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Interactive comment on "Potential for the use of reconstructed IASI radiances in the detection of atmospheric trace gases" *by* N. C. Atkinson et al.

Anonymous Referee #2

Received and published: 15 April 2010

This paper addresses the impact of using principal components compression of IASI hyperspectral infrared observations on the detection of four trace gases for which nearreal time processing is needed. IASI Level 1C products disseminated via EUMETCast contribute significantly to the data volume on this service. In order to accommodate further products EUMETSAT has proposed a data reduction of the IASI L1C product based on Principal Components Analysis (PCA). However, studies need to be carried out to fully assess the impact of truncated IASI spectra on the various user services. In that respect, this paper deals with a very timely and pressing question.

However, I have a few major concerns about the paper itself, both in terms of clarity and presentation, that need to be properly addressed before considering this paper for publication.

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Major comments

My main concern is with the generality of the conclusions drawn here. The authors only consider detection of trace gases (not retrievals) as stated in the title of the paper. Therefore, the authors should be more cautious in the abstract and conclusion before giving general conclusions concerning the use of PC scores for chemical and climate purposes: their results might be promising in terms of detection, but the lonely retrieval case presented here - without details on the retrieval procedure and with somehow limited results, is not sufficient to fully grasp the impact of using PC scores. Only a few case studies are presented, when a much longer trial and evaluation period, over all seasons and areas, would be needed before judging the merits of using reconstructed radiances for chemistry and climate applications. The authors should try to present their arguments for what they are, without overselling their results.

Referring to the chemistry and climate community, the authors state "there is a concern that the signatures of trace gases may not be retained in the reconstructed spectra". One of the major concerns of this community is indeed that the signatures of trace gases may not be retained in the reconstructed spectra. This question is partially addressed in this paper. However, this is by far not the only worrying point. Most pressing questions are: -To what extent are the signatures entirely retained in the reconstructed spectra, especially for weak signatures? -What would be the impact of using PC scores on both the precision and the accuracy of trace gas retrievals? -Another major concern is what is called noise reduction: in a PCA, the diagonal noise is indeed reduced, but to the cost of increasing off-diagonal terms, something that could be seen as "noise spreading". -In terms of retrieval, and not only detection, most techniques take advantage of the correlation existing between channels. This correlation will certainly be affected by the compression and will certainly depend on the training set used to compute the eigenvectors. These points should be mentioned and addressed in the paper.

Many trace gases (CO2, CH4, N2O, etc) are characterized by strong seasonal cycles.

Any compression scheme should thus be evaluated over at least one year, and periodically checked to account for any evolution of the instrument or of the atmospheric state. Accordingly, the IASI Sounding Science Working Group, which is the scientific advisory body to both CNES and EUMETSAT for all matters related to IASI, recognized that any set of eigenvectors "needs to be tested over a long time period (of order one year), in order to evaluate the impact of the data truncation on the user services. There is a risk that the data truncation based on a distinct threshold will be rejected and that a truncation of the data with a new threshold will have to be tested for another trial period, with an unpredictable outcome." Such a statement should be added in the paper.

The paper strongly lacks a detailed description of the technique used to compute the principal components. Section 2 describes the general methodology but the authors do not explain how they adapted it to process IASI data. In particular, what noise normalisation matrix did they use? Did they work on apodized spectra? How was the scanning angle taken into account? Were the eigenvectors generated for each angle or not? A general description of the characteristics of IASI instruments (3 spectral bands, spectral and spatial resolutions, number of FOVs, etc) should be given at some point and linked to the choices the authors made to compute the principal components.

The choice of the eigenvectors is quite mysterious, and not clear at all for the average reader. Some information should be given on the way the training sets and the number of eigenvectors have been chosen. This is particularly true for sets 2 and 3, since neither reference nor detail is given for them. Concerning set 4, described in Section 4, some precision on the iterative selection of outliers should be given to fully grasp how the set is built. Since it is said that this set works better than the 3 previous ones, results obtained with this set should be presented (at least in terms of score) for all the cases studied before. This is particularly the case for SO2 since the authors claim in Section 3.2 that set 4 improves the residual structures found with set 3, but do not refer to it at all in Section 4.

 $\label{eq:concerning the figures, I find it particularly hard-and dangerous, to only compare raw$

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radiances in one panel with reconstructed radiances in another. A better way to present the results would be to plot the differences between raw radiances and reconstructed radiances. This would reveal to what extent the intensities of the plumes are similar, and the denoising of the radiances would be highlighted.

Specific comments

Abstract

p. 502, l. 7: "the technique can also be used to generate reconstructed radiances in which random instrument noise has been suppressed."

This is an overstatement. The noise is reduced to some extent, but at the cost of spreading the noise from diagonal terms to off-diagonal terms and changing the correlation between channels.

p. 502, I. 17-19: Some features of the chemical signatures are retained in the reconstructed radiances, but it is not clear from the results presented in the paper, to what extent the whole signatures are actually retained. Even a slight under/over-estimation could have huge impact on the precision and accuracy of the retrievals based on these signatures.

p. 502, l. 22-23: "The paper describes the generation of the reference eigenvectors for this new service."

Since this paper aims at being the reference for one part of the new EARS-IASI service, the generation of the eigenvectors should be more described in Section 4 (see above).

Introduction

p. 503, l. 14: could the authors specify whether the same subset of channels is used by all NWP centres or not, and, if not, what the differences are? In case these NWP centres used principal components, would they use the same set?

p. 503, l. 17-24: MACC is the atmospheric service of the European GMES programme.

