SUMMARY

Sea surface temperature (SST) is a fundamental quantity to understand weather and climate dynamics. Modern ocean observing systems monitor SST using multiple platforms and instruments – including satellite-borne sensors. However, the interpretation of estimated trends and anomalies or the integration or assimilation of observations from multiple sources into ocean/atmosphere numerical models requires that we understand the retrieval error and uncertainty of SSTs from each instrument or measurement system. This poster investigates the errors in SST observations from three different sources: two infrared radiometers (MODIS-Aqua and VIIRS-Suomi NPP) and in situ sensors (drifting and moored buoys). We start with the triple collocation (TC) error estimation technique to assess the relative quality of SST retrievals derived from each source. However, a fundamental assumption of the TC method is that errors between sources must be independent. Because the two satellite SST retrievals have similar characteristics, this assumption is probably not valid and, as expected, TC estimation of errors gave counter-intuitive results. We use simulated data with known errors to explore the implications of correlated errors on TC estimates of variability from the different SST sources. We find that in the simulated dataset *TC estimated SDs (TC-SDs) were only correct when correlation among all sources was zero* and a higher correlation between satellite errors (buoy errors were always independent) led to *increasingly overestimated TC-SDs for buoys and underestimated TC-SDs for satellite SSTs. Given an estimate for the correlation between errors in MODIS and VIIRS SSTs, we use the proportion of over/underestimation in TC-SDs for that level of correlation discovered from the simulated dataset to correct the counter-intuitive MODIS, VIIRS, and in-situ TC-SDs.*

TC estimation of errors gave counter-intutitive results. These are probably tied to the correlation between VIIRS and AQUA errors. Because the two satellite SST retrievals have similar characteristics, the assumption of independence of errors required by TC is probably not valid. We use simulated data with known errors to explore the implications of correlated errors on TC estimates of variability from the different SST sources. We find that the TC method produces correct estimates of variability for each source only when the correlation among errors is zero for all sources. The higher the correlation between satellite errors (buoy errors are always independent), the *triple collocation SDs for buoys are increasingly overestimated.* Conversely, the higher correlation results in *increasingly underestimated errors for satellite SSTs. We use the trends discovered between correlation and TC estimated SDs (TC-SDs) in the simulated dataset to correct for the effect of correlation on the counter-intuitive VIIRS, MODIS, and in-situ TC-SDs.*

MOTIVATION

Sea surface temperature (SST) is a key climate and weather measurement routinely used in atmospheric, oceanographic, fisheries, climate, and other sciences. The synoptic, repeated coverage of satellite remote sensing provides the best method of deriving accurate global SSTs on daily to decadal periods.

Calibration and validation of global satellite SSTs rely mostly on in situ SST observations from moored or drifting buoys. This approach can have limitations. First, in situ observations have sparse temporal and geographic distributions that bias estimates towards regions and conditions sampled most

frequently. Despite increasing coverage (see Fig. 1), there are still relatively undersampled ocean regions. Second, error estimation is complicated by the nature of measurements: buoy SSTs are point measurements averaged over minutes, whereas satellite retrievals are instantaneous but averaged over a larger footprint. Finally, differences in observation times and depths (skin versus bulk SSTs) and inaccuracies of in situ measurements may contribute to faulty interpretations of validation results.

To address these limitations, the triple collocation method has been proposed to estimate simultaneously the error structure and the cross-calibration of a set of at least three linearly related datasets. O’Carroll (2008) studied errors in SSTs from the Advanced Along-Track Scanning Radiometer (AATSR, an infrared or IR radiometer) and the Advanced Microwave Scanning Radiometer (AMSR-E, a microwave radiometer). Gentemann (2014) compared SSTs from buoys, the AMSR-E and the Moderate-resolution Imaging Spectroradiometer (MODIS) aboard Aqua (one of the SST sources used here).

