# Information content of radiance climatologies for advanced infra-red sounders

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## Abstract

When assimilating observations into numerical weather prediction (NWP) models, it is usually assumed that there are two sources of information: the observations and the NWP background field. Current research to improve the exploitation of advanced infra-red sounder data is making use of "radiance climatologies", i.e. large ensembles of "historical" radiances from the same instruments. The leading principal components (PCs) of the covariances of such ensembles are being used to make the processing and assimilation of these data more efficient - in both the forward (radiative transfer) computation and the inverse (retrieval/assimilation) component - and to reduce the noise in the measured spectra. These radiance climatologies therefore constitute a potential third source of information for retrieval/assimilation processes.

We consider here, from a theoretical perspective, the status of this third source of information and its implications for retrieval/analysis accuracy. We compare two methods of applying PCs to the processing of IASI spectra: simple PC truncation and optimal radiance estimation. We show why it is possible to reduce the noise in IASI Level 1C data considerably (by a factor ~3), yet this does not lead to comparable reductions in retrieval/analysis error. We also present the theory required to consider whether it is possible, with information from the radiance climatology, to reduce the retrieval error at all.

## 1. Introduction

Advanced hyper-spectral infra-red instruments for sounding the atmosphere provide thousands of observations in each measured radiance spectrum. For example, the Infra-red Atmospheric Sounding Interferometer (IASI) (Siméoni et al. 1997) on the Metop satellite series has 8461 channels, and the Atmospheric InfraRed Sounder (AIRS) (Pagano et al. 2003) on the Aqua satellite has 2378 channels. The length of this radiance vector greatly exceeds the number of independent atmospheric variables for which the observations carry information. For the atmospheric temperature and humidity profiles, this number is measured in tens and is related to the vertical resolution of the measurement and to measures of information content such as degrees of freedom for signal (See Collard 2007, Prunet et al. 1998, Rabier et al. 2002). In addition to the variables needed to represent adequately the temperature and humidity information, many more are required to explain fully the effects of clouds, aerosols, surface emissivity, etc., and the effects of nonlinearities. However, altogether the total number is probably in the range 200-300; studies have found that this is the number of principal components (PCs) of the covariance of a large climatological set of radiance vectors that are needed to reconstruct any radiance vector to within the instrument noise (Goldberg et al. 2003, Hultberg 2009).

Therefore the information content of each measurement vector is highly redundant. This raises the question: is it possible to exploit this feature to improve the interpretation of the observations? In this paper, we examine the nature of the information contained in “radiance climatologies” (RCs), by which we mean large, representative samples of past measurements from the same instrument, and we explore how such RCs can be used to improve the extraction of atmospheric information from the data. We also draw attention to the limitations of this approach.

Truncated PC representations of multi-spectral radiance observations have been used for many years, e.g. Smith and Woolf (1976), to reduce the dimension of the observation vector and thus to make data processing more efficient. In more recent years, they have been applied to spectra from hyper-spectral sounders, for which the efficiency gains are potentially much greater. They have been used with aircraft interferometer data, in anticipation of their use with satellite data (Huang and Antonelli 2001, Antonelli et al. 2004), with AIRS data (Goldberg et al. 2003) and with IASI data both pre- and post-launch (e.g. Aires et al. 2003, Hultberg 2009, EUMETSAT 2010, Collard et al. 2010, Atkinson et al. 2010). In these studies and applications, the data compression and noise reduction properties of PC representations, and of radiance spectra reconstructed from them, have been demonstrated, and the use of PC scores as input to retrievals and for quality control has been discussed.

In this paper, we step back from previous work on truncated PCs to take a fresh look at role of RCs from the perspective of optimal estimation (OE) theory, and we consider the use of truncated PCs as a special case of a more general use of RCs. It is clear from previous work that, via truncated PC representations of the spectrum, RCs offer a much improved efficiency in processing of hyper-spectral data. In this paper, we address the following questions: in obtaining this increased efficiency, (1) is there a small (perhaps insignificantly small) loss of information, as suggested by the truncated PC formulation, or (2) do the RCs provide additional information which allows us to make improved retrievals (perhaps insignificantly improved), or (3) do they make no difference to retrieval skill, if the various sources of information, error covariances, etc., are all handled optimally?

