National Aeronautics and Space Administration

Decision-Theoretic Uncertainty Quantification for Remote Sensing Inverse Problems

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Objectives:

This project will develop decision-theoretic uncertainty quantification (DTUQ) into a practically useful alternative to contemporary Bayesian UQ methods for remote sensing inverse problems, specifically focused on carbon flux inversion.

Specific objectives:

1. Develop a theoretic, algorithmic and practical understanding of the DTUQ 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 DTUQ intervals in GEOS-Chem carbon flux inversion.
4. Investigate extensions of DTUQ methods to handle uncertain forward models motivated by these challenges in GEOS-Chem flux inversions

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 DTUQ 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:

We approach DTUQ from two complementary perspectives:

1. *Prior-optimized intervals*: a decision-theoretic approach to compute confidence intervals that have both frequentist coverage and optimal length with respect to a prior distribution.
2. *Minimax intervals*: utilize a game-theoretic perspective on zero-sum games for a worst-case scenario approach to uncertainty quantification.

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

We developed the prior-optimized intervals and compared to other functional confidence interval methods via a one-dimensional density deconvolution problem (Fig. 1) in a paper submitted to the Journal of Instrumentation [A].

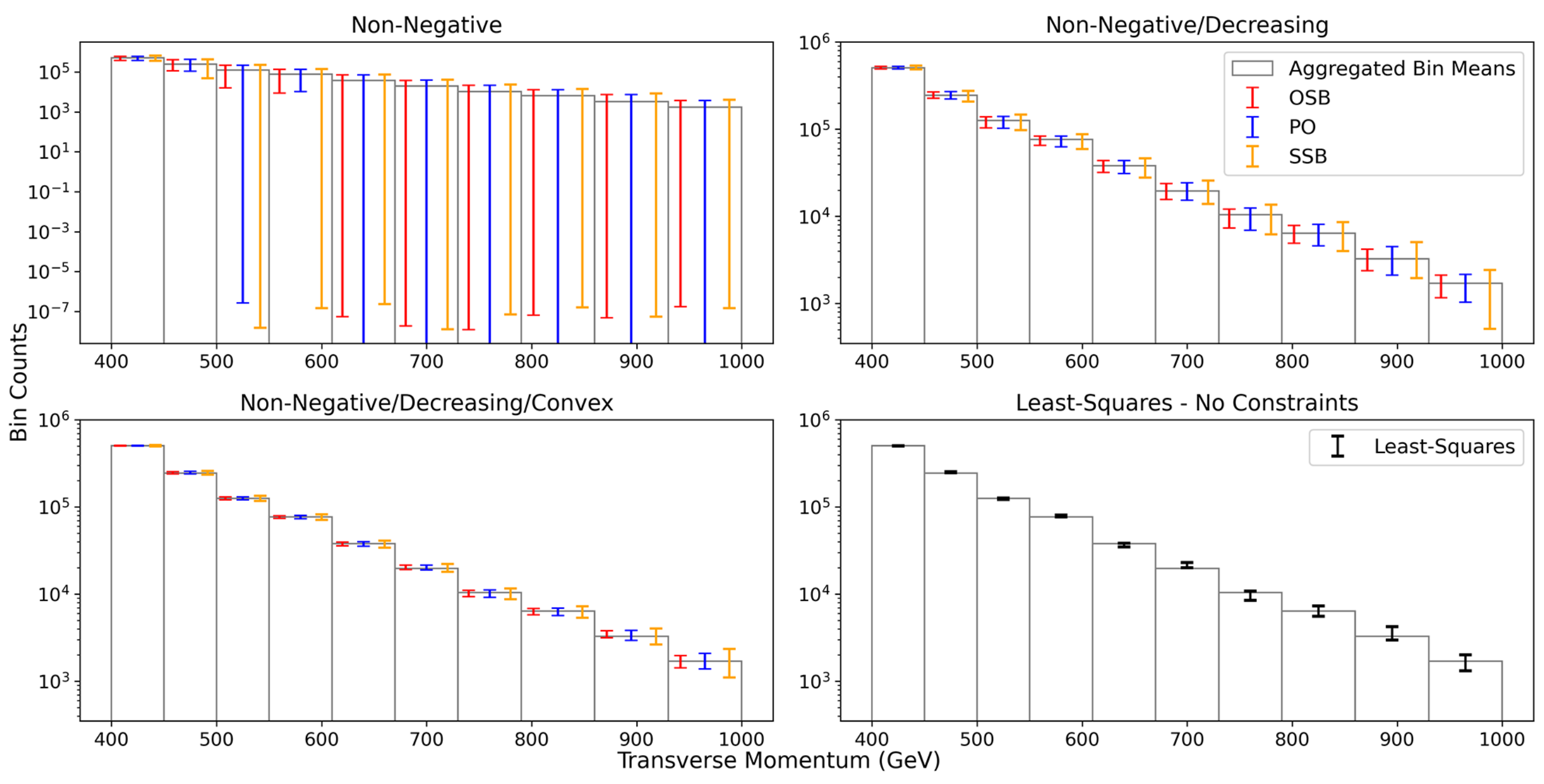

Figure 1: *Uncertainty interval (vertical bars) comparisons on a one-dimensional deconvolution problem in high energy physics. Top left to top right to bottom left represents increased number of included constraints on the parameter space. More constraints provide more regularization resulting in smaller width confidence intervals while maintaining correct frequentist coverage. Figure from [A].*

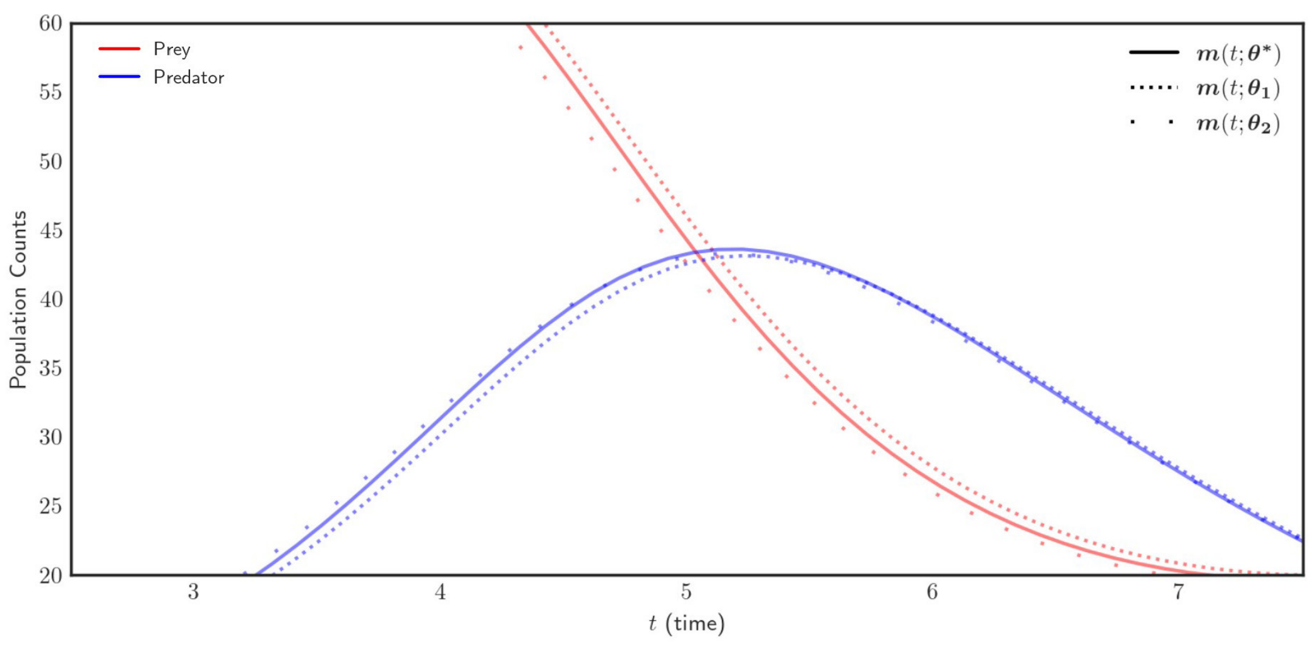

Figure 2: *Implementation of the minimax interval method on the Lotka-Volterra predator prey model. The minimax estimate (solid line) of the true predator-prey population dynamics for parameters is shown with point-wise interval uncertainties (dotted lines). Figure from [B].*

We finalized the implementation of minimax intervals on a two-dimensional predator-prey problem (Fig. 2), providing a critical contribution to [B]. This method can be interpreted as inference with respect to a “least favorable prior” and provides a conservative alternative to the subjective prior choice in a classical Bayesian approach.

