MEASURES 2017 Data Fusion

Algorithm Theoretical Basis Document

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1 Introduction

This Algorithm Theoretical Basis Document (ATBD) describes the theoretical basis of the algorithm used to generate the fused data products for the Making Earth Science Data Records for Use in Research Environments project (MEaSUREs '17: Records of Fused and Assimilated Satellite Carbon Dioxide Observations and Fluxes from Multiple Instruments. The description of outputs for the data files (e.g., format, variable types, etc.) is covered in the Data User Guide. This ATBD is divided into three parts:

- Description of data sources (Section 2)

- Description of fusion approach (Section 3)

- Description of kriging equations (Section 4)

An overview of the goals and objective of this MEaSUREs project can be found at (INSERT URL). The fused outputs could be obtained at (INSERT URL).

2 Data Sources for Fusion

The Orbiting Carbon Observatory-2 (OCO-2) is NASA's first Earth remote sensing instrument dedicated to studying carbon dioxide's global distribution. It was launched on July 2, 2014, and it uses three high-resolution grating spectrometers to acquire observations of the atmosphere in three observation modes: nadir, glint, and target. In nadir mode, the instrument points to the local nadir to collect data

directly below the spacecraft. Nadir mode does not provide adequate signal-to-noise ratio over the dark ocean surface, and thus over ocean OCO-2 uses glint mode. In that mode, OCO-2 points its mirrors at bright glint spots where the solar radiation is specularly reflected from the surface. Finally, in target mode the instruments locks its view onto specific surface locations (usually a ground-based TCCON station or observational tower) while flying overhead. OCO-2 has a repeat cycle of sixteen days and a sampling rate of about one million observations per day, making it a high-density and high-resolution complement to GOSAT. The CO_2 concentrations in an atmospheric column are inferred from the observed spectra through optimal estimation (Crisp et al., 2010). The outputs are available as 20-dimensional CO_2 profiles and column-averaged CO_2 concentrations. The latter is derived from the former using a pressure weighting function, which is a 20-dimensional vector of weights derived from local atmospheric conditions. A pressure weighting function is convolved with the 20-dimensional CO_2 vector in a linear combination to form the column-averaged estimate (O'Dell et al., 2012).

GOSAT is a polar-orbiting satellite dedicated to the observation of carbon dioxide and methane, both major greenhouse gases, from space. It flies at approximately 665 kilometers (km) altitude, and it completes an orbit every 100 minutes. The satellite returns to the same observation location every three days (Morino et al., 2011). NASA's Atmospheric CO_2 Observations from Space (ACOS) team uses the raw-radiance data from GOSAT to estimate the column-average CO_2 mole fraction in ppm, extending from the surface to the satellite over a base area corresponding to the instrument's footprint. In this article, we will be using GOSAT retrievals

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that are processed by the ACOS team to yield Level 2 column-average CO_2 data (see Crisp et al., 2012, for more details), which were available to us through NASA's Goddard Earth Sciences Data and Information Services Center. Hereafter, we refer to these as ACOS data. Since the ACOS product is produced at the Jet Propulsion Laboratory by the same team behind the OCO-2 instruments, much of the retrieval characterization (e.g., priors, choice of pressure levels, forward models, etc.) are the same between the two products.

2.1 Data version and quality filter

For our fusion products, we use ACOS Version 7 data, which are produced by the Jet Propulsion Lab at NASA. These data are available at `https://disc.gsfc.nasa.gov/datacollection/ACOS_L2_Lite_FP_7.3.html`. For the OCO-2 Level 2 data, we use the Version 9 data, which are available at `https://disc.gsfc.nasa.gov/datasets/OCO2_L2_Lite_FP_9r/summary`. The User Data Guide for ACOS V7.3 can be found at `https://docserver.gesdisc.eosdis.nasa.gov/public/project/OCO/ACOS_v7.3_DataUsersGuide-RevF.pdf`, and the Data User Guide for OCO-2 Version 9 can be found at `https://docserver.gesdisc.eosdis.nasa.gov/public/project/OCO/OCO2_DUG.V9.pdf`.

