## NASA

# Application of Inverse Methods to Atmospheric Remote Sensing

### Kevin W. Bowman

Jet Propulsion Laboratory, California Institute of Technology Joint Institute for Regional Earth System Science and Engineering, University of California, Los Angeles

### Patriarch of Atmospheric Trace Gas Retrievals

Dr. Clive D. Rodgers (Oxford University Emeritus) has had an indelible impact on atmospheric retrievals.

He brought estimation theory from statistics and electrical engineering into the trace gas remote sensing community.

Most modern trace gas satellite retrieval algorithms utilize this theory, e.g. TES, MOPITT, IASI, OMI, MLS, etc. Series on Atmospheric, Oceanic and Planetary Physics --- Vol. 2

#### INVERSE METHODS FOR ATMOSPHERIC SOUNDING Theory and Practice









### Remote sensing of the atmosphere



Atmospheric remote sensing is based upon radiative transfer, which quantifies the molecular absorption and scattering of electromagnetic radiation at different wavelengths through the atmosphere.

## Radiation Transfer: thermal infrared

In the nadir (down-looking) thermal infrared, gases absorb and emit spectral radiation (wavelengthdependent **v**).

The radiation that is emitted to space is the sum of the transmittance T and the Planck emission B at layer *i* and temperature  $T_{i}$ .

The layer transmittance is a function of optical depths, which are defined in terms of gas aborption,  $\kappa^{j}$ , and gas amount **x**<sup>*j*</sup>.



# Setting the stage: from physics to math

#### **The Forward Problem**



#### **The Inverse Problem**





# Posing your problem

•An inverse problem is the inference of parameters (or functions) of a system given observables of that system.

• How do I infer the vertical distribution of ozone given observations of infrared spectral radiances?

•Inverse problems are frequently ill-posed

The notion of ill-posed problems is attributed to J. Hadamard through the definition of a wellposed problem:

- 1. A solution exists
- 2. The solution is unique
- 3. The solution depends continuously on the data



Goal of inverse methods is to develop regularization approaches that transform an illposed problem to a well-posed problem.

# Tripartite Challenge



The retrieval problem can decomposed into 3 components:

- 1. Forward Problem: What is the relationship between what can be measured and what we want to know?
- 2. Inverse Problem: How to determine what I want to know given what can be measured.
- 3. What is the relationship between what has been estimated ("retrieved") with what I want to know?



# The Forward Model



$$\mathbf{y} = \mathbf{F}(\mathbf{x}) + \mathbf{n}$$

•y what you measure.

- •F is the forward model
- •x is the state vector (what you want to know)
- •n is the noise vector (the precision of your measurement)

Inverse methods hinge upon an understanding of the functional properties of **F** and *a priori* knowledge of **x** and **n** 

 $\hat{\mathbf{x}} = \mathbf{R}(\mathbf{y})$ 

# How to be sensitive: the Jacobian

We start by representing the equation of radiative transfer as a vector valued non-linear function:

$$\mathbf{F}(\mathbf{x}) = \begin{bmatrix} f_1(\mathbf{x}) \\ f_2(\mathbf{x}) \\ \vdots \\ f_M(\mathbf{x}) \end{bmatrix} \quad f_m(\mathbf{x}) : \mathbb{R}^N \to \mathbb{R}$$

We will focus on the Taylor series expansion of the forward model

$$\mathbf{F}(\mathbf{x} + \delta \mathbf{x}) \approx \mathbf{F}(\mathbf{x}) + \nabla \mathbf{F}(\mathbf{x}) \delta \mathbf{x}$$

For linear problems,  $\nabla F$  does not depend on x. For, nonlinear problems it does.

# How to be sensitive: the Jacobian

The Jacobian can be written more explicitly as



where  $x_n = [{f x}]_n$  for compactness, we'll redefine the Jacobian as  $abla {f F}({f x}) = {f K}_{f x} = {f K}({f x})$ 

The Jacobian describes how much an observable will change if the state changes.

### Test case: ozone

NA SA

Characterization of the vertical distribution of ozone is critical to understanding its role in atmospheric chemistry and climate



### Jacobians and the greenhouse gas effect





# Filling the columns



define the sensitivity of the radiances to ozone at a *specific* altitude



In the thermal infrared, vertical resolution is obtained by exploiting the pressure dependence of spectral lines

At a spectral resolution of 1.43 cm<sup>-1</sup>, At the spectral radiances respond the *in the same way* to changes to the vertical distribution of ozone dis

At a spectral resolution of 0.07 cm<sup>-1</sup>, the spectral radiances respond differently to changes in the vertical distribution of ozone.