In Section 2, we show how the true (noise-free) radiance vector associated with a single measurement may be estimated in an optimal way from the measured radiances and a climatology of prior radiance measurements. We examine the relationship between this optimal estimate and an estimate obtained using a truncated PC representation of the spectrum, and we draw attention to some of the matrix ill-conditioning problems that arise. These ideas are illustrated with calculations for IASI spectra.

In Section 3, we present the theory for using these new estimates of the radiance vector (derived optimally or through PC truncation) for the retrieval of the atmospheric state. This represents the first part of a study to assess the questions: could the use of information in RCs have advantages in terms of reduced retrieval error and, if so, could these reductions be significant?

Section 4 presents a summary of the results and conclusions to date.

## 2. Optimal estimation of radiance vectors

### 2.1 Basic optimal estimation theory

Whenever we make a new observation, the information available to us in the radiance space is:

- the observed radiance vector, $y^o$, and its error covariance (instrument noise), N, and
- the RC obtained from previous observations.

Let us characterise the RC of the true (noise-free) radiances by its mean radiance, $y^m$, and its covariance, C.

We assume here that N is independent of the measurement itself and is constant in time. For real hyper-spectral instruments this should be valid, at least approximately, if the measurements are expressed as radiances (but not as brightness temperatures).

We can combine this new measurement with the RC to give an optimal estimate, y', of the true radiance vector and its error covariance, Q, using simple linear OE theory:

$$y' = Q\,(N^{-1}\,y^o + C^{-1}\,y^m) \ , \tag{2.1}$$

$$Q^{-1} = N^{-1} + C^{-1} \ , \tag{2.2}$$

Equations (2.1) and (2.2) can be rearranged in many ways, e.g.

$$y' = y^m + C\,(C+N)^{-1}\,(y^o - y^m) \ , \tag{2.3}$$

$$y' = y^o + N\,(N+C)^{-1}\,(y^m - y^o) \ , \tag{2.4}$$

$$Q = N\,(N+C)^{-1}\,C = N - N\,(N+C)^{-1}\,N = C - C\,(C+N)^{-1}\,C \ . \tag{2.5}$$

Note that the climatological covariance obtained from a large set of measurements is not C but $C^o$: the sum of the true (noise-free) radiance covariance and the noise covariance:

$$C^o = C + N \ . \tag{2.6}$$

Combining equations (2.3) and (2.6):

$$y' = y^m + (C^o - N)\,(C^o)^{-1}\,(y^m - y^o) \ . \tag{2.7}$$

This provides the optimal estimate of the radiance vector with an error covariance given by eq.(2.5).

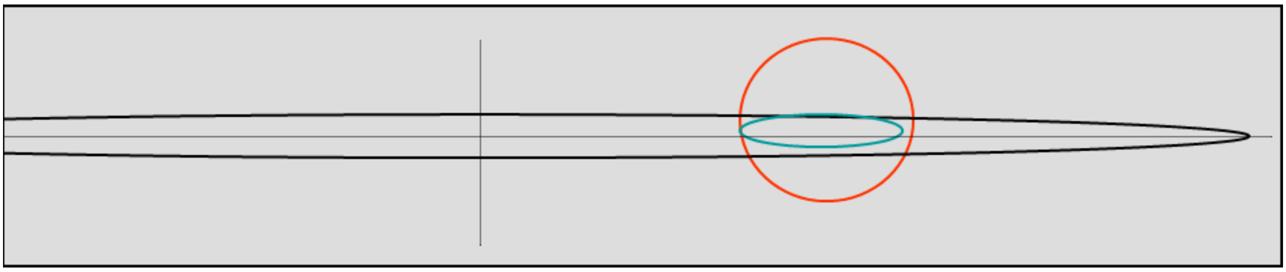

**Fig.1.** Illustrating noise reduction through optimal radiance estimation. The PDFs of the observed radiances, the radiance climatology and the optimal estimate are given by the (red) circle, the large (black) ellipse and the small (green) ellipse respectively. The centre of the cross is the mean of the radiance climatology.

