VOLUME 7

NUMERICAL ANALYSIS OF PARAMETRIZED NONLINEAR EQUATIONS

WERNER C. RHEINBOLDT

UNIVERSITY OF ARKANSAS LECTURE NOTES IN THE MATHEMATICAL SCIENCES

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Preface

This monograph represents an expanded version of the series of invited lectures I gave as principal speaker of the Seventh Annual Lecture Series in the Mathematical Sciences at the University of Arkansas, Fayetteville, in the Spring of 1983.

The theme of the lecture series was the numerical analysis of nonlinear equations involving a finite number of parameters. Such equations arise typically in connection with static equilibrium problems in science and engineering. The aim of these notes is to discuss some of the recent developments in this area. They are not meant to provide a survey of any kind; rather, this monograph reflects very much my own view of the topic. Moreover, the lectures were supposed to cover some of my related research results, and hence the presentation has a decidedly personal flavor.

In my opinion, the theory of parametrized equations has strong roots in modern differential geometry and should be considered in the setting of differentiable manifolds. Most of the numerical studies in the area, notably those on continuation methods, utilize this theoretical foundation very little.

In these notes I have tried to show how a numerical analysis of parametrized equations may be developed on a differential geometric basis. The first three sections are intended to set the scene; Section 1 provides some general comments about the problem area; Section 2 illustrates the area with several typical model problems; and, finally, Section 3 summarizes some background material from nonlinear analysis in a form needed later.

The next three sections form an introduction to the theoretical aspects of the problem. Section 4 provides a rudimentary discussion of the theory of differentiable manifolds and its use in the study of the solution manifolds of parametrized equations. Section 5 presents some recent results about a priori estimates of the errors between the solution manifold of an equation and the corresponding manifold defined by one of its discretizations. Essentially all available computational methods for analyzing the solution manifold of an equation consist of some form of continuation process for the computational trace of one-dimensional submanifolds. Section 6 introduces the one-distribution concept used in defining these submanifolds and considers some of the connections with augmented forms of the equations.

Section 7 begins the discussion of the numerical aspects of the problem area; it describes the design of the continuation package PITCON for which a FORTRAN listing is included in an appendix to the monograph. Section 8 discusses the use of this package, and Section 9 gives an overview of various algorithms which have been proposed for the computation of limit points, including the method used in PITCON itself.

The last two sections address further related material. Section 10 summarizes some recent results about differential-algebraic equations that are based on interpreting them as differential equations on a manifold. Finally, Section 11 outlines a new approach for the computation of a posteriori estimates of the errors considered in Section 5.

As noted before, the presentation has a very personal flavor and hence is certainly uneven in its emphasis on the various topics and ideas. In particular, there exists additional material that could have been included or at least mentioned. For example, I deliberately touched only in passing upon the rich subject of bifurcation theory. There are already a number of excellent books in that area and within the framework of this monograph it would have been impossible to do any justice to the wealth of relevant topics.

I would like to express my special thanks to the organizers of the lecture series for their fine planning and personal attention, which made it a very enjoyable experience. It is also a pleasure to acknowledge the support of the National Science Foundation under grants MCS-78-05299 and MCS-83-09926, as well as that of the Office of Naval Research under contract N-00014-80-C-9455, for the parts of my own research which are covered in these notes.

Werner C. Rheinboldt
Pittsburgh, Pennsylvania
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1. INTRODUCTION

parameter
Greek: para - besides
metron - measure

In every computational application we encounter various parameters. They may measure intrinsic properties of the physical system under consideration or they may represent external quantities which influence its behavior. The aim of a scientific computation is to draw conclusions, or derive implications about the system. For instance, in engineering the computed data may have to provide a basis for a decision about a proposed design, while in a scientific study the intent may be to develop predictions of the system's behavior for experimental verification. Accordingly, the computation has to give information about the response of the system under variation of specific parameters; that is, we are interested in the effects of changes of the values of these parameters upon the computed results.

