

Principal component and reconstructed radiance based assimilation techniques

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Motivation for the exploitation of assimilation techniques based on principal components or reconstructed radiances.

- To date, the preferred option for the assimilation of observations from hyper-spectral infrared sounders is the use of selected channels.

However:

- 1) This approach is computationally inefficient and as we seek to exploit an increasing proportion of the full measured spectrum from multiple hyper-spectral sounding instruments it will become computationally prohibitive.
- 2) There is strong evidence that data providers will evolve to the dissemination of PC scores to improve efficiency.

- It is thus timely and opportune to investigate the feasibility of directly assimilation PC scores or reconstructed radiances into NWP models.

A brief review of the theory of Principal Component Analysis (PCA)

- PCA is a method that allows the reduction of the dimensionality of a data set by exploiting the interrelation between the variables contained in the data set.
- The reduction of the dimension of the data set is obtained by replacing the original set of correlated variables with a smaller number of uncorrelated variables called Principal Components (PCs).
- The *first few PCs* are ordered so that they retain most of the variation present in *all of the original* variables. Hence, PCA theory provides a tunable mechanism to efficiently represent the information in the data set.

A brief review of the theory of Principal Component Analysis (PCA)

- In our context, the data set consists of a sample of l spectra of n radiances, \mathbf{r} , arranged into a l by n data matrix \mathbf{R} .
- If \mathbf{C} in the n by n covariance matrix of \mathbf{R} , we can form a matrix \mathbf{A} using the eigenvectors of the covariance matrix arranged as row vectors in descending order according the magnitude of their eigenvalues. The eigenvectors represent the direction of maximum variance in the data.
- The PCs, \mathbf{p} , of the vector population can be written as:

$$\mathbf{p} = \mathbf{A} \mathbf{r} \quad (1)$$

The values of the PCs associated to each spectrum are known as **PC scores**.

A brief review of the theory of Principal Component Analysis (PCA)

- The first PC is the linear combination that explains as much variation in the original data as possible.
- The second PC is the linear combination that explains as much variation not present in the first PC and so on.
- A number of PCs, m , fewer than n can often represent most of the variation in the data. The choice of m is based on the total variation accounted for by the leading PCs and it will in general depend on specific aspects of the original dataset.

A brief review of the theory of Principal Component Analysis (PCA)

■ For any new radiance spectrum, \mathbf{r}^* , we can compute the equivalent PC scores by projecting the radiances upon the full set of eigenvectors derived from the covariance matrix of the training data set.

■ The vector of m truncated PC scores, \mathbf{p}^* , will then convey most of the information about the atmospheric state

$$p_i^* = \sum_{k=1}^n A_{ik} r_k^* \quad (2)$$

where $i=1, m$

■ *The truncated PC scores may be regarded as an efficient encapsulation of the original data and may be used for storage, transmission or (and this is the focus of today's talk) assimilation. For instance, most of the information contained in a full IASI spectrum made of 8461 channels can be encapsulated in typically no more than 200~300 PCs.*

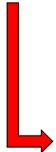
A brief review of the theory of Principal Component Analysis (PCA)

■ In addition to reducing the dimension of the data set, the value of m can also be tuned to achieve filtering of the data. By retaining only the leading PC scores we can separate variations of the atmospheric signal from variations of the random instrument noise. Optimal noise filtering can be achieved by noise normalising the spectra.



For interferometer instruments whose radiances have been apodised, it is important that spectra are normalised using the full instrument error covariance matrix.

■ Take must be taken in truncating the PC scores for this purpose because small-scale and small-amplitude atmospheric features which can be source of rapid forecast error growth in NWP might be removed if the truncation is too severe.



The importance of the noise reduction aspect of the problem should not be overemphasized, though. The total error budget can in fact still be dominated by forward model error, quality control error, representivity error, etc.

A brief review of the theory of Principal Component Analysis (PCA)

■ If required, the truncated PC scores may be used to reconstruct a new radiance vector, \mathbf{r}^{rec} ,

$$r_i^{rec} = \sum_{k=1}^m A_{ki} p_k^* \quad (3)$$

where $i=1,n$

■ Any subset of n_r reconstructed radiances will contain the same information present in the m principal components as long as $n_r \geq m$.

 *However, if $n_r \geq m$ the covariance matrix of the reconstructed radiances is in general not invertible although it is theoretically possible to find a subset of m reconstructed radiances whose covariance matrix can be inverted.*

■ The reconstructed radiances are noise filtered but they generally have channel-correlated errors even in the case when the original radiance errors are not correlated.

