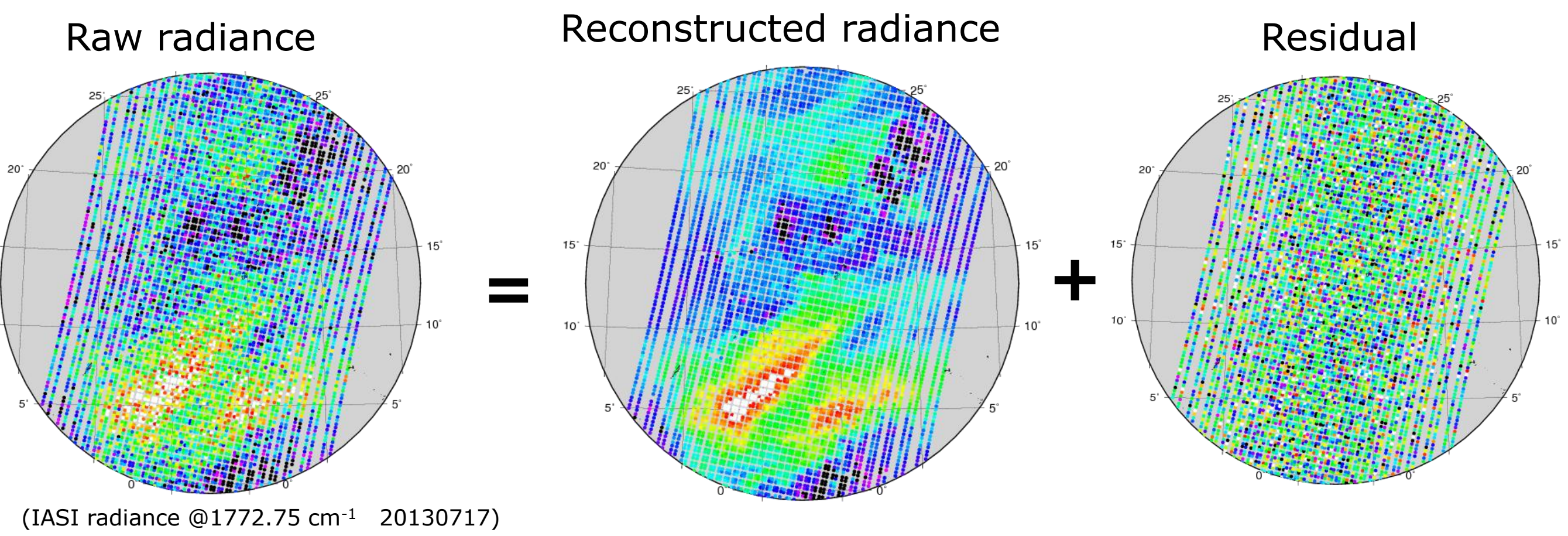
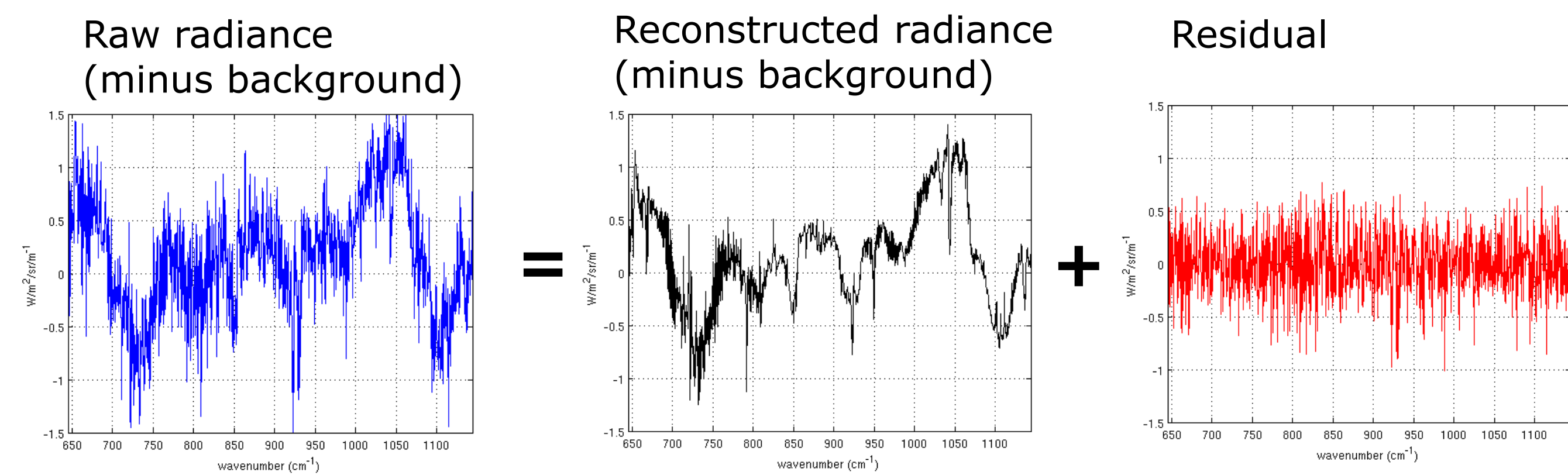


