Jari Kaipio
E. Somersalo

Applied Mathematical Sciences 160

Statistical and Computational Inverse Problems

With 102 Figures

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To Eerika, Paula, Maija and Noora

Between the idea
And the reality
Between the motion
And the act
Falls the Shadow

T.S. Eliot

Preface

This book is aimed at postgraduate students in applied mathematics as well as at engineering and physics students with a firm background in mathematics. The first four chapters can be used as the material for a first course on inverse problems with a focus on computational and statistical aspects. On the other hand, Chapters 3 and 4, which discuss statistical and nonstationary inversion methods, can be used by students already having knowldege of classical inversion methods.

There is rich literature, including numerous textbooks, on the classical aspects of inverse problems. From the numerical point of view, these books concentrate on problems in which the measurement errors are either very small or in which the error properties are known exactly. In real-world problems, however, the errors are seldom very small and their properties in the deterministic sense are not well known. For example, in classical literature the error norm is usually assumed to be a known real number. In reality, the error norm is a random variable whose mean might be known.

Furthermore, the classical literature usually assumes that the operator equations that describe the observations are exactly known. Again, usually when computational solutions based on real-world measurements are required, one should take into account that the mathematical models are themselves only approximations of real-world phenomena. Moreover, for computational treatment of the problem, the models must be discretized, and this introduces additional errors. Thus, the discrepancy between the measurements and the predictions by the observation model are not only due to the "noise that has been added to the measurements." One of the central topics in this book is the statistical analysis of errors generated by modelling.

There is rich literature also in statistics, especially concerning Bayesian statistics, that is fully relevant in inverse problems. This literature has been fairly little known to the inverse problems community, and thus the main aim of this book is to introduce the statistical concepts to this community. As for statisticians, the book contains probably little new information regarding, for example, sampling methods. However, the development of realistic observation models based, for example, on partial differential equations and the analysis of the associated modelling errors might be useful.

As for citations, in Chapters 1–6 we mainly refer to books for further reading and do not discuss historical development of the topics. Chapter 7, which discusses our previous and some new research topics, also does not contain reviews of the applications. Here we refer mainly to the original publications as well as to sources that contain modifications and extensions which serve to illustrate the potential of the statistical approach.

Chapters 5–7, which form the second part of the book, focus on problems for which the models for measurement errors, errorless observations and the unknown are really taken as *models*, which themselves may contain uncertainties. For example, several observation models are based on partial differential equations and boundary value problems. It might be that part of the boundary value data are inherently unknown. We would then attempt to model these boundary data as random variables that could either be treated as secondary unknowns or taken as a further source of uncertainty and compute its contribution to the discrepancy between the observation model and the predictions given by the observation model.

In the examples, especially in Chapter 7 that discusses nontrivial problems, we concentrate on research that we have carried out earlier. However, we also treat topics that either have not yet been published or are discussed here with more rigor than in the original publications.

We have tried to enhance the readibility of the book by avoiding citations in the main text. Every chapter has a section called "Notes and Comments" where the citations and further reading, as well as brief comments on more advanced topics, are given.

We are grateful to our colleague and friend, Markku Lehtinen, who has advocated the statistical approach to inverse problems for decades and brought this topic to our attention. Much of the results in Chapter 7 have been done in collaboration with our present and former graduate students - as well as other scientists. We have been privileged to work with them and thank them all. We mention here only the people who have contributed directly to this book by making modifications to their computational implementations or otherwise: Dr. Ville Kolehmainen for Sections 7.2 and 7.9, Dr. Arto Voutilainen for Section 7.4, Mr. Aku Seppänen for Sections 7.5 and 7.7 and Ms. Jenni Heino for Section 7.8. We are also much obliged to Daniela Calvetti for carefully reading and commenting the whole manuscript and to the above-mentioned people for reading some parts of the book. For possible errors that remain we assume full responsibility.

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much of the novel material in this book was conceived during the authors' visits there.

Helsinki and Kuopio
June 2004

Jari P. Kaipio
Erkki Somersalo

Contents

1

Inverse Problems and Interpretation of Measurements

Inverse problems are defined, as the term itself indicates, as the inverse of direct or forward problems. Clearly, such a definition is empty unless we define the concept of direct problems. Inverse problems are encountered typically in situations where one makes indirect observations of a quantity of interest. Let us consider an example: one is interested in the air temperature. Temperature itself is a quantity defined in statistical physics, and despite its usefulness and intuitive clarity it is not directly observable. A ubiquitous thermometer that gives us information of the air temperature relies on the fact that materials such as quicksilver expand in a very predictable way in normal conditions as the temperature increases. Here the forward model is the function relating the volume of the quicksilver as a function of the temperature. The inverse problem in this case is trivial, and therefore it is not usually considered as a separate inverse problem at all, namely the problem of determining the temperature from the volume measured. A more challenging inverse problem arises if we try to measure the temperature in a furnace. Due to the high temperature, the traditional thermometer is useless and we have to use more advanced methods. One possibility is to use ultrasound. The high temperature renders the gases in the furnace turbulent, thus changing their acoustic properties which in turn is reflected in the acoustic echoes. Now the forward model consists of the challenging problem of describing the turbulence as a function of temperature plus acoustic wave propagation in the medium, and its even more challenging inverse counterpart of determining the temperature from acoustic observations.

