LAS LLAMADAS TECNICAS DE ESTABILIZACION PERMITEN ESTABILIZAR PROBLEMAS QUE, EN PRINCIPIO, SON INESTABLES.

ES DECIR PERMITEN TRATAR PROBLEMAS MAL CONDICIONADOS

SEGUN P. LINZ THEORETICAL NUMERICAL ANALYSIS
ACTUAN EN DOS ETAPAS DIFERENTES DEL DESARROLLO DEL **P.I.**

LOS LLAMADOS METHODOS DE EXPANSIÓN EN EL MOMENTO DE LA CONSTRUCCIÓN DEL **ALGORITMO** QUE CONSTRUIMOS PARA FORMULAR NUMERICAMENTE EL **P.I**

LAS LLAMADAS TECNICAS DE REGULARIZACION
EN EL MOMENTO DEL TRATAMIENTO DEL PROBLEMA NUMÉRICO UNA VEZ QUE EL **P.I.** HA SIDO FORMULADO
ACTUAN MODIFICANDO LA NATURALEZA DEL PROPIO PROBLEMA QUE TRATAMOS DE RESOLVER (ACEPTANDO, A PRIORI, UNA APROXIMACIÓN)

THEORETICAL NUMERICAL ANALYSIS. Peter LINZ John Wiley & Sons 1979

9 THE SOLUTION OF IMPROPERLY POSED PROBLEMS

We have so far considered only problems which were well-posed. It seems intuitively reasonable that equations arising from physical situations should be well-posed since the parameters entering the equations are usually derived from actual measurements and therefore inexact to some extent. It would be unreasonable to expect the physical situation to change drastically if we were to change the parameters by a small amount; if our equation does indeed model the real world, then we would expect it to be insensitive to experimental errors. This reasoning is fairly sound and most of the problems we deal with are indeed well-posed. Nevertheless, certain mathematical descriptions of actual situations lead to improperly or ill-posed formulations, as we shall see shortly by a simple example.

The prototype for this situation is the *Fredholm equation of the first kind*

$$\int_0^1 k(s,t)x(t)\,dt = y(s), \qquad 0 \le s \le 1. \tag{9.1}$$

If we assume that $k(s,t)$ is differentiable in $[0,1]\times[0,1]$, then it is easy to see that this problem in not well-posed. Take the function $x_n(t)=\sin nt$; then

$$\int_0^1 k(s,t)x_n(t)\,dt = O(1/n),$$

which follows from an elementary argument. This according to Theorem 4.7, shows that the operator does not have a bounded inverse. Another way of saying this is that a small perturbation of size $O(1/n)$ on the right-hand side can generate a change with norm of order unity in the solution. Since

we can make n as large as we want the problem cannot be well-posed. Of course, we can write down any equation we want; it does not follow that there is an actual physical situation modeled by such an equation. For (9.1), however, there is a corresponding physical problem.

Consider a simple optical system consisting of an object O, a lens L, and an image I. If we denote by $x(s)$ and $y(s)$ the light intensities of O and I, respectively, then we can think of the lens as represented by an operator L mapping x into y, or $Lx=y$. What form might this operator L have? If the lens were perfect, then the image intensity at some point s would depend only on the intensity at a single corresponding point in the object; if the lens is not perfect, then a certain amount of "smearing" will occur and $y(s)$ will depend on some sort of weighted average of the object intensity. Mathematically, this weighted average can be represented as an integral with a certain weight function; if we call this weight function $k(s,t)$, then we get exactly (9.1).

We may note at this point that if we take the Dirac delta "function" as $k(s,t)$, then $x(s)=y(s)$ (perfect lens case), and the problem is certainly well-posed. On the other hand, as we have indicated, when $k(s,t)$ is smooth then the problem is ill-posed. We are thus led to the somewhat unexpected situation that a poorly behaved kernel defines a solution more satisfactorily than a smoother kernel.

While we have taken a somewhat oversimplified physical situation in this discussion, equations of this type often arise in physical systems where the nature of an object is to be inferred from indirect and experimental observations. For a discussion of other types of ill-posed problems arising in mathematical physics see (Lavrentiev, 1967).

When solving ill-posed problems numerically we must certainly expect some difficulties, since any errors act as a perturbation on the original equation and so may cause arbitrarily large changes in the solution. Since errors can never be completely avoided the prospects look rather dim; if we are to make any progress we must reexamine our notion of the solution of an equation. To provide some insight into this, let us return to the simple physical model above. Suppose that the light intensity in the object oscillates rapidly from dark to bright. When this input is smeared by an imperfect lens the image will look uniformly grey. Therefore, if we observe a uniformly grey image it may be the result of an object composed of rapidly alternating dark and bright spots. On the other hand, it may also be the image of a uniformly grey object. Without any further assumptions we cannot tell the difference. If we were to encounter this in an actual experimental situation we would probably rule out the first alternative as uninteresting or implausible and ask instead what regularly behaved object could have caused the observed image.

