Verification, Validation, and Uncertainty Quantification (VVUQ) for Global Imaging Spectroscopy

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Agenda

• Motivation and Elements of VVUQ
• Example: The OCO-2 Mission
• VVUQ for imaging spectroscopy
• UQ for requirements definition
Elements of VVUQ

Calibration

Observations

Physical Earth

Measurement Uncertainty
Elements of VVUQ

- Theoretical Models
- Observations
- Physical Earth
- Validation
- Model Uncertainty
- Measurement Uncertainty
- Calibration
Elements of VVUQ

- Calibration
- Theoretical Models
- Observations
- Physical Earth
- Model Uncertainty
- Measurement Uncertainty
- Discretization, Approximation, Bugs
- Verification
- Validation

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Elements of VVUQ

Calibration

Observations

Physical Earth

Theoretical Models

Verification

Computational Models

Validation

Uncertainty

Model Uncertainty

Discretization, Approximation, Bugs

Measurement Uncertainty

Uncertainty Quantification with statistical modeling
Why is VVUQ important?

- Prerequisite for hypothesis testing and model comparison
- Achieves a more complete understanding of the observation/retrieval system
- Enables data fusion across sensors, times, regions, atmospheres
- Provides accurate uncertainty estimates for policymakers and downstream analysts
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Why is VVUQ important?

• It predicts future instrument performance to validate instrument requirements
Example: OCO-2 Mission

• Level 2 product is the column-averaged dry air mole fraction for CO$_2$ ($X_{CO_2}$)
Example: OCO-2 Mission

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• The retrieval algorithm finds a maximum a posteriori (MAP) solution within an optimal estimation (OE) framework
  – Physics-based radiative transfer model
  – Input is calibrated radiances and meteorology
Example: OCO-2 Mission

• **Validation** compares retrieved $X_{\text{CO}_2}$ to ground station measurements from the Total Column Carbon Observing Network (TCCON) throughout phase E
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- **Verification** uses software functional unit tests, end-to-end regression tests, and a forward-to-inverse tool
Example: OCO-2 Mission

• **Validation** compares retrieved $X_{\text{CO}_2}$ to ground station measurements from the Total Column Carbon Observing Network (TCCON) throughout phase E

• **Verification** uses software functional unit tests, end-to-end regression tests, and a forward-to-inverse tool

• **Uncertainty Quantification** uses the OE framework for estimating posterior uncertainty from measurement error and a priori knowledge of quantity of interest.
  – Linear sensitivity studies
  – Monte Carlo simulation studies of operational or alternative retrieval configurations
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Imaging spectroscopy case study

[Thompson et al., Remote Sensing of Environment 2018]

• AVIRIS-NG remote data
• In-situ Reagan sunphotometers
• In-situ ASD spectrometers
• Six validation sites at three locations
• Diverse surfaces, altitudes and solar illuminations
Iterative Maximum A Posteriori


Optimal estimation: A statistically-rigorous inversion incorporates prior and measurement distributions across the full spectral range. Enables rigorous uncertainty accounting.

\[ y = F(x) + \epsilon \]

Predict radiance
Iterative Maximum A Posteriori


**Optimal estimation:** A statistically-rigorous inversion incorporates prior and measurement distributions across the full spectral range. Enables rigorous uncertainty accounting.

\[
\chi^2(x) = (F(x) - y)^T S_{\epsilon}^{-1} (F(x) - y) + (x - x_a)^T S_{a}^{-1} (x - x_a)
\]

- **Cost**
- **Model match to measurement**
- **Bayesian prior**

\[
y = F(x) + \epsilon
\]
Model components

Instrument: AVIRIS-NG

Atmosphere: MODTRAN 6.0 RTM

Surface: Multi-component Multivariate Gaussians
Model components

Instrument: AVIRIS-NG
- Instrument model with Wavelength- and signal-dependent SNR
- Photon shot & read noise

Atmosphere: MODTRAN 6.0 RTM
- DISORT MS, Correlated-k
- Rural aerosol model

Surface: Multi-component Multivariate Gaussians

Pre-defined
Model components

**Instrument**: AVIRIS-NG
- Instrument model with Wavelength- and signal-dependent SNR
- Photon shot & read noise
- Uncorrelated calibration uncertainty
- Systematic calibration / RT uncertainty

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- Unmodeled unknowns, including H₂O absorption coefficients

**Surface**: Multi-component Multivariate Gaussians
- Prior based on universal library, highly regularized to permit accurate retrieval of arbitrary shapes

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Pre-defined
Statistical, fit to data
**Model components**

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Statistical, fit to data
Retrieved in the inversion

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- Unmodeled unknowns, including H₂O absorption coefficients
- H₂O, AOD retrieved

