New physically based sea surface temperature retrievals for NPP VIIRS

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Activities

• Data
  – VIIRS & MODIS L1B
  – VIIRS & MODIS GHRsst SST
  – NCEP GFS
  – Aerosol climatology (CMIP5)

• Working with matchups
  – Time-space matches with *in situ*
  – iQUAM data (drifting & moored buoys)
  – Allows quantitative assessment of algorithm adjustments

• Channel selection
  – Check observed BTs against output from CRTM
  – For now, only use channels which agree “well”
    ➢ *Ad hoc* bias correction risks corrupting signal, or distorting physical model
    ➢ Best to identify and fix issues at source
    ➢ Experiments with GOES indicate bias correction can degrade retrieval
Physical Retrieval

• Reduces the problem to a local linearization
  – Dependent on ancillary data (NWP) for an initial guess
  – More compute-intensive than regression – not an issue nowadays
    Ø Especially with fast RTM (e.g. CRTM)

• Widely used for satellite sounding
  – More channels, generally fewer (larger) footprints

• Start with a simple reduced state vector
  – $x = [\text{SST, TCWV}]^T$
    – *N.B.* Implicitly assumes NWP profile shape is more or less correct

• Selection of an appropriate inverse method
  – Ensure that satellite measurements are contributing to signal
  – Avoid excessive error propagation from measurement space to parameter space
    Ø If problem is ill-conditioned
History of Inverse Model

- **Forward model:** \( Y = KX \)
- **Simple Inverse:** \( X = K^{-1}Y \) (measurement error)

- **Legendre (1805) Least Squares:**
  \[
  X = X_{ig} + (K^T K)^{-1} K^T (Y_\delta - Y_{ig})
  \]

- **MTLS:**
  \[
  X = X_{ig} + (K^T K + \lambda R)^{-1} K^T (Y_\delta - Y_{ig})
  \]

- **OEM:**
  \[
  X = X_a + (K^T S_e^{-1} K + S_a^{-1})^{-1} K^T S_e^{-1} (Y_\delta - Y_a)
  \]
Uncertainty Estimation

Physical retrieval

Normal LSQ Eqn: \[ \Delta x = (K^T K)^{-1} K^T \Delta y \quad [= G \Delta y] \]

MTLS modifies gain: \[ G' = (K^T K + \lambda I)^{-1} K^T \]

Regularization strength: \[ \lambda = (2 \log(\kappa)/\|\Delta y\|) \sigma^2_{\text{end}} \]

(\sigma^2_{\text{end}} = \text{lowest singular value of } [K \Delta y])

Total Error

\[ \|e\| = \|(M RM - I)\Delta x\| + \|G'\|\langle\|\Delta y - K\Delta x\|\rangle \]

N.B. Includes TCWV as well as SST
“Optimized” OE

• \([S_e], S_a = \begin{bmatrix} \sigma^2 \text{ is an overestimate…} \\ 0 \text{ …or an underestimate} \end{bmatrix}\)

• Perform experiment – insert “true” SST error into \(S_a^{-1}\)
  – Can only be done when truth is known, e.g. with matchup data
DFS/DFR and Retrieval error

- Retrieval error of OEM higher than LS
- More than 75% OEM retrievals are degraded w.r.t. a priori error
- DFR of MTLS is high when a priori error is high

The retrieval error of OEM is good when a priori SST is perfectly known, but DFS of OEM is much lower than for MTLS.
Improved cloud detection

- Use a combination of spectral differences and RT
  - Envelope of physically reasonable clear-sky conditions
- Spatial coherence (3×3)
- Also check consistency of single-channel retrievals
- Flag excessive TCWV adjustment & large MTLS error

- Almost as many as GHRSSST QL3+, but with greatly reduced leakage
VIIRS Initial Results

- Data are ordered according to MTLS error
  - Reliable guide for regression as well as MTLS
  - Trend of initial guess error is expected
MODIS Initial Results

- Note improvement from discarding MTLS error “last bin”
  - Irrespective, MTLS is quite tolerant of cloud scheme
- Recalculated SST4 coefficients produce quite good results

NASA MODIS-VIIRS ST Meeting, May 18 – 22, 2015
Status & Plans

• “Initial cut” MTLS shows promise with VIIRS
  – Well-calibrated instrument, with reliable* fast RTM available
  – Error calculation useful quality indicator
  – MODIS offers more possibilities