Use of reconstructed radiances in EUMETSAT's IASI Level 2 processor

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It is well known that hyper-spectral infrared radiances, like IASI measurements, can be represented by a small number of principal component (PC) scores, with almost no loss of atmospheric information. The same is true for a small subset of radiances, reconstructed from these PC scores, provided that the subset is selected in such a way that the corresponding sub-matrix of the PC's is invertible. We show how to make this selection and efficiently extract the atmospheric information in the measurements by optimal estimation retrieval based on a small subset of reconstructed radiances. A second reconstruction, using forward model PC's, is applied to the radiances in order to suppress instrument artefacts, which, although being small, do otherwise affect the retrievals negatively.

First PC filtering for noise suppression



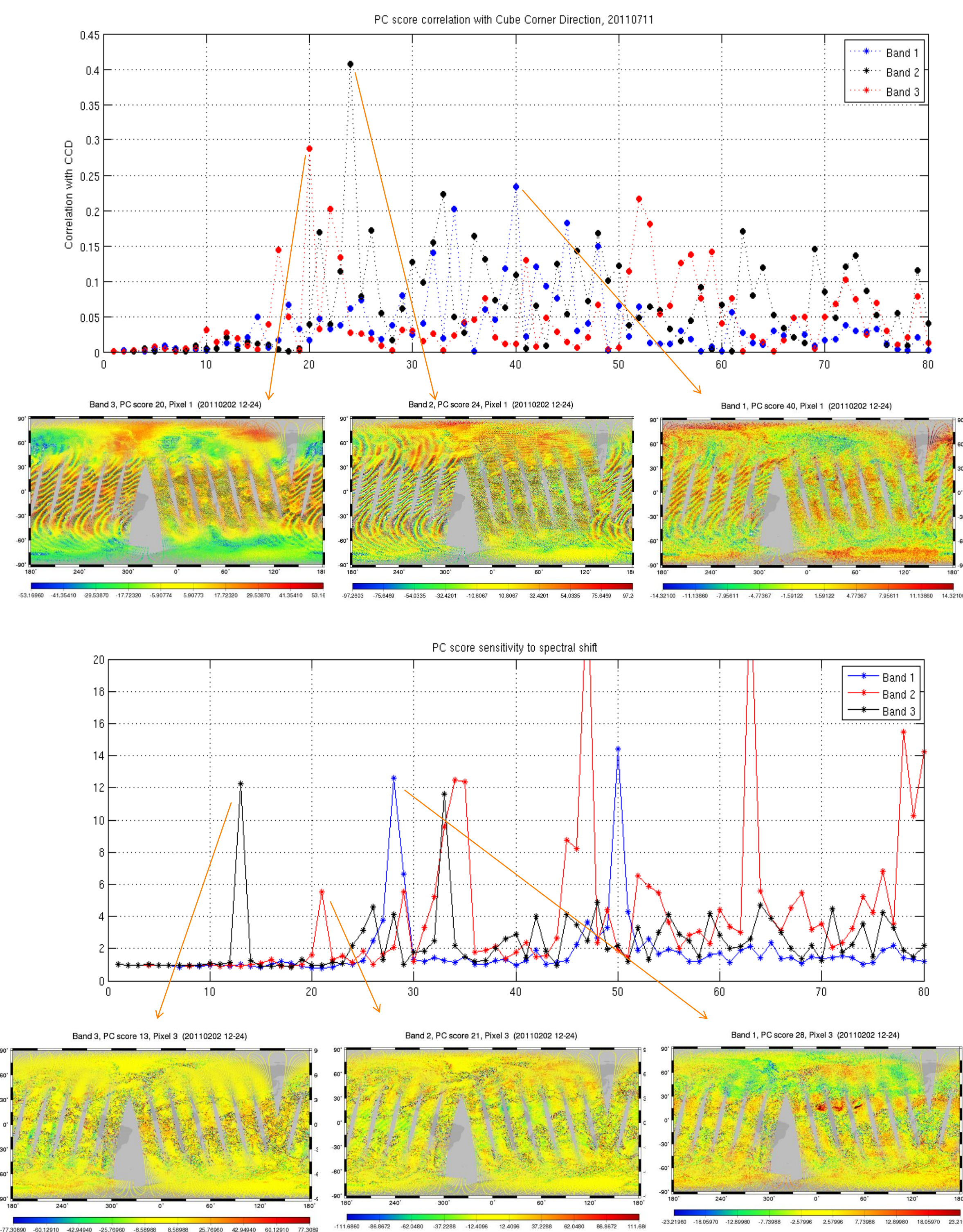
Compression works by suppressing redundant data – no redundancy, no compression. Random noise has no redundancy. Hyper-spectral infrared satellite measurements can be seen as a sum of atmospheric signal, which typically has a high degree of spectral correlation (hence redundancy), and random noise originating from measurement errors. Since this second part can't be compressed, the overall compression rate which can be achieved for hyper-spectral infrared satellite measurements is limited, unless some of the random noise is removed. One way to do so is called quantisation and consists in rounding the radiances to the nearest multiple of a predefined quantity which depends on the standard deviation of the noise in each channel. This approach makes no attempt to distinguish between signal and noise, but since the magnitude of the signal is typically higher than the magnitude of the noise, the relative effect is typically highest for the noise. It is perfectly possible for the quantisation to remove weak but spectrally correlated atmospheric signal which could have been detected and retained with principal component (PC) analysis. Therefore quantisation should never be applied prior to PC compression.