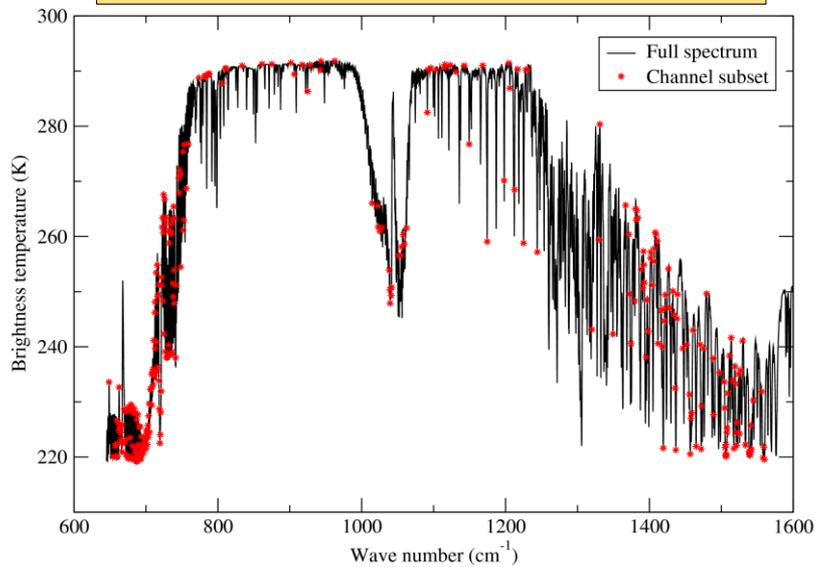
A brief review of the theory of Principal Component Analysis (PCA)

- At a theoretical level, the assimilation of PC scores or reconstructed radiances can arguably be considered equivalent (if we do everything correctly).
- The successful introduction of either of these approaches in a operational NWP environment will eventually depend on how well the various elements of the assimilation system can be practically implemented and tuned.

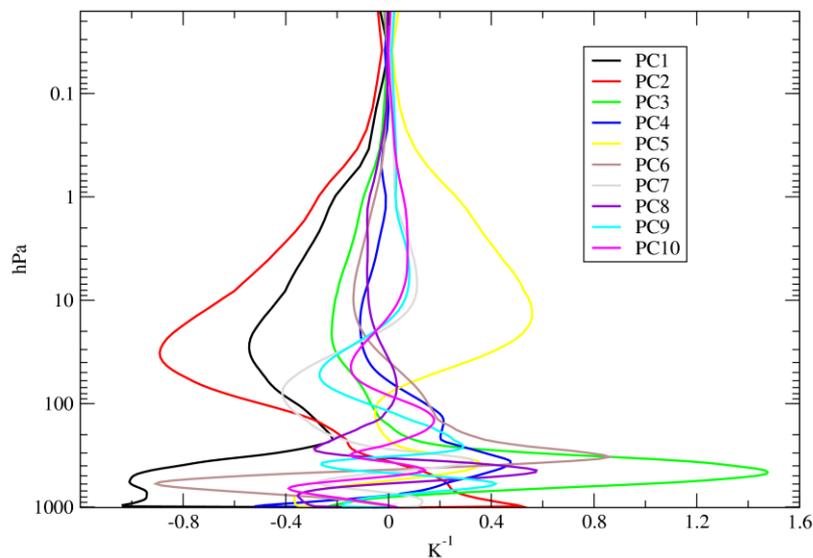
Potential issues with the direct assimilation of PC scores

When compared to spectral radiances, the physical interpretation of PC score observations is less intuitive.

Subset of the IASI spectrum



The temperature Jacobian for the first ten PC scores



PC skin temperature Jacobian

Potential issues with the direct assimilation of PC scores

Handling of clouds in PC space

What we do in radiance space

We operationally assimilate clear channels above clouds.

Analogue in PC space

There is no analogue in PC space because due to the non-local nature of the PC Jacobians it is not possible to find PC score observation insensitive to the presence of clouds.

We could try:

Option 1) We predetermine a set of IASI channels that are always unaffected by clouds as the eigenvector basis and use this fixed basis for cloudy scenes only.

Option 2) We identify which subset of clear channels can be used in a particular cloud affected scene. We re-compute (on the fly) a dedicated eigenvector basis and project the measured spectrum to produce cloud free PC scores for this scene.

Potential issues with the direct assimilation of PC scores

Handling of clouds in PC space

What we do in radiance space

We assimilate data in overcast scenes.

Analogue in PC space

In principle, no significant obstacles are foreseen to reproducing the functionality and benefits of overcast radiance assimilation in PC space. To this end we have developed a PC based model (PC_CLD_RTTOV) that is capable of simulating cloud affected PC scores.

Potential issues with the direct assimilation of PC scores

Handling of clouds in PC space

What we might be doing in radiance space

ECMWF is studying the assimilation of radiance data in any cloud conditions (the so called all-sky approach). Challenges related to the extreme nonlinearity of the observation operators and the difficulty in reconciling the spatial scales of the NWP model and the observations could mean that an operational implementation is still several years away.

Analogue in PC space

A PC based fully cloudy fast RT model exists. If a solution can be found for the assimilation of infrared radiance data in any cloud conditions, a PC implementation would not be far behind.

Potential issues with the direct assimilation of PC scores



Handling of clouds in PC space

■ The handling of clouds could be more straightforward if the Jacobians of the PCs were more localised in the vertical. In principle this could be achieved by imposing locality as a constraint upon the calculation of the projection. However, it is not yet clear how this could be done.

