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Abstract

The Optimal Estimation (OE) approach based on Bayesian inversion gained popularity in the satellite sea surface temperature (SST) retrieval community with the promise of improving accuracy over the traditional non-linear SST (NLSST) retrieval algorithms, especially overcoming their problem with regional biases. OE, however, has its own problems typically related to insufficient knowledge of prior state, too few degrees of freedom, too crude forward model or insufficient measurement accuracy.

We applied the OE approach to SST retrievals using in two IR MODIS channels at 11 and 12 μm and found that the OE approach is not always better than the NLSST retrieval.

Bayesian inversion concepts

Conceptually, the Bayesian approach can be summarized as follows:

- 1) we have some knowledge of the state before the measurement is made and the prior knowledge is expressed by a prior *pdf* of the state variables.
- 2) we have a forward model that maps the state variable into the measurement space.
- 3) we know the *pdf* of the measurement errors.
- 4) we can calculate posterior *pdf* by augmenting the prior *pdf* of the state vector with the measurement.

If the forward model is \mathbf{F} , the prior state is x_a and the measurements is y then for Gaussian *pdfs* the expected value of posterior *pdf* of state variables is given by:

$$x = x_a + \left(K^T S_e^{-1} K + S_a^{-1} \right)^{-1} K^T S_e^{-1} (y - F(x_a)) \quad (1)$$

where \mathbf{K} is a Jacobian of \mathbf{F} and the covariance matrix of the posterior state is:

$$S^{-1} = K^T S_e^{-1} K + S_a^{-1} \quad (2)$$

The OE Approach

Satellite Dataset

We apply the OE retrieval to a subset of MODIS Collection 6 (R2014) Match-Up Data Base (MUDB), for 2015 and 2016 from the North Atlantic Ocean and the Mediterranean Sea (Figure 2). The MUDB includes the 11 and 12 μm radiance measurements (channels 31 and 32). The error specification is 0.05K, corresponding to a radiance of $\sim 0.007 \text{ W/m}^2\text{-}\mu\text{m}\text{-sr}$. Each MUDB record includes assessment of the confidence in the retrieved value expressed as the *quality flag* (*qf*). The bests match-ups have *qf*=0 and the slightly worse *qf*=1. Quality flags > 1 typically indicate contaminated pixels and are not used here.

Prior knowledge

The MODIS NLSST (Kilpatrick et al, 2015) is based on the radiance measured in channels 31 and 32 being sensitive to the SST, and the channel radiance difference being sensitive to the Total Column Water Vapor (TCWV). Given two measurements, at best two components of the state vector can be retrieved, so we use a reduced state vector: $x = [\text{SST}, \text{TCWV}]$.

Prior knowledge is the SST and TCWV fields is taken from the European Centre for Medium-Range Weather Forecasts (ECMWF) ERA5 dataset. We assume that the prior *pdf* of x is Gaussian with mean $[SST_0, TCWV_0]$ given by ERA5, and some prior variance that we have to specify. The ERA5 SST corresponds to a subsurface temperature measured at a buoy level. This temperature differs from the skin SST obtained by satellite measurements and the average offset has been estimated at -0.17 K (Donlon et al., 2002), so we subtract this from ERA5 SST to estimate skin SST. For the forward radiative transfer modelling we use the ERA5 atmospheric profiles of temperature, water vapor, and ozone. The spatial resolution is $0.4^\circ \times 0.4^\circ$ and the temporal resolution for 6 hours for the atmospheric profiles and 24 hours for the SST.

Forward model

We use the Radiative Transfer for TOVS (RTTOV) v12.1 (Hocking et al., 2018). The ERA5 data are interpolated to the time and position of the match-up data point. Using RTTOV we simulate MODIS channel 31 and 32 radiances as well as the Jacobian matrix, \mathbf{K} . The forward model is only an approximation and thus is an additional source of error.

