The sensitivity of the suboptimal NWP analysis system to the representation of hyperspectral data

Fiona Hilton and John Eyre
Met Office
FitzRoy Road, Exeter, EX1 3PB
fiona.hilton@metoffice.gov.uk

Abstract

Satellite data are usually assimilated in the numerical weather prediction (NWP) system via variational analysis schemes based on optimal estimation theory. This theory will only give an optimal analysis if the assumed observation and background errors are correct. In practice, the analysis is suboptimal, as observation error correlations and the synoptic dependence of background errors are usually ignored.

This paper tests the hypothesis that the form of the response of the observations to changes in the atmospheric profile (in other words, the shape of the Jacobian) may affect the sensitivity of the analysis to misspecification of the background error covariance matrix, **B**. This question is particularly relevant to the assimilation of hyperspectral data, where significant research effort has already been put into the assimilation of principal components (PCs) of measured spectra. PC Jacobians, which are very different in shape from radiance Jacobians, are highly nonlocalised in the vertical. It has been conjectured that the increased nonlocalisation may give rise to greater sensitivity to the misspecification of the background error. The hypothesis is tested in a one-dimensional variational (1D-Var) context with idealised Jacobian forms, and also with typical Infrared Atmospheric Sounding Interferometer (IASI) Jacobians in radiance and principal component form.

Experiments with idealised Jacobians suggest that the narrowness of the weighting function is important in minimising the effects of misspecification of background error covariances. The results also suggest that if the full profile space is evenly spanned, increasing the number of overlapping channels will not mitigate against the misspecification. Experiments with IASI Jacobians in radiance space suggest that using the full spectrum as opposed to a small subset of channels may help to produce a more robust analysis in the event of errors in **B**. There is no evidence that the representation of the full spectral information as PCs increases the degradation of the analysis, in an unbiased system. Further experiments are required to understand the implications of misspecification of observation error and the introduction of bias into the system.

1 Introduction

Data assimilation schemes in numerical weather prediction (NWP) systems, for example four-dimensional variational assimilation (4D-Var), are usually based on optimal estimation theory (e.g. Rodgers, 2000). The analysis generated will only be optimal if all assumptions made in the underlying theory hold true. Many of the assumptions are quite reasonable for satellite data assimilation techniques. For example the requirement that the observation response to changes in the atmospheric profile is linear to small perturbations about the background state is a fair assumption for certain analysis problems such as temperature profile determination, although it does not hold for cloudy analysis. It is also assumed that the background and observation errors are uncorrelated, which is true for direct radiance assimilation. However, the assumption that the observation and model are unbiased with respect to the true atmosphere does not generally hold, as we find residual biases between observations and model even after bias correction. Also fundamental to an optimal analysis is that the background and observation error covariance statistics are well-characterised.

One of the major conclusions of the 2009 ECMWF/EUMETSAT NWP-SAF "Workshop on the Assimilation of IASI in NWP" was that observation errors for hyperspectral sounders are not well characterised, and it is not clear that they can be estimated with sufficient accuracy to ensure an optimal analysis (Garand et al., 2009). Recent work by Bormann and Bauer (2010), Bormann et al. (2010) and Stewart (2010) has begun to address the form of the observation error covariance structure and its influence on the optimality of the NWP analysis.

Of equal importance in establishing the correct weighting of observations and background to produce an optimal analysis is the background error covariance matrix, which will be referred to as $\mathbf{B}$. The form of $\mathbf{B}$ is generally estimated using a procedure such as the so-called National Meteorological Center (NMC) method (Parrish and Derber, 1992) or via the use of an ensemble forecasting system (e.g. Fisher, 2003). These methods are usually used to produce a statistical estimate of the error in the background state, which results in a mismatch between the assumed $\mathbf{B}$, here referred to as $\mathbf{B_A}$, and the true $\mathbf{B}$ for a given point in time and space. Hybrid methods, combining a statistical estimate with a flow-dependent component usually derived from an ensemble of forecast states, attempt to reduce this mismatch. However, background errors can only ever be approximated and so misspecification is likely to remain an issue.

Eyre and Hilton (2010) investigate the potential effects of misspecifying $\mathbf{B_A}$. One possible outcome is that the analysis may have larger errors than the true background error. The purpose of the current work, of which the initial stages are presented here, is to establish an assimilation system for infrared hyperspectral sounders which is less sensitive to misspecification of $\mathbf{B_A}$. It is thought that the shape of the observation Jacobian may play an important part in defining a robust assimilation system with minimal sensitivity to errors in $\mathbf{B_A}$.

2 The assimilation of infrared hyperspectral observations

Operational NWP centres have for several years assimilated radiances from AIRS and IASI (e.g. McNally et al., 2006; Hilton et al., 2009; Collard and McNally, 2009). Typically, less than 200 channels are assimilated operationally, out of the several thousand available. The most important reason for choosing such a small subset of channels is that the information content of the full spectrum is well below the number of channels, and most of the information can be retained in a well-chosen channel subset (e.g. Collard, 2007) which is computationally affordable to process.

One alternative technique proposed for operational assimilation schemes is to transform the data into orthogonal pieces of information using principal components (PCs) and then to assimilate a truncated set of PC scores (Antonelli et al., 2004; Liu et al., 2007). This would preserve even more of the information content of the full spectrum, give faster radiative transfer calculations, and moreover reduce the random noise in the observation. The assimilation of PC-transformed data seems an ideal solution, but there are some practical difficulties with the use of the data in an operational system (Hilton and Collard, 2009; Collard et al., 2010). One particular concern is the shape of PC Jacobians, which are highly nonlocalised in the vertical (see Figure 8). Problems have been observed in the Met Office operational system with AIRS channels that have distinct peaks in the stratosphere and troposphere; occasional erroneous increments in the troposphere were attributed to a poorly specified background in the stratosphere. If the background errors were perfectly known, this result should not occur statistically, as the larger background error in the stratosphere should allow for the profile increment to be retained at the correct height.

The work presented here tests the hypothesis that the nonlocalisation of the Jacobian form makes the analysis more susceptible to misspecification of $\mathbf{B_A}$, allowing errors which are not correctly specified to be transferred to other parts of the profile. This process of error transfer may potentially result in an analysis that is worse than its forecast background.

3 The suboptimal NWP analysis

The theory of the suboptimal analysis system, where $\mathbf{B_A} \neq \mathbf{B}$ is described fully in Eyre and Hilton (2010). The optimal analysis error at a given $\mathbf{B}$ is given by:

$$\mathbf{A_{opt}}(\mathbf{B}) = (\mathbf{I} - \mathbf{KH})\mathbf{B}(\mathbf{I} - \mathbf{KH})^T + \mathbf{KRK}^T \tag{1}$$

where $\mathbf{A_{opt}}$ is the optimal analysis error, $\mathbf{K}$ is the Kalman gain, or the weight given to the observations in the linear analysis, $\mathbf{H}$ is the observation Jacobian, and $\mathbf{I}$ is the identity matrix. In the suboptimal case, the true analysis error, $\mathbf{A}$, is greater than $\mathbf{A_{opt}}(\mathbf{B_A})$ because the weight, $\mathbf{K}$, is evaluated at $\mathbf{B_A}$, which is denoted in equation 2 by subscript $\mathbf{B_A}$:

$$\mathbf{A}(\mathbf{B}) = (\mathbf{I} - \mathbf{K_{B_A}H})\mathbf{B}(\mathbf{I} - \mathbf{K_{B_A}H})^T + \mathbf{K_{B_A}RK_{B_A}}^T \tag{2}$$

The analysis is always calculated using $\mathbf{B_A}$ to define the weights, because this is the known quantity in the variational assimilation system, while true $\mathbf{B}$ is unknown. Equation 2 can be rewritten in terms of the optimal analysis error at $\mathbf{B_A}$, and a background sensitivity component resulting from the difference between $\mathbf{B}$ and $\mathbf{B_A}$:

$$\mathbf{A}(\mathbf{B}) = \underbrace{(\mathbf{I} - \mathbf{K_{B_A}H})(\mathbf{B} - \mathbf{B_A})(\mathbf{I} - \mathbf{K_{B_A}H})^T}_{\text{background sensitivity}} + \underbrace{(\mathbf{I} - \mathbf{K_{B_A}H})\mathbf{B_A}(\mathbf{I} - \mathbf{K_{B_A}H})^T + \mathbf{K_{B_A}RK_{B_A}}^T}_{\mathbf{A_{opt}}(\mathbf{B_A})} \tag{3}$$

If the background sensitivity is small, the analysis is relatively insensitive to misspecification of $\mathbf{B_A}$. Even if it is relatively large, only certain criteria will result in a degradation of $\mathbf{A}$ to the extent that $\mathbf{A} > \mathbf{B}$ (see Eyre and Hilton, 2010, for a description of the “Danger Zone”). The analysis presented in the following sections examines: whether Jacobian shape is an important factor in the sensitivity to misspecified $\mathbf{B_A}$; whether the vertical density of Jacobians helps to mitigate against a large background sensitivity; and whether a PC representation of the IASI spectrum is likely to lead to a degraded analysis.

