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Independent uncertainty estimates for coefficient based sea surface temperature retrieval from the Along-Track Scanning Radiometer instruments

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ABSTRACT

We establish a methodology for calculating uncertainties in sea surface temperature estimates from coefficient based satellite retrievals. The uncertainty estimates are derived independently of in-situ data. This enables validation of both the retrieved SSTs and their uncertainty estimate using in-situ data records. The total uncertainty budget is comprised of a number of components, arising from uncorrelated (e.g. noise), locally systematic (e.g. atmospheric), large scale systematic and sampling effects (for gridded products). The importance of distinguishing these components arises in propagating uncertainty across spatio-temporal scales. We apply the method to SST data retrieved from the Advanced Along Track Scanning Radiometer (AATSR) and validate the results for two different SST retrieval algorithms, both at a per pixel level and for gridded data. We find good agreement between our estimated uncertainties and validation data. This approach to calculating uncertainties in SST retrievals has a wider application to data from other instruments and retrieval of other geophysical variables.

1. Introduction

Uncertainty is inherent in all geophysical measurements and must be appropriately characterized for their scientific application. Data providers have a responsibility to communicate the levels of uncertainties associated with their products and inform data users of the correct methodology for using uncertainty information provided. Within the Sea Surface Temperature Climate Change Initiative (SST CCI) project (Hollman et al., 2013; Merchant et al., 2014) we aim to provide an uncertainty budget for every SST value provided in products (skin temperature, SST at 0.2 m depth and spatially averaged SST). We aim to derive uncertainty estimates independently of SST validation datasets, allowing validation of both the SST values and their associated uncertainty.

The terms 'error' and 'uncertainty' are sometimes used interchangeably, but have distinct standard definitions that will be adhered to throughout this paper. Error is the difference between a measured value and the true value of the measurand (JCGM, 2008; Kennedy, 2014). In practice we know neither the true value nor therefore the error for a particular measurement. However the distribution of the errors can often be estimated and this distribution characterizes the uncertainty in the measured value. Formally, uncertainty is a parameter characterizing the dispersion of values that could reasonably be attributed to the measured value (JCGM, 2008). To quantify uncertainty in this paper we quote one standard deviation of the error distribution.

It is common to provide generic uncertainty estimates for remotely sensed SST derived via comparison with in-situ datasets during validation activities. The standards of the Group for High Resolution Sea Surface Temperature (GHRSST) specify the provision in all datasets of single sensor error statistics (SSES). For pragmatic reasons, SSES are defined to comprise the mean difference and standard deviation of remotely sensed SST matched to a 'reference' dataset (GHRSST Science Team, 2010). Drifting buoy SSTs are often used as the 'reference'. Mean and standard deviation validation statistics are often provided as globally invariant dataset specific values (Casey & Cornillon, 1998; May, Parmeter, Olszewski, & McKenzie, 1997; Reynolds, Rayner, Smith, Stokes, & Wang, 2002). An additional field indicating the retrieval quality level can be specified at pixel resolution providing information on the likelihood of cloud contamination, noise amplification at extreme satellite zenith angles or input data quality (Donlon et al., 2007; Kilpatrick, Podestá, & Evans, 2001). An extension of this approach is the MODerate Resolution Infrared Spectrometer (MODIS) algorithm, which provides validation-based uncertainty information stratified by season, latitude, surface temperature, satellite zenith angle, a selected brightness temperature difference, SST quality level and day/night (Castro et al., 2010).

Sources of uncertainty in remotely sensed SST are intrinsic to the retrieval process and the data utilized. Uncertainties vary from pixel to pixel due to local changes in instrument noise, satellite viewing geometry and atmospheric conditions. We present here a method of estimating SST

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retrieval uncertainty that accounts for these factors at the pixel level. There are a number of sources of uncertainty in SST measurement and the need to differentiate the effects of random, and systematic errors has been previously noted (Casey & Cornillon, 1998; Kennedy, 2014; Merchant et al., 2012; Reynolds et al., 2002). Gridding of products introduces sampling uncertainties and a number of studies have considered these when constructing global or regional SST datasets from in-situ observations (Brohan, Kennedy, Harris, Tett, & Jones, 2006; Folland et al., 2001; Jones, Osborn, & Briffa, 1997; Morrissey & Greene, 2009; Rayner et al., 2006; She, Hoyer, & Larsen, 2007).

In this paper, we consider uncorrelated and locally systematic effects contributing to SST uncertainty. The random or uncorrelated effects arise from noise in the satellite brightness temperature, which propagates into the retrieved SST. Locally systematic effects cause errors that are correlated on synoptic scales of atmospheric variability and are related to the retrieval method itself interacting with changes in atmospheric properties (Barton, 1998; Embury & Merchant, 2012; Le Borgne, Roquet, & Merchant, 2011; Merchant et al., 2012; Minnett, 1986; Minnett & Corlett, 2012). We also discuss uncertainties from large scale systematic effects (spatially coherent on larger scales than synoptic features). In a companion paper (Bulgin et al., 2016-in this issue) we derive a method for calculating sampling uncertainty in gridded products due to incomplete sampling of observations in each grid cell, primarily as a result of cloud cover. In this paper, we use results from Bulgin et al. (2016-in this issue), and, for completeness, show how sampling uncertainty combines with other components of uncertainty in gridded products.

