Interactive comment on “Limb scatter ozone retrieval from 10 to 60 km using a Multiplicative Algebraic Reconstruction Technique” by D. A. Degenstein et al.

Anonymous Referee #2

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General comments:

This is a useful contribution to the toolkit of geophysical inversion algorithms. In my opinion the paper should be published after the authors have revised the manuscript in the light of the general and specific comments below.

1) The Odin spacecraft is in a terminator orbit (see line 49), and the solar zenith angle varies along the atmospheric line of sight to OSIRIS. Also, at high altitudes, where photochemistry is rapid, the along-LOS gradient of the Solar Zenith Angle will induce a slight gradient in the concentration of ozone. Did those effects have to be accounted
for, e.g., in the forward model, or was the variation unimportant?

2) According to the abstract, and to lines 32-34 and 87-88, “This technique allows for the consistent merging of the absorption information from radiance measurements at wavelengths in the Chappuis and the Hartley-Huggins bands at each iteration of the inversion.” Admittedly, some inversion algorithms do not achieve that. But other algorithms that have been used widely for years do merge that type of information quite well. In particular, the Minimum Mean Square Error “Optimal” Estimation algorithm, in e.g., Rodgers’ formulation of it, can smoothly and consistently merge information from quite different spectral regions. In the present case, that would be achieved by using all of the relevant spectral channels simultaneously during each iteration of the inversion for ozone, but smoothly varying the diagonal elements of the measurement noise covariance matrix as a function of wavelength and tangent altitude to shade out the influence of the UV channels at low altitudes and of the VIS channels at high altitudes. That ought to be mentioned. The consistent merging of diverse spectral information is indeed demonstrated by this paper to be a virtue of SaskMART, and it is worthy of mention, but it is not a virtue of SaskMART alone, and it seems to be over-emphasized throughout the paper.

3) An averaging kernel must exist for MART. Displaying it would make clear the true vertical resolution of the measurement, which is likely to be less fine than the somewhat arbitrary vertical sampling of the input lines of sight and the vertical grid used for the numerical inversion.

4) Do the calculated tangent altitudes include the effects of refraction? Refraction should be significant below about 30 km.


6) Typo in line 329: “Homstein” => “Hornstein”
7) The wording in line 85 is confusing. It states that “the pair and triplet definitions given above are the inverse of those used in previous work”. But the pairs and triplets are not being chosen differently, the measurement vector is. The authors meant to say that the measurement vector defined here is such that the “ref” and “abs” factors are assigned to the numerator and denominator of the argument of the logarithm in a way that is opposite to what previous authors have done.

8) Lines 81-83. It would be helpful to the reader to state explicitly that iterations are needed only because of the nonlinearity of the exact forward problem. That is hinted at in line 83, but is easy to miss, since the main point of the sentence that begins in line 83 is something else, namely a positivity condition.

8) How is the first guess profile $x^\odot(0)$ chosen? To what extent does the result of the iteration depend on the first guess, when measurement noise is present?

9) Typo in line 97: “modelled” should be “modeled”.

10) In line 115, “distinguish” would be clearer than “indicate”.

11) The least systematic feature of SaskMART seems to be in choosing the $W_{kji}$. The $W$ are plotted in Fig. 4, and are discussed in Section 3.4. Lines 125-131 indicate that the $W$s are guessed at via trial and error. It also indicates that they are taken to have fixed values, independent of the true atmosphere and of the data. Because the true forward problem is nonlinear, the reader will expect the $W_{kji}$ to depend on the atmosphere ($x$ vector), and thence to depend somewhat on the data vector $y$. But apparently that is not necessary. That is delightful, but puzzling. The choosing of the $W_{kij}$ is discussed further in point 16), below.

12) Lines 150-154 state that “The Hartley-Huggins band pairs are normalized at successively higher tangent altitudes such that the maximum value of the pair, which occurs at the minimum altitude, is approximately 1.0. In an approximate sense, this represents a distance of one optical depth from the normalization altitude to the minimum
altitude.". This doesn’t seem plausible. If the optical depth were 1 at the normalization altitude, then it would be about 2 at the minimum altitude, which would be far from optically thin, and might well be below the knee.

