Jet Propulsion Laboratory
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Simulation-Based Uncertainty Quantification for Infrared Sounder Atmospheric Retrievals

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Outline

Outline

- NASA Earth Science Data Products
- UQ Perspective
- Infrared Sounders: AIRS
- Simulation-Based UQ
- Extensions

NASA Earth Science

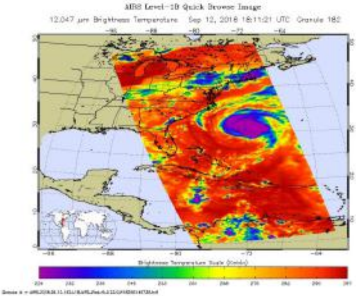
https://science.nasa.gov/earth-science/earth-missions

See also: NASA’s Eyes on the Earth

Data Products

Data product pipeline for NASA Earth-observing satellites

- Level 1: Instrument data (radiance spectra) that have been processed to sensor units
- Level 2: Derived geophysical variables at the same resolution and location as Level 1 source data.
- Level 3: Variables mapped on uniform space-time grid scales, usually with some completeness and consistency.
- Level 4: Model output or results from analyses of lower-level data



AIRS Level 1 product airs.jpl.nasa.gov

Data Products

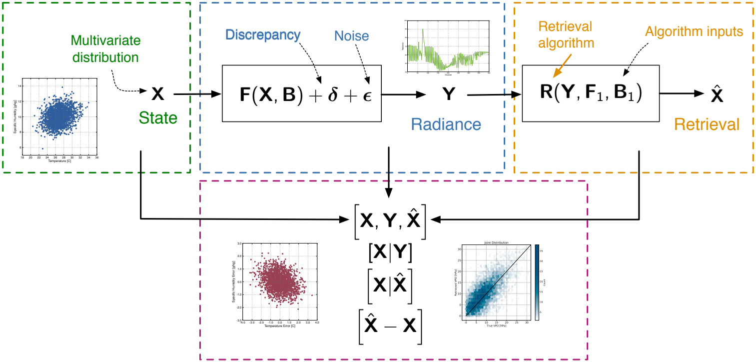
UQ Perspective on Data Product Pipeline

- Level 1 $\rightarrow$ Level 2 is an inverse problem known as a *retrieval*
  - UQ approach: Braverman, et al. (2021)
  - IR sounder implementation in current work
- Level 2 $\rightarrow$ Level 3 requires characterization of L2 uncertainty
  - Multiple Platforms: Kalmus et al. (2022)
- Level 2 (or L3) $\rightarrow$ Level 4 is another inverse problem, often data assimilation

Uncertainty

- Uncertainty represents lack of knowledge about a geophysical quantity of interest (QOI) *after observing relevant data*.
- The true value of the QOI, $\mathbf{X}$, is generally unknown, so plausible/likely values must be characterized.
- Probability offers a coherent framework for representing the distribution of the QOI, or the plausible error $\hat{\mathbf{X}} - \mathbf{X}$, given an estimate $\hat{\mathbf{X}}$ based on observed data.
- Earth science data records are relying on increasingly complex methods for constructing estimates $\hat{\mathbf{X}}$.
    - Remote sensing retrievals (Level 1 $\rightarrow$ Level 2) using satellite radiances and radiative transfer models
    - Data assimilation using Earth system models and multiple data sources

OSUE



- Observing system uncertainty experiment (Turmon and Braverman, 2019) characterizes joint distribution of complex observing system

AIRS

- The Atmospheric Infrared Sounder (AIRS) on Aqua has provided remote sensing data for weather and climate since 2002
- Growing constellation of IR sounders on multiple platforms
- 3×3 array of AIRS *fields of view* (FOV) within AMSU *field of regard* (FOR)

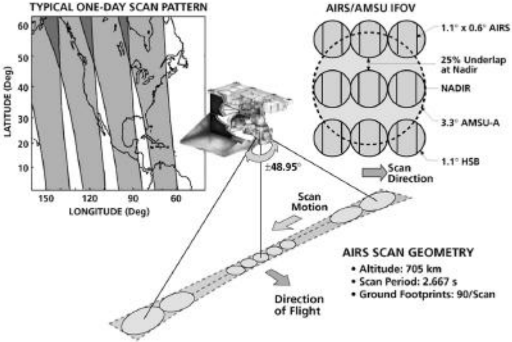


Fig. 1 from Aumann et al. (2003)