# Filling the rows



The rows of the Jacobian define the sensitivity of a *specific* radiance to ozone for each altitude.



# The Inverse Problem



How often does that happen? From physics to statistics.

Let's say that we made some guess,  $\mathbf{x}_0$ , about ozone at a particular place, e.g., Boulder. What would we see at the instrument?

$$\mathbf{y} - \mathbf{F}(\mathbf{x_0}) \approx \mathbf{K}(\mathbf{x} - \mathbf{x_0}) + \mathbf{n}$$

We know about the sensitivities, K

To determine **x**, we need to know something about **x** and **n** 

If we can statistically characterize **x** and **y** in general, we can estimate **x** in particular given a measurement **y**.

### Bayes' Theorem

We want to know the probability of the atmospheric state **x**, e.g., ozone, given a measurement **y**, e.g., radiances:  $p(\mathbf{x}|\mathbf{y})$  How do we calculate it?

Start with the joint probability distribution function (pdf):  $p(\mathbf{x}, \mathbf{y})$ 

The conditional pdf is:

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

The marginal distribution is

$$p(\mathbf{x}) = \int p(\mathbf{x}, \mathbf{y}) d\mathbf{y}$$



### Bayes' Theorem

The joint pdf can be written two ways:

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

Substituting these into the conditional pdf leads to *a posteriori distribution* from the Bayes' Theorem:



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

#### Let's break it down:

 $p(\mathbf{x})$  A priori knowledge of the state

 $p(\mathbf{y}|\mathbf{x})$  Observation given knowledge of the state (data distribution)

$$\mathcal{D}(\mathbf{y})$$
 Marginal distribution. Need integration of the joint pdf

# The Multivariate Gaussian case



The data mean and covariance can be defined as

 $E[\mathbf{n}] = \bar{\mathbf{n}} = \mathbf{0} \quad E[(\mathbf{n} - \bar{\mathbf{n}})(\mathbf{n} - \bar{\mathbf{n}})^{\top}] = \mathbf{S}_n$ 

The data model assumes measurement noise statistics are known

### Climbing the hill: MAP solution

Algebraic manipulation:

 $\ln p(\mathbf{x}|\mathbf{y}) \propto \ln p(\mathbf{y}|\mathbf{x}) + \ln p(\mathbf{x}) + \operatorname{const}_{\operatorname{purposes of estimating } \mathbf{x}}^{\operatorname{In practice } p(\mathbf{y}) \operatorname{can ignored for the}}$ 

$$\ln p(\mathbf{x}|\mathbf{y}) \propto \|\mathbf{y} - \mathbf{F}(\mathbf{x})\|_{\mathbf{S}_n^{-1}}^2 + \|\mathbf{x} - \mathbf{x}_a\|_{\mathbf{S}_a^{-1}}^2$$

 $p(\mathbf{x}|\mathbf{y})$  is the sum of Gaussians—and also a Gaussian—and has a maximum: The most probable value of  $\mathbf{x}$  given  $\mathbf{y}$ .

The Maximum A Posteriori (MAP) solution is consequently found from

$$\frac{dp(\mathbf{x}|\mathbf{y})}{d\mathbf{x}}|_{\mathbf{x}=\hat{\mathbf{x}}} = \mathbf{0} \qquad \qquad \hat{\mathbf{x}} = \int \mathbf{x}p(\mathbf{x}|\mathbf{y})d\mathbf{x}$$

The MAP solution can be written as a numerical problem:

$$\min_{\mathbf{x}} \left\{ (\mathbf{y} - \mathbf{F}(\mathbf{x}))^{\top} \mathbf{S}_n^{-1} (\mathbf{y} - \mathbf{F}(\mathbf{x})) + (\mathbf{x} - \mathbf{x}_a)^{\top} \mathbf{S}_a^{-1} (\mathbf{x} - \mathbf{x}_a) \right\}$$

