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Comment on "Synergetic use of IASI and TROPOMI space borne sensors for generating a tropospheric methane profile product"

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Abstract. A great interest is growing about methods that combine measurements from two or more instruments that observe the same species either in different spectral regions or with different geometries. Recently, a method based on the Kalman filter has been proposed to combine IASI and TROPOMI methane products. We show that this method is equivalent to the
 Complete Data Fusion method. Therefore, the choice between these two methods is driven only by the advantages of the different implementations. From the comparison of the two methods a generalization of the Complete Data Fusion formula,

which is valid also in the case that the noise error covariance matrices of the fused products are singular, is derived.

1 Introduction

Schneider et al. (2021) presented a method for the combined use of the individual retrieval products of IASI and TROPOMI.

15 The method is based on the Kalman filter (Rodgers, 2000) and, as stated by the authors, is largely equivalent to using the spectra of the different sensors together in a single retrieval procedure (simultaneous retrieval). This method was already presented in Warner et al. (2014) and used to combine CO products of AIRS and TES as well of AIRS and MLS. The purpose of this comment is to study the relationship between the method presented in Schneider et al. (2021) and the

Complete Data Fusion (CDF) method presented in Ceccherini et al. (2015). CDF too uses the output of the individual

20 retrievals and, in the case that the linear approximation holds in the range of the retrieved products, provides products equivalent to those of the simultaneous retrieval.

Given the similarities between the two methods, it is reasonable to expect a close relationship between them and in effect in Section 2 we prove their equivalence. Conclusions are drawn in Section 3.

2 Equivalence between data fusion with Kalman filter and CDF

25 In this Section, we prove the equivalence of the method proposed in Schneider et al. (2021) and the CDF method proposed in Ceccherini et al. (2015).

We start from Eq. (A9) of Schneider et al. (2021):

$$\hat{\mathbf{x}}^{a} = \hat{\mathbf{x}}^{b} + \mathbf{M} \begin{bmatrix} \hat{\mathbf{x}}^{o} - \mathbf{H} \hat{\mathbf{x}}^{b} \end{bmatrix}, \tag{1}$$

where $\hat{\mathbf{x}}^{a}$ is the analysis state, $\hat{\mathbf{x}}^{b}$ is the background state, $\hat{\mathbf{x}}^{o}$ is the new observation, **M** is the Kalman gain matrix and **H** is the measurement forward operator.

30 We substitute in Eq. (1) the different quantities as given in Appendix A2.3 of Schneider et al. (2021). From Eq. (A14), (A15) and (A13) we have, respectively:

$$\hat{\mathbf{x}}^b = \hat{\mathbf{x}}_1 - \mathbf{x}_a \,, \tag{2}$$

$$\hat{\mathbf{x}}^o = \hat{\mathbf{x}}_2 - \mathbf{x}_a \tag{3}$$

$$\mathbf{H} = \mathbf{A}_2, \tag{4}$$





where $\hat{\mathbf{x}}_1$ and $\hat{\mathbf{x}}_2$ are the two individual retrieval products, \mathbf{x}_a is the a priori state vector and \mathbf{A}_2 is the averaging kernel matrix of $\hat{\mathbf{x}}_2$. The Kalman gain matrix \mathbf{M} is given by Eq. (A17) that using Eq. (A4) becomes:

$$\mathbf{M} = \left(\mathbf{F}_{1} + \mathbf{F}_{2} + \mathbf{S}_{a}^{-1}\right)^{-1} \left(\mathbf{F}_{2} + \mathbf{S}_{a}^{-1}\right),\tag{5}$$

where S_a is the a priori covariance matrix (CM) and we have introduced the Fisher information matrices (Fisher, 1935; 35 Ceccherini et al., 2012):

$$\mathbf{F}_{i} = \mathbf{K}_{i}^{T} \mathbf{S}_{\mathbf{y}_{i},n}^{-1} \mathbf{K}_{i} = \mathbf{A}_{i}^{T} \mathbf{S}_{\hat{\mathbf{x}}_{i},n}^{-1} \mathbf{A}_{i} = \mathbf{S}_{\hat{\mathbf{x}}_{i}}^{-1} \mathbf{A}_{i} \qquad i = 1, 2,$$
(6)

 \mathbf{K}_{i} being the Jacobian matrices of the forward models, $\mathbf{S}_{\mathbf{y}_{i},n}$ the CMs for noise on the measured radiances \mathbf{y}_{i} , $\mathbf{S}_{\hat{\mathbf{x}}_{i},n}$ the noise error CMs of the retrieved states and $\mathbf{S}_{\hat{\mathbf{x}}_{i}}$ the a posteriori CMs. In the case that the matrices $\mathbf{S}_{\hat{\mathbf{x}}_{i},n}$ are singular, Eq. (6) is still valid replacing the matrices $\mathbf{S}_{\hat{\mathbf{x}}_{i},n}^{-1}$ with the generalized inverse matrices (Kalman, 1976) $\mathbf{S}_{\hat{\mathbf{x}}_{i},n}^{+}$, as shown in the appendix of Ceccherini et al. (2012).