Here, we use the triple collocation error estimation technique to assess the relative quality of SST retrievals derived from in situ sensors (drifting and moored buoys) and from two infrared radiometers, the Moderate-resolution Imaging Spectroradiometer (MODIS) instrument aboard the AQUA satellite, and the Visible Infrared Imaging Radiometer Suite (VIIRS) flying on the Suomi National Polar-Orbiting Partnership (Suomi NPP) spacecraft.

An important assumption in the triple collocation approach is that SST errors from different instruments are uncorrelated. This is a reasonable assumption when comparing SSTs from buoys, microwave and infrared instruments, as these measurements have very different physical foundations.

However, the two IR radiometers that we study here (VIIRS and MODIS) (i) use similar technologies and wavelengths, (ii) collect data close in time from one another and with a comparable footprint, and (iii) share common sources of error such as undetected clouds or fog, or unusual atmospheric profiles. However, MODIS is a heritage instrument of VIIRS and ensuring compatibility and comparison between the two data sources is necessary for continuity in satellite SST validation (?) and Climate Data Records (?). For these reasons, we explore the validity of the assumption of independence of errors and its implications on results from the triple collocation method and ultimately use this understanding to derive corrected triple collocation estimates of errors in MODIS, VIIRS, and in-situ SSTs.

(Figure 1)

COLLOCATED DATA

We used SST data from the MODIS and VIIRS instruments. SST derivation is similar for VIIRS and MODIS. Both estimates are based on measurements of top of the atmosphere (TOA) brightness temperatures (BT) at wavelengths where the atmosphere is relatively transparent to IR radiation: we use the “atmospheric window” in the long-wave, thermal infrared (λ=10-12 μm) spectral intervals.

Matchup Databases. To generate the collocated data, we use matchup databases (MDBs) for VIIRS and MODIS originally assembled for calibration and validation of SST algorithms. The MDBs include temporally (±30 min) and spatially (within 10 km) coincident measurements of (i) buoy SSTS from moored and drifting buoys and (ii) satellite quantities: brightness temperatures from IR channels, viewing geometry, and “skin” SSTs estimated using operational algorithms.

Buoy SST as common element in both MDBs. There are many cases in which the same buoy observation is included in both VIIRS and MODIS MDBs. Consequently, the buoy ID is the common element that allows us to join the two MDBs to produce the triple collocations. The collocated data span the period from XX October 2012 to XX March 2016.

Filtering collocated records. Various filters were applied to collocated data. Only nighttime satellite data were used to reduce diurnal warming effects. MODIS and VIIRS records were limited to being an hour apart from each other to ensure that both instruments were viewing the ocean through similar atmospheres. Records with the highest SST quality were selected to limit contamination by clouds. Only drifting and moored buoys were used as in-situ SST measurements and the MODIS and VIIRS buoy measurement times had to be less than 1 minute and 100 meters apart. Both MODIS and VIIRS measure IR radiation emitting from a few micrometers below the surface of the ocean so we add 0.17°C (the average skin effect) to VIIRS and MODIS SSTs to convert “skin” SSTs into “bulk” SSTs (i.e., what buoys measure).

The collocated set included 65,545 records. The satellite SST residuals (satellite minus buoy) are displayed on Figure 2. The residuals are unbiased. Robust standard deviations of residuals (interquartile range / 1.328) are 0.333°C and 0.293°C for AQUA and VIIRS, respectively.

(Figure 2)

TRIPLE COLLOCATION METHOD

The three-way error analysis was developed for validation of wind speeds by Stoffelen (1998) and used for SST validation by Blackmore et al. (2007), O’Carroll et al. (2008) and Gentemann (2014). The standard deviation and bias for each observation type is determined using collocations of the three different data types. The standard deviation for each of the three observation types is calculated as:

(Eqn. 1)

where 1, 2 and 3 indicate observation types and V12 is the variance of the difference between observation types 1 and 2 and so forth. For more details, a derivation and discussion is included in the Appendix of O’Carroll et al. (2008).

