

Author comments for RC2:

We would like to thank the reviewer for the valuable feedback and efforts in reviewing the manuscript.

This manuscript presents a multi-objective optimization trained to increase GOSAT sounding availability in the sparsely observed regions of the high latitudes with minimal increase in error when compared to TCCON. Overall, the paper is well written, and the approach will have great impact for further science from the GOSAT mission, therefore the manuscript is appropriate for AMT and nearly ready for publication. However, a few questions should be addressed:

1. The authors provide good setup in section 3 for why the problem should be treated with multi-objective heuristic approach but do not give reason for selecting a genetic algorithm over other multi-objective optimization approaches e.g., Bayesian methods like Hypervolume Improvement which can find optimal regions much faster. Additionally it would be nice to see a brief comparison/discussion to the Genetic Algorithm used for OCO-2 and GOSAT XCO₂ filtering presented in Mandrake et al. 2009 (<https://amt.copernicus.org/articles/6/2851/2013/>) and a hybrid heuristic and machine learning approach presented in Keely et al. 2025 that also aimed to increase sounding availability in the high latitudes and cloud affected regions (<https://agupubs.onlinelibrary.wiley.com/doi/10.1029/2025EA004329>).

We agree with the reviewer that genetic algorithms are not the only possible approach to this kind of a multi-objective problem. Several approaches have previously been explored to address this type of multi-objective optimisation problem. Bayesian multi-objective optimisation, including methods based on hypervolume improvement can be highly sample efficient as they use probabilistic surrogate models to minimise the number of evaluations needed, particularly when each objective evaluation is computationally expensive (such as e.g., full-physics forward-model runs). A Bayesian multi-objective optimisation together with a random forest, non-linear, interpretable machine learning technique is recently demonstrated for the optimisation of OCO-2 quality filtering (Mauceri et al., 2025; Keely et al., 2025). However, in the present study, each candidate solution consists of fundamentally eight filter parameters that can be evaluated directly by applying the thresholds to the existing GOSAT XCH₄ data set with acceptable run time of around 10 to 15 minutes. When the objective evaluations are computationally cheaper, a genetic algorithm can be a reasonable straight forward choice and NSGA-II returns a full, diverse non-dominated population without the use of trained surrogate models, the objective functions can be evaluated directly using the existing GOSAT–TCCON dataset making this approach suitable for the present problem.

GA has also been applied earlier by Mandrake et al. (2013), who presented a GA-based sounding selection strategy for OCO-2 retrievals, tested using GOSAT ACOS XCO₂ retrievals, which involved a multi-stage procedure, where they have used a large number of input candidate features, including spectral parameters, geometry and signal to noise, to generate large ensemble of optimised filters. It generated warning levels and spatial-coverage selection for soundings, which later on, was discontinued due to its operational complexity (Keely et al., 2025; Mandrake et al., 2015). The present study addresses a more focused optimisation problem by applying NSGA-II to optimise thresholds within an existing GOSAT Proxy XCH₄ filtering framework. Our objectives are directly focused on increasing data density while maintaining data quality, whereas Mandrake et al. aimed to reduce retrieval scatter, maximise the data throughput, and minimise the filter complexity which involved a more elaborate and complex process.

This discussion is added at the end of Section 3 in the revised manuscript.

Keely, W., Mauceri, S., Nelson, R., Laughner, J., O'Dell, C. W., Massie, S., et al. (2025). Uncertainty-aware machine learning bias correction and filtering for OCO-2: 2. *Earth and Space Science*, 12, e2025EA004329. <https://doi.org/10.1029/2025EA004329>

Mauceri, S., Keely, W., Laughner, J., O'Dell, C. W., Massie, S., Nelson, R., et al. (2025). Uncertainty-aware machine learning bias correction and filtering for OCO-2: 1. *Earth and Space Science*, 12, e2025EA004328. <https://doi.org/10.1029/2025EA004328>

Mandrake, L., Frankenberg, C., O'Dell, C. W., Osterman, G., Wennberg, P., and Wunch, D.: Semi-autonomous sounding selection for OCO-2, *Atmos. Meas. Tech.*, 6, 2851–2864, <https://doi.org/10.5194/amt-6-2851-2013>, 2013.

Mandrake, L., et al. "Orbiting Carbon Observatory-2 (OCO-2) Warn Level, Bias Correction, and Lite File Product Description." *Jet Propulsion Laboratory. California Institute of Technology, Pasadena Retrieved from http://disc.sci.gsfc.nasa.gov/OCO-2/documentation/oco-2-v7/OCO2_XCO2_Lite_Files_and_Bias_Correction_0915_sm.pdf* (2015).

