

Abstract

In order to avoid problems connected with the content of a priori information in volume mixing ratio vertical profiles measured with the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS), a user-friendly representation of the data has been developed which will be made available in addition to the regular data product. In this representation, the data will be provided on a fixed pressure grid coarse enough to allow a virtually unconstrained retrieval. As to avoid data interpolation, the grid is chosen to be a subset of the pressure grids used by the Chemistry Climate Model Initiative and the Data Initiative within the Stratosphere-troposphere Processes And their Role in Climate (SPARC) project as well as the Intergovernmental Panel of Climate Change climatologies and model calculations. For representation, the profiles have been transformed to boxcar base functions, which means that volume mixing ratios are constant within a layer. This representation is thought to be more adequate for comparison with model data. While this method is applicable also to vertical profiles of other species, the method is discussed using ozone as an example.

1 Introduction

The often ill-posed nature of inverse problems in remote sensing of the atmosphere is typically fought by formal regularization. The most common of such methods is optimal estimation (e.g. Rodgers, 1976) which later has been renamed maximum posteriori retrieval (Rodgers, 2000). Another common regularization method is that developed independently by Tikhonov (1963), Twomey (1963) and Phillips (1962). While all these problems provide profiles which are in some sense optimal, the major drawback is that the data product contains a certain amount of a priori information. This a priori content can precisely be characterized and quantified by the averaging kernel, which is the derivative of the retrieved atmospheric state with respect to the true atmospheric state. Some problems, however, still remain: (a) the need to communicate averaging kernels

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to the data user multiplies the amount of data to be transmitted; (b) many data users are not willing to consider averaging kernels in their analysis and prefer to take the data as they are, ignoring their content of prior information; (c) averaging kernels vary with time, which leads to unsolved problems in trend analysis (e.g. Yoon et al., 2013) or analysis of annual cycles (e.g. Hegglin et al., 2013). On the other hand, every statistics toolbox offers solutions to deal with varying error bars. Thus, it appears desirable to offer an alternative representation of the data which is user-friendly in a sense that the data user has not to care about averaging kernels, and no averaging kernels have to be provided to the user. Further, all variation of the information content of the measurement shall solely be reflected by the error bar, while the altitude resolution shall remain constant with time. In this paper we present a retrieval scheme which provides vertical abundance profiles of atmospheric constituents measured with the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) in a maximum likelihood representation. After a description of the MIPAS instrument and observations (Sect. 2), we introduce the retrieval scheme along with related terminology and describe how the maximum likelihood representation is achieved (Sect. 3). In Sect. 4 resampling on a user-friendly profile representation is discussed. Recommendations on the adequate use of the resampled data are given in Sect. 5, while in Sect. 6 we show examples of MIPAS retrievals and compare the maximum likelihood representation to the regular data version. Finally, in Sect. 7, we critically discuss the benefits and caveats of the new representation of the MIPAS data.

2 MIPAS

As a test case for the method suggested and for purposes of demonstration, measurements obtained with the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) are used. MIPAS is a limb viewing mid-infrared Fourier transform spectrometer (Fischer et al., 2008). From June 2002 to April 2012 it was used to globally measure spectrally resolved atmospheric emission from a polar orbit from 4.1 to 14.7 μm (685–

enough sampling of the atmosphere and applying some prior assumptions how the atmosphere behaves between the sampling points, or in an explicit formal way.

Constant values within layers or linear interpolation between adjacent levels are two common options to implement prior assumptions in the ML case. The ML-estimator $\hat{\mathbf{x}}_{\text{ml}}$ of the true state $\hat{\mathbf{x}}$ is

$$\hat{\mathbf{x}}_{\text{ml}} = \mathbf{x}_0 + \left(\mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K} \right)^{-1} \mathbf{K}^T \mathbf{S}_y^{-1} (\mathbf{y} - \mathbf{f}(\mathbf{x}_0)) \quad (1)$$

where \mathbf{K} is the Jacobian $\partial \mathbf{y} / \partial \mathbf{x}$, \mathbf{S}_y is the measurement error covariance matrix, \mathbf{y} is the vector of measurements, $\mathbf{f}(\mathbf{x}_0)$ are the simulated measurements as calculated for an initial guess atmospheric state \mathbf{x}_0 , and where T indicates a transposed matrix. Variants of this estimator in the context of Newtonian iteration exist but are ignored for the moment because they are not relevant to the current discussion.