PC compression works by projecting the measurements onto the subspace generated by the leading eigenvectors of the noise normalised measurement covariance matrix. The noise normalisation is essential, because it ensures that the random noise is equally distributed among all possible directions and therefore makes eigenvector directions carrying even a very weak signal in addition to the noise distinguishable from directions carrying only noise. This is true, even in the unlikely case that a signal is not spectrally correlated, in other words if the signal only affects a single channel. In practice what would happen in such a case is that the unit vector corresponding to this channel would be included in the subspace spanned by the leading eigenvectors. The signal would therefore be preserved, but there would be no noise reduction for this particular channel. It comes as a surprise for many that a single set of eigenvectors is suitable to serve, equally well, as a basis for the representation of measurements over Antarctica and Australia (for example). The lack of regional biases is easy to verify by examination of the residuals. ("The residuals" is the term for the difference between the measured radiances and the radiances reconstructed from the compressed representation).

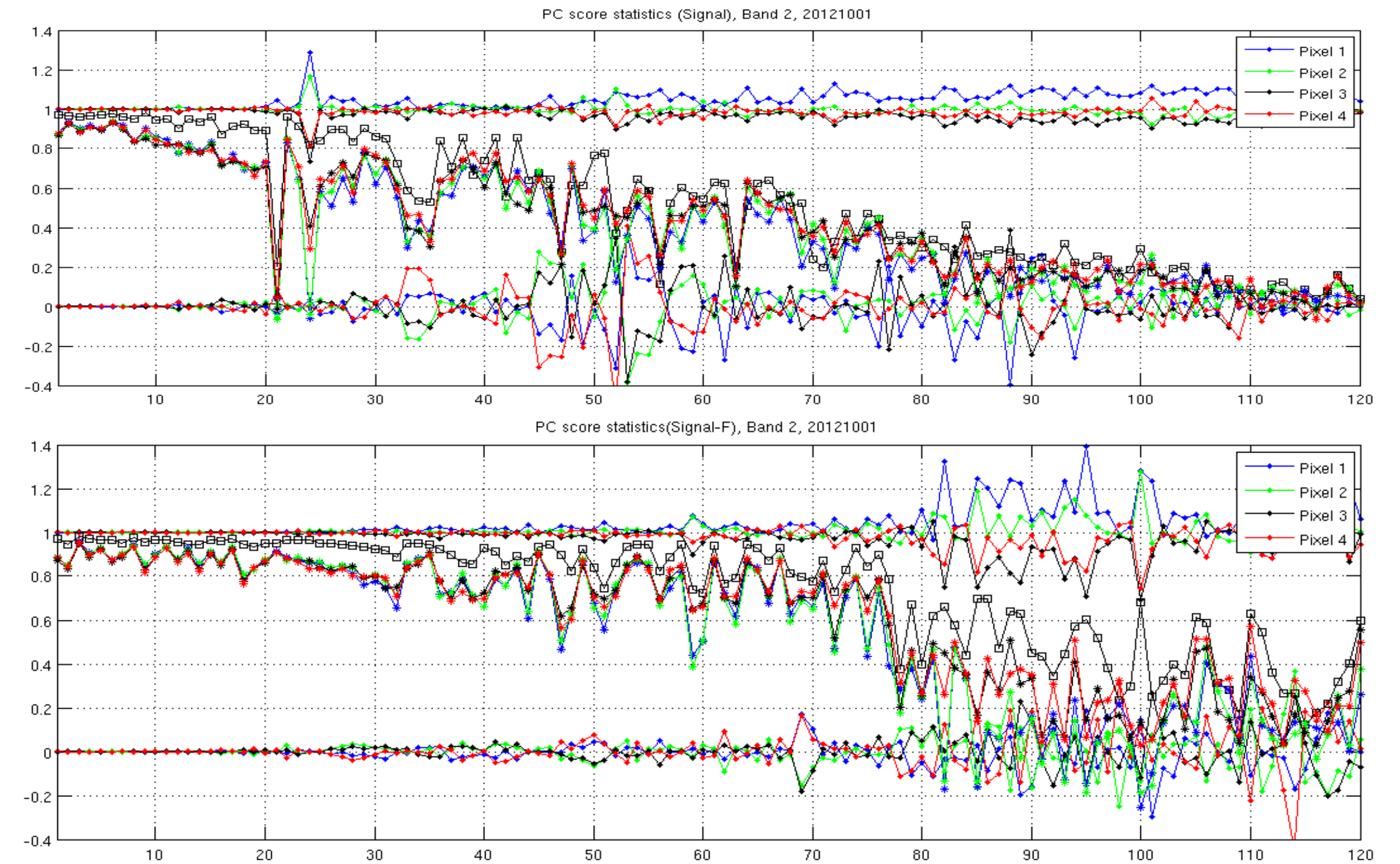
While PC compression with proper noise normalisation is capable of retaining both very weak and spectrally narrow features, it will not retain features which have not been included in the training set. Instead, measurements with such previously unseen spectral features will be identified by an anomalous residual.

Although the usefulness could be debated, some users have expressed a preference for "full radiances". One way of delivering this, originally suggested in a study by Tony Lee, is to disseminate quantised (and Huffman encoded) residuals in addition to the truncated set of PC scores. It is argued here that the additional dissemination of the complementary PC scores would be a better option for getting "full radiances" to the users, for two reasons: 1) the residuals are guaranteed to fit in a subspace of dimension equal to the number of channels minus the number of scores, so it is wasteful to represent them in channel-coordinates, and more importantly 2) the quantisation of the residuals is likely to destroy weak but spectrally correlated signal which could possibly be retained in the complementary PC scores even when these are also quantised.