Next, we consider the selection of α which controls the overall magnitude of the regularization effect. From one point of view we would like to make α as large as possible. Since for $\alpha=0$ the problem is ill-posed it seems reasonable to require α to be large. Although the set in which the minimum lies is compact for all $\alpha>0$, we run into ill-conditioning in the numerical minimization when α is very small. To see this, let us try to define a condition number for the minimization of a given functional $H(x)$. A condition number is essentially a measure of how well we can tell the solution from a near-solution; thus if we perturb the solution x by Δx we would like to see an appreciable change in $H(x)$. By a Taylor expansion we have

$$H(x+\Delta x) \cong H(x) + H'(x)\Delta x + \tfrac{1}{2}H''(x)(\Delta x)^2. \tag{9.8}$$

If x minimizes H, then $H'(x)=0$, so that the perturbation Δx causes a change of $\frac{1}{2}H''(x)(\Delta x)^2$ in H. Thus we can think of

$$1/\inf \frac{\|H''(x)(\Delta x)^2\|}{\|\Delta x\|^2} \tag{9.9}$$

as a condition number which we want to keep small. Since J'' involves a term $\alpha\varphi''$ it appears that a large α will tend to make the minimization of J well-conditioned.

Of course, we also have to remember that minimizing J does not yield the solution of (9.3) unless $\alpha=0$, so for this reason we want to keep α small. If x is a solution of (9.3) and $\hat{x}$ minimizes J, then we have

$$\begin{aligned} J(\hat{x}) &\le J(x) \\ &= \|Lx-y\| + \alpha\varphi(x) \\ &\le \alpha\varphi(x), \end{aligned}$$

from which we get

$$\begin{aligned} \|L\hat{x}-y\| + \alpha\varphi(\hat{x}) &\le \alpha\varphi(x) \\ \|L\hat{x}-y\| &\le \alpha\varphi(x). \end{aligned} \tag{9.10}$$

Thus, while $\hat{x}$ is not a solution it will be a good approximate solution if α is small. If we are permitted an error ϵ in the sense of (9.2), then we must have $\alpha\varphi(x)\le\epsilon$. A reasonable choice of α appears then to be

$$\alpha = \epsilon/\varphi(x), \tag{9.11}$$

although because of the various inequalities this may not be the optimal choice.

Conditions (a) and (b) which we imposed on φ were chosen, somewhat arbitrarily, for the sake of discussion. Other types of regularization functionals can and have been used. The proper choice of φ obviously depends on L; furthermore we would like to choose it so that $\varphi(x)$ is very small when x is the sought solution and so that it is large for those near-solutions we want to eliminate. The more information we have about the solution the better we will be able to do this. What the formal properties of φ should be is an open question.

9.2 EXPANSION METHODS

In the regularization method we control the unwanted near-solutions by imposing a heavy penalty on them through the functional $\varphi(x)$. Another approach is to eliminate these undesirable solutions altogether by an *a priori* choice of the space of the permitted solutions. For this we choose a finite-dimensional space X_n and look for solutions in this space; generally there will, of course, not exist an exact solution, so that we can solve (9.3) only approximately. If $\{\varphi_{ni}\}$ is a basis for X_n, then we look for a solution of the form

$$x_n = \sum_{i=1}^{n} \alpha_i \varphi_{ni} \tag{9.12}$$

such that

$$Lx_n \cong y. \tag{9.13}$$

This is essentially what we did in Section 4.2 for well-posed problems, although here we are not able to prove convergence since this concept is not very meaningful when the problem is ill-posed. In any case the observation suggests that it is possible to adapt Galerkin and least squares type methods for ill-posed problems.

Let us assume that X and Y are Hilbert spaces. If we use the Galerkin approach, then we want to make $Lx_n - y$ orthogonal to span $\{\varphi_{n1}, \varphi_{n2}, \cdots, \varphi_{nn}\}$, which leads as before to the matrix equation

$$A\boldsymbol{\alpha} = \mathbf{b}, \tag{9.14}$$

with $a_{ij}=(L\varphi_{ni}, \varphi_{nj})$, $b_i=(\varphi_{ni}, y)$.