The estimator using a formal constraint is

$$\hat{\mathbf{x}}_c = \mathbf{x}_a + \left(\mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K} + \mathbf{R} \right)^{-1} \mathbf{K}^T \mathbf{S}_y^{-1} (\mathbf{y} - \mathbf{f}(\mathbf{x}_a)), \quad (2)$$

Where \mathbf{R} is a constraint matrix which in one way or the other pushes the estimate $\hat{\mathbf{x}}_c$ towards the priori assumption \mathbf{x}_a . Commonly used constraints are $\mathbf{R} = \mathbf{S}_a^{-1}$ where the inverse a priori covariance matrix \mathbf{S}_a^{-1} pushes the estimate towards the prior information and yields an optimal estimate in a Bayesian sense (e.g. Rodgers, 2000), or setting \mathbf{R} a squared first order finite differences operator (Tikhonov, 1963; Twomey, 1963; Phillips, 1962) and $\mathbf{x}_a = \mathbf{0}$ where the estimate will be a smoothed version of the true profile (Steck and von Clarmann, 2001; von Clarmann et al., 2009). The presence of a formal constraint term implies that the grid on which the atmospheric state is represented can be chosen finer than the ML-grid without running into problems of singular matrices.

The advantage of ML-representation of vertical profiles is that the averaging kernel matrix, which includes the partial derivatives of the retrieved profile values at altitude

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i with respect to the true profile values at altitude j is the unity matrix, at least when represented on the grid on which the retrieval is made (this issue will be critically discussed below). The price to pay is that the ML representation of vertical profiles is only possible if the altitude grid is coarse enough to allow a stable retrieval. A fine vertical grid in an unregularized retrieval will lead to ill-posed retrieval problems which boosts the error bars (see, e.g. Rodgers, 2000 for a more detailed discussion). The most user-friendly altitude grid is that one the data user works with, because this avoids interpolation problems and saves the data user from transforming the unity averaging kernel to the new grid. For this reason, we use for our retrievals a well-established pressure grid as a “master vertical grid”, which has been used (except for some tropospheric, mesospheric and thermospheric gridpoints newly added) in the context of the SPARC Chemistry Climate Model Validation activities (e.g. Eyring et al., 2006, 2007, or Hegglin et al., 2010) or the SPARC Data Initiative (Hegglin and Tegtmeier, 2011). The pressure gridpoints of the master grid are 1000, 700, 500, 400, 300, 250, 200, 170, 150, 130, 115, 100, 90, 80, 70, 50, 30, 20, 15, 10, 7, 5, 3, 2, 1.5, 1, 0.7, 0.5, 0.3, 0.2, 0.15, 0.1, 0.03, 0.01, 0.003, 0.001, 0.0003, 0.00003, 0.00001 hPa.

This master vertical grid, however, is still too fine to allow stable unregularized retrievals. In order to avoid any unnecessary interpolation, the actual retrieval grid is chosen to be a subset of the master grid. The approximate allowed minimum gridwidth is determined with the method presented by von Clarmann and Grabowski (2007), who allow one vertical gridpoint for the ML retrieval per altitude range over which the sum of the diagonal of the averaging kernel of a preceding regularized fine-grid retrieval is unity. Since our ML data product is only an alternative representation to the already available regularized product, it is generated by only one iteration where the regular product is used as initial guess. Technically, the ML-product is also generated with the same processor which generates the regular product, and the only difference is the altitude grid and the regularization. The regularization of the new product uses a Tikhonov-type (Tikhonov, 1963) first order smoothing constraint matrix with altitude-dependent regularization strength. Over a wide part of the profile the regularization strength is set

because they represent the true atmosphere better than the staircase profiles with their discontinuities at the layer boundaries. To avoid related inaccuracies in the radiative transfer calculations, we consider the triangular base functions as more appropriate and accept the additional effort implied by the transformation to the rectangular base functions.

5 How to use the ML-data

In cases when the ML-data are sampled exactly on the model grid, direct comparison of observations and model data without any transformation is possible and adequate. It is sufficient that the grids match in the altitude range considered for the intercomparison. Occasionally, the observations will, for reasons discussed above, be represented on a subset of the master-grid. In these cases a mass-weighted mean of the respective two or more contiguous model layers will be the adequate quantity to be compared with the observation. This approach, while still simple and intuitive, is roughly equivalent with the application of the averaging kernel evaluated on the master grid, assuming linearity in a sense that the instrument is equally sensitive to the target gas regardless of its actual distribution within the combined retrieval layer.