AIRS Spectra

- AIRS observes at 2378 visible and infrared (IR) spectral channels
- Thermal IR spectra sensitive to thermal emission from the atmosphere and surface
- Water vapor absorption
- Additional trace gas absorption: O_3, CO, CO_2, CH_4, among others

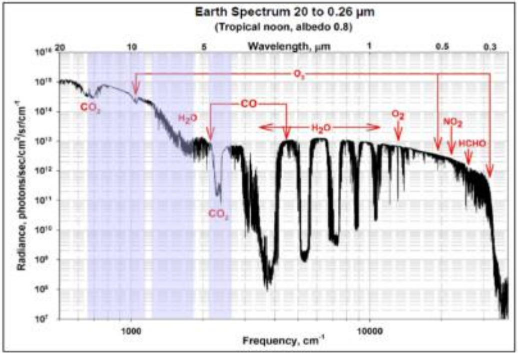
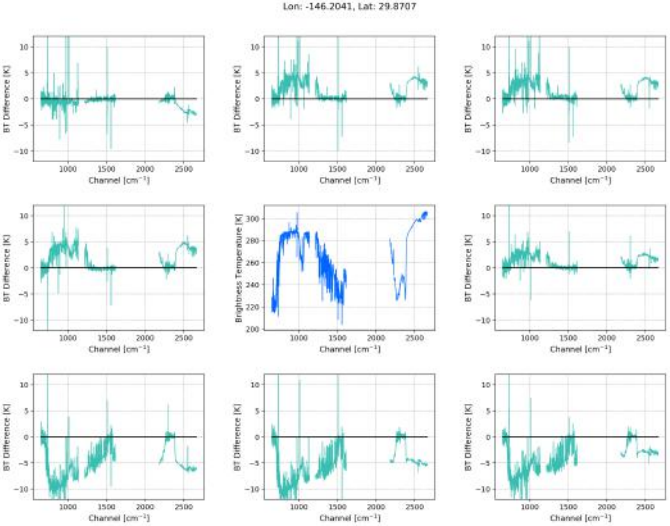


Figure credit: J. McDuffie and ReFRACtor team

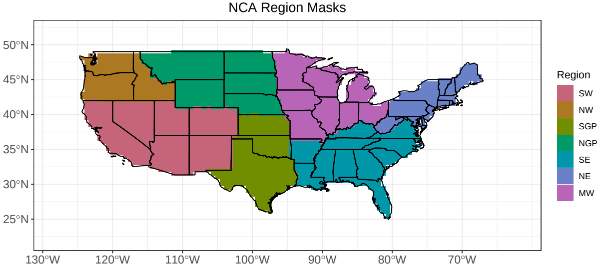
Clouds

- Variability among FOVs due to variable cloud cover



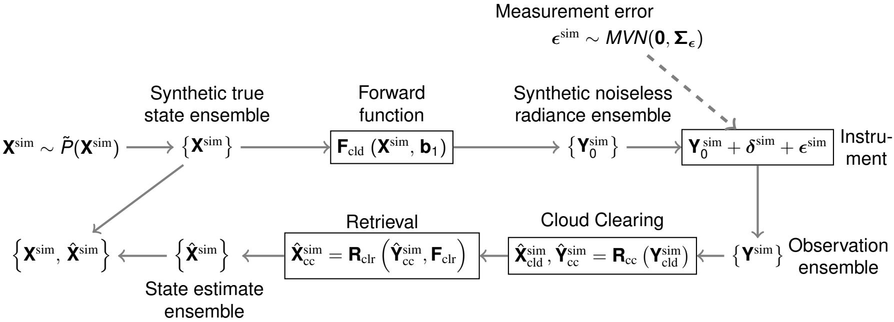
Templates

- UQ experiments performed under a specific set of atmospheric and observing conditions: a *geophysical template*.
  - Range of times, locations, observing conditions
  - Reference data (reanalysis, in situ data)
- AIRS templates motivated by applications: data fusion and downstream use of temperature and humidity retrievals (Behrangi et al., 2016)