40 In analogy with Eqs. (2) and (3), we introduce the quantity $\hat{\mathbf{x}}_{f}$ such as the analysis state $\hat{\mathbf{x}}^{a}$ is the difference between $\hat{\mathbf{x}}_{f}$ and \mathbf{x}_{a} :

$$\hat{\mathbf{x}}^a = \hat{\mathbf{x}}_f - \mathbf{x}_a \,. \tag{7}$$

Substituting Eqs. (2-5) and (7) in Eq. (1), we obtain:

$$\hat{\mathbf{x}}_{f} - \mathbf{x}_{a} = \hat{\mathbf{x}}_{1} - \mathbf{x}_{a} + \left(\mathbf{F}_{1} + \mathbf{F}_{2} + \mathbf{S}_{a}^{-1}\right)^{-1} \left(\mathbf{F}_{2} + \mathbf{S}_{a}^{-1}\right) \left[\hat{\mathbf{x}}_{2} - \mathbf{x}_{a} - \mathbf{A}_{2}\left(\hat{\mathbf{x}}_{1} - \mathbf{x}_{a}\right)\right].$$
(8)

Using Eqs. (A2-A3) of Schneider et al. (2021) and Eq. (6), we have:

$$\mathbf{A}_{i} = \left(\mathbf{F}_{i} + \mathbf{S}_{a}^{-1}\right)^{-1} \mathbf{F}_{i} \qquad i = 1, 2,$$
(9)

therefore, Eq. (8) can be written as:

$$\hat{\mathbf{x}}_{f} - \mathbf{x}_{a} = \left[\mathbf{I} - \left(\mathbf{F}_{1} + \mathbf{F}_{2} + \mathbf{S}_{a}^{-1}\right)^{-1} \mathbf{F}_{2}\right] (\hat{\mathbf{x}}_{1} - \mathbf{x}_{a}) + \left(\mathbf{F}_{1} + \mathbf{F}_{2} + \mathbf{S}_{a}^{-1}\right)^{-1} \left(\mathbf{F}_{2} + \mathbf{S}_{a}^{-1}\right) (\hat{\mathbf{x}}_{2} - \mathbf{x}_{a}) = \\ = \left(\mathbf{F}_{1} + \mathbf{F}_{2} + \mathbf{S}_{a}^{-1}\right)^{-1} \left[\left(\mathbf{F}_{1} + \mathbf{S}_{a}^{-1}\right) (\hat{\mathbf{x}}_{1} - \mathbf{x}_{a}) + \left(\mathbf{F}_{2} + \mathbf{S}_{a}^{-1}\right) (\hat{\mathbf{x}}_{2} - \mathbf{x}_{a}) \right]$$
(10)

45 Consistently with Eq. (3) of Ceccherini et al. (2015), we introduce the α_i quantities, such as:

$$\hat{\mathbf{x}}_i - \mathbf{x}_a = \mathbf{a}_i - \mathbf{A}_i \mathbf{x}_a \qquad i = 1, 2 \tag{11}$$

and Eq. (10) becomes:

$$\hat{\mathbf{x}}_{f} - \mathbf{x}_{a} = \left(\mathbf{F}_{1} + \mathbf{F}_{2} + \mathbf{S}_{a}^{-1}\right)^{-1} \left[\left(\mathbf{F}_{1} + \mathbf{S}_{a}^{-1}\right) \left(\boldsymbol{\alpha}_{1} - \mathbf{A}_{1}\mathbf{x}_{a}\right) + \left(\mathbf{F}_{2} + \mathbf{S}_{a}^{-1}\right) \left(\boldsymbol{\alpha}_{2} - \mathbf{A}_{2}\mathbf{x}_{a}\right) \right] = \\ = \left(\mathbf{F}_{1} + \mathbf{F}_{2} + \mathbf{S}_{a}^{-1}\right)^{-1} \left[\left(\mathbf{F}_{1} + \mathbf{S}_{a}^{-1}\right) \boldsymbol{\alpha}_{1} + \left(\mathbf{F}_{2} + \mathbf{S}_{a}^{-1}\right) \boldsymbol{\alpha}_{2} - \mathbf{F}_{1}\mathbf{x}_{a} - \mathbf{F}_{2}\mathbf{x}_{a} \right] = , \qquad (12)$$
$$= \left(\mathbf{F}_{1} + \mathbf{F}_{2} + \mathbf{S}_{a}^{-1}\right)^{-1} \left[\left(\mathbf{F}_{1} + \mathbf{S}_{a}^{-1}\right) \boldsymbol{\alpha}_{1} + \left(\mathbf{F}_{2} + \mathbf{S}_{a}^{-1}\right) \boldsymbol{\alpha}_{2} + \mathbf{S}_{a}^{-1}\mathbf{x}_{a} \right] - \mathbf{x}_{a}$$

where we have used Eq. (9).