6 Results

Here we compare the differences between the regular and the ML representation of typical ozone retrievals on the basis of zonal mean volume mixing ratio cross-sections (Fig. 3). The distributions are virtually equivalent with respect to amounts and morphology. No differences in information content or atmospheric state are discernable except at the ozone peak in equatorial latitudes. Slightly lower peak values are a typical characteristic of the staircase representation. The mass within a layer, however, is the same as that resulting from integration over a layer with altitude-dependent volume mixing ratios.

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7 Discussion and conclusion

Admittedly the statement that the averaging kernel of the ML-retrieval is unity can be challenged: While algebraically this is certainly true when the averaging kernel is calculated on the coarse ML retrieval grid, the correct sensitivity of the retrieval with respect to the true atmospheric state would require consideration of atmospheric variability on a finer scale (Rodgers, 2000, Sect 10.1). The fact that the ML averaging kernel is unity only on a coarse grid implies that it does not represent the response of the retrieval to true atmospheric structures of scales too fine to be represented on the coarse grid. These finer structures, however, cannot be seen by the instrument anyway, because the coarse grid has been chosen as fine as possible to allow an unconstrained retrieval. From the fact that any finer grid would lead to an ill-posed retrieval problem, we conclude that the respective rows of the Jacobian are linearly dependent and that the coarse-grid averaging kernel thus is a sufficiently accurate approximation to the true averaging kernel. This concept is referred to as “weak gridding criterion” by von Clarmann (2014).

For each species the altitude-grid is chosen time-invariant. Thus, the altitude resolution, which in an ML retrieval is determined solely by the vertical grid chosen, does not vary with time either. Variations of the information content of the measurements with time thus change only the error bars while the vertical resolution remains constant. Variable error bars, however, can be handled by any advanced statistical toolbox, as opposed to varying averaging kernels. In consequence, problems in time series analysis encountered by Yoon et al. (2013) or Hegglin et al. (2013) are avoided.

In the upcoming version of MIPAS data, both representations of the data will be made available: the regular retrievals will be available along with the usual diagnostics including averaging kernels and error estimates. The easy-to-use ML data product will be made available as an alternative, for applications where related problems cannot easily be solved by application of the averaging kernels (amplitudes of annual variation; trends) or for data users who have no experience in working with data containing

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priori knowledge. It must be mentioned that for some species the ML-representation is inadequate. Abundances of species like CO, NO or NO₂ vary locally by orders of magnitudes and it is not possible to define a global grid on which a reasonable unconstrained profile retrieval is always possible. For these species the data user will have to use the regular data product.

Our method is initially targeted at trace gas distributions measured with the limb sounding technique and should be applicable to a wide range of instruments measuring limb emission or solar/stellar/lunar occultation. Application to nadir viewing instruments could be more difficult because of their limited vertical resolution. Nevertheless, similar efforts were made in the context of the nadir-looking Tropospheric Emission Spectrometer (TES) by Payne et al. (2009).

Appendix: Staircase resampling

The column density of gas *g* in a layer between altitudes z_{below} and z_{above} is

$$\begin{aligned} c_g &= \int_{z_{\text{below}}}^{z_{\text{above}}} \rho(z) \text{vmr}_g(z) dz \\ &= \int_{z_{\text{below}}}^{z_{\text{above}}} \frac{\rho(z)}{R_L(z)T(z)} \text{vmr}_g(z) dz; \end{aligned} \tag{A1}$$

where ρ is air density, vmr is volume mixing ratio, p is pressure, R_L is the specific gas constant of air, and T is temperature. Assuming an isothermal layer and constant molar mass of air within the layer, we have

$$c_g = \frac{1}{R_L T} \int_{z_{\text{below}}}^{z_{\text{above}}} \rho(z) \text{vmr}_g(z) dz. \tag{A2}$$

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This holds for all vertical profile shapes $\text{vmr}(z)$, thus also for an altitude-constant profile segment $x(z) = \text{const.} = x$ and a profile segment $y(z)$ which varies linearly with altitude. In order to get the representative mixing ratio x which corresponds to the same column density as the profile segment $y(z)$, we have to solve the following equation:

$$5 \quad \frac{1}{R_L T} \int_{z_{\text{below}}}^{z_{\text{above}}} \rho(z) x dz = \frac{1}{R_L T} \int_{z_{\text{below}}}^{z_{\text{above}}} \rho(z) y(z) dz \quad (\text{A3})$$