The study of the influence of parameters upon the behavior of mathematical models is one of the basic problems of applied mathematics. Usually, we are interested in systems which are locally stable in the sense that their qualitative behavior does not change under small variations of the parameters. Here, some form of perturbation theory may be the appropriate tool, or we may bring to bear some theoretical results about the structural stability of mappings. Before this, dimensional analysis may have to be applied to identify the dimensionless parameters upon which a particular practical problem depends. In turn, the choice of properly scaled dimensionless variables is important for the specification of meaningfully small parameters needed in the perturbation analysis. This list of relevant fundamental techniques of applied mathematics is easily extended.

While the determination of local stability is highly important in practice, it is equally essential to understand those variations of the parameters which produce a change of the behavior. In particular, there may be a change in the stability properties. For instance, a mechanical structure may buckle or collapse, or a laminar fluid flow may turn turbulent. Loosely speaking, the parameter values, where such stability changes occur, define the set of bifurcation points of the problem. The general study of these points is the topic of bifurcation theory, a field with a burgeoning literature. But, in practice, and especially in connection with complex engineering problems, many of these theoretical results turn out to be difficult to apply. Moreover, for experimental comparisons we often need to know explicitly the properties of the solutions for a large region of physical significance. Then interest centers on computational methods for determining quantitatively the form of specific segments of the solution set. As noted in the Preface, that is the topic of this monograph.

The mathematical models for describing the systems considered here are formed by nonlinear equations, including algebraic, differential, or integral equations. All of them involve several parameters, and hence have the generic form

$$F(z,\lambda) = 0. \tag{1.1}$$

Here z varies in some space Z and characterizes the state of the system while λ denotes the parameter variable allowed to vary in a space Λ. Hence the nonlinear operator F is defined on a set in the product space $Z \times \Lambda$.

In line with the earlier comments, it does not suffice to determine solution states z of (1.1) only for a few specified values of λ. Instead, we want to assess how these states change when the parameters vary in some prescribed subset of Λ. In other words, we have to look at the solutions of (1.1) as points (z,λ) in the product space $Z \times \Lambda$.

Under rather general conditions, this solution set has the structure of a differentiable manifold. Broadly speaking, our task then is the numerical determination of the principal features of this manifold. In order to identify some of the relevant questions, it may be useful to consider a very simple model problem, namely, the cubic equation

$$z^3 - \lambda z - \mu = 0. \qquad (1.2)$$

Here $z \in R^1$ is the state variable, and the parameter vector $(\lambda,\mu) \in R^2$ is two-dimensional. The solution set of (1.2) in R^3 is easily drawn and constitutes a two-dimensional surface of the form shown in Figure 1.1. This figure also includes projections onto two planes parallel to certain coordinate axis. This identifies some interesting features. The λ-axis together with the parabola $z^2 = \lambda$ forms a so-called pitchfork bifurcation diagram in the (z,λ)-plane. The cusp line $\mu^2 = (4/27)\lambda^3$ represents the projection onto the (λ,μ)-plane of the line of fold points $(z,3z^2,-2z^3)$, $z \in R^1$. If the surface were made of translucent plastic and illuminated along the direction of the z-axis, the cusp line then would be its apparent image on a projection screen orthogonal to that axis.

The example already suggests some of the tasks involved in a numerical study of the solution manifold of an equation of the form (1.1). First of all, we are certainly interested in calculating suitable sequences of solution points. Usually this means that we wish to compute points along specified paths on the manifold. For instance, in the case of (1.2) such a path might be defined by the

