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Optimal Estimation for Earth Science Imaging Spectroscopy with Multivariate Uncertainty Analysis

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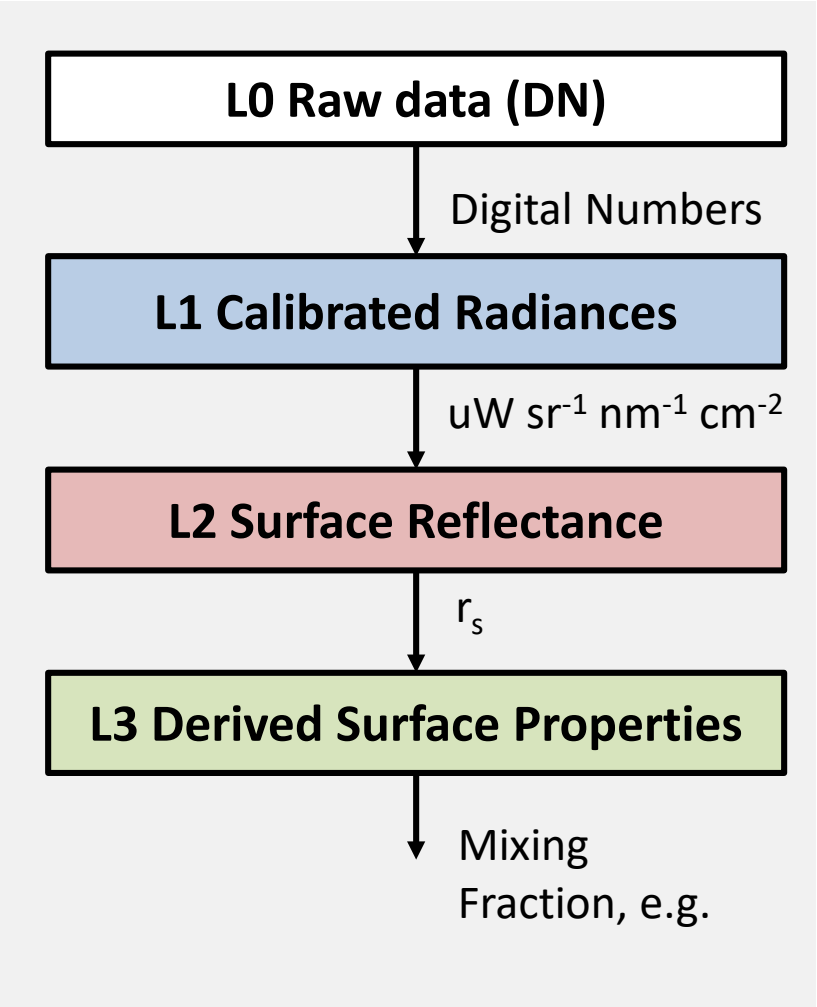
Measurements are statistical objects



