# Post-hoc Uncertainty Quantification for Remote Sensing Observing Systems

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# Outline

- Introduction
- Remote sensing observing systems
- Orbiting Carbon Observatory 2 (OCO-2) mission, science, and data
- Statistical model of the observing system and uncertainty
- Methodology
- Application to OCO-2
- Summary and discussion points

# Introduction

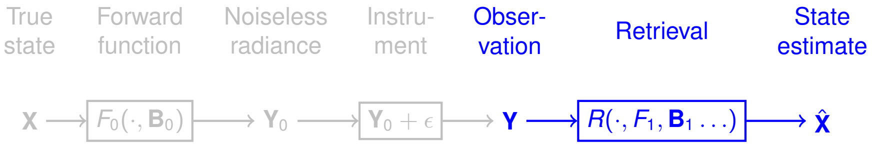
Remote sensing levels of data processing:

- Level 0: raw photon counts direct from satellite
- Level 1: georectified and calibrated radiances
- **Level 2: estimates of geophysical state**
- Level 3: “statistical summaries" of Level 2 on uniform space-time grid
- Level 4: output of models or data assimilation

*Level 2 “data" aren’t “data"; they are inferences!*

How do we calculate uncertainties of the point estimates provided by remote sensing observing systems?

## Remote sensing observing system:




Retrieval is an inference problem: estimate **X** when you only get to see **Y**.

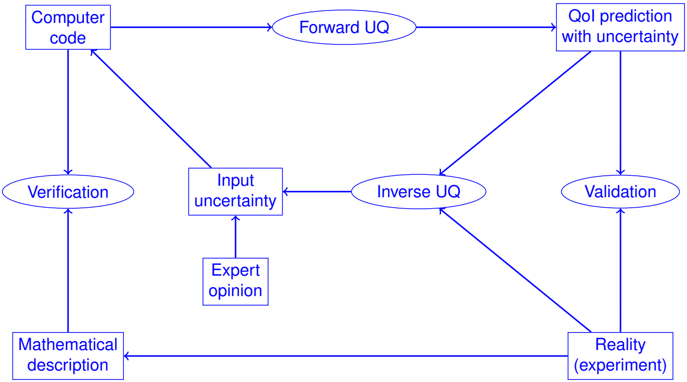
$F_0$ = nature's true forward function; $\mathbf{B}_0$ = other true quantities.

$F_1$ = forward model used in retrieval, $R$; $\mathbf{B}_1$ = other retrieval inputs.

$\epsilon$ = instrument measurement error.

$\ldots$ = other retrieval algorithm inputs.

## Uncertainty quantification:

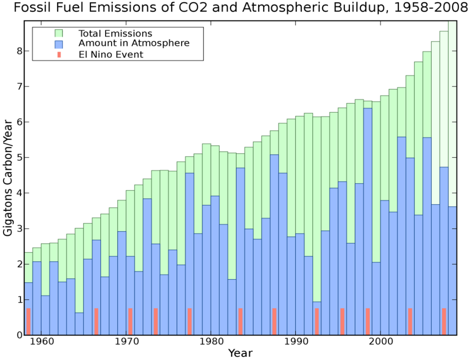



Adapted from Wu et al, (2018). DOI: 10.1016/j.nucengdes.2018.06.004.

# Introduction

- Uncertainty quantification (UQ) provides a formalism for understanding uncertainty in the output of computational models.
- Remote sensing data processing utilizes complex computational models.
- But:
    - we lack information about uncertainty of known inputs
    - there are many unknown unknowns (e.g., interaction effects)
    - computational artifacts must be taken into account
    - analysis must be performed after the fact and be computationally feasible

# OCO-2 mission and science




Graphic courtesy of Annmarie Eldering.

- Less than half of the carbon is staying in the atmosphere.
- Where are the sinks that are absorbing more than half of this $CO_2$?
- Why does $CO_2$ build-up vary from year to year with nearly uniform emission rates?
- How will $CO_2$ sinks respond to climate change?

# OCO-2 mission and science

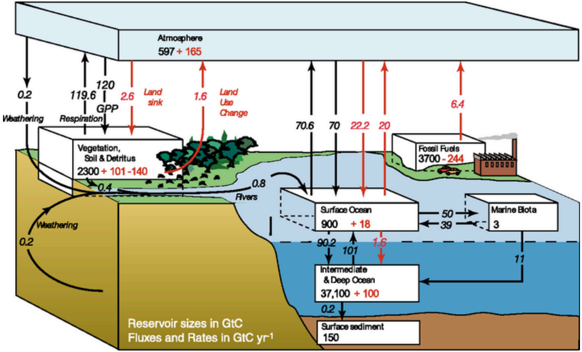
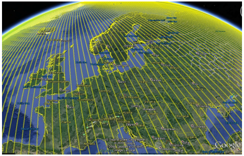



Figure 7.3 from *Climate Change 2007: Working Group I: The Physical Science Basis.*

- Benefit of space-based greenhouse-gas measurement is coverage and resolution.
- Challenge is the need for high-precision measurements to detect small changes in flux against large background variations.
- A primary objective of OCO-2 is to find and study the natural sinks.

