A Computationally Efficient Retrieval Algorithm For Hyperspectral Sounders Incorporating A Priori Information

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Abstract—In this letter we describe a novel implementation scheme for the inversion of the radiative transfer equation as encountered in satellite remote sensing and incorporating a priori information. Unlike traditional MAP approaches, the new algorithm does not require the use of a forward model tangent linear and does not pay a large computational time penalty in the use of numerical derivatives. Using spectral data from EUMETSAT’s IASI sensor, we provide a demonstration of the algorithm and comparison to the NOAA operationally available product using carbon monoxide as target gas.

Index Terms—Infrared measurements, inverse problems, matrices, remote sensing, satellites.

I. INTRODUCTION

A. Background

Orbiting 800km above the surface of the Earth, the Infrared Atmospheric Sounding Interferometer (IASI) makes globally representative spectral measurements 2 times per day. Spectral measurements from IASI contain information on the distribution of tropospheric trace gases such as CO, CH₄, CO₂, as well as stratospheric trace gases such as HNO₃ and O₃ [1]. NOAA currently operationally processes 100% of IASI data from calibrated and apodized L1C spectral measurements to geophysical L2 products and distributes these products to NOAA/Comprehensive Large Array-data Stewardship System (CLASS) (available at http://class.ngdc.noaa.gov). The algorithm used to produce the L2 products from IASI is largely based on the AIRS science team (AST) algorithm [2] including the fast Radiative Transfer Algorithm (RTA) [3], fast eigenvector regression [4], [5], as well as cloud-cleaning and physical retrieval methodologies [6] and is described in the IASI L2 Algorithm Theoretical Basis Document (ATBD) available at http://www.orbit2.nesdis.noaa.gov/smcd/spb/iosspdt/iosspdt.php.

B. Retrieval Theory

In addition to the AST algorithm currently used to produce AIRS and IASI products at NOAA, various other methods exist that are capable of solving for trace gas abundances and temperatures via inversion of the IR radiative transfer equation. For instance, Equation 1 gives the expression for the Maximum A Posteriori or MAP method [7], [8]:

\[
\hat{x}_{i+1} = x_a + (K_i^T W K_i + S_a^{-1})^{-1} K_i^T W \left[ (R - R(x_i, b)) + K_i (\hat{x}_i - x_a) \right].
\]

In Equation 1, \( \hat{x}_{i+1} \) is the retrieved profile for iteration \( i \); \( x_a \epsilon \mathbb{R}^L \) is the a priori profile; \( K_i \epsilon \mathbb{R}^{n \times L} \) are the channel, \( n \), by level/layer, \( L \), derivatives of the radiative transfer [3], [9] with respect to \( x \) for iteration \( i \); and \( W \epsilon \mathbb{R}^{n \times n} \) is the channel by channel noise covariance matrix including both systematic (e.g. forward model error) and instrument error terms (e.g. from cloud clearing). We have also defined \( S_a \epsilon \mathbb{R}^{L \times L} \), which is the a priori error covariance matrix; \( R \epsilon \mathbb{R}^n \), which are the observed instrument radiances; and \( R(x_i, b) \epsilon \mathbb{R}^n \), which are the calculated radiances for the current estimate of the retrieved state, \( x \) and background states, \( b \). In Equation 1 we did not explicitly include an iteration index, \( i \), on \( W \) however, \( W \) may also be allowed to vary as a function of iteration.

A more computationally efficient methodology can be derived by first diagonalizing the error covariance \( S_a \) (see for instance, [8] Section 5.8.3, or for a remote sensing application [10]), by making the substitutions:

\[
\hat{\mathbf{x}} = U^T x \quad (2)
\]

\[
\hat{\mathbf{K}} = KU \quad (3)
\]

In Equations 2 and 3, \( U \epsilon \mathbb{R}^{L \times L} \) are the eigenvectors of the a priori covariance matrix \( S_a \); that is,

\[
\Sigma = U^T S_a U \quad (4)
\]

and \( \Sigma \epsilon \mathbb{R}^{L \times L} \) is a diagonal matrix of eigenvalues containing the variances of \( U \) (i.e., \( \Sigma = \text{diag}(\sigma_i) \)). These transformations yield an equation for our desired change:

\[
\Delta \hat{x}_{i+1} = U \left( \tilde{K}_i^T \tilde{W} \tilde{K}_i + \Sigma^{-1} \right)^{-1} \tilde{K}_i^T \tilde{W} \left[ \Delta R + \tilde{K}_i (\hat{x}_i - \hat{x}_a) \right],
\]

which can be written in a more compact form:

\[
\Delta \hat{x}_{i+1} = G \left[ \Delta R + \tilde{K}_i (\hat{x}_i - \hat{x}_a) \right],
\]

where we defined the contribution function, \( G \epsilon \mathbb{R}^{L \times n} \), which describes to first-order how the retrieval changes with changes in the measurement vector. At this point it is useful to define...
the averaging kernel, \( A = GK \), which describes to first order how the retrieval changes with respect to changes in the true atmospheric state.