# The geometry of Bayes

Bayes Theorem provides a statistical justification for the least squares problem

$$\begin{split} \min_{\mathbf{x}} \left\{ (\mathbf{y} - \mathbf{F}(\mathbf{x}))^{\top} \mathbf{S}_{n}^{-1} (\mathbf{y} - \mathbf{F}(\mathbf{x})) + (\mathbf{x} - \mathbf{x}_{a})^{\top} \mathbf{S}_{a}^{-1} (\mathbf{x} - \mathbf{x}_{a}) \right\} \\ \hat{\mathbf{x}} &= \mathbf{x}_{a} + (\mathbf{K}^{\top} \mathbf{S}_{n}^{-1} \mathbf{K} + \mathbf{S}_{a}^{-1})^{-1} \mathbf{K}^{\top} \mathbf{S}_{n}^{-1} (\mathbf{y} - \mathbf{F}(\mathbf{x}_{a})) \\ \hat{\mathbf{S}} &= (\mathbf{K}^{\top} \mathbf{S}_{n}^{-1} \mathbf{K} + \mathbf{S}_{a}^{-1})^{-1} \end{split}$$

Example: Let  $\mathbf{x} \in \mathbb{R}^3$   $\mathbf{y} \in \mathbb{R}^2$ 

- Large ellipsoid is a contour of the prior pdf
- Cylinder is a contour of the pdf of the state given only the measurement
- Small ellipsoid is a contour of the posterior pdf:



### The optimal estimate





## Characterization

# The Third Pillar: Characterization

A powerful part of this methodology is the characterization of the estimate relative to the true state.

Consider the approximation

 $\mathbf{y} - \mathbf{F}(\mathbf{x}_a) pprox \mathbf{K}(\mathbf{x} - \mathbf{x}_a) + \mathbf{n}$  substitute into the estimate

$$\hat{\mathbf{x}} = \mathbf{x}_a + (\mathbf{K}^{\top} \mathbf{S}_n^{-1} \mathbf{K} + \mathbf{S}_a^{-1})^{-1} \mathbf{K}^{\top} \mathbf{S}_n^{-1} (\mathbf{K} (\mathbf{x} - \mathbf{x}_a) + \mathbf{n})$$

$$\hat{\mathbf{x}} = \mathbf{x}_a + \mathbf{A}(\mathbf{x} - \mathbf{x}_a) + \mathbf{Gn}$$

Gain matrix

G

Averaging kernel matrix

$$= \frac{\partial \mathbf{\hat{x}}}{\partial \mathbf{F}} = (\mathbf{K}^{\top} \mathbf{S}_n^{-1} \mathbf{K} + \mathbf{S}_a^{-1})^{-1} \mathbf{K}^{\top} \mathbf{S}_n^{-1}$$

 $\mathbf{A} = \frac{\partial \hat{\mathbf{x}}}{\partial \mathbf{x}} = \mathbf{G}\mathbf{K}$ 

The optimal estimate (retrieval) is related to the true (but unknown state) by the averaging kernel matrix.



# Averaging Kernel

The averaging kernel matrix, **A**, is one of the most important characterizations of the estimate

$$\mathbf{A} = rac{\partial \hat{\mathbf{x}}}{\partial \mathbf{x}} = \mathbf{G}\mathbf{K}$$

The averaging kernel matrix describes the change in the estimate due to the change in the true state. This relationship can be further described by looking at the rows and columns of **A** with respect to the estimate.

Averaging kernel

 $\frac{\partial \hat{x}_i}{\partial \mathbf{x}} = \langle \mathbf{a}_{i,*}, \delta \mathbf{x} \rangle$ 

Impulse response

$$\frac{\partial \mathbf{\hat{x}}}{\partial x_i} = \delta x_i \mathbf{a}_{*,i}$$

## **Averaging Kernel Matrix**

The averaging kernel and the impulse response provide complimentary information about the estimate.

NA SA



The averaging kernel describes how the true state changes the estimate at a particular altitude,  $x_i$ , whereas the impulse response describes how the entire estimate changes to the true state a particular altitude,  $x_i$ .



## Where is it? Resolution

The averaging kernel provides a means of defining the vertical *resolution* of the estimate, i.e., how well can the estimate (ozone) at one altitude be distinguished from another?

The resolution can be calculated from full-width half height.



A more robust, but more abstract definition of resolution is the degrees of freedom for signal (dofs), which is the trace of the averaging kernel matrix: dofs = Trace(A)

The dofs provides a measure of the independent information that can be determined from an estimate. It can be calculated over subsets of the atmospheric state

#### The what and where of vertical resolution

The averaging kernel is a function of the sensitivity, which includes spectral resolution, precision, the inherent variability of the atmospheric state.

Different instrument designs can achieve resolution at different altitudes by making trade-offs such as spectral resolution and precision.

Sensitivity to ozone in the lower most troposphere requires much higher spectral resolution than the upper troposphere.