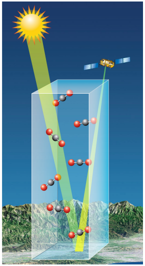
# OCO-2 mission and science



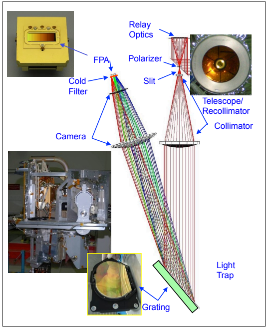
Ground tracks

OCO-2 in polar orbit at 705 km. 16-day ground-track repeat cycle (14.57 orbits per day).

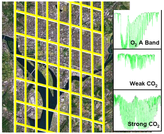
Longitude offset between orbits = 25 degrees; 1.5 degrees between tracks after 16 days.



Measurement principle




Measurement technology




Ground footprints

Eight 1.29 x 2.25 km footprints cross-track.

Three co-bore-sighted high-resolution grating spectrometers, observing in oxygen-A, weak CO2 and strong CO2 bands (3024 wavelengths).

- For each footprint, OCO-2 measures a $3048 \times 1$ vector of radiances, **Y** (Crisp, 2015).
- The retrieval uses **Y** to estimate the $45 \times 1$ atmospheric state vector, **X**, which includes CO2 dry air mole-fraction at 20 altitudes.

# OCO-2 mission and science

Greatest interest lies in the scalar quantities,

$$\hat{\mathrm{X}} \approx \mathrm{E}(\mathbf{h}'\hat{\mathbf{X}}_{1:20}|\mathbf{Y}), \quad \hat{\mathrm{S}} \approx \mathrm{var}(\mathbf{h}'\hat{\mathbf{X}}_{1:20}|\mathbf{Y}),$$

where $\mathbf{X}_{1:20}$ is the first 20 elements of the OCO-2 state vector (the CO2 vertical profile), and $\mathbf{h}$ is the 20-element pressure weighting function.

OCO-2 uses the Optimal Estimation (OE; Rodgers 2000) method to "retrieve" the maximum a posteriori estimate, $\hat{\mathrm{X}}$, and then computes $\hat{\mathrm{S}}$ as a linear function of $\hat{\mathrm{X}}$, all under Gaussian assumptions.

- $\hat{\mathrm{X}}$ is treated as the posterior mean total column mole-fraction of CO2.
- $\hat{\mathrm{S}}$ is treated as the posterior variance of total column mole-fraction of CO2.

# Statistical model

| True state | Forward function | Noiseless radiance | Instru-ment | Obser-vation | Retrieval | State estimate |
| --- | --- | --- | --- | --- | --- | --- |
| $\mathbf{X}$ | $F_0(\cdot, \mathbf{B}_0)$ | $\mathbf{Y}_0$ | $\mathbf{Y}_0 + \epsilon$ | $\mathbf{Y}$ | $R(\cdot, F_1, \mathbf{B}_1 \ldots)$ | $\hat{\mathbf{X}}$ |

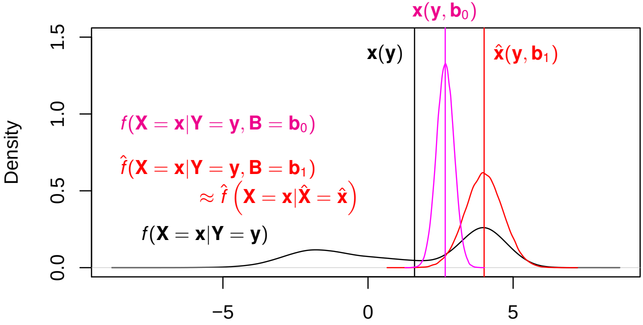
$$\mathbf{X} \longrightarrow \boxed{F_0(\cdot, \mathbf{B}_0)} \longrightarrow \mathbf{Y}_0 \longrightarrow \boxed{\mathbf{Y}_0 + \epsilon} \longrightarrow \mathbf{Y} \longrightarrow \boxed{R(\cdot, F_1, \mathbf{B}_1 \ldots)} \longrightarrow \hat{\mathbf{X}}$$

Uncertainty is quantified by conditional distributions.

- OE: $P(\mathbf{X}|\mathbf{Y})$; only source of uncertainty is $\epsilon$.
- Our view: $P(\mathbf{X}|\hat{\mathbf{X}})$; uncertainty induced by mismatches of $F_1$ to $F_0$, $\mathbf{B}_1$ to $\mathbf{B}_0$, non–Gaussianity, computational artifacts (e.g., discretization, definition of vertical grid, etc.), and unknown interactions among all these sources.
- How to proceed given that we can't even enumerate all sources of uncertainty?