We get

$$x = \frac{\int_{z_{\text{below}}}^{z_{\text{above}}} \rho(z) y(z) dz}{\int_{z_{\text{below}}}^{z_{\text{above}}} \rho(z) dz} \quad (\text{A4})$$

10 If the staircase profile segment x was meant to represent the same altitude range as the linear profile segment $y(z)$ we were done and z_{below} as well as z_{above} could simply be chosen as gridpoints of the underlying altitude grid. But between n gridpoints representing n independent mixing ratios between which the profiles varies linearly, there are only $n - 1$ layers characterized by $n - 1$ x values. Thus the information corresponding to one full degree of freedom would be lost. Thus we define the staircase in a way that each of the altitude gridpoints of the y representation is characterized by
 15 a constant profile segment. Around each altitude gridpoint i we have

$$y(z) = y_i + (z - z_i) \frac{y_i - y_{i-1}}{z_i - z_{i-1}} = y_i + (z - z_i) a_{\text{lo}} \quad (\text{A5})$$

for the lower branch and

$$y(z) = y_i + (z - z_i) \frac{y_{i+1} - y_i}{z_{i+1} - z_i} = y_i + (z - z_i) a_{\text{hi}} \quad (\text{A6})$$

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for the upper branch, where z_i is the altitude of gridpoint i . The ranges around z_i in which these interpolations shall be applied will be discussed later. For isothermal lower and upper segments of hydrostatic pressure profiles we have

$$\rho(z) = \rho_{lo} e^{b_{lo} z} \quad (A7)$$

5 and

$$\rho(z) = \rho_{hi} e^{b_{hi} z} \quad (A8)$$

where

$$\rho_{lo} = \rho(z_{i-1}) \left(\frac{\rho(z_i)}{\rho(z_{i-1})} \right)^{\frac{-z_{i-1}}{z_i - z_{i-1}}}, \quad (A9)$$

$$\rho_{hi} = \rho(z_i) \left(\frac{\rho(z_{i+1})}{\rho(z_i)} \right)^{\frac{-z_i}{z_{i+1} - z_i}}, \quad (A10)$$

$$10 \quad b_{lo} = \frac{\ln \frac{\rho(z_i)}{\rho(z_{i-1})}}{z_i - z_{i-1}}, \quad (A11)$$

and

$$b_{hi} = \frac{\ln \frac{\rho(z_{i+1})}{\rho(z_i)}}{z_{i+1} - z_i}. \quad (A12)$$

Equation (A4) for a constant layer from z_{below} to z_{above} around the altitude z_i now reads

$$x_i = \frac{\int_{z_{below}}^{z_i} \rho(z) y(z) dz + \int_{z_i}^{z_{above}} \rho(z) y(z) dz}{\int_{z_{below}}^{z_i} \rho(z) dz + \int_{z_i}^{z_{above}} \rho(z) dz}. \quad (A13)$$

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Using Eqs. (A5)–(A8) we get

$$x_i = \frac{\int_{z_{\text{below}}}^{z_i} \rho_{\text{lo}} e^{b_{\text{lo}} z} (y_i + (z - z_i) a_{\text{lo}}) dz}{\int_{z_{\text{below}}}^{z_i} \rho_{\text{lo}} e^{b_{\text{lo}} z} dz + \int_{z_i}^{z_{\text{above}}} \rho_{\text{hi}} e^{b_{\text{hi}} z} dz} + \frac{\int_{z_i}^{z_{\text{above}}} \rho_{\text{hi}} e^{b_{\text{hi}} z} (y_i + (z - z_i) a_{\text{hi}}) dz}{\int_{z_{\text{below}}}^{z_i} \rho_{\text{lo}} e^{b_{\text{lo}} z} dz + \int_{z_i}^{z_{\text{above}}} \rho_{\text{hi}} e^{b_{\text{hi}} z} dz}. \quad (\text{A14})$$

