

### Introduction to Imaging Spectroscopy

Dr. David R. Thompson Jet Propulsion Laboratory, Imaging Spectroscopy Group 27 August, 2019





### Agenda

Imaging spectroscopy measurement and instruments Example missions, phenomena and results for Earth and Planetary exploration Algorithms: easy and hard, monolithic and parallelizable, stochastic and probabilistic

# The nebulae promise: Increase the *effective science yield* for a given bandwidth limit



### Remote science has stringent requirements

**High accuracy:** e.g. sub-percent surface reflectance

Quantitative physical interpretability: Output reported in physical units of quantities measurable *in situ*, and traceable to rigorous physical models

**Principled uncertainty propagation:** Respect input noise, report confidence intervals

**Generalizability:** should apply across different new locales, new spatiotemporal sampling



### **Dramatis Persone**



# Measurement process – 100s of parallel spectrometers



### Imaging spectroscopy vs. multiband analysis



### Multiband

Typically built with optical filters

1-10s of bands

Image-space (morphological) analyses

Band math, thresholds, trees

Often mathematically underdetermined

Analyses are often qualitative

Empirical modeling

### Imaging Spectroscopy

Uses dispersive elements (e.g. gratings)

100s of channels

Spectroscopy using each pixel independently

Feature fitting and shape matching

Often mathematically overdetermined

Quantitative measurement with uncertainties

Empirical or physics-based modeling

Dolomite CaMg(CO3)2

010[(OH)8

2200

2500

### Imaging spectroscopy at JPL



First Imaging Spectrometer AIS flights in 1982

AVIRIS imaging spectrometer >1000 refereed journal articles

NIMS imaging spectrometer to Jupiter

VIMS imaging spectrometer to Saturn

MICAS Miniature Integrated Camera and Imaging Spectrometer to Comet

Hyperion-Earth, CRISM-Mars and ARTEMIS-Earth imaging spectrometers (gratings, designs, calibration, science)

NASA Moon Mineralogy Mapper (M3)

> 7 Airborne/Rover-type Imaging Spectrometer operating at cryogenic temperature and in a vacuum (2005-2015)















### Lunar Trailblazer Mission

Faustini crater PSR from terrain-scattered light (Cisnaros et al., 2016)



OH/H2O absorption

(blue) at 3-µm from M3

(Pieters et al., 2009)

PI: Bethany Ehlmann, Caltech



### Map of lunar water from 85 degree latitude

From [Milliken and Li, 2017]







### Agriculture and Terrestrial Ecosystems

**Geology, Soils, Surface Composition** 

# Example: Geologic Mapping via absorption fitting



## Salton Sea, CA (AVIRIS instrument)

### Courtesy NASA/JPL/Roger Clark

## Salton Sea, CA (AVIRIS instrument)



### **Cloud optical properties at high spatial resolution**

Important for sub-gridsquare GCM parameterizations and glaciation rates of mixed clouds



### **Cloud optical properties at high spatial resolution**

[Thompson et al., JGR 2016]



Tan and Storelvmo, Journal of the Atmospheric Sciences, 2016



**RGB** Image

lce Liquid Vapor



### Localized greenhouse sources



### CH<sub>4</sub> in California

[Duren et al. *Nature,* in press); Thorpe et al., 2016; Thompson et al. 2015 & 2016]





## Natural CH<sub>4</sub> emissions in the Arctic

Elder, Thompson, et al. [in preparation]





L0: Raw

**Numbers** 

Digital



## **Typical data** volumes

~15 Tb/day

possible

per day of

L2 data

L3: ? GB per Tetracorder 3.3 product Iron Oxides acquisition second Reflectance Spectrum 0.5 L2: 3 GB per 0.4 Reflecta acquisition is easily 0.3 acquisition 0.2 second 0.1 1000 1500 Wavelength (nm) 2000 2500 500 over 50 TB of data **Radiance Spectrum** L1: 3 GB per uncompressed L0acquisition second 2000 500 1000 1500 Wavelength (nm) 2500 Raw Spectrum 5000 L0: 3 GB per Value (DN) 4000 acquisition 3000 second 2000 1000

100

200 3 Band Number

300

400

Cuprite, Nevada AVIRIS 1995 Data USGS

Clark & Swayze

Hematite

Hematite Large-grained hematite

nanocrystalline

Fine-grained to medium-grained Band arithmetic or dot products (trivial)

**Closed form** linear algebra (fast)

Iterative nonlinear optimization (slower)

\*Possible external dependencies

## **Algorithms**

Fit reflectance signatures **Band ratios** Least squares **Matched filter** M.A.P model inversion

Calculate surface signal

**Topographic corrections\*** 

Iterative thermal estimation\*

**PSF** Corrections

**Radiation correction** 

**Bad pixel inference** 

**Radiometric calibration\*** 

M.A.P. model inversion\*

**Calibration** 

I/F division (standard)









