Response to the referee (RC1)

In-Flight Estimation of Instrument Spectral Response Functions Using Sparse Representations

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We would like to thank the Editor and the referees and community members for their careful and thoughtful comments about our paper. We really appreciate the time and effort that has gone into their reviews. All the comments have been considered as detailed below. A detailed answer to the comments can be found in the following pages.

Response to Referee (RC1)

Comment 1

The paper focus on the instrument spectral response functions estimation based on sparse methodologies. This is an interesting paper with a new proposed method that reveals to be competitive and outperforms the state of the art, specifically, the parametric based strategies as the Gaussian and Generalized Gaussian.

Response:

We thank the referee for his/her appreciation of our work.

Comment 2

How confident are you in the reference spectrum obtain using a radiative transfer model and/or the ground characterization for each instrument and what would be the impact of a possible mismatch on such transfer model/ ground characterization?

Response:

In practical applications, the instrument is calibrated using the measured spectra for some specific scenes whose reference spectra are well-characterized (Sun, Moon, uniform scenes such as deserts, etc). Illustrations of the impact of potential mismatches have been included in Section 5.4 of the manuscript, including the figures 1, 2 and 3 below. In a first experiment, a Gaussian noise was introduced to the reference spectrum (with signal-to-noise ratios of 20 dB and 80 dB, cf. Fig. 1). In a second experiment, Gaussian noise is introduced into one-third of the ISRFs used to create the dictionary, with signal-to-noise ratios of 40 dB and 80 dB (cf. Fig. 2). As can be observed in the results presented in Fig. 3, when the noise level increases, the errors in approximating the ISRFs increase, as expected. Nonetheless, the overall error remains lower than those obtained when using parametric models. Furthermore, when the dictionary is constructed from these noisy ISRFs, the noise modifies the form of the atoms, thereby degrading the estimation of the ISRFs. However, note that during ISRF on-ground measurements, the laser is of high precision, and such noisy ISRF measurements with SNR = 20dB are unlikely to occur.

A mismatch may also arise if the instrument undergoes motion during flight, resulting in disparate in-flight ISRFs when compared to those characterized on-ground. This phenomenon was partially examined in our work when when we analyzed the ISRF's dependence on the scene. We showed in Sect. 5.4.3 of the paper that incorporating three additional ISRFs from non-uniform scenes is effective to address the mismatch and sufficient to obtain good ISRF estimation performance. Future work related to these issues will be pointed out in the conclusion of the manuscript.

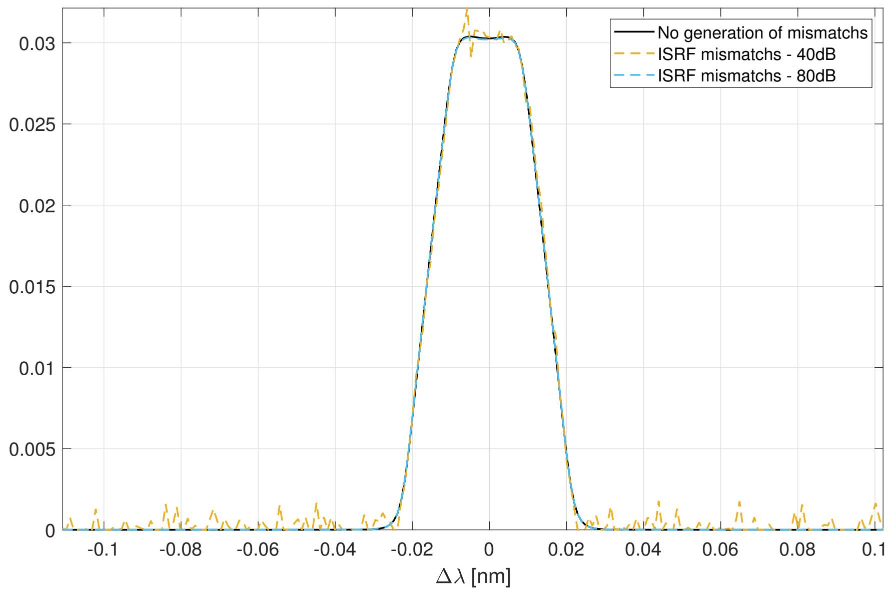

Figure 1: Representation of possible ISRF mismatches by adding different levels of noise (SNR of 40dB or 80dB) versus true associated ISRF.