For the integration we use

$$f(q) = qe^{\alpha q} \Rightarrow F(q) = \frac{\alpha q - 1}{\alpha^2} e^{\alpha q} \quad (\text{A15})$$

and get

$$x_i = y_i \quad (\text{A16})$$

$$\begin{aligned} & \frac{z_i a_{\text{lo}} \frac{\rho_{\text{lo}}}{b_{\text{lo}}} e^{b_{\text{lo}} z_{\text{below}}} - \rho_{\text{lo}} \frac{a_{\text{lo}}}{b_{\text{lo}}^2} e^{b_{\text{lo}} z_i}}{\frac{\rho_{\text{lo}}}{b_{\text{lo}}} (e^{b_{\text{lo}} r_i} - e^{b_{\text{lo}} z_{\text{below}}}) + \frac{\rho_{\text{hi}}}{b_{\text{hi}}} (e^{b_{\text{hi}} z_{\text{above}}} - e^{b_{\text{hi}} z_i})} \\ & - \frac{\rho_{\text{lo}} a_{\text{lo}} \frac{z_{\text{below}}}{b_{\text{lo}}} e^{b_{\text{lo}} z_{\text{below}}} - \rho_{\text{lo}} \frac{a_{\text{lo}}}{b_{\text{lo}}^2} e^{b_{\text{lo}} z_{\text{below}}}}{\frac{\rho_{\text{lo}}}{b_{\text{lo}}} (e^{b_{\text{lo}} r_i} - e^{b_{\text{lo}} z_{\text{below}}}) + \frac{\rho_{\text{hi}}}{b_{\text{hi}}} (e^{b_{\text{hi}} z_{\text{above}}} - e^{b_{\text{hi}} z_i})} \\ & - \frac{z_i a_{\text{hi}} \frac{\rho_{\text{hi}}}{b_{\text{hi}}} e^{b_{\text{hi}} z_{\text{above}}} - \rho_{\text{hi}} a_{\text{hi}} \frac{z_{\text{above}}}{b_{\text{hi}}} e^{b_{\text{hi}} z_{\text{above}}}}{\frac{\rho_{\text{lo}}}{b_{\text{lo}}} (e^{b_{\text{lo}} r_i} - e^{b_{\text{lo}} z_{\text{below}}}) + \frac{\rho_{\text{hi}}}{b_{\text{hi}}} (e^{b_{\text{hi}} z_{\text{above}}} - e^{b_{\text{hi}} z_i})} \\ & - \frac{\rho_{\text{lo}} \frac{a_{\text{hi}}}{b_{\text{hi}}^2} e^{b_{\text{hi}} z_{\text{above}}} - \rho_{\text{hi}} \frac{a_{\text{hi}}}{b_{\text{hi}}^2} e^{b_{\text{hi}} z_i}}{\frac{\rho_{\text{lo}}}{b_{\text{lo}}} (e^{b_{\text{lo}} r_i} - e^{b_{\text{lo}} z_{\text{below}}}) + \frac{\rho_{\text{hi}}}{b_{\text{hi}}} (e^{b_{\text{hi}} z_{\text{above}}} - e^{b_{\text{hi}} z_i})} \end{aligned}$$

For best agreement with model grids, the following choices were made for the new profile segments where the mixing ratio is constant with altitude:

$$\rho(z_{\text{below}}) = \frac{\rho_j + \rho_{j-1}}{2} \quad (\text{A17})$$

and

$$\rho(z_{\text{above}}) = \frac{\rho_j + \rho_{j+1}}{2}. \quad (\text{A18})$$

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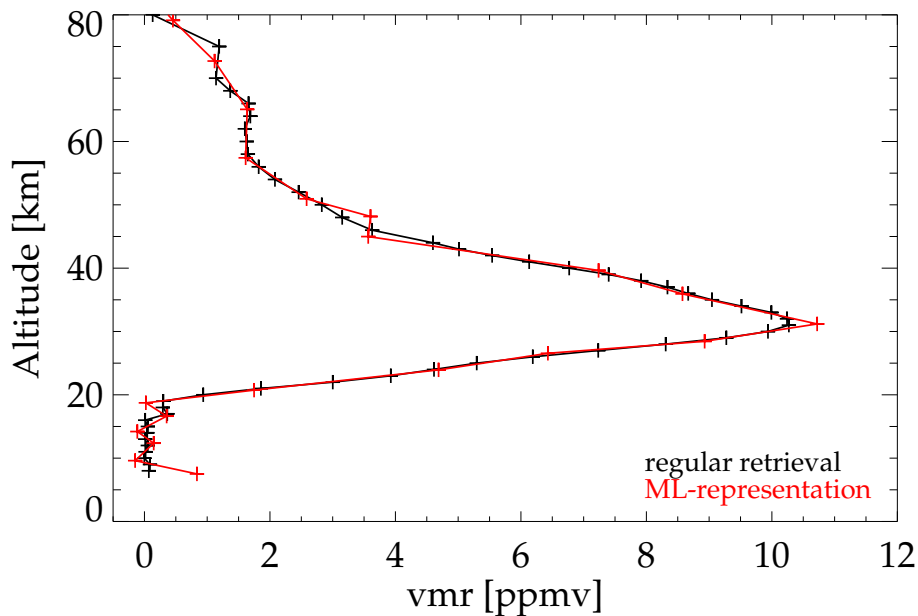