It is the legacy of Newton, Leibniz and others that laws of nature are often expressed as systems of differential equations. These equations are *local* in the sense that at a given point they express the dependence of the function and its derivatives on physical conditions at that location. Another typical feature of the laws is *causality*: later conditions depend on the previous ones. Locality and causality are features typically associated with direct models. Inverse problems on the other hand are most often *nonlocal* and/or *noncausal*. In our example concerning the furnace temperature measurement, the acoustic echo observed outside depends on the turbulence everywhere, and due to the finite signal speed, we can hope to reconstruct the temperature distribution in a time span prior to the measurement, i.e., computationally we try to go upstream in time.

The nonlocality and noncausality of inverse problems greatly contribute to their instability. To understand this, consider heat diffusion in materials. Small changes in the initial temperature distributions smear out in time, leaving the final temperature distribution practically unaltered. The forward problem is then stable as the result is little affected by changes in the initial data.

Going in the noncausal direction, if we try to estimate the initial temperature distribution based on the observed temperature distribution at the final time, we find that vastly different initial conditions may have produced the final condition, at least within the accuracy limit of our measurement. On the one hand, this is a serious problem that requires a careful analysis of the data; on the other hand we need to incorporate all possible information about the initial data that we may have had *prior* to the measurement. The *statistical inversion theory*, which is the main topic of this book, solves the inverse problems systematically in such a way that all the information available is properly incorporated in the model.

Statistical inversion theory reformulates inverse problems as problems of statistical inference by means of Bayesian statistics. In Bayesian statistics all quantities are modeled as random variables. The randomness, which reflects the observer's uncertainty concerning their values, is coded in the probability distributions of the quantities. From the perspective of statistical inversion theory, the solution to an inverse problem is the probability distribution of the quantity of interest when all information available has been incorporated in the model. This distribution, called the *posterior distribution*, describes the degree of confidence about the quantity after the measurement has been performed.

This book, unlike many of the inverse problems textbooks, is not concerned with analytic results such as questions of uniqueness of the solution of inverse problems or their a priori stability. This does not mean that we do not recognize the value of such results; to the contrary, we believe that uniqueness and stability results are very helpful when analyzing what complementary information is needed in addition to the actual measurement. In fact, designing methods that incorporate all prior information is one of the big challenges in statistical inversion theory.

There is another line of textbooks on inverse problems, which emphasize the numerical solution of *ill-posed problems* focusing on regularization techniques. Their point of view is likewise different from ours. Regularization techniques are typically aimed at producing *a reasonable estimate* of the quantities of interest based on the data available. In statistical inversion theory, the solution to an inverse problem is not a single estimate but a probability distribution that can be used to produce estimates. But it gives more than just a single estimate: it can produce very different estimates and evaluate their reliability. This book contains a chapter discussing the most commonly used regularization schemes, not only because they are useful tools for their own right but also since it is informative to interpret and analyze those methods from the Bayesian point of view. This, we believe, helps to reveal what sort of implicit assumptions these schemes are based on.

1.1 Introductory Examples

In this section, we illustrate the issues discussed above with characteristic examples. The first example concerns the problems arising from the noncausal nature of inverse problems.

Example 1: Assume that we have a rod of unit length and unit thermal conductivity with ends set at a fixed temperature, say 0. According to the standard model, the temperature distribution $u(x,t)$ satisfies the heat equation

$$\frac{\partial^2 u}{\partial t^2} - \frac{\partial u}{\partial t} = 0, \quad 0 < x < 1,\ t > 0,$$

with the boundary conditions

$$u(0,t) = u(1,t) = 0$$

and with given intial condition

$$u(x,0) = u_0(x).$$

The inverse problem that we consider is the following: Given the temperature distribution at time $T > 0$, what was the initial temperature distribution?

Let us write first the solution in terms of its Fourier components,

$$u(x,t) = \sum_{n=1}^{\infty} c_n e^{-(n\pi)^2 t} \sin n\pi x.$$

The coefficients c_n are the Fourier sine coefficients of the initial state u_0, i.e.,

$$u_0(x) = \sum_{n=1}^{\infty} c_n \sin n\pi x.$$

Thus, to determine u_0, one has only to find the coefficients c_n from the final data. Assume that we have two initial states $u_0^{(j)}$, $j = 1, 2$, that differ only by a single high-frequency component, i.e.,

$$u_0^{(1)}(x) - u_0^{(2)}(x) = c_N \sin N\pi x,$$

for N large. The corresponding solutions at the final time will differ by