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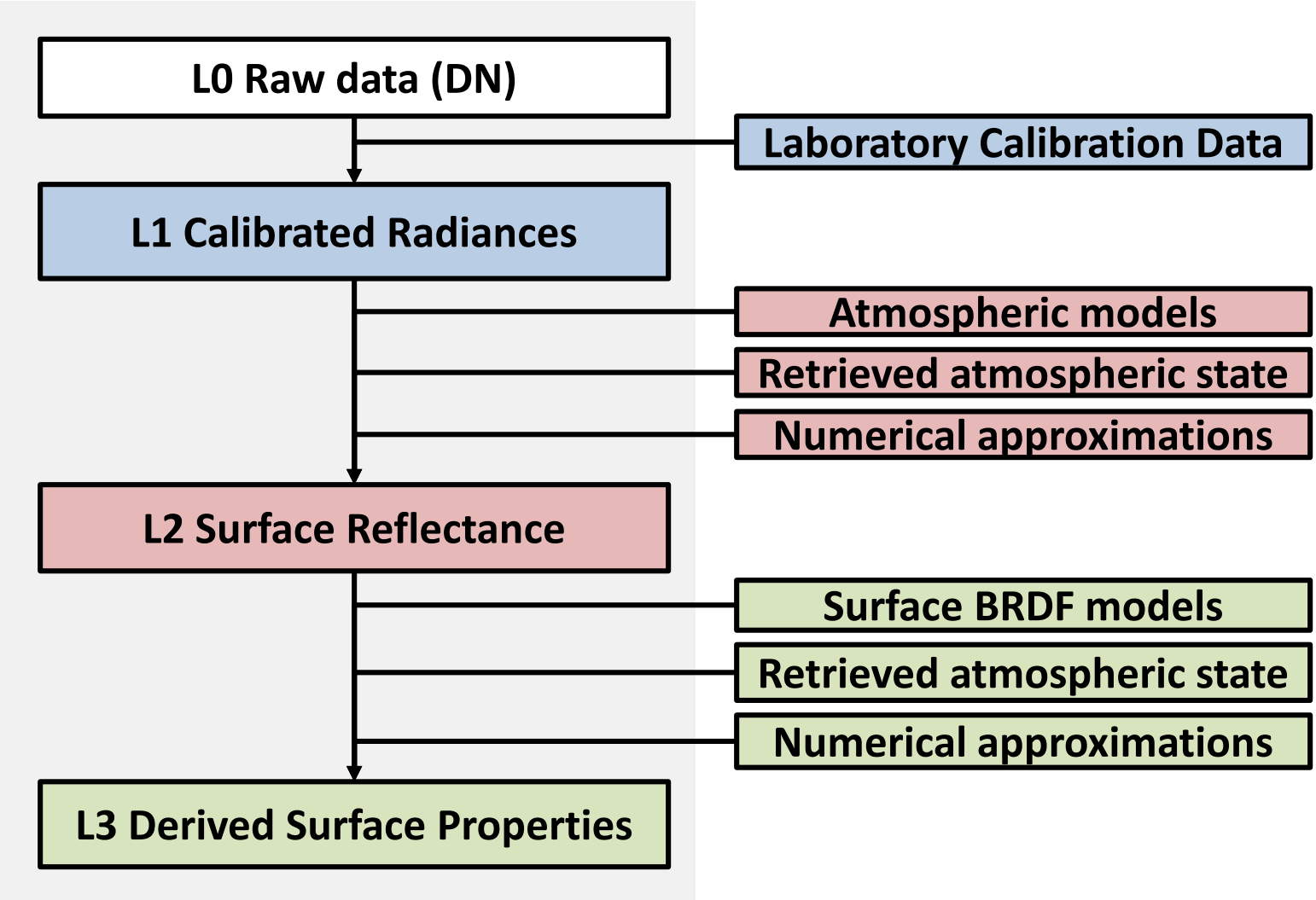
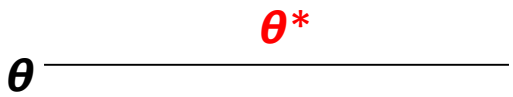
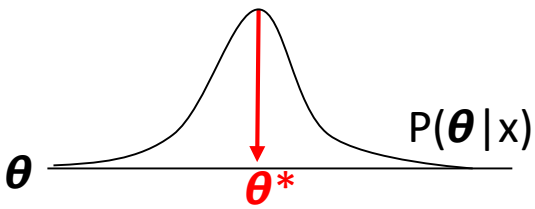


How much information should we carry across product levels?

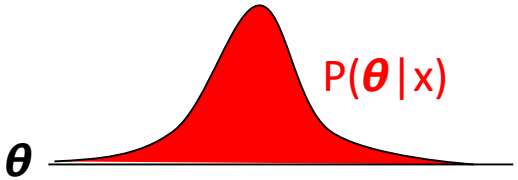
Point estimate of geophysical variable $\boldsymbol{\theta}$ given measurement x