Second PC filtering for instrument artefact suppression



Principal component compression of hyper-spectral infrared observations works by projecting measured radiances onto a lower dimensional linear subspace. The part of the observations which is orthogonal to this subspace consists mainly of random instrument noise and only a negligible amount of atmospheric signal and is discarded. This subspace (the signal subspace) is spanned by a truncated set of eigenvectors of the observation covariance matrix. Similarly the forward model subspace, for a given forward model, can be determined from a large set of representative forward model spectra. For some forward models, the so called PC forward models, the restriction to a lower dimensional subset is even guaranteed by construction. We can analyse the similarities and differences between the IASI observation and RTTOV forward model subspaces by computing the canonical angles and corresponding directions between the two. In this way features found in the IASI observations which are originating from instrument artefacts and are not seen in the forward model spectra can be identified and removed if desired. Instrument artefacts can be observed directly in plots of some of the PC scores (which, as we recall, are nothing but linear combinations of the measured radiances). Many present a cool zebra-striped look, which is not believed to correspond to anything in the observed geo-physics. These PC scores present a high degree of correlation with the IASI cube corner direction, which further highlights the instrument artefact origin of these patterns. It is conjectured that they are related to the so called Ghost-effect, but the day/night difference has hitherto not been explained. Another easily observed artefact is the non-uniform scene ILS effect in inhomogeneous fields of view. The affected PCs typically have a high sensitivity to spectral shift. PCs affected by instrument artefacts can also be identified by studying differences in statistics between the four detectors both in terms of mean and standard deviation as well as spatial correlation. But instead of identifying individual directions we obtain a pair of new bi-orthogonal bases for the signal and forward model subspaces, in which similar directions in the two spaces are "moved forward". Truncation can be used to filter out components of the measurements which are not found in the forward model space and vice versa. For our retrievals we keep 62 basis vectors in Band 1 and 77 basis vectors in Band 2 (corresponding to canonical angles lower than 60 degrees).



The signal and model subspaces

$E_S \in \mathbb{R}^{m \times p}$ $E_F \in \mathbb{R}^{m \times p}$
Spanned by truncated sets of eigenvectors
Intersection of the two subspaces is empty →
Compute principal angles between the two subspaces

