Predicted vs observed results for different channel combinations, information content and operational error for multi-sensors SST retrievals

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## **Basic of Physical Inverse Model**

- Forward model: Y = KX; dY = KdX
- Inverse:  $d\mathbf{X} = \mathbf{K}^{-1}d\mathbf{Y}$  (measurement error)
- Lengendre (1805) developed Least Squares stochastically, but the deterministic form  $\mathbf{X} = \mathbf{X}_{ig} + (\mathbf{K}^{T}\mathbf{K})^{-1}\mathbf{K}^{T}d\mathbf{Y}_{\delta}; \quad dY_{\delta} = \mathbf{Y}_{\delta} - \mathbf{Y}_{ig}$

Last 30~40 years:  $\delta X \leq \kappa \, \delta E; \kappa = \text{cond}(\mathbf{K})$ 

• Two ways can be addressed:

 $dY_{\delta} - \delta Y = \mathbf{K} dX \quad then, \quad LS$  $\frac{\min}{\|\delta K\|, \|\delta Y\|, X} \{ \|\delta K\|^{2} + \|\delta Y\|^{2} \} \quad \text{subject to } (K - \delta K) \, dX = dY_{\delta} - \delta Y$ 



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### **Deterministic & Stochastic**

#### Determinitic

#### Stochastic/Probabilistic

$$\mathbf{X}_{rg} = \mathbf{X}_{ig} + (\mathbf{K}^{\mathrm{T}}\mathbf{K} + \lambda \mathbf{I})^{-1}\mathbf{K}^{\mathrm{T}}d\mathbf{Y}_{\delta}$$

$$= X_{ig} + K_{ps}^{inv} dY_{\delta}$$

$$\mathsf{TLS:} [\mathbf{u} \,\sigma \,\mathbf{v}] = [\mathbf{K} \quad d\mathbf{Y}_{\delta}]$$

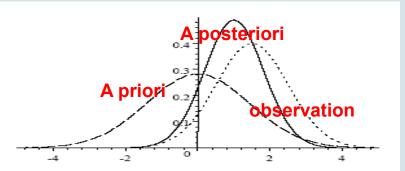
$$\mathsf{MTLS:}$$

$$\lambda = (2\log(\kappa) / \left\| d\mathbf{Y}_{\delta} \right\|^{2}) \sigma_{end}^{2}$$

$$\mathsf{Total Error:} \| \mathbf{X}_{true} - \mathbf{X}_{mtls} \|$$

$$\| (\mathbf{K}_{ps}^{inv} \,\mathbf{K} - \mathbf{I}) \mathbf{X}_{true} \| + \| \mathbf{K}_{ps}^{inv} (d\mathbf{Y}_{\delta} - \mathbf{K}\mathbf{X}_{mtls}) \|$$

Model Resolution Matrix:  $\mathbf{M}_{rm} = \{ (\mathbf{K}^{T}\mathbf{K} + \lambda \mathbf{R})^{-1}\mathbf{K}^{T} \} \mathbf{K}$ Degree freedom in Retrieval:  $DFR_{nor} = trace(\mathbf{M}_{rm}) / \min(m, n)$   $\mathbf{X}_{rtv} = \mathbf{X}_{ig} + (\mathbf{K}^{\mathrm{T}} \delta \mathbf{Y}^{-2} \mathbf{K} + d\mathbf{X}^{-2})^{-1} \mathbf{K}^{\mathrm{T}} \delta \mathbf{Y}^{-2} d\mathbf{Y}_{\delta}$ 



**OEM:** A set of measurement  $\mathbf{X}_{oem} = \mathbf{X}_{ap} + (\mathbf{K}^{\mathrm{T}} \mathbf{S}_{e}^{-1} \mathbf{K} + \mathbf{S}_{a}^{-1})^{-1} \mathbf{K}^{\mathrm{T}} \mathbf{S}_{e}^{-1} d\mathbf{Y}_{\delta}$ Chi-Square test:  $\chi_{resd} = \mathbf{K} \mathbf{X}_{oem} - d\mathbf{Y}_{\delta}$   $\chi = \chi_{resd}^{T} (\mathbf{S}_{e} (\mathbf{K}^{\mathrm{T}} \mathbf{S}_{a} \mathbf{K} + \mathbf{S}_{e})^{-1} \mathbf{S}_{e})^{-1} \chi_{resd}$ Averaging Kernel:  $\mathbf{A} = \{ (\mathbf{K}^{\mathrm{T}} \mathbf{S}_{e}^{-1} \mathbf{K} + \mathbf{S}_{a}^{-1})^{-1} \mathbf{K}^{\mathrm{T}} \mathbf{S}_{e}^{-1} \} \mathbf{K}$  $DFS_{nor} = trace(\mathbf{A}) / \min(m, n)$ 