# Statistical model

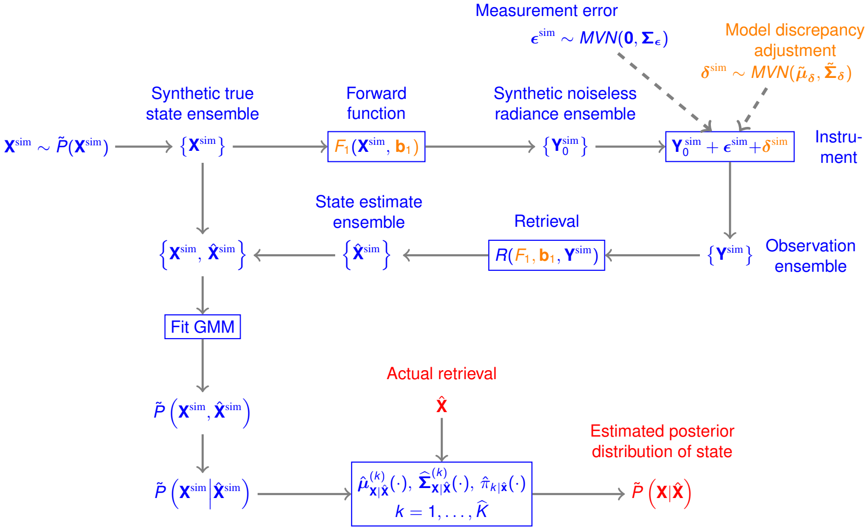
$$\mathbf{X} \sim P_{\mathbf{X}}(\mathbf{x};\theta), \quad \mathbf{Y}_0 = F_0(\mathbf{X}, \mathbf{b}_0), \quad \mathbf{Y} = \mathbf{Y}_0 + \epsilon, \quad \epsilon \sim MVN(\mathbf{0}, \mathbf{\Sigma}_\epsilon),$$
$$\theta_{\mathbf{X}} = \{\mu_{\mathbf{X}}, \mathbf{\Sigma}_{\mathbf{X}}, \ldots\}, \quad \text{and} \quad \hat{\mathbf{X}}(\mathbf{Y}, \mathbf{b}_1) = R(\mathbf{Y}, F_1, \mathbf{b}_1).$$



# Methodology

- "Top-down" approach: simulate the *entire* observing system, and compare retrieved states to synthetic truth over a representative ensemble of conditions.
- Treats the observing system/retrieval as an estimator and focuses on quantifying its mechanistic properties.
- Quanfity mechanistic performance via $P(\mathbf{X}|\hat{\mathbf{X}})$; this distribution is the most complete description of uncertainty in $\mathbf{X}$ after observing $\hat{\mathbf{X}}$.

# Methodology



# Methodology

- Model $P(\mathbf{X}|\hat{\mathbf{X}})$ as a Gaussian mixture model (GMM; McLachlan and Peel, 2000) derived from $P(\mathbf{X}, \hat{\mathbf{X}})$.
- Estimate the parameters of $P(\mathbf{X}|\hat{\mathbf{X}})$ from realistic, simulated data.
- Estimate the (conditional) GMM for a new (actual) $\hat{\mathbf{X}}$:
  - plug the new $\hat{\mathbf{X}}$ into the formulas for regression means and variances for all components in the GMM
  - simulate from the conditional GMM

# Methodology

The Gaussian mixture density for a multivariate random vector **V** is,

$$f_{\mathbf{V}}(\mathbf{v}) = \sum_{k=1}^{K} \pi_k \, \phi\left(\mathbf{v}; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right), \quad \sum_{k=1}^{K} \pi_k = 1,$$

where:

$\phi\left(\mathbf{v}; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right)$ = the multivariate normal density function with mean vector $\boldsymbol{\mu}_k$ and covariance matrix $\boldsymbol{\Sigma}_k$, evaluated at $\mathbf{v}$;

$\pi_k$ = the (mixing) weight of component $k$,

$K$ = the total number of components.

We abbreviate this density by,

$$\mathbf{V} \sim \mathrm{GMM}\left(K, \{\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k, \pi_k\}_{k=1}^{K}\right).$$

# Methodology

The parameters of this model are,

$$\left\{ \widehat{K}, \hat{\boldsymbol{\mu}}_1, \ldots, \hat{\boldsymbol{\mu}}_{\widehat{K}}, \widehat{\boldsymbol{\Sigma}}_1, \ldots, \widehat{\boldsymbol{\Sigma}}_{\widehat{K}}, \hat{\pi}_1, \ldots, \hat{\pi}_{\widehat{K}} \right\}.$$

We use the R package mclust (Scrucca et al., 2016 ) to estimate them.

# Methodology

Partition $\mathbf{V} = (\mathbf{W}', \mathbf{U}')$.

The regression mean function for component $k$ evaluated at $\mathbf{U} = \mathbf{u}$ is,

$$\hat{\mu}^{(k)}_{\mathbf{W}|\mathbf{U}}(\mathbf{u}) = \hat{\mu}^{(k)}_{\mathbf{W}} + \widehat{\boldsymbol{\Sigma}}^{(k)}_{\mathbf{WU}} \left( \widehat{\boldsymbol{\Sigma}}^{(k)}_{\mathbf{UU}} \right)^{-1} \left[ \mathbf{u} - \hat{\mu}^{(k)}_{\mathbf{U}} \right],$$

where $\widehat{\boldsymbol{\Sigma}}^{(k)}_{\mathbf{V}}$ is the estimated covariance matrix for component $k$, which is partitioned as,

$$\widehat{\boldsymbol{\Sigma}}^{(k)}_{\mathbf{V}} = \left[ \begin{array}{c|c} \widehat{\boldsymbol{\Sigma}}^{(k)}_{\mathbf{WW}} & \widehat{\boldsymbol{\Sigma}}^{(k)}_{\mathbf{WU}} \\ \hline \widehat{\boldsymbol{\Sigma}}^{(k)}_{\mathbf{UW}} & \widehat{\boldsymbol{\Sigma}}^{(k)}_{\mathbf{UU}} \end{array} \right].$$