Figure 1. A MIPAS ozone profile from the regular processing (black) and the same profile in a maximum likelihood representation where linear interpolation of vmr between altitude grid-points was assumed (red). This particular example is a measurement at 21.33° S 84.25° W on 2 October 2009. The original retrieval has 20.6 degrees of freedom, yielding 20 steps in the maximum likelihood representation.

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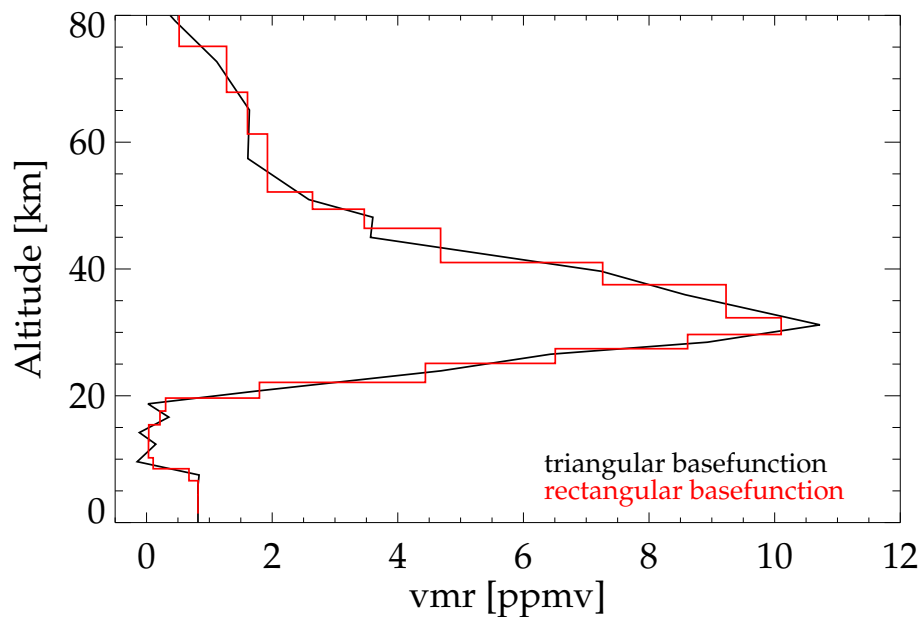


Figure 2. An ozone profile represented in triangular (black) and rectangular (red) base functions.

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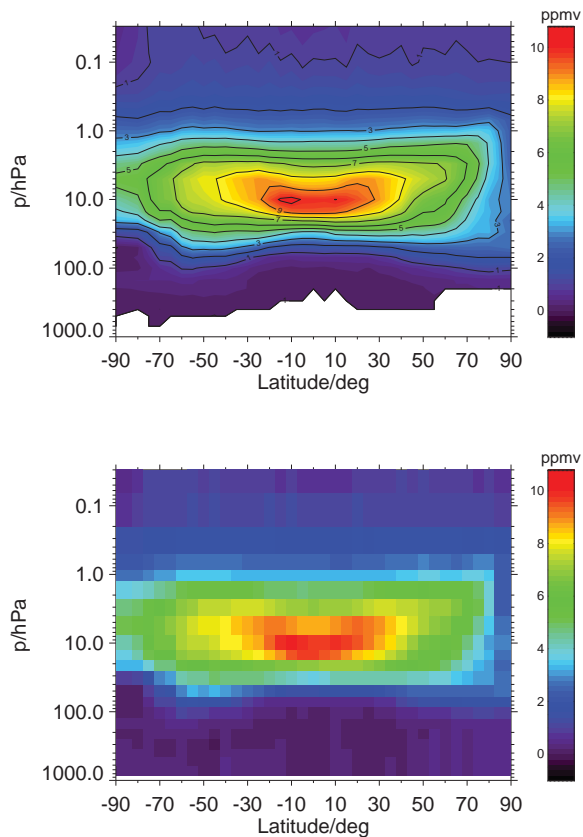


Figure 3. Zonal mean ozone distributions from the regular retrieval on a fine grid (top panel) and the maximum likelihood staircase representation on a coarse grid (bottom panel).

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