Roles of L2 SSES in a L4 production case

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- L2 Single Sensor Error Statistics (**"bias"** and **"std"**) ...
  ... (potentially) used heavily in L4 analysis production.

- This presentation: how SSES are used/abused in a particular case of MUR SST (L4) production.

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MUR (L4) Summary

- $0.01^\circ \times 0.01^\circ$ grid ($\sim$1 km resolution) daily analysis, featuring **MODIS** (high-resolution, wide-swath) L2P data sets.

- Also include: microwave (**AMSR-E, WindSAT**), lower-resolution global infra-red (**AVHRR-18G, -19G**), ice-concentration (OSI SAF), and in-situ (iQuam) data sets.

  To be included in the future: **VIIRS**, **AMSR2**, ...

- Uses only night-time data (for *bulk-temperature analysis*).

- Covers Aqua satellite-period: mid-2002 to present.

$\Rightarrow$ **a fairly standard daily L4 gridded SST product, maybe except for the high spatial resolution .....**

MUR Analysis Requirements and Approach

- Processing of data sets with highly variable resolutions: $\sim$1-km (MODIS), $\sim$10-km (AVHRR, ice), $\sim$25-km (microwave), to even sparser (in-situ data).

  Difficulty: smaller features move faster (within a daily span).

- Approach: multiple "stages" of analysis at different scales (e.g., the last paragraph, Reynolds et al. 2013).

- MUR uses *Multiresolution Analysis* (MRA; cf. wiki) for multi-scale signal decomposition using a wavelet basis:

$$T^{\mathrm{MUR}} = \bar{T}^{(L_0)} + T'^{(L_0)} + T'^{(L_1)} + \cdots + T'^{(L_{max})}$$

  Duration (time window) of the input data is dependent on the scale/resolution (L_i).

MUR Analysis Approach: Multi-scale analysis

MUR Analysis Approach: Input time windows

Narrower time-windows for higher resolution analysis stages:

Examples: with/without multi-scale analysis

AMSR-E (red) and MODIS (blue) samples

Interpolation at 40km scale (L=7)

Interpolation at 10km scale (L=9)

Multi-scale Interpolation (L=2~11)

Core Analysis Procedure, MUR (and others?)

- MUR analysis method uses:
  - multiple stages of scale-specific analysis.
  - a "mesh-less", continuous function (wavelet) basis (no nearest-neighbor gridding, preserves geolocations info).
  - time-weights which are scale dependent.

- However, each stage is a *familiar* OI estimation, like this:

$$T'^{(L)} \longleftarrow \min_{\mathbf{x}} \left\|\mathbf{x} - \mathbf{x}^b\right\|^2_{\mathbf{B}^{-1}} + \|\mathbf{y} - \mathbf{H}\mathbf{x}\|^2_{\mathbf{R}^{-1}}$$

an optimal combination of (assumed) background $\mathbf{x}^b$ and observations $\mathbf{y}$ based on their respective error covariance matrices $\mathbf{B}$ and $\mathbf{R}$.

$\Rightarrow$ **How MUR depends on L2P parameters (including SSES) maybe similar to how other L4 products rely on them.**

Potential uses of L2P SSES (in L4 analysis)

1. **Quality control**
   Which L2P pixels are actually used as the inputs to L4?

2. **Bias corrections**

   - finding the target "SST" (e.g., *foundation SST*)
   - inter-sensor bias

3. **Data weights**
   The key parameters in OI & Bayesian estimation methods.

4. **Posterior error estimation**
   The required `analysis_error` field of L4.

1. Quality control in MUR

- Quality-flags are the primarily means of pixel segregation.
- Geo-location (lat,lon) is checked for inland pixels.
- Currently, MUR doesn't use a background SST field (e.g., climatology, previous day's analysis) for outlier detection.
- *SSES standard_deviation* is checked for large values (e.g., $> 1^{\circ}C$).

