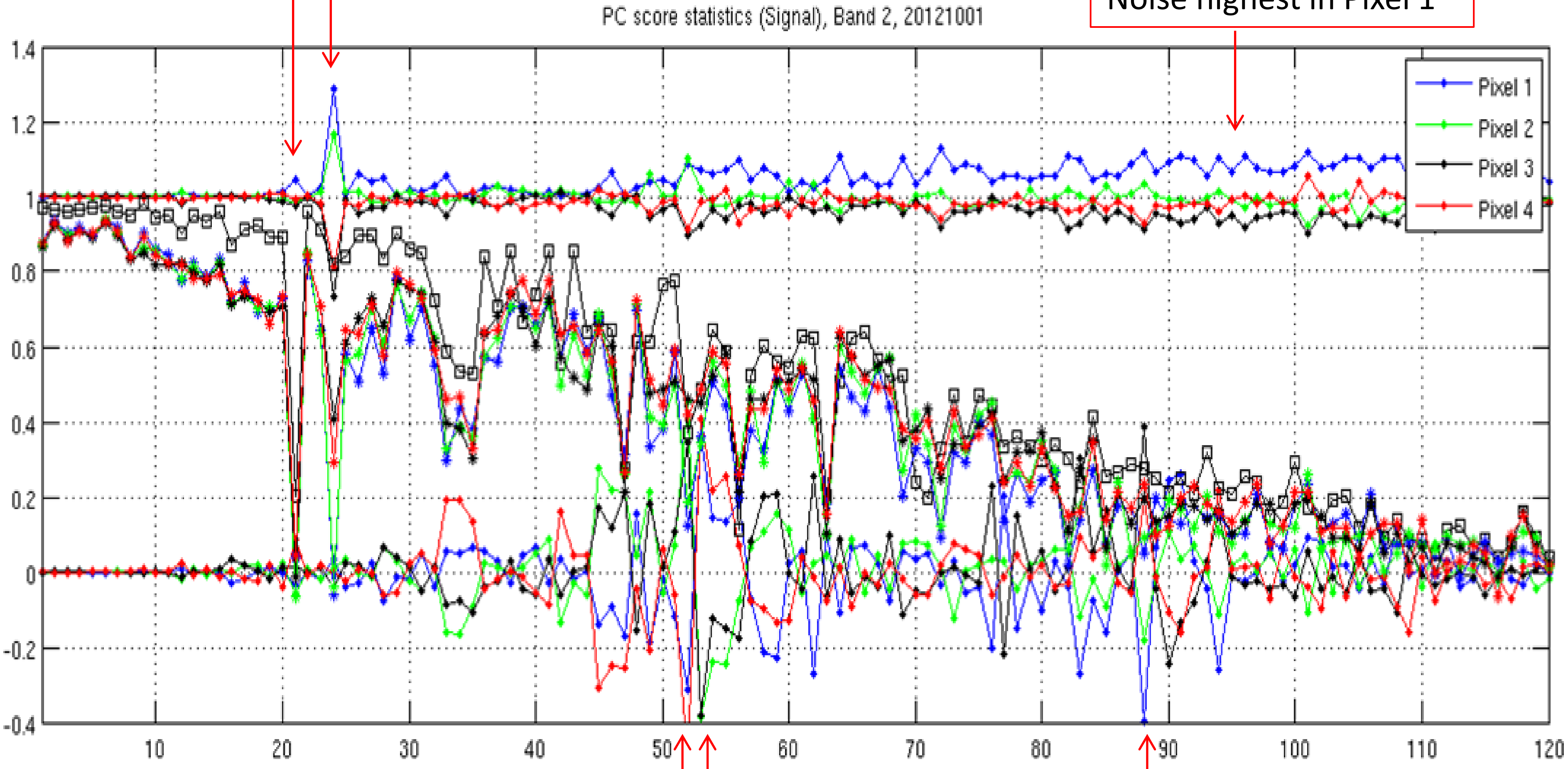

Band 2, PC score 24, Pixel 4 (20110202 12-24)

Evidence of instrument artefacts and inter-pixel differences ➔ identify the affected directions by plotting the means and standard deviations of the scores computed individually for each detector (normalised because of highly variable dynamic range of the scores)

- PC score standard deviation in each pixel (divided by average standard deviation)
- Mean of PC score in each pixel (minus average mean and divided by average standard deviation)
- Spatial correlation of PC score in each pixel
- Inter EFOV spatial correlation of PC score







Very low spatial correlation for score 21 and 24

Noise highest in Pixel 1

Several directions with very different means in the 4 pixels

The signal and forward model subspaces

$$E_S \in R^{m\times p} \qquad E_F \in R^{m\times p}$$

Spanned by truncated sets of eigenvectors

Intersection of the two subspaces is empty ➔ Compute principal angles between the two subspaces

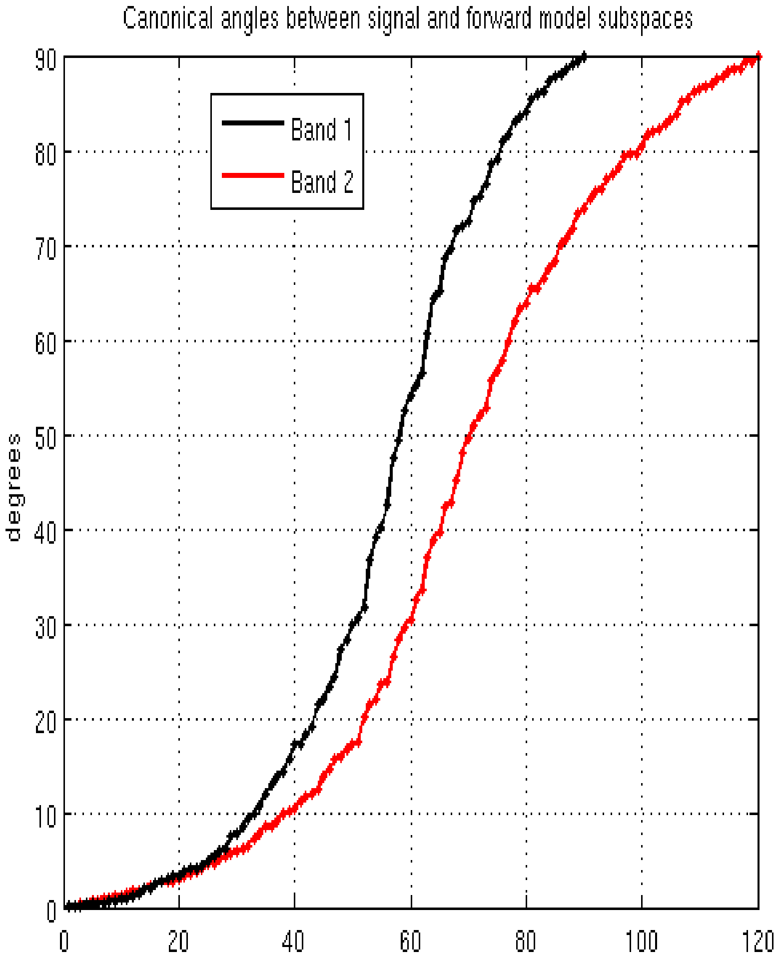
$$E_S{}^T E_F = USV^T$$

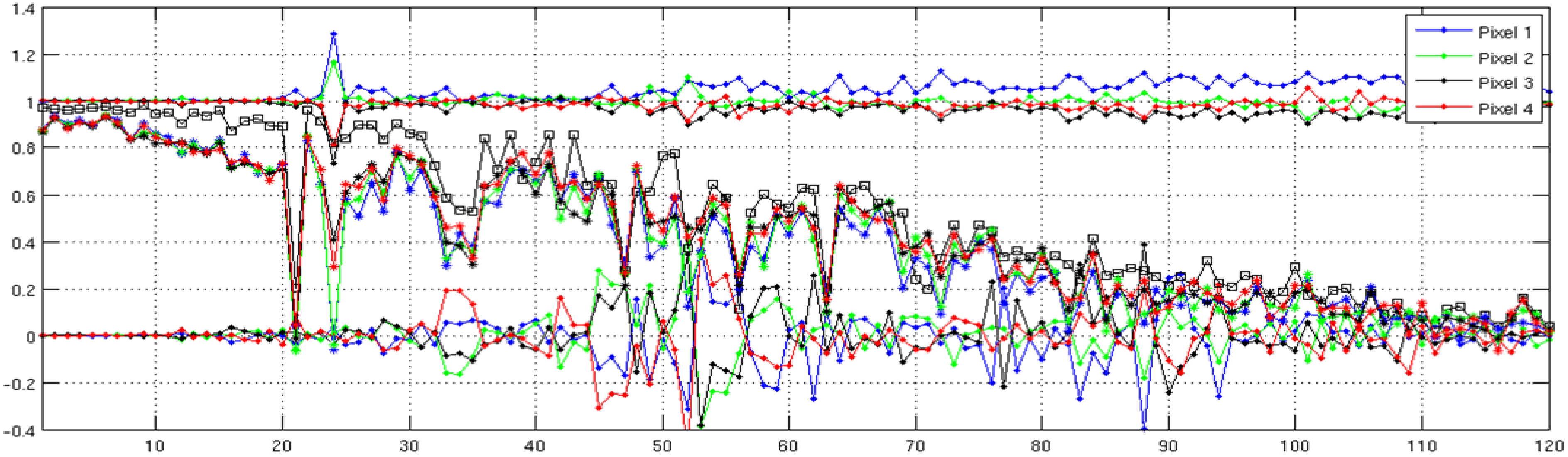
$$\widehat{E_S} = E_S U \qquad \widehat{E_F} = E_F V$$

