FY23 Topic Areas Research and Technology Development (TRTD)

New Bayesian Retrieval Methods at Scale

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Strategic Focus Area: Uncertainty Quantification

Objectives: The objective of this work is to develop and implement methods for rigorous large-scale spatio-temporal Bayesian inference to reduce errors and bias in retrievals of hyperspectral data from instruments such as AVIRIS-NG, EMIT, and SBG.

Background: Visible-shortwave infrared (VSWIR) imaging spectrometers have experienced rapid growth in use for Earth science, with instruments including EMIT and the Surface Biology and Geology (SBG) investigation, and multiple orbital instruments by other space agencies. These sensors aim to measure reflectance properties of the surface, but they only directly observe the light incident at the sensor which is influenced by local atmospheric conditions. Consequently, in the analysis (1) at-sensor radiances are analyzed to simultaneously estimate the atmospheric state and reflectance of the surface, after which (2) the retrieved reflectance spectra are used to infer biogeophysical properties across a wide range of science disciplines. The end products, including ecosystem functional traits, surface composition, and snow state, will be a cornerstone of SBG's contribution to NASA's Earth System Observatory in the coming decade. However, current operational retrievals ignore a key feature of imaging spectroscopy data which is the spatially-dense nature of the acquisition. Moreover, they treat each acquisition independently, ignoring the repeated biweekly observations that will accrue from sun-synchronous orbiters like SBG. In short, they treat all spectra independently and either under-utilize or do not utilize spatiotemporal covariance information. Accounting for this covariance information will dramatically reduce error in the retrievals.

Approach and Results: We formulate the hyperspectral spatio-temporal L2 surface reflectance retrieval as probabilistic graphical model for looking at joint probabilities and the conditional independence structure of a collection of random variables. Assuming a spatio-temporal field of instrument-measured high-dimensional radiances, we model the atmosphere as a spatially smooth field, and surface as a temporally slowly-changing field. We use the new Accelerated Optimal Estimation formalism within a Julia-based retrieval framework for the inference, with test data based on the recent SHIFT measurement campaign in the Santa Barbara region.

Significance/Benefits to JPL and NASA: We have for the first time demonstrated that carrying out spatio-temporal hyperspectral surface reflectance retrievals is computationally feasible, and that the uncertainty reduction that we obtain is substantial and hence highly significant. The results will help guide future uncertainty quantification efforts of hyperspectral missions. This work will help reinforce the leadership of JPL in the arena of large-scale hyperspectral retrievals. The results and algorithms may be adapted to other missions and retrieval frameworks. The team is working towards introducing / enhancing the spatial and spatio-temporal modeling in upstream operational retrievals based on the lessons learned from developing the algorithms and software.

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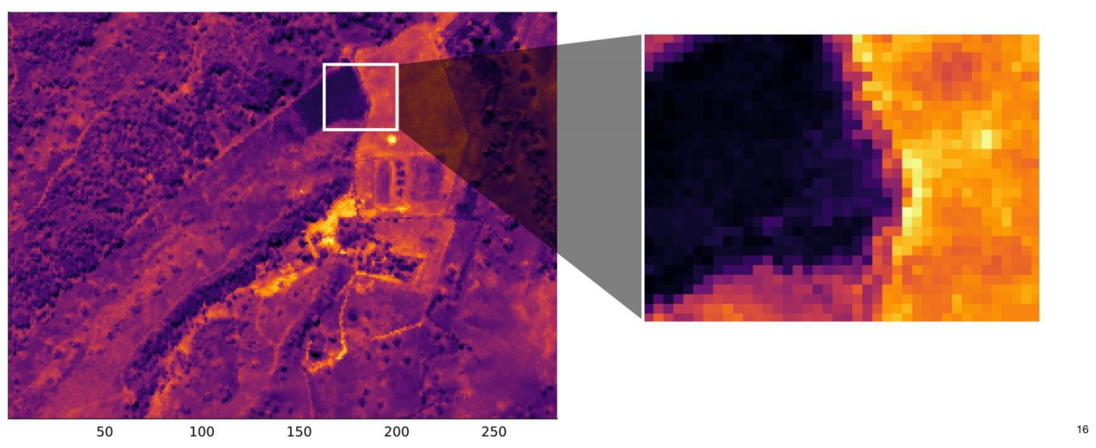
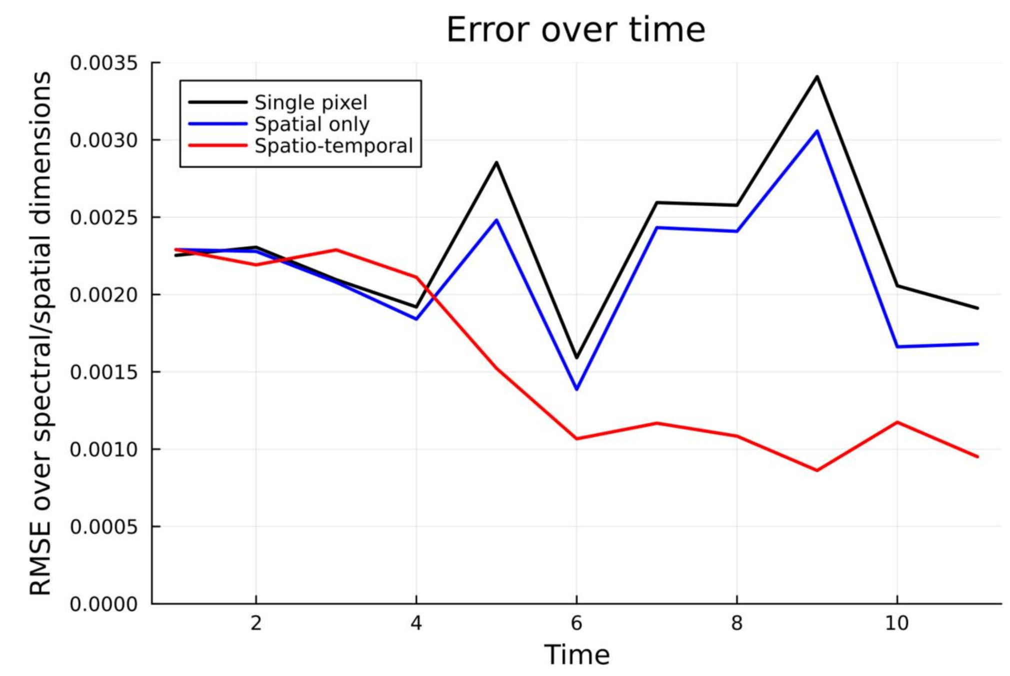
Right: The data that we use comes from the SHIFT campaign. We use the SHIFT (AVIRIS-NG instrument) radiances to generate ground truth states.