**Surface:** Multi-component Multivariate Gaussians
- Prior based on universal library, highly regularized to permit accurate retrieval of arbitrary shapes
- Reflectance estimated independently in every channel
Radiance model vs. measurement

Ivanpah Radiance

Model Estimate
Remote measurement

Green Artificial Turf Radiance

Red Artificial Turf Radiance

Lawn Radiance

Parking Lot Radiance

Dirt Track Radiance

Wavelength (nm)

μW nm⁻¹ sr⁻¹ cm⁻²

Reflectance

Inset
Reflectance estimate vs. in situ
[Thompson et al., Remote Sensing of Environment 2018]
Posterior uncertainty compared to actual discrepancies

[Thompson et al., Remote Sensing of Environment 2018]
Linear sensitivity analysis vs. Markov Chain Monte Carlo

Surface state vector elements

AVIRIS-NG at Karnataka, India 10 January 2016, Courtesy Manoj Mishra (ISRO/SAC)
Linear sensitivity analysis vs. Markov Chain Monte Carlo

Surface state vector elements

Atmospheric state vector elements

AVIRIS-NG at Karnataka, India 10 January 2016, Courtesy Manoj Mishra (ISRO/SAC)
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Forward models predict instrument performance

1. Forward-simulate observations under specific conditions
2. Perform retrievals and compare against the truth
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**Example:** For what aerosol optical depths can AVIRIS-NG achieve a required reflectance accuracy (**spectral angle < 0.03**) for the Pasadena scene?
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Example: For what aerosol optical depths can AVIRIS-NG achieve a required reflectance accuracy (spectral angle < 0.03) for the Pasadena scene?

[Graphic from Thompson et al., Remote Sensing of Environment 2018]

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Forward models predict instrument performance

[Graphic from Thompson et al., Remote Sensing of Environment 2018]
Quantifying Science Yield

**Basic**

1. **Instrument Spec** - “Back of Napkin” based on analogy to prior investigations, spectral/spatial coverage, resolution

**Refined**
Quantifying Science Yield

1. **Instrument Spec** - “Back of Napkin” based on analogy to prior investigations, spectral/spatial coverage, resolution

2. Retrieval uncertainty for representative observations

Refined
Quantifying Science Yield

1. **Instrument Spec** - “Back of Napkin” based on analogy to prior investigations, spectral/spatial coverage, resolution

2. Retrieval uncertainty for representative observations

3. Retrieval uncertainty for realistic distribution of observations
Quantifying Science Yield

1. **Instrument Spec** - “Back of Napkin” based on analogy to prior investigations, spectral/spatial coverage, resolution