The individual errors (expressed as standard deviations) for each buoy measurement type were determined and are shown in Table 1.

(Table 1)

The results seem counter-intuitive and differ from those ofsimilar studies, as the largest error (0.320°C) is assigned to the buoy measurements, and smaller errors result for VIIRS and AQUA retrievals (0.183°C and 0.236°C, respectively). [Provide citations and numbers which explicitly disagree with our results] We suspect that these counterintuitive results may be tied to a failure in the assumption of uncorrelated errors.

We plot (a) VIIRS minus buoy SST differences versus (b) AQUA minus buoy SST differences (Figure 3). As we are subtracting the same buoy SST from each of the satellite retrievals, we assume that these differences represent the errors associated with each satellite radiometer. When we plot the differences against each other, it is clear that the association between errors is far from being negligible: the correlation coefficient is 0.698. Next, we explore the implications of assumption failure on TC-SD estimates for each source.

SIMULATED TC RESULTS

To explore the implication of a failure in the assumption of uncorrelated errors on triple collocation estimates, we simulated data with similar characteristics to those of the collocated observations. Each simulated set was built and analyzed as follows:

1. A total of 65,000 values (approximately the size of the collocated data) with a uniform distribution between 0 and 32°C were generated for each of 3 data sources.

2. Error terms were generated: (a) we generated random normally distributed values (65,000 for each source) with mean 0°C and SDs of 0.25, 0.40, and 0.40°C for buoys, VIIRS and MODIS, respectively (consistent with observed SDs). (b) Random errors were then transformed to impose a given correlation between simulated VIIRS and MODIS errors. Correlations ranged from 0.00 (no correlation) to 0.99 (very high). In contrast, buoy errors were assumed to have zero correlation with both VIIRS and MODIS.

3. Using the TC method, we estimated SDs for each source (noted as TC-SDs) in a simulated data set. To facilitate visualization, TC-SDs were scaled to the TC-SD for each source when correlation among all sources was 0.0. For example, if the TC-SD for VIIRS was 0.40°C when correlation was 0 and 0.20°C when correlation was 0.5, the scaled value in the second case was 0.5.

4. Steps 1-3 were repeated 100 times for each value of imposed correlation between VIIRS and AQUA errors. We calculated the median value of scaled TC-SDs for the 100 simulations. Results are displayed in Figure 4, that shows the scaled TC-SDs (median of 100 simulations) as a function of simulated correlation between VIIRS and AQUA errors.

(Figure 4)

Results are displayed in Figure 4, that shows the scaled TC-SDs (median of 100 simulations) as a function of simulated correlation between VIIRS and AQUA errors.

The TC-estimated SDs are correct only when the correlation among errors for all SST sources are zero (i.e., the assumption in the method is satisfied). As correlations among VIIRS and MODIS errors increase (buoys have zero correlation with satellite SST errors), the TC-SD for buoys is increasingly overestimated, and TC-SDs for VIIRS and AQUA are increasingly underestimated.

However, we can use the proportion of “true” SD estimated in our simulation dataset for a certain correlation value to correct TC-SDs for VIIRS, MODIS, and in-situ in our real MDB. First, we identify what proportion of “true” SD the TC method estimates at a correlation value of 0.7 between VIIRS and MODIS errors. We then take the TC-SD estimations for VIIRS, MODIS, and in-situ (speculated to be erroneous because failure in the assumption of independent errors) and divide it by that proportion. This “re-scaling” procedure uses the patterns of over and under-estimation found in the simulated dataset to correct the erroneous TC-SD estimation for VIIRS, MODIS, and in-situ in the real MDB. Table 2 shows the corrected TC-SD estimations

(Table 2)

CONCLUSION

[Need summary + something a little more]

There are more complicated TC calculations for situations when correlations among errors cannot be assumed to be negligible. This will be the topic of future work.

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REFERENCES