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The direct assimilation of principal components of IASI spectra

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The assimilation of high-resolution radiances measured by the Infrared Atmospheric Sounding Interferometer (IASI) has produced a significant positive impact on forecast quality (*Collard & McNally*, 2009). The operational use of IASI radiances at ECMWF is currently restricted to a selection of temperature sounding channels in the long-wave and short-wave regions of the spectrum and to a small number of ozone and humidity sounding channels. In principle, to exploit the full information content of IASI, the number of channels used in the assimilation could be increased to cover the full spectrum.

Currently, NWP users have to assimilate less than the full IASI spectrum because of the high computational cost, but it is also known that the independent information on the atmosphere contained in an IASI spectrum is significantly less than the total number of channels. There is thus a need to find a more efficient way of communicating the measured information to the analysis system than simply increasing the number of channels. Similarly, satellite agencies are seeking a more efficient means of near-real-time data dissemination for instruments such as IASI because the traditional practice of transmitting full spectral data at full spatial resolution is likely to become prohibitively expensive in the future (as instruments are flown on multiple polar and geostationary platforms).

Principal Component Analysis (PCA) is a classic statistical method for the efficient encapsulation of information from voluminous data (*Joliffe*, 2002). As such, it has been proposed as a solution to the problems associated with the assimilation and dissemination of high spectral resolution data although, while noting that the two issues are quite similar, the requirements are quite separate. There are strong indications that data providers will start to disseminate principal component (PC) scores (i.e. the values of the PCs associated to each observation) to improve efficiency. It is thus timely and opportune to investigate the feasibility of directly assimilating PC scores into NWP models.

In this article we document the development and the functionality of a global four-dimensional variational assimilation system (4D-Var) based on the direct use of PC data. The primary aim is to develop an efficient use of the entire measured IASI spectrum that could not be achieved by traditional radiance assimilation.

A brief review of Principal Component Analysis

PCA is a method that allows the reduction of the dimensionality of a dataset by exploiting the interrelations between all the variables contained in the dataset. This is achieved by replacing the original set of correlated variables with a smaller number of uncorrelated variables called principal components. Because the new derived variables retain most of the information contained in the original data, PCA provides a tuneable mechanism to efficiently represent the information in the data.

In our case, the original variables are n radiances of the IASI spectrum. A number of PCs, which is less than n, can often represent most of the variation in the data. This means that we can replace the n radiances with the first m PCs (referred to as reducing the 'dimension' of the data). In many applications the choice of the number of dimensions is based on the total variation accounted for by the m leading PCs and it will in general depend on specific characteristics of the data. The truncated PC scores may be regarded as an efficient encapsulation of the original set of observations that may be used for storage, transmission or indeed assimilation.

In addition to reducing the dimension of the observed data, the value of m can also be tuned to achieve noise filtering of the observations, using PCA to separate variations of the atmospheric signal from variations of the random instrument noise. Of course great care must be taken if the PC scores are truncated for this specific purpose. Small-scale and small-amplitude atmospheric features can be important sources of rapid growth of forecast error. However, such features might not be strongly correlated across the measured spectrum and could potentially be confused with noise. Consequently, a truncation that is too severe should be avoided because it could potentially remove atmospheric features.

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The IASI long-wave channels and derived PC scores

To demonstrate PC-score assimilation it is assumed that we have access to the full IASI measured spectrum and that we are only investigating the suitability of PCA as a mechanism for efficiently presenting this information to an assimilation system. As such we are deliberately separating this from the potential application of PCA to the logistical issue of compressed data dissemination.

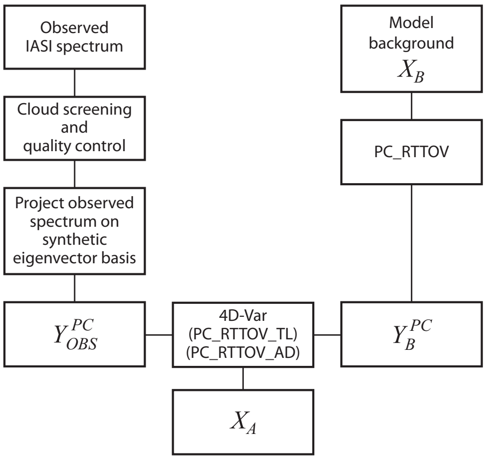
In this article we consider the assimilation of PC scores derived from radiances in the long-wave region of the IASI spectrum. The radiances we have employed are a subset of those used operationally at ECMWF. This subset comprises 165 long-wave channels in IASI band 1 and has been obtained by removing from the operational data the channels located in the water vapour absorption band and in the short-wave region of the spectrum. Excluding radiances with a strong sensitivity to water vapour allows us to run assimilation experiments in more controlled conditions using sounding channels with a primary sensitivity to temperature and the surface.