Templates for CONUS Climate Regions

AIRS Implementation

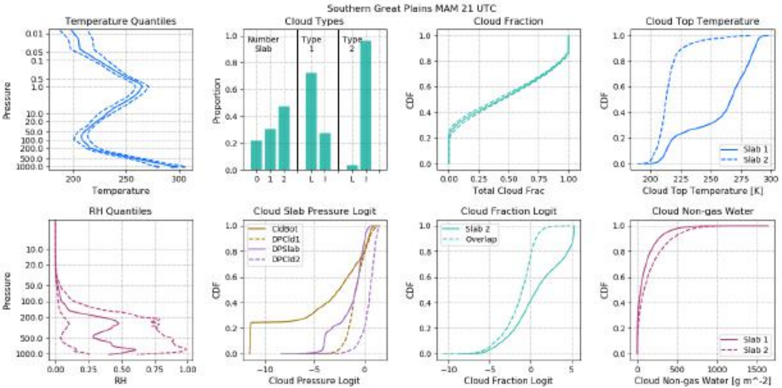


- $\mathbf{F}_{\mathrm{clr}}$: Stand-alone AIRS Radiative Transfer Algorithm (SARTA)
- $\mathbf{F}_{\mathrm{cld}}$: Two-slab SARTA (DeSouza-Machado et al., 2018)

State Vector

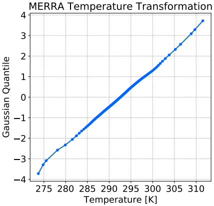
- State vector includes temperature, humidity, clouds, and surface properties
- General state vector setup for IR sounding

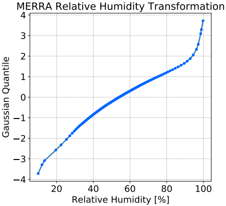
$$\mathbf{X} = \begin{bmatrix} \mathbf{X}_T & \mathbf{X}_{WV} & \mathbf{X}_{sfc} & \mathbf{X}_{gas} & \mathbf{X}_{cfrac} & \mathbf{X}_{cphys} \end{bmatrix}^T$$

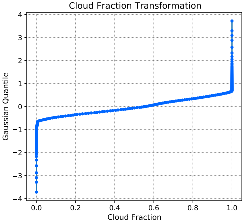


Probability Model

- State vector ensembles can be informed by reanalysis, model nature run, and actual retrievals.
- Develop probabilistic representation using mixture modeling.
  - Apply quantile (normal score) transformation to preserve physical/logical constraints.
  - Monte Carlo Expecation Maximization (MCEM) to estimate joint distribution.
- Synthetic states randomly generated from fitted model.



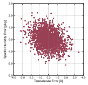




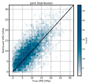
Probability model: Gaussian mixture with quantile transformation

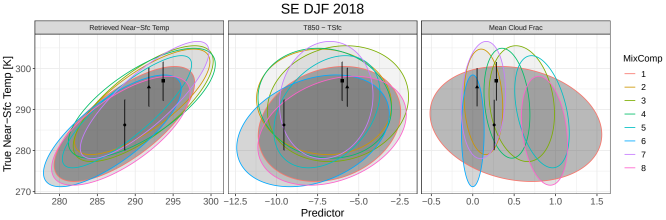
Analysis

- Experiment yields joint distribution for true $\mathbf{X}^{\mathrm{sim}}$ and retrieved $\hat{\mathbf{X}}^{\mathrm{sim}}$ states and any derived QOIs (e.g. near-surface temperature).
- Inference may focus on conditional distribution, $\left[\mathbf{g}(\mathbf{X}^{\mathrm{sim}})|\hat{\mathbf{X}}^{\mathrm{sim}}\right]$
- Construct single-sounding prediction intervals, possibly bias-corrected (Braverman et al., 2021)



$$\left[\mathbf{X}, \mathbf{Y}, \hat{\mathbf{X}}\right]$$
$$\left[\mathbf{X}|\mathbf{Y}\right]$$
$$\left[\mathbf{X}|\hat{\mathbf{X}}\right]$$
$$\left[\hat{\mathbf{X}} - \mathbf{X}\right]$$

