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Guest Editors' introduction to the special section on statistical and computational issues in inverse problems

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Abstract

In the words of D D Jackson, the data of real-world inverse problems tend to be inaccurate, insufficient and inconsistent (1972 *Geophys. J. R. Astron. Soc.* **28** 97–110). In view of these features, the characterization of solution uncertainty is an essential aspect of the study of inverse problems. The development of computational technology, in particular of multiscale and adaptive methods and robust optimization algorithms, has combined with advances in statistical methods in recent years to create unprecedented opportunities to understand and explore the role of uncertainty in inversion. Following this introductory article, the special section contains 16 papers describing recent statistical and computational advances in a variety of inverse problem settings.

Statistical and coqmputational issues in inverse problems

This special issue of *Inverse Problems* presents statistical and computational ideas and tools for the understanding and quantification of uncertainty in the solution of applied inverse problems.

At an appropriate level of abstraction, many scientific questions are inverse problems. Solving those inverse problems is an intrinsically interdisciplinary task: in order to make estimates or draw inferences, experiments must be designed; instruments designed, fabricated and deployed; mathematical descriptions of the measurement process formulated; hypotheses posited; data collected; theory and algorithms developed; and data processed. Often these steps are performed by disjoint groups of researchers who are not aware of the complexity, limitations and opportunities in the steps performed by others. Assumptions made in one step may contradict or fail to account for assumptions and constraints in other steps, limiting the accuracy and utility of the overall process.

How can we assess the reliability of images and inferences, taking into account realistic stochastic and systematic error, approximations to the forward problem, approximations in the representation of the unknown, algorithmic and numerical instabilities and uncertainties, finite computational resources, and the fact that only finitely many observations are available? How can prior knowledge be incorporated into inferences to reduce the true uncertainty—without understating the uncertainty by imposing artificial constraints? How can appropriate physics be incorporated in a computational feasible way, without imposing yet more artificial constraints? How should we assess the relative merits of different methods and algorithms? What measures of the performance are scientifically interesting? Is there an estimator or approach that performs 'best', in some scientifically interesting sense, for a given forward mapping, and reasonable assumptions or constraints on the unknown function and the model and data errors? If so, how can we compute it, given the frequently vast ranges of scales and very large extents of faithful numerical representations? How well does the estimator perform if the assumptions are wrong? Constraints on the unknown function and assumptions about the data errors are sometimes matters of science and sometimes matters of mathematical or computational convenience or expressions of a subjective preference. The influence of untested assumptions on the inferences and the uncertainty of those inferences should be studied and quantified.

The over-arching problem of understanding the accuracy and limitations of mathematical and computational models of complex systems has acquired the name 'uncertainty quantification' (UQ) in recent years. UQ is becoming recognized as an important facet of inverse problems, with applications ranging from assessing the reliability of the power grid to validating the strong motion potential of earthquake-prone basins.

Some of the statistical tools rely on asymptotics, distributional assumptions, or assumptions about the function to be recovered that are hard (if not impossible) to test, and some may overlook hard questions, such as the bias of estimators. Others are at a level of abstraction rather removed from application. Such is the state of the art. Nonetheless, the core ideas and framework are important and hold promise for real problems. On the computational side, multiscale and/or data-adaptive methods promise to enable simulation and inversion algorithms of unprecedented physical fidelity and efficiency.

There is still much left to do to bridge the gap between what practitioners need to compute, to properly quantify uncertainty in the solution of inverse problems, and what can be computed today. This special section illustrates some of the most promising current approaches to closing this gap.

Overview of the special section

We proceed to provide a brief summary of the papers in the special section:

Biros and Dogan [1] describe a multilevel method for an elliptic inverse source problem in which the first-order conditions for an optimum source estimate amount to a Fredholm operator equation. They construct a multilevel preconditioner by solving a constant coefficient approximating problem and use the known spectral decomposition of this approximating problem to construct a hierarchy of subspaces. The target problem is then solved by a conjugate gradient iteration.

Bangerth and Joshi [2] show how adaptive multilevel finite elements may be used to construct efficient solution methods for inverse problems in optical tomography. They give an extensive discussion of the biomedical background and a careful definition of the inverse problem. Synthetic fluorescence tomography experiments based on photogrammetric reconstruction of animal tissue illustrate the capabilities of the approach and underline the essential contribution of adaptive meshing.

Bissantz and Holzmann [3] discuss asymptotic properties of some nonparametric methods for density estimation, regression and density deconvolution, and how those asymptotic properties can be used to construct asymptotic confidence intervals or confidence envelopes, and confidence bounds for the number of modes of a distribution. They illustrate some of the methods using a astrophysical problem—estimating the distribution of heliocentric escape velocities in the Centaurus galaxy cluster.

Calvetti and Somersalo [4] present a hierarchical Bayesian framework for image reconstruction. They show that for a suitable hyperprior, the Bayes estimate is equivalent to some previous regularization techniques, providing a unified treatment of superficially rather disparate methods. They also show how to organize the computations to implement their approach efficiently using Markov chain Monte Carlo methods.