2. Retrieval uncertainty for representative observations

3. Retrieval uncertainty for realistic distribution of observations

4. Posterior uncertainty in main objective, under a realistic simulated mission (full OSSE)
SBG AGU Session

Abstract ID# 416875: A Floating Vegetation Index (FVI) formed with three near-IR channels in the 1.0 – 1.24 micron spectral range for detecting vegetation floating over water surfaces
Abstract ID# 439379: Aerosol atmospheric correction of hyperspectral image data collected in India
Abstract ID# 424185: Airborne Imaging Spectroscopy of Coral Reef Condition
Abstract ID# 369132: (Invited) Change Temporary Title and Complete Invited Paper 369132
Abstract ID# 370344: Close-Range Hyperspectral Imaging of Dynamic Vegetation Communities in a High Arctic Tundra Ecosystem
Abstract ID# 399601: Compact Hyperspectral Prism Spectrometer: Recent Flight Campaign and Applications to the Future of Sustainable Land Imaging
Abstract ID# 370208: Constraining physically-based climate modeling with snow spectroscopic measurements from the Surface Biology and Geology concept
Abstract ID# 406039: DESIS on ISS, first results from commissioning phase
Abstract ID# 360017: Detection & Instrument Characterization Using Spatial Statistical Models
Abstract ID# 441816: Determining the Photosynthetic fAPARChl Canopy Fraction with EO-1 Hyperion Images
Abstract ID# 380013: Drought Response of Urban Vegetation using Airborne Imaging Spectroscopy
Abstract ID# 400233: Enabling a Threshold-Selection Algorithm for Excising Cloud-Contaminated Data Onboard Orbital Imaging Spectrometers
Abstract ID# 420163: Fast and reliable gas path-concentration inversion for thermal InfraRed (IR) hyperspectral imaging data obtained from downward looking sensors.
Abstract ID# 396086: Flight Research Techniques That Bring Results Using NASA Armstrong Airborne Science ER-2, G3, and DC-8 Aircraft
Abstract ID# 395924: High spectral resolution datasets of in situ aquatic inherent and apparent optical properties
Abstract ID# 381643: High-throughput phenotyping of photosynthetic capacities: an ensemble approach based on multiple machine learning models
Abstract ID# 426594: Hyperspectral based Mapping of Hydrothermal Altered Minerals using AVIRIS-NG Data and Machine Learning Algorithms in Hutti-Maski Gold Deposit Region, India
Abstract ID# 404173: Hyperspectral Imaging Automobile Campaign (VNIR-SWIR-TIR) in South Africa – Mineral resources applications
Abstract ID# 415403: Hyperspectral measurements identify contrasting physiological effects of different pathogens in crops
Abstract ID# 435577: Hyperspectral Remote Sensing of Optically Shallow Waters: Radiometric Challenges and Strategies
Abstract ID# 450761: HypMap: a web-based application for hyperspectral data visualization
Abstract ID# 423338: Imaging Spectroscopy Applications for Assessing Wetland Vegetation Distributions and Coastal Resiliency in Louisiana
Abstract ID# 449442: Improving Accuracy of Salt Marsh Aboveground Biomass using High-Spatial Resolution, Multi-View Hyperspectral Imaging Systems
Abstract ID# 368996: (Invited) Insights from the Decadal Survey process: Advancing global thermal infrared imaging for improved surface biology and geology science
Abstract ID# 382667: Inversion Strategies to Retrieve Snow Albedo and Temperature from Spectrometers and Multispectral Sensors
Abstract ID# 400279: Mapping REE-mineralogy using AVIRIS-NG hyperspectral data at the Mountain Pass Mine, California USA
Abstract ID# 447361: Mapping Vegetation Cover Fractions using Brightness Corrected Hyperspectral Image Mosaics and Machine Learning Regression
Abstract ID# 444240: Neural Network Radiative Transfer for Imaging Spectroscopy
Abstract ID# 382341: Prioritizing aquatic science and applications needs in the Chesapeake Bay for a space-borne hyperspectral mission
Abstract ID# 403352: Quantifying Methane Leak Emissions by Fused Airborne Imaging Spectroscopy with in situ Surface Mobile and Airborne Observations of a California Producing Oil Field
Abstract ID# 368449: Quantifying the Information Content of Global Imaging Spectroscopy
Abstract ID# 422126: Remote Detection of Plant Drought Stress Using Airborne Imaging Spectrometer Data Over a Three Year Period of Progressive Drought
Abstract ID# 455355: Seasonal and diurnal drone and ground-based thermal, multispectral and hyperspectral imaging to quantify responses of California oak woodland productivity and evapotranspiration ...
Abstract ID# 433755: Soil Color: the Spectral Soil Line
Abstract ID# 440822: Spatio-temporal Variations of CDOM in Shallow Inland Waters from a Semi-analytical Inversion of Landsat-8
Abstract ID# 408667: Spatiotemporal Rice Phenology and Imaging Spectroscopy
Abstract ID# 410193: Structure and Function of Ecosystems – a Smallsat Compliment to SBG
Abstract ID# 370934: Surface-independent Aerosol Retrieval from Hyperspectral Imagery
Abstract ID# 436010: The Impending Flood of Imaging Spectroscopy Data: Is Ecosystem Science Ready?
Abstract ID# 393836: Thermal footprints preceding volcanic eruptions
Abstract ID# 456505: Thermal Infrared Science and Applications from HyTES and ECOSTRESS in Support of Surface Biology and Geology Science
Abstract ID# 408167: Using AVIRIS-NG Imagery to Map Agricultural Systems with Binary Classifiers and Limited Field Data
Abstract ID# 449208: Using Hyperspectral Imagery and Vegetation Indices to Predict Tree Mortality in a Northeastern American Forest
Abstract ID# 360859: Utilizing Spectral Imagery to Examine High Latitude Ecosystem Function and Diversity
Abstract ID# 413454: Visible/Shortwave and Thermal Infrared Measurements at Cuprite, Nevada: Complementary or Corroborating?
Thanks!

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JPL Research and Technology Development program

NASA Program NNH16ZDA001N-AVRSN, “Utilization of Airborne Visible/Infrared Imaging Spectrometer – Next Generation Data from an Airborne Campaign in India.” Program manager Woody Turner
Backup
Posterior Error decomposition

\[ \hat{S} = GS_\varepsilon G^T + (I - A)S_a(I - A)^T \]

\[ = S_n + S_m \]

Uncertainty due to observation noise

Uncertainty due to resolution of the retrieval
Posterior Error decomposition

\[ \hat{S} = G S_\epsilon G^T + (I - A) S_a (I - A)^T \]

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Uncertainty due to observation noise

Uncertainty due to resolution of the retrieval

Vegetation spectrum

Soil spectrum

[Graphic from Thompson et al., Remote Sensing of Environment 2018]

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