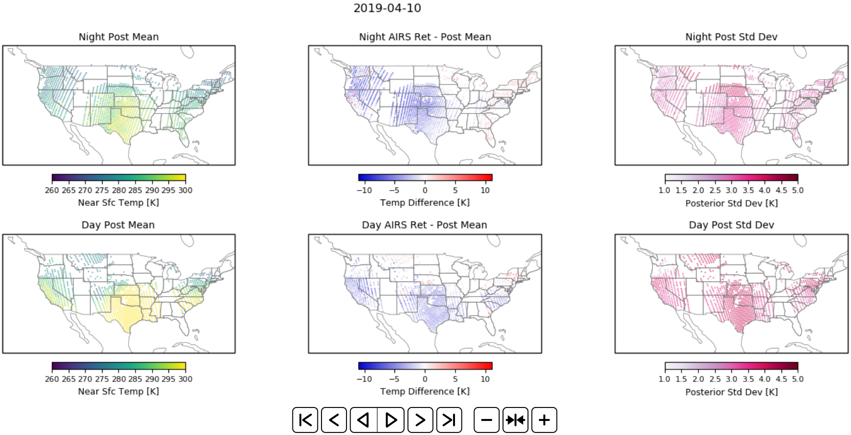




Gaussian mixture model for $\left[\mathbf{g}(\mathbf{X}^{\mathrm{sim}})|\hat{\mathbf{X}}^{\mathrm{sim}}\right]$

AIRS Operational Retrievals

- GMM estimated from simulation applied to operational AIRS retrievals, $\left[\mathbf{g}(\mathbf{X})|\hat{\mathbf{X}}\right]$

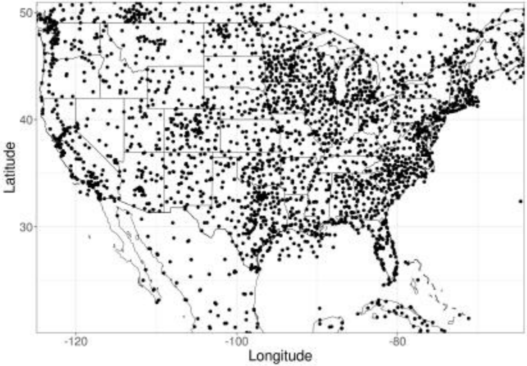


ISD Evaluation

- Evaluate *predictive distributions* for near-surface temperature
  - AIRS: Gaussian centered at retrieval with error estimate as std dev
  - UQ: Produces a full distribution (samples can be drawn)
- Validation with colocated surface observations from Integrated Surface Database (ISD)
- Figures of merit
  - PIT: Probability integral transform; predictive CDF evaluated at ISD value; result a value between 0 and 1; uniform distribution desirable
  - CRPS: Continuous ranked probability score; probabilistic extension of mean absolute error; result in units of quantity of interest (e.g. Kelvin)
- Example densities and results for selected individual retrievals

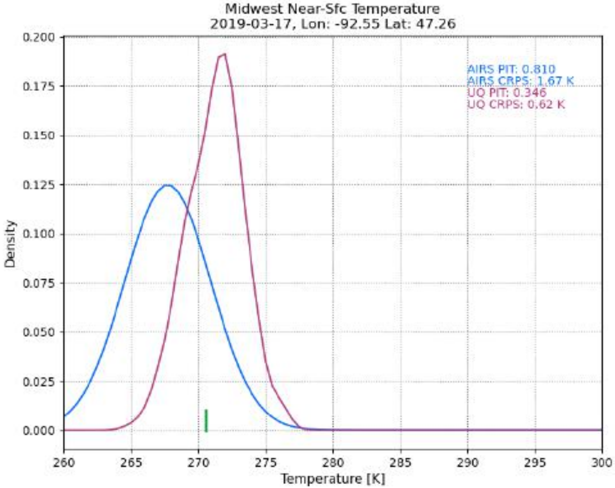
ISD

- Integrated Surface Database (ISD) ground station data available from NOAA
- Stations provide hourly or finer
- Spatial matchups to AIRS retrievals where available
- Additional uncertainty due to representativeness



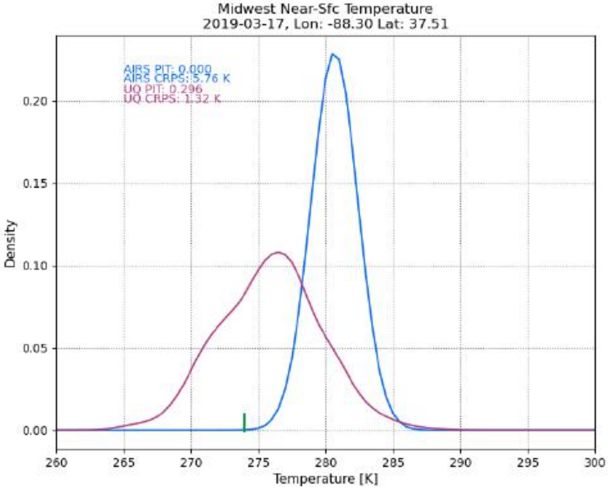
ISD surface station locations over CONUS (Kalmus et al., 2022)

Example 1



Predictive probability density plots for AIRS operational retrieval and simulation-based UQ. Green bar depicts ISD validation near-surface temperature.