■ *Although in principle the same approaches of handling clouds in radiance space could be adopted in PC space, in practice, however, this is considered too much technically demanding to find a viable application in an operational data assimilation system.*

Potential issues with the direct assimilation of PC scores



New fast radiative transfer (RT) models are required

- PC based fast RT models have been developed by several authors.
- In these models the simulated PC scores are expressed as a linear combination of a selected number of either monochromatic (Liu et al. 2006, Havemann 2006, or, as in the case of PC_RTTOV (Matricardi 2010), polychromatic radiances.
- PC based models are trained using the PC scores derived from the eigenvectors of the covariance matrix of a large dataset of synthetic noise-free radiances calculated using an accurate line-by-line model.
- The number of predictor variables used in the regression algorithm is a tuneable parameter in the model.

Potential issues with the direct assimilation of PC scores

- ***Bias correction:*** the removal of biases originating in the stratosphere could potentially impact the troposphere via correlations introduced by the non locality of PC scores.
- ***Quality control:*** the non locality of PC scores might result in error correlations that could allow errors from residual cloud contamination propagating through the entire atmospheric column.
- ***Monitoring :*** the routine monitoring of radiance biases provides useful feedback on the forecast model, the RT model and instrument problems. Can we preserve this diagnostics if the NWP community moved away from assimilating radiance data?

The assimilation of reconstructed radiances

- Arguably, the use of reconstructed radiances is simpler to implement than the direct use of PC scores because NWP centres already know to deal with raw radiances.
- The use of reconstructed radiances would not require any of the significant technical and scientific investment needed to develop a system to directly assimilate PC scores.
- The techniques developed for handling clouds in assimilation systems based on raw radiances should be in principle applicable to reconstructed radiances.

Potential issues with the assimilation of reconstructed radiances



Selection of a subset of reconstructed radiances

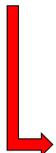
- If we want to reduce the dimensionality of the data we must select a number, n_r , of reconstructed radiances less than the number, n , of raw radiances.
- However, if we want to assimilate all the information in the reconstructed spectrum, poor conditioning may be unavoidable (the reconstructed radiances are linearly dependent).
 - ↳ In principle, we could avoid poor conditioning if we could find a subset of m linearly independent reconstructed radiances although it is very unlikely this can be achieved in practice.
- Eventually, to avoid poor conditioning, we may have to use a number, n_r , of reconstructed radiances less than the number, m , of principal components. To reduce the consequent loss of information, the number of reconstructed radiances should be as close as possible to the number of principal components.

Potential issues with the assimilation of reconstructed radiances



Reconstructed radiances as a proxy for original radiances?

- The observation operator used for the simulation of the reconstructed radiances should reproduce the true (i.e. multichannel) nature of each reconstructed radiance channel. This could be done using a conventional (e.g. RTTOV) forward model but it would be prohibitively expensive.
- Could we approximate the simulated reconstructed radiances with simple, e.g. RTTOV, calculations of the corresponding real channels?
- PC based forward models can directly and efficiently simulate reconstructed radiances but they are trained using synthetic eigenvectors whereas the training set used to derive the observed reconstructed radiances is based on observed data.



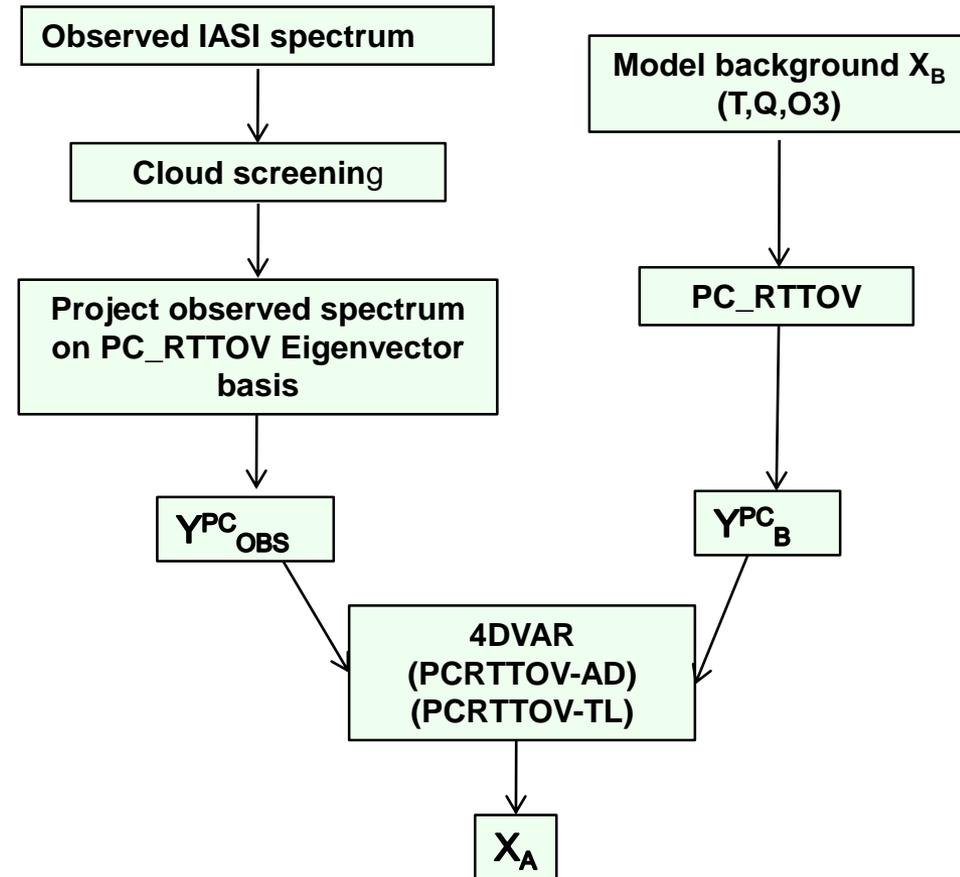
However, simulations and observations could be reconciled by projecting the reconstructed radiances on the eigenvector basis used by the forward model.

