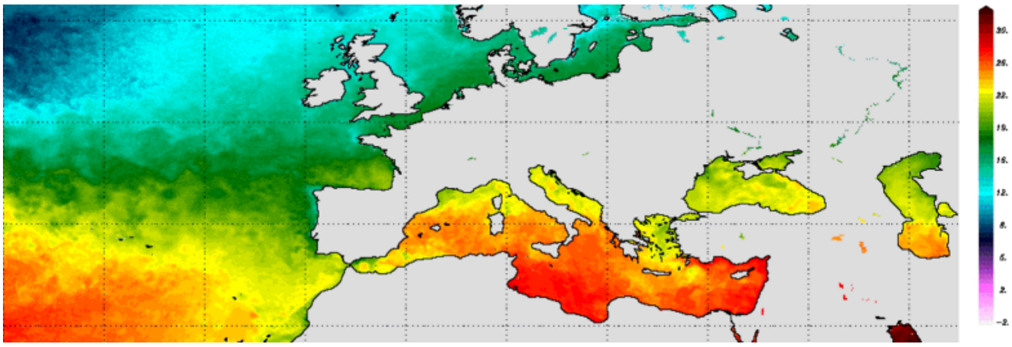
ESA CCI+ Phase 1 Sea Surface Temperature (SST)



Uncertainty Characterisation (E3UB) D2.2 v1

31 March 2020

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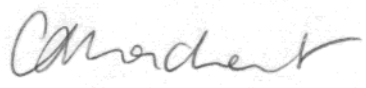

Prof Chris Merchant (UoR)

Address : University of Reading,
Whiteknights,
Reading,
Berkshire,
RG6 6AH,
United Kingdom

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List of Acronyms

AVHRR	Advanced Very High Resolution Radiometer
CCI	Climate Change Initiative
CDR	Climate Data Record
E3UB	End-to-end Error and Uncertainty Budget
ESA	European Space Agency
FIDUCEO	Fidelity and Uncertainty In Climate Data Records from Earth Observation
NWP	Numerical Weather Prediction
OE	Optimal Estimation
RTTOV	Radiative Transfer for TOVS
SST	Sea Surface Temperature
TBC	To be confirmed

1. SCOPE

This is a report in preparation for a comprehensive report on Uncertainty Budget (formally, End-to-End Error Evaluation and Uncertainty Budget, E3UB) that will be completed to describe the Sea Surface Temperature Climate Change Initiative Version 3 Climate Data Record (SST CCI v3 CDR). The full E3UB will be document E3UB D2.2 v3.

The form of content of this interim E3UB report is:

- mathematical development of an improved three-component uncertainty estimation model for optimal estimation retrievals

This development arose as part of preparations towards optimal estimation passive microwave SST retrievals for potential inclusion in the CDR (in CDR v3 or v4, TBC). However, it is applicable also to infrared SSTs, and the method will be implemented across the full processing suite.

A further interim E3UB report (D2.2 v2) will be prepared describing any further developments for SST uncertainty, due at month 18 of the project. The validation of the developments will be presented in D2.2 v3, as obtained in the v3 CDR.

2. UNCERTAINTY MODEL FOR OPTIMAL ESTIMATION

2.1 Introduction

Optimal estimation SST is used for AVHRR 2- and 3-channel retrievals in SST CCI in order to achieve known and satisfactory levels of SST sensitivity, by explicitly using prior NWP to address deficits in the window-channel information about the atmospheric influence on brightness temperatures. The OE solution is obtained in one step, because the retrieval context is adequately linear.

SST CCI (in phase 1) recognised that climate data record (CDR) uncertainties are complex in that contributing errors have a mix of spatio-temporal correlation length scales, and pioneered the principle of modelling uncertainty in three components:

(1) independent (also known as "random"), which is the component for which there is no correlation of errors between different SSTs; a typical source is the error from instrumental noise

(2) locally correlated, which is the component for which errors are strongly coupled for SSTs that are close in space and time, but become independent at large separations; a typical source is the error from ambiguity in retrieval under the specific atmospheric conditions observed

(3) large-scale correlated (including "systematic" or "common" errors), for which errors are coupled at large separations, including across the whole mission; a typical source is calibration error

Optimal estimation is a retrieval framework that provides an uncertainty estimate per retrieval. However, in previous SST CCI datasets, we have not been able simply to use these OE uncertainties, because their correctness relies on the OE being performed with realistic error covariance matrices, which, hitherto, have been poorly estimated. Somewhat ad hoc work-arounds have therefore been used.