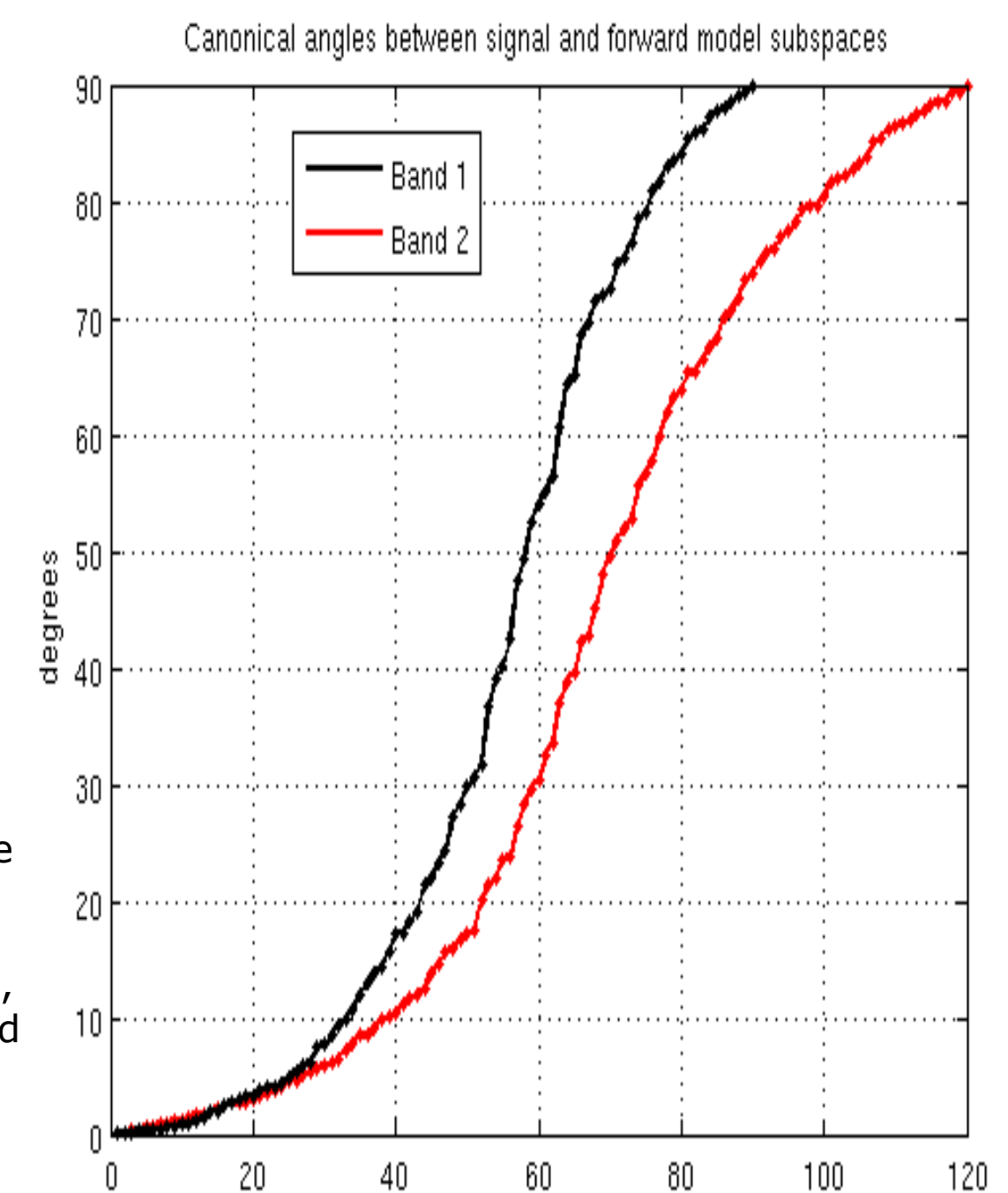
$$E_S^T E_F = USV^T$$

$$\widehat{E}_S = E_S U \quad \widehat{E}_F = E_F V$$

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

The principal angles between the two subspaces are given by $\cos^{-1}(S_i)$ 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



Channel selection for reconstructed radiances and equivalence to PC scores Ruminations on IASI-A vs. IASI-B

It is well accepted that IASI spectra can be represented by a small number of PC scores with only a minor loss of information. The same is true about the representation by a small number of reconstructed radiances. In fact it is easy to go from one representation to the other provided that the channel subset of reconstructed radiances is chosen such that the corresponding sub-matrix of the eigenvector matrix is non-singular. (That this is always possible follows directly from the fundamental theorem of linear algebra.) In order to make the transformation from a subset of reconstructed radiances to PC scores numerically stable and be able to preserve all the information available in the PC scores, it is important that the channel subset is chosen such that the condition number of this sub-matrix is kept low. In practice the condition number is heuristically minimized by choosing linearly independent rows of the eigenvector matrix with either Gaussian elimination or a Gram-Schmidt process, in which the pivot element in each step is chosen to be numerically large.