Figure 1 illustrates geometrically the properties of the optimal estimate. If a radiance vector is represented by a point in an M-dimensional hyperspace, then probability density functions (PDF) of the radiances can be represented by hyper-ellipsoids in this space. If we normalise the radiance in each channel by the standard deviation of the instrument noise, then equi-probable surfaces for the observations will be hyper-spheres in this space. In Fig.1 we show a 2D section through this hyperspace passing through the observation, where the axes of the section are chosen such that: in one direction the variance of the climatology of the (noise-free) radiances is much greater than the instrument noise, and in the other it is much less. In this way, the circle represents the PDF of the observation and the large ellipse represents the PDF of the noise-free climatology (which is not in general co-centred with the observation). The small ellipse then represents the PDF of the optimal estimate. It is only slightly smaller than the circle in one direction but much smaller in the other. Thus the optimal estimate is an improved estimate of the radiances, but only significantly so in those directions for which the variance of the RC is comparable to or smaller than the instrument noise.

## 2.2 Relationship to PC truncation

What is the relationship between this optimal estimate and the estimate given by PC truncation? In the process of PC truncation (Goldberg et al. 2003, Hultberg 2009), it is usual to noise-normalise $C^o$ and then calculate its eigenvectors, E, and eigenvalues, $\lambda_j$ (which are diagonal elements of the diagonal matrix, $\Lambda$):

$$N^{-½}\, C^o\, N^{-½} \;=\; E\, \Lambda\, E^T \;. \qquad (2.8)$$

Therefore,

$$C^o \;=\; N^{½}\, E\, \Lambda\, E^T\, N^{½} \;, \qquad (2.9)$$

and $$(C^o)^{-1} \;=\; N^{-½}\, E\, \Lambda^{-1}\, E^T\, N^{-½} \;. \qquad (2.10)$$

From eq.(2.7) and (2.10):

$$y' \;=\; y^m + \{N^{½}\, E\}\, (\Lambda - I)\, \Lambda^{-1}\, \{E^T\, N^{-½}\}\, (y^o - y^m) \;, \qquad (2.11)$$

The matrix $(\Lambda\text{-I})\Lambda^{-1}$ is a diagonal matrix with diagonal elements

$$q_i = (\lambda_i - 1) / \lambda_i \,. \qquad (2.12)$$

We call the values $q_i$ the "PC weights".

Equation (2.12) represents the following set of operations:

- noise-normalise the observed radiance departures from the mean radiance, and project them on to the eigenvectors (i.e. form the PC scores),
- scale each PC score by its PC weight,
- project the scaled PC scores back into the radiance space,
- add these increments from the mean radiance to form the optimal estimate.

This is similar to the method of PC truncation. The difference is that here the PC scores are not simply accepted or rejected but scaled by their PC weights. The effect will be to "accept" ($q_i \approx 1$) all the modes that are predominantly signal and to "reject" ($q_i \approx 0$) all the modes that are predominantly noise, with a smooth transition in between. Moreover, the noise in the accepted modes will remain almost unchanged whereas the noise in the rejected modes will be reduced to zero.

## 2.3 Ill-conditioning problems

Combining equations (2.6) and (2.9), we obtain:

$$C = N^{½} E (\Lambda - I) E^T N^{½} \,, \qquad (2.13)$$

or $$C^{-1} = N^{-½} E (\Lambda - I)^{-1} E^T N^{-½} \,, \qquad 2.14)$$

where I is a unit matrix.