However, as explained in Merchant et al. (2020a) and Merchant et al. (2020b), we now have a theoretical basis on which to estimate proper error covariance matrices for OE. As well as putting Bayesian cloud detection and SST retrieval on a firmer footing, this is expected to enable us to use the OE uncertainty framework in the CDR v3. (These developments should also be widely applicable across remote sensing where OE is used.)

Some further work is necessary, however. The classic OE formulation doesn't consider error correlation length scales or how to partition uncertainty into the three components. The solution to those needs is presented in this report.

2.2 Assumptions

Problem: the uncertainty components for OE retrievals in the SST CCI v2.1 CDR are not being optimally distributed between the correlation components (uncorrelated, locally correlated, large-scale correlated), since an interim coding solution was implemented previously to ensure uncertainties were realistic. Now that more realistic error covariance matrices will be available for the OE retrieval, the proper solution for correct distribution of uncertainty components is derived here.

The logic follows Rodgers (2000, chapter 3) but applies it to the specific case of SST retrieval.

Assume that the observations can be described as a true model of the physics and instrument (perfectly calibrated), $\boldsymbol{f}$, given the true state, $\boldsymbol{x}$, plus measurement error, ϵ_m. The measurement error consists of noise (uncorrelated between pixels) and other errors: $\epsilon_m = \epsilon_\mathrm{n} + \epsilon_\mathrm{o}$. We have

$$\boldsymbol{y} = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{b}') + \epsilon_m \qquad \text{Eq. 1}$$

where $\boldsymbol{b}'$ is the complete set of true model parameters not included in the state.

Assume the retrieval method used is bias-corrected optimal estimation (OE) using a reduced state vector, but running the forward model with a full state vector. The forward model is an approximation, and therefore equals the observation to within some error, ϵ_F. (Rodgers puts this error on the other side of and calls it $\Delta\boldsymbol{f}$.):

$$\boldsymbol{F}(\boldsymbol{x}) + \boldsymbol{\beta} = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{b}') + \epsilon_F \qquad \text{Eq. 2}$$

where $\boldsymbol{F}(\boldsymbol{x})$ is RTTOV (we do not represent or question any internal parameters of RTTOV) and $\boldsymbol{\beta}$ are ideal bias corrections of the forward model.

2.3 Derivation of OE total uncertainty

The retrieval is

$$\hat{\boldsymbol{z}} = \boldsymbol{z}_a + (\boldsymbol{K}^\mathrm{T}\boldsymbol{S}_\epsilon^{-1}\boldsymbol{K} + \boldsymbol{S}_a^{-1})^{-1}\boldsymbol{K}^\mathrm{T}\boldsymbol{S}_\epsilon^{-1}\left(\boldsymbol{y} - \left(\boldsymbol{F}(\boldsymbol{x}_a) + \hat{\boldsymbol{\beta}}\right)\right) \qquad \text{Eq. 3}$$

where: any correction for prior bias has been absorbed into the prior and its error covariance matrix; we are using standard OE symbols with $\boldsymbol{z}$ is a reduced state vector. Note that we don't have the ideal bias correction parameters, we have estimates of these, $\widehat{\boldsymbol{\beta}}$ from a bias-aware OE procedure (Merchant et al., 2020a). For convenience, define the gain, $\boldsymbol{G}$:

Eq. 4

$$\hat{\boldsymbol{z}} = \boldsymbol{z}_a + \boldsymbol{G}\left(\boldsymbol{y} - \left(\boldsymbol{F}(\boldsymbol{x}_a) + \widehat{\boldsymbol{\beta}}\right)\right)$$

Using the relationships above, we can substitute for the observations:

Eq. 5

$$\hat{\boldsymbol{z}} = \boldsymbol{z}_a + \boldsymbol{G}\left(\boldsymbol{F}(\boldsymbol{x}) + \boldsymbol{\beta} - \epsilon_F + \epsilon_m - \boldsymbol{F}(\boldsymbol{x}_a) - \widehat{\boldsymbol{\beta}}\right)$$