A detailed description of the PC assimilation methodology can be found in *Matricardi & McNally* (2013) and the methodology is outlined in Box A.

PC assimilation methodology

A

The methodology adopted for the direct 4D-Var assimilation of PC scores is shown schematically in the figure (refer to *Matricardi & McNally, 2013, Q. J. R. Meteorol. Soc.*, **140**, 573–582, for more details).



The observed IASI spectra are first screened for the presence of clouds and contaminated spectra are discarded. This must be done before assimilation as the PC training has been performed with only completely clear data and none of the eigenvectors correspond to cloud signals. The clear spectra are then converted into a vector of observed PC scores Y_{OBS}^{PC}.

Each vector of observed PC scores has length *n,* but crucially we assimilate only the first *m* of these, preferentially retaining highest rank PC scores that convey most information about the atmospheric state. The *m* observed PC scores are then provided as input to the 4D-Var. Trajectory estimates of the atmospheric state (*X*) are used as input to the observation operator to compute model equivalents of the *m* PC scores, Y_B^{PC} (*X*). The thPC score observation operator used in our tests is PC_RTTOV *(Matricardi, 2010, Q. J. R. Meteorol. Soc.,* **136**, 1823–1835) which has been available as part of the operational RTTOV observation operator since the release of RTTOV version 10.

During the minimization of the 4D-Var cost function, perturbations of the atmospheric state are mapped into the observation (PC) space by the tangent linear of the observation operator PC_RTTOV_TL. Likewise, gradients of the cost function with respect to the PC scores are evaluated and mapped into gradients with respect to the atmospheric state by the adjoint of the observation operator PC_RTTOV_AD. The atmospheric state X_A that minimizes the above cost function is referred to as the *analysis* and the departures of this from the background atmospheric state X_B are referred to as analysis increments defined at the start of the 4D-Var window.

The 4D-Var cost function involves the specification of the error covariance matrix of PC scores, *R,* which should describe the combined error of the observations (PC scores) and observation operator (PC_RTTOV). An initial estimate of the diagonal elements of R can be obtained by computing the standard deviation of the observed minus background departures. Of course these values are not optimal in that they contain a contribution from the uncertainties in the background state and as such can only be regarded as an upper bound upon the required error. To separate the contribution of the observation error and the background error in the departure statistics we have used the techniques proposed by *Hollingsworth & Lönnberg* (1986, *Tellus,* **38A**, 111–136) and *Desroziers et al.* (2005, *Q. J. R. Meteorol. Soc.,* **131**, 3385–3386) which should give a refined estimate of the observation error (for details see *Bormann & Bauer,* 2010, *Q. J. R. Meteorol. Soc.,* **136**, 1036–1050).

PC-based quality control

Currently, the assimilation of PC scores is restricted to clear-sky conditions utilising a dedicated cloud detection scheme that uses three separate tests applied to uncorrected radiance departures and seeks to identify only fully clear IASI pixels. In conjunction with the new cloud detection scheme, an additional PC-based quality control is used and acts as an extra check for residual cloud contamination.

Because the first principal component (PC1) has similar characteristics to an infrared window channel showing a heightened sensitivity to the surface emission and the presence of clouds, positive observed minus background departures of the observed PC1 score from the clear-sky computed value are an indication that the observation is affected by clouds. Using a visual inspection of AVHRR imagery overlaid with IASI pixels it was found that a threshold of 40 (in dimensionless units) applied to the departure in the long-wave PC1 is sufficient to reject most cases of residual cloud contamination.

Bias correction for PCs

In the ECMWF PC-based assimilation system, biases in the PC observations and systematic errors in the PC-based radiative transfer model and cloud screening are removed using the variational bias correction scheme (VarBC). This is an adaptive correction algorithm used operationally at ECMWF for all satellite data, including IASI radiances (and indeed some in situ observations, such as from aircraft), where the bias is expressed as a linear combination of pre-defined atmospheric predictors. For consistency with radiance observations, but also because PC scores are likely to be influenced by rather similar sources of systematic error, we have applied the same multi-predictor bias correction scheme for the assimilation of the PC scores.