A disadvantage to traditional MAP retrieval implementations is that the application of the previous equations (e.g., Equations 1-6), requires calculation of \( L \) (a possibly large number) forward model derivatives. In addition, IR sounder measurements have finite vertical resolution and limited information content with respect to trace gases; therefore, a direct application of the previous equations does not take advantage of \( a \) \( a \) priori \( a \) knowledge about the vertical sensitivity of the sounding instrument to the target parameters. For instance, the fact that IR sounder kernel functions are generally peaked functions with finite width over a finite vertical extent implies that the instrument cannot “see” all of the vertical correlations within the \( a \) priori \( a \) information.

A solution to this information mismatch proceeds by selecting \( t \) leading eigenvectors of \( U: U_{t} \in R^{L \times t} \), \( t < L \), thus enabling tuning the number of independent variables determined in the retrieval. If \( t \) is large enough, \( i.e., assuming \) that the higher order \( t \) terms will have low magnitude, but non-zero variability such that their contribution to the inversion vanishes) we reduce the dimensionality of the problem from an \( L \) dimension problem to a \( t \) dimension problem thus decreasing the computational burden.

The NOAA IASI algorithm is in various stages of validation for temperature and moisture retrievals, and just beginning validation stages for the trace gas products. In this letter our aim is not to provide validation to the CO retrieval, but to show both \( d \) \( t \) and \( t \) as a function of the number of terms, \( t \), selected is large enough to reproduce most of the variability in \( S_{a} \).

We should not expect these scalar quantities to change as a function of the number of terms, \( t \), carried through the calculation in Equation 10. Therefore analysis of the \( d_{a} \) and \( H \) as a function of \( t \) also enables the determination of an adequate number of terms to propagate through the retrieval.

An example of using \( d_{a} \) and \( H \) is shown in Figure 1 using the system setup described in Section III. In Figure 1 we show both \( d_{a} \) and \( H \) as a function of the number of terms allowed to propagate through the retrieval, \( t \). Even though only \( \approx 90\% \) of the variance is explained, \( d_{a} \) and \( H \) do not vary with \( t \geq 3 \) terms indicating that at minimum, the retrieval should require \( t + 1 = 4 \) calls per channel to the RTA to calculate derivatives. Due to the use of 9 retrieval basis functions, the current implementation of the operational algorithm for IASI

In Equation 8, \( a_{0} \) is a multiplicative constant used to ensure linearity in the derivatives as discussed in Section II-A2 and also to add units between the state vector \( x \) and the unitless eigenfunctions, \( u_{i} \). In practice, we choose derivatives with a unitless denominator, that is we drop the \( u_{i} \) on the right hand side of Equation 8.

\[ \text{percent of total variance} = \frac{\sum_{i=1}^{t} \sigma_{i}}{\sum_{i=1}^{L} \sigma_{i}} \] (9)

for various \( t \). In addition, defining the noise-normalized (pre-whitened), atmospheric variability weighted Jacobians, \( \bar{K} \in R^{n \times t} \):

\[ \bar{K} = W^{-1/2} K U_{t} \Sigma_{t}^{-1/2} U_{t}^{T} \] (10)

and requiring that the minimum signal-to-noise (S/N) for each element \( t \) is greater than or equal to some number, \( r \), will enable truncation of even more terms. Generally speaking, selecting channels and retrieved parameters such that we maximize the number of parameters with a minimum S/N \( \geq 1 \) (e.g. setting \( r \approx 1 \)) is advantageous for efficient and high information content IR sounder retrievals. Nevertheless, parameters with \( r \leq 1 \) should also be allowed as over restriction on \( r \) (i.e., setting \( r \) to be too large) will cause our retrieval to be overly dependent on \( a \) \( a \) priori \( a \). In any case, care must be taken to ensure that the number of terms, \( t \), selected is large enough to reproduce most of the variability in \( S_{a} \).

Performing a singular-value decomposition of Equation 10 enables study of the information content of a particular instrument given a \( a \) \( a \) priori \( a \) information [8]. For instance, the singular values, \( \gamma_{i} \), and singular vectors, \( \bar{U} \) and \( \bar{V} \), of Equation 10 enables the determination of the information content, \( H \),

\[ H = \frac{1}{2} \sum_{i=1}^{t} \log_{e} (1 + \frac{\gamma_{i}^{2}}{1 + \gamma_{i}^{2}}), \] (11)

and the degrees of freedom for signal, \( d_{a} \),

\[ d_{a} = \sum_{i=1}^{t} \frac{\gamma_{i}^{2}}{(1 + \gamma_{i}^{2})}. \] (12)

We should not expect these scalar quantities to change as a function of the number of terms, \( t \), carried through the calculation in Equation 10. Therefore analysis of the \( d_{a} \) and \( H \) as a function of \( t \) also enables the determination of an adequate number of terms to propagate through the retrieval.