$\hat{E}_F$ and $\hat{E}_S$ are bi-orthogonal bases for the two subspaces

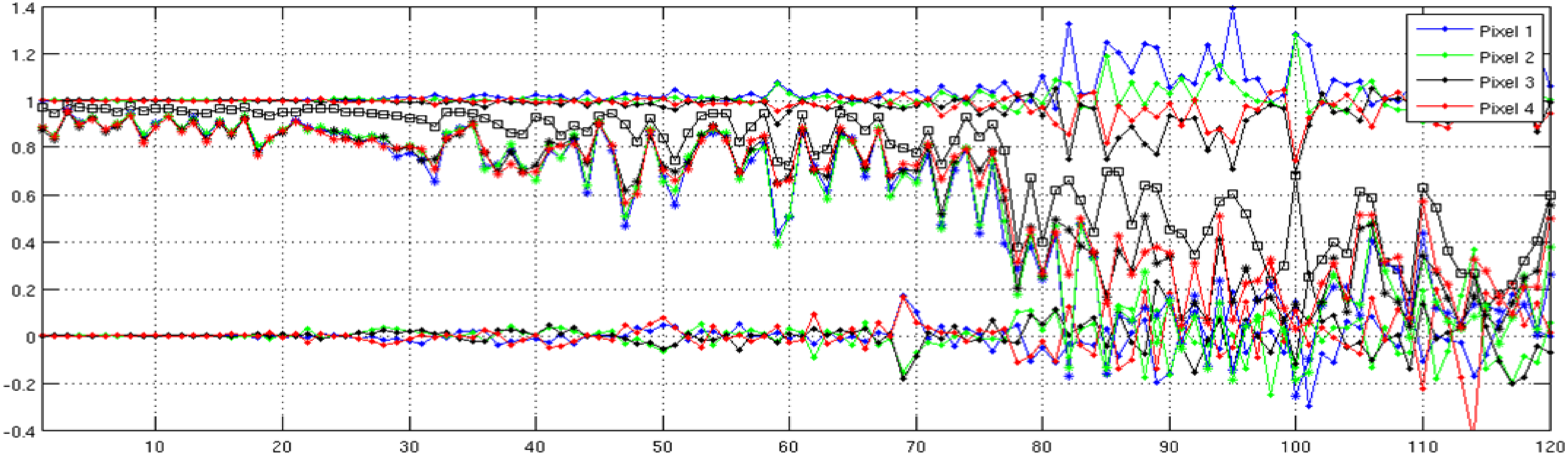
The principal angles between the two subspaces are given by $\cos^{-1}(S_{ii})$ in ascending order

New bases for the signal and forward model spaces, in which similar directions are identified and ordered according to their degree of similarity

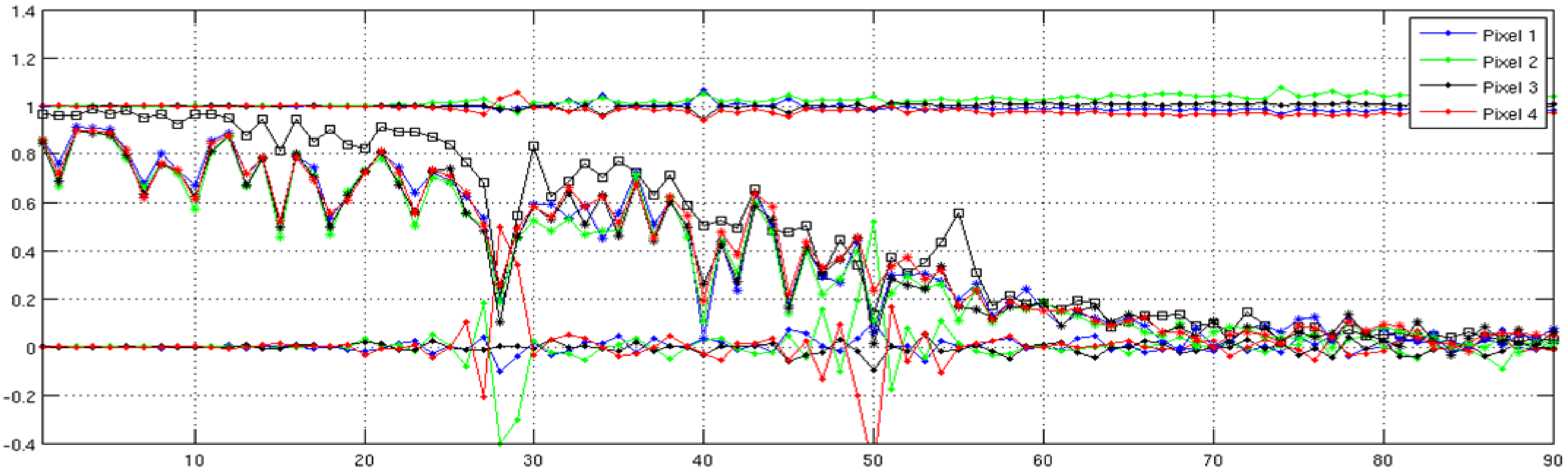


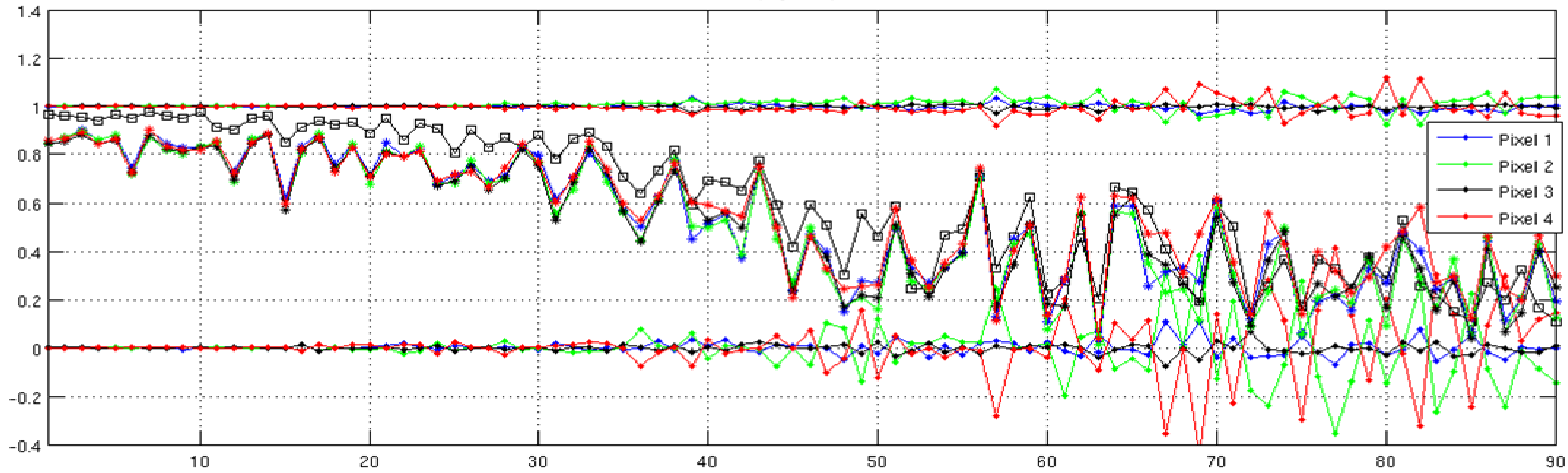


PC score statistics (Signal), Band 2, 20121001



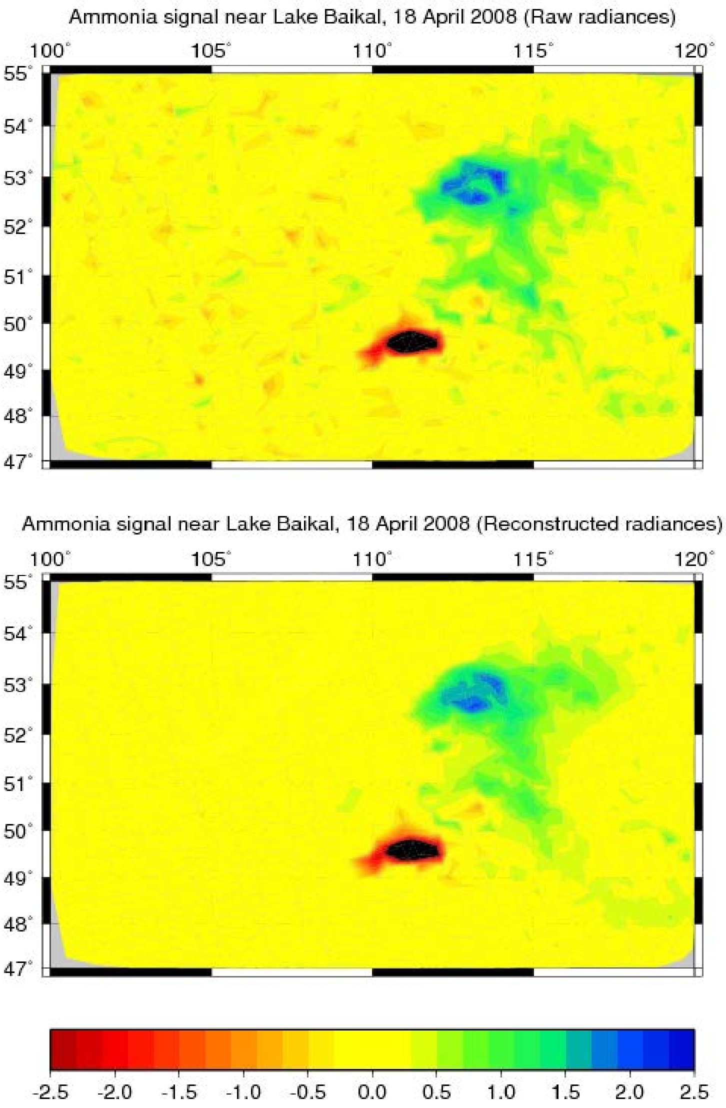
PC score statistics(Signal-F), Band 2, 20121001