We investigated a Monte Carlo (MC) method for estimating posterior variance in linear data assimilation that characterizes additional uncertainty arising from the MC method itself, particularly motivated by carbon flux inversion (Fig. 3).

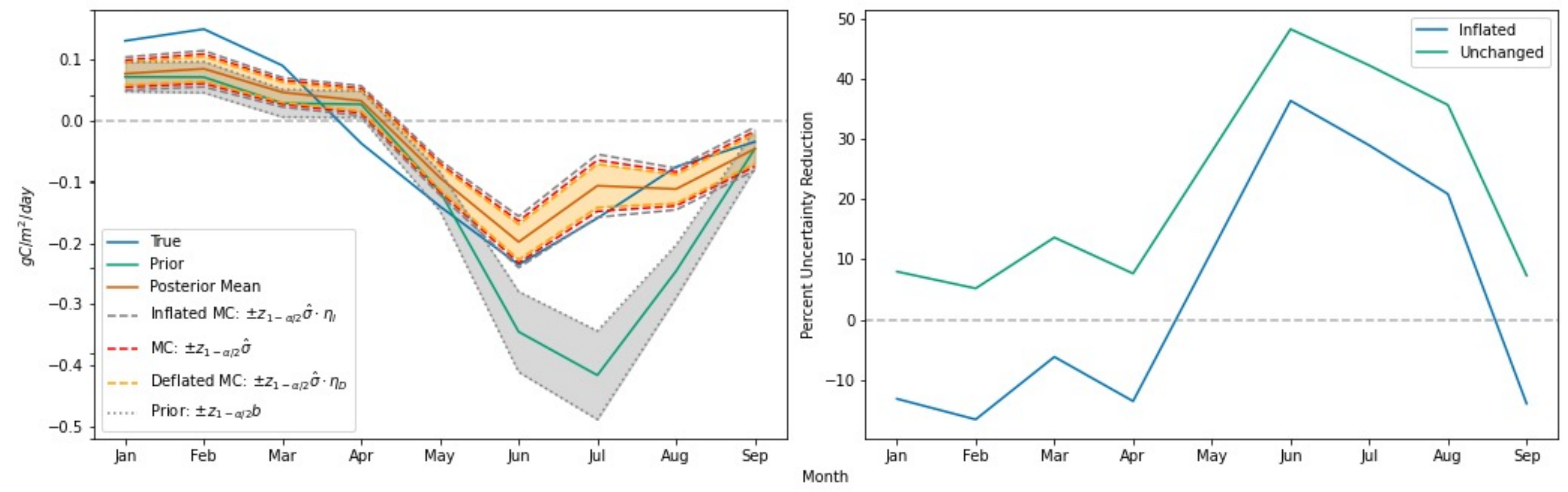

Figure 3: *(Left) Bayesian posterior credible intervals (orange) from 4D-Var global carbon flux inversion are subject to bias induced by the prior distribution (green/grey intervals). This results in overly optimistic intervals that miss the truth (blue line) for large portions of the considered time frame. (Right) Posterior uncertainty reduction both with and without accounting for Monte Carlo uncertainty.*

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Publications:

[A] M. Stanley, et al., “Uncertainty quantification for wide-bin unfolding: one-at-a-time strict bounds and prior-optimized confidence intervals,” Submitted to the *Journal of Instrumentation* (2022)

[B] H. Bajgiran, et al., “Uncertainty Quantification of the 4th kind; optimal posterior accuracy-uncertainty tradeoff with minimum enclosing ball,” Accepted at *The Journal of Computational Physics* (2022).

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