Typically, OCO-2 and ACOS L2 data vary in retrieval quality due to different atmospheric conditions (e.g., contamination of the radiance by clouds or uncertainties in the atmospheric aerosols). Hence, the OCO-2 team recommends that the Level XCO2 data be filtered to eliminate potential 'bad' data. Here, we make use of the 'xco2_quality_flag' quality flag from the Lite products. From the OCO-2 Level 2 Data

Quality Guide:

"xco2_quality_flag [...] is simply a byte array of 0s and 1s. This filter has been derived by comparing retrieved XCO2 for a subset of the data to various truth proxies, and identifying thresholds for different variables that correlate with poor data quality. It applies a number of quality filters based on retrieved or auxiliary variables that correlate with excessive XCO2 scatter or bias."

For the fusion product, we filter both ACOS and OCO-2 L2 product by selecting only values for which xco2_quality_flag == 0. Both data products employ a bias correction process, which is a post-processing algorithm that applies a small offset to each retrieved XCO2 value to correct for instrument biases. For our fusion, we make use of the bias-corrected XCO2 values from both ACOS and OCO-2 products.

2.2   Data fusion output modes

OCO-2 instruments have three primary observation modes: glint, nadir, and target modes. The nadir mode consist of observations where the surface solar zenith angle is less than 85 degrees, and the glint mode consist of observation at latitudes where the solar zenith angle of the glint spot is less than 75 degrees. Finally, target mode consists of very localized observations are conducted over selected OCO-2 validation sites. The three modes differ in their quality and biases. They also differ in their spatial coverage. Nadir mode, for instance, is only collected over land, while glint mode can collect observations over both land and ocean.

It has been shown that the bias correction process for ACOS and OCO-2 still demonstrate residual bias, which depends on surface type, latitude, and scattering by aerosol Wunch et al. (2017). One significant factor in determining the residual bias is whether the surface is land or ocean. Therefore, many flux inversion studies opt for assimilate the XCO2 data separately for land and ocean. Consequently, we stratify our fusion products into 4 different products, as seen in the table below: In the fusion

Table 1: Fusion output modes

Product	Description
Land Only	Uses only Land observations from ACOS and OCO-2 (Land Nadir)
Ocean Only	Uses only Ocean observations from ACOS and OCO-2 (Land Glint and Ocean Glint)
Land and Ocean	Uses all ACOS observations and OCO-2 Glint and Nadir modes
Target	Uses only Target observations from OCO-2

outputs, these different modes can be identified by the variable 'source_data_mode', which is an integer ranging from 1 to 4, where 'Land Only' = 1, 'Ocean Only' = 2, 'Land and Ocean' = 3, and 'Target' = 4.

3   Fusion approach

The data fusion approach based on kriging is well developed in the literature, specifically for Level 3 XCO2 generation (e.g. Nguyen et al., 2012). However, this MEaSUREs project is specifically geared towards producing data that could be incorpo-

rated into flux inversion studies, and hence the approach needs to be modified. The key difference between Level 3 XCO2 generation and flux inversion is the number of variables required for the outputs. Assuming that we have N retrievals, the variables that the flux modelers use include the following: longitude, latitude, pressure levels (which varies at each footprint), pressure weighting functions, XCO2, time in UTC , prior mean, and column averaging kernel. For using the naming convention of the OCO-2 Lite files and the fusion output files, these variables are described in the table below:

Table 2: Variables required for flux inversion

Name	Dimension	Description
longitude	1x1	The longitude at the center of the sounding field-of-view
latitude	1x1	The latitude at the center of the sounding field-of-view
xco2	1x1	The bias-corrected XCO2 (in units of ppm)
time	1x1	The time of the sounding in seconds since 1970-01-01
co2_profile_apriori	20x1	The prior mean profile of CO2 in ppm
xco2_averaging_kernel	20x1	The normalized column averaging kernel for the retrieved XCO2
pressure_levels	20x1	The retrieval pressure level grid for each sounding in hPa
pressure_weight	20x1	The pressure weighting function on levels used in the retrieval