13) The normalization altitudes should have been listed. Admittedly, they can be estimated from lines 157-158 together with Fig. 4. Since Fig. 4 shows that $W$ for 331 nm vanishes above about 37.5 km, the corresponding normalization altitude must be about 5 km more than that, so it is about 42.5 km. The normalization altitudes can also be found from the fact stated in lines 160 and 165, namely, as the upper altitude at which the relevant curve in Fig. 2 meets the vertical axis. In agreement with the above, that seems to be at about 42.5 km for 331 nm. Indeed, line 179 says that the normalization altitude is 42 km for 331 nm. But the discrepancy between my estimate and the true value shows that listing the normalization altitudes would be more accurate, and would also avoid unnecessary tedious labor for the reader.

14) Minor typo in line 173: “low altitude” was written as “low altitudes”.

15) The finding stated in lines 185-187, on the need for a smooth altitude variation for the contribution from each pair and triplet, should be of widespread interest to the inverse estimation community.

16) Overall, the least satisfactory aspect of this approach is the lack of a systematic way of choosing the weights $W$. Lines 200-201 indicate that the optimal weights are defined by a minimum that is broad in some directions in $W$-space, but which might be sharp in the other directions. How does that relate to lines 222-223, which says that increasing the number of pairs and triplets is beneficial? Is it always? What about the effective number of degrees of freedom? Does the redundancy from using more pairs or triplets than the number of degrees of freedom usefully suppress the effect of noise, or does it eventually destabilize the algorithm by introducing linear dependence?

17) Lines 226-230: Do these extrapolations introduce a bias? The extrapolations above the highest retrieved tangent altitude have an obvious use, since the lines of sight for all
of the retrieved tangent altitudes pass through those higher altitudes, and so the ozone concentration at those altitudes must be known. But it might be worthwhile to point out why the extrapolations below the lowest retrieved tangent altitude are needed. They are needed because in limb scattering, in contrast to solar occultation, the radiation upwelling from below a line of sight influences the radiance received from that line of sight.

18) Lines 233-237 indicate that ozone, aerosols, and NO2 are retrieved separately rather than in a single retrieval for all three. Overlapping extinction features would make separate retrievals impossible without assuming some profile for the concentration of the atmospheric ingredient whose extinction overlaps that of the retrieved ingredient. Aerosol extinction has such a broad spectrum that it certainly overlaps that from ozone and NO2. NO2 absorption near 440 nm overlaps some ozone and aerosol extinction. Are the aerosol and NO2 profiles obtained from climatology, or are the iterations in the retrievals of aerosol and of NO2 interleaved with those of ozone, so that each iteration in each retrieval can take advantage of the best current estimate of the other species?

19) Line 238 says that cloud top is detected by using an IR channel. For nadir viewing sensors it has recently been discovered that using IR-based cloud top altitudes leads to an error, because the effective cloud top in the UV can be significantly lower than that in the IR. The errors might be much smaller in limb viewing mode, but I do not know whether that is the case.

20) In these particular profiles, OSIRIS measures more ozone than does SAGE II at low altitudes when the latitude is 44.1 degrees, and the opposite occurs at -66.1 degrees. Fig. 6 shows that, averaged over the 196 comparison profiles, OSIRIS systematically measures more ozone than does SAGE II at low altitudes, and less at high altitudes. Line 272 asserts that the bias at low altitudes is due to the larger variability there. Variability would increase the RMS (and does so), but should not significantly affect the averages, and hence the bias. So that explanation does not seem plausible.
21) In the comparison of the tropical zonal averages, the explanation (lines 283-284) in terms of the higher tropopause in the tropics is plausible, especially since the sharp increase in the mean difference begins at the average height of the tropical tropopause, and, as noted in line 285, the increased variability when descending to that altitude confirms that the tropopause begins at the altitude where the mean difference increases sharply. The RMS in the SAGE II measurements of the zonal averages agrees with that in the OSIRIS measurements. So the increase in the difference in the zonal means at low altitudes must be caused by a difference in the longitudes sampled by SAGE II and OSIRIS during the single day considered. Although solar occultation usually spans the full span of longitudes over a single day, it does so discretely, with large gaps between successive samples, and that might have introduced a bias.

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