The ECMWF 4DVar PC score assimilation system

Methods

- 1) Develop a PC based fast model (PC_RTTOV).
- 2) Develop a cloud scheme for the detection of cloudy scenes.
- 3) Modify the IFS to allow the ingestion of PC data.
- 4) Develop a PC based quality control to filter out residual cloud contamination.
- 5) Monitor the proper functionality of VARBC in PC space.
- 6) Finely tune the number of PCs to be used in the assimilation.
- 7) Finely tune the observation errors in PC space.

PC analysis system design



In 4DVar we minimise the cost function $J(X)$

$$J(X) = [X - X_B]^T B^{-1} [X - X_B] + [Y_{OBS}^{PC} - Y^{PC}(X)]^T R^{-1} [Y_{OBS}^{PC} - Y^{PC}(X)]$$

The ECMWF 4DVar PC score assimilation system



Evolution of the system

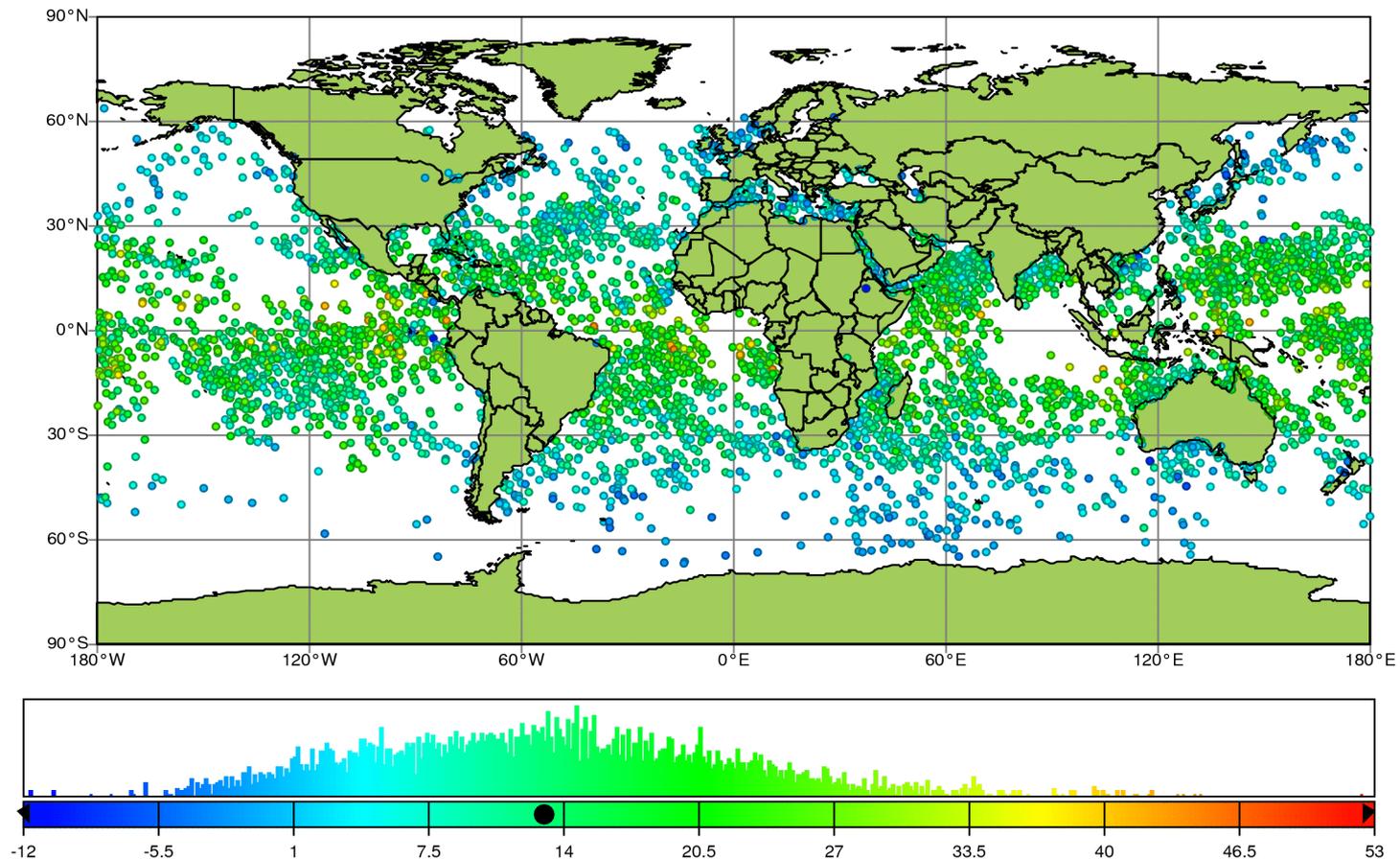
- 1) **Prototype system (only conventional and IASI observations):** assimilation of PC scores derived from channels in the short wave band of IASI.
- 2) **Full data assimilation system (all operational observations - satellite and conventional):** assimilation of PC scores derived from the 191 long wave IASI channels used in ECMWF operations.
- 3) **Revised full data assimilation system :** we focused on maximising the spectral information of IASI assimilating PC scores derived from 305 IASI channels obtained by augmenting the 191 operational channels with additional surface, ozone, and water vapour sounding channels.

