OPTIMAL ESTIMATION FOR RETRIEVING SEA SURFACE TEMPERATURE

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Proposition: Despite the evident success of coefficient-based retrievals of sea surface temperature (SST) during the AVHRR era, there are significant benefits in using optimal estimation (OE) instead.

What are the benefits of OE? Reduced regional biases, reduced noise, better quality information.

Any disadvantages? OE is more difficult than using coefficients (fast forward modelling is required), but is feasible for operational centres and re-analysis projects.

Is OE worth the extra effort? Judge for yourself from the case study of METOP-A below …

THE THEORETICAL BACKGROUND

The NLSST that is used as a benchmark here against which the OE performance is assessed has the form:

$$\hat{x} = (a_1 + a_2 s) + \begin{bmatrix} a_3 + a_4 s + a_5 x_c \\ -a_4 s - a_5 x_c \end{bmatrix}^{T} \begin{bmatrix} y_{11} \\ y_{12} \end{bmatrix}$$

in which the SST estimate, x, is a nearly linear combination of the brightness temperatures y, the combination being controlled by coefficients, a, the secant of the satellite zenith angle via s, and a climatological SST x_c. The order of magnitude of performance for the NLSST is similar to that of other commonly used options, such as the MCSST, linear retrieval covering two SST ranges, etc.

All such nearly-linear retrieval are subject to biases intrinsic to their formalism: prior error and non-linearity error[3].

Optimal estimation is a generic name for categories of satellite retrieval that have long been used for atmospheric sounding[4], etc. The particular OE estimator whose results are shown here is the **maximum a posteriori** (MAP) estimate.

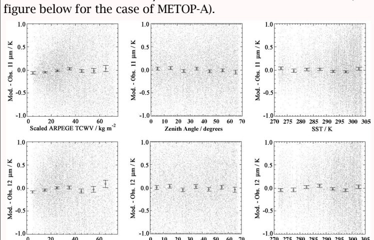
We take NWP fields, $\mathbf{x}_a$, from Meteo France and use the fast radiative transfer model RTTOV to calculate prior estimates of the brightness temperatures expected, $\mathbf{F}(\mathbf{x}_a)$. The retrieval is of a reduced state vector, $\mathbf{z}$, comprising the SST, x, and the total column water vapour (TCWV), w. The MAP estimate is then

$$\hat{\mathbf{z}} = \mathbf{z}(\mathbf{x}_a) + \left(\mathbf{K}^T\mathbf{S}_\varepsilon^{-1}\mathbf{K} + \mathbf{S}_a^{-1}\right)^{-1}\mathbf{K}^T\mathbf{S}_\varepsilon^{-1}\left(\mathbf{y}_o - \mathbf{F}(\mathbf{x}_a)\right)$$

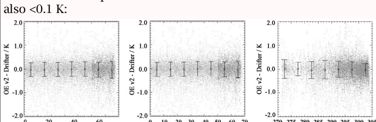
where $\mathbf{y}_o$ are the observed BTs and

$$\mathbf{K} = \left[\frac{\partial \mathbf{F}(\mathbf{x}_a)}{\partial \mathbf{z}}\right] = \begin{bmatrix} \partial y_{11}/\partial x & \partial y_{11}/\partial w \\ \partial y_{12}/\partial x & \partial y_{12}/\partial w \end{bmatrix} \quad \mathbf{S}_\varepsilon = \begin{bmatrix} e_{11}^2 & 0 \\ 0 & e_{12}^2 \end{bmatrix} \quad \mathbf{S}_a = \begin{bmatrix} e_{xa}^2 & 0 \\ 0 & e_{wa}^2 \end{bmatrix}$$

The forward model[5] RTTOV is adapted somewhat to give good bias correction of observed and modelled radiances. First, a skin effect is modelled to relate NWP and radiometric SST. Second, some dependencies between BT residuals and TCWV, latitude and zenith angle are parameterized and removed. As a result, the modelled minus observed BTs have systematic variations less than 0.1 K (see figure below for the case of METOP-A).



The functional dependencies of OE SST minus drifter SST are then also <0.1 K:



The expression for the cost used here to assess the goodness of fit of the OE SST is

$$\hat{\chi}^2 = \left(\mathbf{K}\hat{\mathbf{z}}' - \mathbf{y}'\right)^T\left(\mathbf{S}_\varepsilon\left(\mathbf{K}\mathbf{S}_a\mathbf{K}^T + \mathbf{S}_\varepsilon\right)^{-1}\mathbf{S}_\varepsilon\right)^{-1}\left(\mathbf{K}\hat{\mathbf{z}}' - \mathbf{y}'\right)$$

where $\mathbf{y}' = \mathbf{y} - \mathbf{F}(\mathbf{x}_a)$ $\quad \hat{\mathbf{z}}' = \hat{\mathbf{z}} - \mathbf{z}_a$

Lastly, note that the validation statistics have a contribution from drifter error. If we assume that drifter error is 0.2 K, the true OE SST retrieval for an SD of (say) 0.37 K is $\sqrt{0.37^2 - 0.20^2}$ =0.31 K.