# Methodology

The regression covariance function for component $k$ evaluated at $\mathbf{U} = \mathbf{u}$ is,

$$\widehat{\boldsymbol{\Sigma}}^{(k)}_{\mathbf{W}|\mathbf{U}}(\mathbf{u}) = \widehat{\boldsymbol{\Sigma}}^{(k)}_{\mathbf{WW}} - \widehat{\boldsymbol{\Sigma}}^{(k)}_{\mathbf{WU}} \left(\widehat{\boldsymbol{\Sigma}}^{(k)}_{\mathbf{UU}}\right)^{-1} \widehat{\boldsymbol{\Sigma}}^{(k)}_{\mathbf{UW}}.$$

The (posterior) mixing weights are,

$$\hat{\pi}_{k|\mathbf{u}} = \tilde{P}(\kappa = k|\mathbf{U} = \mathbf{u}) = \frac{\hat{\pi}_k\, \phi\left(\mathbf{u}; \hat{\boldsymbol{\mu}}^{(k)}_{\mathbf{W}|\mathbf{U}}(\mathbf{u}), \widehat{\boldsymbol{\Sigma}}^{(k)}_{\mathbf{W}|\mathbf{U}}(\mathbf{u})\right)}{\sum_{l=1}^{\widehat{K}} \hat{\pi}_l\, \phi\left(\mathbf{u}; \hat{\boldsymbol{\mu}}^{(l)}_{\mathbf{W}|\mathbf{U}}(\mathbf{u}), \widehat{\boldsymbol{\Sigma}}^{(l)}_{\mathbf{W}|\mathbf{U}}(\mathbf{u})\right)},$$

for $k = 1, \ldots, \widehat{K}$.

$\kappa$ indicates component membership: the probability that $\mathbf{V}$ comes from component $k$ is $\hat{\pi}_k$ before observing $\mathbf{U}$, and $\hat{\pi}_{k|\mathbf{u}}$ after seeing $\mathbf{U} = \mathbf{u}$.

# Methodology

Conditional distribution of $\mathbf{W}$ given $\mathbf{U} = \mathbf{u}^*$:

$$[\mathbf{W}|\mathbf{U} = \mathbf{u}^*] \sim \mathrm{GMM}\left(\widehat{K}^{\mathrm{sim}}, \left\{\hat{\boldsymbol{\mu}}^{(k)}_{\mathbf{W}|\mathbf{U}}(\mathbf{u}^*), \widehat{\boldsymbol{\Sigma}}^{(k)}_{\mathbf{W}|\mathbf{U}}(\mathbf{u}^*), \hat{\pi}_{k|\mathbf{u}^*}\right\}_{k=1}^{K}\right).$$

Approximate this distribution by simulating from it $B$ times:

1. Let $\kappa_b$ be a univariate random variable taking values in the set $\{1, \dots, \widehat{K}^{\mathrm{sim}}\}$ with,

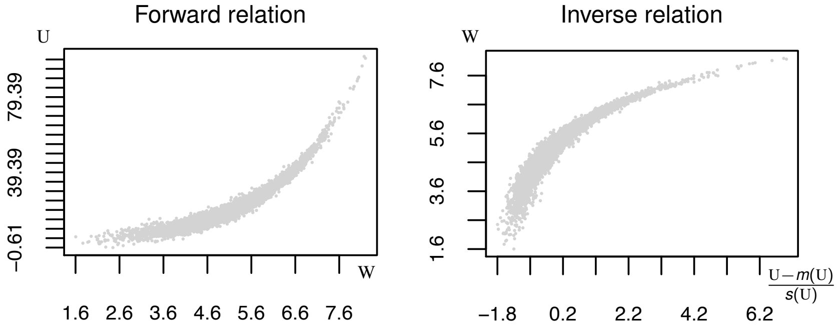
$$P(\kappa_b = k) = \hat{\pi}_{k|\mathbf{u}^*}, \quad k \in \{1, \dots, \widehat{K}^{\mathrm{sim}}\}.$$

2. Draw $B$ random variables,

$$\mathbf{W}^*_b \sim \mathrm{N}\left(\hat{\boldsymbol{\mu}}^{(\kappa_b)}_{\mathbf{W}|\mathbf{U}}(\mathbf{u}^*), \widehat{\boldsymbol{\Sigma}}^{(\kappa_b)}_{\mathbf{W}|\mathbf{U}}(\mathbf{u}^*)\right), \quad b = 1, \dots, B.$$

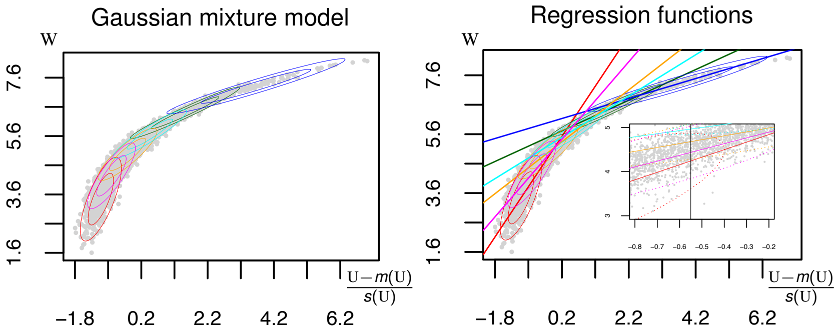
3. Fit kernel density estimate to $(\mathbf{W}^*_1, \dots, \mathbf{W}^*_B)$.