The ECMWF 4DVar PC score assimilation system



Quality control for residual cloud contamination

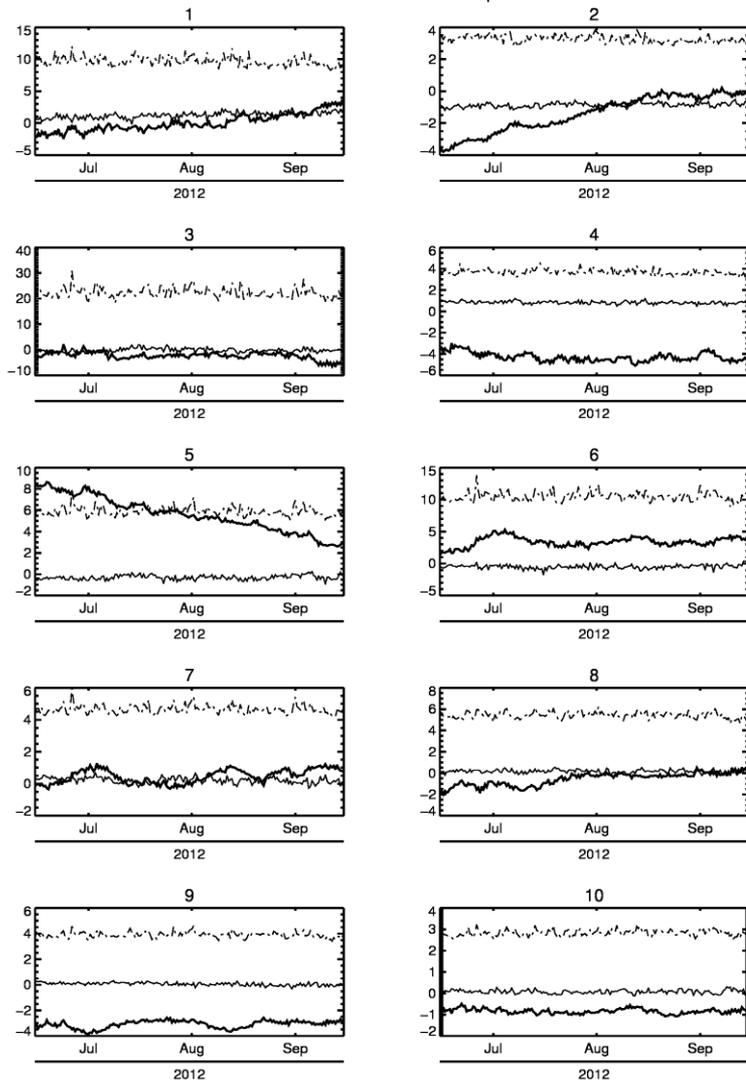
PC#1 has similar characteristics to an infrared window channel. Large positive departures of the observed PC#1 score from the clear-sky computed value are an indication that the observation is affected by clouds.



The ECMWF 4DVar PC score assimilation system

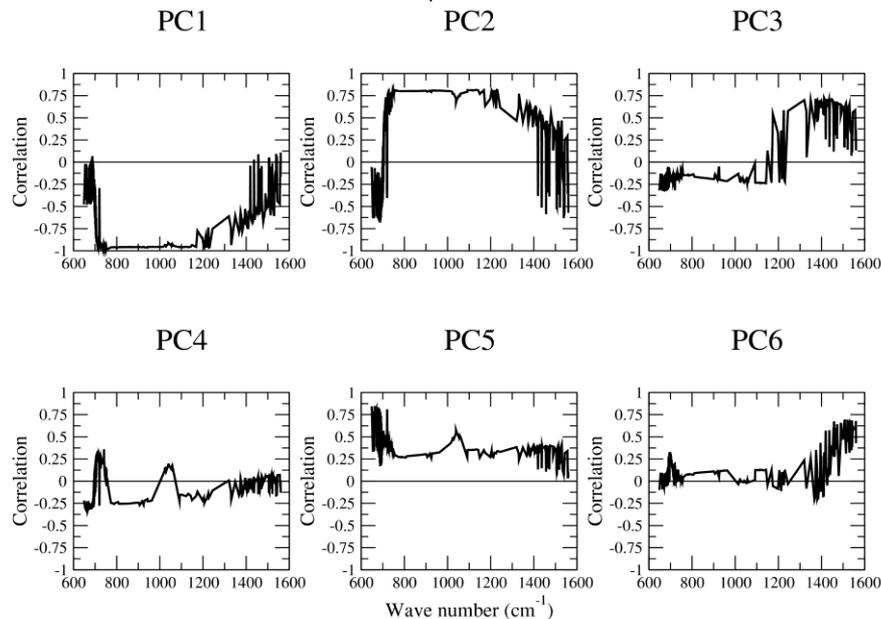
The monitoring of the adaptive VARBC bias corrections in PC space