Prior covariance S_a and Measurement error covariance S_e

The covariance matrices are:

$$S_a = \begin{bmatrix} e_{SST}^2 & 0 \\ 0 & e_{TCWV}^2 \end{bmatrix} \quad S_e = \begin{bmatrix} e_{31}^2 & 0 \\ 0 & e_{32}^2 \end{bmatrix}$$

where e_i is uncertainty of the prior state variables for S_a and measurement uncertainty in channels 31 and 32 of MODIS (0.05K) combined with an estimate of the forward model uncertainty (0.1K) for S_e . For retrievals discussed here $e_{SST} = 0.5 \text{ K}$, and $e_{TCWV} = 25\%$.

Results

The Table shows in the 1st row the state of prior knowledge as the difference between the prior ERA5 SST and in situ measurements, ΔSST , for daytime and night-time measurements, for quality 0 and 1 pixels; numbers in brackets are robust values. The 2nd row shows results of OE retrieval, ΔSST_{OE} , row 3 the NLSST retrieval, ΔSST_{NL} and row 4 shows results of OE retrieval with a modified prior SST. Two main results are:

- 1) For the night-time match-ups, OE delivers better results than NLSST, particularly for the lower quality data.
- 2) NLSST outperforms OE in the daytime.

The poorer performance of the OE approach for the daytime data indicates that the OE process is not strong enough to overcome the -0.26K average bias of the prior SST. We thought the bias might be related to the fact that the ERA5 SST field does not contain diurnal component of SST variation. The amplitude of diurnal variation can be quite large, sometimes exceeding 1K. We introduced a simple method of estimating the diurnal bias in the ERA5 data as a linear function of the cosine of solar zenith angle, *msolz*, and attempt the OE retrieval with the improved prior SST. Figure 1 shows as a contour plots of ΔSST vs *msolz* before (a) and after the diurnal bias correction for *qf*=0 data in the daytime. The bias correction for *qf*=0 data is calculated with *qf*=1 data as the diurnal bias should be independent of the quality of the satellite matchup and to keep the correction independent of the data field being corrected.

	Day <i>qf</i> =0		Day <i>qf</i> =1		Night <i>qf</i> =0		Night <i>qf</i> =1	
	Mean	Std.	Mean	Std.	Mean	Std.	Mean	Std.
ΔSST	-0.26 (-0.24)	0.73 (0.56)	-0.24 (-0.23)	0.67 (0.51)	-0.04 (-0.03)	0.71 (0.49)	-0.04 (-0.04)	0.74 (0.52)
ΔSST_{OE}	-0.18 (-0.15)	0.68 (0.45)	-0.19 (-0.18)	0.63 (0.58)	0.01 (0.03)	0.66 (0.47)	-0.06 (-0.04)	0.70 (0.51)
ΔSST_{NL}	0.03 (0.03)	0.63 (0.58)	-0.08 (-0.04)	0.76 (0.74)	-0.10 (-0.08)	0.53 (0.53)	-0.32 (-0.29)	0.75 (0.79)
ΔSST_{OE^*}	0.05 (0.08)	0.67 (0.53)	0.07 (0.09)	0.63 (0.50)	0.04 (0.06)	0.66 (0.47)	-0.03 (-0.01)	0.70 (0.51)