# Methodology



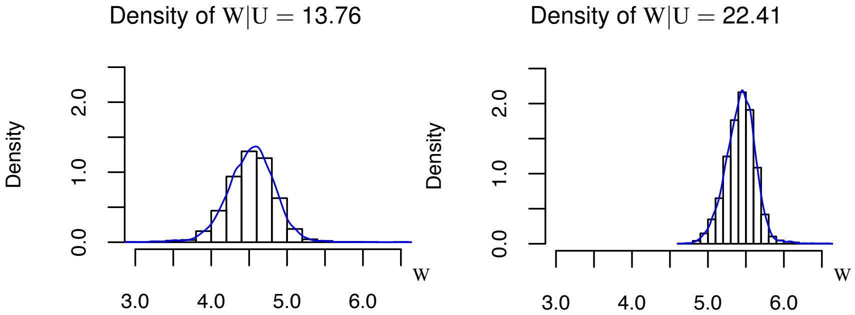

$$W \sim N(5,1), \quad U = (1.75)^{W} + \epsilon, \quad \epsilon \sim N(1,2).$$

# Methodology

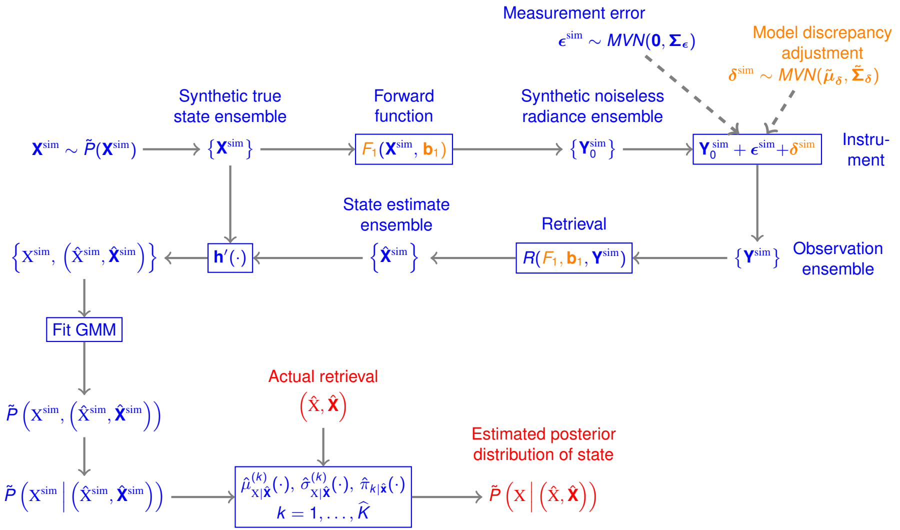



For any $\mathrm{U} = \mathrm{u}^*$, obtain mean, variance, and mixing weight for each component from its regression functions, and simulate.

# Methodology



# Application to OCO-2



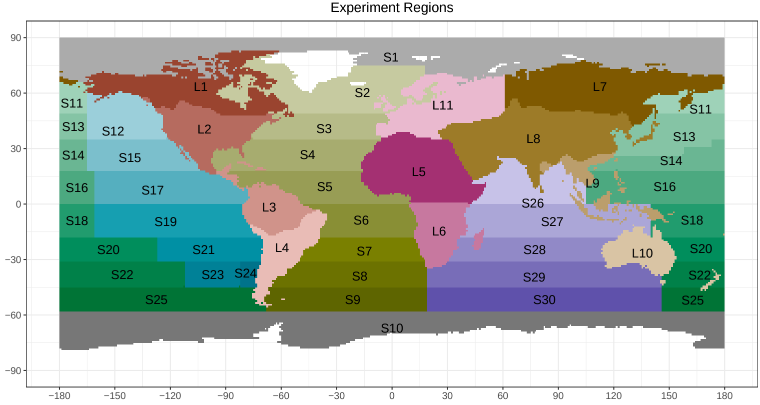
# Application to OCO-2

Synthetic true state ensemble, $\tilde{P}(\mathbf{X}^{\text{sim}})$:

- Ocean and land treated separately– land discussed here.
- Actual OCO-2 retrievals partitioned into 11 land regions by week-long time periods.
- Gaussian mixture model fit (by mclust) separately to each region-week ("template").
- Make 5000 iid draws from each template GMM.

The strategy is similar to a semi-parametric bootstrap.