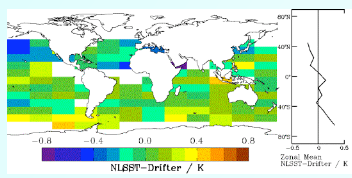
THE CASE STUDY[1] – SST FROM METOP-A

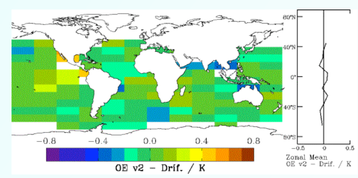
METOP-A is the first European polar-orbiter carrying an AVHRR. This case study was undertaken with the operational team at Meteo-France, and was sponsored by EUMETSAT within the Ocean and Sea Ice Satellite Application Facility.

Data: 32175 matches with *in situ* drifters between April and July 2007: All results are based on
- the nearest single pixel (so we see the true pixel level noise)
- night-time matches (no confounding by diurnal variability[2])

In situ measurements probably have error between 0.2 and 0.25 K

Comparison: OE-based retrieval compared to the operational non-linear SST (NLSST) – i.e., 11 and 12 μm "split window" retrieval. The NLSST used has near-zero bias and near-minimum error (for its formalism).

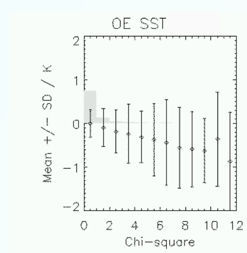




Biases: Regional biases are intrinsic to the NLSST algorithm, and only **33%** of cells (above left) have mean AVHRR-drifter difference less than 0.1 K. With OE (above right), there is less regional bias, with **64%** of cells less than 0.1 K.

Noise: The table below shows the validation statistics for all data. The conventional standard deviation (SD) is shown together with a robust standard deviation (RSD, insensitive to non-Gaussian outliers). Both for "All data" and for "Best data" (those cases where the processing gives highest confidence to results), the retrieval noise is significantly improved.

Case	Mean / K	SD / K	RSD / K	N
All data: NLSST	0.00	0.72	0.53	32175
All data: OE	-0.06	0.44	0.32	32175
"Best" data: NLSST	0.12	0.59	0.44	11908
"Best" data: OE	-0.04	0.42	0.31	11908
Low χ^2 data: OE	-0.03	0.37	0.30	30831



Quality control: For a small extra effort, the OE can calculate a "cost", χ^2, of the retrieved solution. Here, the fit between retrieved and observed brightness temperatures is used as the measure of cost. The figure above shows that retrieval quality is a strong function of the χ^2. This is powerful for quality control, as shown in the last row of the table above. While identifying a far greater proportion of matches as best quality, the SD and RSD are still significantly improved on the values obtained using the operational flag for "best data", if low cost is used instead to identify the best results.

Final comment: If you are wondering "What if the 3.7 μm is being used in addition to the split window channels?", the bottom line is that the retrieval noise (SD) is reduced from 0.44 to 0.38 K by using OE on all data, and that for the 80% of data with lowest cost, it is 0.26 K (i.e., most of the apparent error is probably contributed by the drifter!).

1. Merchant C J, P Le Borgne, A Marsouin and H Roquet, Optimal estimation of sea surface temperature from split-window observations, Rem. Sens. Env., in press, 2008. doi:10.1016/j.rse.2007.11.011

2. The only difference between radiometric SST as seen by satellite and the in situ SST measured at depth is then the skin effect. See, for example, Donlon C, I Robinson, K Casey, J Vasquez, E Armstrong, et al., The Global Ocean Data Assimilation Experiment (GODAE) High Resolution Sea Surface Temperature Pilot Project (GHRSST-PP), Bull. Am. Met. Soc, 88 (8), 1197-1213, 2007.

3. Merchant, C. J., Horrocks, L. A., Eyre, J., & O'Carroll, A. G. (2006). Retrievals of sea surface temperature from infra-red imagery: origin and form of systematic errors, *Quarterly J. Royal Meteorological Society*, 132, 1205-1223.

4. Rodgers, C. D. (1990). Characterization and error analysis of profiles retrieved from remote sounding measurements, *J. Geophysical Research*, 95 (D5), 5587-5595.

5. Saunders, R. W., Brunel, P., Chevallier, F., DeBlonde, G., English, S. J., Matricardi, M., & P. J. Rayer (2002), RTTOV-7 – Science and Validation Report, NWP Technical Report No. 387, Met Office, UK.

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