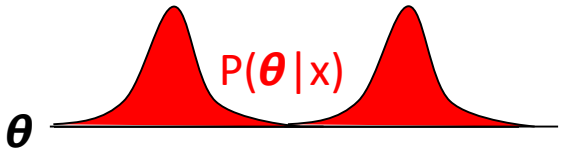
Maximum A Posteriori estimate



Full or Constrained Gaussian



Full Posterior Distsribution



Example state vector

Parameter	Degrees of Fredom	True Distribution
Radiometric gain	1	Gaussian
Radiometric offset	1	Gaussian
Spectral FWHM	1	Gaussian
Lorentzian PSF fraction	1	Gaussian
Aerosol Optical Depth	1	Exponential
Water vapor	1	Exponential
Constituents	~3	Multinomial discrete
Mixing Fractions	~2	Dirichlet
Total for $P(L_3 \mid L_0, L_2, L_3)$	**15**	**Fully connected graph?**

Conditional independence permits factorization of probability distributions

$$P(L_3|L_0) = \int_{L2} \int_{L1} \underbrace{P(L_3|L_2) \quad P(L_2|L_1) \quad P(L_1|L_0)}_{\text{Retrieval of geophysical quantities}} \quad dL_1 \quad dL_2$$

Conditional independence permits factorization of probability distributions

$$P(L_3|L_0) = \int_{L2} \int_{L1} P(L_3|L_2) \quad P(L_2|L_1) \quad P(L_1|L_0) \quad dL_1 \quad dL_2$$

$$P(L_3|L_0) = \int_{L2} \underbrace{P(L_3|L_2)}_{\text{Retrieval of geophysical quantities}} \int_{L1} \underbrace{P(L_2|L_1)}_{\text{Atmospheric correction}} \underbrace{P(L_1|L_0)}_{\text{Radiometry}} \quad dL_1 \quad dL_2$$

Conditional independence permits factorization of probability distributions

Probability distributions can be encapsulated in products permitting *exact* L3 posterior distributions.

$$P(L_1|L_0)$$

Radiometry

$$P(L_2|L_0) = \int_{L1} P(L_2|L_1) \; P(L_1|L_0) \; dL_1$$

L1 Product

Atmospheric correction

$$P(L_3|L_0) = \int_{L2} P(L_3|L_2) \; P(L_2|L_0) \; dL_2$$

L2 Product

Retrieval of geophysical quantities

Experimental Hypotheses

1. **There is measurable off-diagonal covariance structure in uncertainty**
   - Cross-channel correlations could be communicated in products
2. **Incorporating covariance structure at every product level can improve retrievals**

Method

Synthesize complete retrievals

1. L1 with added noise simulating HyspIRI [Dennison et al.] and Lorentzian PSF tails
2. L2 using LibRadTran calculation of variable
3. L3 based on nonnegative least squares of P, NPV, GV endmembers

Use three alternative estimation methods:

1. No error estimate (point mass probabilities)
2. Multivariate Gaussians, diagonal covariance
3. Multivariate Gaussian distributions, full covariance

Weight error functions by inverse error distribution

Modify spectrum fitting to account for the full uncertainty distribution

Standard least squares fitting error

$$err(x,\theta) = \frac{1}{n}\sum_{\lambda}(\hat{x} - x)^2$$

Mahalanobis distance – weight by inverse of error distribution

$$err(x,\theta) = \frac{1}{n}\sum_{\lambda}((\hat{x} - x) - \mu)^T C^{-1} ((\hat{x} - x) - \mu)$$