### The many flavors of error

The total error can be split into two useful terms:  $\hat{\mathbf{S}} = (\mathbf{K}^{\top} \mathbf{S}_n^{-1} \mathbf{K} + \mathbf{S}_a^{-1})^{-1}$ smoothing and measurement error

$$\hat{\mathbf{S}} = (\mathbf{I} - \mathbf{A})\mathbf{S}_a(\mathbf{I} - \mathbf{A})^{\top} + \mathbf{G}\mathbf{S}_n\mathbf{G}^{\top}$$

Smoothing error

measurement error

<u>Smoothing error:</u> error in the estimate from the lack of resolution (as defined by the averaging kernel).

Note that the smoothing error is dependent on the variability of the state: CO2 will be different than O3.

<u>Measurement error:</u>error from random noise.



# Putting it together

#### TES observations during the NOAA TEXAQS 2006 campaign

Pressure (hPa)

http://tes.jpl.nasa.gov/TexAQS\_2006/browse\_run4911.html



TES Nadir Retrieval Result: Ozone, 2006–08–23 Cross Section Along Orbit Track: RunID=4911, Seq=1–1, Scan=0–124, UTClime=19:34:40–19:48:31 

TES Nadir Retrieval Result: CO, 2006-08-23

Cross Section Along Orbit Track: RunID=4911, Seg=1-1, Scan=0-124, UTCtime=19:34:40-19:48:31



TES retrievals of elevated ozone and CO are seen near Houston on Aug 23<sup>rd</sup>, 2006.

How do we characterize this retrievals?



The primary driver of sensitivity for thermal instruments is surface temperature and clouds.

The TES-retrieved cloud optical depth is high off the coast of Texas but low directly on land.

The diagonal of the ozone averaging kernel shows high sensitivity in the lower troposphere.



### Where is the pollution?

**O3 AK** 

CO AK



- O3 and CO between the surface and 680 hPa and 18-20N is driven by the a priori.
- At 680 hPa, the retrievals are influenced by the true atmosphere from near surface to about 300 hPa.
- Poleward of 40N, upper tropospheric O3 sensitivity at 215 hPa increases because of decreasing tropopause height.

### **Observation operators:**

#### connecting measurements to assimilation







$$\hat{\mathbf{x}} = \mathbf{x}_a + \mathbf{A}(\mathbf{x} - \mathbf{x}_a) + \mathbf{G}\mathbf{n}$$







## **Conclusions/Future Directions**

- Atmospheric trace gas retrievals are built on 3 pillars:
  - Forward Model (atmospheric radiative transfer)
  - Inverse Model (optimal estimation)

NASA

- Characterization/Error Analysis (averaging kernels, dofs, etc.)
- Observation operators—constructed from averaging kernels—are powerful tools to compare remote sensing estimates to other data, e.g., sondes, and to assimilation systems
- Non-Gaussian, non-linear approaches, e.g., Markov Chain Monte Carlo (MCMC), will become increasingly important.



Backup

## BACKUP



# **Multi-Spectral Remote Sensing**

Image: NASA

### Two eyes are better than one: IR and UV

ASA



UV and IR measurements provide complimentary sensitivity to ozone. Worden et al, GRL, 2007 and Landgraff and Hasekamp, JGR, 2007 showed the feasibility of estimating boundary layer ozone. Fu et al, ACP, 2013 and Cuesta et al, ACP, 2013 have demonstrated the potential for TES and IASI.

# AIRS/OMI--Aug 23rd, 2006



- The TES optimal estimation retrieval algorithm was applied to the combination of AIRS and OMI radiances to infer O3 and CO.
- Elevated CO and O<sub>3</sub> in Pacific NW associated with biomass burning.
- DOFS show skill in separating upper and lower troposphere.
- DOFS and Cloud OD show the British Columbia obscured by clouds
- Elevated Texan LT ozone associated with agricultural burning and antrhopogenic emissions

Diagnosis of synthetic retrievals



# OLR bias in chemistry-climate models



ZM ozone vs TES / ppbv (acchist; 2000 slice mean)

The Atmospheric Chemistry-Climate Model Intercomparison Project (**ACCMIP**) estimated historic radiative forcing (RF) and future response using consistent emissions for the IPCC 5<sup>th</sup> assessment. (Lamarque et al, 2013)



In the tropics, discrepancies lead to over 300 mWm<sup>-2</sup> for individual models and up to 100 mWm<sup>-2</sup> for the ACCMIP ensemble.

-100

-200

mW/m2

Ó

100

200