• Cloud detection can be aided by RTM
  – “Single-channel” retrieval consistency, MTLS error calculation

• Plans
  – Take advantage of SIPS!
    ➢ Liaise w/ RSMAS on matchups
  – Take advantage of differing length scales to reduce atmospheric noise
  – Perhaps combine with sounder for more local atmospheric information
  – Refine fast RTM, iteration
  – Tropospheric aerosols…
Deterministic & Stochastic

<table>
<thead>
<tr>
<th>Deterministic</th>
<th>Stochastic/Probabilistic</th>
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<tbody>
<tr>
<td><strong>MTLS/RTLS/Tikhonov</strong>: Single pixel</td>
<td><strong>OEM</strong>: A set of measurement</td>
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<tr>
<td>$dX = K^{-1}dY$</td>
<td>A posteriori</td>
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<tr>
<td>measurement error</td>
<td>A priori</td>
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<tr>
<td>Lengendre (1805)</td>
<td>observation</td>
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<td>Least Squares:</td>
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<tr>
<td>$X_{ls} = X_{ig} + (K^T K)^{-1} K^T dY_\delta$; $dY_\delta = Y_\delta - Y_{ig}$</td>
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<tr>
<td>Last 30~40 years $\delta X \leq \kappa \delta E$; $\kappa = \text{cond}(K)$</td>
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<tr>
<td>$X_{rg} = X_{ig} + (K^T K + \lambda R)^{-1} K^T dY_\delta$</td>
<td></td>
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<tr>
<td>$= X_{ig} + K_{ps}^{-1} dY_\delta$</td>
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<tr>
<td><strong>MTLS</strong>: $[u , \sigma , v] = [K , \begin{bmatrix} dY_\delta \end{bmatrix}]$; $R = I$</td>
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<tr>
<td>$\lambda = (2 \log(\kappa) / |dY_\delta|^2) \sigma^2_{end}$</td>
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<tr>
<td>Total Error: $\left| X_{true} - X_{mls} \right|$</td>
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<tr>
<td>$\left| (K_{ps}^{-1} K - I) X_{true} \right| + \left| K_{ps}^{-1} (dY_\delta - K X_{mls}) \right|$</td>
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<tr>
<td>Regression: A set of measurement</td>
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<td>Historical heritage in SST retrieval using Window channels.</td>
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<td>Coefficient Vector/matrix: $C \quad X_{reg} = CY_\delta$</td>
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<td>Main concerns: Correlation &amp; Causation</td>
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Recent update to Geo-SST

- Physical retrieval based on Modified Total Least Squares
- Improved bias and scatter *cf.* previous regression-based SST retrieval

**GOES-15**

![GOES15 Day 2013](image1)

![GOES15 Night 2013](image2)

**Daytime**

**Nighttime**

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How sensitive is retrieved SST to true SST?

- If SST changes by 1 K, does retrieved SST change by 1 K?
- CRTM provides tangent-linear derivatives

\[ \frac{\partial T_{11}}{\partial \text{SST}_{\text{true}}} \quad \frac{\partial T_{12}}{\partial \text{SST}_{\text{true}}} \]

Response of NLSST algorithm to a change in true SST is…

\[ \frac{\partial \text{NLSST}}{\partial \text{SST}_{\text{true}}} = \left( a_1 + a_2 \times \text{SST}_{bg} + a_3 \times \{\sec(ZA) - 1\} \right) \times \frac{\partial T_{11}}{\partial \text{SST}_{\text{true}}} \]

\[ - \left( a_2 \times \text{SST}_{bg} + a_3 \times \{\sec(ZA) - 1\} \right) \times \frac{\partial T_{12}}{\partial \text{SST}_{\text{true}}} \]

Sensitivity to true SST

Sensitivity often <1 and changes with season
Sensitivity to true SST
Air – Sea Temperature Difference

Jul

(1 - Sensitivity)\times ASTD (K)
Seasonal Geographic Distribution of Bias

Dec

SST Bias / K

-0.75  -0.50  -0.25  0.00  0.25  0.50  0.75
Characteristics of different cloud detections

- The data coverage of new cloud (NC) 50% more than OSPO
- # cloud free pixels for high SZA is sparse – maybe OSPO & OSI-SAF regression form are not working for this regime

• There is no physical meaning from RT for a regression variable of SSTg multiplied with (T11-T12).