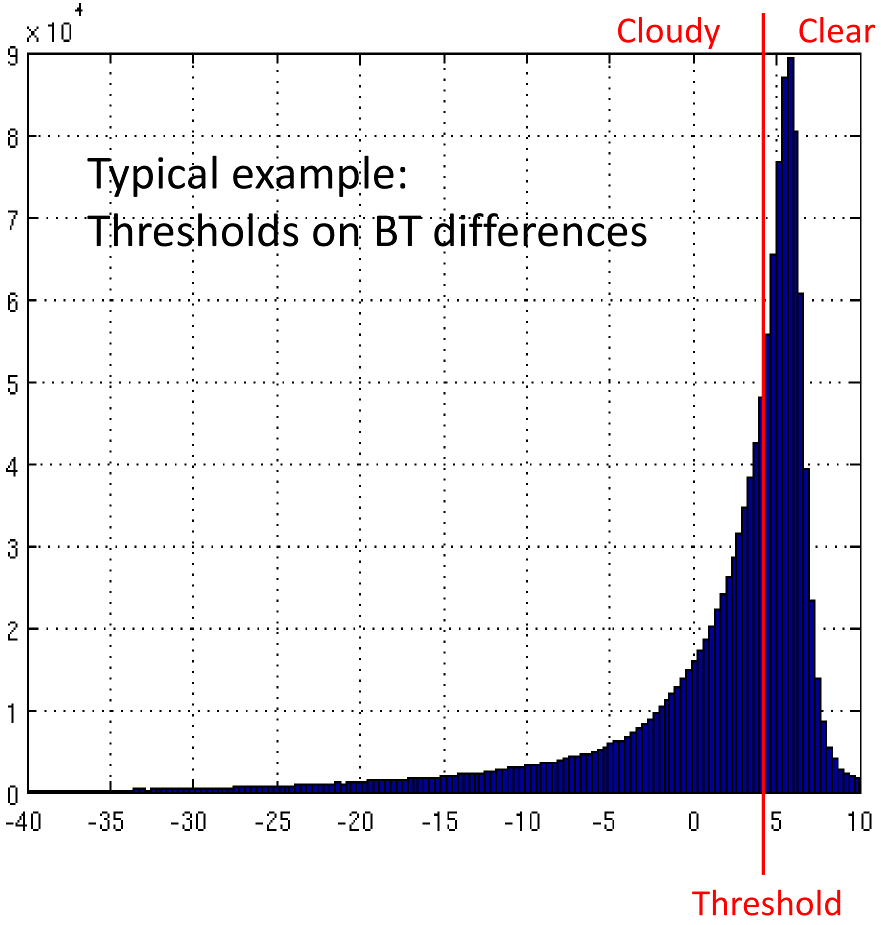

PC score statistics (Signal), Band 1, 20121001


PC score statistics (Signal-F), Band 1, 20121001

IASI data are not fully exploited

- Often better results could be obtained simply by using reconstructed instead of raw radiances
- The problem is that people expect the same results and get disappointed when in fact they get better (but different) results





Typical example:
Thresholds on BT differences

More cases close to and above the threshold than close to and below the threshold ➔ Number of cases classified as cloudy decreases after noise filtering.

Neural network retrievals taking subset of IASI channels as input

- make retrievals with raw radiances
- make retrievals with reconstructed radiances
- compare the two ➔ differences “too big” ➔ reconstructed radiances are bad (**?!**)

Should instead compare the two retrievals with an independent “truth”

➢ Due to the non-linearity of NN the best solution would be to train with reconstructed radiances

Using subset of reconstructed radiances instead of PC scores for retrieval or assimilation

The two cost functions are identical if

1. **The forward model space is a subspace of the signal space, or alternatively, the reconstructed radiances are projected onto the forward model space.**
2. **The channel subset of reconstructed radiances is chosen such that the corresponding sub-matrix of the eigenvectors is invertible**.

\+ easy to reject “contaminated channels”

\+ faster than using current PC forward models

(-) need dense linear algebra for the observation error covariance, but really you always need it

“We want to get raw radiances because we want use our own PC’s!”

-Good reasons to use own (forward model) PC’s

-But does that mean that radiances should not be disseminated using another set of PC’s?

To answer this question we look at the difference between the two scenarios:

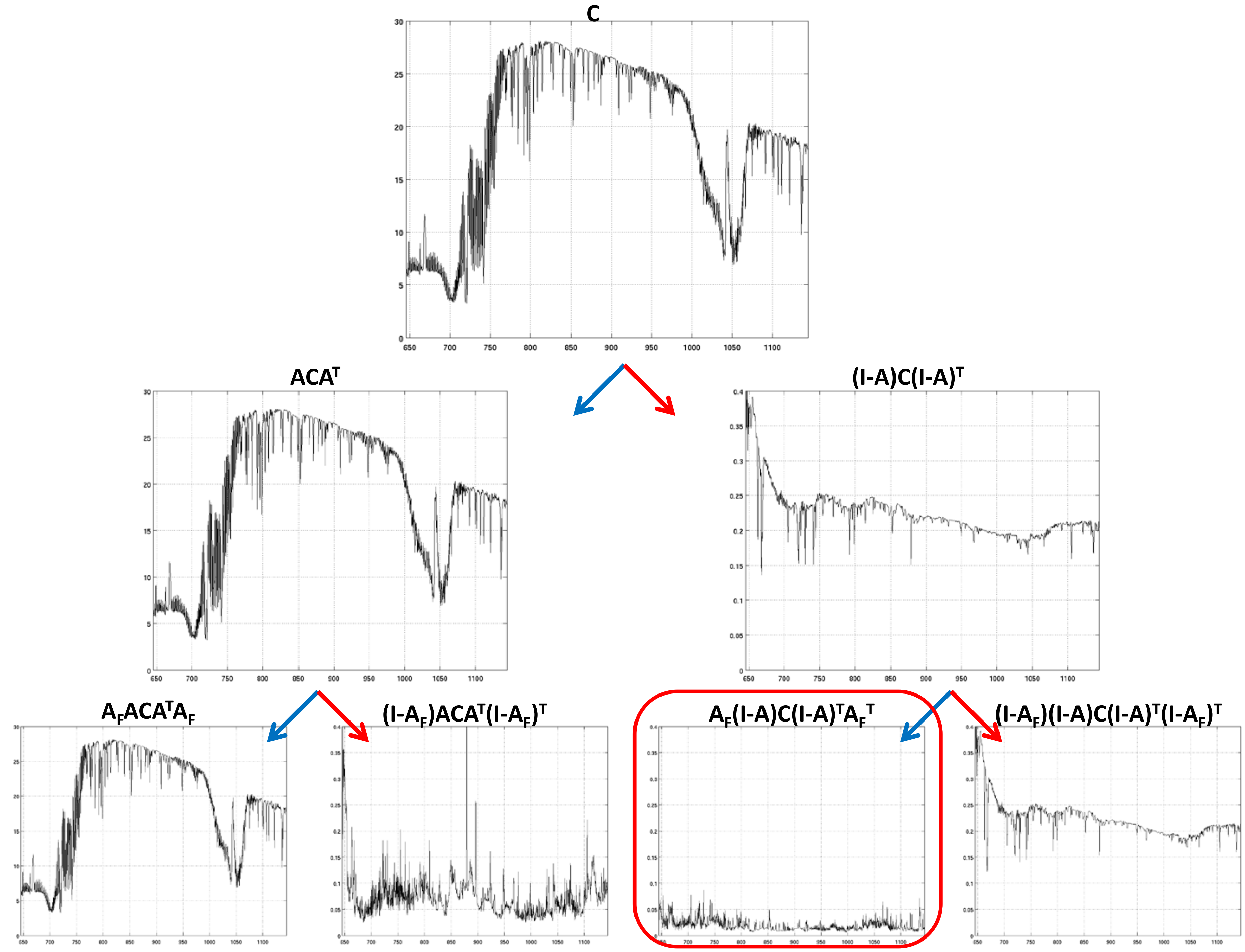
1. Projecting raw radiances onto forward model space
2. Projecting raw radiances onto signal space and then onto forward model space

- ➢ Clearly if the forward model space was a subspace of the signal space there would be no difference.
- ➢ However, this is not the case in practise! (➔ forward model produce features never seen in any real measurements)

Two interpretations of this:

a) Forward model errors

b) Signal outside the signal space (i.e. reconstruction error)