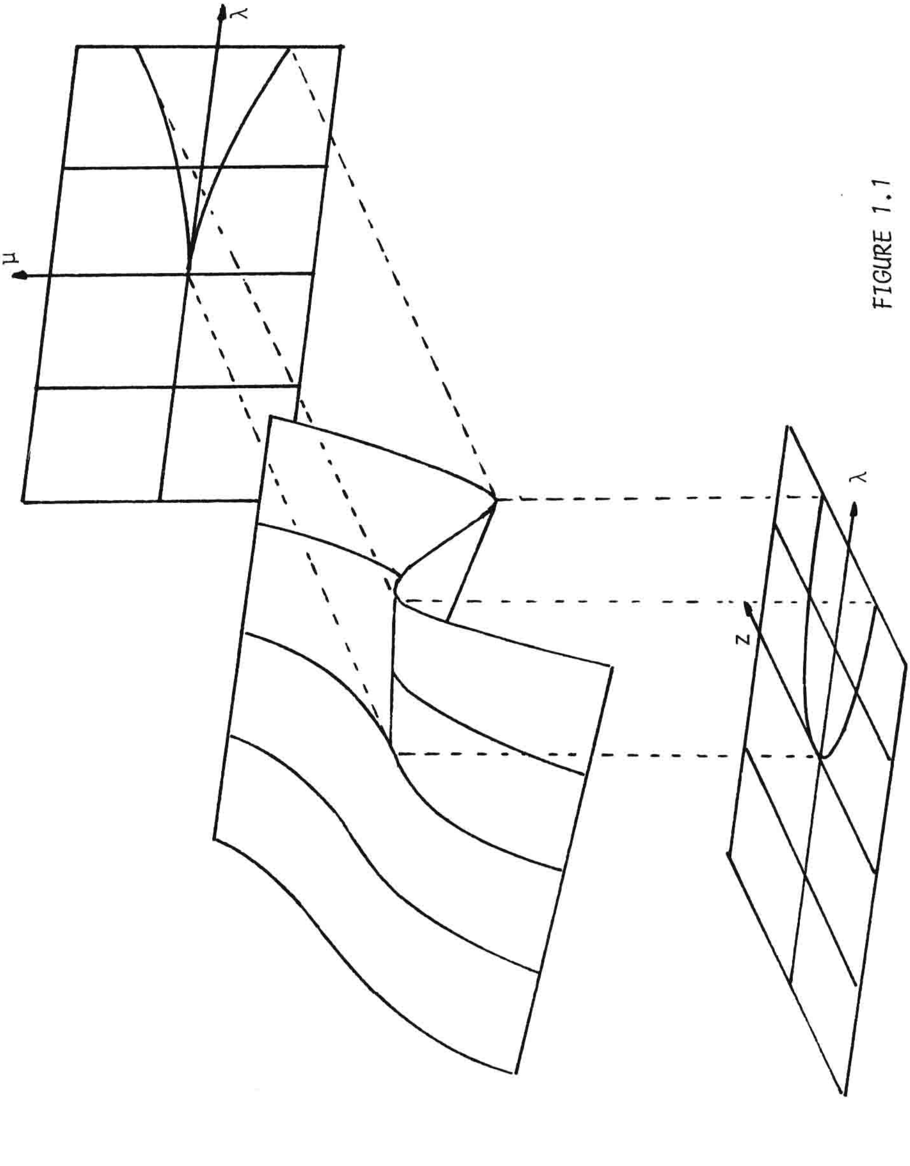

FIGURE 1.1

condition μ = constant. As the model problem of Section 1.2 below will illustrate, fold lines often constitute the locus of points where the stability behavior changes. Hence the determination of such points clearly is another task for our numerical study. Such fold points might be determined one by one, say as extrema on paths of the form λ = constant. Alternately, we may want to design numerical processes which are capable of following a fold line directly.

In our example, the origin constitutes a so-called simple bifurcation point while the other points on the fold lines are simple limit points or turning points. This identifies two of the most basic types of singular points on such solution manifolds. As indicated earlier, the general study of the changes in equilibrium behavior at singular points is a topic of bifurcation theory. For our purposes we are interested in devising methods for locating and computing such points and for determining the form of the manifold near them.

These are only some of the many computational tasks before us. Some others do not occur in our simple example (1.2). For instance, when (1.1) is a differential or integral equation then we need to introduce a suitable discretization before we can proceed with the actual numerical calculation. In other words, we do not solve the original equation but some approximate form. This in turn leads to the question of estimating the approximation error between the solution manifold of the given equation and that of its discretization. Moreover, we are interested in determining whether any features on the original manifold, such as limit points or bifurcation points, correspond to analogous features on the approximating manifold.