Linearising the RTTOV simulation of the (unknown) true state, $\boldsymbol{z}$, around the prior, $\boldsymbol{x}_a$, obtains

Eq. 6

$$\hat{\boldsymbol{z}} = \boldsymbol{z}_a + \boldsymbol{G}\left(\boldsymbol{F}(\boldsymbol{x}_a) + \boldsymbol{K}(\boldsymbol{z} - \boldsymbol{z}_a) + \boldsymbol{\beta} - \epsilon_F + \epsilon_m - \boldsymbol{F}(\boldsymbol{x}_a) - \widehat{\boldsymbol{\beta}}\right)$$

The unknown error in the retrieved value is therefore

Eq. 7

$$\hat{\boldsymbol{z}} - \boldsymbol{z} = -(\boldsymbol{z} - \boldsymbol{z}_a) + \boldsymbol{GK}(\boldsymbol{z} - \boldsymbol{z}_a) + \boldsymbol{G}\left(\boldsymbol{\beta} - \widehat{\boldsymbol{\beta}}\right) + \boldsymbol{G}(\epsilon_m - \epsilon_F)$$

$$= (\boldsymbol{GK} - \boldsymbol{I})(\boldsymbol{z} - \boldsymbol{z}_a) + \boldsymbol{G}\left(\boldsymbol{\beta} - \widehat{\boldsymbol{\beta}}\right) + \boldsymbol{G}(\epsilon_m - \epsilon_F)$$

There error covariance of the solution is therefore

Eq. 8

$$\boldsymbol{S} = (\boldsymbol{GK} - \boldsymbol{I})\boldsymbol{S}_a(\boldsymbol{GK} - \boldsymbol{I})^{\mathrm{T}} + \boldsymbol{G}\boldsymbol{S}_{\widehat{\boldsymbol{\beta}}}\boldsymbol{G}^{\mathrm{T}} + \boldsymbol{G}\boldsymbol{S}_{\boldsymbol{\epsilon_n}}\boldsymbol{G}^{\mathrm{T}} + \boldsymbol{G}\boldsymbol{S}_{\boldsymbol{\epsilon_o}}\boldsymbol{G}^{\mathrm{T}} + \boldsymbol{G}\boldsymbol{S}_{\boldsymbol{\epsilon_F}}\boldsymbol{G}^{\mathrm{T}}$$

Compared to the standard expression without bias correction parameters, this is identical except that the beta term is new, given that $\boldsymbol{S}_{\boldsymbol{\varepsilon}}$ represents our estimate of $\boldsymbol{S}_{\boldsymbol{\epsilon_n}} + \boldsymbol{S}_{\boldsymbol{\epsilon_o}} + \boldsymbol{S}_{\boldsymbol{\epsilon_F}}$. We assume we have means to estimate $\boldsymbol{S}_{\boldsymbol{\epsilon_n}}$ such as from the noise level when calibrating the instrument against on-board references**;** FIDUCEO-style analyses (Mittaz et al., 2019) can support an estimate of $\boldsymbol{S}_{\boldsymbol{\epsilon_o}}$; $\boldsymbol{S}_{\widehat{\boldsymbol{\beta}}}$ is estimated in the process of bias-aware OE ; the observation-simulation error covariance estimated from optimising OE is $\boldsymbol{S}_{\widehat{\boldsymbol{\beta}}} + \boldsymbol{S}_{\boldsymbol{\epsilon_n}} + \boldsymbol{S}_{\boldsymbol{\epsilon_o}} + \boldsymbol{S}_{\boldsymbol{\epsilon_F}}$ combined.

Note that $\boldsymbol{S}_{\widehat{\boldsymbol{\beta}}}$ is estimated in the process for optimising OE and will be available to the processor as an auxiliary data file (ADF).

2.4 Partitioning of uncertainty

To partition the uncertainty components by correlation characteristics means we need to put each term into "uncorrelated", "locally correlated" or "large-scale correlated" categories.