Compression Lossless 4x in real time



## Iterative model inversion methods

[Thompson et al., Remote Sensing of Environment 2018, 2019a, 2019b]



### Parallelizability

### **Global scale**

 L4+ Planetary Maps and Global Models at low res

### Multiple scenes, one domain

- Region-wide Analyses
- Time series
- Possibly lower spatial resolution

### Multiple spectra, one scene

- Region of interest analysis
- Some atmospheric studies

## Independent spectra or aggregated spectra

• ALL standard products



AVIRIS-C RGB and H<sub>2</sub>O field from [Thompson et al., *Surveys in Geophys.* 2019]



### Jet Propulsion Laboratory

California Institute of Technology

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## Delta-X EV-S mission PI: Marc Simard

**Urgency:** If ignored, Relative Sea Level Rise (RSLR) will very soon have devastating consequences on the livelihood of the half billion people that live in these low-lying coastal regions. Nearly all the world's major river deltas are threatened along with the services they provide: flood protection, carbon sequestration, biodiversity and food supply.



**Delta-X Science Question:** Will river deltas completely drown, or some parts of these deltas accumulate sufficient sediments and produce enough plants to keep pace with RSLR ?





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## NASA's CORAL Mission



Thompson et al., *Remote Sensing of Environment* 2017



Hochberg et al., *Remote Sensing of Environment* 2003 08/28/2019

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### Water-leaving Reflectance

### Rb

### **Benthic Cover**

### Depth













## Agenda

- Overview and upcoming missions
- **Deep Dive 1:** Instrument characterization
- Deep Dive 2: CH<sub>4</sub> leaks, other greenhouse point sources
- Deep Dive 3: Optimal Estimation for surface/atmosphere retrievals



## **PSF** Characterization

Subtle tails of the Focal Plane point spread function can:

- Disrupt fine atmospheric structure
- Create unwanted spatial blur



## **Measurement model**





## Posit the functional forms of the CRF and SRF Optimize free parameters to match observation

1.

Method

3. Optimize free parameters to match observations via:

### 

4. Correct future data using the following linear transformation:

Find well-constrained properties of scenes' true radiance

$$L_{corr} = ((C^{T})^{+} ((S^{T})^{+} L_{meas}^{T})^{T})^{T}$$

Here, <sup>+</sup> represents the Moore-Penrose inverse, e.g.

$$C^{+} = (C^{T} C)^{-1} C^{T}$$
  $C^{+}C = I$ 




Methods include:

- Comparisons vs. lab measurements
- Pressure altitude predictions vs. DEMs
- Surface reflectance fidelity



Results from Thompson et al., RSE 2018





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# Localized greenhouse sources



# Fugitive CH<sub>4</sub> emissions at Four Corners, NM

Frankenberg, Thorpe, Thompson et al., PNAS 2016







### Aliso canyon gas storage leak

EO-1 Spacecraft at LEO, 1/1/2016

ER-2 at 6.6 km altitude, 1/12/2016



Thompson et al., *Geophys. Res. Lett.* (2016)



# CH<sub>4</sub> in California, (in review), Thorpe et al. (2015), Thompson et al. (2015)





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# Algorithms for CH<sub>4</sub> detection

The matched filter aims to detect a perturbing signal **t** against a background distribution defined by a mean vector and covariance matrix,  $\mu, \Sigma$ 

For a radiance vector **x** it discriminates two hypotheses:

$$H_0: \mathbf{x} \sim \mathcal{N}(\mu, \Sigma) \qquad H_1: \mathbf{x} \sim \mathcal{N}(\mu + \alpha \mathbf{t}, \Sigma)$$
(pure background) (background plus target)



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# Algorithms for CH<sub>4</sub> detection

The matched filter is written:

$$\hat{\alpha}(\mathbf{x}) = \frac{(\mathbf{x} - \mu)^T \Sigma^{-1} \mathbf{t}}{\mathbf{t}^T \Sigma^{-1} \mathbf{t}}$$

For interpretability, the target signature **t** is defined as the change in radiance caused by an additional unit absorption of  $CH_4$  above background.

$$\mathbf{t} = \frac{\partial \mathbf{x}}{\partial \ell} = -\mu e^{-\kappa \ell} \kappa = -\mu \kappa$$
Absorption path length
Absorption
Coefficient



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# Challenge #1: Multi-modality

The background distribution is seldom uniform. This can lead to undesirable "clutter" effects and reduction of sensitivity in general.

Sources of nonuniformity include:

- Variability in surface substrate materials
- Structured instrument effects, e.g. calibrations for pushbroom spectrometers.



