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Numerical Regularization for Atmospheric Inverse Problems

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Preface

The retrieval problems arising in atmospheric remote sensing belong to the class of the so-called discrete ill-posed problems. These problems are unstable under data perturbations, and can be solved by numerical regularization methods, in which the solution is stabilized by taking additional information into account.

The goal of this research monograph is to present and analyze numerical algorithms for atmospheric retrieval. The book is aimed at physicists and engineers with some background in numerical linear algebra and matrix computations. Although there are many practical details in this book, for a robust and efficient implementation of all numerical algorithms, the reader should consult the literature cited.

The data model adopted in our analysis is semi-stochastic. From a practical point of view, there are no significant differences between a semi-stochastic and a deterministic framework; the differences are relevant from a theoretical point of view, e.g., in the convergence and convergence rates analysis.

After an introductory chapter providing the state of the art in passive atmospheric remote sensing, Chapter 2 introduces the concept of ill-posedness for linear discrete equations. To illustrate the difficulties associated with the solution of discrete ill-posed problems, we consider the temperature retrieval by nadir sounding and analyze the solvability of the discrete equation by using the singular value decomposition of the forward model matrix.

A detailed description of the Tikhonov regularization for linear problems is the subject of Chapter 3. We use this opportunity to introduce a set of mathematical and graphical tools to characterize the regularized solution. These comprise the filter factors, the errors in the state space and the data space, the mean square error matrix, the averaging kernels, and the L-curve. The remaining part of the chapter is devoted to the regularization parameter selection. First, we analyze the parameter choice methods in a semi-stochastic setting by considering a simple synthetic model of a discrete ill-posed problem, and then present the numerical results of an extensive comparison of these methods applied to an ozone retrieval test problem. In addition, we pay attention to multi-parameter regularization, in which the state vector consists of several components with different regularization strengths. When analyzing one- and multi-parameter regularization methods, the focus is on the pragmatic aspects of the selection rules and not on the theoretical aspects associated with the convergence of the regularized solution as the noise level tends to zero.

At first glance, it may appear that Chapter 4, dealing with statistical inversion theory, is an alien to the main body of the textbook. However, the goal of this chapter is to reveal the similitude between Tikhonov regularization and statistical inversion regarding the regularized solution representation, the error analysis, and the design of regularization parameter choice methods. The marginalizing method, in which the auxiliary parameters of the retrieval are treated as a source of errors, can be regarded as an alternative to the multi-parameter regularization, in which the auxiliary parameters are a part of the retrieval.

Chapter 5 briefly surveys some classical iterative regularization methods such as the Landweber iteration and semi-iterative methods, and then treats the regularizing effect of the conjugate gradient method for normal equations (CGNR). The main emphasis is put on the CGNR and the LSQR implementations with reorthogonalizations. Finally, we analyze stopping rules for the iterative process, and discuss the use of regularization matrices as preconditioners.

The first five chapters set the stage for the remaining chapters dealing with nonlinear ill-posed problems. To illustrate the behavior of the numerical algorithms and tools we introduce four test problems that are used throughout the rest of the book. These deal with the retrieval of O_3 and BrO in the visible spectral region, and of CO and temperature in the infrared spectral domain.

In Chapter 6 we discuss practical aspects of Tikhonov regularization for nonlinear problems. We review step-length and trust-region methods for minimizing the Tikhonov function, and present algorithms for computing the new iterate. These algorithms rely on the singular value decomposition of the standard-form transformed Jacobian matrix, the bidiagonalization of the Jacobian matrix, and on iterative methods with a special class of preconditioners constructed by means of the Lanczos algorithm. After characterizing the solution error, we analyze the numerical performance of Tikhonov regularization with a priori, a posteriori and error-free parameter choice methods.

Chapter 7 presents the relevant iterative regularization methods for nonlinear problems. We first examine an extension of the Landweber iteration to the nonlinear case, and then analyze the efficiency of Newton type methods. The following methods are discussed: the iteratively regularized Gauss–Newton method, the regularizing Levenberg–Marquardt method and the Newton–CG method. These approaches are insensitive to overestimations of the regularization parameter, and depend or do not depend on the a priori information. Finally, we investigate two asymptotic regularization methods: the Runge–Kutta regularization method and the exponential Euler regularization method.

In Chapter 8 we review the truncated and the regularized total least squares method for solving linear ill-posed problems, and put into evidence the likeness with the Tikhonov regularization. These methods are especially attractive when the Jacobian matrix is inexact. We illustrate algorithms for computing the regularized total least squares solution by solving appropriate eigenvalue problems, and present a first attempt to extend the total least squares to nonlinear problems.

Chapter 9 brings the list of nonlinear methods to a close. It describes the Backus–Gilbert method as a representative member of mollifier methods, and finally, it addresses the maximum entropy regularization.

For the sake of completeness and in order to emphasize the mathematical techniques which are used in the classical regularization theory, we present direct and iterative methods for solving linear and nonlinear ill-posed problems in a general framework. The analysis is outlined in the appendices, and is performed in a deterministic and discrete setting. Although discrete problems are not ill-posed in the strict sense, we prefer to argue in this setting because the proofs of convergence rate results are more transparent, and we believe that they are more understandable by physicists and engineers.

Several monographs decisively influenced our research. We learned the mathematical fundamentals of the regularization theory from the books by Engl et al. (2000) and Rieder (2003), the mathematical foundation of iterative regularization methods from the recent book by Kaltenbacher et al. (2008), and the state of the art in numerical regularization from the book by Hansen (1998). Last but not least, the monograph by Vogel (2002) and the book by Kaipio and Somersalo (2005) have provided us with the important topic of regularization parameter selection from a statistical perspective.

This book is the result of the cooperation of more than six years between a mathematically oriented engineer and two atmospheric physicists who are interested in computational methods. Therefore, the focus of our book is on practical aspects of regularization methods in atmospheric remote sensing. Nevertheless, for interested readers some mathematical details are provided in the appendices.

The motivation of our book is based on the need and search for reliable and efficient analysis methods to retrieve atmospheric state parameters, e.g., temperature or constituent concentration, from a variety of atmospheric sounding instruments. In particular, we were, and still are, involved in data processing for the instruments SCIAMACHY and MIPAS on ESA's environmental remote sensing satellite ENVISAT, and more recently for the spectrometer instruments GOME-2 and IASI on EUMETSAT's MetOp operational meteorological satellite. This resulted in the development of the so-called DRACULA (aDvanced Retrieval of the Atmosphere with Constrained and Unconstrained Least squares Algorithms) software package which implements the various methods as discussed in this book. A software package like DRACULA, complemented by appropriate radiative transfer forward models, could not exist without the support we have received from many sides, especially from our colleagues at DLR in Oberpfaffenhofen. To them we wish to address our sincere thanks.

Finally, we would like to point out that a technical book like the present one may still contain some errors we have missed. But we are in the fortunate situation that each author may derive comfort from the thought that any error is due to the other two. In any case, we will be grateful to anyone bringing such errors or typos to our attention.

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