2. The choice to use the raw column averaged gas as a filtering variable could allow for the filter to overfit or potentially remove good data given the binary selection of threshold. In addition to the requested discussion above it would be useful to see further validation of the filter variable selection and why other retrieved surface or atmospheric state parameters as is described in O'Dell et al. 2018 (<https://amt.copernicus.org/articles/11/6539/2018/>).

We agree that using the retrieved XCH₄ and XCO₂ values as filtering variables may lead to the rejection of valid observations if the selected filters are too restrictive. But the optimised lower XCH₄ threshold is substantially lower than the original threshold, making this criterion less restrictive and allowing additional observations to be retained (figure 6). Figure 6 provides further insight into the optimised filter thresholds. The thresholds that matter settle tightly and neatly stabilised while lower threshold χ^2 wanders, that don't have much impact on the optimisation. This behaviour indicates that the algorithm is finding genuine, physically meaningful optimal bounds rather than over-fitting to noise.

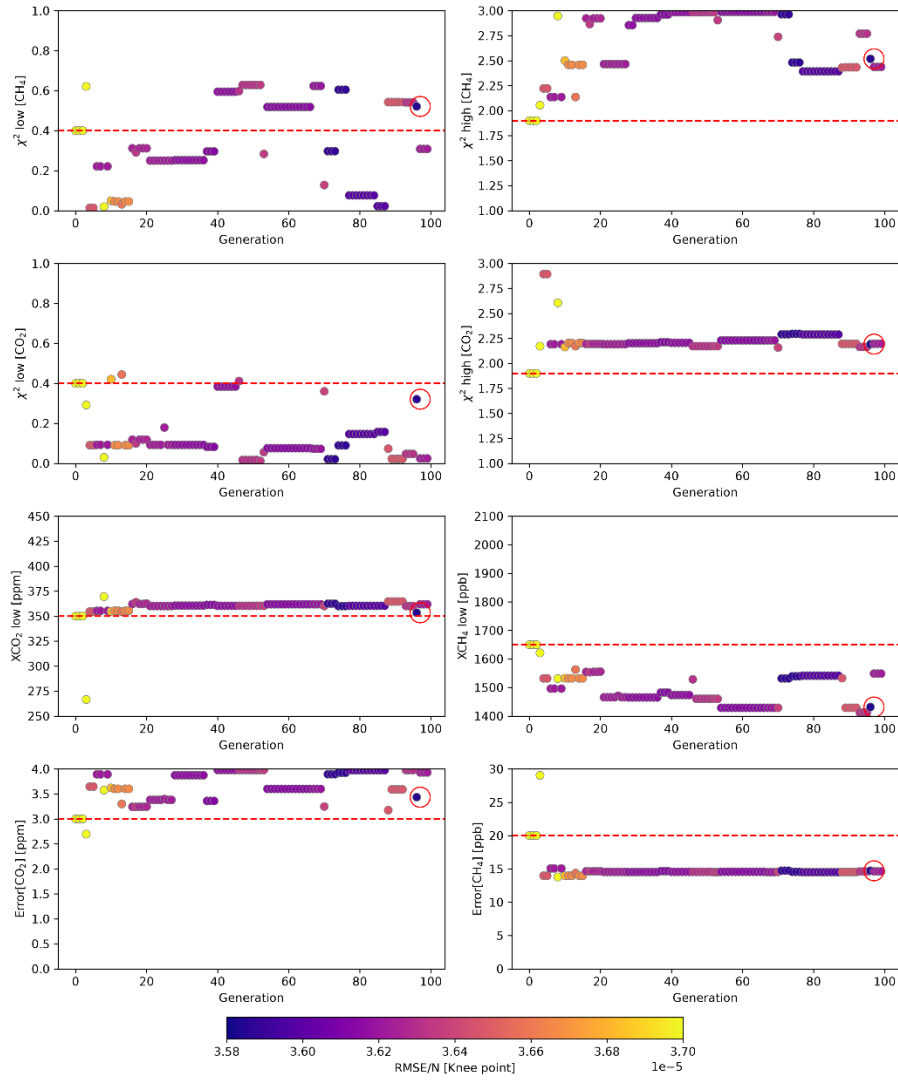


Figure 6. Evaluation of decision variables (filter values as given in Table 1) with generations. Red dotted line shows the initial standard filters. The red circle shows the selected optimised filter values correspond to the generation of minimum of the ratio of RMSE to N.

We chose to retain these set of filter variables as they are already part of the existing UoL GOSAT proxy methane product's post-retrieval filtering process, so that the original and optimised datasets are consistent for direct comparison (Parker et al., 2020). We agree that testing the GA using additional atmospheric and surface state parameters following the ACOS quality filter screening of O'Dell et al. (2018), would be a valuable extension. However, it is to be noted that UoL GOSAT Proxy methane retrieval state vector contains CH_4 and CO_2 profiles, H_2O and temperature scaling, surface albedo and spectral dispersion and not aerosols as the scattering-induced light-path modification is cancelled by taking the XCH_4/XCO_2 ratio (Parker et al., 2011). Thus, aerosol optical depth and similar quantities are not available as filter variables (Parker et al., 2011; 2020).