# Multi-modal covariance options

Original data cube



Partition spatially (Funk et al., 2001)

Pushbroom column partitioning (Thompson et al.,



Combined pushbroom and spatial partitioning





# Multi-modal covariance estimates

Partitioning that accounts for instrument effects can mitigate deviations from calibration model assumptions



Greenhouse gas point source retrievals improved by columnwise covariance estimattion (Thompson et al., 2015)



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# Multi-modal covariance estimates

Coupling k-means background clustering with the column-wise MF provides improved robustness to background changes



AVIRIS-NG Four Corners 2015

Column-wise Matched Filter (MF) Column-wise MF with multi-modal background model



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# Challenge #2: Sample sizes

- As the number of partitions increases, it becomes increasingly difficult to estimate the covariance matrix reliably.
- This is also an issue for small flightlines.
- Poor covariance estimation reduces sensitivity.



# Approach

Shrinkage estimation regularizes the sample covariance matrix, shifting it toward a stable prior (such as a diagonal covariance matrix).



We adopt a method from Theiler et al. (Proc. SPIE, 2012) to select the optimal weighting using a closed form for cross-validation error





## Remote wind speed estimation

2 3

4 5 6 7

Plume Width (m)





Wind Speed (m/s) Large Eddy Simulations reveal a stochastic relationship between plume shape and windspeed, enabling flux estimates (Jongaramrungruang et al., in prep.)

8 9 10



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# From radiance to reflectance



GE 1266/200109 npson@jpl.nasa.gov

"AVIRIS Classic" imaging spectrometer, visible wavelengths



Retrieved Water vapor [Thompson et al., *Surv. Geohysics,* 2018]









### Global spectroscopy missions are an atmospheric correction challenge



Annual average AOD



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Thompson et al., (in review)

### Global spectroscopy missions are an atmospheric correction challenge





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Thompson et al., (in review)

Optimal Estimation Theory [Rodgers 2000]: Simultaneous estimation of surface and atmosphere

- A true spectroscopic retrieval that can exploit information distributed across the spectrum, helping to disentangle surface and atmosphere
- A rigorous probabilistic formulation incorporates prior knowledge via Bayes' rule
- Comprehensive uncertainty estimates can inform downstream analyses and global maps
- Flexible state vectors that might be more robust for difficult observing conditions
- Elegant, conceptually simple 1-step estimation



### The "forward problem"





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### The "inverse problem"





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### Maximum A Posteriori solution

$$p(\mathbf{x}|\mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{x})p(\mathbf{x})}{p(\mathbf{y})}$$

### Maximum A Posteriori solution

$$p(\mathbf{x}|\mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{x})p(\mathbf{x})}{p(\mathbf{y})}$$

The *Maximum A Posteriori* estimation is equivalent to the optimization:

$$\chi^{2}(\mathbf{x}) = (\mathbf{F}(\mathbf{x}) - \mathbf{y})^{T} \mathbf{S}_{\epsilon}^{-1} (\mathbf{F}(\mathbf{x}) - \mathbf{y}) + (\mathbf{x} - \mathbf{x}_{a})^{T} \mathbf{S}_{a}^{-1} (\mathbf{x} - \mathbf{x}_{a})$$
Cost
Model match to
Bayesian prior
measurement

... we can solve it by conjugate gradient descent.

# Maximum A Posteriori estimation







### Iterative simultaneous estimation of atmosphere and surface





# Case study

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

- In-situ AOD via Reagan sunphotometers
- In-situ surface reflectance via ASD Fieldspec

#### Ivanpah Playa



#### **Jet Propulsion Laboratory**



#### California Institute of





08/28/2019 From Thompson et al., RSE 2018. david.r.thompson@jpl.nasa.gov



# Model components

#### Statistical, fit to data Retrieved in the inversion

#### Instrument: AVIRIS-NG

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

#### Atmosphere: MODTRAN 6.0 RTM

- DISORT MS, Correlated-k
- Rural aerosol model
- broad prior uncertainties
- Unmodeled unknowns, including H<sub>2</sub>O absorption coefficients
- H<sub>2</sub>O, 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



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# Reflectance estimate vs. in situ

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



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# Posterior uncertainty compared to actual discrepancies



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


### High aerosol loading in India campaign





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High aerosol loading in India campaign

"Averaging Kernels" for H<sub>2</sub>O, and absorbing and scattering aerosol particles





### High aerosol loading in India campaign



Right: A dataset of 29 flightlines shows uniform improvements in spectral quality metrics vis a vis the AVIRIS-NG standard reflectance product. AOD estimates align with MODIS AOD retrievals from the same day (correlation coefficient r = 0.83). Left: different surfaces provide varying levels of aerosol information for the retrieval. Green vegetation is particularly well-constrained We use the most confident 5% of retrievals to form the flightline-wide estimate.