4 Method

Various forms of misspecification of $\mathbf{B_A}$ have been tested, from a simple scaling of variance to the use of a new matrix with completely different structure from $\mathbf{B}$. The following sets of experiments were performed, using two different matrices, $\mathbf{B_1}$ and $\mathbf{B_2}$. In each case, we take $\mathbf{B} = \mathbf{B_1}$ and make the following modifications to $\mathbf{B_A}$:

- Scale all the variances of $\mathbf{B_1}$ by a factor to make $\mathbf{B_A}$ larger (experiments a and b)
- Scale all the variances of $\mathbf{B_1}$ by a factor to make $\mathbf{B_A}$ smaller (experiments c and d)
- Use the eigenvectors of $\mathbf{B_1}$ to make $\mathbf{B_A}$, but take the eigenvalues from $\mathbf{B_2}$ (experiment e)
- Use the eigenvectors of $\mathbf{B_2}$ to make $\mathbf{B_A}$, but take the eigenvalues from $\mathbf{B_1}$ (experiment f)
- Use the correlation structure of $\mathbf{B_2}$ to make $\mathbf{B_A}$, but take the variances from $\mathbf{B_1}$ (experiment g)
- Use $\mathbf{B_2}$ for $\mathbf{B_A}$ (experiment h)

These experiments were performed for univariate temperature and water vapour retrievals. Water vapour retrievals are performed in units of ln(g/kg).

For $\mathbf{B_1}$, the matrix chosen is that used in the Met Office's operational 1D-Var preprocessor for satellite radiances. This is a matrix dating from around 2000, and as such represents a 1D estimate of the 3D-Var error covariance matrix used at the time. For $\mathbf{B_2}$, a 1D estimate of the Met Office's operational 4D-Var error covariance from December 2009 was calculated. The matrix was calculated by taking the covariance of a set of column profiles of temperature and water vapour representing random perturbations consistent with the original statistics (using a method following Andersson et al., 2000). In both cases, the matrix is calculated on 43 RTTOV fixed pressure levels (Saunders, 2002), on which the operational 1D-Var preprocessor is run. $\mathbf{B_1}$ only has the lowest 26 levels defined for water vapour analysis and is set to zero above this. $\mathbf{B_2}$ has much lower errors for temperature, but the water vapour components do not differ as greatly (Figure 1).

The background sensitivity was calculated in each case, for a variety of Jacobian shapes:

- Delta function
- Idealised 20-channel weighting functions following Rodgers (2000)
- Idealised 150-channel weighting functions following Rodgers (2000)
- IASI Jacobians for the US Standard Atmosphere, 314 channel set (Collard, 2007)
- IASI Jacobians for the US Standard Atmosphere, full channel set
- IASI Jacobians for the US Standard Atmosphere transformed to PC space (assuming eigenvectors of apodised IASI observations as used in Hilton and Collard, 2009)

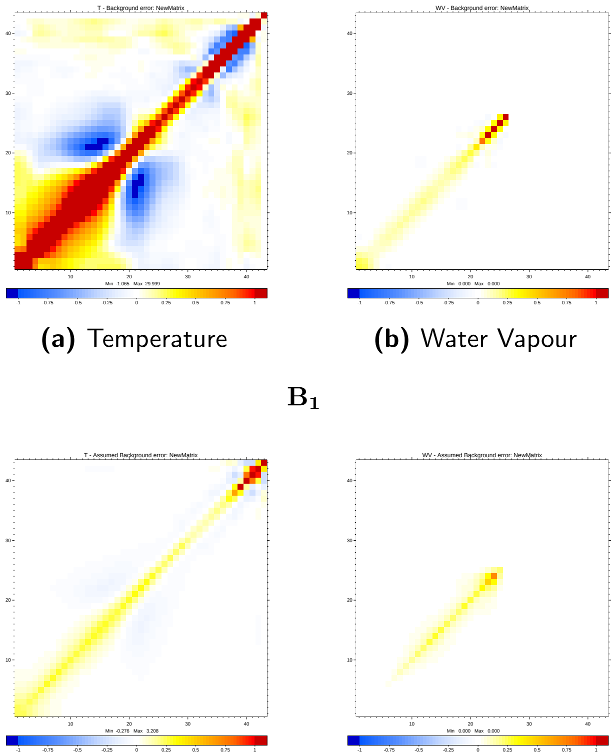
The background sensitivity components were plotted to determine whether particular Jacobian shapes showed greater sensitivity to changes in $\mathbf{B_A}$. For some combinations of $\mathbf{B_A}$ and Jacobian, the quantity $\mathbf{A}-\mathbf{B}$ was also plotted in order to determine whether a particular background sensitivity component was likely to lead to a degraded analysis.

5 Results

The experiments attempt to answer three questions:

1. Does the width of the weighting function affect the sensitivity of the analysis to errors in $\mathbf{B_A}$?
2. Do highly overlapping weighting functions mitigate against errors in $\mathbf{B_A}$?
3. Do highly nonlocalised weighting functions show more sensitivity to errors in $\mathbf{B_A}$?

The first two questions are addressed by the experiments with synthetic weighting functions, and the third using IASI Jacobians in channel and PC space.



(a) Temperature **(b)** Water Vapour

$\mathbf{B_1}$

(c) Temperature **(d)** Water Vapour

$\mathbf{B_2}$

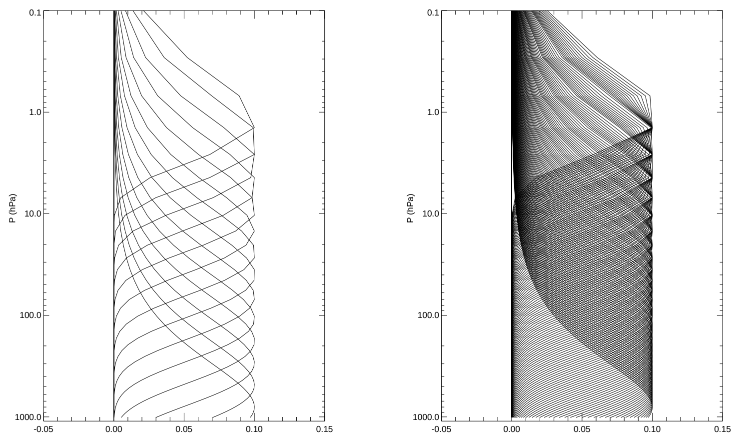
Figure 1: Background error covariance matrices used in calculations of background sensitivity. Level 1 in the lower left corner is the surface level, and level 43 in the top right is the topmost stratospheric level. Colour scales run from -1 in blue to +1 in red.

5.1 Idealised weighting functions

Two forms of idealised Jacobian have been investigated: a set of delta functions defined on RTTOV levels, and idealised, evenly-spaced weighting functions equivalent to those used by Rodgers in his example calculations (Rodgers, 2000). For temperature analysis, two idealised instruments were set up: one with 20 channels and one with 150 channels, with both sets of channels spanning the full atmospheric column (Figure 2). For water vapour, the 20-channel idealised instrument spanned the troposphere only, and no 150 channel instrument was used. For both delta function and idealised weighting functions, the observation error was set to $\sigma = 0.5$K.

Figures 3 and 4 show background sensitivity components for a delta function for temperature and water vapour respectively. A delta function Jacobian is virtually insensitive to the misspecification of $\mathbf{B_A}$. Simple incorrect scaling of the matrix has almost no effect on the analysis increment—only when $\mathbf{B_A}$ is completely unrelated to $\mathbf{B}$ or when the eigenvalues are decreased significantly is there a moderate background sensitivity component.

Figures 5 and 6 show the background sensitivity, for temperature and water vapour, for the 20 channel synthetic instrument. They show that a wider instrument response similar to a satellite weighting function is more sensitive to misspecification of $\mathbf{B_A}$, resulting in a larger background sensitivity for each experiment in both temperature and water vapour. The background sensitivity is furthermore correlated (or anticorrelated) between layers, particularly for temperature. The experiments which altered the mag-



(a) 20 channels **(b)** 150 channels

Figure 2: Idealised weighting functions defined on 43 RTTOV levels

nitude of $\mathbf{B_A}$ (large scale factors, new eigenvalues, or a new matrix) gave a larger background sensitivity than the other experiments.