# Application to OCO-2

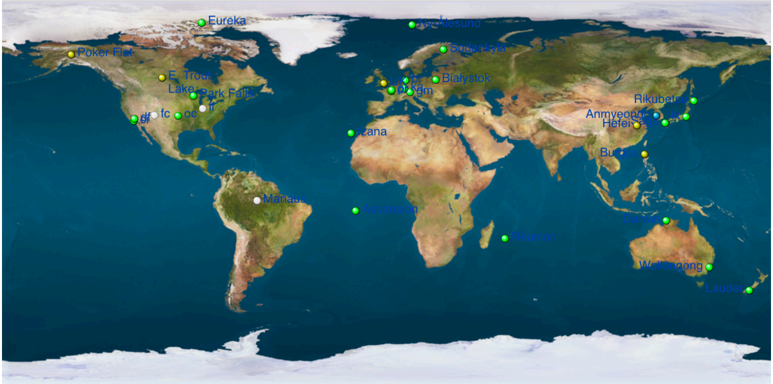


# Application to OCO-2

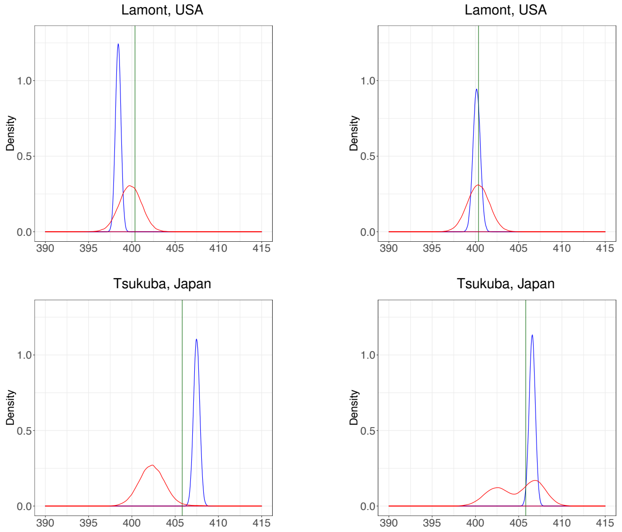
How well does this work?

- Evaluate simulation-based distributions using "ground-truth" (Total Carbon Column Observing Network; TCCON, Wunch et al., 2017) where it exists.
- Consider OCO-2 footprints that contain TCCON sites during four months: August 2015, November 2015, February 2016, and May 2016.
- Also evaluate operationally derived distributions: $\mathrm{N}(\hat{\mathrm{X}}, \hat{\mathrm{S}})$.
- Two metrics: centrality of the TCCON value in the reported distribution, and bias of the distribution mean relative to the TCCON value.

## Total Carbon Column Observing Network (TCCON)



# Application to OCO-2




TCCON value

Operational distribution

Simulated distribution

# Application to OCO-2

Metrics for evaluating simulated and operational distributions.

Metric 1:

$$G_{op}(\mathrm{X}_T) = P_{op}(\mathrm{X} \leq \mathrm{X}_T) \approx \Phi\left(\mathrm{X}_T; \hat{\mathrm{X}}, \hat{\mathrm{S}}\right),$$

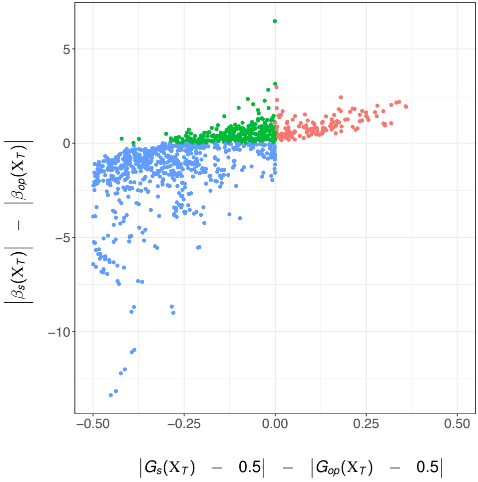
$$G_s(\mathrm{X}_T) = P_s(\mathrm{X} \leq \mathrm{X}_T) \approx \frac{1}{B}\sum_{b=1}^{B} \mathcal{I}\left(\mathrm{W}_b^* \leq \mathrm{X}_T\right).$$

Metric 2:

$$\beta_{op}(\mathrm{X}_T) = (\hat{\mathrm{X}} - \mathrm{X}_T) \quad \text{and} \quad \beta_s(\mathrm{X}_T) = \left(\frac{1}{B}\sum_{b=1}^{B} \mathrm{W}_b^*\right) - \mathrm{X}_T.$$

$\mathrm{X}_T$ denotes the TCCON value, subscropts *op* and *s* denote operational and simulated quantities, respectively.

# Application to OCO-2




$N = 944$

63.1%

25.7%

11.2%

# Application to OCO-2

## Checking interval coverage...

- Let $Q^s_{\alpha/2}$ and $Q^s_{1-\alpha/2}$ denote the lower and upper $\alpha/2$ quantiles of the simulated distribution.
- Let $Q^{op}_{\alpha/2}$ and $Q^{op}_{1-\alpha/2}$ denote the lower and upper $\alpha/2$ quantiles of the operational (Gaussian) distribution.
- Then $\left[Q^s_{\alpha/2}, Q^s_{1-\alpha/2}\right]$ and $\left[Q^{op}_{\alpha/2}, Q^{op}_{1-\alpha/2}\right]$ are $(1-\alpha)100\%$ confidence intervals.
- Compute

$$p^s_{1-\alpha} = \frac{1}{N_r}\sum_{n=1}^{N_r} \mathcal{I}\left(\mathrm{X}_T \in \left[Q^s_{\alpha/2}, Q^s_{1-\alpha/2}\right]\right), \text{ and}$$