The data fusion approach in Nguyen et al. (2012) provides a framework for fusing scalar quantities such as XCO2 or aerosols, however, the presence of multivariate

profiles (e.g., co2_profile_apriori, xco2_averaging_kernel) requires extra care. In principle, one approach would be to apply the scalar fusion method to all fields in Table 1 individually for each pressure level. However, we note that certain variables such as time and co2_profile_apriori are deterministic functions, and as such do not conform to assumptions of a statistical spatial dependence model (i.e., a semi-variogram model such as that described in 4.1).

Our approach in this section is a generalization of a common technique called the '10 second average' that is used in many flux inversion (e.g., Basu et al., 2018). There, the approach is to simply take the average of all the fields in Table 1 in 10 seconds intervals. Here, we generalize the approach by using a spatial statistics approach (specifically local krigin) to provided a weighted vector of coefficients, which we then apply to the fields in Table 1 to get the fused outputs.

The Bayesian Optimal Estimation framework, as formalized in Rodgers (2000), is popular for inverse problems in remote sensing and it is the method of choice for OCO-2 retrievals (Crisp et al., 2010). In this section, we will review the background of Optimal Estimation (OE), and then discuss how our fusion approach is consistent with the OE formulation. For ease of exposition, we will consider the inverse problem where the forward model is linear.

3.1 Background

Consider the case where an N-dimensional radiance vector $\mathbf{y}$ is related to the r-dimensional (hidden) true state $\mathbf{x}$ by the following data model:

$$\mathbf{y} = \mathbf{F}(\mathbf{x}) + \boldsymbol{\epsilon}, \tag{1}$$

where $\mathbf{F}(\,\cdot\,)$ is the forward model, $\mathbf{x}$ is the r-dimensional true state with true mean $\mathbf{x}_T$ and true covariance matrix $\mathbf{S}_T$, and $\boldsymbol{\epsilon}$ is the N-dimensional measurement-error vector with mean $\mathbf{0}$ and covariance matrix $\mathbf{S}_\epsilon$. That is, $\mathbf{x} \sim N_r(\mathbf{x}_T, \mathbf{S}_T)$ and $\boldsymbol{\epsilon} \sim N_N(\mathbf{0}, \mathbf{S}_\epsilon)$. The true mean $\mathbf{x}_T$ is defined at a set of r pressure levels $\mathbf{p}$ that will change from observation to observation. Since we assume that the forward model is linear, the general data model in (1) becomes,

$$\mathbf{y} = \mathbf{c} + \mathbf{K}\mathbf{x} + \boldsymbol{\epsilon},$$

where $\mathbf{K}$ is the Jacobian of the forward model, and $\mathbf{c}$ is an N-dimensional constant vector.

Without lack of generality, we can assume that $\mathbf{c} = \mathbf{0}$ (since $\mathbf{c}$ is known and hence in principle could be subtracted from $\mathbf{y}$). Our data model then becomes,

$$\mathbf{y} = \mathbf{K}\mathbf{x} + \boldsymbol{\epsilon}. \tag{2}$$

Rodgers (2000) proposed a loss function that is the negative logarithm of the posterior

distribution of $\mathbf{x}$ given $\mathbf{y}$, dropping constant terms,

$$L(\mathbf{x}) \equiv -2\mathrm{log}P(\mathbf{x}|\mathbf{y}) = (\mathbf{y} - \mathbf{Kx})' \mathbf{S}_\epsilon^{-1} (\mathbf{y} - \mathbf{Kx}) - (\mathbf{x} - \mathbf{x}_T)' \mathbf{S}_T^{-1} (\mathbf{x} - \mathbf{x}_T). \qquad (3)$$