This means that, as eigenvalues of $N^{-½}C^oN^{-½}$ tend to 1, then the equivalent eigenvalues of $N^{-½}CN^{-½}$ will tend to 0. As discussed in section 1, the IASI spectrum contains only ~200 pieces of independent information in ~8000 channels. This means that, in the geometric representation of Fig.1, in most directions $C^o$ represents only instrument noise and so C is vanishingly small; the hyper-ellipsoid becomes a "hyper-disc". In eq.(2.9) and (2.13), $\lambda_j \approx 1$ for most j, and so $(\Lambda - I)$ and hence C will be highly ill-conditioned. Also, through eq.(5), Q will also be highly ill-conditioned as can be seen from Fig.1. This will lead to computational problems in any calculation involving $C^{-1}$ or $Q^{-1}$ or $(\Lambda - I)^{-1}$.

We can address these ill-conditioning problems by transforming the measurement into a new space, i.e. the eigenspace of the noise-normalised RC, and truncating it appropriately. We define the observation in the new space as:

$$z_{tr} = E_{tr}^{\ T} N^{-½} (y^o - y^m) \,, \qquad (2.15)$$

where subscript tr denotes an appropriately chosen truncation of the full set of eigenvectors.

In this space the RC has a mean value of 0 and a covariance of $(\Lambda_{tr} - I_{tr})$. The optimally estimated measurement in the new space, equivalent to equations (2.11) or (2.12) is:

$$z_{tr}' = Q_{tr} E_{tr}^T N^{-½} (y^o - y^m) , \qquad (2.16)$$

where $Q_{tr} = (\Lambda_{tr} - I_{tr}) \Lambda_{tr}^{-1}$ (2.17)

and is the error covariance of $z_{tr}'$. $Q_{tr}$ is a diagonal matrix with the truncated PC weights as its diagonal elements.

## 2.4 Application to IASI data

We start our computations from observed IASI "climatological" covariance matrices supplied by EUMETSAT and used by EUMETSAT to compute operational PC scores (Hultberg 2009, EUMETSAT 2010). They are supplied separately for the 3 IASI bands: band 1, channels 1-1997 (645-1144 $cm^{-1}$); band 2, channels 1998-5116 (1144.25-1923.75 $cm^{-1}$); band 3, channels 5117-8461 (1924-2760 $cm^{-1}$). Each covariance matrix is formed from ~100000 spectra. We noise-normalise these matrices using a full matrix N which takes account of the apodisation of IASI Level 1C data, using an apodisation matrix as described by Lee and Bedford (2004).

The eigen-decomposition of the noise-normalised matrix then gives the values of $\lambda_i$ (eq. 2.8) and then the PC weights (eq. 2.18). The PC weights for IASI band 1 are shown in Fig.2.

