National Aeronautics and Space Administration

FY24 Strategic University Research Partnership (SURP)

Decision-Theoretic Uncertainty Quantification for Remote Sensing Inverse Problems

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Objectives:

Develop new, optimization-based uncertainty quantification (UQ) methods for remote sensing inverse problems, with specific focus on carbon flux inversion, to serve as practical, objective alternatives to contemporary Bayesian UQ methods.

Specific objectives:

1. Develop a theoretic, algorithmic and practical understanding of the UQ approaches through demonstration on well-understood toy problems.
2. Develop open-source software implementation of the methods to make them accessible to practitioners.
3. Demonstrate the use and benefits of the UQ intervals in GEOS-Chem carbon flux inversion.
4. Extend methodology to OCO-2 carbon flux inversion and perform optimization-based UQ for a collection of regional fluxes of scientific interest.

Background:

Statistical solutions to UQ for carbon flux estimation and other remote sensing inverse problems are primarily built upon the Bayesian paradigm in which prior knowledge is updated with new measurements. For remote sensing inverse problems, Bayesian methods can suffer from well-documented issues with bias and coverage due to dependency on the specification of the prior distribution. These issues can expose the resulting Bayesian estimates and uncertainties to both miscalibration and inefficiency. The proposed UQ methods are built upon the idea of guaranteeing frequentist coverage and are therefore a potential answer to the statistical issues of the usual Bayesian procedures.

Significance/Benefits to JPL and NASA:

This project represents a significant research effort to enhance statistical uncertainty quantification in remote sensing inverse problems, specifically in carbon flux inversion, through both theoretical and applied development. Establishing coverage guarantees for uncertainty intervals is vital for accurate scientific inference, as such guarantees have the potential to provide more objective UQ than traditional Bayesian methods. Well-calibrated UQ estimates for remote sensing retrievals are needed to enhance scientific understanding and should provide more informed forecasts for decision-making. This work could be instrumental for future NASA remote sensing retrieval designs and will contribute to making JPL a leader in UQ for JPL/NASA missions.

Approach and Results:

Our approach provides UQ by obtaining the (1-α)% confidence interval for a quantity of interest through direct optimization of the interval endpoints.

- Interval optimizations are constructed by representing the UQ problem as the inversion of a constrained likelihood ratio test.

In contrast to purely Bayesian methods, our methods rely on constraints rather than prior distributions to regularize inverse problems.

Figure 1 illustrates uncertainty intervals of continental US target flux using a GEOS-Chem OSSE framework. Compared to Bayesian 4D-var methods that require a subjective choice of prior, our methods are only informed by the data and parameter constraints and therefore provide a more conservative (wider) and less biased quantification of uncertainty.

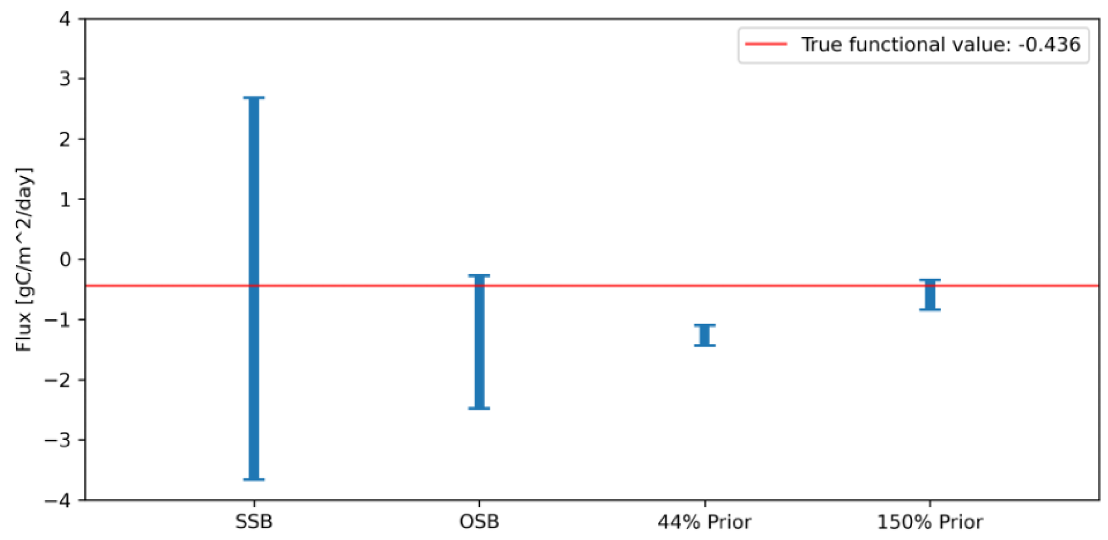

Figure 1: *Two optimization-based UQ intervals, SSB (Simultaneous Strict Bounds) and OSB (One-at-a-time Strict Bounds), for continental US June 2010 biospheric flux compared to Bayesian UQ intervals for two different prior specifications (44% vs 150%).*

We have developed two numerical optimization algorithms to obtain estimates of the UQ interval endpoints:

- **OSB-Primal:** optimizes the end points from the *"inside-out"* – computationally practical, but cannot guarantee full theoretical coverage.
- **OSB-Dual**: optimizes the end points from the *"outside-in"* – provides a theoretically valid interval estimate endpoint but is more computationally challenging.