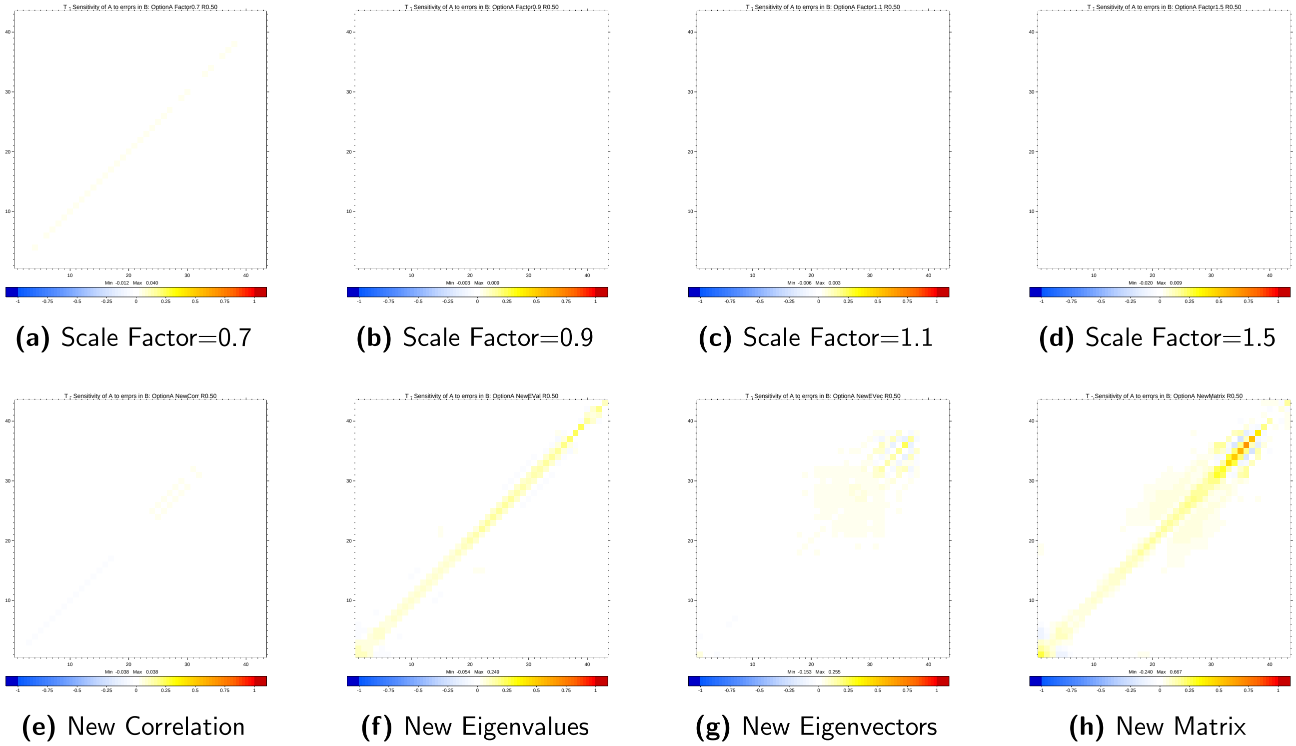
The number of channels spanning the retrieval space seems to have little effect on the size of the background sensitivityt, demonstrated for the 150 channel synthetic instrument for temperature in figure 7. This last result is perhaps somewhat unexpected—intuitively one might think that a larger number of channels would allow better differentiation between adjacent retrieval levels and that this might result in a lower sensitivity to errors in $\mathbf{B_A}$. This result is explored further in section 5.2.

For most of the water vapour experiments, the largest effect is at the top of the water vapour profile between levels 20 (286 hPa) and 26 (122 hPa), where $\mathbf{B}$ is largest and the numerical discrepancy between $\mathbf{B}$ and $\mathbf{B_A}$ is greatest. Replacing the eigenvectors or using a completely new matrix affected the whole column. Changing the eigenvalues had a large effect on the temperature retrieval, but the greater similarity in magnitude of diagonal elements between $\mathbf{B_1}$ and $\mathbf{B_2}$ is probably the reason that this experiment does not produce a particularly large background sensitivity component for water vapour.

The results presented in this section show a very narrow vertical response function is relatively insensitive to misspecification of $\mathbf{B_A}$. A wider response function is more sensitive, and the resulting analysis is further from the optimal analysis. More highly overlapping weighting functions do not seem to mitigate to any great extent against this (although see results in section 5.2 regarding how well-spanned the column is). The effect of the degree of localisation on the size of the background sensitivity component is tested in section 5.2 using IASI Jacobians.

5.2 IASI Jacobians in channel and PC space

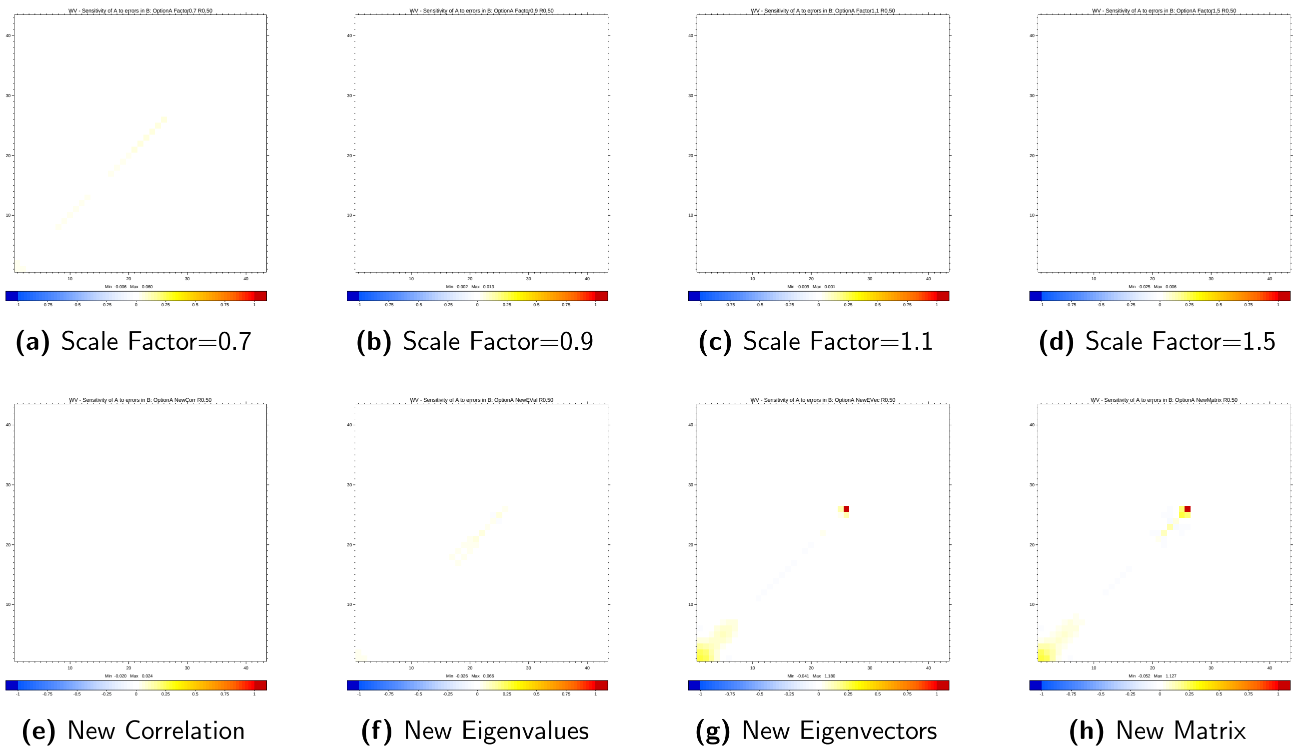
As a method of optimising hyperspectral data assimilation, principal component compression is gaining support as a way to increase the computational efficiency and maximise the information content. Before it can be used in an operational context, the implications of the PC-transform on the analysis problem must be understood. It is therefore important to consider whether the degree of localisation of the Jacobians affects the sensitivity of the analysis to misspecification of $\mathbf{B_A}$. Figure 8 shows the first 10 temperature Jacobians for the US Standard Atmosphere, for a set of PCs derived from real IASI data. The PC Jacobians not only span broad regions of the atmospheric column, but are also multiply peaked rather than



(a) Scale Factor=0.7 (b) Scale Factor=0.9 (c) Scale Factor=1.1 (d) Scale Factor=1.5