The maximum a posteriori solution (also the posterior mean in our linear forward model case) is then given by,

$$\hat{\mathbf{x}}_T = \mathbf{x}_T + \mathbf{G}_T(\mathbf{y} - \mathbf{Kx}_T), \qquad (4)$$

where $\mathbf{G}_T$ is called the gain matrix and is given by $\mathbf{G}_T = (\mathbf{S}_T^{-1} + \mathbf{K}'\mathbf{S}_\epsilon^{-1}\mathbf{K})^{-1}\mathbf{K}'\mathbf{S}_\epsilon^{-1}$. The uncertainty on $\hat{\mathbf{x}}$ is then given by,

$$\boldsymbol{\Sigma}_T \equiv \mathrm{Var}(\hat{\mathbf{x}} - \mathbf{x}) = (\mathbf{S}_T^{-1} + \mathbf{K}'\mathbf{S}_\epsilon^{-1}\mathbf{K})^{-1}. \qquad (5)$$

The relationship in (4) is sometimes expressed as a relationship between the true state, the retrieved state, and the prior mean state as follows,

$$\hat{\mathbf{x}}_T = \mathbf{x}_T + \mathbf{A}_T(\mathbf{x} - \mathbf{x}_T) + \epsilon_x, \qquad (6)$$

where $\mathbf{A}_T \equiv (\mathbf{S}_T^{-1} + \mathbf{K}'\mathbf{S}_\epsilon^{-1}\mathbf{K})^{-1}\mathbf{K}'\mathbf{S}_\epsilon^{-1}\mathbf{K}$ is a $r \times r$ matrix called the averaging kernel. Typically, the column CO_2 amount is not used in flux inversion, and a linear combination is applied to this state vector to compute what is called the total-column CO_2 (XCO$_2$). That is, $x_{xco2} = \mathbf{h}'\hat{\mathbf{x}}$, where $\mathbf{h}$ is the pressure weighting vector. Note that the averaging kernel can be interpreted as a derivative with respective to the

true state $\mathbf{x}$ as follows,

$$\mathbf{A}_T = \frac{d\hat{\mathbf{x}}}{d\mathbf{x}} \qquad (7)$$

Finally, flux inversion also requires a quantity called column averaging kernel $\mathbf{c}$, which is given as

$$\mathbf{c} = (\mathbf{h}'\mathbf{A}_T) \oslash \mathbf{h}', \qquad (8)$$

where $\oslash$ denotes element-wise division.

3.2 Fusion approach

Let's consider the case of OCO-2 and GOSAT, both of which provide all the information required above. The main difficulty is that the data fusion methodology we develop should also produce *fused* quantities for all the variables above. We have explored methodologies for fusing scalars (e.g., Nguyen et al., 2012), but some of these variables (e.g., pressure levels, prior means, and column averaging kernel) are r-dimensional vectors.

We take a similar approach as the 10-second average (Basu et al., 2018). Since the fused estimate is a linear combination of the two individual datasets, we can perform a scalar data fusion on XCO_2, and then use the linear coefficients therefrom to form linear combination of the remaining quantities. For instance, let the XCO2 data vector and time vector be indicated by $\mathbf{Z}_i$ and $\mathbf{T}_i$ for $i = 1, 2$. Our fused estimate for

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XCO$_2$ is $Z_F = \mathbf{a}'_1 \mathbf{Z}_1 + \mathbf{a}'_2 \mathbf{Z}_2$, and the fused UTC time would then be $T_F = \mathbf{a}'_1 \mathbf{T}_1 + \mathbf{a}'_2 \mathbf{T}_2$, where $\mathbf{a}'_1$ and $\mathbf{a}'_2$ are derived from the XCO_2 fusion.