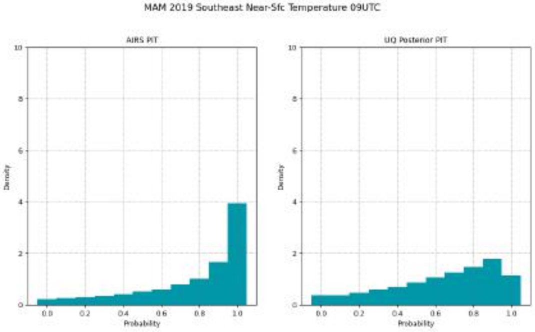
Example 2



Example with UQ making a favorable bias correction. Additionally, UQ produces asymmetric or multi-modal predictive distribution.

ISD Evaluation

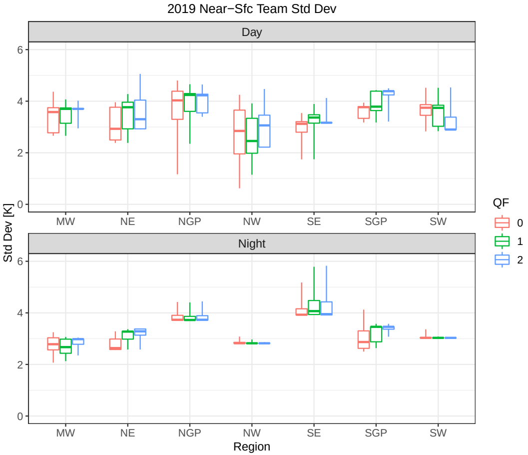
- ISD evaluation particularly favorable for simulation-based UQ for night (descending); mixed results for day (ascending)
- Specification of model discrepancy δ vital for reproducing regional patterns of bias
- Modification involving distribution of $\mathbf{F}_{\mathrm{clr}}(\hat{\mathbf{X}})$ under investigation



Summary of single-retrieval PIT values for AIRS operational intervals (left) and simulation-based UQ GMM distributions (right) for the CONUS Southeast region.

Extensions

- Regional and diurnal patterns in conditional variabiility are evident
- Science investigations and applications can make use of uncertainty estimates
  - Level 3-4 products
- UQ can supplement additional product information on data quality



Summary of GMM conditional standard deviations

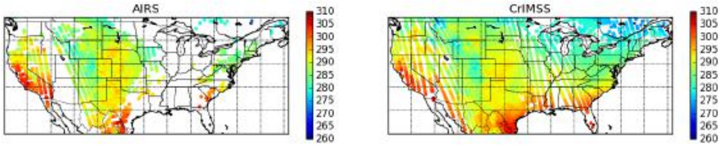
Extensions

- Additional vertical temperature information available from AIRS
- Retrieval quality and precision generally worst near surface
- Spatio-temporal modeling and prediction can be aided by sounding-specific information (Konomi, et al. 2023)

Temperature predictions with a quality-aware spatial model (top) versus single-parameter (bottom), from Konomi, et al. 2023

Data Fusion

- Spatial statistical data fusion methodology for combining multiple instruments into Level 3 products (Kalmus, et al. 2022)
  - Exploit/account for spatial dependence
  - Enable continuity of data records
- Instruments, retrievals, and internal "error estimates" likely different



Near-surface air temperature retrievals from AIRS (left) and CrIMSS (right)

Discussion

- Lessons Learned
  - Geophysical templates and experimental design targeted to a specific hypothesis, application, or product
  - Distinguish between known but variable and unknown inputs
  - Importance of forward model misspecification or discrepancy, δ^{sim}
  - Case-specific enumeration of true state for each instance is critical
- Ongoing/Future Work
  - Model discrepancy specification
  - Application to other sounder observing systems and retrievals (SNPP CrIS), enabling use with multi-instrument data fusion
  - Incorporating multiple retrievals/footprints in the presence of spatial correlation

- Suggestions and contributions from Bill Irion, Maggie Johnson, Brian Kahn, Bjorn Lambrigtsen, Ben Smith, and Mike Turmon are appreciated.

Questions?

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