C

ACA^T

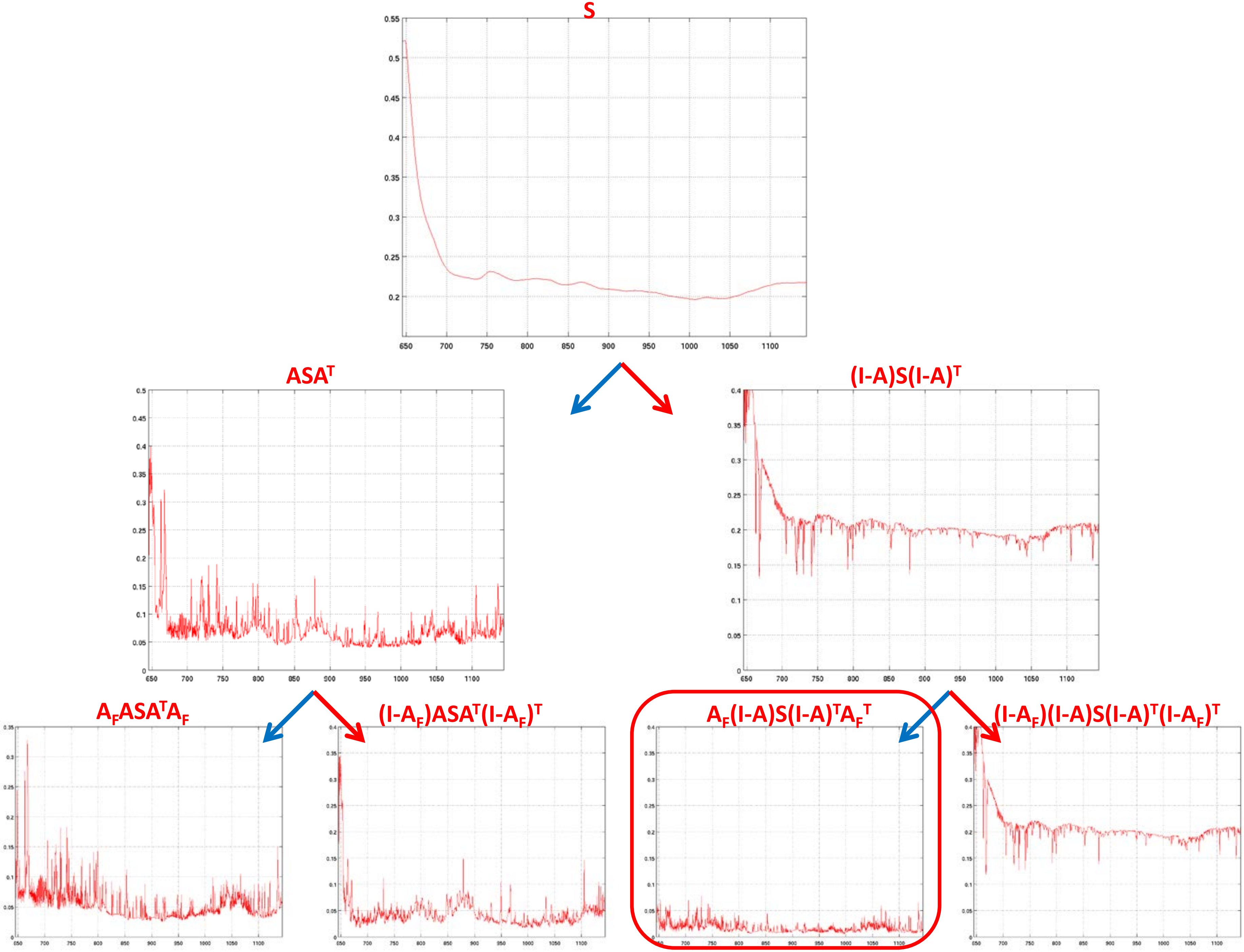
$(I-A)C(I-A)^T$

$A_FACA^TA_F$

$(I-A_F)ACA^T(I-A_F)^T$

$A_F(I-A)C(I-A)^TA_F^T$

$(I-A_F)(I-A)C(I-A)^T(I-A_F)^T$



S

ASA^T

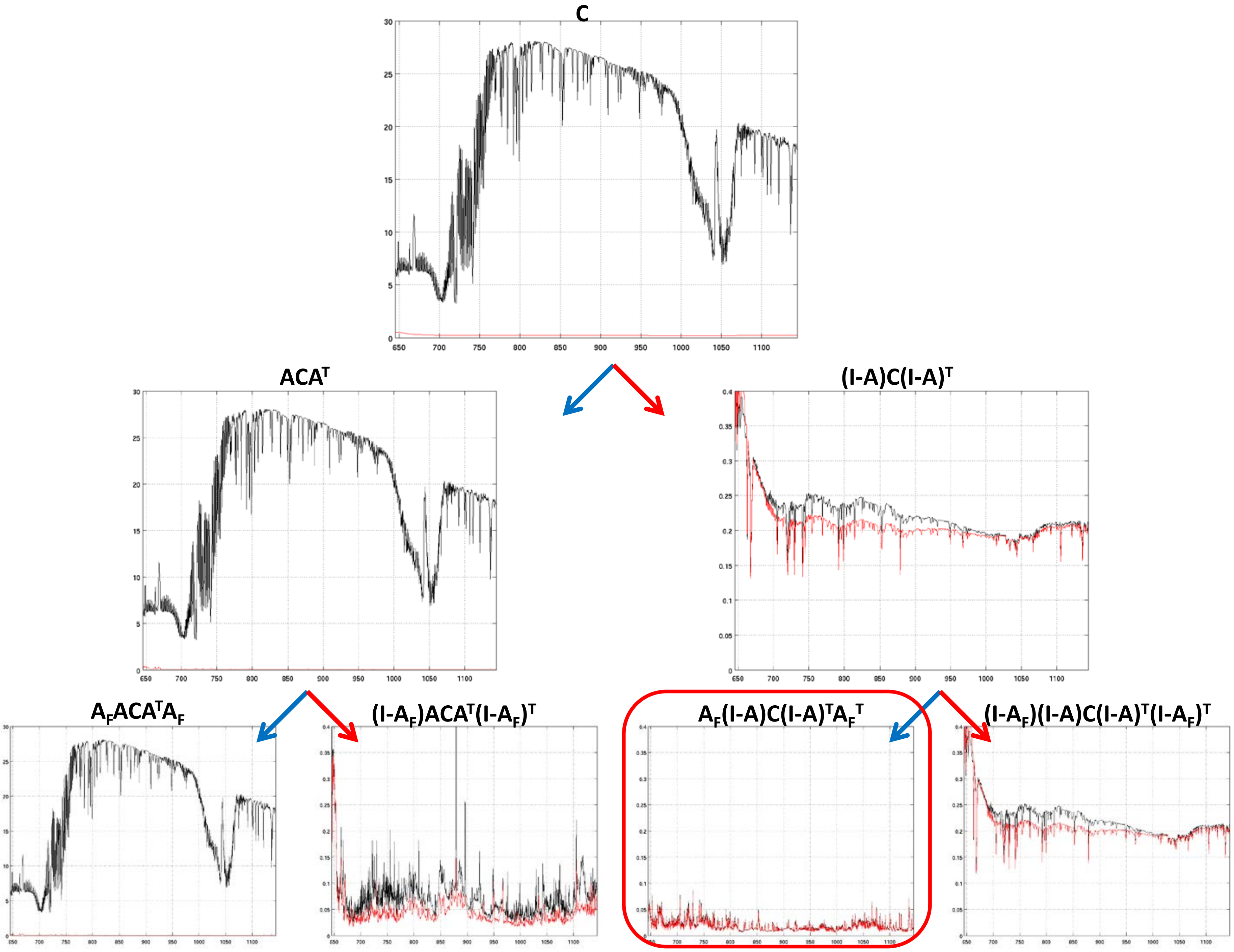
$(I-A)S(I-A)^T$

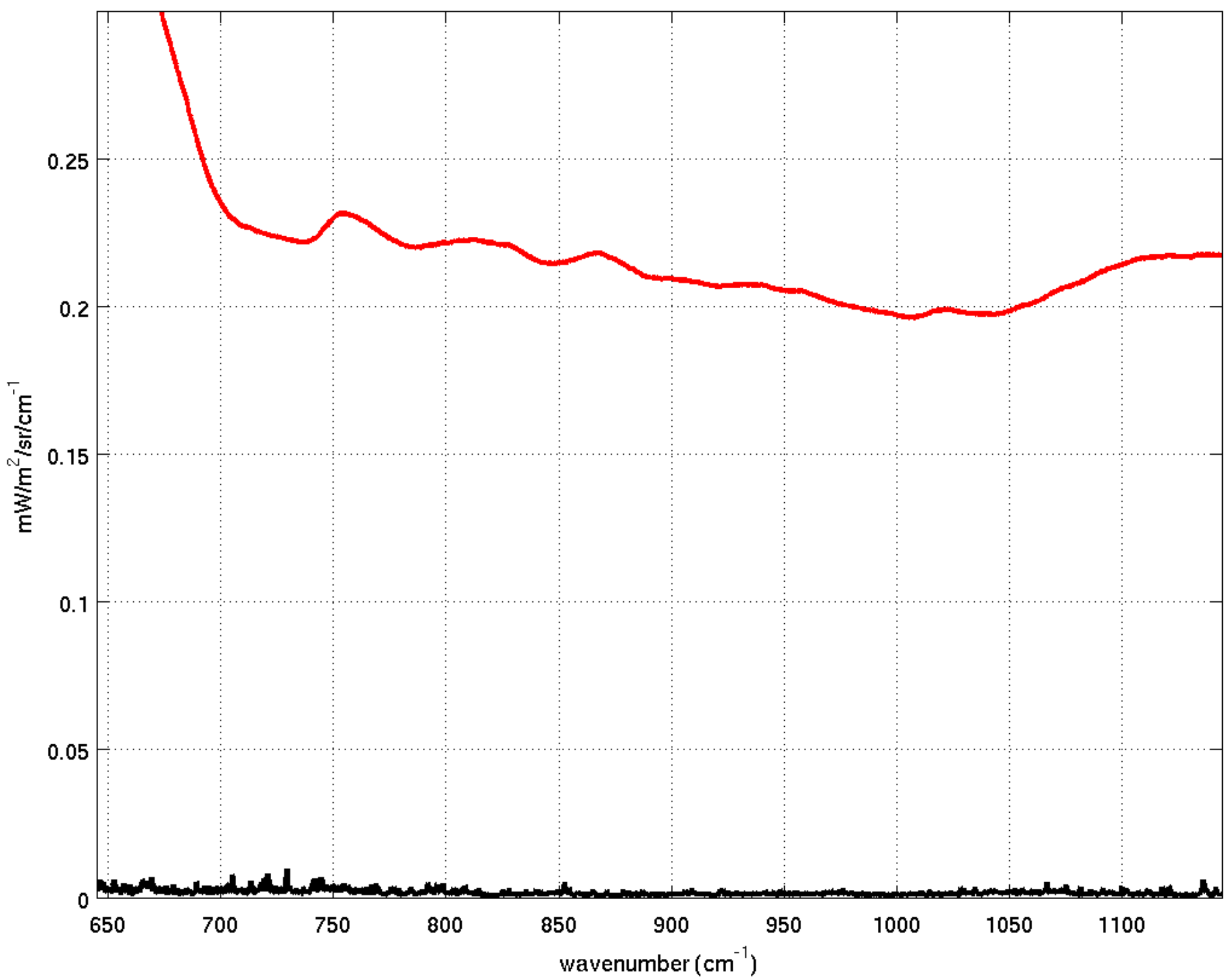
$A_F ASA^T A_F$

$(I-A_F)ASA^T(I-A_F)^T$

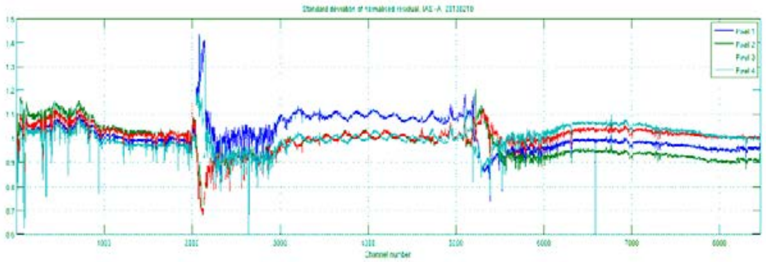
$A_F(I-A)S(I-A)^T A_F^T$

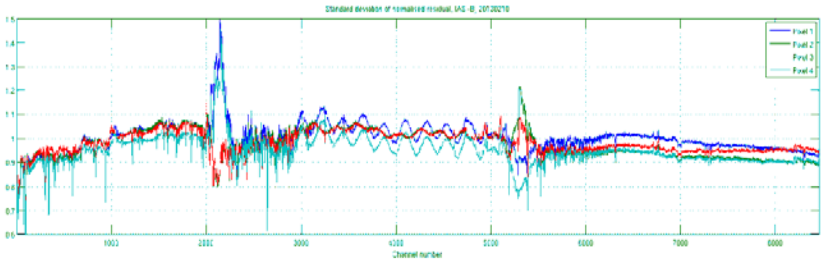