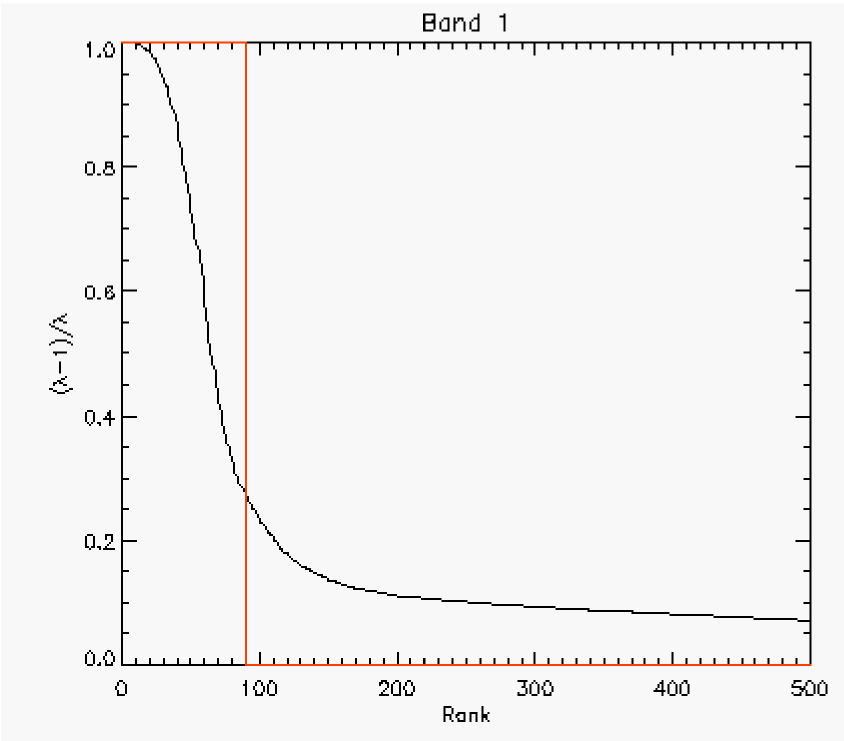


**Fig. 2.** PC weights (black line) for the leading 500 PCs for IASI band 1, and equivalent PC weights (red line) for simple PC truncation at the 90th PC.

Figure 2 illustrates the relationship between optimally estimated radiances and simple PC truncation; in the latter the PC weight equals one for each leading PC and zero beyond the truncation point, whereas for the former the reduction in PC weights is gradual.

Diagonals of N and of Q in the original radiance space are shown for IASI band 1 in Fig.3.

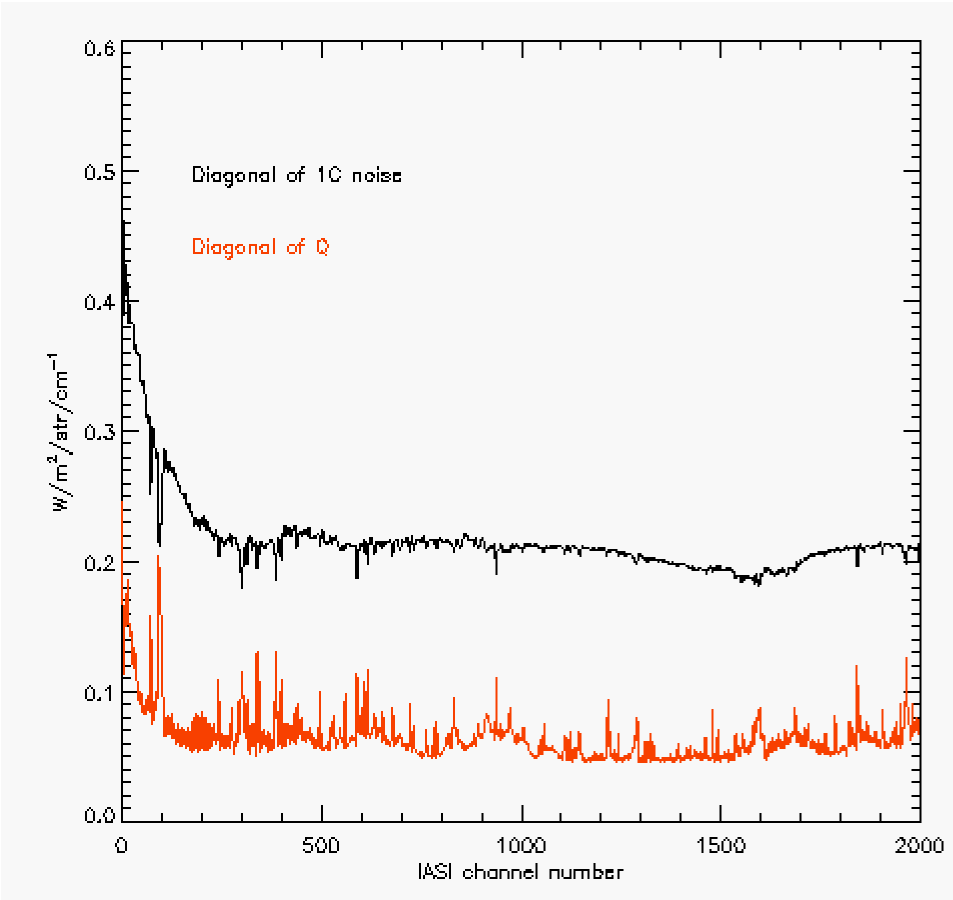


**Fig.3.** Noise standard deviations (square roots of the diagonals of covariance matrices) for channels in IASI band 1. Upper line (black): Level 1C radiances; lower line (red): optimally estimated radiances.