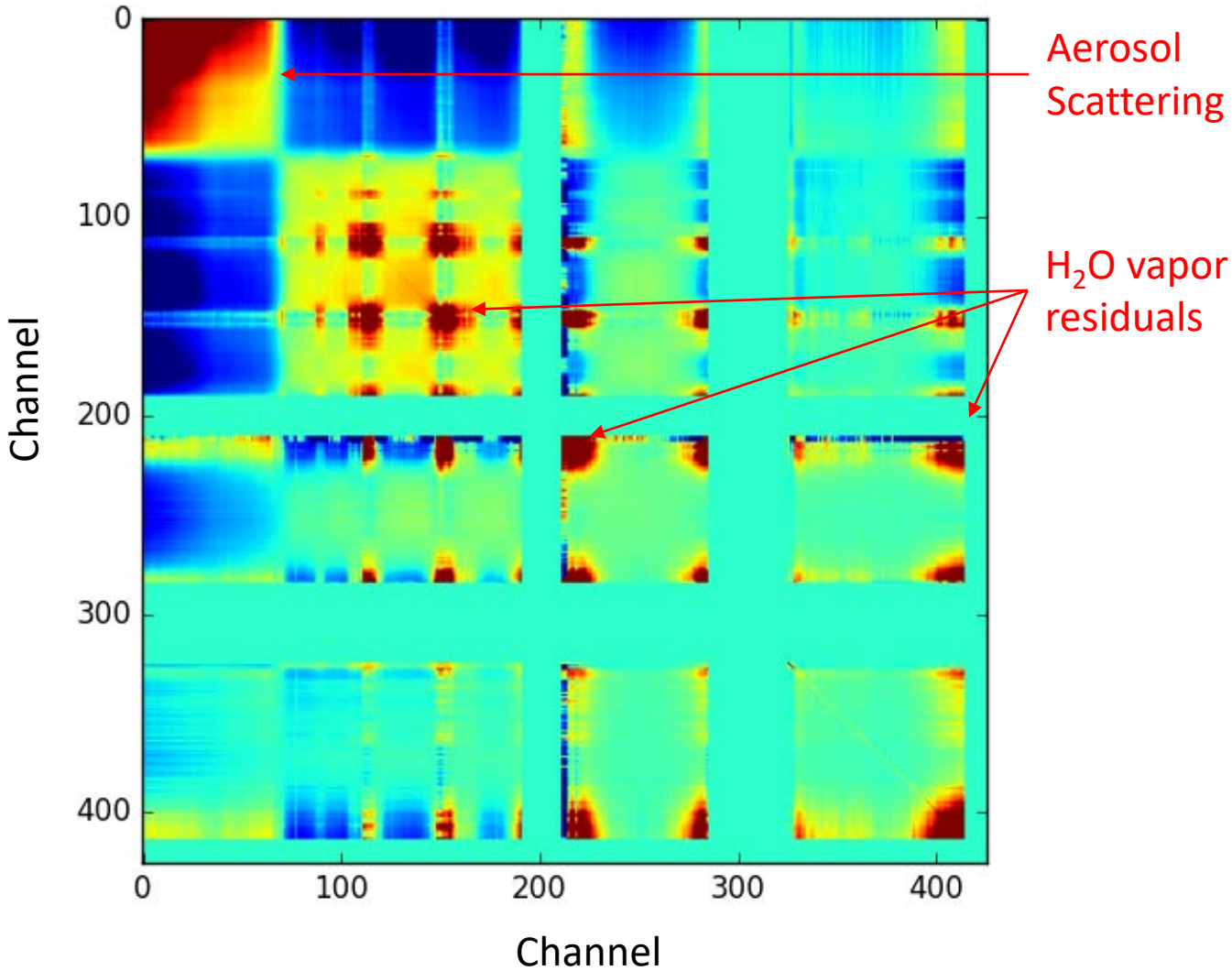
$$\frac{1}{n}\sum_{\lambda}[((\hat{x} - \mu)C^{-1/2} - (x - \mu)C^{-1/2})]^2$$

Amounts to a whitening pre-transformation of libraries and reflectance.