After an initial training phase of typically two to three weeks, it is found that the bias correction for PC scores performs extremely well – it becomes very stable in time and removes almost all systematic differences between the observations and the analysis. An exception to this are the corrections computed for a small number of PC scores that are slower to stabilize and tend to drift slightly over time, most likely because these PCs are affected by the same processes that cause drifts in radiance biases (time varying model error and feedback with quality control). While this slow variation of bias corrections is undesirable and certainly warrants further investigation, previous experience with radiances, confirmed by tests with PC scores, suggests that it is not a significant source of quality degradation in the assimilation.

Set-up of the assimilation experiments

To quantify the performance of the PC-score assimilation system we have designed a basic set of 4D-Var assimilation experiments that consist of a baseline experiment (BASE), a radiance assimilation control experiment (RAD) and a PC-score experiment (PC-SCORE).

- BASE uses all operational observations (satellite and conventional) with the exception of IASI data.
- RAD is identical to BASE, but additionally assimilates 165 IASI radiances.
- PC-SCORE is identical to BASE, but additionally assimilates 20 PC scores derived from the 165 IASI radiances.

Note that in the RAD and PC-SCORE experiments the use of IASI data is restricted to fully clear pixels over the ocean. All experiments have been run using a reduced horizontal resolution version (T511, ~40 km) of cycle 38r2 of ECMWF's Integrated Forecasting System (IFS) with 137 vertical levels for the period from 1 June to 15 September 2012.

For the PC assimilation testing we have retained only the first 20 PC scores because it was found that beyond around that number there was no discernible improvement in performance (as measured by the fit of the analysis to other observations).

Impact on the assimilation

Analysis increments

Figure 1 shows the difference between zonally-averaged root-mean-square temperature analysis increments between RAD and BASE (left) and PC-SCORE and BASE (right) evaluated over the three-month assimilation period. Analysis increments (defined as the change to the initial conditions at the beginning of the 4D-Var analysis window) are a good indication of how much and where the background errors are corrected by the assimilation of observations.

It can be seen in Figure 1 that above 400 hPa the RAD and PC-SCORE display similar patterns of analysis increments. In other areas, for example in the tropics and at high latitudes, PC-SCORE has slightly larger adjustments than RAD. It is likely that the differences can be attributed to the slightly greater weight assigned to the PC scores than to the IASI radiances and to differences in data coverage. However, the most important conclusion is that in these statistics there is no evidence of any anomalous or spurious behavior in the analysis increments produced by the PC-SCORE experiment.

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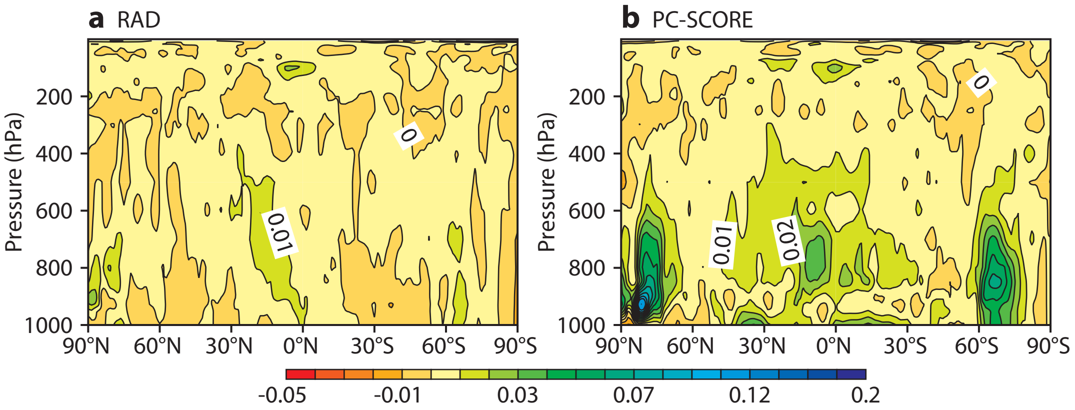

Figure 1 The difference between zonally-averaged root-mean-square temperature analysis increments for (a) RAD and BASE experiments and (b) PC-SCORE and BASE experiments. The results are evaluated over three months of assimilation for June to September 2012.