(e) New Correlation (f) New Eigenvalues (g) New Eigenvectors (h) New Matrix

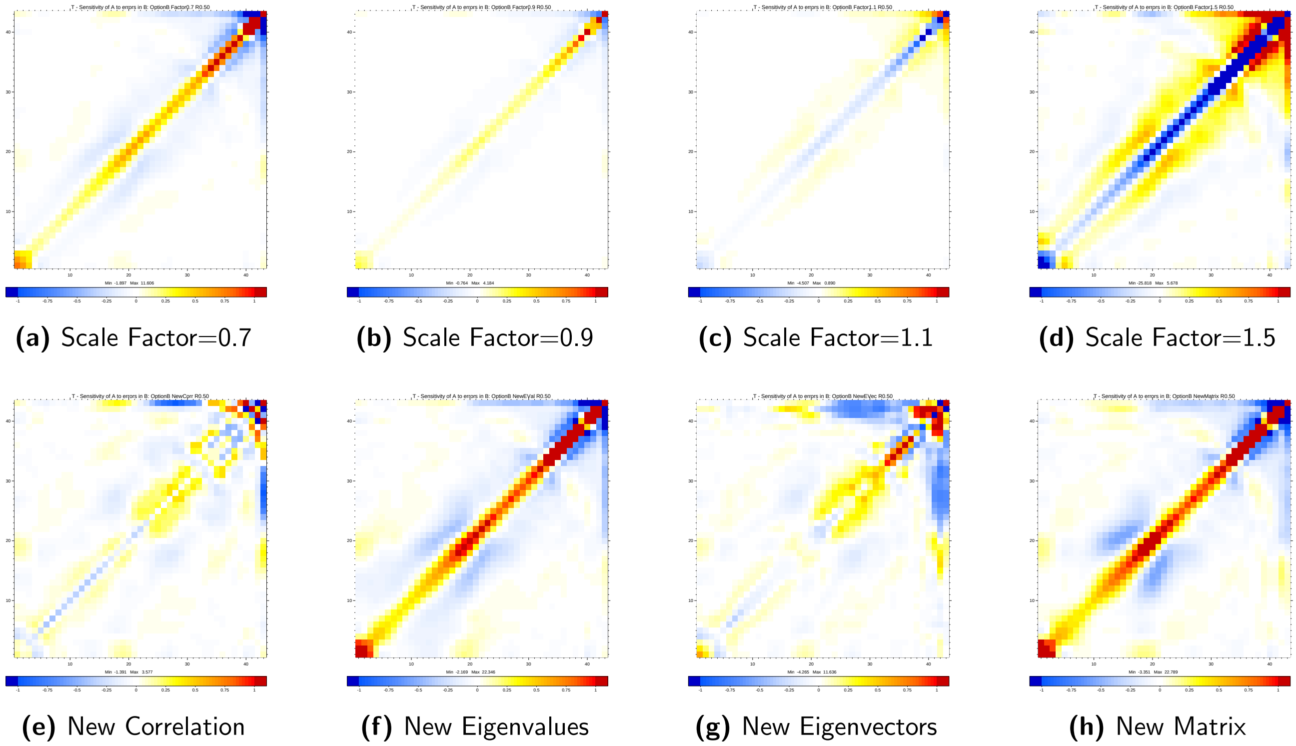
Figure 3: Delta Function temperature background sensitivity. Level 1 in the lower left corner is the surface level, and level 43 in the top right is the topmost stratospheric level. Colour scales run from -1 in blue to +1 in red.



(a) Scale Factor=0.7 (b) Scale Factor=0.9 (c) Scale Factor=1.1 (d) Scale Factor=1.5

(e) New Correlation (f) New Eigenvalues (g) New Eigenvectors (h) New Matrix

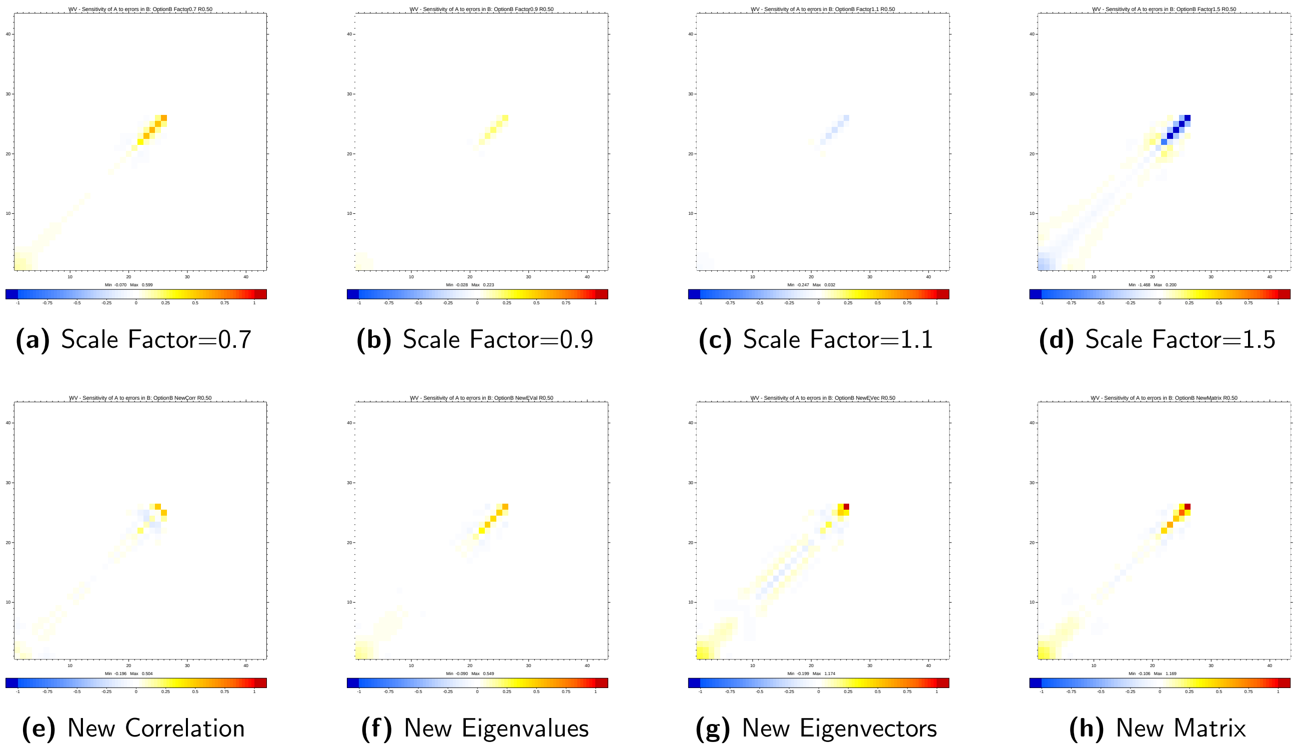
Figure 4: Delta Function water vapour background sensitivity. Level 1 in the lower left corner is the surface level, and level 43 in the top right is the topmost stratospheric level. Colour scales run from -1 in blue to +1 in red.



(a) Scale Factor=0.7 (b) Scale Factor=0.9 (c) Scale Factor=1.1 (d) Scale Factor=1.5

(e) New Correlation (f) New Eigenvalues (g) New Eigenvectors (h) New Matrix

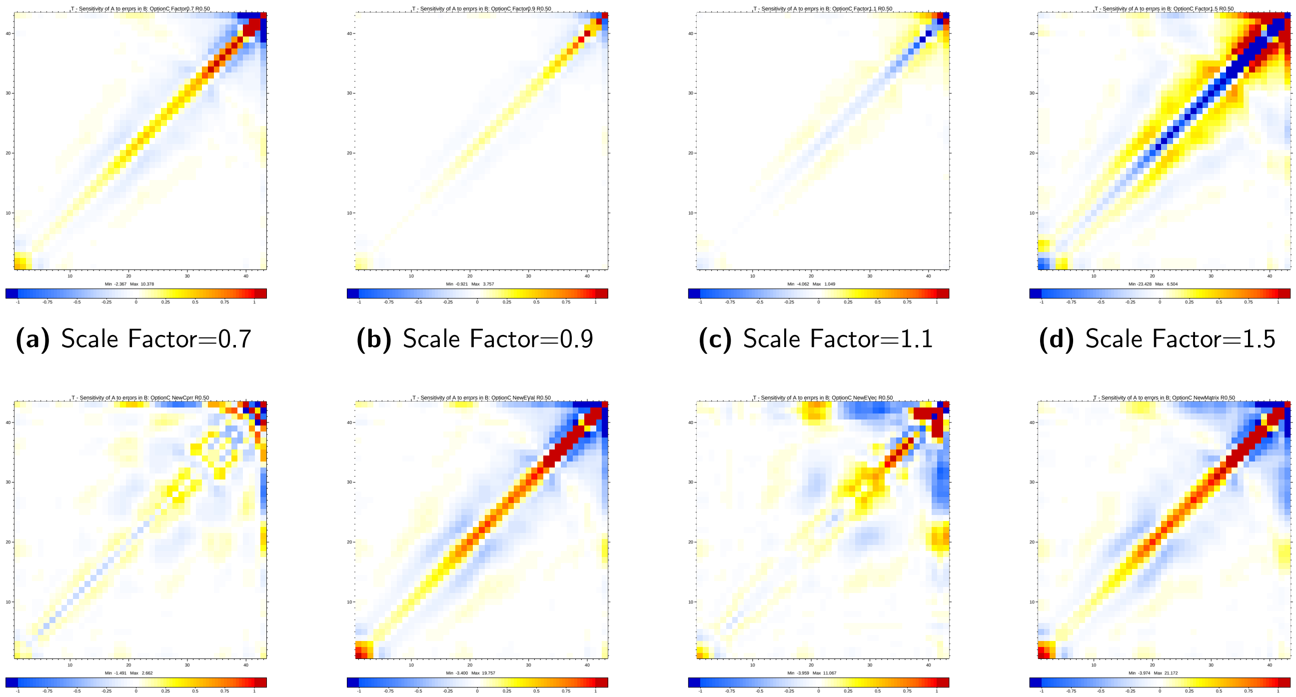
Figure 5: 20 channel idealised weighting functions temperature background sensitivity. Level 1 in the lower left corner is the surface level, and level 43 in the top right is the topmost stratospheric level. Colour scales run from -1 in blue to +1 in red.