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## Characteristics of Inverse Methods

Elements	Deterministic	Stochastic
Measurement/s	True value + error	Expected value + uncertainty
Physical model	Necessary	Not always (e.g. regression)
Parameters	True value	Random variables
Inversion	Single pixel	A set of measurements
Validation(for a set of measurements)	RMSE= Systematic + Random	Bias (stability) + SD (uncertainty)
Names	Tikhonov, L-M, G-N, LS, TLS, RTLS, TSVD etc.	OE, M-L, Id-var, Regression
EOS/Satellite inversion	A little known	Widely used



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## Information Content

Based on Shannon & Weaver (1949) information content study based on stochastic assumptions:

 Rodgers stated (p. 34-37, 2000): information of measurement is the changing of entropy of the state space before and after measurement and it is given for remote sensing radiative transfer inverse problem as:

$$\mathbf{H} = \mathbf{S}(\mathbf{p}_1) \cdot \mathbf{S}(\mathbf{p}_2)$$

• After simplification final form for information:

$$H = -\frac{1}{2} \ln |I - A|$$
 For LS, A=I, H=0!



# Data and Forward model specifications

- Forward model using ver. CRTM2. I
- Monthly matchups pixel collocated data
- Buoy (coastal, Moore & drifters)
- □ Sensors: GOES13, MTSAT2, MODIS-A, VIIRS
- iQUAM quality control data
- Using GFS ancillary data (NRT operational)
- Night time scenarios
- CMIP5 climatology standard aerosol
- □ OEM error covariance: difficult in operation
- Cloud detection is major issue
- Bias for Skin-bulk, forward model and measurement



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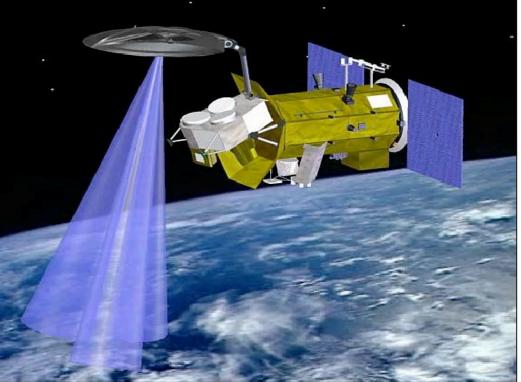
## **OEM** error covariances

VIIRS (3.7 4.0 11 12): Ambiguities 0.12 0.04 0.03 0.03 (Boryana Efremova et al JGR 2014) 0.065 0.078 0.038 0.070 (JPSS ATBD 474 474-00048) MTSAT2: http://www.wmo-sat.info/oscar/instruments MODIS-A: Xiaoxiong Xiong IEEE TGRS, 47, 2009 GOES13: NOAA Technical Report NESDIS 131 Fast forward model (CRTM2.1) error. It is very difficult to estimate correct forward model error. We assumed: ~0.2K near 4  $\mu$  m channels (due to many absorbers in this region, which is considered in CRTM2.1) and  $\sim 0.1$  K for other channels.



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## **Clear Sky Assumptions**



### **Experimental Filter**

$$rtv_{3.9} = (T_{3.9} - BT_{3.9}) / K_{3.9}$$
$$abs(SSTb - rtv3.9) < 1$$



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### Systematic Errors for various model

- I. Forward model biases (SRF, approximation RT equations, Parameterizations, profiles etc.
- 2. Instrument biases (calibration, recalibration, drifting etc.)
- 3. References biases (systematic skin-bulk error)

**Experimental set up**: Bias correction  $(BC_{ls})$  is made based on the mean difference between the LS solution and SST<sub>b</sub>. MTLS or TLS based algorithm minimizes the cost function using orthogonal LS, as compared to ordinary LS equally weights all measurement..Thus MTLS bias correction is made:

$$BC_{mtls} = \frac{\sum_{i=1}^{m} \omega_i}{m \times \max(\omega_i)} BC_{ls}; \quad \omega = K_{s.}$$

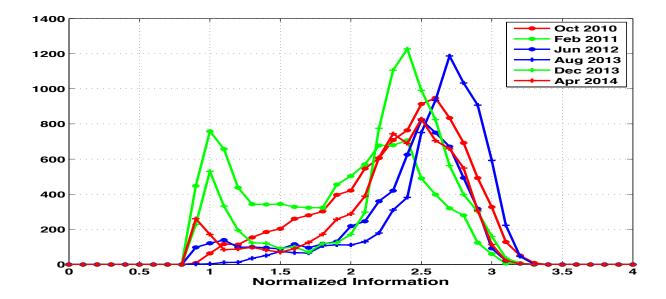
Bias is an error. It generates from Models errors and should be objectively corrected at source.



