Uncertainty Quantification for Remote Sensing Retrievals: Monte Carlo Experiments for the Orbiting Carbon Observatory-2

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Uncertainty Quantification

- IPCC Working Group I report provides estimates of the anthropogenic impact on the Earth's energy balance (Myhre, et al., 2013).
- Contributions are not perfectly estimated, and plausible values are reflected as probability distributions.
- Uncertainty arises because the climate system is nonlinear with many feedback mechanisms.
- Uncertainty quantification (UQ) targets identifying and reducing uncertainties for quantities of interest associated with complex systems (Smith, 2014).

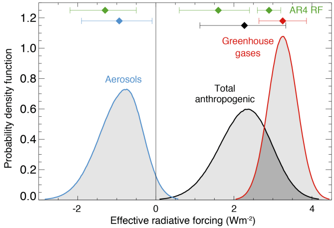


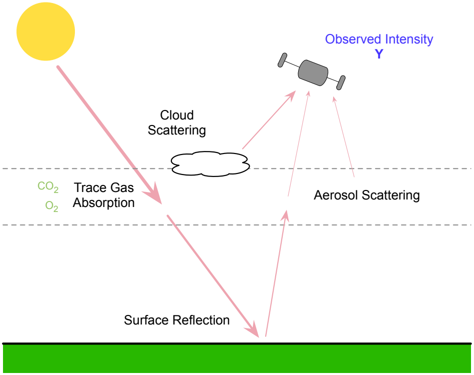
Figure 8.16 from IPCC AR5 Working Group I report

OCO-2

- Carbon cycle scientists combine data on carbon dioxide (CO_2) concentrations with process models to infer carbon sources and sinks.
- Estimates of CO_2 from satellites such as the Orbiting Carbon Observatory-2 (OCO-2) provide substantial spatial and temporal coverage.
- Satellite observations are indirect so UQ is challenging.
- Reported uncertainties, or standard errors, dictate relative weight of data in flux estimation.

http://oco.jpl.nasa.gov

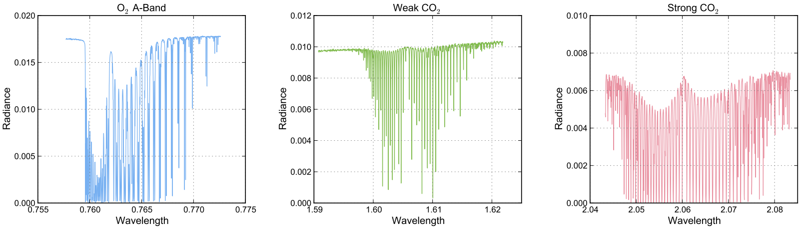
OCO-2 Measurement



- Key **state variables**, **X**, for OCO-2 include
  - CO_2 concentration
  - Pressure
  - Scattering particles
  - Surface albedo
- Observed **radiance**, **Y**, is a function of the state.

OCO-2 Measurement

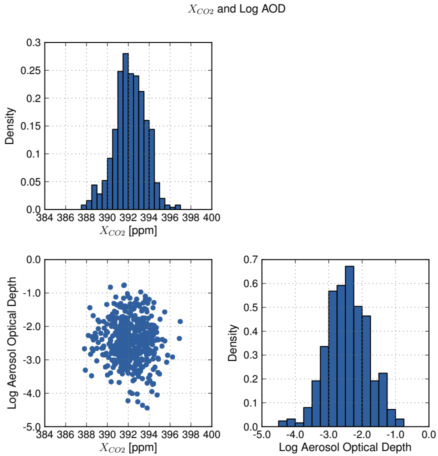
- OCO-2 observation **Y** includes radiances at 1016 wavelengths in each of three spectral bands.
- Objective is to estimate X_{CO2}, the total column CO_2 concentration, given observed radiances **Y**. The estimate's uncertainty should also be quantified.
- Inference utilizes a **forward model**, a mathematical representation of the relationship between **X** and **Y**.



Uncertainty Quantification

- Uncertainty quantification (UQ) relies on a probabilistic treatment of sources of uncertainty (Smith, 2014).
    - Inherent variability in the state or measurement process
    - Lack of complete knowledge about fixed parameters or the physical model of the process
- Monte Carlo simulation is a tool for propagation of uncertainty through a model.
- Alternatives can be necessary depending on simulation scope and computational expense.

Monte Carlo



Randomly generated ensemble of X_{CO2} and log aerosol optical depth.

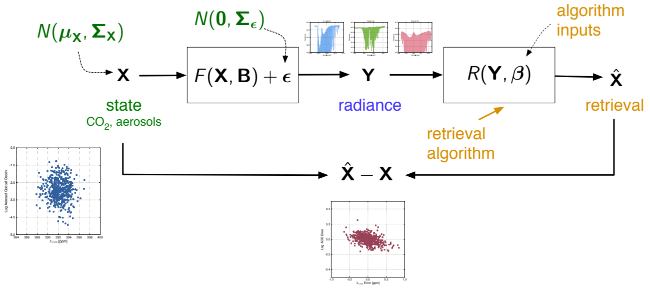
- For illustration, suppose X_{CO2} and log aerosol optical depth have a bivariate Gaussian distribution,

$$\mathbf{X} \sim \mathrm{N}(\boldsymbol{\mu}_{\mathbf{X}}, \boldsymbol{\Sigma}_{\mathbf{X}})$$

- Monte Carlo investigation begins by randomly generating state vectors **X**.
- The forward model is evaluated for each state, yielding synthetic radiances **Y**.

