Numerical Data Fitting in Dynamical Systems

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Numerical Data Fitting in Dynamical Systems

A Practical Introduction with Applications and Software

by

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Preface

Real life phenomena in engineering, natural, or medical sciences are often described by a mathematical model with the goal to analyze numerically the behaviour of the system. Advantages of mathematical models are their cheap availability, the possibility of studying extreme situations that cannot be handled by experiments, or of simulating real systems during the design phase before constructing a first prototype. Moreover, they serve to verify decisions, to avoid expensive and time consuming experimental tests, to analyze, understand, and explain the behaviour of systems, or to optimize design and production.

As soon as a mathematical model contains differential dependencies from an additional parameter, typically the time, we call it a dynamical model. There are two key questions always arising in a practical environment:

1 Is the mathematical model correct?

2 How can I quantify model parameters that cannot be measured directly?

In principle, both questions are easily answered as soon as some experimental data are available. The idea is to compare measured data with predicted model function values and to minimize the differences over the whole parameter space. We have to reject a model if we are unable to find a reasonably accurate fit.

To summarize, parameter estimation or data fitting, respectively, is extremely important in all practical situations, where a mathematical model and corresponding experimental data are available to describe the behaviour of a dynamical system.

The main goal of the book is to give an overview of numerical methods that are needed to compute parameters of a dynamical model by a least squares fit. The mathematical equations that must be provided by the system analyst are explicit model functions or steady state systems in the simplest situations, or responses of dynamical systems defined by ordinary differential equations, differential algebraic equations, or one-dimensional partial differential equations. Many different mathematical disciplines must be combined, and the intention is to present at least some fundamental ideas of the numerical methods needed, so that available software can be applied successfully.

It must be noted that there are two alternative aspects not treated in this book. First, we do not emphasize statistical analysis, which is also known as *nonlinear regression* or *nonlinear parameter estimation.* Moreover, we do not investigate the question whether parameters of a dynamical model can be identified at all, and under which mathematical conditions. It is supposed that a user is able to prepare a well-defined model, where the dynamical system is uniquely solvable and where the parameters can be identified by a least squares fit. There exist numerous qualified textbooks for both topics mentioned, from which additional information can be retrieved.

It is assumed that the typical reader is familiar with basic mathematical notation of linear algebra and analysis, as for example learned in elementary calculus lectures. No additional knowledge about mathematical theory is required. New concepts are presented in an elementary form and are illustrated by detailed analytical and numerical examples.

Extensive numerical results are included to show the efficiency of modern mathematical algorithms. We also discuss possible pitfalls in the form of warnings that even the most qualified numerical algorithms we know today can fail or produce unacceptable responses. The practical progress of mathematical models and data fitting calculations is illustrated by case studies from pharmaceutics, mechanical, electrical or chemical engineering, and ecology.

To be able to repeat all numerical tests presented in the book and to *play* with algorithms, data, and solution tolerances, an interactive software system is included that runs under Windows 95/98/NT4.0/2000. The program contains the mathematical algorithms described in the book. The database consists of 1,000 illustrative examples, which can be used as benchmark test problems. Among them is a large number of real life models (*learning by doing*).

The book is the outcome of my research activities in this area over the last 20 years with emphasis on the development of numerical algorithms for optimization problems. It would have been impossible to design applicable mathematical algorithms and to implement the corresponding software without intense discussions, contacts, and cooperation with firms, for example Boehringer Ingelheim Pharma, BASF Ludwigshafen, Siemens Munich, Schloemann-Siemag Hilchenbach, EADS Munich, Bayer Sarnia, Dornier Satellite Systems Munich, and many research institutions at universities. Particularly, I would like to thank Dr. M. Wolf from the University of Bonn, Department of Pharmaceutics, for providing many dynamical models describing pharmaceutical applications, and for encouraging the investigation of models based on partial differential equations. Part of my research was supported by projects funded by the BMBF research program *Anwendungsbezogene Verbundprojekte in der Mathematik* and the DFG research program *Echtzeit-Optimierung großer Systeme.*

Klaus Schittkowski