$(I-A_F)(I-A)S(I-A)^T(I-A_F)^T$

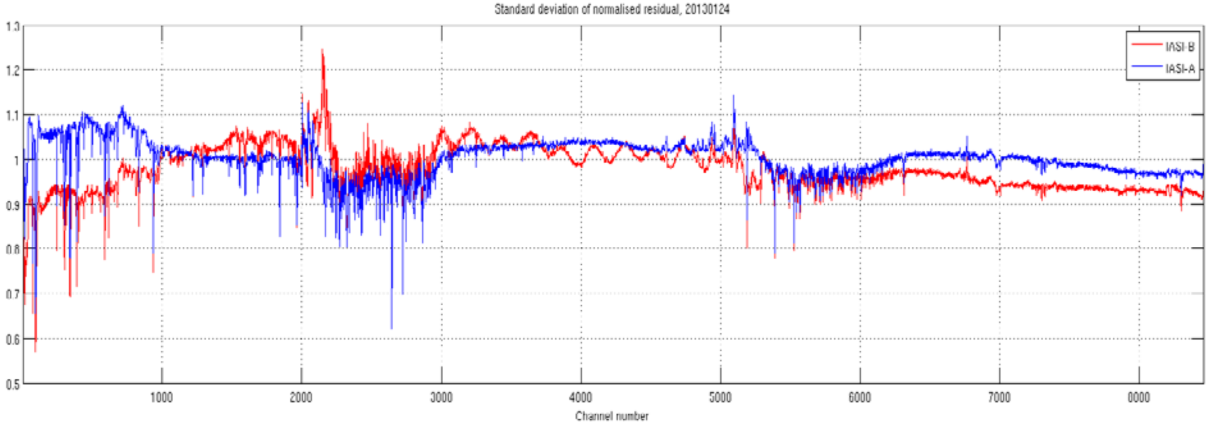


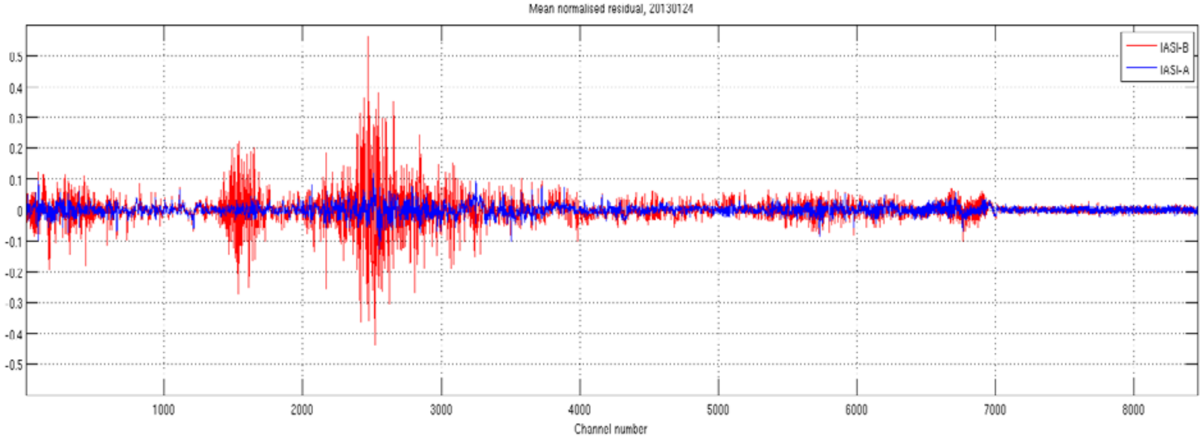

0.25
0.2
0.15
0.1
0.05
0
mW/m^2/sr/cm^{-1}
650
700
750
800
850
900
950
1000
1050
1100
wavenumber (cm^{-1})

Can PC's obtained from IASI-A spectra be used for dissemination of IASI-B spectra?



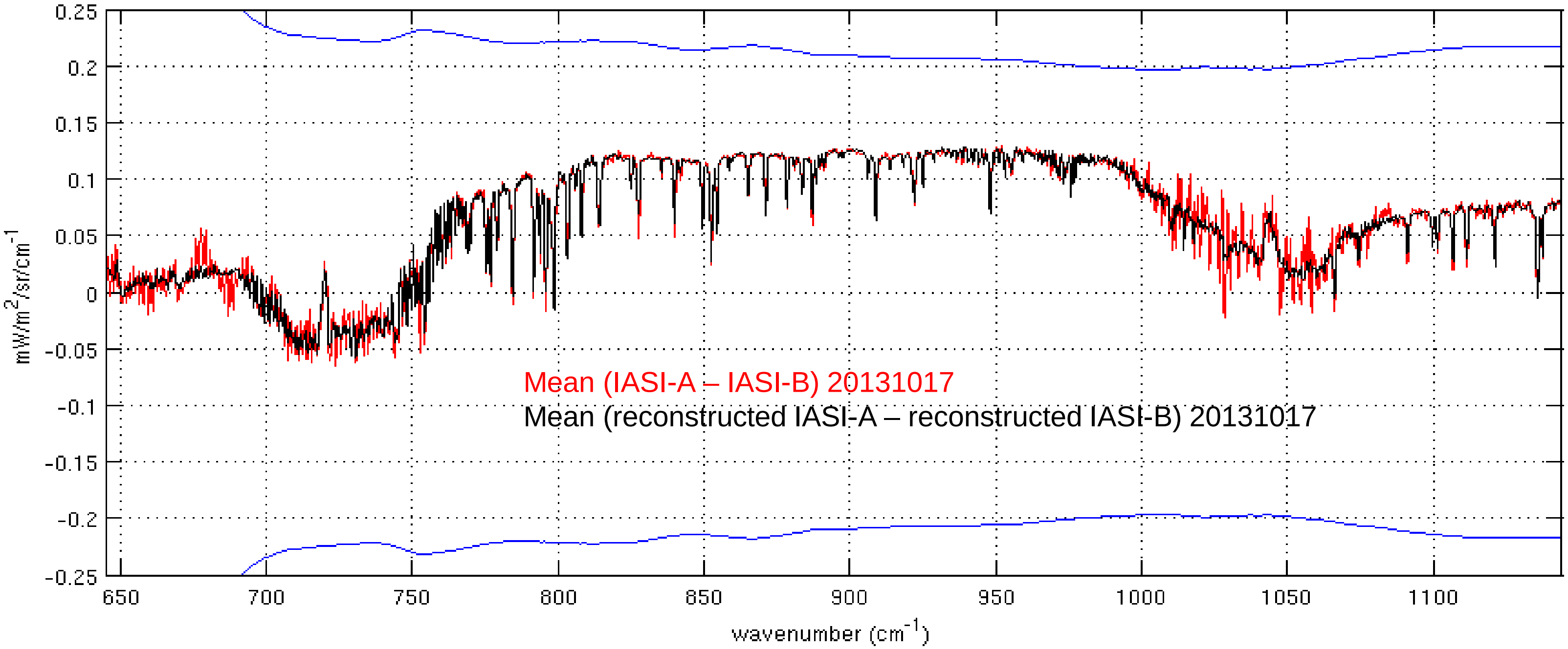




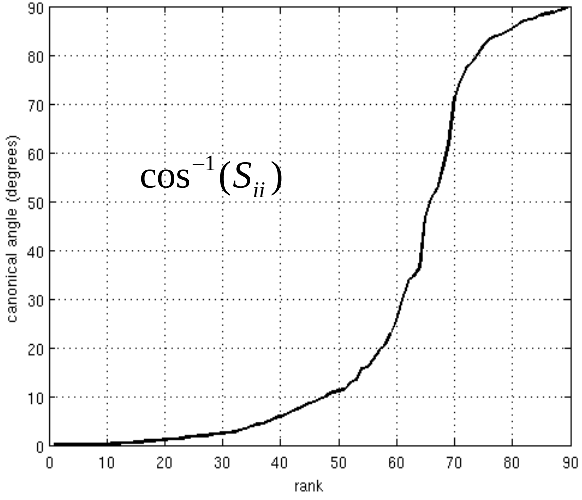


Yes. That's what we're doing and it works fine.