Analysis departure mean (solid) and standard deviation (dot-dash) and bias (thick)
Instrument(s): IASI Area(s): S.Hemis
From 00Z 15-Jun-2012 to 12Z 15-Sep-2012



Thick line: Bias correction
Solid line: mean value of analysis departure
Dot-dashed line: standard deviation of analysis departure

Correlation between PCs and IASI channels



The ECMWF 4DVar PC score assimilation system



Assimilation of PC scores derived from 305 IASI channels: diagnosed observation errors

Estimate of the total observation error: Desroziers and Hollingsworth/Lönnerberg methods have been used to separate the contribution of the observation and background error.

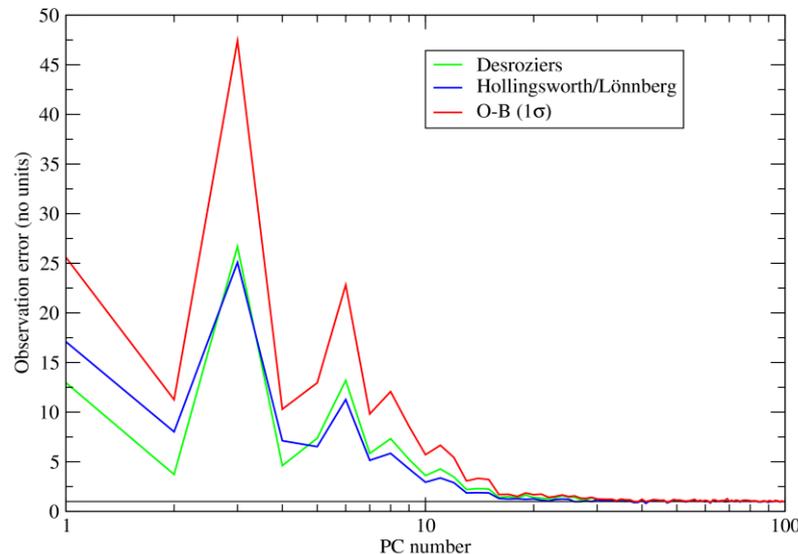
Hollingsworth/Lönnerberg assumptions:

background errors are spatially uncorrelated, observation errors are spatially uncorrelated, and, background and observation errors are uncorrelated.

Desroziers assumptions:

background and observation errors are uncorrelated, the weights that are assigned to the observations in the analysis agree with the true background and observation error covariances.

Diagnosed PC score observation errors (i.e. diagonal elements of the diagnosed PC error covariance matrix)