This formulation is consistent with the derivation of averaging kernels above. That is, if we consider the original space of the state vector $\mathbf{x}$,

$$
\begin{aligned}
\mathbf{x}_F = \ & a_{11}\hat{\mathbf{x}}_{11} + a_{12}\hat{\mathbf{x}}_{12} + \ldots + a_{1N_1}\hat{\mathbf{x}}_{1N_1} + \ldots \\
& + a_{21}\hat{\mathbf{x}}_{21} + a_{22}\hat{\mathbf{x}}_{22} + \ldots + a_{2N_1}\hat{\mathbf{x}}_{2N_2},
\end{aligned}
$$

Then the averaging kernel of this fused estimate is given as

$$
\begin{aligned}
\mathbf{A}_F = \ & \frac{d\hat{\mathbf{x}}_F}{d\mathbf{x}} \\
= \ & a_{11}\frac{d\hat{\mathbf{x}}_{11}}{d\mathbf{x}} + a_{12}\frac{d\hat{\mathbf{x}}_{12}}{d\mathbf{x}} + \ldots + a_{1N_1}\frac{d\hat{\mathbf{x}}_{1N_1}}{d\mathbf{x}} + \ldots \\
& + a_{21}\frac{d\hat{\mathbf{x}}_{21}}{d\mathbf{x}} + a_{22}\frac{d\hat{\mathbf{x}}_{22}}{d\mathbf{x}} + \ldots + a_{2N_2}\frac{d\hat{\mathbf{x}}_{2N_2}}{d\mathbf{x}}, \\
= \ & a_{11}\mathbf{A}_{11} + a_{12}\mathbf{A}_{12} + \ldots + a_{1N_1}\mathbf{A}_{1N_1} + \ldots \\
& + a_{21}\mathbf{A}_{T21} + a_{22}\mathbf{A}_{T22} + \ldots + a_{2N_1}\mathbf{A}_{2N_2}.
\end{aligned}
\tag{9}
$$

The theoretical basis for fusing XCO2 based on their geospatial dependence is well-explored in the literature (e.g., Hammerling et al., 2012; Nguyen et al., 2012). In the next section we will describe the motivation and implementation details for the fusion of XCO2 from OCO-2 and ACOS.

4 Kriging equations

Here, we will take the approach of Hammerling et al. (2012) and fuse the XCO2 field
('/xco2' from the OCO-2 Lite product and the ACOS product) using a form of local
kriging based on the exponential semivariogram. For ease of reference, we provide a
review of kriging below.

Assume that we have observed CO2 data in the following form:

$$\mathbf{Z} = (Z(\mathbf{s}_1), Z(\mathbf{s}_2), \ldots, Z(\mathbf{s}_N))',$$

$$Z(\mathbf{s}_i) = Y(\mathbf{s}_i) + \epsilon(\mathbf{s}_i)$$

Under this formulation, the (linear unbiased) optimal interpolation can be written
as

$$\hat{Y}(\mathbf{s}_0) = \mathbf{a}_0'\mathbf{Z}$$

where $\mathbf{a}_0$ is a N-dimensional vector of kriging coefficients at location $\mathbf{s}$.

We wish to find the vector $\mathbf{a}$ that minimizes,

$$
\begin{aligned}
E(Y(\mathbf{s}) - \hat{Y}(\mathbf{s}))^2 &= \text{Var}(Y(\mathbf{s}) - \mathbf{a}_0'\,\mathbf{Z}), \\
&= \text{Var}(Y(\mathbf{s})) - 2\mathbf{a}_0'\,\text{Cov}(\mathbf{Z}, Y(\mathbf{s})) + \mathbf{a}_0'\,\text{Var}(\mathbf{Z})\,\mathbf{a}_0, \quad (10)
\end{aligned}
$$

with respect to $\mathbf{a}_0$, subject to the unbiasedness constraint,

$$1 = \mathbf{a}_0' \mathbf{1},$$

Note that this vector of kriging coefficient $\mathbf{a}_0$ is precisely the one required for forming linear combinations of the fields in Table 1 (also see Section 3.2). We can solve the minimization problem above for the optimal $\mathbf{a}_0$ using the method of Lagrange multiplier.