(a) Scale Factor=0.7 (b) Scale Factor=0.9 (c) Scale Factor=1.1 (d) Scale Factor=1.5

(e) New Correlation (f) New Eigenvalues (g) New Eigenvectors (h) New Matrix

Figure 6: 20 channel idealised weighting functions water vapour background sensitivity. Level 1 in the lower left corner is the surface level, and level 43 in the top right is the topmost stratospheric level. Colour scales run from -1 in blue to +1 in red.



(a) Scale Factor=0.7 **(b)** Scale Factor=0.9 **(c)** Scale Factor=1.1 **(d)** Scale Factor=1.5

(e) New Correlation **(f)** New Eigenvalues **(g)** New Eigenvectors **(h)** New Matrix

Figure 7: 150 channel idealised weighting functions temperature background sensitivity. Level 1 in the lower left corner is the surface level, and level 43 in the top right is the topmost stratospheric level. Colour scales run from -1 in blue to +1 in red.

smoothly tapering as infrared sounder channel Jacobians tend to be. In the Met Office system, problems with assimilation of double-peaked AIRS channels led to their exclusion from operational assimilation. One possibility is that the double peaks interacted with a misspecified background error covariance matrix to produce an erroneous analysis increment; the innovation (observation minus forward-modelled profile) implied an ambiguous increment which was applied in the wrong part of the profile.

If this hypothesis is correct, then in a system where the background errors are misspecified, the transformation of spectra into PC space could result in Jacobians which are more sensitive to an incorrect $\mathbf{B_A}$. If the assimilation system were to be more unstable in this respect, any advantages of the PC assimilation, such as increased information content and faster processing time, may be outweighed.

The hypothesis that PC Jacobians are more sensitive to misspecification of $\mathbf{B_A}$ than those of individual channels is tested here for the US Standard Atmosphere. Jacobians were calculated in brightness temperature units for the full spectrum using RTTOV9 on 43 levels. The Jacobians were converted from brightness temperature to radiance, normalised by the level 1c instrument noise and then transformed into truncated PC space retaining 150 PC scores. These PC Jacobians were used to calculate the background sensitivity using an observation error equal to the identity matrix (for an explanation of PC observation errors see Collard et al., 2010). The results can be seen in Figures 9 and 10 for temperature and water vapour respectively. The background sensitivity was also calculated for the spectral radiance Jacobians, for the Met Office operational 1D-Var channel selection (Hilton et al., 2009), with an observation error equal to level 1c instrument noise converted to brightness temperatures at the scene temperature (figures 11 and 12).

The PC Jacobian background sensitivity is for the most part smaller in magnitude than for the 183 channel assimilation system, and in fact is virtually zero for temperature in the troposphere away from

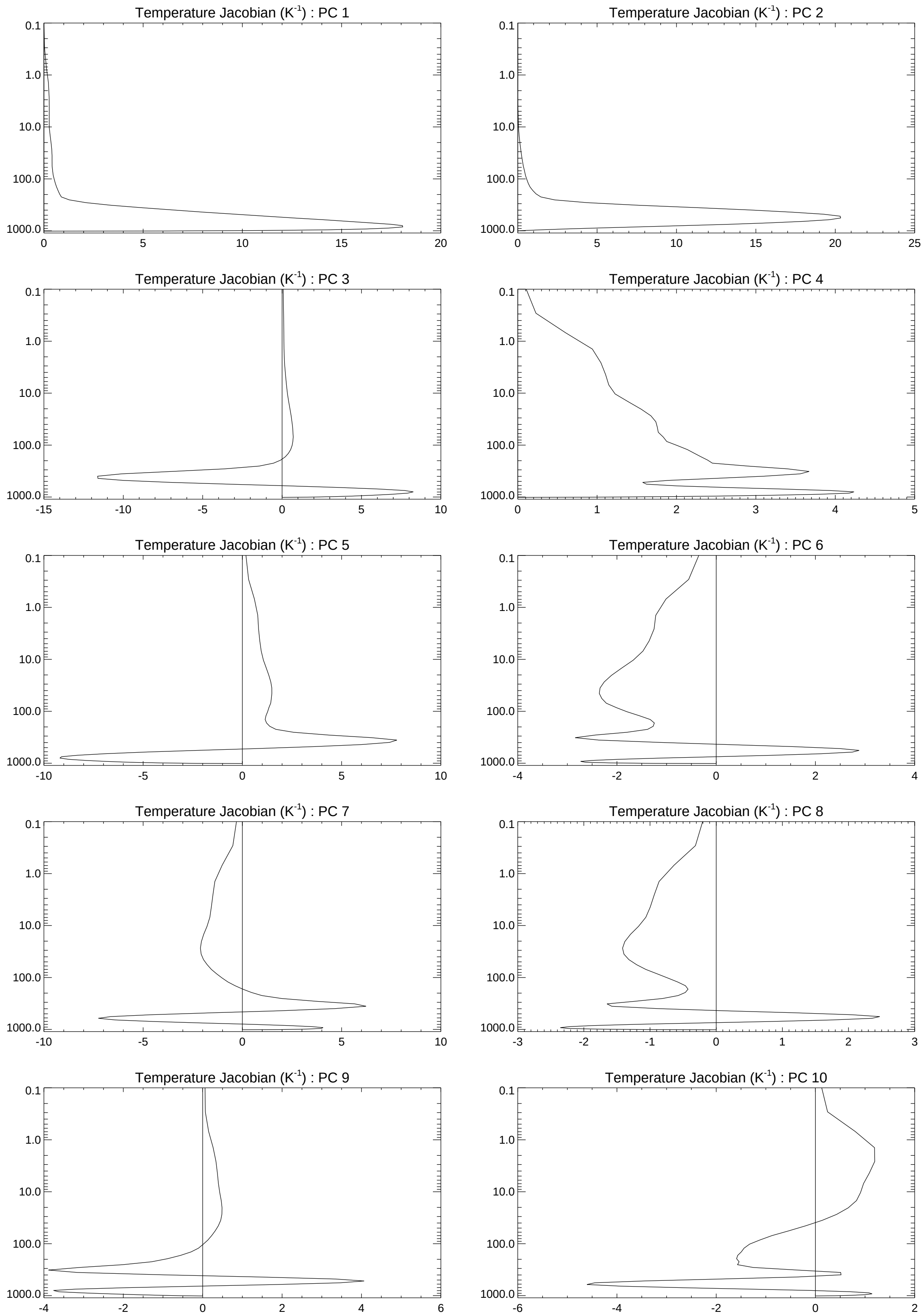
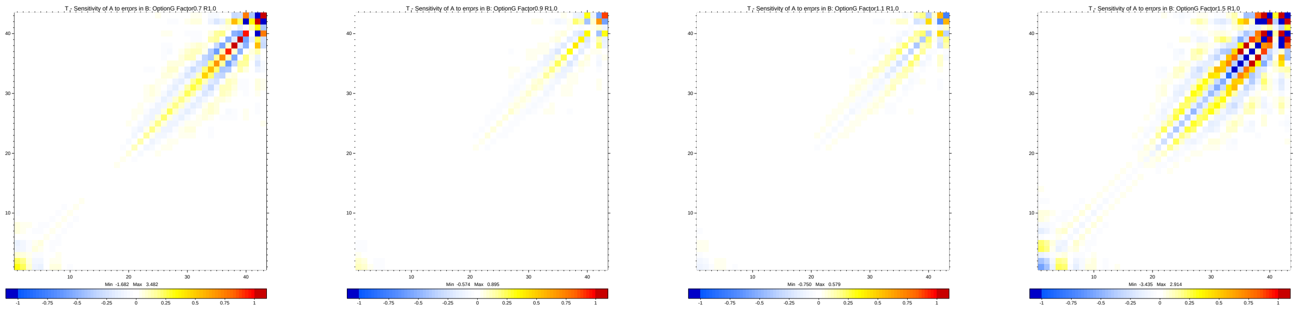
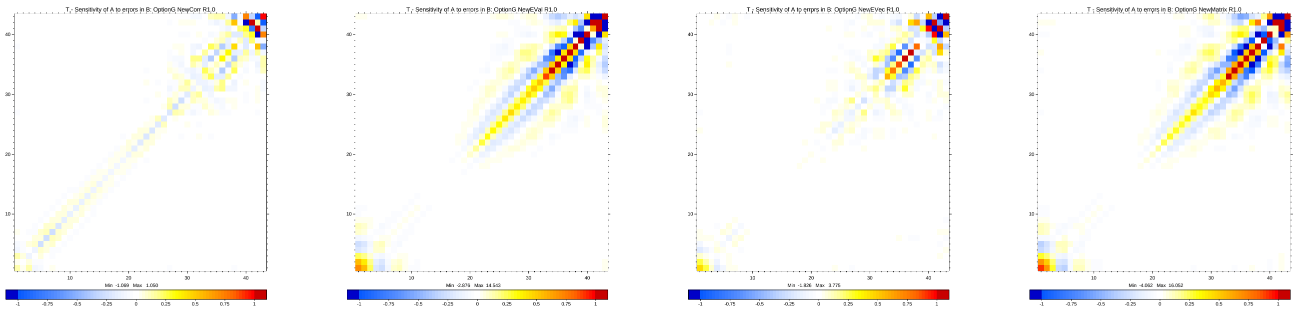