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# Normalized Information for SST retrieval from GOES13 using OEM

• NI=H/min(m,n)



One measurement cannot produce more than one piece of information.



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## **Degree of Freedom**

 $DFR_{nor} = trace(\mathbf{M}_{rm}) / \min(m, n)$  $DFS_{nor} = trace(\mathbf{A}) / \min(m, n)$  $\mathbf{A} = \{ (\mathbf{K}^{T} \mathbf{S}_{e}^{-1} \mathbf{K} + \mathbf{S}_{a}^{-1})^{-1} \mathbf{K}^{T} \mathbf{S}_{e}^{-1} \} \mathbf{K}; \quad \mathbf{M}_{rm} = \{ (\mathbf{K}^{T} \mathbf{K} + \lambda \mathbf{R})^{-1} \mathbf{K}^{T} \} \mathbf{K} \}$ 

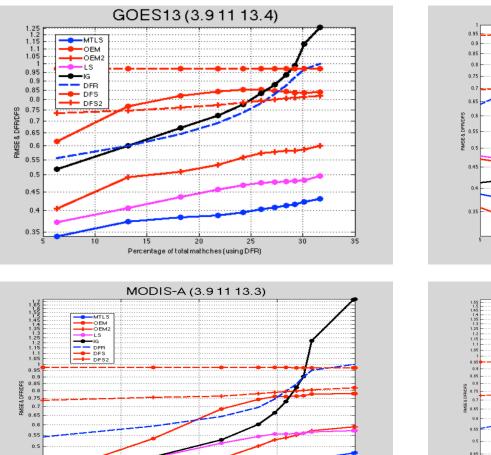
### □ Normalized DFS/DFR of LS is one.

Thus we add LS in comparison study of MTLS & OEM as a reference.

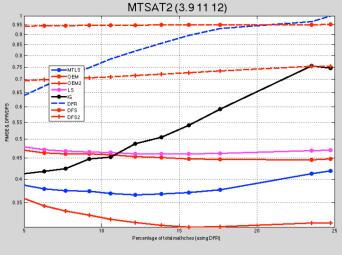


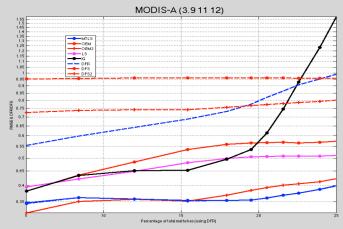
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## DFS/DFR and Retrieval error using three sensors for the month of June 2014



Percentage of total mathches (using DFR)

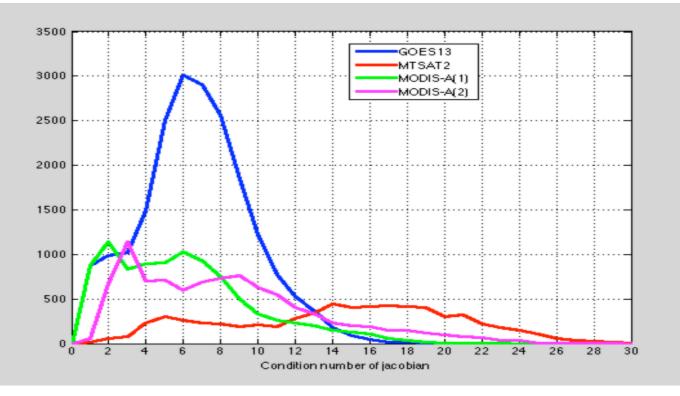






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## **Distribution of Condition number**