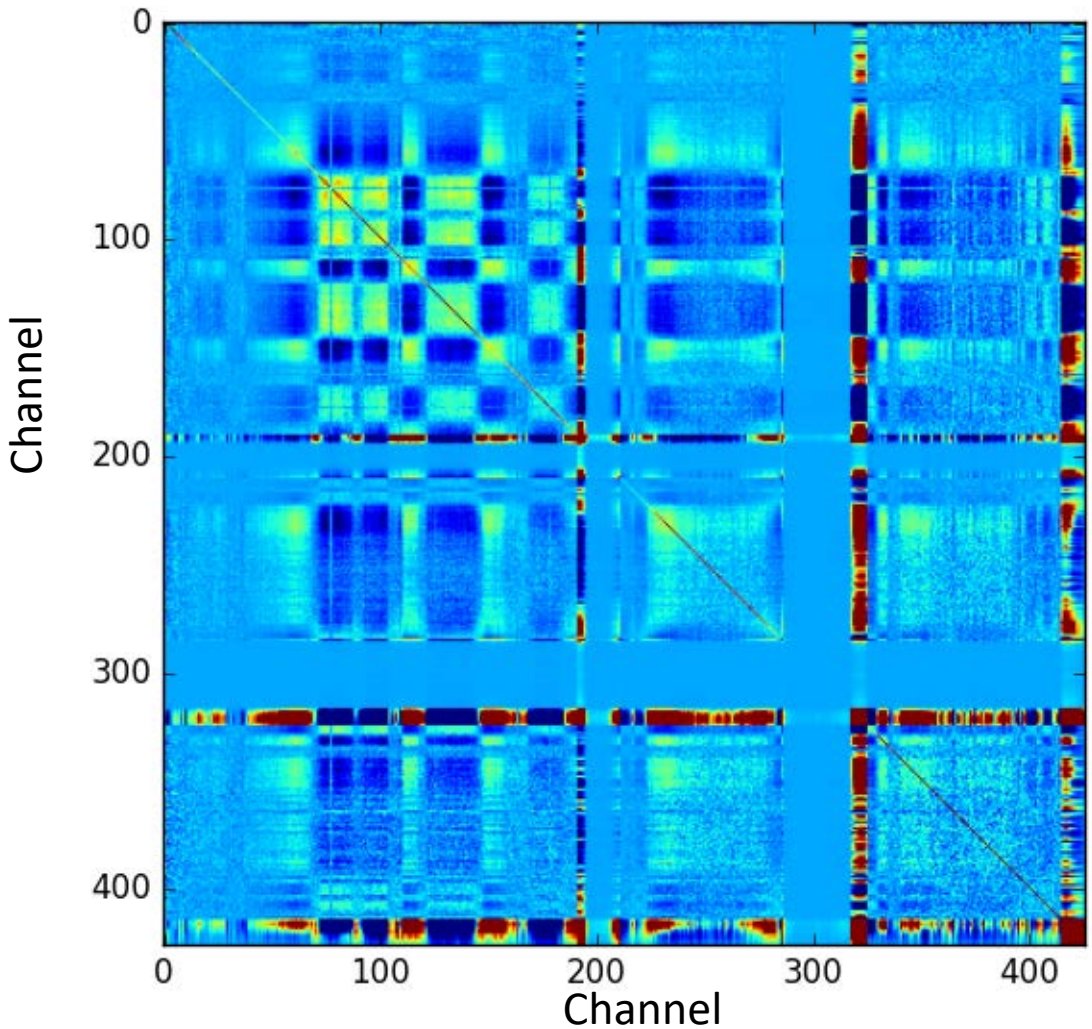
Retrieval approach

- **Linear radiometric calibration** including slope, offset terms [Green et al., 1998]
- **Parametric atmospheric correction** [Gao et al., 1993; Thompson et al., 2015]
- **MESMA unmixing** [Roberts et al., 2008]