Figure 8: The first 10 temperature Jacobians for a set of PCs derived from real IASI data

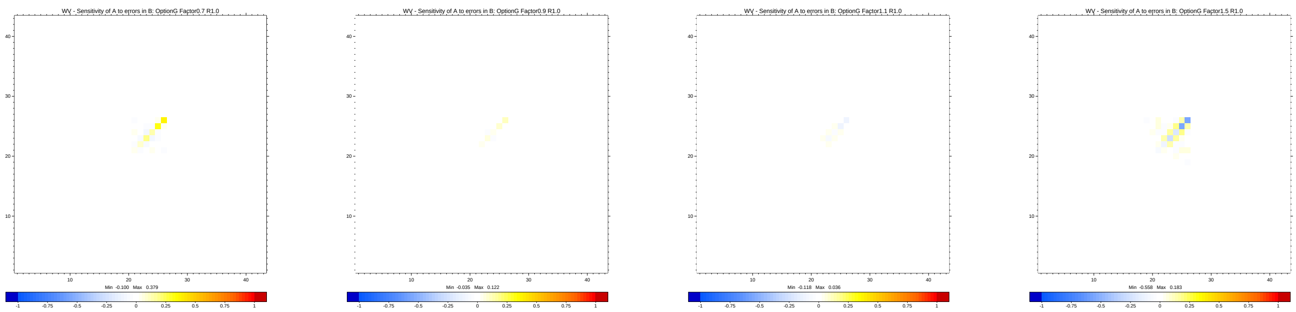


(a) Scale Factor=0.7 **(b)** Scale Factor=0.9 **(c)** Scale Factor=1.1 **(d)** Scale Factor=1.5

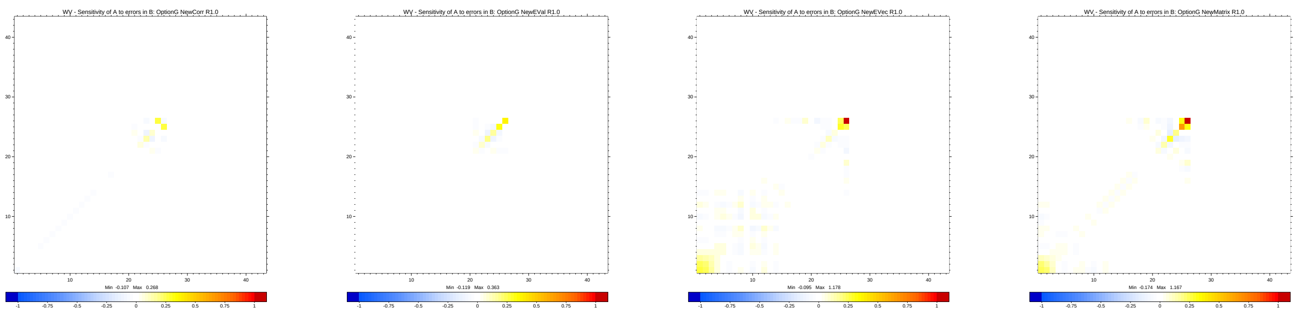


(e) New Correlation **(f)** New Eigenvalues **(g)** New Eigenvectors **(h)** New Matrix

Figure 9: IASI PC Jacobian temperature background sensitivity. Level 1 in the lower left corner is the surface level, and level 43 in the top right is the topmost stratospheric level. Colour scales run from -1 in blue to +1 in red.

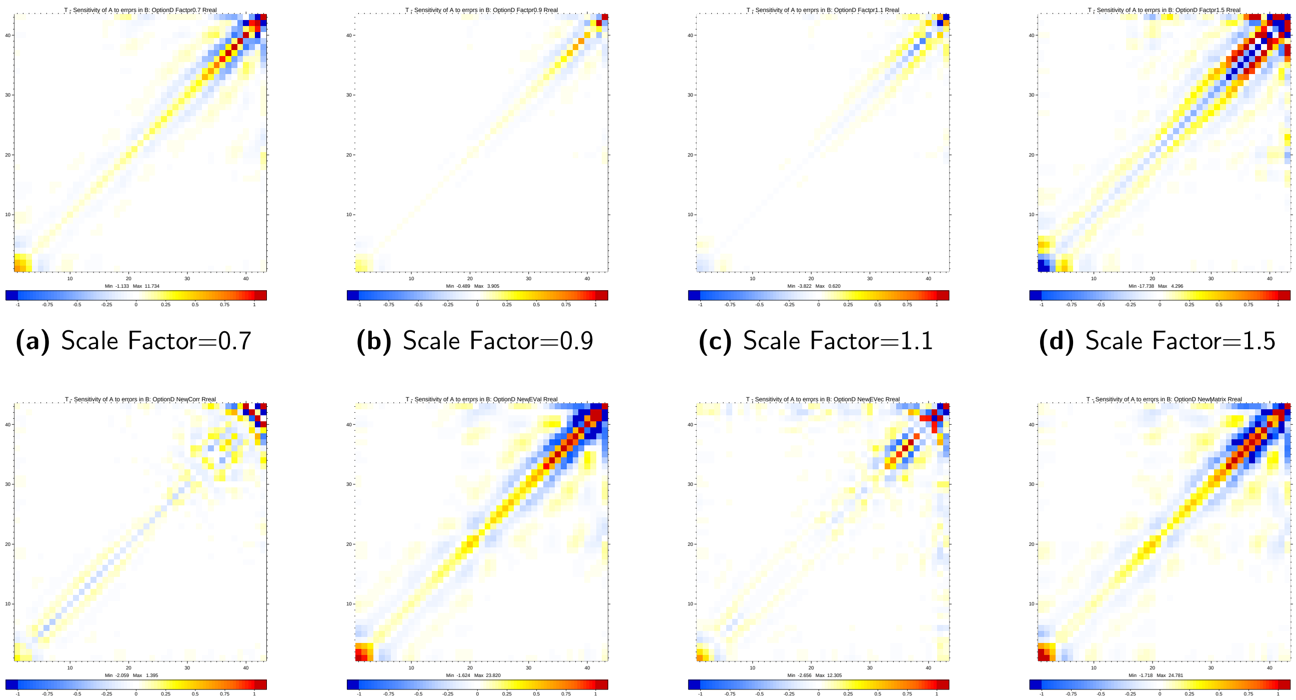


(a) Scale Factor=0.7 **(b)** Scale Factor=0.9 **(c)** Scale Factor=1.1 **(d)** Scale Factor=1.5



(e) New Correlation **(f)** New Eigenvalues **(g)** New Eigenvectors **(h)** New Matrix

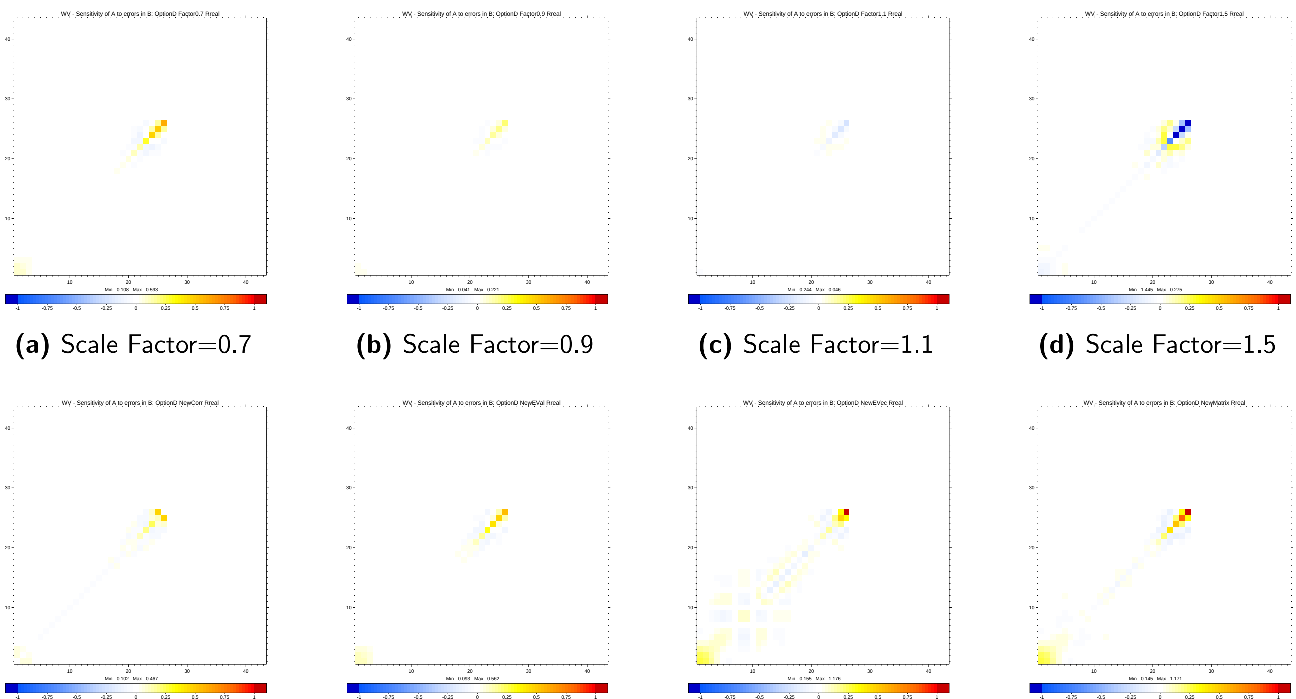
Figure 10: IASI PC Jacobian water vapour background sensitivity. Level 1 in the lower left corner is the surface level, and level 43 in the top right is the topmost stratospheric level. Colour scales run from -1 in blue to +1 in red.