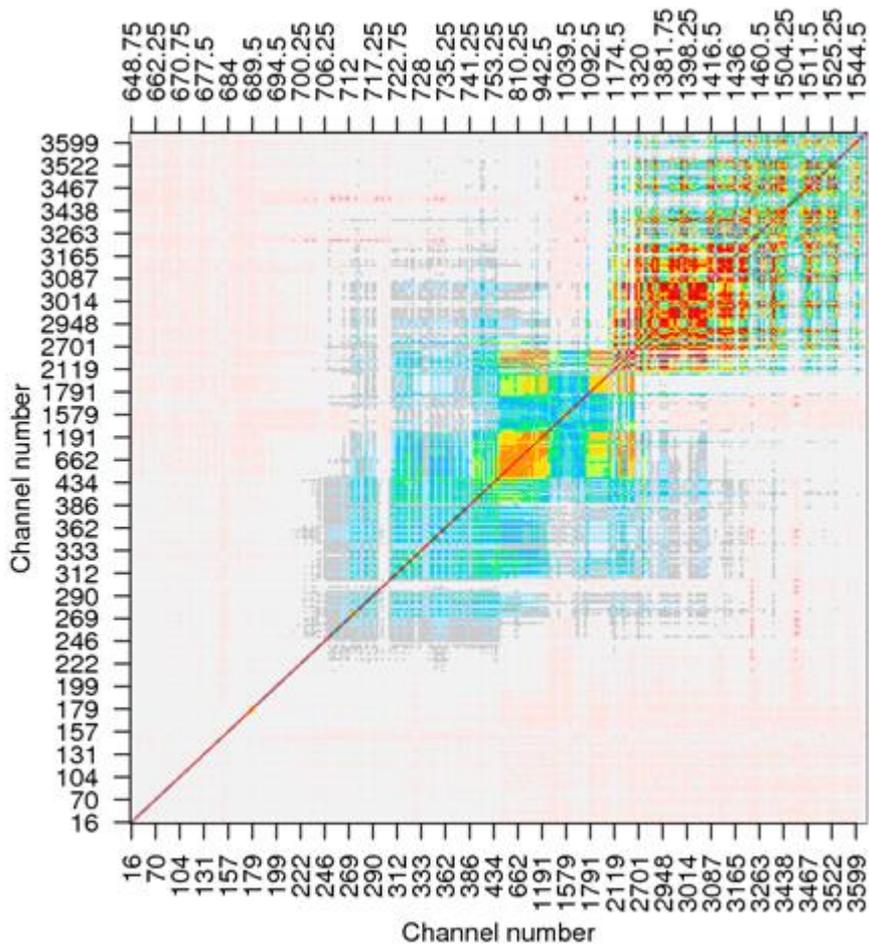


The ECMWF 4DVar PC score assimilation system

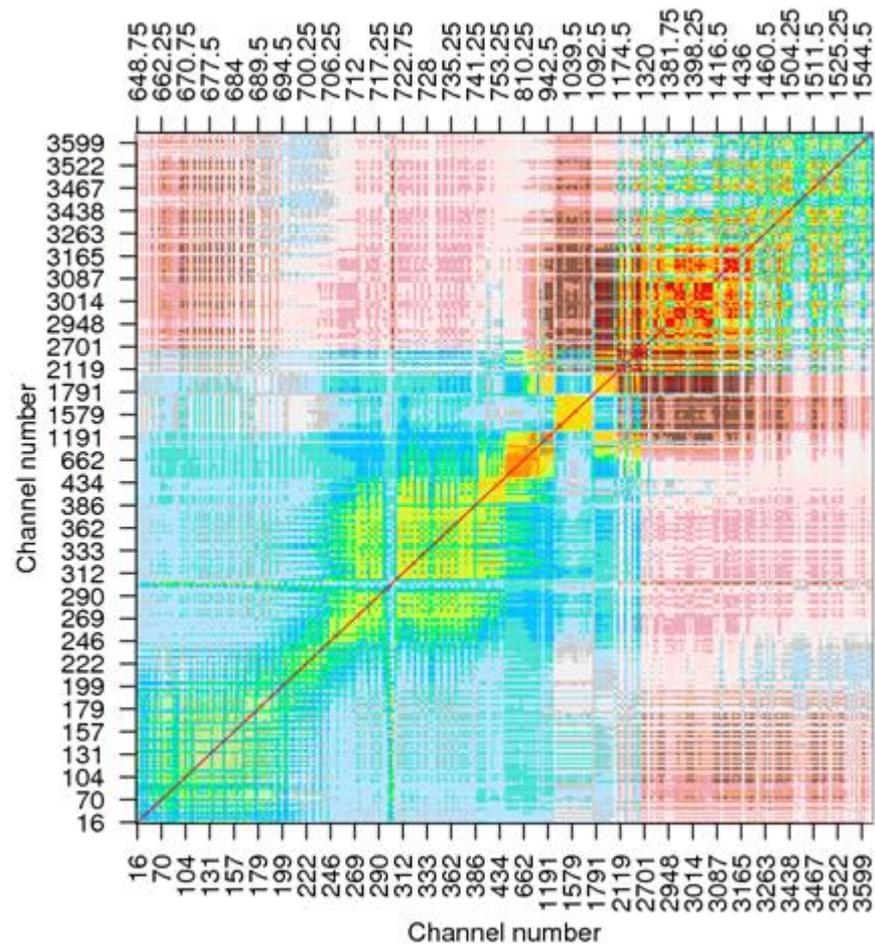


Assimilation of PC scores derived from 305 IASI channels: diagnosed error correlations

Full PC correlation matrix is converted into radiance space



Diagonal PC correlation matrix is converted into radiance space



The ECMWF 4DVar PC score assimilation system



Assimilation of PC scores derived from 305 IASI channels: experiment design

To assess the performance of the PC based assimilation system we have devised the following experiment design:

- 1) **BASE:** we use all operational observations (satellite and conventional) with the exception of IASI data.
- 2) **RAD:** identical to BASE but additionally assimilates 191 channels used in the operational 4D-Var.
- 3) **PC:** identical to BASE but additionally assimilates 50 PC scores derived from 305 IASI channels.

Experiments (cycle 38R2 – T511- 137 L) have been carried out for the period 15 June 2012-15 December 2012.

NOTE: in the PC experiment we assimilate only cloud-free scenes whereas in the RAD experiment we assimilate fully overcast scenes and channels not affected by clouds.