In the revised manuscript we have added this discussion in two different parts. The following clarification is added in section 3.1.

'We chose to retain these variables as they are already part of the existing UoL GOSAT proxy methane product's post-retrieval filtering process, so that the original and optimised datasets are consistent for direct comparison (Parker et al., 2020). Aim of the study is to demonstrate the capability of GA for enhancing the satellite GHG throughput rather than filter selection for quality filtering. Testing the GA using additional atmospheric and surface state parameters following the ACOS quality filter screening of O'Dell et al. (2018), would be a valuable extension. However, it is to be noted that UoL GOSAT Proxy methane retrieval state vector contains CH_4 and CO_2

profiles, H₂O and temperature scaling, surface albedo and spectral dispersion and not aerosols as the scattering-induced light-path modification is cancelled by taking the XCH₄/XCO₂ ratio (Parker et al., 2011). Thus, aerosol optical depth and similar quantities are not available as filter variables (Parker et al., 2011; 2020).'

We have added the following part of the discussion to section 4.2 where figure 6 is cited.

'Using lower thresholds for the retrieved XCH₄ and XCO₂ values as filtering variables may lead to the rejection of valid observations if the selected filters are too restrictive. But the optimised lower XCH₄ threshold is substantially lower than the original threshold, making this criterion less restrictive and allowing additional observations to be retained (figure 6). Figure 6 provides further insight into the optimised filter thresholds. The thresholds that matter settle tightly and neatly stabilised while lower threshold χ^2 wanders, that don't have much impact on the optimisation. This behaviour indicates that the algorithm is finding genuine, physically meaningful optimal bounds rather than over-fitting to noise.'

O'Dell, C. W., Eldering, A., Wennberg, P. O., Crisp, D., Gunson, M. R., Fisher, B., Frankenberg, C., Kiel, M., Lindqvist, H., Mandrake, L., Merrelli, A., Natraj, V., Nelson, R. R., Osterman, G. B., Payne, V. H., Taylor, T. E., Wunch, D., Drouin, B. J., Oyafuso, F., Chang, A., McDuffie, J., Smyth, M., Baker, D. F., Basu, S., Chevallier, F., Crowell, S. M. R., Feng, L., Palmer, P. I., Dubey, M., García, O. E., Griffith, D. W. T., Hase, F., Iraci, L. T., Kivi, R., Morino, I., Notholt, J., Ohyama, H., Petri, C., Roehl, C. M., Sha, M. K., Strong, K., Sussmann, R., Te, Y., Uchino, O., and Velasco, V. A.: Improved retrievals of carbon dioxide from Orbiting Carbon Observatory-2 with the version 8 ACOS algorithm, *Atmos. Meas. Tech.*, 11, 6539–6576, <https://doi.org/10.5194/amt-11-6539-2018>, 2018.

Parker, R. J., Webb, A., Boesch, H., Somkuti, P., Barrio Guillo, R., Di Noia, A., Kalaitzi, N., Anand, J. S., Bergamaschi, P., Chevallier, F., Palmer, P. I., Feng, L., Deutscher, N. M., Feist, D. G., Griffith, D. W. T., Hase, F., Kivi, R., Morino, I., Notholt, J., Oh, Y.-S., Ohyama, H., Petri, C., Pollard, D. F., Roehl, C., Sha, M. K., Shiomi, K., Strong, K., Sussmann, R., Té, Y., Velasco, V. A., Warneke, T., Wennberg, P. O., and Wunch, D.: A decade of GOSAT Proxy satellite CH₄ observations, *Earth Syst. Sci. Data*, 12, 3383–3412, <https://doi.org/10.5194/essd-12-3383-2020>, 2020.

Parker, R., et al. (2011), Methane observations from the Greenhouse Gases Observing SATellite: Comparison to ground-based TCCON data and model calculations, *Geophys. Res. Lett.*, 38, L15807, doi:[10.1029/2011GL047871](https://doi.org/10.1029/2011GL047871).

3. Relying on TCCON as the sole truth proxy for training the GA leaves open the potential for circularity. Keely et al. 2025 address this by evaluating on additional truth proxies such as XGas fields from flux inversion models and use an epistemic uncertainty metric derived from the ML models to assess when to trust data that is far away from TCCON sites in state space. Could such a distance metric be derived using the GA approach given that TCCON sites are sparse in the high latitudes? Discussion of this would be of great use to the community for the strengths and tradeoffs between approaches (e.g., as the authors already mention the lack of need to use large, labelled training data for GA methods).