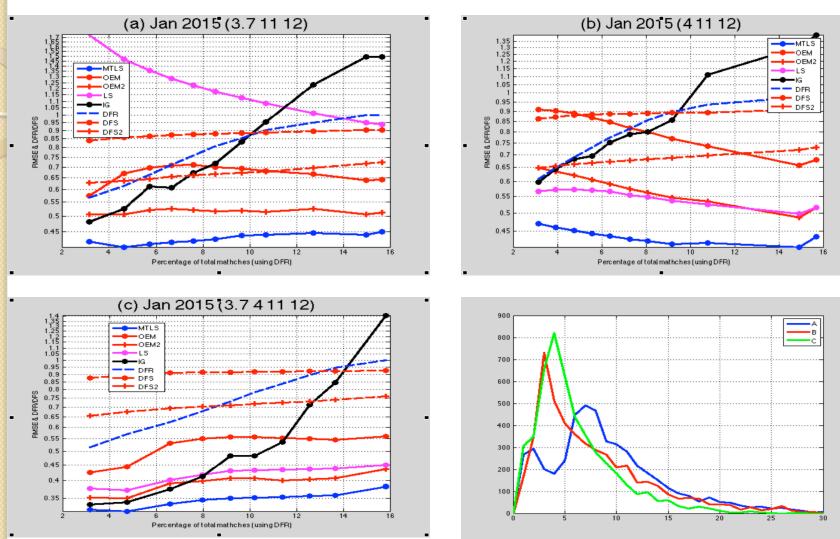


Condition number of jacobian containing 13.4  $\mu$  m hannel is lesser than the same of 12  $\mu$  m channel.



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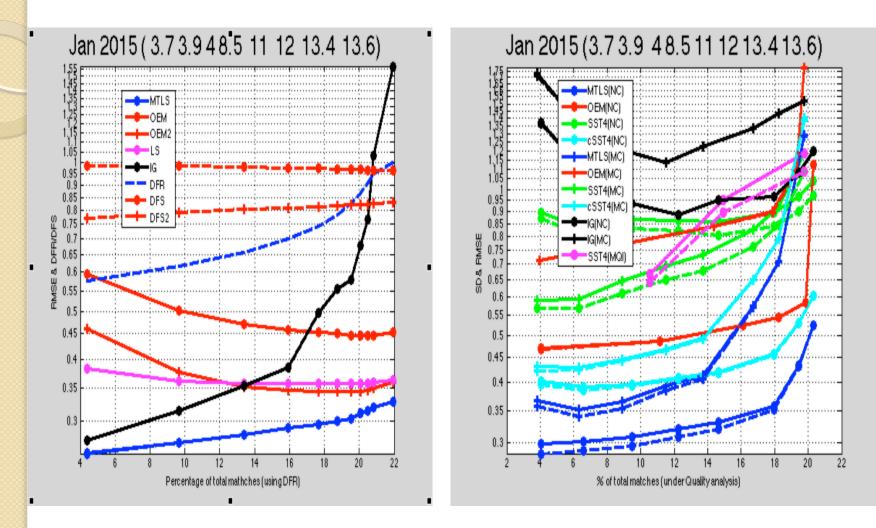
### DFR/DFS of VIIRS for various channels combinations





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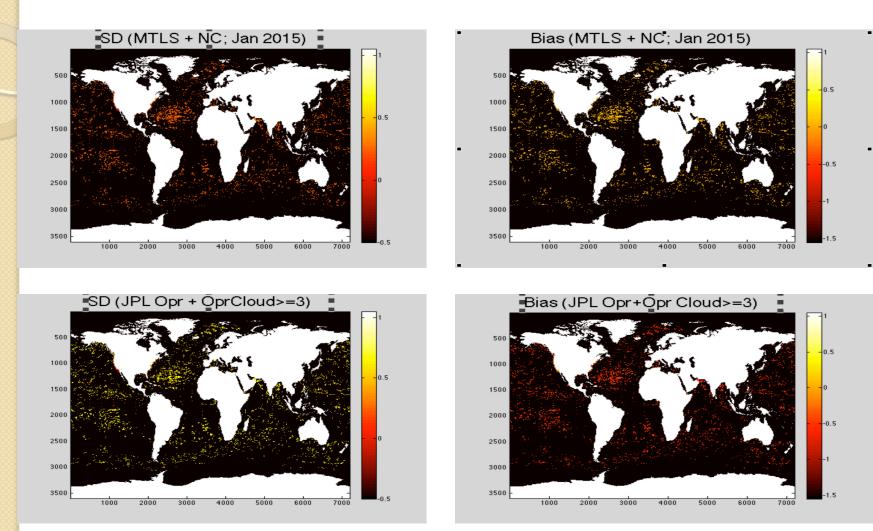
### **Results of MODIS-A for multichannels**





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### Validation Map for MODIS-A SST





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## Summary and conclusions

- Developmental history of inverse algorithms and sensitivity study.
- In our study, MTLS shows the best performance
- This study also shows that for majority of cases, OEM solutions contain higher error than that of a priori.
- Additionally, whether OEM outperforms LS or vice versa depends on the condition number of the problem in hand. (discussed theoretically at the beginning, and shown practically)
- Sensitivity study shows that: a low DFR/DFS does not necessarily mean a more accurate product. In other words, DFR alone is inadequate to characterize the true sensitivity.
- The success of MTLS is attributed to its data-driven regularization, i.e., when IG error is high, regularization is low and vice versa.

## THANKS!