The ECMWF 4DVar PC score assimilation system



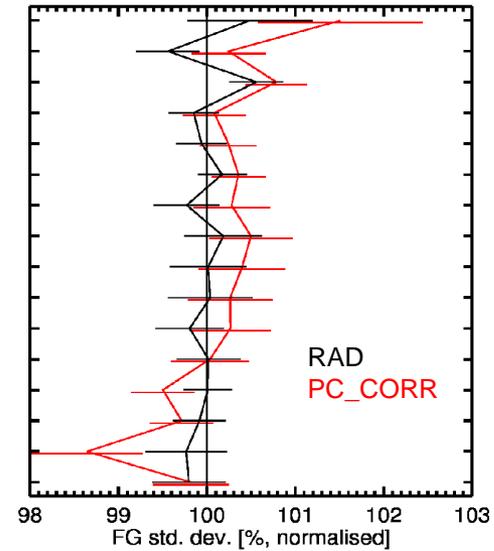
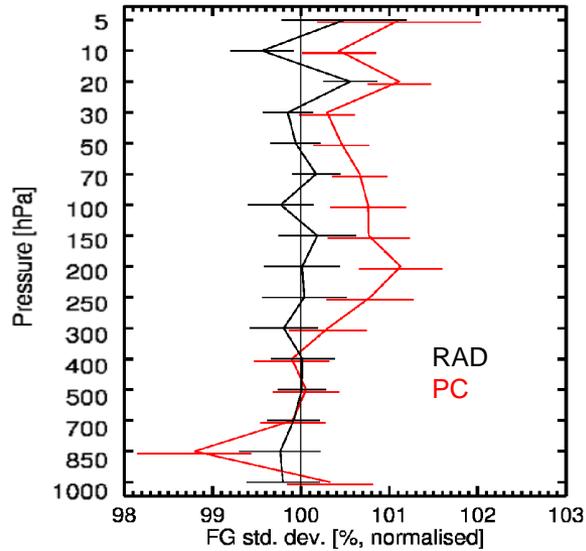
Performance of the PC score assimilation system

- *Results suggest that the current PC assimilation system (in clear sky only) performs as well as – and in some respects slightly better than – the current operational IASI radiance assimilation that also uses radiances peaking above clouds and overcast scenes.*

- *In addition, significant improvements in the performance of the assimilation have been obtained when correlated error between different PCs is taken into account.*

- *Crucially, the PC score system uses substantially less computer resources (during the 4D-var minimization) compared to the radiance based system.*

Verification against radiosondes: Temperature in the Tropics



Forecast rms errors for the 850 hPa relative humidity in the Tropics

Control normalised: base (ope) minus rad (ope)

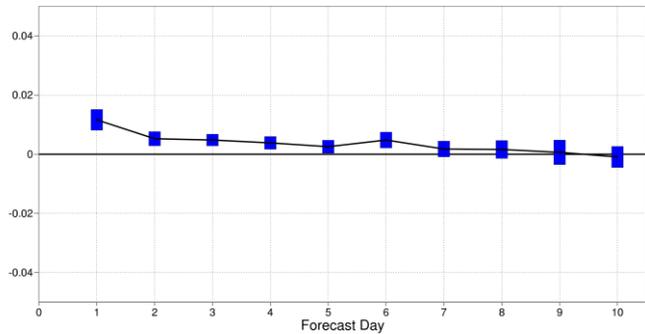
850hPa relative humidity

Root mean square error

Tropics (lat -20.0 to 20.0, lon -180.0 to 180.0)

Date: 20120615 00UTC to 20121215 00UTC

00UTC T+24 T+48 ... T+240 | Confidence: [95.0] | Population: 184



Control normalised: base (ope) minus pc (ope)

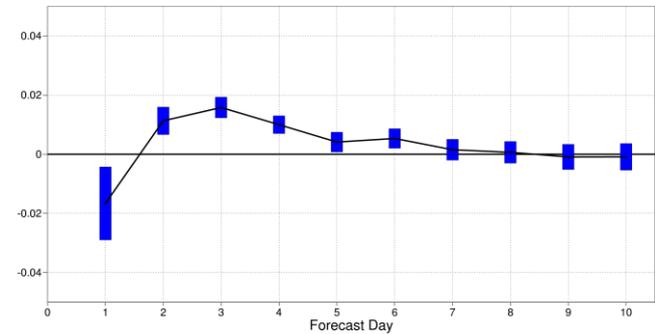
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00UTC T+24 T+48 ... T+240 | Confidence: [95.0] | Population: 184



■ The assimilation of AIRS and IASI reconstructed radiances has been carried at ECMWF by Collard et al. (2010) and at the Met Office by Hilton and Collard (2009) respectively.

Points to note:

- Reconstructed radiances were used as proxy of raw radiances.
- A diagonal error covariance matrix was used although an inflated observation noise was utilized to reduce the influence of errors arising from unmodelled inter-channel correlations.
- No attempt was made to reduce the dimension of the data using a subset of reconstructed radiances.
- The difference in forecast impacts between experiments using raw radiances and reconstructed radiances was statistically neutral.

Summary

- The viability of direct PC assimilation in NWP has been demonstrated for cloud-free scenes.
- NWP centres should begin serious testing of the reconstructed radiances approach making an efficient use of them (i.e. assimilate a subset of the full reconstructed radiance spectrum) and compare the results with those obtained from the direct assimilation of PC scores.