(a) Scale Factor=0.7 **(b)** Scale Factor=0.9 **(c)** Scale Factor=1.1 **(d)** Scale Factor=1.5

(e) New Correlation **(f)** New Eigenvalues **(g)** New Eigenvectors **(h)** New Matrix

Figure 11: IASI 183 Channel selection temperature background sensitivity. Level 1 in the lower left corner is the surface level, and level 43 in the top right is the topmost stratospheric level. Colour scales run from -1 in blue to +1 in red.



(a) Scale Factor=0.7 **(b)** Scale Factor=0.9 **(c)** Scale Factor=1.1 **(d)** Scale Factor=1.5

(e) New Correlation **(f)** New Eigenvalues **(g)** New Eigenvectors **(h)** New Matrix

Figure 12: IASI 183 Channel selection water vapour background sensitivity. Level 1 in the lower left corner is the surface level, and level 43 in the top right is the topmost stratospheric level. Colour scales run from -1 in blue to +1 in red.

the surface. A PC-based assimilation system would, from this result, seem to be less sensitive to errors in $\mathbf{B_A}$ than a channel-based assimilation system. The calculations certainly suggest that the hypothesis—that multiply peaked Jacobian systems are more sensitive to errors in $\mathbf{B_A}$—is incorrect. It is possible that the problems seen with the use of dual-peaked AIRS channels are instead related to an inability to resolve the ambiguous response of these channels owing to incomplete spanning of the full atmospheric column by the selected channels.

In fact, the reduced background sensitivity for the PC analysis relative to the 183 channel assimilation system is a result of the channel selection itself. The selection is chosen to maximise the information content of the analysis via the use of a small number of channels, and there are inevitably gaps in the vertical content of the assimilated information. If the full spectrum of 8461 channels is used, the background sensitivity of the channel-based assimilation is nearly identical to that of the PC-based system (they are not strictly identical as the PCs were truncated reducing the random noise in the observation). Although the full spectrum will produce a background sensitivity component near-identical to that of the PCs, the clear advantage of the PC-based system is the processing time of each observation. Even discounting the computational cost of the forward model and Jacobian calculation, the inversion of an 8461×8461 matrix is extremely slow relative to a 150×150 matrix.

The sensitivity of the analysis to using the full information content of the spectrum as opposed to a subset of this information suggests that spanning the largest possible vertical range of the atmosphere is important. This result does indicate that using the full information content of the IASI spectrum would result in a more robust analysis, which is less sensitive to misspecification of $\mathbf{B_A}$, particularly for the tropospheric temperature analysis.

In order to determine the significance of any improvement in the size of the background sensitivity component, the quantity $\mathbf{A} - \mathbf{B}$ was calculated for the most extreme case of an error in $\mathbf{B_A}$, where the matrix is completely incorrect (experiment h). If this quantity is negative, the analysis error is smaller than the background error, regardless of $\mathbf{A}$ being larger than $\mathbf{A_{opt}}$. A positive $\mathbf{A} - \mathbf{B}$ would indicate that the analysis is degraded relative to the background as a result of misspecification of $\mathbf{B_A}$. In a further experiment, the matrices used to represent $\mathbf{B}$ and $\mathbf{B_A}$ were swapped, to test the effects of assuming a $\mathbf{B_A}$ much larger than $\mathbf{B}$. For the reverse case, $\mathbf{B} = \mathbf{B_2}$ and $\mathbf{B_A} = \mathbf{B_1}$.

Figure 13 shows $\mathbf{A} - \mathbf{B}$ for both temperature and water vapour for the operational channel selection and for the PC-based system (which is nearly identical to the use of the full spectrum). Along the diagonal, in blue are shown areas where the analysis has a lower error than the background and in yellow areas where it has a higher error. The blue areas off-diagonal show a lower covariance than the background and yellow indicates a higher covariance.

Plots a–d show the results for the standard case where $\mathbf{B} = \mathbf{B_1}$ and $\mathbf{B_A} = \mathbf{B_2}$. In this case, for temperature, $\mathbf{B}$ is very large and $\mathbf{B_A}$ is much smaller. There is a large reduction in analysis error covariance over the background error covariance and the background sensitivity component is relatively small in comparison. The only area in which the analysis error is substantially improved by using the full spectral information via the PC analysis is at the surface. For water vapour, the results indicate an improvement in the analysis, regardless of whether the full spectral information or just a channel selection is used, again a consequence of the fact that the background sensitivity component is much smaller than the overall reduction in analysis error from the assimilation of the observation.

Plots e–h show the results for the reverse case where $\mathbf{B} = \mathbf{B_2}$ and $\mathbf{B_A} = \mathbf{B_1}$. Here, $\mathbf{B}$ is much smaller than $\mathbf{B_A}$ for temperature, and slightly smaller for water vapour; the results reflect the smaller improvement of the analysis over the more accurate background. The smaller tropospheric background sensitivity for the PC Jacobians is now reflected in a slightly more negative $\mathbf{A} - \mathbf{B}$ along the diagonal. Both 183 channel

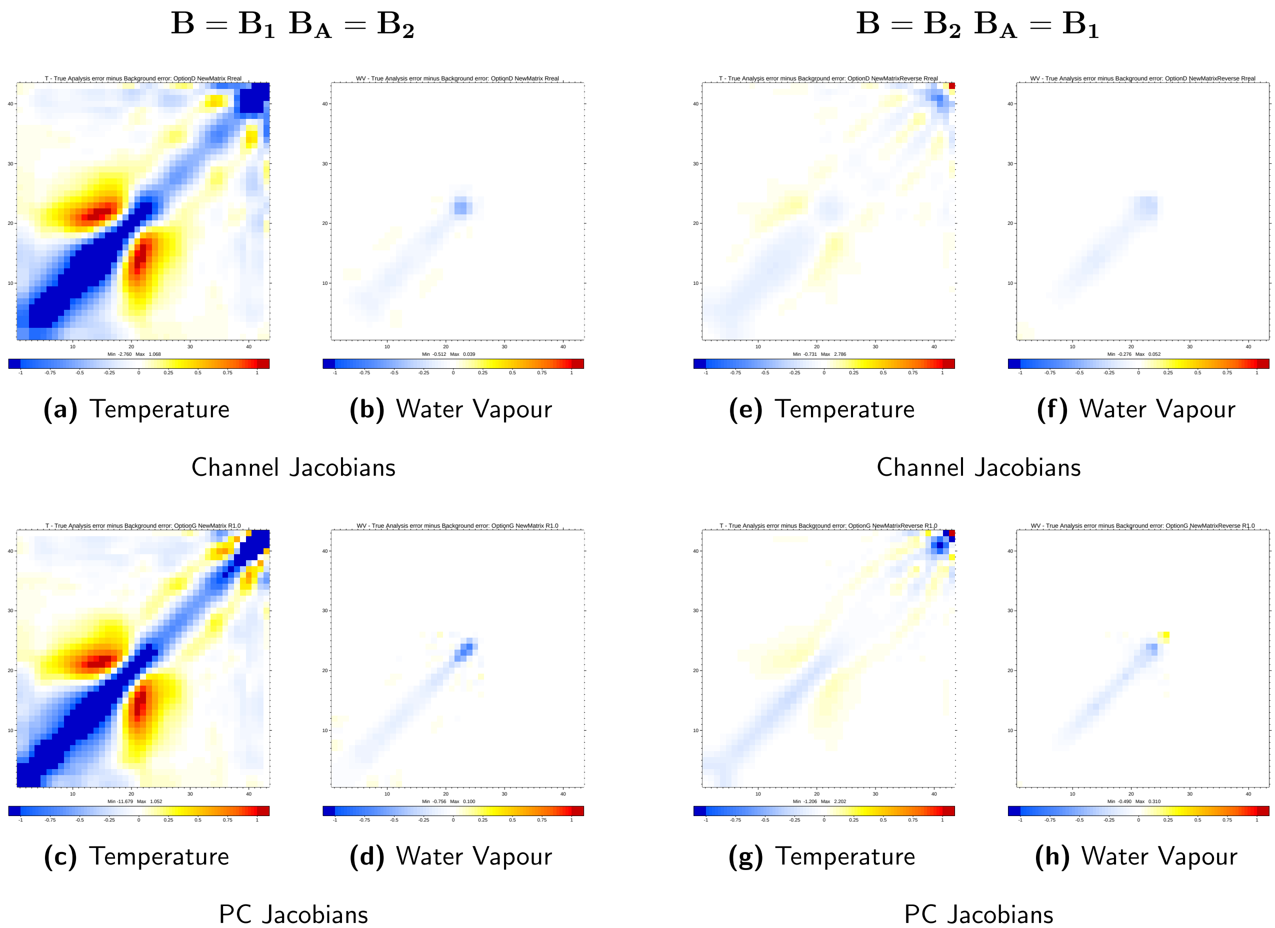


Figure 13: $\mathbf{A} - \mathbf{B}$ for two cases of a completely incorrect $\mathbf{B_A}$. Level 1 in the lower left corner is the surface level, and level 43 in the top right is the topmost stratospheric level.