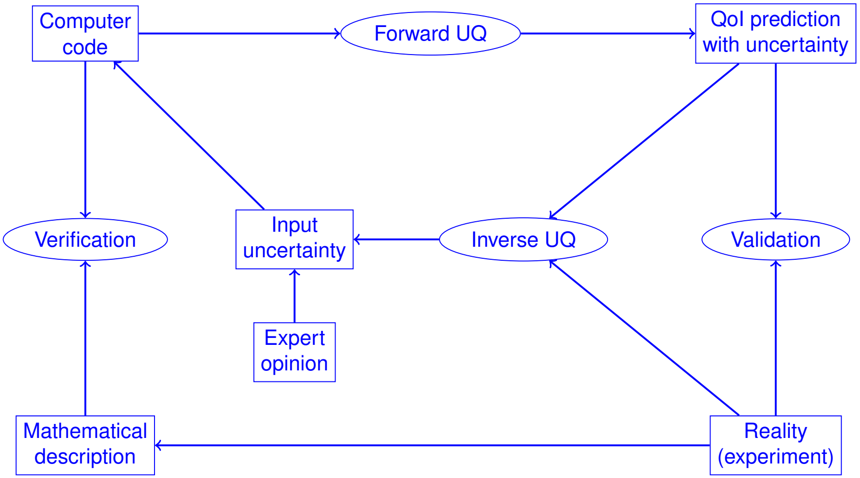
$$p^{op}_{1-\alpha} = \frac{1}{N_r}\sum_{n=1}^{N_r} \mathcal{I}\left(\mathrm{X}_T \in \left[Q^{op}_{\alpha/2}, Q^{op}_{1-\alpha/2}\right]\right),$$

where $N_r$ is the number of OCO-2 footprints.

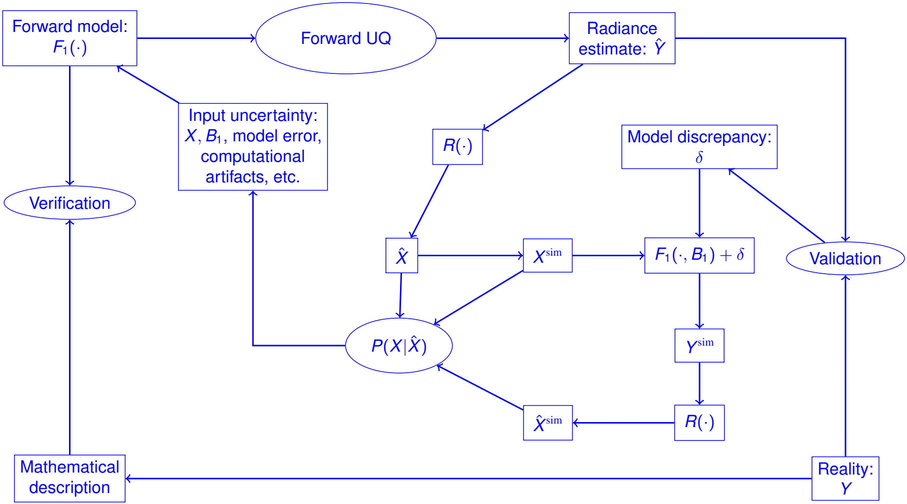
# Application to OCO-2

| Site | Week | $p^{op}_{.95}$ | $p^{op}_{.50}$ | $p^{s}_{.95}$ | $p^{s}_{.50}$ | $N_r$ |
|---|---|---|---|---|---|---|
| Bialystok, Poland | 2016-02-17 | 0.013 | 0.000 | 1.000 | 1.000 | 80 |
| Darwin, Australia | 2015-08-10 | 0.663 | 0.366 | 0.970 | 0.782 | 202 |
| Lamont, OK USA | 2015-11-02 | 0.288 | 0.143 | 1.000 | 0.909 | 132 |
| Lauder, New Zealand | 2016-02-29 | 0.449 | 0.170 | 0.932 | 0.441 | 118 |
| Orleans, France | 2015-11-02 | 0.627 | 0.322 | 0.746 | 0.661 | 59 |
| Sodankyla, Finland | 2015-08-20 | 0.533 | 0.133 | 0.600 | 0.267 | 15 |
| Tsukuba, Japan | 2016-05-13 | 0.390 | 0.169 | 0.974 | 0.818 | 77 |
| Wollongong, Australia | 2015-11-24 | 0.272 | 0.115 | 0.973 | 0.778 | 261 |

# Summary and discussion



# Summary and discussion



# Summary and discussion points

- The challenge was to develop a practical method to assign uncertainties to every estimate produced by a remote sensing obsreving system.
- Uncertainty is defined by the conditional distribution of the true state given the operationally produced state estimate.
- Our method is similar to the bootstrap bias correction (Davison and Hinkley, 1997), but goes further: we correct the entire distribution (not just the mean).
- Simulation-based confidence intervals are usually valid, but not always efficient.
- Operational confidence intervals are rarely valid.

# Summary and discussion points

- Method appears to perform relatively well in this study, but there are indications that we need to adjust the stratification so that the model is more globally representative.
- The most computationally intensive stage in building the model is the retrieval on the simulated radiances.
- Once the model is built, it is very fast to apply to new/actual retrieved estimates.

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# Acknowledgements

We would like to thank the Orbiting Carbon Observatory-2 Project for sponsoring this work.