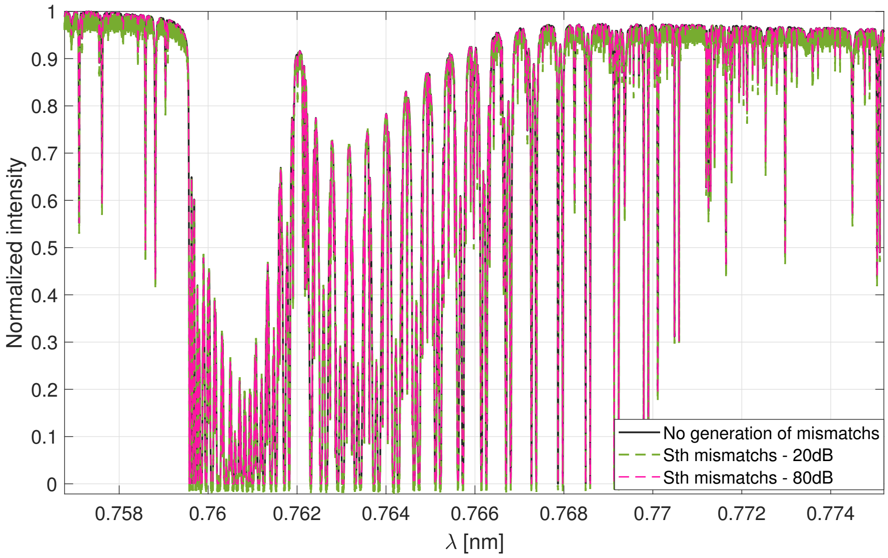

Figure 2: Representation of possible mismatches regarding the reference spectrum by adding different levels of noise (SNR of 20dB or 80dB) versus true associated reference spectrum.

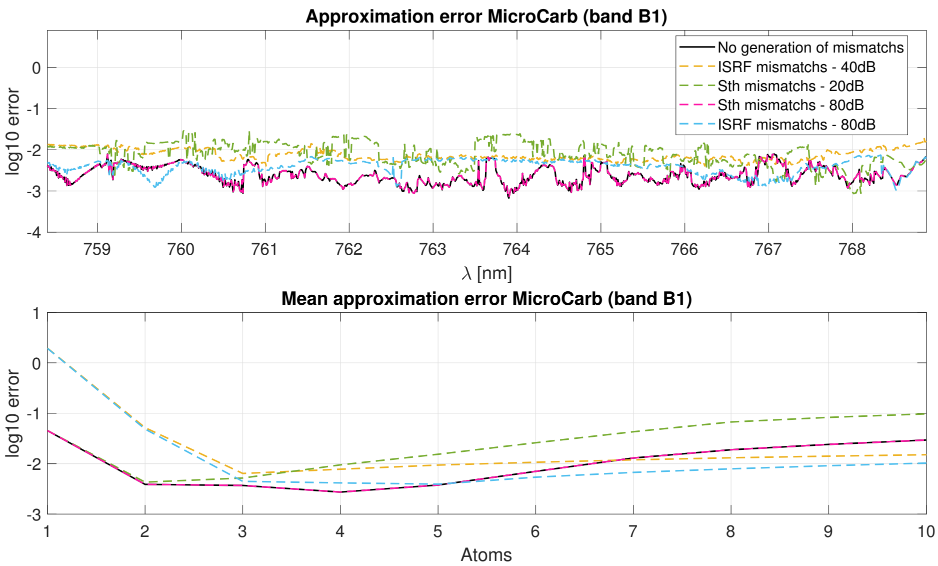

Figure 3: Results obtained using SVD and OMP for the different scenarios of ISRF and reference spectrum mismatches.

Comment 3

What is the number of representatives ISRF examples used in the simulation part? Can you discuss (at least numerically) the minimum number that leads to an error below of the required 1%?

Response:

The number of representative ISRFs used in the simulation part depends on the spectrometer. Approximately 10% of the total number of ISRFs within the band was selected to construct the dictionary. This number is sufficient to yield the performances reported in our work.

We would further argue that the question is less about the minimum number of representative ISRFs used to yield good results, but rather about that there is enough diversity in the ISRFs used to construct the dictionary so the atoms thereof are capable of representing the ISRFs encountered in the estimation problem. Indeed, if all the representative ISRFs are taken from the same part of the spectra (end or beginning), performance will degrade. A similar observation is given in Section 5.4.3, taking into account the ISRF dependency on the scene: if the atoms in the dictionary can not properly represent the asymmetric shapes of some ISRFs, the resulting ISRF estimates will be inaccurate.

Comment 4

From fig 1 it is clear that the plotted ISRF cannot be accurately modeled by bell-shaped Gaussian distribution nor the generalized Gaussians one. Nevertheless, it seems that a mixture of Gaussians can be a good fit. Can you elaborate more on this option (the number of mixtures can be estimated using BIC or AIC)?

Response:

We thank the reviewer for this interesting observation. Indeed, the ISRF could be modeled using a mixture of Gaussians. This approach was not considered in the present article, and the authors are unaware of any previous work on the use of a mixture of Gaussians in this context[a].

One possible drawback of the use of a mixture of Gaussians could be the potentially larger number of parameters to be estimated, contrary to the proposed sparse representations of ISRFs in a dictionary that use only a small number of atoms (typically around four). Nevertheless, we believe that a study of the use of mixtures of Gaussians in this context could be an interesting future research direction. This perspective will be included in the conclusion of the paper.