Using Eqs (A2) and (A5) of Schneider et al. (2021), we can write the noise error CMs as:

$$\mathbf{S}_{\hat{\mathbf{x}}_{i},\mathbf{n}} = \left(\mathbf{F}_{i} + \mathbf{S}_{a}^{-1}\right)^{-1} \mathbf{F}_{i} \left(\mathbf{F}_{i} + \mathbf{S}_{a}^{-1}\right)^{-1} \qquad i = 1, 2.$$
(13)

In the case that $S_{\hat{x}_{r,n}}$ are not singular matrices, from Eq. (9) it results:

$$\mathbf{A}_{i}^{T}\mathbf{S}_{\hat{\mathbf{x}}_{i},\mathbf{n}}^{-1} = \left(\mathbf{F}_{i} + \mathbf{S}_{a}^{-1}\right) \qquad i = 1,2$$

$$(14)$$

50 and, using Eqs. (6) and (14), from Eq. (12) we obtain:





$$\hat{\mathbf{x}}_{f} = \left(\mathbf{A}_{1}^{T}\mathbf{S}_{\hat{\mathbf{x}}_{1},n}^{-1}\mathbf{A}_{1} + \mathbf{A}_{2}^{T}\mathbf{S}_{\hat{\mathbf{x}}_{2},n}^{-1}\mathbf{A}_{2} + \mathbf{S}_{a}^{-1}\right)^{-1} \left[\mathbf{A}_{1}^{T}\mathbf{S}_{\hat{\mathbf{x}}_{1},n}^{-1}\boldsymbol{\alpha}_{1} + \mathbf{A}_{2}^{T}\mathbf{S}_{\hat{\mathbf{x}}_{2},n}^{-1}\boldsymbol{\alpha}_{2} + \mathbf{S}_{a}^{-1}\mathbf{x}_{a}\right],$$
(15)

which is the equation of the CDF reported in Eq. (5) of Ceccherini et al. (2015), proving the equivalence of the Kalman filter method reported in Schneider et al. (2021) with the CDF method reported in Ceccherini et al. (2015). In the case that $\mathbf{S}_{\hat{\mathbf{x}}_{j,n}}$ are singular matrices, we cannot write Eq. (15). However, using Eq. (A4) of Schneider et al. (2021) and

Eq. (6), from Eq. (12) we obtain:

$$\hat{\mathbf{x}}_{f} = \left(\mathbf{S}_{\hat{\mathbf{x}}_{1}}^{-1}\mathbf{A}_{1} + \mathbf{S}_{\hat{\mathbf{x}}_{2}}^{-1}\mathbf{A}_{2} + \mathbf{S}_{a}^{-1}\right)^{-1} \left[\mathbf{S}_{\hat{\mathbf{x}}_{1}}^{-1}\boldsymbol{\alpha}_{1} + \mathbf{S}_{\hat{\mathbf{x}}_{2}}^{-1}\boldsymbol{\alpha}_{2} + \mathbf{S}_{a}^{-1}\mathbf{x}_{a}\right].$$
(16)

55 Eq. (16) is valid also when $\mathbf{S}_{\hat{\mathbf{x}}_{i,n}}$ are singular matrices and fully maintains the equivalence with the method proposed in Schneider et al (2021), furthermore, it is equivalent to Eq. (15) when $\mathbf{S}_{\hat{\mathbf{x}}_{i,n}}$ are not singular matrices. Therefore, Eq. (16) is more general than Eq. (15) proposed for the CDF in Ceccherini et al. (2015).

3 Conclusions

The equivalence between the method for the synergetic use of data acquired by different instruments proposed in Schneider

- 60 et al. (2021) and the CDF method proposed in Ceccherini et al. (2015) has been proved. However, the original CDF formula can only be used in the case that the noise error CMs of the fused products are not singular and the full equivalence of the two methods exists only in the case of the revised CDF formula that has been here derived, and given in Eq. (16). The CDF method was also proved (Ceccherini, 2016) to be equivalent to the measurement space solution data fusion method (Ceccherini et al., 2009) that explicitly considered the case of measurements made in an incomplete space. Case that
- 65 corresponds to having singular matrices. Therefore, the three methods are equivalent among themselves and, for linear and moderately nonlinear problems, they are all equivalent to the simultaneous retrieval. Consequently, we expect that the choice of which among these three methods can be more efficiently used in an operational data fusion depends only on the implementation advantages. Studies that assess the implementation convenience of the three methods for different data fusion problems would be very useful.

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Competing interests. The author declares that he has no conflict of interest.

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