Figure 3 shows the effect of optimal estimation on the measurements when they are projected back into the original radiance space. The noise is reduced by a factor of ~3-4. The values for simple PC truncation (not shown) are similar. [For unapodised spectra, for which the noise power is expected to be distributed equally amongst all the PCs, simple PC truncation is expected to reduce the noise power by the ratio of the total number of channels to the number of PCs retained. For IASI band 1, this would be 1997/90 = 22.2 for noise variance, or 4.7 for its standard deviation. This value is expected to be reduced for Level 1C spectra because of the adopisation process.]

## 3. Consequences for the retrieval of atmospheric variables

The noise reduction possible through optimal estimation of the radiances or through PC truncation is very great, but to what extent are we able to benefit from this when retrieving atmospheric variables? We now explore this question from two theoretical perspectives.

### 3.1 Radiance climatology as prior information on the observations

It is instructive to return to the Bayesian probability theory from which optimal estimation can be derived (see Rodgers 1976). The conditional probability of the atmospheric state x given the measurements $y^o$ is given by:

$$P(x|y^o) = P(y^o|x)\, P(x) / P(y^o) \quad , \qquad (3.1)$$

where P(x) is the prior probability of x, $P(y^o)$ is the prior probability of $y^o$, and $P(y^o|x)$ is the conditional probability of $y^o$ given x.

The most probable value of x is obtained by maximising $P(x|y^o)$ with respect to x. This is equivalent to maximising $\ln\{P(x|y^o)\}$ which, with the addition of a constant, gives the usual "cost function" J(x) used in variational analysis (see Lorenc 1988):

$$J(x) = k_1 - \ln\{P(x|y^o)\} = k_1 - \ln\{P(y^o|x)\} - \ln\{P(x)\} + \ln\{P(y^o)\} \quad . \qquad (3.2)$$

If the probability functions are Gaussian, the terms in the cost function will take their normal quadratic form, but eq.(3.2) shows how to obtain the appropriate cost function if the probabilities are other than Gaussian.

The final term in eq.(3.2) is usually absorbed into the constant and ignored. This is because the prior probability of the observations, $P(y^o)$, is usually assumed to be constant across the range of values for which it is physically possible for the instrument to record values (and to be zero outside this range).

Now, if we have prior knowledge of $y^o$ through a RC, then it is possible to replace the constant $P(y^o)$ by a Gaussian of the form:

$$\ln\{P(y^o)\} = k_2 - \{(y^o - y^m)^T (C^o)^{-1} (y^o - y^m)\} \quad , \qquad (3.3)$$

where $y^o$, $y^m$ and $C^o$ are as defined in Section 2, and $k_2$ is a normalising constant.

The use of eq.(3.3) for $\ln\{P(y^o)\}$ clearly changes the form of the cost function, and it will change the value of J(x) for a given $y^o$. This may be important whenever the value of J(x) itself is used as part of the retrieval/analysis process, e.g. in quality control. However $\ln\{P(y^o)\}$, although no longer constant, is not a function of x. When we seek the optimal value of x by differentiating eq.(3.2) with respect to x, the term involving $\ln\{P(y^o)\}$ is lost, and so it can have no effect on the optimal value of x.

Therefore, from this perspective, i.e. with a mathematical statement of the problem to be solved represented by equations (3.1)-(3.3), we conclude that: the additional information contained in the RC, whilst it allows us to improve certain components of our estimate of the radiance vector, does not allow us to improve our estimate of x.

### 3.2 Radiance climatology as a third source of information

In Section 2 we have shown how a measurement $y^o$, with expected error covariance N, may be combined with a climatological estimate $y^m$, with expected error covariance C, to provide an improved estimate of the radiance vector y' with expected error covariance Q. We can now use this improved estimate to obtain an estimate of the atmospheric state.