II. IMPLEMENTATION

A. Efficient Calculation of the Forward Model Derivatives

In the absence of the availability of an accurate analytic forward model Jacobian, the execution time required for explicit calculation of \( K \) is prohibitive. For instance, a one-sided derivative requires \( L + 1 \) calls to the RTA for each channel (two-sided derivatives require \( 2L + 1 \) calls per channel). In order to maximize computational efficiency we expand the forward model in a Taylor series about an arbitrary state, \( (x, b) \), and drop all but the linear term to yield:

\[ \Delta R = R(x + \delta x, b) - R(x, b) \approx K \cdot \delta x \] (7)

Writing our transformation of the derivatives in Equation 3 in the same manner yields the computationally efficient form:

\[ \bar{K} = K U_{t} \approx (R(x + a_{0} \cdot u_{i}, b) - R(x, b)) \cdot u_{i}, \quad i = 1, t \] (8)
model sensitivities in temperature, moisture as well as trace gas species (CO, O$_3$, CH$_4$, CO$_2$, etc.). For the retrieval of CO we selected 33 channels in the 4.5 $\mu$m region of the 1-0 vibration-rotation CO fundamental based on their signal-to-noise ratio (including geophysical uncertainties) and vertical extent of sensitivity.

III. COMPARISON OF AIRS SCIENCE TEAM RETRIEVAL TO MAP RETRIEVAL METHODOLOGY USING IASI DATA

In the following, we compare and contrast IASI retrievals for 10/19/2007 over the tropical range (latitudes between $\pm$ 30 degrees) using both the AST retrieval methodology and the MAP methodology described in previous sections.

A. Averaging Kernels and Error Estimates

Figure 2 shows a comparison of the AST (purple) and MAP (green) retrieval algorithms at 500 hPa as a function of latitude (top panel) and shown as a function of pressure as a scattergram (bottom panel). Immediately apparent from the bottom panel, the most notable differences are for the upper and lower layers at 50 hPa and 900 hPa. These differences are due to the smoothing constraints on the retrievals.

In the case of the AST approach, the primary smoothing constraint is the use of trapezoidal basis functions [12]. For the MAP retrieval, eigenvectors of $S_a$, $U_i$, serve as the primary smoothness constraint. As shown in Figure 2, at 50 hPa the AST retrieval basis functions correlate instrument sensitivity from layers below such that the variability introduced in the stratosphere is unphysical. For instance, in the most extreme cases (between -15 and -5 degrees latitude) the retrieval modifies the prior by almost 100%. Near the surface, the AST retrieval relaxes back to its a priori, due to the algorithm’s lack of an a priori smoothing constraint. The MAP retrievals behave in an opposite manner. Instrument sensitivity at 5 km is correlated with the prior constraint in $U_i$ to enable the retrieval to move the bottom of the atmosphere.

Fig. 2. Comparison of AST (purple) and MAP (green) retrieval algorithms at 500 hPa as a function of latitude (top panel) and shown as a function of pressure as a scattergram (bottom panel). Colored dotted lines in the bottom panel show uncertainty envelopes for theoretically calculated error estimates (see text). The individual pressures are plotted as various symbols and colors.
the MAP retrievals relax back to the \textit{a priori} due to the combination of low magnitude prescribed variability in $U_i$ and lack of instrument sensitivity.

Propagation of error techniques [8] provide a better gauge to the similarities and differences between the two retrieval algorithms. For instance, in the bottom panel of Figure 2 we show theoretically calculated total uncertainties (sum of spectrally interfering species as well as instrument $N E \Delta T$ and averaging kernel smoothing) for a nominal tropical atmosphere. For background species, we used 1K errors for surface temperature, and formed error covariances using Equation 13 and coarse layer surface temperature, and formed error covariances using Equation 13 and coarse layer $\sigma$’s and pressures for temperature and moisture as defined in Table II with correlation parameters: $\delta P = 700 \text{hPa}$ for temperature and $\delta P = 300 \text{hPa}$ for moisture. Coarse layer $\sigma$’s in Table II were estimated using our current knowledge of temperature and moisture uncertainty from IASI as matched to an operational radiosonde database [13], [14].