$\Rightarrow$ *Reliance on the L2P quality flags, mostly.*

2. Bias corrections in MUR

- Can *SSES bias* be used to determine the "bulk SST"?
  - Operating assumption:

    SSES bias *and* **standard_deviation** *are the mean and* $\sqrt{variance}$ *statistics of the difference between L2P and match-up data base (buoy) SSTs.*

  - Good assumption? (What exactly are SSES's?)
    - How are such statistics made available for *each* pixel?
    - What is the accuracy of the *SSES bias*?

2. Bias corrections in MUR

RMS [°C]	SST	SST−bias
AMSRE	0.065	0.047
AVHRR18G	0.062	0.055

Use of SSES bias improves self consistency ... slightly.

2. Bias corrections in MUR

- SSES bias are applied for most input L2P data sets.
- MUR co-estimates bias b_s for each sensor s (with noise ϵ_s):

$$T_s^{\text{L2P}} = T^{\text{MUR}} + b_s + \epsilon_s$$

except $b_s = 0$ when s is "in situ" (for bulk temperature).

$\longrightarrow$ *simultaneously attains bulk temperature and corrects for inter-sensor bias*

$\Rightarrow$ *in situ* data set (iQuam) plays a key role in bias correction.

3. Data weighting in MUR

- Importance of respecting pixel-to-pixel correlations (e.g., Kaplan et al 2003; "super-obs").

- MUR assumes a constant correlation coefficient for each grid-box. → SSES variance values are discounted according to the pixel density. Example: Fig. 8 from Chin et al 2014

AMSR-E + MODIS on 2006/200: (a = reference; b = bad; c = good)

- Also, time-window weights (a previous slide) are applied.

⇒ *SSES std (variance) values are heavily altered !*

4. Posterior error statistics in MUR

- Background error model (covariance matrix, variational constraints, etc) typically affects the L4's own error estimate.

  Posterior variance values can become too low
  (often not an ideal Bayesian scenario).

- L4 ensemble statistics can be useful,
  e.g., GMPE standard-deviation correlates well with buoy-ΔSST, Fig.5 of Martin et al 2012.

- MUR uses the latter to correct the former by scaling.

$\Rightarrow$ *SSES std values are altered beyond the Bayesian formula.*

— MUR also needs a separate (experimental) flag to indicate the MODIS pixel locations, because posterior error doesn't locate them well.

Uses of L2P SSES in MUR L4 analysis

1. **Quality control** (which L2 pixels are actually used?)

   SSES std is looked at, but L2P quality flag is relied on.

2. **Bias corrections** (target "SST" and inter-sensor bias)

   SSES bias is applied, but bias is then co-estimated.

3. **Data weights** (basis of OI & Bayesian estimation methods)

   SSES std is used but altered (beyond recognition).

4. **Posterior error statistics** (`analysis_error` field of L4)

   The altered SSES std is used, and output is scaled.

MUR's reliance on L2P quality parameters

in the order of importance/impact:

1. *Quality flag*
2. *SSES standard deviation*
3. *SSES bias*

However, *SSES bias* has a potential to play a much larger role, because it applies directly to the SST values.

Summary and Comments

- Gridding is a harsh environment for L2P SSES parameters.
  - a non-ideal Bayesian scenario
    (prior models, correlations, biases, data density, ...)
  - "bin-averaging" does NOT avoid issues (e.g., correlation)
- Still, "data products" should (?) inherit error estimates (mostly) from the upstream data sets, i.e., L4/L3 from L2P.
  - consider alternatives to use L2P SSES better:
    e.g., direct gridding/interpolation of *SSES std* values.
- Potential impacts of *SSES bias* on L4 seems large.
  - can reduce inter-sensor bias and reach target SST (skin/bulk).
  - What's the reference? (What's "SST−bias"?) Accuracy?
  - Definitions? Documentations?
- *Quality flag(s)* could be included in SSES discussions.