Ruminations on IASI-A vs. IASI-B



Canonical angels between
IASI-A and IASI-B signal spaces

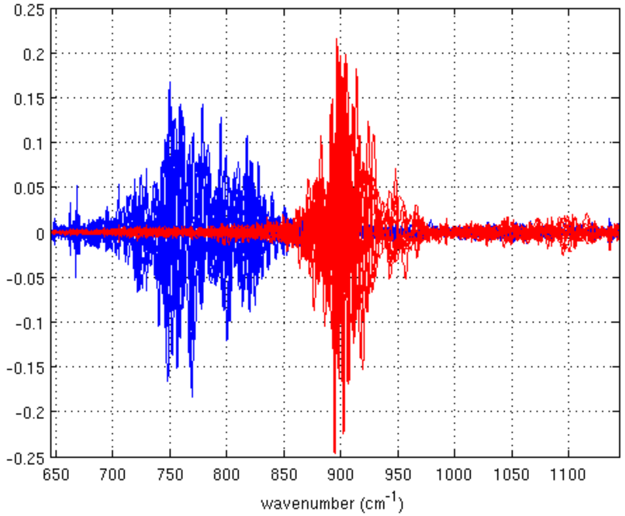


$$E_A^T E_B = U S V^T$$

$$\hat{E}_A = E_A U \qquad \hat{E}_B = E_B V$$

Eigenvectors E_A and E_B based on the covariance of a complete day of measurements from IASI-A and B

Last 10 vectors of $\hat{E}_A$
Last 10 vectors of $\hat{E}_B$



http://www.eumetsat.int/website/home/Data/Products/Level1Data/

***IASI Level 1 PCC Product Generation Specification*, EUM.OPS-EPS.SPE.08.0199**

***IASI Level 1 PCC Product Format Specification*, EUM.OPS-EPS.SPE.08.0195**

IASI Principal Component Compression (IASI PCC) FAQ

Eigenvectors shared with EARS-IASI (NWPSAF collaboration(Nigel Atkinson, Fiona Smith))

Dissemination of Metop-A IASI PC scores on EUMETCast since 2010.08.05

- **IASI PCC Eigenvector files - Band 1,2 and 3 (HDF5) 1.3**
- ***EPS Product Validation Report: IASI L1 PCC PPF (Part 1),* EUM/OPS-EPS/REP/10/0148**

Metop-A IASI PC scores product operational since 2011.02.22

- **IASI PCC Eigenvector files - Band 1,2 and 3 (HDF5) 1.4**
- ***EPS Product Validation Report: IASI L1 PCC PPF (Part 2),* EUM/OPS-EPS/REP/11/0036**

Metop-B IASI PC scores product operational since 2013.03.12

- ***Product validation report. IASI PCC for Metop-B,* EUM/RSP/TEN/13/691073**

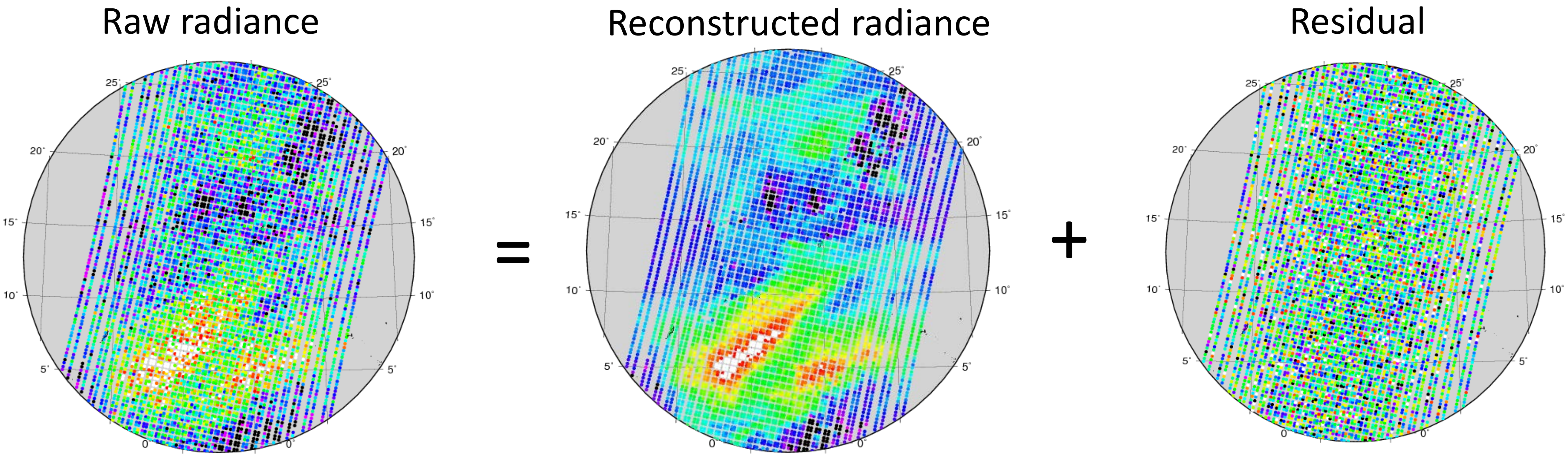
Conclusions

- no serious compression without noise removal ➔ danger of removing signal as well ➔ however except for extremely rare cases detected by the residual RMS and 5 channels around 667.75 cm very little sign of this can be found in the residuals

- quality control of L1C spectra possible with the residual RMS

- decomposing spectra in the directions of the eigenvectors reveals small but undesired artefacts very clearly

- IASI measurements not exploited to their full potential, because users (of channel subsets) insist on keeping all the noise


Raw radiance = Reconstructed radiance + Residual

(IASI radiance @1772.75 cm^{-1} 20130717)

The end

Extra slides →

Why do we use separate PC’s for each of the three IASI bands?

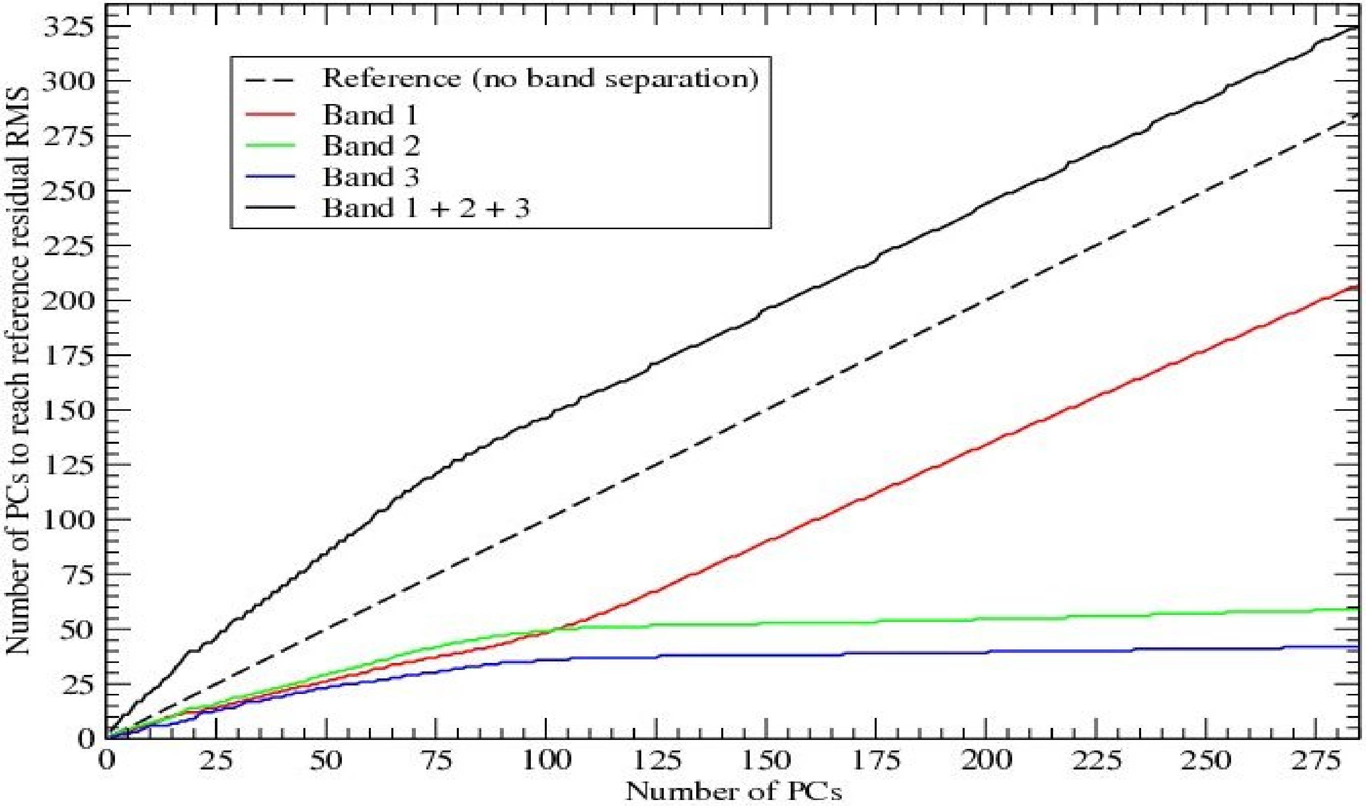
➔If one band (typically band 3) is of bad quality we can disseminate good PC scores from the other bands

\+ Compression/decompression is faster

\- About 40 extra PC scores are needed

```
Band 1  channel#    0 to 1996 (1997)      Band 1:  645.00 – 1144.00 cm-1
Band 2  channel# 1997 to 5115 (3119)      Band 2: 1144.25 - 1923.75 cm-1
Band 3  channel# 5116 to 8460 (3345)      Band 3: 1924.00 – 2760.00 cm-1
```

Experiments show that about 40 PC scores less would be needed to reach the same level of residual RMS as with band separation ➔