The literature which relates to our topic spans a wide spectrum. The mathematical foundations include, in particular, the theory of stable mappings and their singularities. The origin of this theory may be found in the fundamental results of Hassler Whitney and Marston Morse which in part formed a basis of René Thom's development of catastrophe theory. Broadly speaking, a mapping is stable if every nearby mapping is identical with it after suitable coordinate changes in the domain and range. For some presentations of stability theory and the classification of the singularities of stable mappings we refer, for instance, to Arnold (1968), Golubitsky and Guillemin (1973), Gibson (1979), or Martinet (1982), where many further references may be found. For an overview of some of the applications of catastrophe theory see Poston and Stewart (1978).

In practical applications the topological approaches of modern singularity theory are often replaced by approximate analytical techniques based on linearizations at singular points and the earlier mentioned methods of perturbation theory and asymptotics. This is, for instance, the approach of elastic stability theory as presented by Thompson and Hunt (1973).

As noted earlier, the term bifurcation theory usually refers to the study of the solution set of parametrized equations, especially in the neighborhoods of points where the structure of this set does change. Here, one needs to distinguish two situations. The static case involves the structure of the set of zeros of a parameterized function. On the other hand, in the dynamic case one is interested in the structure of the limit sets of solutions of differential equations as the parameters vary. For some monographs in the area see, for instance, Iooss and Joseph (1980), Marsden and McCracken (1976), and, especially, Chow and Hale (1982), where numerous references are given.

The numerical analysis of our general area developed from a number of different roots. One of these is the study of continuation methods which in turn has several evolutionary lines. In the numerical analysis literature, probably beginning with Lahaye (1934) and Davidenko (1953), much emphasis has been placed on constructing a zero of a nonlinear function by connecting that function homotopically with another function for which the zeros are known. The numerical procedure then consists in following the corresponding homotopy path of zeros. For some survey of such methods see, for example, Wacker (1978), or Garcia and Zangwill (1981). In the engineering literature continuation procedures developed under the name of incremental methods or methods of incremental loading. In general, these are methods for determining a path of equilibrium solutions of a structure when some intrinsic parameter, such as a load intensity, is changed. For some overviews of these approaches see, e.g., Oden (1972) and Rheinboldt and Riks (1983). Discussions of computational aspects of continuation methods may be found, for instance, in Allgower and Georg (1980), Deuflhard et al (1976), Deuflhard (1979), Haselgrove (1961), Kearfott (1981), Kubicek (1976), Kubicek et al (1981), Burkardt and Rheinboldt (1983), Watson (1979), and Watson and Fenner (1980).

Parallel with this work on continuation procedures, the study of the constructive aspects of bifurcation theory and of the numerical solution of bifurcation problems has evolved. Here some of the fundamental results are due to H. B. Keller, who also contributed significantly to the study of continuation methods (see e.g. Keller (1970), Keener and Keller (1973), Keller (1973), and Keller (1978)). For some overviews we refer, for instance, to Kubicek and Marek (1983) and the recent conference proceedings edited by Kuepper, Mittelmann, and Weber (1984).

These brief historical comments are intended only to sketch the broad areas of the literature which relate to our topic, and, as noted in the Preface, no survey of this literature will be given here.

2. SOME SAMPLE PROBLEMS

This chapter presents several sample problems involving parametrized equations. They are intended to illustrate the principal concepts and some of the questions that are to be considered. Further examples are included throughout the text.

2.1. A SIMPLE FRAMEWORK

In order to focus the discussion, we begin with a simple example involving a two-dimensional solution manifold in R^3 (see also Poston and Stewart (1978)). The planar framework shown in Figure 2.1 consists of two rigid rods of length 1 each. The rods are pin-jointed and the spring between them tries to keep the framework in the straight reference configuration. Two loads λ, ν are applied as indicated. The deformation can be characterized by the angle y and, clearly, any deformation y lengthens the spring by $2y$. If the spring is assumed to be linear it will then contain the elastic energy $(1/2)k(2y)^2$ where k is the given spring constant.