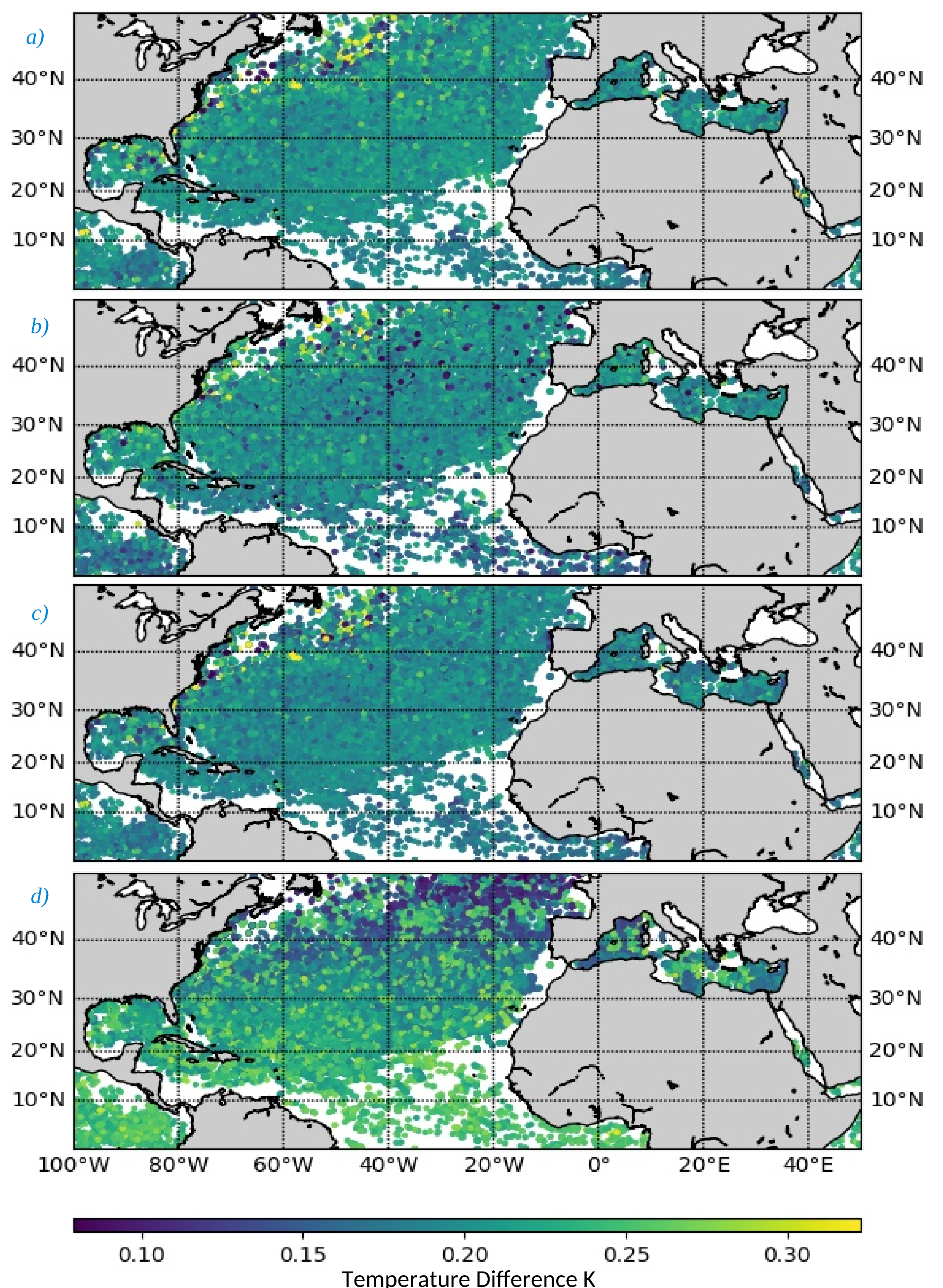
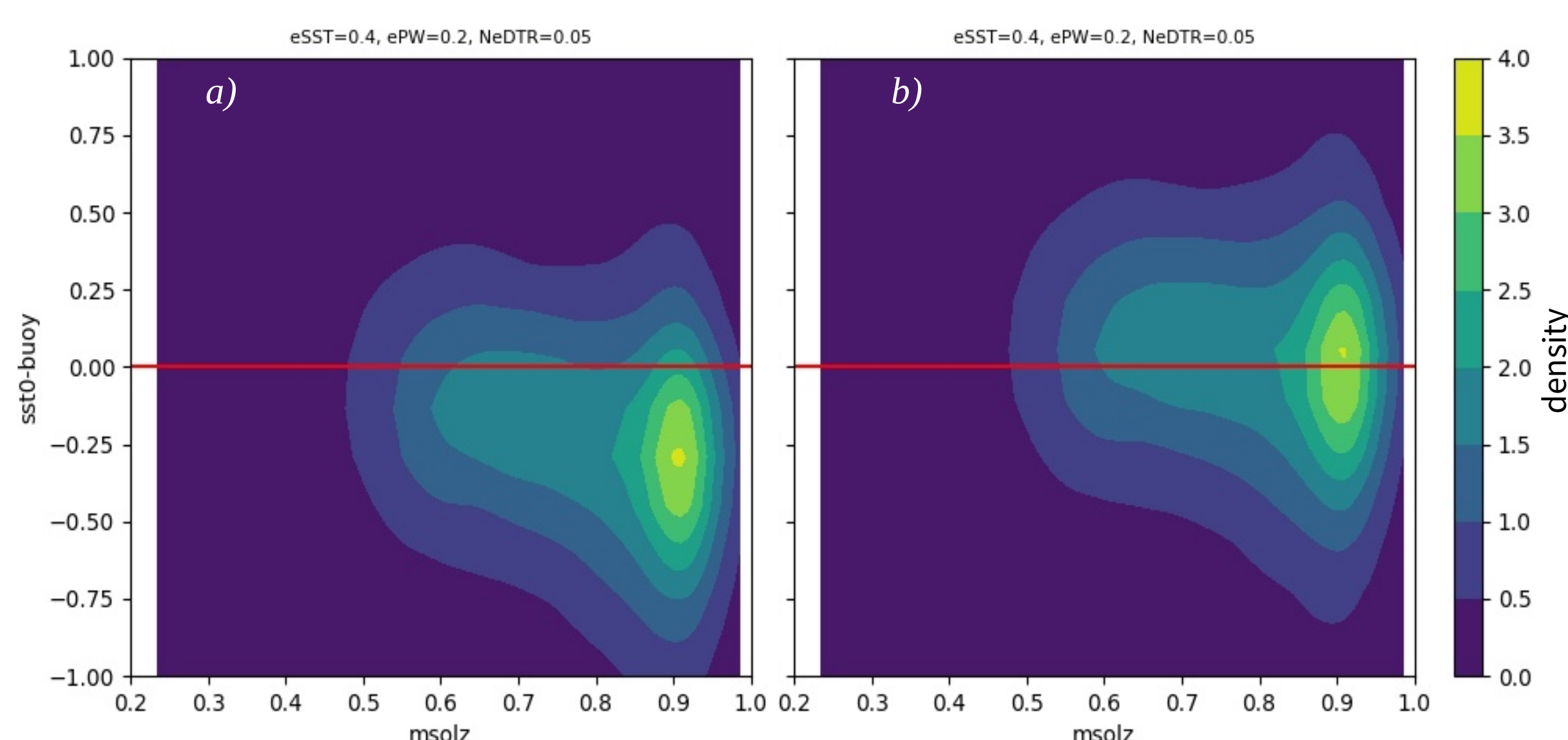


Figure 2. Maps of the retrieval domain: a) prior knowledge minus buoy temperature corrected by the skin effect SST; b) NLSST - SST; c) unmodified OESST SST; and d) the difference between the original OESST and the modified OESST* with the SST prior corrected for diurnal signals.

Summary and Conclusions

- The accuracy of the OESST is limited by that of the prior *pdf* of SST and seemingly cannot overcome biases of 0.1 K or more. This means our prior knowledge of SST has to already be in a range of 0.1 K or better.
- The unmodified OESST only improves on the prior ERA5 SST by about 30% in bias reduction with respect to buoy measurements.
- Simple diurnal correction improves the performance of OE significantly for the daytime data but even then the NLSST performs better.
- The selection of the prior SST is crucial for performance of OE, not so for NLSST.
- For night-time data, OE outperforms NLSST in all cases. Due to the lack of input from the visible channels the night-time data are in general more susceptible to being contaminated by clouds, and that would be even more so for lesser quality data so perhaps it is not surprising that NLSST performs worse for this category.
- One might ask if we already have accurate and unbiased prior, as is there necessary for the OE is there a point of performing the retrieval at all?

References

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