Cavalier [5] reviews some theoretical tools that are useful for comparing the asymptotic behavior of estimators and deriving bounds on the (asymptotically) best possible performance in some idealized inverse problems. He presents definitions and results relating to constraint classes, estimators and measures of statistical performance such as ellipsoids in normed spaces, regularization, rates of convergence, adaptivity, oracle inequalities and empirical estimates of risk.

Epanomeritakis *et al* [6] present a finite element approach to elastic modeling and inversion of the Earth's crust, and progress toward using these tools to understand the structure of major sedimentary basins such as that underlying Los Angeles. The enormous size of these problems mandates careful problem formulation and algorithm selection, use of cutting-edge high-performance computing resources, and very careful software engineering. A key feature of the core simulation methodology is the use of a multilevel adaptive mesh, organized via the octree data structure.

Image registration is the process of creating a correspondence between points in multiple images referencing the same points on a physical object. This problem arises in many biomedical imaging modalities, such as computerized x-ray tomography and magnetic resonance imaging, in which multiple views of the same subject must be correlated spatially. Fischer and Modersitzki [7] review the image registration problem. The authors present a general mathematical model for image registration, permitting the classification of most currently used approaches. They also describe the difficult numerical issues arising in this category of inverse problems.

Gu [8] describes modifications to regularization to account for non-Gaussian errors or correlated errors by using an appropriate likelihood function to measure fit to the data. He discusses cross validation for selecting the tradeoff between model fit and model complexity, and the connections among regularization methods, spline-like models and functional analysis of variance. He also points to some computational tools in the public domain.

Hintermüller [9] describes an approach to inverse problems based on elliptic variational inequalities, an important class of problems which includes contact problems in mechanics and rheology and the Black–Scholes model in computational finance. An unavoidable feature of these problems is the dependence of the computational domain on the data—a feature which arises in many other problems but which in this setting cannot be suppressed. Hintermüller uses mesh coarsening to regularize the problem, and includes an application to a lubrication problem.

Mesh smoothing is an important task in computer graphics, which may be formulated as an inverse problem. Huang and Ascher [10] treat the mesh smoothing problem with an adaptive multilevel algorithm based on construction of an anisotropic mesh-adaptive Laplacian operator. The chief difficulty in these problems is to avoid oversmoothing, which destroys important texture information. The authors illustrate that their method preserves such intrinsic texture, even in the presence of mesh sampling irregularity.

Lukas [11] introduces a variant of generalized cross validation (GCV) for selecting the tradeoff parameter between fit to the data and model complexity in regularization estimates. The new merit function, R_1GCV, adds a term (and a new tradeoff parameter for that term) that measures the influence of each point on the complexity of the estimate, an idea from robust estimation. He shows the asymptotic equivalence of some variants of GCV, and that R_1GCV has desirable asymptotic properties. In simulations he presents, regularization estimates perform better when the tradeoff parameter is selected by R_1GCV instead of GCV.

O'Sullivan *et al* [12] develop a novel iterative regularization method to reconstruct water wave height fields from refraction or reflection data (which are sensitive to surface gradients) to estimate wave front shapes and periodicities. Their treatment involves a physically motivated representation of the solution in terms of solutions to an approximate physical problem: they express the solution as a superposition of plane waves, and they develop a tomographic approximation to choose the number of degrees of freedom for a generalized cross validation function. Their approach may be useful to construct regularization estimates for other multidimensional problems.

Plessix and Mulder [13] describe the imaging of the Earth's interior using controlled source electromagnetic data. This imaging mode has received considerable attention in recent years: while it does not threaten the dominance of reflection seismology in petroleum prospection, it does open up the possibility of mapping rock characteristics largely complementary to those estimated by seismic means. Unlike reflection seismic data, controlled source electromagnetic data offer few visible clues to its meaning in its raw state, and must be viewed through the lens of inversion. This communication describes the experimental methodology and modeling in detail, and develops a numerical approach to the inverse problem set as a least squares data fitting exercise. Synthetic and field data examples illustrate the state of the art.

Rust and O'Leary [14] present a method to choose the regularization parameter that balances the tradeoff between data misfit and model complexity in Tikhonov regularization. They apply some basic tools from time series analysis to analyze the residuals of the fit. The basic idea is to choose the parameter that makes the periodogram of the residuals consistent with the distribution of the original errors. They compare the performance of their method to that of generalized cross validation and the *L* curve.

Stark [15] generalizes the Backus–Gilbert notion of 'resolution' to nonlinear inverse problems, to inverse problems with constraints, to nonlinear parameters, to nonlinear and biased estimators, and to measures of risk other than variance—which lead to definitions of minimax and Bayes resolution, generalizations of minimax and Bayes estimation. He also introduces design resolution, which allows the measurements to be selected optimally to make sharper inferences. Design resolution generalizes a problem in information-based complexity.

Optimal control and inverse problems intersect in many ways. von Winckel and Borzi [16] discuss an optimal control problem in quantum mechanics. They show that the functional-analytic setting of these problem, i.e. the choice of (inequivalent) norms in infinite-dimensional model spaces, can have a determining influence on the convergence of iterative optimization methods.

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