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### Aerosol mapping examples (Hawaii campaign)



AVIRIS-C f170127t01p00r16 (subset, visible bands)



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#### Combined estimate of H<sub>2</sub>O vapor, AOT, surface reflectance and





# Maximum A Posteriori vs. MCMC





# With due thanks to:

- Kevin Bowman (JPL), for much of the source material in these slides
- **Clive D. Rogers,** for theoretical foundations, approach and notation (e.g. *Inverse Methods for Atmospheric Sounding, Theory and Practice*, 2000).
- NASA Earth Science for sponsorship of AVIRIS-NG and the AVIRIS-NG India investigation and analysis.
- The JPL Research and Technology Development and NASA Center Innovation Fund Programs
- The JPL Office of Chief Scientist and Technologist
- Other coinvestigators, coauthors and colleagues including Amy Braverman, Jonathan Hobbs, Robert Spurr, Steven Massie, Bruce Kindel, Manoj Mishra, et cetera.



### Backup



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Colocasia esculenta
Polygonum punctatum/Forbs
Senesced Nelumbo/Floating Vegetation
Phragmites australis
Other Grasses



### Coastal ecosystems: wetland [Daniel Jensen, *TGARS* 2018 Control of Water" 8x SRTD

	Nelumbo	Polygonu m/ Forbs	Colocasia	Salix/ Forest	Grasses	
In Situ Points	50	19	18	30	16	
Correct Points	46	10	13	23	8	
Percent Correct	92.0	52.6	72.2	76.7	50.0	



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# Intrinsic dimensionality

- The degrees of freedom in a process under study
- Quantifies the measurable diversity in a dataset





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Laplacian Eigenmap code via Kye Taylor, Mathworks file exchange

# Dimensionality estimates must account for measurement noise



# High Intrinsic Dimensionality







NASA

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# Variability due to measurement noise vs. unknown state parameters



# Measurement noise (instrument effects)

- Photon noise
- Read noise
- Dark current noise

# Unknown parameters in the observation system

- Sky view factor
- H<sub>2</sub>O absorption coefficient intensity
- Systematic radiative transfer error
- Uncorrelated radiative transfer error

# Measuring subpixel coverage









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83/28/2000ppson@jpl.nasa.gov Yosemite Mosaic 1130503 (no color blending applied) Liquo/Ice Melting

Clouds 🍂

Half dome

[Thompson et al., RSE 2015

1 Million

CAN SELLA







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# Coincident multi-aircraft measurement







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# In situ corroborates remote data



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### Remote sensing of cloud phase



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# Example of b<sub>b</sub> endmember library





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# Example of K<sub>d</sub> endmember library





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# Case studies

- Instrument characterization PSF fitting
- Gases CH<sub>4</sub> monitoring
- Liquids Bathymetry and Benthos
- Solids- Optimal Estimation



# Performance drivers

- **Stability:** Careful temperature control and low-noise instrument electronics
- **Uniformity:** Single-detector designs, curved gratings for low-distortion and high throughput
- Alignment: Micron-level adjustment of optical components
- **Calibration:** Accurate characterization of spectral response





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Grating



Optimize via Levenberg Maquardt, minimizing:



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Posit the relation [Maritorena et al., 1994]:

$$\operatorname{Rrs}_{0} = \operatorname{R_{inf}}_{\uparrow} + (\operatorname{R_{b}}_{-} - \operatorname{R_{inf}^{-2K_{d}}})^{d} \operatorname{e}_{\text{Depth}}$$



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#### **Problem: underdetermined**

 $K_d$ , bb, and  $R_b$  yield (3N + 1) parameters for just N measurements



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#### **Problem: underdetermined**

 $K_d$ , bb, and  $R_b$  yield (3N + 1) parameters for just N measurements

#### **Solution: represent as linear mixtures**

Parameterize  $K_d$ , bb, and  $R_b$  as nonnegative linear combinations of endmember spectra, and retrieve mixing coefficients (~20 DOF)



# Airborne (2019 – 2024): Delta-X

**Urgency:** If ignored, Relative Sea LevePRisea (RSSR) and (dPLs) bon have devastating consequences on the livelihood of the half billion people that live in these low-lying coastal regions. Nearly all the world's major river deltas are threatened along with the services they provide: flood protection, carbon sequestration, biodiversity and food supply.



**Delta-X Science Question:** Will river deltas completely drown, or some parts of these deltas accumulate sufficient sediments and produce enough plants to keep pace with RSLR ?



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# Airborne (2016 – 2019): CORAL



NASA

Hochberg et al., *Remote Sensing of Environment* 2003 08/28/2019

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Thompson et al., *Remote Sensing of Environment* 2017

> 10 5

#### Water-leaving Reflectance

#### Rb

#### **Benthic Cover**

#### Depth















# Airborne (2020 - 2024): S-MODE

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## R<sub>rs</sub> vs. bottom reflectance result







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