Variational theory (e.g. see Lorenc 1988, Rodgers 1976) provides us with a framework for combining new observational information with prior information on the atmospheric state, in the form of an estimate $x_b$ with expected error covariance B, to give a new estimate $x_a$ with expected error covariance A.

Consider first the estimation of x from the original observations $y^o$. Starting from Bayesian theory, we derive a cost function of the form:

$$J(x) = (x - x_b)^T B^{-1} (x - x_b) + \{ (y^o - y(x))^T (N + F)^{-1} (y^o - y(x)) \} , \quad (3.4)$$

where y(x) is the “observation operator”, which computes the radiances expected given the state x, and F is the error covariance of the observation operator.

By linearising the problem it can be shown that the error covariance of the solution, A, is given (exactly, in the linear limit) by:

$$A = B - B H^T (H B H^T + N + F)^{-1} H B , \quad (3.5)$$

or

$$A^{-1} = B^{-1} + H^T (N + F)^{-1} H , \quad (3.6)$$

where H is the radiance Jacobian, i.e. the gradient of y(x) with respect to x.

Now, when $y^o$ and its error covariance N are replaced by the new estimates, y' and Q, the equivalent equation for the error covariance is:

$$A' = B - B H^T (H B H^T + Q + F)^{-1} H B . \quad (3.7)$$

or

$$A'^{-1} = B^{-1} + H^T (Q + F)^{-1} H , \quad (3.8)$$

The evaluation of equation (3.7) or (3.8) is problematic because of the ill-conditioning problems discussed in section 2.3. These can be addressed by working in the transformed, truncated radiance space described in that section. In transformed space, the Jacobians are given by:

$$H_{PC} = E^T N^{-½} H , \quad (3.9)$$

and in the truncated, transformed space by:

$$(H_{PC})_{tr} = E_{tr}^T N^{-½} H \ . \qquad (3.10)$$

In the limit of F=0, the equations for error covariances are as follows:

for all channels or all PCs: $$A^{-1} = B^{-1} + H^T N^{-1} H = B^{-1} + H_{PC}^T H_{PC} \ , \qquad (3.11)$$

for truncated PCs: $$A^{-1} = B^{-1} + (H_{PC})_{tr}^T (H_{PC})_{tr} \ , \qquad (3.12)$$

for optimally estimated radiances: $$A^{-1} = B^{-1} + (H_{PC})_{tr}^T Q_{tr}^{-1} (H_{PC})_{tr} \ . \qquad (3.13)$$

The limit of F=0 is, of course, unrealistic for assimilation/retrieval with real data. If the forward model error F has been absorbed, such that N and Q are estimates of total error (i.e. including forward model error), then equations 3.11-3.13 would be valid. However, note that now the noise-normalisation based on instrument noise only is not optimal; a renormalisation including the effects of forward model error would be appropriate for the retrieval/analysis problem.

## 4. Summary and conclusions

PCs of radiance climatologies have demonstrated “engineering” advantages – for data compression and for efficient radiative transfer calculations, with consequent efficiencies for retrieval and assimilation operations. The work presented here is the first part of a study to explore the questions: do PCs of radiance climatologies have additional scientific advantages in terms of reduced retrieval error and, if so, are the reductions significant?

We have introduced the context of optimal radiance estimation and shown its relationship to a truncated PC representation of the spectrum. We have shown that optimally-estimated radiances (as with radiances reconstructed from truncated PCs) give a large reduction in noise compared with the original radiances. However, noise is removed mainly in “directions” (in radiance space) that contain no atmospheric information, and so this reduction is not expected to lead to dramatic reductions in retrieval error.

Nevertheless, it is interesting to quantify what reductions, if any, will be possible in retrieval error, and further work is planned on this quantification for IASI using the theory presented in section 3.

## Acknowledgements

This work has benefited considerably from discussions with Andrew Collard, Sean Healy, Fiona Hilton and Tim Hultberg. Tim Hultberg also provided the IASI radiance covariance data on which our calculations are based.

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