Together, the two approaches provide the numerical range in which the true interval endpoint is guaranteed to lie – the Dual-Primal Gap.

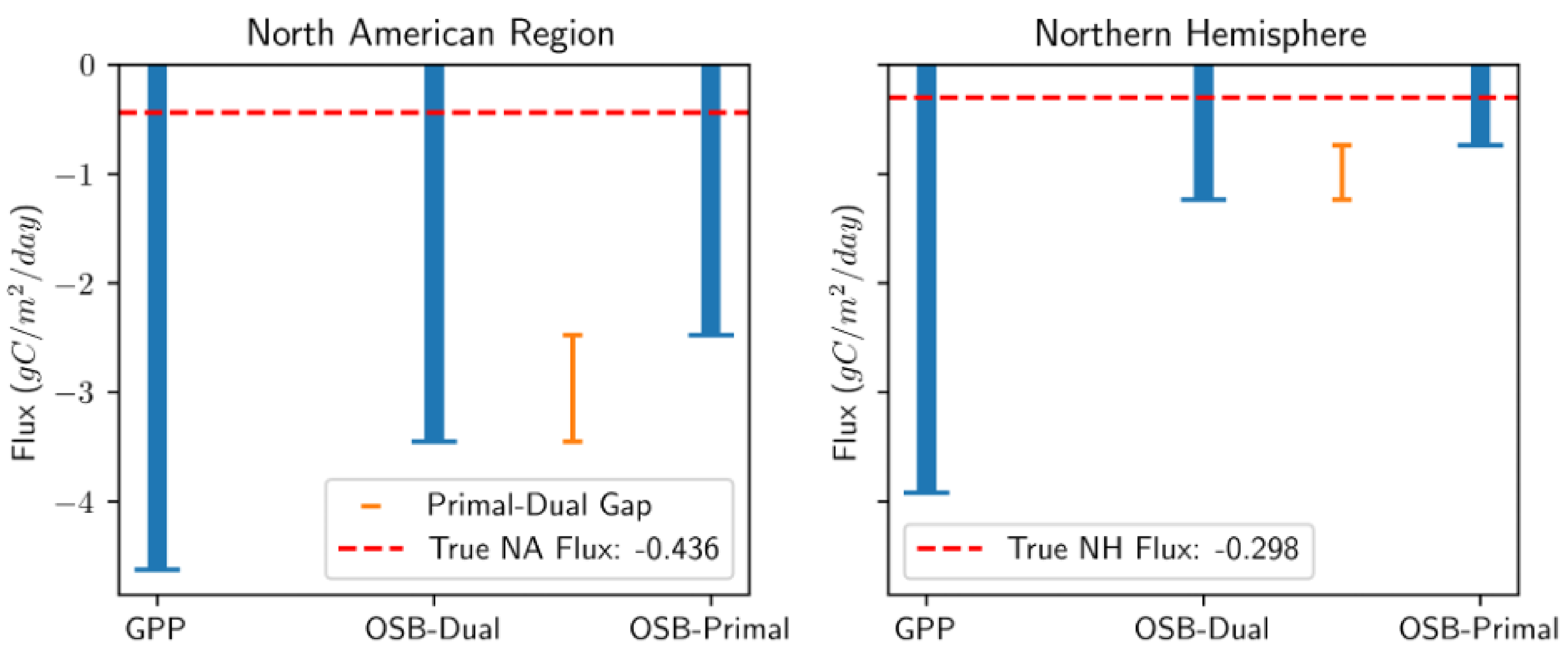

Figure 2: *OSB primal and dual one-sided 97.5% confidence intervals for carbon flux compared to the lower bound from gross primary productivity (GPP) constraints alone. Intervals for North American (NA) June 2010 biospheric flux (**left**) are compared to Northern Hemisphere (NH) June 2010 biosphere flux (**right**).*

Figure 2 shows one-sided 97.5% confidence intervals of regional flux for two regions, North America (NA) and the larger Northern Hemisphere (NH) using GEOS-Chem assimilating XCO2 data. OSB-primal and –dual interval endpoints are compared to the lowest possible flux given known constraints from GPP.

- The true interval endpoint lies within the dual-primal gap, shown by orange bars.
- The interval endpoint optimization improves the GPP-only flux lower bound by **26-46%** for NA flux and **68-81%** for the NH flux.

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Publications:

- Stanley, M., et al. (2024+) "Confidence intervals for functionals in constrained inverse problems via data-adaptive sampling-based calibration." *In prep for Biometrika.*
- Batlle, P. Patil, P., Stanley, M, …, "Optimization-based frequentist confidence intervals in constrained inverse problems: Resolving the Rust-Burrus conjecture" (2024+). *In prep for Annals of Statistics.*
- Stanley, M. (2024) "Uncertainty Quantification for Ill-Posed Inverse Problems in the Physical Sciences: Confidence Intervals via Optimization and Sampling" *PhD Dissertation*.
- Stanley, M., et al. (2024) "Technical note: Posterior uncertainty estimation via a Monte Carlo procedure specialized for 4D-Var data assimilation" *Atmospheric Chemistry and Physics,* 24, 9419-9433.

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