National Aeronautics and Space Administration

FY23 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 by 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.***

For GEOS-Chem carbon flux inversion, we used an initial *"inside-out"* optimization implementation to obtain intervals for a continental US target flux (Fig. 1). Compared to traditional, 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.

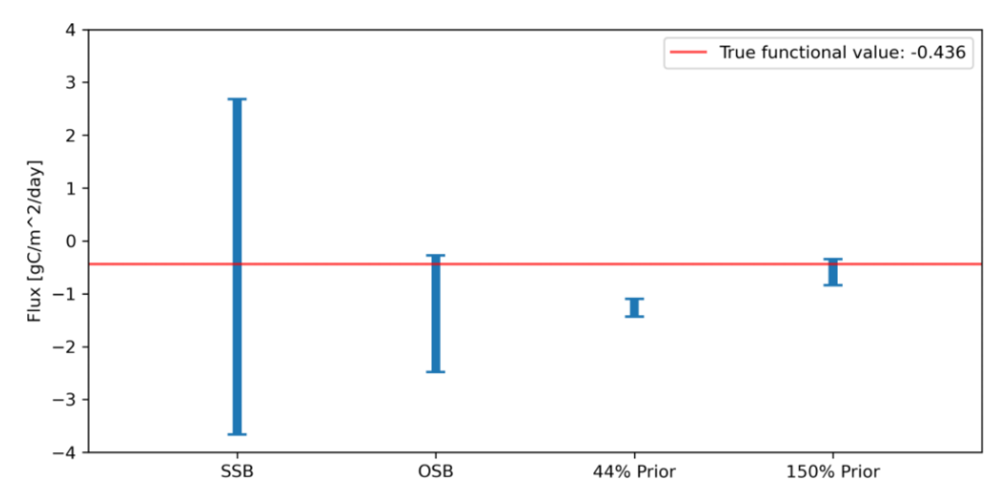


***Figure 1:*** *Two optimization-based UQ intervals, SSB (Simultaneous Strict Bounds) and OSB (One-at-a-time Strict Bounds), for continental US June 2010 biospheric flux compared to Bayesian UQ intervals for two different prior specifications (44% vs 150%).*

While the first "inside-out" optimization provides a practical implementation, we cannot guarantee the optimization has converged and therefore cannot fully guarantee optimality of the resulting interval (Fig. 2).

- A second "outside-in" implementation is currently in development which would guarantee the obtained intervals have the correct coverage (Fig. 3).

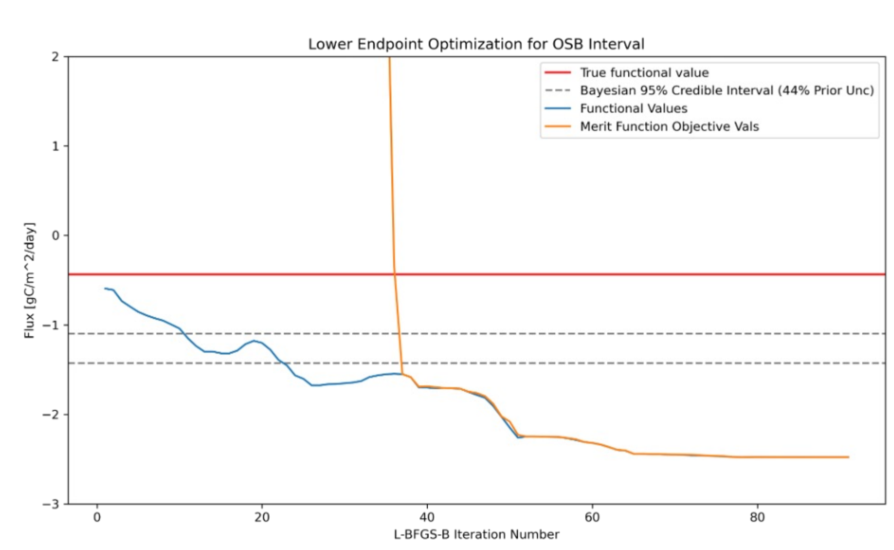


***Figure 2:*** *Trajectory of the "inside-out" optimization for the lower interval endpoint. The optimizer appears to reach "reasonable" convergence, but we cannot fully guarantee the optimizer has reached the "outside" of the interval.*