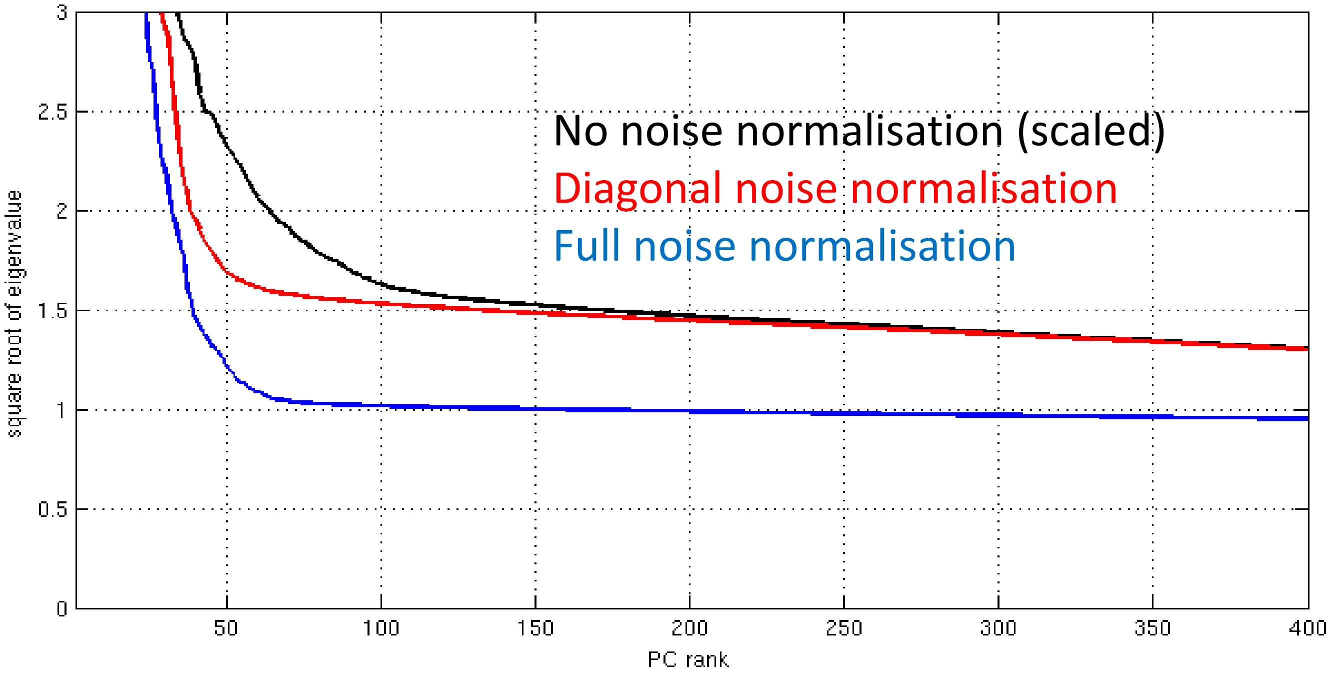
Noise normalisation

Diagonal noise normalisation matrix.

- noise does not get de-correlated ☹
- it works, but is suboptimal and should be changed (Nigel Atkinson, Fiona Hilton)

N equal to the matrix square root of the instrument noise covariance matrix.

- the correlated L1C noise gets normalised and de-correlated.
- equivalent to de-apodising prior to compression
- ensures that same amount of noise is carried by all eigenvectors ☺



$y = y_0 + \varepsilon_y$ Measured radiances = “true radiances” + noise

$p = E^T N^{-1}(y - \bar{y})$ PC scores

$\tilde{y} = NEp + \bar{y}$ Reconstructed radiances

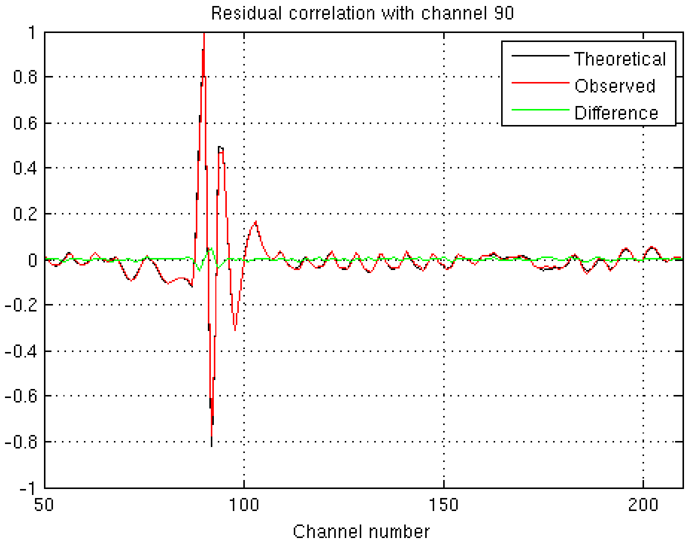
$A_y = NEE^T N^{-1}$ (short hand notation)

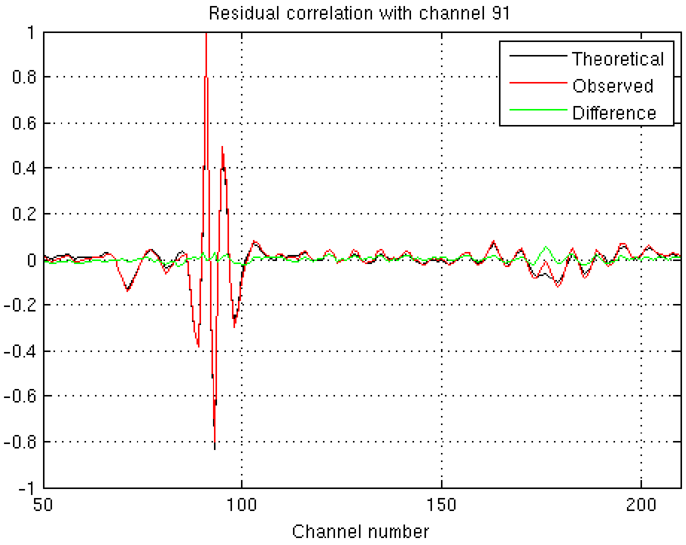
$$\tilde{y} = A_y(y - \bar{y}) + \bar{y} = A_y y + (I - A_y)\bar{y}$$

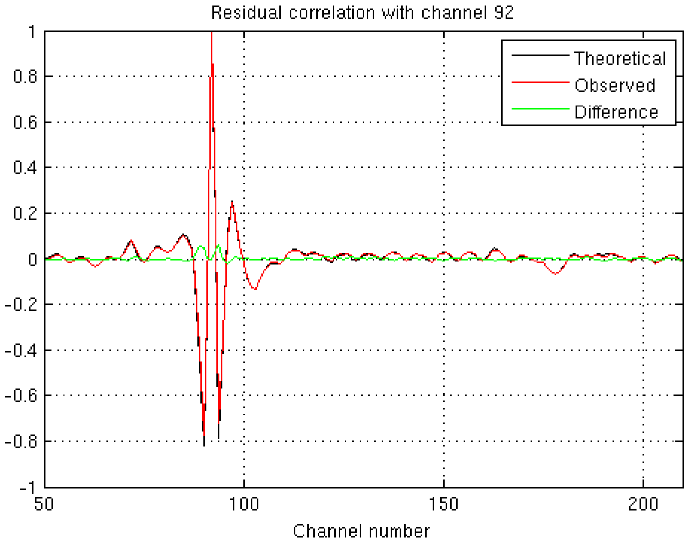
a projection (a linear transformation *P* from R^{8461} to itself such that $P^2 = P$)

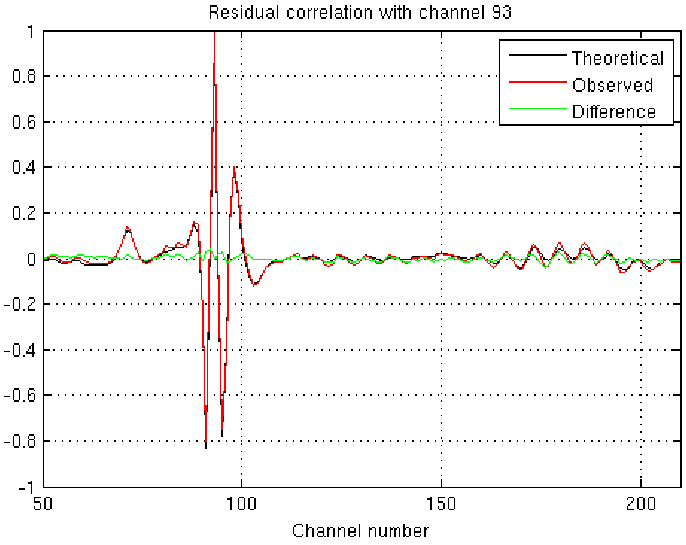
two orthogonal subspaces providing a unique decomposition of each spectrum

range(P) *Signal space*
kernel(P) *Noise space*


Residual correlation with channel 90


Residual correlation with channel 91


Residual correlation with channel 92


Residual correlation with channel 93

Practical issues

- Execution speed

  Compress/reconstruct many spectra simultaneously, i.e. use matrix-matrix multiplications instead of matrix-vector multiplications