With the exception of the extremely high CO abundances (biomass burning regions), Figure 2 shows that both retrieval methodologies give similar results between 300-700hPa altitude. The differences for the large values could be due to either underconstrained AST retrievals or overconstrained MAP retrievals. Total column retrievals (not shown) show good agreement, which indicate the opposite magnitude differences as a function of altitude between each of the retrieval methodologies counteract each other resulting in better agreement in the integral CO abundance.

Figure 3 shows example retrieved CO profiles for each algorithm over Brazil as well as corresponding averaging kernels, A. A, describe the sensitivity of each retrieval algorithm to changes in “true” CO and further illustrate the differences in the retrieval algorithm constraints. The degrees of freedom, $dof$ for the AST algorithm [12] and the degrees of freedom for signal, $dfs$, for the MAP retrieval algorithm [8] are listed at the top of the right panel.

Differences in the vertical constraints used in the two algorithms are further evident from the left panel in Figure 3 where the enhanced CO retrieved from the AST algorithm (blue line between 8 and 5 km) is partially offset by the enhancement in the MAP retrieved CO (red line below 2 km). For pressures below 200hPa, the uncertainty curves in Figure 2 act as envelopes to the differences between the two algorithms indicating that the differences are within expected retrieval uncertainty. At 200hPa and 50hPa, the differences between the two retrieval algorithms are outside of the uncertainty curves for 6% and 55% of cases. This behavior can be best understood through inspection of the averaging kernels shown in Figure 3.

Above 200hPa, middle tropospheric averaging kernels for the AST algorithm decay toward zero slower than middle tropospheric averaging kernels for the MAP algorithm and indicate that the smoothness constraints in the AST algorithm, namely the use of trapezoidal basis functions, impart large vertical scale correlations between the middle troposphere and higher altitudes. The fact that our uncertainty curves were calculated for a MAP algorithm, which does does not include the ability to characterize the correlation of the AST algorithm, explains that discrepancy between the uncertainty curves and the difference between the AST and MAP algorithms above 200hPa.

<table>
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<th>Pressure (hPa)</th>
<th>1100</th>
<th>800</th>
<th>600</th>
<th>400</th>
<th>200</th>
<th>100</th>
<th>50</th>
<th>10</th>
<th>1</th>
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<td>$\sigma$ (%)</td>
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<td>40.0</td>
<td>40.0</td>
<td>33.3</td>
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<td>10.0</td>
<td>6.67</td>
<td>3.33</td>
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**TABLE I**

COARSE PRESSURES AND PERCENT VARIABILITIES, $\sigma$, USED TO DEFINE THE \textit{AD HOC} \textit{A PRIORI} COVARIANCE, $S_a$.

The general agreement between the two unrelated retrieval methodologies in mixing ratios between 300-700 hPa and total column abundances, strengthens the indication from the $dof$ and $dfs$ in Figure 3 that the sensitivity of IASI measurements to CO variability is limited to around 1 degree of freedom in the vertical weighted toward 300-700hPa.

**IV. CONCLUSIONS AND OUTLOOK**

In this letter we have described a novel and fast approach to the implementation of the MAP method for the derivation of CO from IASI cloud-cleared measurements. Although the algorithm demonstration and comparison contained in this letter focused on the use of IASI data to derive CO, the algorithm is flexible enough for use with any hyperspectral sounder dataset (e.g. AIRS, IASI, or CrIS) and target parameter where \textit{a priori} information is available. For instance, we have successfully applied the algorithm principles to retrievals of temperature, ozone and CO$_2$ and are currently preparing manuscripts for consideration for publication in various journals.
Using a theoretical analysis of IASI sensitivities we have shown that for CO the expectation of performance is approximately 10-15% in the middle troposphere with slightly larger errors near the surface. Comparing the MAP retrieval with the AST retrieval on real data, we find that both retrieval methodologies yield answers within this precision estimate in the middle troposphere; however, although well constrained by theoretical error estimates (see Figure 2), the differences between the algorithms are larger approaching the surface and in the upper troposphere. These facts indicate that both the IASI algorithms are currently sensitive to approximately 1 piece of information highly weighted toward the middle troposphere. Nevertheless, it is our expectation that higher sensitivities will tend toward the surface in regions of strong thermal gradients between tropospheric and surface temperatures and in strictly clear scenes.

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REFERENCES


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<th>10</th>
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<th>600</th>
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<tr>
<td>σ (K)</td>
<td>1.25</td>
<td>1.0</td>
<td>1.0</td>
<td>1.25</td>
<td>1.5</td>
<td>1.5</td>
<td>1.75</td>
<td>20</td>
<td>30</td>
<td>30</td>
<td>60</td>
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TABLE II COARSE PRESSURES AND PERCENT VARIABILITIES, σ, USED TO DEFINE THE AD HOC COVARIANCE MATRICES FOR TEMPERATURE AND MOISTURE, Sσ.