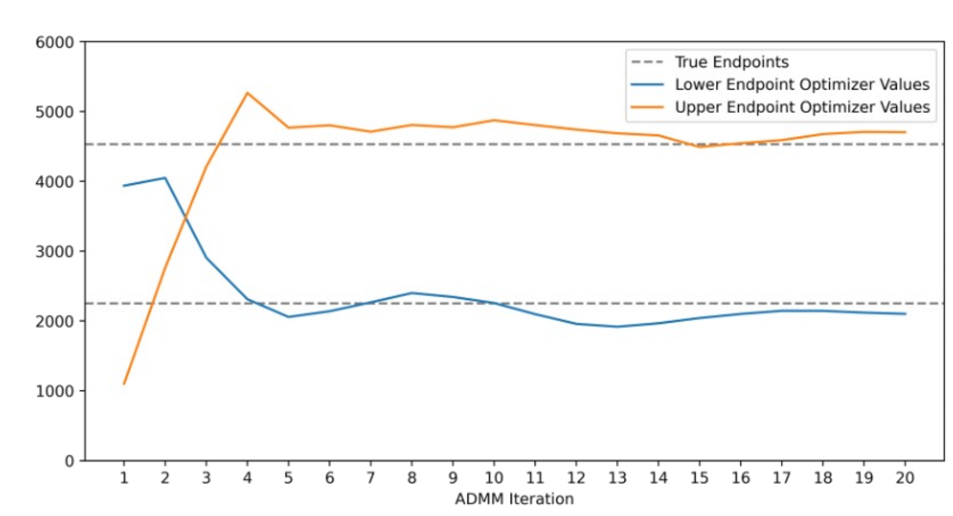


***Figure 3:*** *Lower and upper endpoint optimization trajectories for the "outside-in" optimization on a lower-dimensional inverse problem shows rapid convergence to the true interval endpoints.*

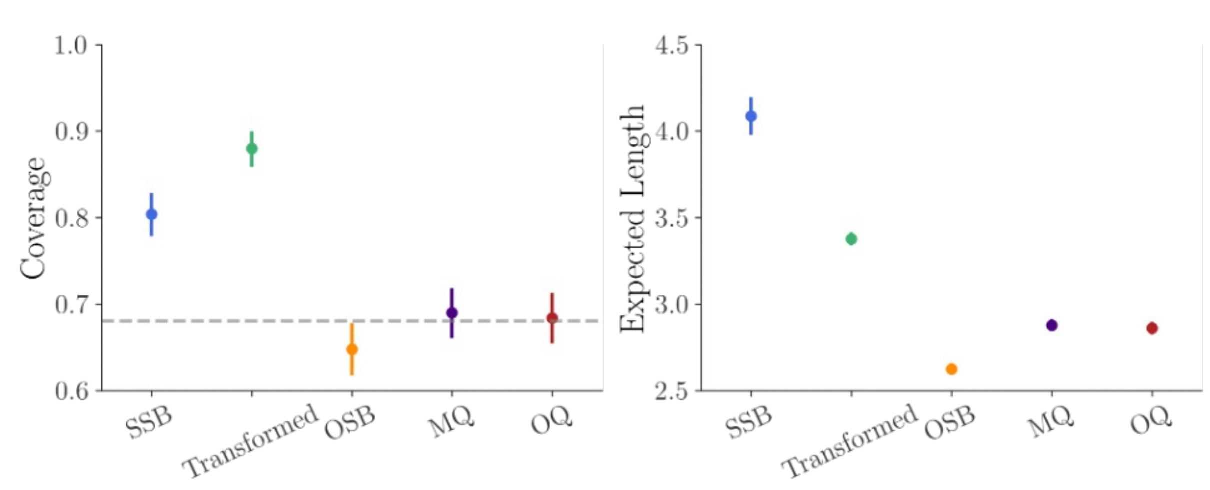


***Figure 4:*** *Results of new calibrated confidence intervals (MQ) methodology under development. Preliminary results indicate that this new method, Maximum Quantile (MQ), is able to achieve better coverage and interval length characteristics relative to the originally developed intervals (OSB/SSB).*

Parallel, ongoing research focuses on extending the methodology to allow for the relaxation of a variety of previous assumptions (e.g., linear forward models, Gaussian errors, and linear quantity of interest), see Fig. 4.

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## Publications:

[A] M. Stanley, et al., "Estimating Posterior Uncertainty via a Monte Carlo Procedure Specialized for Data Assimilation" (2023). *To be submitted to the Quarterly Journal of the Royal Meteorological Society*.

[B] P. Batlle, …, M. Stanley, et al., "Optimization-based frequentist confidence intervals in constrained inverse problems: Resolving the Rust-Burrus conjecture" (2023). *To be submitted to the Journal on Uncertainty Quantification.*

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