Comment on egusphere-2022-806
Anonymous Referee #1

Referee comment on "Use of machine learning and principal component analysis to retrieve nitrogen dioxide (NO2) with hyperspectral imagers and reduce noise in spectral fitting" by Joanna Joiner et al., EGUsphere, https://doi.org/10.5194/egusphere-2022-806-RC2, 2022

Review of Joiner et al "Use of machine learning to retrieve nitrogen dioxide with hyperspectral imagers in the ultraviolet and blue spectral rang" submitted to Atmospheric Measurement Techniques.

Joiner et al. presented a new method based on machine learning to retrieve NO2 from low spectral resolution instruments. This is an interesting study and the authors demonstrated well the potential of this approach for forthcoming missions with high spatial resolution. The paper is very well written and structured and there is little to say on the content. It should be published in AMT, after few (mostly minor) corrections. Overall, the quality of the figures is quite poor, and it would be needed to improve the resolution of all figures.

Comments

My main reservation is that the paper covers two things: (1) the retrieval of NO2 from instruments with lower spectral resolution, (2) the retrieval of NO2 using machine learning. What I would like to see is a DOAS-type retrieval of NO2 for the lower spectral resolution data so that one can evaluate the benefit of the machine learning approach directly. I realize that this is probably quite some work but it would be nice to understand if machine learning can improve the retrievals or not. It is understood that machine learning is interesting in terms of computational time but from the results shown here it is not clear if it is the only advantage.

-Section 2:
A small section introducing OCI and GLIMR is missing here. Details on instruments (spectral range, sampling, performance, etc) should be added (e.g., as a form of a table).

It would be good to refer to past studies of low spectral resolution NO2 retrievals attempts.

line 89 reads ‘..a retrieval would likely need to make use of the broad continuum absorption..’. Not sure what is meant here. Is the author meaning a large wavelength range to better constrain the fit or is it really the broadband contribution of the NO2 absorption which is targeted? Please clarify.

p8, line 179 ‘...to half the number of spectral elements was sufficient to capture the spectral information associated with NO2 while providing some noise reduction’. I don’t understand why this should provide a noise reduction. Could you elaborate?

p9, 275: the use of the logarithm of the NO2 SCD does not correspond to anything physical. Could you clarify why this was used? Is there a justification for this, other than it gives good results.

p10, line 237: about the NN ability to capture the wavelength dependence of the SNR. What about wavelengths cross-correlations? It is this information available from the OCI and GLIMR? I guess not but could it affect the performance of the NN approach?

-Section 3

for figs 5,6,9, it is not always clear to what settings they correspond. E.g., what wavelength range was used, noise added or not, etc. I propose to detail this in all figure captions.

Table 1: why is the bias larger for the case where the wavelength range is close to that of OMI NO2 (400-470 nm)? In general, the SCDs in different windows should not be identical (because of the AMF wavelength dependence). I find this aspect is not discussed enough.

P14, l 313: it is mentioned that the 'largest errors occur over highly polluted areas'. Could it be because the NN is not sufficiently trained for these conditions? Could the
situation improve by adding such highly polluted scenes in the training set? If yes, what would be the weight of such scenes in the training set?

*p14, l 328 : ‘..but rather the VCD’. Why? SCD is the actual signal, not the VCD.

* In general, how frequent should the NN be trained? Have you tried the algorithm for periods affected by the row anomaly of older data in the OMI mission? How is the data quality affected?

*p19, line 392: it would be good to add these results in SI.

Typos

-P1, line4: S5P resolution is 3.5 km x 5.5 km (not 3.5 km x 5 km)

-p4, line94: 'gloyoxal'-> 'glyoxal'

-p4, line94: 'spectral imprint' -> unclear what is meant by 'imprint'