[a] If the referee has any reference on this approach applied to the ISRF estimation, we would be grateful for the opportunity to conduct a comparative analysis with our proposed approach.

Comment 5

The authors said that the analysis of concentrations from two spectrometers could provide a better understanding of the carbon cycle. Nevertheless, it seems that the analysis in the paper has been done separately (ie., per instrument). Is it possible to use data fusion in this case in order to have a more accurate results?

Response:

We thank the reviewer for this remark. The associated sentence was misleading, and we corrected it into: “Note that OCO-2 and MicroCarb aim to provide a better understanding of the carbon cycle". The two spectrometers are used for the same purpose. However their design is different and the associated ISRFs to be estimated are different. Thus, the analyses are conducted separately for these two spectrometers.

Comment 6

The authors should add a supplementary material, or annex in order to elaborate more on the algorithm, specifically, in page 6, it is not clear how the matrix S is constructed, how we compute the “appropriate" error matrix ... A pseudo code would be much appreciated from the readers

Response:

Following the reviewer comment, we have added a pseudo-code for the K-SVD algorithm in Appendix A. The appendix also describes the computation of the associated error matrix, based on the algorithm defined in [1], and is given below.

Algorithm 1 Construction of the dictionary using the K-SVD algorithm.

Input: Matrix of selected ISRFs $\boldsymbol{I}$, number of selected ISRFs L, size of the dictionary N_{obs}, Dictionary $\boldsymbol{\Phi}$ obtained using SVD in Algorithm (2), sparsity parameter K

Output: New dictionary of ISRFs $\boldsymbol{\Phi}$.

while not convergence **do**
  Sparse coding step: $\boldsymbol{x}_l = \text{OMP}(\boldsymbol{I}_l, \boldsymbol{\Phi}, K)\ \forall\ l = 1, ..., L$
  Dictionary update:
  for $j = 1, ..., N_{\text{obs}}$ **do**
    Define the group of examples that uses the j-th colum of the dictionary j, $w_j = \{l | 1 \leq l \leq N, \boldsymbol{x}_T^j(l) \neq 0\}$
    Compute the overall representation error matrix, $\boldsymbol{E}_j = \boldsymbol{I} - \sum_{i \neq j} \boldsymbol{\phi}_i \boldsymbol{x}_T^i$
    Build $\boldsymbol{E}_j^R$ from $\boldsymbol{E}_j$ using the columns corresponding to w_j
    SVD decomposition $[\boldsymbol{U}, \boldsymbol{\Gamma}, \boldsymbol{V}^*] = \text{SVD}(\boldsymbol{E}_j^R)$
    Update the dictionary column $\boldsymbol{\phi}_j$ as the first column of $\boldsymbol{U}$ and the vector $\boldsymbol{x}_R^j$ as the first column of $\boldsymbol{V}\boldsymbol{\Gamma}(1, 1)$.
  end for
end while
return $\boldsymbol{\Phi}$

Comment 7

In page 7, the authors want to assess the robustness of the proposed ISRF. What do you mean exactly by robustness (is it w.r.t. the noise level, a possible mismatch, a possible presence of outliers . . .), can you be more specific?

Response:

The use of the word “robustness" in page 7 was indeed misleading. There, we are not assessing the “robustness" of the proposed method w.r.t. noise levels, mismatches, etc., but we are demonstrating the applicability of the method to different spectrometers. The word “robustness" was thus modified to “applicability".

Comment 8

The caption of some figures is too short and needs more explanation, eg, Fig 1, Fig. 2, Fig 9
Typo in eq 5 (=)

Response:

We thank the referee for this comment. The typo was corrected, and the captions of the figures have been modified in order to include more explanations as:

- "Examples of MicroCarb ISRFs." becomes "Illustration of all the ISRFs simulated for the band B1 of MicroCarb instrument using uniform scenes."
- "Representation of the four first atoms of the dictionary constructed using one SVD (top) or using the K-SVD algorithm (bottom) for the MicroCarb spectrometer (band B1)." becomes "Representation of the four first atoms of the dictionary of ISRFs $\boldsymbol{\Phi}$ constructed using an SVD on the matrix of representative ISRFs (top) or using the K-SVD algorithm using the same matrix of representative ISRFs (bottom) for the MicroCarb spectrometer (band B1)."
- "Examples of ISRFs IN, scene and NU (MicroCarb band 1)." becomes "Examples of ISRFs from uniform scenes (ISRF IN - left) and from different non-uniform scenes displayed in Fig. 10 and FOVs (ISRF scene - right) (MicroCarb band B1)."

References

[1] M. Aharon, M. Elad, and A. Bruckstein, “K-SVD: An algorithm for designing overcomplete dictionaries for sparse representation,” *IEEE Trans. Signal Process.*, vol. 54, no. 11, pp. 4311–4322, 2006.