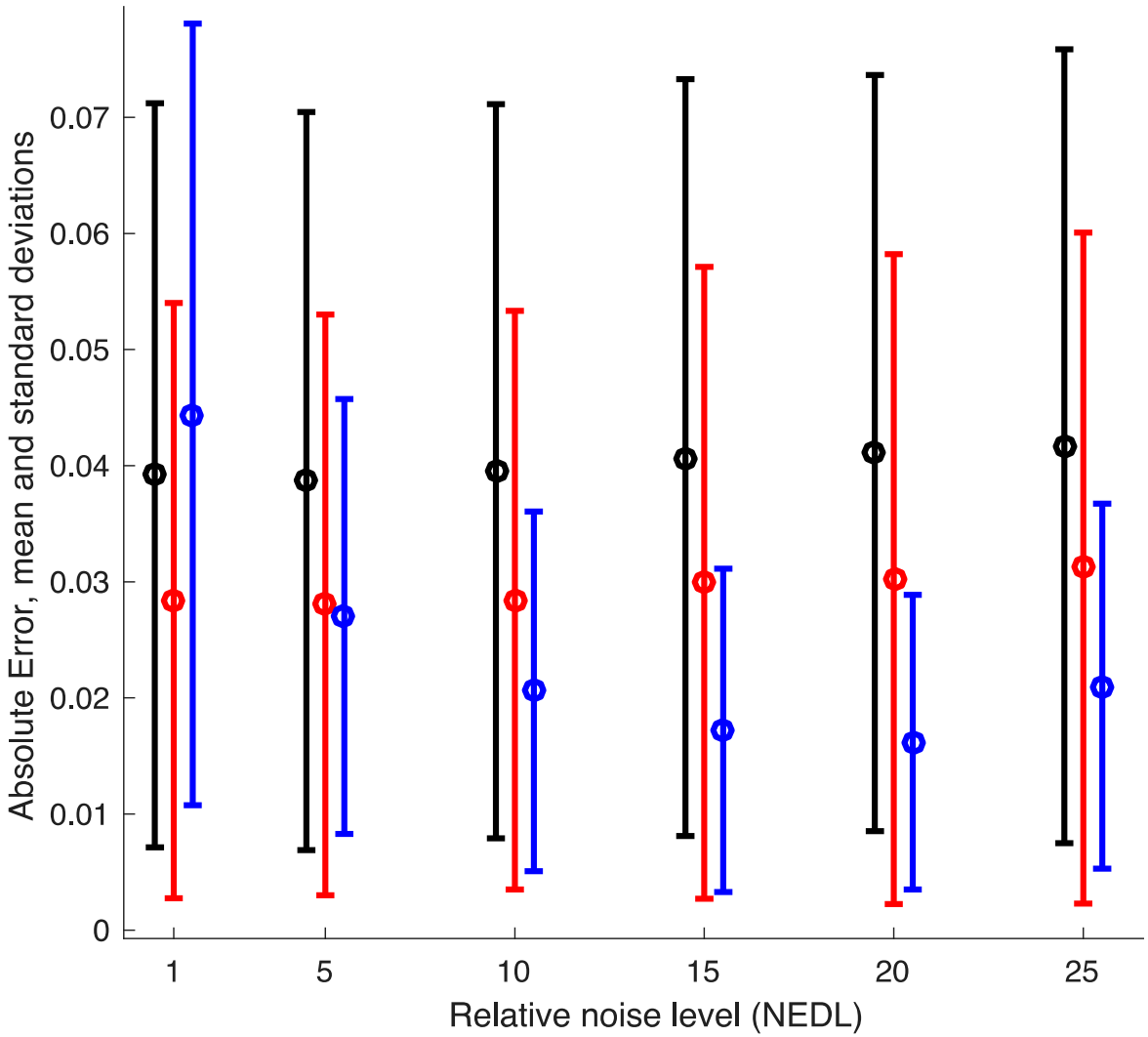
Error covariance matrix: r_s



Error covariance matrix: ρ_{toa}



Initial results for unmixing L3



Point estimate (no accounting for uncertainty)

Diagonal uncertainty covariance

Full uncertainty covariance

Future directions

- Characterize multimodality
- Consider alternative (and more complex) level 3 retrievals
  - Coastal applications
  - Atmospheric applications
- Consider empirical error estimates using field and laboratory calibration data
- Evaluate uncertainty due to modeling error

Thanks!

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- **Scientists at JPL and elsewhere** whose counsel was invaluable throughout the system design process: Andrew Aubrey, Lance Christensen, Dar A. Roberts, Brian Bue.

AVIRIS-C data is available from http://aviris.jpl.nasa.gov.

Hyperion data is available from http://earthexplorer.usgs.gov.