As illustrated to the right, in the context of 1DVar or assimilation, the cost function obtained with both representations are identical, provided that the two forward models are the same, in the sense that the forward modelled PC scores expanded to radiances via pre-multiplication with E_F agree with the forward modelled radiances. In this case the matrix to be inverted is a sub-matrix of the observation error covariance matrix in reconstructed radiance space, $E E^T S_y E E^T$

$$(\text{rank } m) \quad S_y \rightarrow E E^T S_y E E^T \quad (\text{rank } s)$$

In this context, it might therefore be advantageous to base the channel selection on the minimization of the condition number of this sub-matrix. This is equivalent to selecting s linearly independent rows of the matrix square root $E E^T S_y^{1/2}$ (with large pivot elements). The use of reconstructed radiances seem to be easier to implement than PC scores and has the big advantage that screening of channels affected by un-modelled features like trace gases or clouds is feasible. In practise it has also proven to work well, but care must be taken to ensure that numerical issues related to the poorer condition of the observation error covariance matrix are avoided.

$E \in \mathbb{R}^{m \times s}$ Matrix of s leading eigenvectors (rank s)

$E_s \in \mathbb{R}^{s \times s}$ Can always choose s linearly independent rows of E (i.e. such that E_s is invertible)

$$\tilde{y}_s = E_s E^T y \quad \text{subset of reconstructed (noise normalised) radiances}$$

$$y^T E E^T (E_s E^T R E E_s^T)^{-1} E_s E^T y = y^T E E_s^T E_s^{-T} (E^T R E)^{-1} E_s^{-1} E_s^T y = y^T E (E^T R E)^{-1} E^T y$$