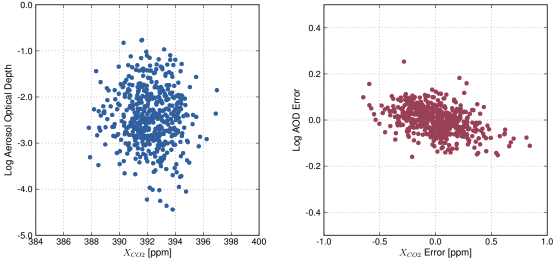
Inverse Problem

- The atmospheric state is the quantity of interest, *inverse inference* is necessary.
- A **retrieval algorithm** to produce an **estimate** is required.
- The simulation framework can interrogate the propagation of uncertainty to the retrieval.



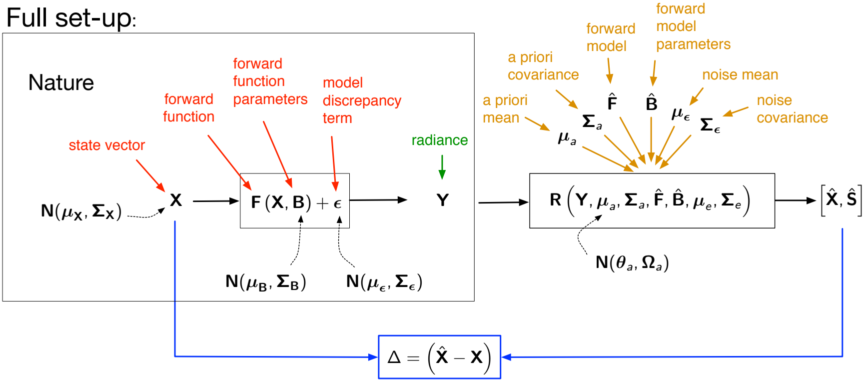
UQ for Retrievals

- Quantify the impact of retrieval choices that are subject to uncertainty on the overall bias and variance of the retrieval errors, $\hat{\mathbf{X}} - \mathbf{X}$.
- The OCO-2 retrieval problem is underdetermined and prior information is utilized in a Bayesian setting (Rodgers, 2000).
- The retrieval algorithm produces an uncertainty estimate $\hat{\mathbf{S}}$.
- The retrieval algorithm requires an **a priori mean** μ_a be input as a guess for the true ensemble mean.

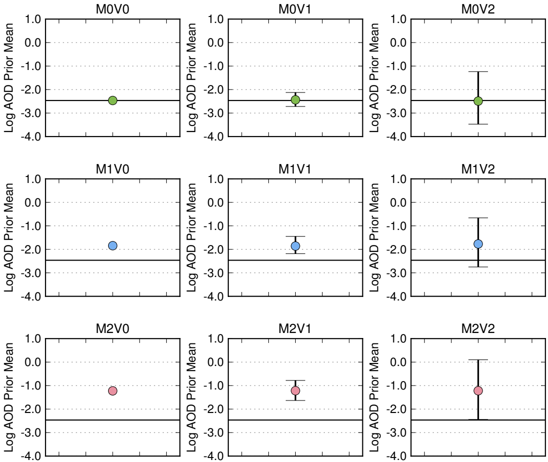


Surrogate Model Experiment

Full set-up:

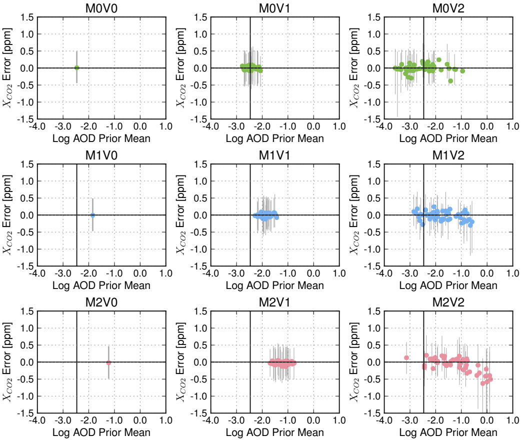


Surrogate Model Experiment



- Quantify the impact of a misspecified, uncertain **a priori mean** μ_a on retrieval bias and error covariance.
- Implement with a computationally efficient **surrogate model**.

X_{CO2} Error



- Error variance in X_{CO2} grows with increasing uncertainty in the parameter $\boldsymbol{\mu}_a$.
- Both systematic and stochastic components interact to produce largest bias in M2V2.

Error distribution for X_{CO2} under different experimental conditions. Points depict the mean and error bars enclose the center 95% of the distribution.

Experiment Summary

- Ratio of error standard deviation to reported retrieval standard deviation

$$\frac{\sqrt{Var(\Delta_{XCO2})}}{\sqrt{E(\widehat{Var}_{XCO2})}}$$

M0V0 1.025	M0V1 1.045	M0V2 1.234
M1V0 1.021	M1V1 1.026	M1V2 1.223
M2V0 0.993	M2V1 1.002	M2V2 1.648

- As uncertainty in μ_a increases, variability in realized errors surpasses the reported uncertainty.
- Bias is also largest for M2V2 treatment.

Discussion/Extension

- A geographically and seasonally comprehensive set of experiments is forthcoming. Spatially and temporally varying marginal distributions $(\boldsymbol{\mu}_{\mathbf{X}}, \boldsymbol{\Sigma}_{\mathbf{X}})$ are required.
- Methodology is general and can be potentially applied for retrievals based on physical or empirical models.
- The approach can be used to provide an estimate of the retrieval error variance when an operational algorithm does not routinely produce an uncertainty estimate.
- Other applications of UQ in inverse problems can incorporate a Monte Carlo approach.
  - Atmospheric data assimilation
  - Hydrologic model calibration

Acknowledgments

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Questions?

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