and PC systems are degrading the analysis in the stratosphere, in particular the analysis of the topmost level. The large background sensitivity in the stratosphere is a reflection of the large difference in value for σ^2 in $\mathbf{B_1}$ relative to $\mathbf{B_2}$. For water vapour, the results show that the PC-based analysis is comparable throughout most of the troposphere to that of the 183 channel analysis but, at levels 25 and 26 (143–122hPa), the PC-based analysis is degraded relative to the background. This is likely to be a consequence of $\mathbf{B_1}$ not having been calculated for levels 27-43 which means that the background is assumed to have zero errors for these levels. Whilst the 183 channel selection analysis can avoid channels which will produce increments correlated across this boundary by using only low-peaking water vapour channels, the use of the Jacobians from the full spectrum generates increments which do span the boundary, and the analysis is therefore affected by lack of knowledge of the background errors higher in the atmosphere.

Figure 13 shows that for a typical IASI assimilation in mid-latitude, with accurately known observation errors and a reasonable range of uncertainty in $\mathbf{B_A}$, we are unlikely to be straying into the "danger zone" identified by Eyre and Hilton (2010) except for stratospheric temperature analysis when $\mathbf{B_A}$ is significantly larger than $\mathbf{B}$. In almost all other levels, and for water vapour, the analysis will improve upon the background regardless of the incorrect specification of $\mathbf{B_A}$, as long as the background errors are specified for the full profile. The results show that grossly overestimating background errors could cause problems in satellite data assimilation, and demonstrate the importance of specifying errors for the full atmospheric profile where increments may be created high in the atmosphere. The results shown do not indicate a large benefit to the level-by-level analysis variance in increasing the amount of spectral information used from IASI. However there is some indication that using the full spectrum mitigates against misspecification of $\mathbf{B_A}$ and may slightly improve tropospheric analysis where $\mathbf{B}$ is much smaller than $\mathbf{B_A}$.

6 Conclusions and Further Work

The work to understand the consequences of nonlocalisation of Jacobians is still in the early stages. Simple artificial experiments using delta functions and evenly spaced artificial weighting functions (section 5.1) suggest that the narrowness of the Jacobian is important in reducing sensitivity to $\mathbf{B_A}$. Analysis using the IASI instrument (section 5.2) does not show any increased sensitivity from a high degree of nonlocalisation and multiply peaked Jacobians. It does, however, suggest that using the full spectral information will help to mitigate against misspecification of $\mathbf{B_A}$ by ensuring the maximum information from throughout the model column is used.

The results of section 5.2 show that comparing 20 channel and 150 channel idealised experiments (section 5.1) did not fully represent the way in which the selection of a set of channels from a full spectrum is typically performed, as the spread of information across the whole atmospheric column was maintained in both idealised cases. However, the general similarity of the form of the results for IASI and idealised Jacobians does suggest that the idealised Jacobian forms can be used for further study to perform clean experiments into the effects of Jacobian shape and their interaction with a biased background state.

This analysis has been done assuming a perfect knowledge of observation errors, and perfect noise-normalisation of spectra before conversion to PC scores. The results may be affected by misspecified observation errors. Furthermore, the analysis assumes no bias between observations and background, and it remains to be investigated whether multiply peaked Jacobians increase sensitivity to differential model biases between different parts of the profile which are greater than the assumed background errors. There has also been no investigations of the effect of misspecification of $\mathbf{B_A}$ on a joint temperature and humidity retrieval system. The results presented do, however, suggest that guarding against large overestimations of background error will help to prevent the analysis being degraded relative to the background.

References

Andersson, E., M. Fisher, R. Munro, and A. McNally (2000). Diagnosis of background errors for radiances and other observable quantities in a variational data assimilation scheme, and the explanation of a case of poor convergence. *Q. J. R. Meteorol Soc.*, Vol. 126, pp. 1455–1472.

Antonelli, P., H. E. Revercomb, L. A. Sromovsky, W. L. Smith, R. O. Knuteson, D. C. Tobin, R. K. Garcia, H. B. Howell, H.-L. Huang, and F. A. Best (2004). A principal component noise filter for high spectral resolution infrared measurements. *J. Geophys. Res.*, Vol. 109, No. D23102. DOI 10.1029/2004JD004862.

Bormann, N. and P. Bauer (2010). Estimates of spatial and interchannel observation-error characteristics for current sounder radiances for numerical weather prediction. I: Methods and application to ATOVS data. *Q. J. R. Meteorol. Soc.*, Vol. 136, pp. 1036–1050. DOI 10.1002/qj.616.

Bormann, N., A. Collard, and P. Bauer (2010). Estimates of spatial and interchannel observation-error characteristics for current sounder radiances for numerical weather prediction. II: Methods and application to AIRS and IASI data. *Q. J. R. Meteorol. Soc.*, Vol. 136, pp. 1051–1063. DOI 10.1002/qj.615.

Collard, A. D. (2007). Selection of IASI channels for use in numerical weather prediction. *Q. J. R. Meteorol. Soc.*, Vol. 133, pp. 1977–1991. DOI 10.1002/qj.178.

Collard, A. D. and A. P. McNally (2009). The assimilation of Infrared Atmospheric Sounding Interferometer radiances at ECMWF. *Q. J. R. Meteorol. Soc.*, Vol. 135, pp. 1044–1058. DOI 10.1002/qj.410.

Collard, A. D., A. P. McNally, F. I. Hilton, S. B. Healy, and N. C. Atkinson (2010). The Use of Principal Component Analysis for the Assimilation of High-Resolution Infrared Sounder Observations for Numerical Weather Prediction. *submitted to Q. J. R. Meteorol. Soc.*

Eyre, J. R. and F. I. Hilton (2010). Beyond Optimal Estimation: Sensitivity Of Analysis Error To The Specification Of Background Error. In *Proceedings of the 17th International TOVS Study Conference, 14-20 April 2010, Monterey, USA*.

Fisher, M. (2003). Background error covariance modelling. In *ECMWF Seminar on Recent Developments in Data Assimilation for Atmosphere and Ocean, 8-12 September 2003*, pp. 45–64. `http://www.ecmwf.int/publications/library/do/references/list/17111`.

Garand, L., N. Baker, and C. Clerbaux (2009). Working group reports. In *ECMWF/EUMETSAT NWP-SAF Workshop on Assimilation of IASI in NWP, 6-8 May 2009*. `http://www.ecmwf.int/publications/library/ecpublications/_pdf/workshop/2009/IASI/`.

Hilton, F. I. and A. D. Collard (2009). Recommendations for the use of principal component-compressed observations from infrared hyperspectral sounders. Met R&D Tech. Rep. 536, Met Office.

Hilton, F., N. C. Atkinson, S. J. English, and J. R. Eyre (2009). Assimilation of IASI at the Met Office and assessment of its impact through observing system experiments. *Q. J. R. Meteorol. Soc.*, Vol. 135, pp. 495–505. DOI 10.1002/qj.379.

Liu, X., D. K. Zhou, A. Larar, W. L. Smith, and S. A. Mango (2007). Case-study of a principal-component-based radiative transfer forward model and retrieval algorithm using EAQUATE data. *Q. J. R. Meteorol. Soc.*, Vol. 133, pp. 243–256. DOI 10.1002/qj.156.

McNally, A. P., P. D. Watts, J. A. Smith, R. Engelen, G. A. Kelly, J. N. Thpaut, and M. Matricardi (2006). The assimilation of AIRS radiance data at ECMWF. *Q. J. R. Meteorol. Soc.*, Vol. 132, pp. 935–957. DOI 10.1256/qj.04.171.

Parrish, D. F. and J. C. Derber (1992). The National Meteorological Center's spectral statistical interpolation analysis system. *Mon. Wea. Rev.*, Vol. 120, pp. 1747–1763.

Rodgers, C. D. (2000). *Inverse Methods for Atmospheric Sounding: Theory and Practice*: World Scientific, Singapore.

Saunders, R. W. (2002). *RTTOV-7 Users Guide.* `http://research.metoffice.gov.uk/research/interproj/nwpsaf/rtm/rttov7_ug.pdf`.

Stewart, L. M. (2010). Correlated observation errors in data assimilation. Ph.D. dissertation, University of Reading, Reading, UK.