The remainder of the paper is structured as follows. Section 2 describes the theory behind the calculation of uncertainties, their propagation and how this is applied to different levels of SST data (orbit data and gridded products). Section 3 describes how an initial uncertainty budget is constructed from errors originating from random, locally correlated and sampling effects. In Section 4 we present a validation of our uncertainty budget and in Section 5 provide a discussion of the results. We conclude the paper in Section 6.

2. Uncertainty calculation and propagation

We construct an uncertainty budget for SST measurements in CCI products comprised of uncertainty components arising from random, locally systematic, large-scale systematic and sampling effects. The full equation for the propagation of uncertainty in a variable y, $(u(y))$, given that y is related to input quantities x_i via $y = f(x_1, \ldots, \ldots, x_n)$, is defined as Eq. (1) in the Guide to the Expression of Uncertainty in Measurement (GUM) (JCGM, 2008).

$$u^2 = \sum_i^n \left(\frac{\partial f}{\partial x_i}\right)^2 u_i^2(x_i) + 2\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\left(\frac{\partial f}{\partial x_i}\right)\left(\frac{\partial f}{\partial x_j}\right) u(x_i, x_j) \tag{1}$$

Uncertainty is expressed with respect to (y) in the GUM, and we reproduce this notation throughout the paper. However, in Earth Observation, we conventionally relate a retrieval estimate x to observations y i.e. $x = f(y)$ which is the reverse convention. The first term in Eq. (1) describes the propagation of uncertainties from uncorrelated errors. These can be added in quadrature with the differential term $(\partial f/\partial x_i)$ defining the sensitivity of the total uncertainty to each uncertainty component. The second term describes the propagation of uncertainty terms arising from correlated errors. This term sums the uncertainty components from correlated errors for each pair of input variables (x_i and x_j) found as the product of the sensitivity for both x_i and x_j and the covariance between them, $u(x_i,x_j)$. The factor of '2' is included, as for each pair, each is equally correlated with the other.

Eq. (1) can also be written in the form of Eq. (2) where the uncertainty is expressed as the sum over all pairs of input variables and the covariance term is expressed as the product of the standard uncertainty in x_i, written u_i, in x_j, written u_j, and of the correlation of errors in x_i and x_j, written r_{ij}.

$$u^2 = \sum_{i=1}^{n}\sum_{j=1}^{n}\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j}u_i u_j r_{ij} \tag{2}$$

Eq. (2) applies fairly generically to any transformation $y = f(x_i, \ldots, x_n)$ for which the sensitivity parameters $(\partial f/\partial x_i)$ are adequately constant over the range $x_i - u_i$ to $x_j + u_j$; it is a first order approximation. Because we will use the results later, we illustrate the use of Eq. (2) for calculating the uncertainty in the mean SST from a number of observations. If $f = \sum_{i=1}^{n} x_i/n$, where each x_i is a contributing SST value, then the sensitivity parameter is $\partial f/\partial x_i = 1/n$ giving:

$$u^2 = \frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}u_i u_j r_{ij}. \tag{3}$$

We can consider three limiting cases. First assume errors are uncorrelated between pixels. We can then put $r_{ij} = \delta_{ij}$, where $\delta_{ij} = 1$ for $i = j$, and $\delta_{ij} = 0$ for $i \neq j$. In this case, the uncertainty in the mean is scaled by the familiar '$\frac{1}{\sqrt{n}}$' reduction in uncertainty, because

$$u^2 = \frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}u_i u_j \delta_{ij} \tag{4}$$

$$= \frac{1}{n^2}\sum_{i}^{n}u_i^2. \tag{5}$$

Second, consider the case $r_{ij} = 1$, which means errors fully correlate between contributing SSTs. Eq. (3) becomes

$$u^2 = \frac{1}{n^2}\sum_{i=1}^{n}\sum_{i=j}^{n}u_i u_j \tag{6}$$

$$= \frac{1}{n^2}\left(\sum_{i=1}^{n}u_i\right)^2 \tag{7}$$

implying $u = \frac{1}{n}\sum_{i=1}^{n}u_i$ i.e. the uncertainty is the average uncertainty of the contributing SSTs.

Third, consider the case $r_{ij} = \delta_{ij} + (1 - \delta_{ij})r$ - all SSTs have the same error correlation with other SSTs. Substituting into Eq. (3) gives

$$u^2 = \frac{1}{n^2}\sum_{i}^{n}\sum_{j}^{n}u_i u_j\left[\delta_{ij} + (1-\delta_{ij})r\right] \tag{8}$$

$$= \frac{1}{n^2}\sum_{i}^{n}\sum_{j}^{n}u_i u_j\left[r + (1-r)\delta_{ij}\right] \tag{9}$$

$$= \frac{r}{n^2}\left(\sum_{i=1}^{n}u_i\right)^2 + \frac{(1-r)}{n^2}\left(\sum_{i=1}^{n}u_i^2\right). \tag{10}$$

This form yields the previous results as special cases ($r = 0$ and $r = 1$). Constant r_{ij} for $i \neq j$ is in practice unlikely to be exact for a real situation, but may be a useful approximation in some cases, avoiding the need to estimate r_{ij} for every contributing pair.

3. Uncertainty budget components

3.1. Uncorrelated effects

Random errors in SST estimation from satellite data arise from noise in the satellite observations. The signal recorded by a typical radiometer is a