Scene from SHIFT data (Sedgwick Reserve)

- 40 x 30 pixel field that includes coyote bush, road, grass field
- 11 time steps from 02/24/2022 to 05/29/2022

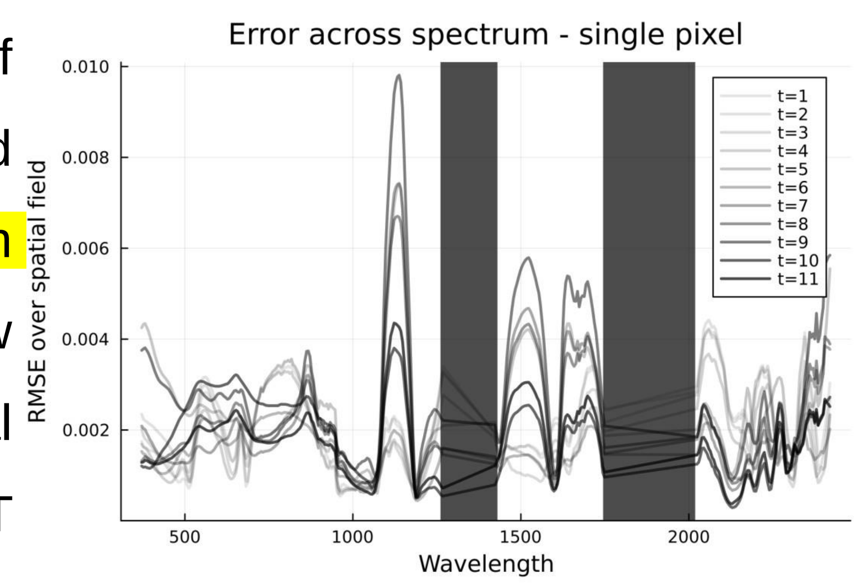


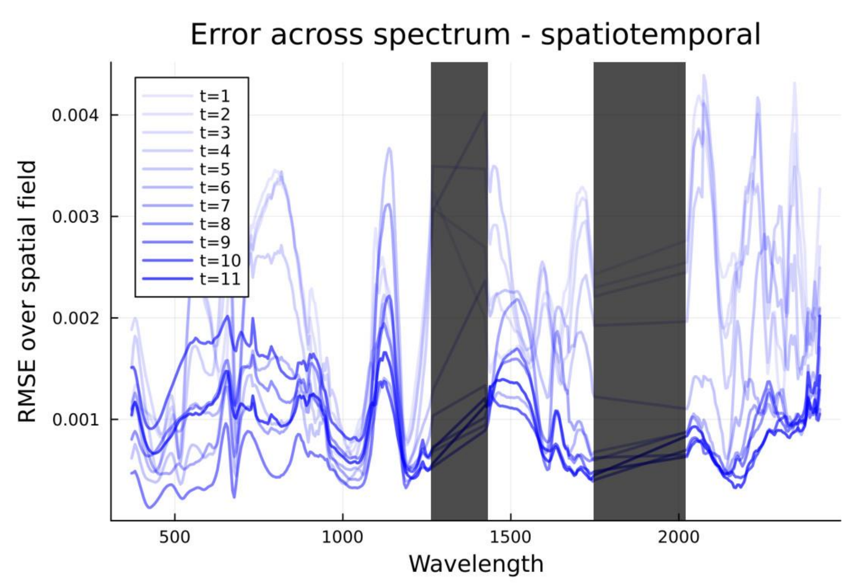


- **Absolute error** *(retrieved reflectance – truth)* normed over all spectral bands and spatial locations
- ***Single pixel*** and ***spatial only*** use the same priors
- ***Spatial only*** and ***spatio-temporal*** condition on the same atmosphere
- Increased smoothness and lower errors when incorporating spatio-temporal correlations

Above: Error decreases over time in the spatio-temporal retrieval whereas pixel-by pixel retrieval error does not really change that much. In this figure the error is averaged over all 1200 pixels in the domain of interest.

Below: Average error per spectral band at each time step for pixel-by-pixel retrievals (left) and spatio-temporal retrievals (right). Note the different y-axis scales. The error goes down for later time steps in the spatio-temporal case, whereas such trend is not visible on the left. This is to be expected. A smoothing step would further improve errors on the right hand side for the early time steps.





- Absolute error normed over spatial locations
- Single pixel has worst performance around 1100 nm (water vapour feature)
- Spatiotemporal smooths out error over the spectrum

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