$$
\begin{pmatrix}
C_{11} & C_{12} & \dots & C_{1N} & 1 \\
C_{21} & C_{22} & \dots & C_{1N} & 1 \\
\vdots & \vdots & \ddots & \vdots & 1 \\
C_{N1} & C_{N2} & \dots & C_{NN} & 1 \\
1 & 1 & \dots & 1 & 0
\end{pmatrix}
\begin{pmatrix}
a_1 \\
a_2 \\
\vdots \\
a_N \\
\lambda
\end{pmatrix}
=
\begin{pmatrix}
C_{10} \\
C_{20} \\
\vdots \\
C_{N0} \\
1
\end{pmatrix}
\tag{11}
$$

where $C_{ij} = \mathrm{Cov}(\mathbf{s}_i, \mathbf{s}_j)$, $\mathbf{a}_0 = (a_1, \dots, a_N)$, and λ is the Langrange multiplier. In our implementation of the data fusion, we prefer to use an alternative measure of spatial dependence called semi-variogram, which is defined between any two location $\mathbf{s}_i$ and $\mathbf{s}_j$ as

$$
\begin{aligned}
\gamma(\mathbf{s}_1, \mathbf{s}_2) &= \frac{1}{2} E(Z(\mathbf{s}_i) - Z(\mathbf{s}_j))^2 \\
&= \frac{1}{2} \mathrm{Var}(Z(\mathbf{s}_i) - Z(\mathbf{s}_j)).
\end{aligned}
$$

It is easy to see that the semi-variogram is related to the covariance by the following:

$$\begin{aligned}
\gamma(\mathbf{s}_1, \mathbf{s}_2) &= \frac{1}{2} \operatorname{Var}(Z(\mathbf{s}_i) - Z(\mathbf{s}_j)) \\
&= \frac{1}{2}(C_{ii} + C_{jj}) - C_{ij}.
\end{aligned} \tag{12}$$

Substituting (12) into (13), we get the following expression in terms of the semi-variograms:

$$
\begin{pmatrix}
\gamma(\mathbf{s}_1, \mathbf{s}_1) & \gamma(\mathbf{s}_1, \mathbf{s}_2) & \cdots & \gamma(\mathbf{s}_1, \mathbf{s}_N) & 1 \\
\gamma(\mathbf{s}_2, \mathbf{s}_1) & \gamma(\mathbf{s}_2, \mathbf{s}_2) & \cdots & \gamma(\mathbf{s}_2, \mathbf{s}_N) & 1 \\
\vdots & \vdots & \ddots & \vdots & 1 \\
\gamma(\mathbf{s}_N, \mathbf{s}_1) & \gamma(\mathbf{s}_N, \mathbf{s}_2) & \cdots & \gamma(\mathbf{s}_N, \mathbf{s}_N) & 1 \\
1 & 1 & \cdots & 1 & 0
\end{pmatrix}
\begin{pmatrix}
a_1 \\ a_2 \\ \vdots \\ a_N \\ \lambda
\end{pmatrix}
=
\begin{pmatrix}
\gamma(\mathbf{s}_1, \mathbf{s}_0) \\
\gamma(\mathbf{s}_2, \mathbf{s}_0) \\
\vdots \\
\gamma(\mathbf{s}_N, \mathbf{s}_0) \\
1
\end{pmatrix}
\tag{13}
$$

The solution to the minimization problem in (10) can easily be found by solving (13) using matrix inversion. This provides the vector of kriging coefficient $\mathbf{a}_0$ required by Section 3.2.

4.1   Implementation

As described in the previous section, we use local kriging to obtain kriging coefficients for the XCO2 field, which we then apply to all remaining fields (e.g., longitude, latitude, pressure levels (which varies at each footprint), pressure weighting functions, XCO2, time in UTC , prior mean, and column averaging kernel) to obtain the fused outputs. The local neighborhood that we consider is a circular region of radius of

300km. That is, for every fusion location $\mathbf{s}_0$, we search for all available ACOS and OCO-2 data within 300km in the same day and use that as our fusion data. The semi-variogram model that we use is the exponential variogram, which has the form

$$\gamma(\mathbf{s}_i, \mathbf{s}_j) = (s - n)\left(1 - e^{-|\mathbf{s}_i - \mathbf{s}_j|/(3r)}\right) + n1_{(0,\infty)}(h) \tag{14}$$

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