Fit to radiosonde data

When we examine how the assimilation of either PC scores or radiances modifies the fit to radiosonde temperature observations, we see that the assimilation of 20 PC scores produces results that are statistically comparable with those obtained from the assimilation of 165 radiances. This is exemplified in Figure 2, which shows results for the extratropical southern hemisphere (90ºS to 20ºN) where the fit to radiosonde data is particularly sensitive to changes in the use of satellite observations and thereby provides a reliable measure of quality. Standard deviations averaged over the three-month assimilation period for RAD and PC-SCORE are shown with respect to the BASE (values are explicitly normalised by the BASE to improve visualization) for the analysis (Figure 2a) and background (Figure 2b). Thus, reduced values indicate the extent to which the assimilation of the IASI satellite data (either using radiances or PC scores) improves the fit to radiosonde data compared to the BASE assimilation.

Computational efficiency

The primary objective of developing a PC-score assimilation system is to improve computational efficiency. Performance tests indicate that the 4D-Var minimization requires 25% less computer resources (elapsed CPU time) when 20 PC scores are used compared to the system that assimilates 165 radiances. This represents a significant saving inside the time-critical processing path for NWP centres, but could potentially be improved even further by tuning the efficiency of calculations for the radiative transfer model used for the simulation of the PCs (PC_RTTOV).

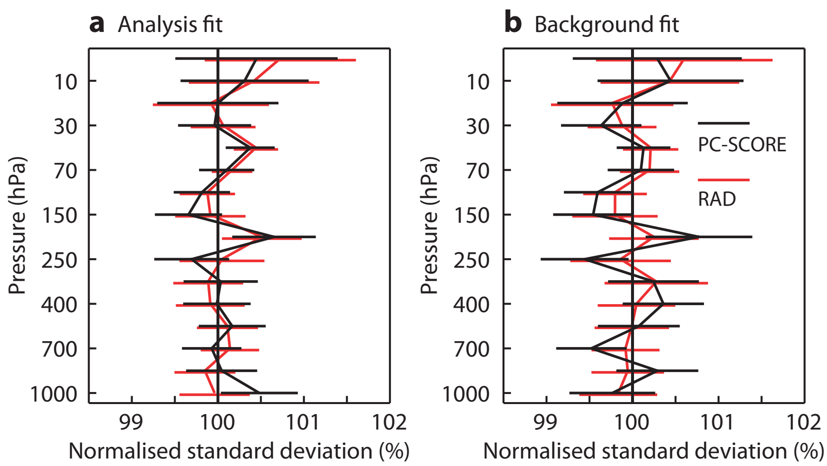

Figure 2 Normalised standard deviation of the fit to radiosonde temperature data of (a) the analysis and (b) background in the southern hemisphere for 15 June to 15 September 2012 are shown for the RAD and PC-SCORE experiments. The error bars indicate the 95% confidence range and thus give an indication of the statistical significance of the results.

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Impact on forecasts

Forecasts have been run from analyses generated by the BASE, RAD and PC-SCORE assimilation systems and verified using ECMWF operational analyses. Forecast scores for 15 June to 15 September 2012 have been computed as the change in the root-mean-square error compared to the BASE with the differences normalised by the forecast error of BASE. While this normalisation is arguably the best way to illustrate the impact on forecast errors in the medium range, it can result in the amplification of small differences in the shorter range (0 to 72 hours) where errors in the verifying analyses may be important.

To verify the forecast, the geopotential is traditionally used as a representative field because it provides a very good measure of the skill to predict large-scale flows and the general weather type. In the tropics, however, because of the different nature of the atmospheric circulation, the geopotential height (and indeed temperature) is not suitable to describe the predictive skill of the forecasting system and it is better to verify the wind vector.

Here we present results in terms of 500 hPa geopotential height for the extratropical northern and southern hemispheres (Figures 3a and 3c) and the 850 hPa wind vector in the tropics (Figure 3b). Results for the RAD experiment are plotted in the left panels while results of the PC-SCORE experiment are plotted in the right panels. A negative value of the forecast score means that the use of IASI data improves forecast accuracy compared to the BASE. Due to the relatively short duration of the experiments, some caution should be exercised when evaluating the results. This said, results suggest that the forecast scores produced by the assimilation of 20 PCs are statistically equivalent to those produced by the assimilation of 165 radiances, confirming the conclusion from the analysis diagnostics. This means that the PC-score assimilation system performs as well as the radiance system.

