Optimization approaches for solving inverse problems must account for uncertainty in both data and downstream decisions

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A major challenge in solving inverse problems for high-consequence science and engineering applications is neglecting to fully account for uncertainties. Some optimization formulations for inverse problems involve objectives that capture uncertainties with the data-generating process; this can be done in the form of statistical likelihoods and treated from both frequentist (e.g., via maximum likelihood estimation) and Bayesian (e.g., via maximum a posteriori estimation) perspectives. Although it is vital to take into account uncertainties in the data, such approaches typically neglect how the inferred parameters will be used in downstream decisions.

One example where it is critical to account for downstream tasks arises from "implementation errors." For example, consider the inverse problem of determining material properties from samples imaged at a DOE light source. If one wants to then replicate this material, or alter it toward a specific aim, then it is important to understand the precision with which the inferred parameters can actually be implemented. In many settings, knowing that a synthesis process can only be implemented within a prescribed precision (e.g., curing temperature within 0.1 degrees Celsius, chemical volume up to 0.001 mL) could significantly alter the "optimal" parameters that should be employed. Our position is that it is vital to account for uncertainties such as implementation errors; not doing so risks prioritizing reduction of forward model mismatches over the actual subsequent uses of the resulting forward model. By moving into the optimization formulation the uncertainties essential to the downstream tasks performed with the inversion parameters, the resulting parameters will be born decision-ready.

Myriad examples exist where this would be a gamechanger. For example, nuclear waste management represents a critical application where parameter sensitivity affects safety outcomes. When characterizing repository sites using inverse methods, uncertainties in geological parameters must be considered alongside downstream operational variability and constraints. Similarly, in agent-based model calibration for energy infrastructure planning, inferred parameters drive decisions about resource allocation and grid resilience that have significant implementation tolerances. Finally, in quantum material design, inferred electronic structure parameters must account for both measurement uncertainty and the precision limitations of synthesis techniques to produce viable energy storage solutions.

A key opportunity exists to pursue robust optimization [1] approaches that ensure optimized parameters are insensitive to perturbations from multiple sources. By explicitly accounting for uncertainties in data acquisition, forward model approximations, and parameter implementation constraints, we can develop inverse methods that deliver solutions with quantifiable reliability bounds. This shift toward decision-aware inverse problems could transform how DOE facilities utilize characterization data by connecting upstream inference directly to downstream decision processes. The impact would be particularly significant for experimental design workflows where the objective is not merely to infer parameters but to guide future experiments or manufacturing processes with well-characterized uncertainty. Successfully addressing these opportunities would reduce costly iteration cycles between characterization and implementation across multiple DOE mission areas.

Several breakthroughs are essential to enable this new paradigm. First, we need computational frameworks that can efficiently handle the inherent nonlinearity introduced when accounting for both data and decision uncertainties simultaneously. Current methods that separately address these sources of uncertainty fail to capture important interactions and trade-offs. Second, hierarchical approaches that strategically decompose the problem structure are needed to navigate the highly nonconvex, multimodal objective function landscapes that arise in these formulations. These approaches must adaptively determine which uncertainties dominate in different regions of parameter space. Finally, developing specialized regularization techniques that reflect implementation constraints rather than just statistical priors would create more practical solutions. These innovations would transform inverse problems from academic inference exercises into practical decision support tools that directly address the gap between characterization and implementation in complex systems.

By considering all the uncertainties that arise in the inverse problem and the ways in which the inversion will be used, optimization-based approaches can directly mitigate failure modes of current practice. Models and methods that instantiate and solve such a capability are crucial for accelerating scientific discovery and improving decision making.

Reference:

[1] S. Leyffer, M. Menickelly, T. Munson, C. Vanaret, & S.M. Wild (2020). A survey of nonlinear robust optimization. INFOR: Information Systems and Operational Research, 58(2), 342–373.