- $E^T N^{-1}$ and NE can be pre-computed

  No execution time penalty for using non-diagonal N / N^{-1}

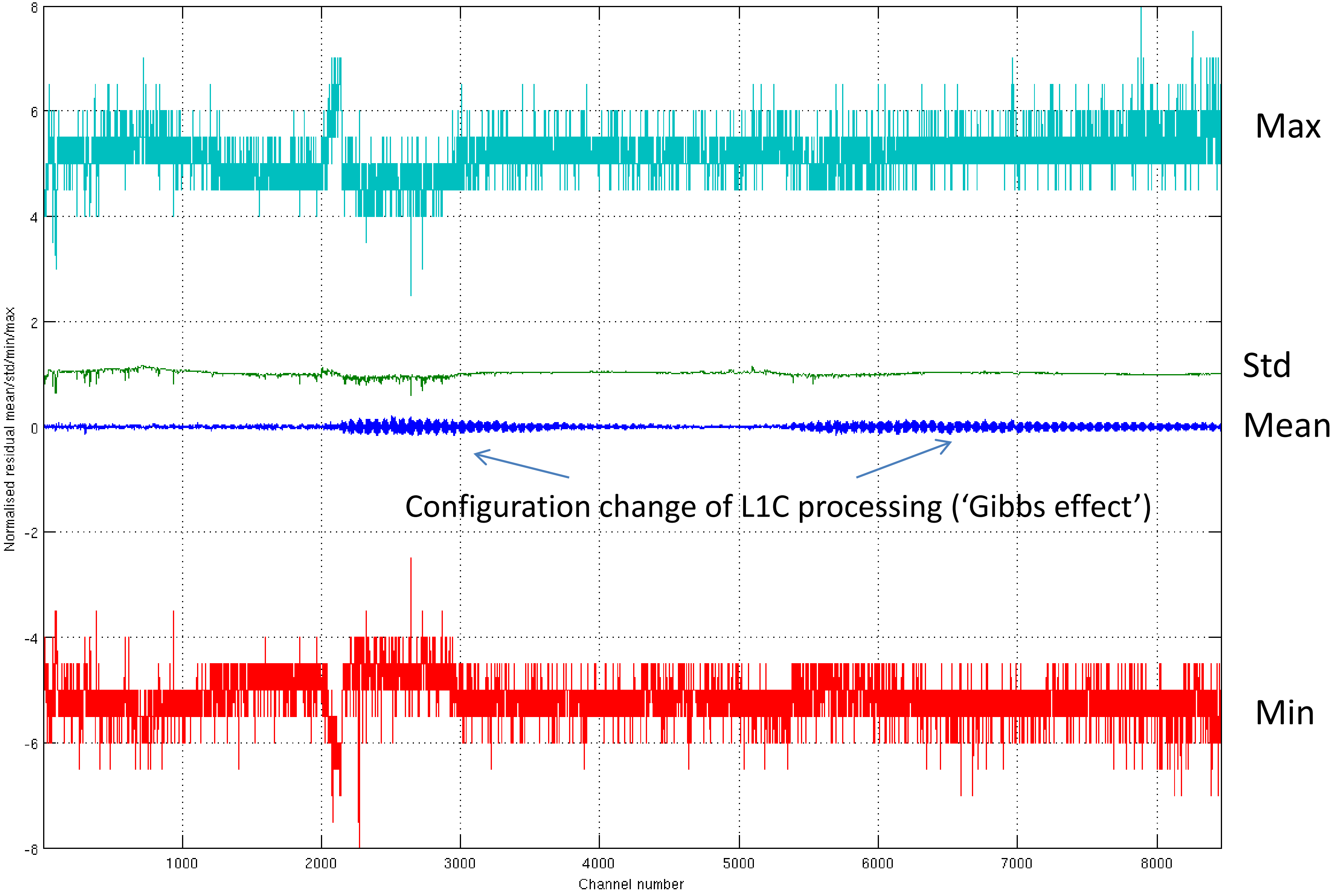
- Quantisation of PC scores

  Dynamic range of PC scores decreases with the rank, most scores can be stored in one byte

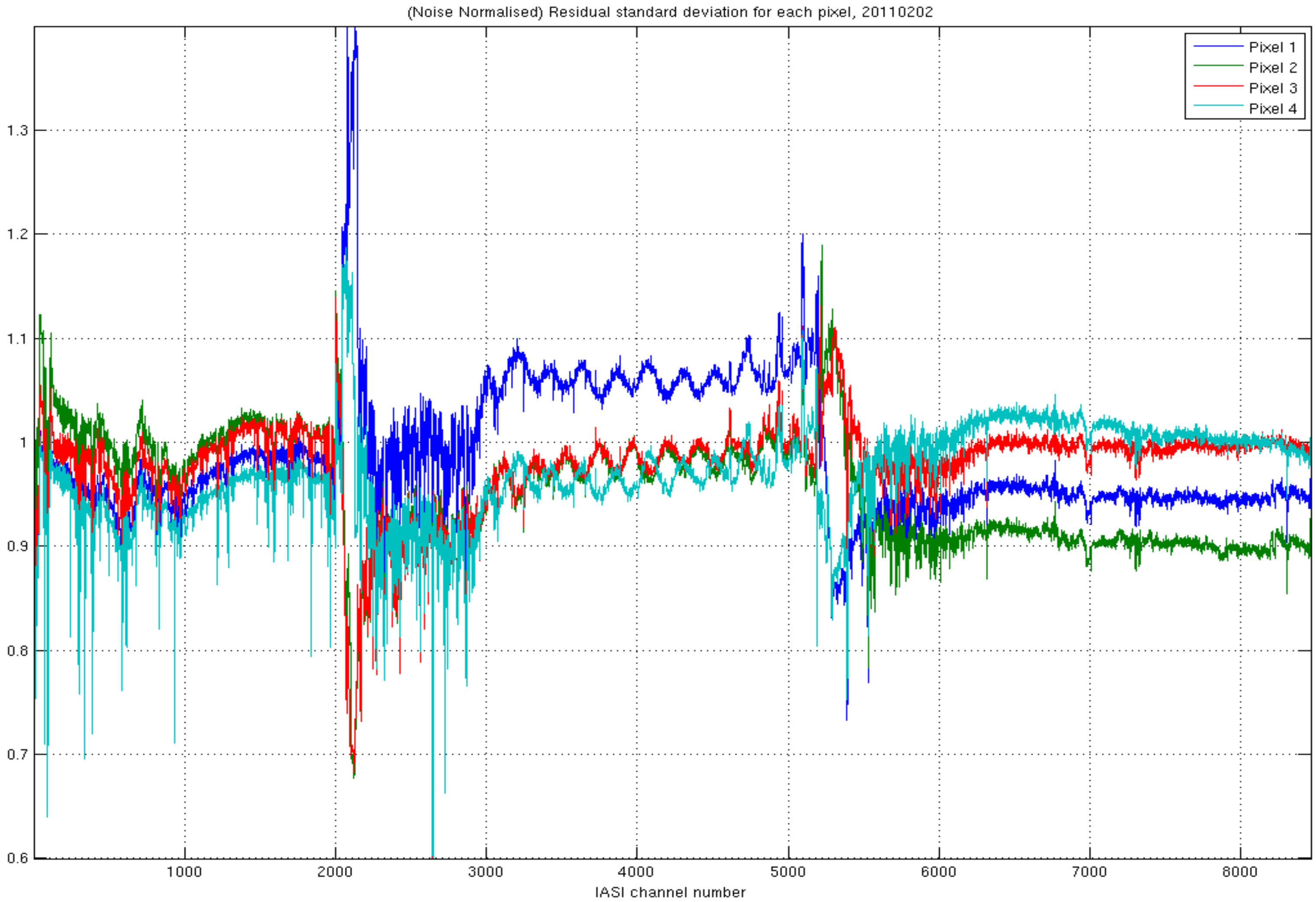
- Use update formulas for covariance matrix

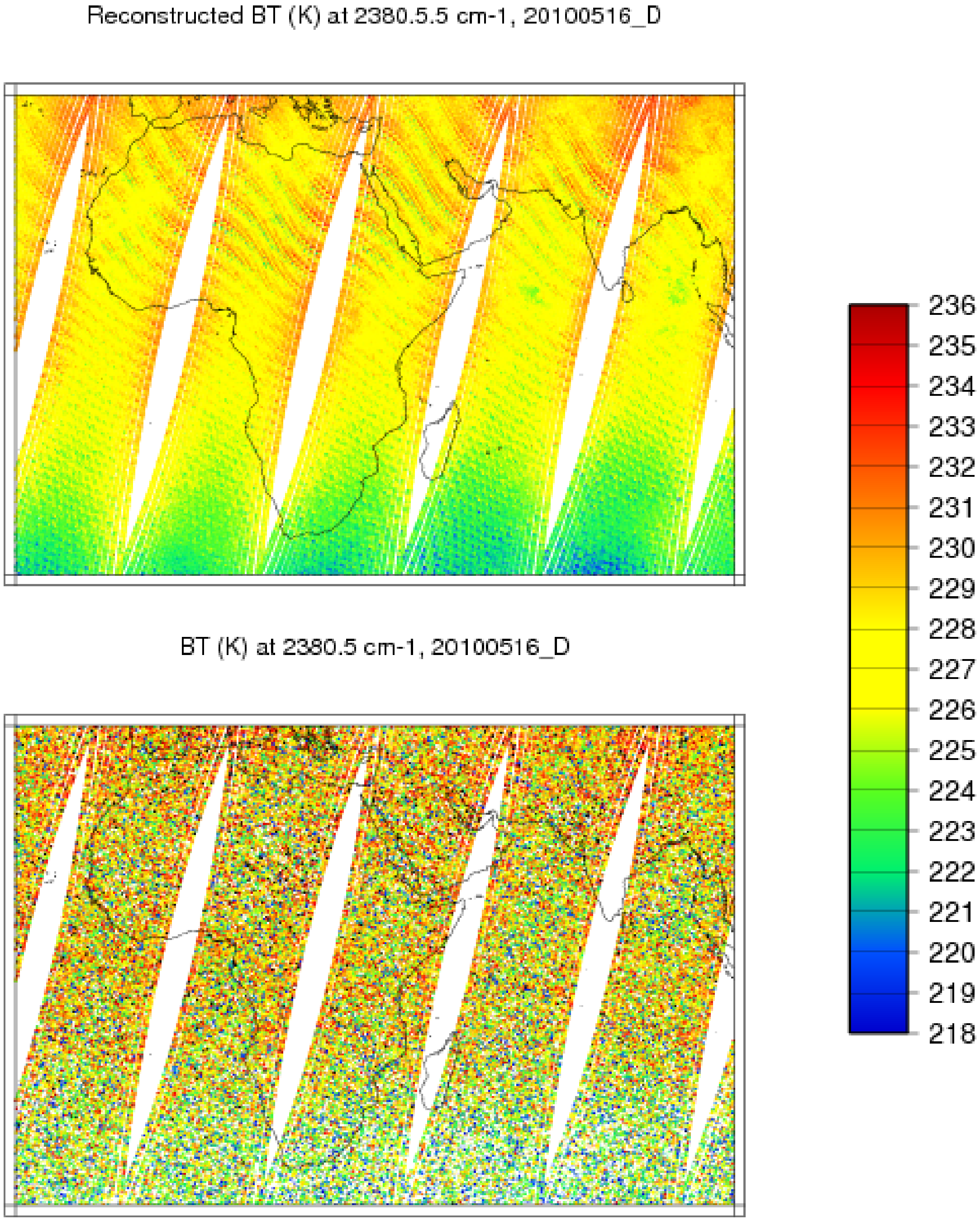
  when adding outlier spectra to the training set

Residual statistics, one full day (20100321)



Configuration change of L1C processing (‘Gibbs effect’)


(Noise Normalised) Residual standard deviation for each pixel, 20110202
Pixel 1
Pixel 2
Pixel 3
Pixel 4
1.3
1.2
1.1
1
0.9
0.8
0.7
0.6
1000
2000
3000
4000
5000
6000
7000
8000
IASI channel number



Reconstructed BT (K) at 2380.5.5 cm-1, 20100516_D

BT (K) at 2380.5 cm-1, 20100516_D