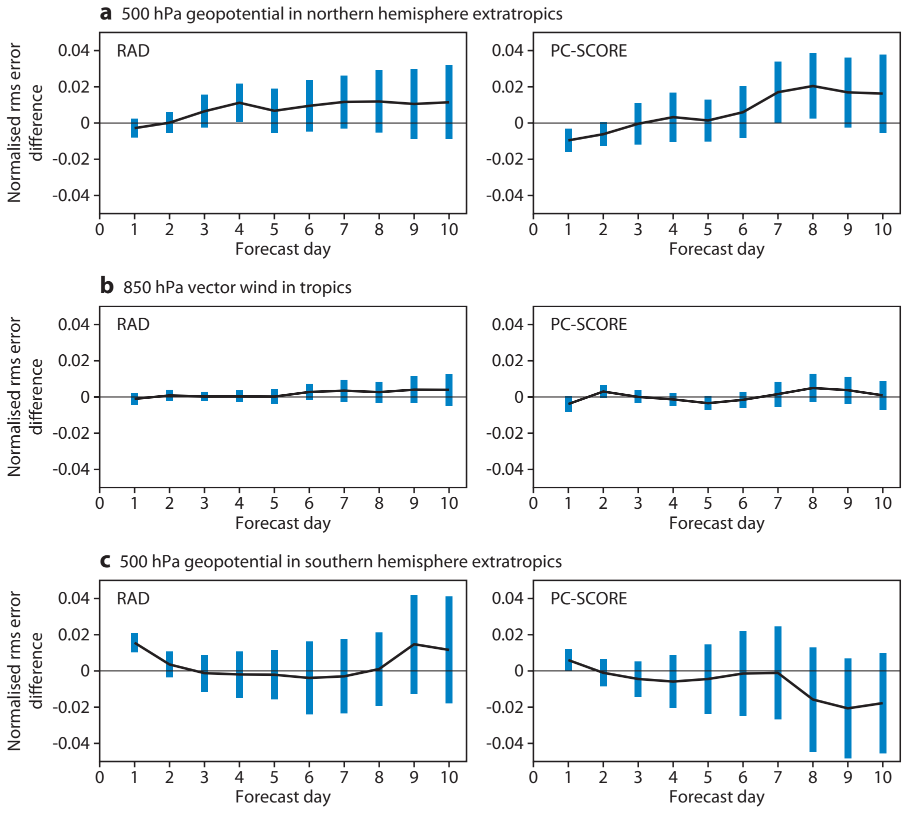

Figure 3 Normalised root-mean-square (rms) error difference for (a) 500 hPa geopotential forecasts in the northern hemisphere extratropics, (b) 850 hPa wind vector forecasts in the tropics and (c) 500 hPa geopotential forecasts in the southern hemisphere extratropics for RAD (left) and PC-SCORE (right) experiments for each forecast day. The forecasts are verified versus the operational analysis for 15 June to 15 September 2012. Error bars indicate the 95% confidence range.

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Summing up

The operational ECMWF 4D-Var has been adapted to allow the direct assimilation of PC scores derived from infrared sounders with a high spectral resolution. The primary aim is to develop an efficient use of the entire measured spectrum that could not be achieved by traditional radiance assimilation. The system presented in this study uses 20 PCs instead of 165 IASI long-wave radiances thereby achieving an eight-fold reduction in data volume and a 25% reduction in the overall cost of assimilation. These figures have been achieved with a rather conservative setting of the tuneable accuracy of the PC_RTTOV radiative transfer model and further computational savings could be achieved.

The new scheme has been extensively tested in a full observing system where IASI observations were used either as PC scores or radiances. Testing over a period of three months suggests that the quality of the analyses produced by the assimilation of 20 IASI PCs is almost identical to that obtained when 165 IASI radiances are assimilated. The verification of forecasts launched from these test analyses further confirms that there is no loss of skill from the assimilation of PC scores compared to that of radiances.

While this study considered only data in the IASI long-wave region, it follows a previous investigation into the use of PC scores to represent the IASI short-wave spectrum. A logical future step is to consider the extraction of information from the dedicated IASI water vapour and ozone bands towards the exploitation of all IASI spectral regions. Furthermore, within each spectral band we aim to use the largest possible number of channels to maximise the exploitation of the IASI instrument.

To summarise, the results obtained from the direct assimilation of IASI PC scores are very encouraging. They demonstrate the viability of an alternative route to radiance assimilation for the exploitation of high spectral resolution data from infrared sounders. Progress in this area is very timely – at the time of writing there were four such instruments in space (i.e. IASI on Metop-A and B, AIRS on AQUA and CrIS on NPP). Work is now needed to take this prototype system forward to a stage where it can be considered as an option for the safe and efficient operational exploitation of these crucial instruments.

Further reading

Collard, A.D. & **A.P. McNally,** 2009: Assimilation of IASI radiances at ECMWF. *Q. J. R. Meteorol. Soc.*, **135,** 1044–1058.

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