We agree that evaluating the final filter using the same six high-latitude TCCON data, that is used in the optimisation process (in the objective function) can cause potential circularity and does not make it a fully independent validation. TCCON was selected for validating the optimised dataset because the validity of the University of Leicester GOSAT Proxy XCH₄ product has been established against TCCON (Parker et al., 2020), and, using the same reference dataset for both the original and optimised datasets provides consistency in comparing the effect of optimised filtering in the new data set. However, the evaluation also includes a global comparison with 15 TCCON sites that were not used in the optimisation. These additional sites provide an independent assessment of the performance of the optimised filter beyond the high-latitude stations used in the objective function. We acknowledge that the evaluation using the six high-latitude stations is not fully independent, but the global comparison provides additional evidence of the filter's performance at sites not involved in the optimisation.

Independent ground-based EM27/SUN observations provide another potential complementary dataset for independent validation of the optimised dataset. These include COCCON observations (Frey et al., 2019), GEMINI-UK network data (Kurganskiy et al., 2025; Humpage et al., 2026) and other coordinated EM27/SUN campaigns (Hase et al., 2015), which provide an opportunity for the independent validation of the optimised dataset. Although these datasets were not used in the present optimisation, their use in future work could

provide an independent evaluation of the optimised filter, particularly at locations where TCCON observations are unavailable.

Keely et al., 2025, have used an ML-derived uncertainty in the predicted OCO-2 -TCCON bias correction to identify soundings that may be unreliable, and they also calculate maximum matching geographical distance between OCO-2 and TCCON soundings to be that corresponds to a cut off of 25% increase in RMSE (Mauceri et al., 2025; Kelly et al., 2025). Since the GA aims at minimising RMSE while maximising the number of observations, it already favours filters that retain observations with better agreement with TCCON without discarding too much data. However, it does not fully address how well the TCCON- satellite soundings are matching in the state space. Another possible extension is to examine how consistently each sounding is retained across the final population of solutions. The fraction of solutions in the final Pareto population that accepts each sounding could be calculated to identify observations whose retention is robust across alternative optimised filter configurations. Additional evaluation against suitable model-derived XGas estimates from flux inversions, could also help assess retrieval performance in regions with sparse TCCON coverage, while accounting for the uncertainties of these alternative references.

WE have revised the manuscript by adding this discussion to section 4.4

Frey, M., Sha, M. K., Hase, F., Kiel, M., Blumenstock, T., Harig, R., Surawicz, G., Deutscher, N. M., Shiomi, K., Franklin, J. E., Bösch, H., Chen, J., Grutter, M., Ohyama, H., Sun, Y., Butz, A., Mengistu Tsidu, G., Ene, D., Wunch, D., Cao, Z., Garcia, O., Ramonet, M., Vogel, F., and Orphal, J.: Building the COllaborative Carbon Column Observing Network (COCCON): long-term stability and ensemble performance of the EM27/SUN Fourier transform spectrometer, *Atmos. Meas. Tech.*, 12, 1513–1530, <https://doi.org/10.5194/amt-12-1513-2019>, 2019.

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Keely, W., Mauceri, S., Nelson, R., Laughner, J., O'Dell, C. W., Massie, S., et al. (2025). Uncertainty-aware machine learning bias correction and filtering for OCO-2: 2. *Earth and Space Science*, 12, e2025EA004329. <https://doi.org/10.1029/2025EA004329>

Citations:

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Keely, W., Mauceri, S., Nelson, R., Laughner, J., O'Dell, C. W., Massie, S., ... & Payne, V. (2025). Uncertainty-aware machine learning bias correction and filtering for OCO-2. 2. *Earth and Space Science*, 12(11), e2025EA004329.

O'Dell, C. W., Eldering, A., Wennberg, P. O., Crisp, D., Gunson, M. R., Fisher, B., Frankenberg, C., Kiel, M., Lindqvist, H., Mandrake, L., Merrelli, A., Natraj, V., Nelson, R. R., Osterman, G. B., Payne, V. H., Taylor, T. E., Wunch, D., Drouin, B. J., Oyafuso, F., Chang, A., McDuffie, J., Smyth, M., Baker, D. F., Basu, S., Chevallier, F., Crowell, S. M. R., Feng, L., Palmer, P. I., Dubey, M., García, O. E., Griffith, D. W. T., Hase, F., Iraci, L. T., Kivi, R., Morino, I., Notholt, J., Ohyama, H., Petri, C., Roehl, C. M., Sha, M. K., Strong, K., Sussmann, R., Te, Y., Uchino, O., and Velasco, V. A.: Improved retrievals of carbon dioxide from Orbiting Carbon Observatory-2 with the version 8 ACOS algorithm, *Atmos. Meas. Tech.*, 11, 6539–6576, <https://doi.org/10.5194/amt-11-6539-2018>, 2018.