Therefore, the sentence should be modified according to: "...in the context of the international efforts under the Global Monitoring for Environment and Security (GMES) initiative, in particular through its atmospheric service designed in the framework of the Monitoring Atmospheric Composition and Climate (MACC) project (http://www.gmes-atmosphere.eu/)."

p. 504, I. 9-12: the authors present the use of principal components as unavoidable. Another possibility to distribute IASI data would be to increase the bandwidth of the communication channels, or to distribute a reduced subset of channels selected by the users.

p. 504, l. 18: "This could occur if the trace gas signal is very weak (significantly below instrument noise level)"

This question has not been addressed in the paper, the authors focusing on rather strong signals, usually well above the noise level. A comment should be added on the performance of PCA for weak signal which are of the same level as the noise (as it is the case for CO2 or N2O for instance).

p. 505, l. 2-6: as explained in Razavi et al., 2009, the nu3 band MAY add information on CH4 but only in specific conditions. The sentence should be rephrase accordingly.

Section 2: PC methodology

p. 506, l. 20: what represents location i?

p. 506, l. 3-4: "To simplify the computation, the noise normalisation matrix is usually assumed to be diagonal."

Is it the case here? What is the reference for this matrix?

p. 506, l. 25: a brief description of the three bands of IASI should be given.

p. 507, l. 10: it would be helpful to explain what an elevated or particularly low value of a Reconstruction Score mean.

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Section 3.1: Detection of ammonia

Fig. 1 and 2: could it be possible to indicate on Fig. 1 the spots used to plot Fig. 2?

p. 508, l. 18-21: "we conclude that the inability of set 1 to detect the ammonia signal is due primarily to a lack of significant ammonia episodes within the relatively small set 1 training set"

This is quite an important comment, which shows a weakness of the methodology: as in any compression/retrieval scheme, the training dataset is a crucial element. If some events (here, signatures of key elements) are missing, the compression will fail. In case that some signatures appear to be missing (especially from unexpected species – let's remind here that one of the biggest discovery made from IASI observations was the ability to detect new species that were generally thought to be out of reach), a new dataset will have to be generated and tested. This should be included in the discussion.

p. 509, I. 2: what are the reconstruction scores obtained in band 1 with sets 2 and 3 and how does it compare with the reconstruction scores obtained with set 1?

p. 509, l. 3-4: "Clearly the inclusion of these outliers is adding an ammonia signal to the eigenvectors."

This sentence is quite vague and leads to the question of how big the added ammonia signal needs to be to add enough information in the data sets. Could it be possible to detail more carefully what is the level of detection that is achievable with IASI using raw radiances or reconstructed radiances?

Section 3.2: Detection of volcanic SO2

Could the authors provide some insights on the reasons for an overestimation of SO2 with set 2?

Section 3.4: Retrieval of carbon monoxide

The results presented in this section are particularly hard to evaluate since the retrieval

scheme is not detailed, nor even published. Details on the retrieval methodology should be given here (prior information, covariance matrices, spectroscopic databases, etc). The choice of the covariance matrices is particularly crucial in such an approach, since retrieval methods based on the so-called optimal method make use of the correlations existing between channels. Now, using principal components changes the covariance between channels. Therefore, the authors should indicate how they dealt with this issue.

Fig. 10: it would be interesting to add the noise level on the right panel to see how the BT difference compares to it.

p. 511, l. 21-25: "The differences between raw and set 3 radiances produce differences in retrieved values which are generally less than 25-50% of the retrieval error."

The typical retrieval error should be indicated, to give a feeling of what 50% of the error stands for in ppb. A striking feature displayed in Fig. 10 that is not addressed in the text, is the shape of the distribution of the error. It seems that there is a negative bias of about -20%, with an associated standard deviation of 25%. Could the author comment on that bias? What would be the implication of such a bias on the retrieved fields?

pp. 511-512: "In both cases, the residual fit is within the instrument noise across the spectral region, indicating that the principal component compression has had no major effect on the behaviour of the retrieval scheme."

This statement seems particularly misleading to me and should be rephrased. As already said, PCA decreases diagonal noise but increases off-diagonal terms of the noise matrix and changes the correlation between channels. Therefore, random noise has been traded for a reconstruction noise with specific characteristics that could influence the results.

Fig. 12: according to Fig. 12, the instrument noise seems constant in the spectral range 2140-2180 cm-1. Is it the case? What is the reference for the instrument noise?

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While brightness temperatures were used in all the other figures, radiances are shown in Fig. 12. For the sake of comparison, it would help the reader to re-plot Fig. 12 using brightness temperature.

Section 4: Further refinement of the eigenvectors

p. 512, l. 8-9: "The previous section has shown that the set of eigenvectors generated through the addition of outliers to the initial training set generally performs well."

This is overstated – it has been shown that some features could still be detected, but with no quantitative evaluation of the level of agreement.

Section 5: Conclusions

As said previously, the conclusions seem rather optimistic and definitive, despite all the questions that remain to be addressed. Here is the wording I object to:

p. 513, l. 23-24: "and additionally reduces the amount of random instrument noise in the reconstructed spectra considerably"

As explained before, the noise reduction has undesirable effects that should also be given here.

p. 514, l. 9: "However, an iterative procedure, involving refinement of a base training set by the addition of outlier spectra, is successful."

I would prefer the wording: ... by the addition of outlier spectra, helps improving the residuals.

p. 514, l. 10: "will be used in the EARS-IASI system".

It should be clearly said that the training set will need to be 1) fully tested by the community; 2) refined on a regular basis to account for unaccounted signatures or for any evolution of the instrument of the atmospheric state.

Interactive comment on Atmos. Meas. Tech. Discuss., 3, 501, 2010.