Term	Comments	Allocation
$\boldsymbol{G}\boldsymbol{S}_{\epsilon_n}\boldsymbol{G}^{\mathrm{T}}$	Instrument noise is assumed uncorrelated.	Uncorrelated
$(\boldsymbol{G}\boldsymbol{K}-\boldsymbol{I})\boldsymbol{S}_a(\boldsymbol{G}\boldsymbol{K}-\boldsymbol{I})^{\mathrm{T}}$	This varies with the spatio-temporal scales of the difference between the prior and true state.	Locally correlated
$\boldsymbol{G}\boldsymbol{S}_{\epsilon_F}\boldsymbol{G}^{\mathrm{T}}$	The forward model error probably varies with the spatio-temporal scales of some (undetermined) properties of the atmosphere which is likely local, although large scale is also conceivable.	Locally correlated
$\boldsymbol{G}\boldsymbol{S}_{\hat{\beta}}\boldsymbol{G}^{\mathrm{T}}$	This is the effect of the inadequacies of the bias correction formulation, which, after fitting bias dependencies, we expect (TBC) to be local rather than large scale.	Locally correlated
$\boldsymbol{G}\boldsymbol{S}_{\epsilon_o}\boldsymbol{G}^{\mathrm{T}}$	This is a combination of locally correlated effects (structured effects in the radiances) plus calibration, which would be a large-scale correlated effect. If we have a FIDUCEO analysis, we can estimate the partitioning. Here, assume large-scale dominates.	Large-scale correlated

The practical application in the case where we have:

1. independent noise estimates (e.g., from calibration cycle), $\boldsymbol{S}_{\epsilon_n}$, which in general is variable through the mission

2. information from FIDUCEO-style analysis, or otherwise a reasoned guess, of the calibration/large-scale error covariance, $\boldsymbol{S}_{\epsilon_c}$
3. an empirical determination of the total observation-simulation error covariance, $\boldsymbol{S}_{\varepsilon}$, under conditions of known noise $\boldsymbol{S'}_{\epsilon_n}$

is as follows.

1. Calculate the non-noise error covariance $\boldsymbol{S}_{\varepsilon}' = \boldsymbol{S}_{\varepsilon} - \boldsymbol{S'}_{\epsilon_n}$ (offline, input to processor along with $\boldsymbol{S}_a$)
2. For the retrieval, use the then-current noise in combination with the non-noise, $\boldsymbol{S}_{\varepsilon}' + \boldsymbol{S}_{\epsilon_n}$ **(**along with $\boldsymbol{S}_a$)
3. Calculate the uncorrelated uncertainty component as root-of-diagonal-term of $\boldsymbol{G}\boldsymbol{S}_{\epsilon_n}\boldsymbol{G}^{\mathrm{T}}$
4. Calculate the locally correlated uncertainty component from
$$(\boldsymbol{GK} - \boldsymbol{I})\boldsymbol{S}_a(\boldsymbol{GK} - \boldsymbol{I})^{\mathrm{T}} + \boldsymbol{G}(\boldsymbol{S}_{\varepsilon}' - \boldsymbol{S}_{\epsilon_c})\boldsymbol{G}^{\mathrm{T}}$$
5. Calculate the large-scale uncertainty component from $\boldsymbol{G}\boldsymbol{S}_{\epsilon_c}\boldsymbol{G}^{\mathrm{T}}$

This is a complete and self-consistent decomposition of uncertainty components. It can be applied whether or not we have bias corrections (and we don't need to know $\boldsymbol{S}_{\hat{\boldsymbol{\beta}}}$ within the processor).

2.5 Variant for maximum-likelihood-like OE

In order to manage the retrieval sensitivity (equal to $\boldsymbol{GK}$), the OE retrieval has in v2.1 and prior SST CCI CDRs been made with a modified prior error covariance matrix, $\boldsymbol{S}_a'$ in which a pessimistic prior SST uncertainty is assumed. This makes the retrieval more sensitive to the satellite observations, and less sensitive to the prior, ensuring the CCI SSTs are maximally independent of in situ observations (which typically inform the prior SST). In this case, $\boldsymbol{S}_a'$ is used in the retrieval, but the uncertainty equations above use the best estimate of the prior error covariance, $\boldsymbol{S}_a$ and are thus unchanged from the above expressions.

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