# Backup slides

# Model discrepancy

- Model discrepancy is $\delta^{\text{sim}} = F_0(\mathbf{X}, \mathbf{b}_0) - F_1(\mathbf{X}, \mathbf{b}_1)$.
- We would like to simulate from the distribuiton of $\delta^{\text{sim}} \sim \mathrm{N}\left(\tilde{\boldsymbol{\mu}}_\delta, \tilde{\boldsymbol{\Sigma}}_\delta\right)$.
- Assume this distribution is Gaussian with mean $\mathrm{E}(\delta^{\text{sim}})$ and covariance matrix $\mathrm{cov}(\delta^{\text{sim}})$.
- But we only have access to $F_1(\hat{\mathbf{X}}, \mathbf{b}_1)$, which motivates the approximation,

$$\delta^{\text{sim}} \approx F_0(\mathbf{X}, \mathbf{b}_0) - F_1(\hat{\mathbf{X}}, \mathbf{b}_1) - \left[F_1(\mathbf{X}^{\text{sim}}, \mathbf{b}_1) - F_1(\hat{\mathbf{X}}^{\text{sim}}, \mathbf{b}_1)\right].$$

# Model discrepancy

- Let $\mathbf{Y} \equiv F_0(\mathbf{X}, \mathbf{b}_0) + \epsilon$, and $\hat{\mathbf{Y}} \equiv F_1(\hat{\mathbf{X}}, \mathbf{b}_1)$. Then,

$$\delta^{\mathrm{sim}} \approx F_0(\mathbf{X}, \mathbf{b}_0) - F_1(\hat{\mathbf{X}}, \mathbf{b}_1) - \left[F_1(\mathbf{X}^{\mathrm{sim}}, \mathbf{b}_1) - F_1(\hat{\mathbf{X}}^{\mathrm{sim}}, \mathbf{b}_1)\right].$$

$$= \left(\mathbf{Y} - \epsilon - \hat{\mathbf{Y}}\right) - \left(\mathbf{Y}_0^{\mathrm{sim}} - \hat{\mathbf{Y}}^{\mathrm{sim}}\right),$$

$$\delta^{\mathrm{sim}} + \epsilon \approx \left(\mathbf{Y} - \hat{\mathbf{Y}}\right) - \left(\mathbf{Y}_0^{\mathrm{sim}} - \hat{\mathbf{Y}}^{\mathrm{sim}}\right).$$

- Expected value:

$$\mathrm{E}(\delta^{\mathrm{sim}} + \epsilon) \approx \mathrm{E}\left(\mathbf{Y} - \hat{\mathbf{Y}}\right) - \mathrm{E}\left(\mathbf{Y}_0^{\mathrm{sim}} - \hat{\mathbf{Y}}^{\mathrm{sim}}\right),$$

$$\tilde{\mu}_\delta + \mathbf{0} \approx \frac{1}{N}\sum_{n=1}^{N}\left(\mathbf{Y}_n - \hat{\mathbf{Y}}_n\right) - \frac{1}{M}\sum_{m=1}^{M}\left(\mathbf{Y}_{0,m}^{\mathrm{sim}} - \hat{\mathbf{Y}}_m^{\mathrm{sim}}\right),$$

where $n = 1, \ldots, N$ indexes actual OCO-2 retrievals, and $m = 1, \ldots, M$ indexes trials of the simulation.

# Model discrepancy

- Covariance:

$$\mathrm{cov}(\boldsymbol{\delta}^{\mathrm{sim}} + \boldsymbol{\epsilon}) \approx \mathrm{cov}\left(\mathbf{Y} - \hat{\mathbf{Y}}\right) + \mathrm{cov}\left(\mathbf{Y}_0^{\mathrm{sim}} - \hat{\mathbf{Y}}^{\mathrm{sim}}\right) - 2\,\mathrm{cov}\left(\mathbf{Y} - \hat{\mathbf{Y}}, \mathbf{Y}_0^{\mathrm{sim}} - \hat{\mathbf{Y}}^{\mathrm{sim}}\right)$$

$$\tilde{\boldsymbol{\Sigma}}_\delta = \mathrm{cov}\left(\boldsymbol{\delta}^{\mathrm{sim}}\right) \leq \mathrm{cov}\left(\mathbf{Y} - \hat{\mathbf{Y}}\right) + \mathrm{cov}\left(\mathbf{Y}_0^{\mathrm{sim}} - \hat{\mathbf{Y}}^{\mathrm{sim}}\right) - \mathrm{cov}(\boldsymbol{\epsilon}),$$

$$\approx \widehat{\mathrm{cov}}\left(\mathbf{Y} - \hat{\mathbf{Y}}\right) + \widehat{\mathrm{cov}}\left(\mathbf{Y}_0^{\mathrm{sim}} - \hat{\mathbf{Y}}^{\mathrm{sim}}\right) - \mathrm{cov}(\boldsymbol{\epsilon}),$$

assuming $\mathrm{cov}\left(\mathbf{Y} - \hat{\mathbf{Y}}, \mathbf{Y}_0^{\mathrm{sim}} - \hat{\mathbf{Y}}^{\mathrm{sim}}\right) \geq 0$, and $\boldsymbol{\epsilon}$ and $\boldsymbol{\delta}^{\mathrm{sim}}$ are independent.