The solvability of this system depends on the choice of $\{\varphi_{ni}\}$. One way which is, at least formally, very simple is to use the eigenfunctions of L as

This gives us a clue for proceeding in general: to solve ill-posed problems we must restrict the type of answer we will accept so that we get only plausible solutions. How we define "plausible" is essentially up to us; different ways of definition lead to different numerical approaches as we see below. Once we have defined an acceptable solution we still have some worries. How do we know that the problem actually has a solution in the defined set? The answer is that it probably has not, but if we are in a real situation the presence of experimental and observational errors makes it unimportant to satisfy the equation exactly. The task of solving an ill-posed problem can then be restated as: find an element x, subject to certain restrictions, such that the equation $Lx=y$ is satisfied approximately, that is, such that

$$\|Lx-y\| \leq \epsilon, \tag{9.2}$$

for some given $\epsilon>0$.

For the rest of this chapter we will not proceed in the usual theorem-proof fashion that we have employed so far; rather we will present a "discussion" of the pertinent problems and results. By this we mean that we will indicate the lines along which a theory can be developed without rigorously carrying out all the proofs. The reader may consider it a challenge to his understanding to see how far he can make precise what we are about to present. The reason for taking this approach is two-fold. First, it seems that at the present there has not yet emerged a commonly accepted approach and it is difficult to see what a general theory will ultimately look like. Also, the theoretical development that does exist involves technical difficulties whose discussion would lead us too far afield. As a second consideration, the reader may find it instructive to see the kind of "plausibility" arguments that are often made in the early stages of research. One often tries to get a "feeling" for the subject before settling down to the task of establishing proofs and a general theory. One must be cautious, however. While this type of treatment can be very helpful to one's understanding, one must not jump to the conclusion that anything has been proved.

9.1 REGULARIZATION TECHNIQUES

We shall restrict ourselves to equations of the form

$$Lx = y, \tag{9.3}$$

where L is a linear operator between two linear spaces X and Y. We also assume that $\mathcal{D}(L)=X$ and $\mathcal{R}(L)=Y$, so that the problem has a solution.

Since we want to consider ill-posed problems we shall assume that L^{-1} is not bounded.

In our discussion of (9.1) we saw that a difficulty was caused by the existence of highly oscillatory functions which, while not actually being solutions, satisfy the equation very closely. Somehow, we want to eliminate such "near-solutions" from consideration. One way to accomplish this is the so-called *regularization method*, which was first systematically developed by Tikhonov (see for example, Tikhonov, 1963). Consider the functional

$$J(x) = \|Lx-y\| + \alpha\varphi(x), \tag{9.4}$$

where $\alpha>0$ and φ is a functional defined on X. Instead of attempting to solve (9.3) we try to minimize J, that is, we look for an $\hat{x}\in X$ such that

$$J(\hat{x}) \leq J(x) \text{ for all } x\in X \tag{9.5}$$

Provided that the *regularization functional* $\varphi(x)$ is properly chosen this minimization problem will be well-posed even if (9.3) is not. How then do we choose φ? Intuitively, we want $\varphi(x)$ to be small for well-behaved x and very large for irregular x. More formally, we might require that φ satisfy

(a) $\varphi(x)\geq 0$ for all $x\in X$

(b) φ is such that for any $M<\infty$ the set $\Phi_M=\{x\in X|J(x)\leq M\}$ is compact.

Example 9.1. Let X be $C^{(1)}[0,1]$ with maximum norm. Let L be given by (9.1) and define φ by

$$\varphi(x) = \|x\|_\infty + \|x'\|_\infty. \tag{9.6}$$

Condition (a) is obviously satisfied. Condition (b) follows from the fact that the functions in Φ_M are uniformly bounded and equicontinuous; hence by the Arzela–Ascoli theorem Φ_M is compact.

The reason for imposing conditions (a) and (b) is that they are sufficient to allow us to look for the minimum of J on a compact set, which is a well-posed problem. We can see this from the following argument. If x is a solution of (9.3), then $J(x)=\alpha\varphi(x)$. If $\hat{x}$ minimizes J, then

$$J(\hat{x}) \leq J(x) = \alpha\varphi(x). \tag{9.7}$$

Thus the minimum, if it is attained, must be in the compact set $\{\bar{x}\in X|J(\bar{x})\leq\alpha\varphi(x)\}$.

expansion functions. If u_i is such that

$$Lu_i = \lambda_i u_i, \tag{9.15}$$

then setting $\varphi_{ni} = u_i$ makes the matrix in (9.14) diagonal and the solution is immediately given by

$$x_n = \sum_{i=1}^{n} \frac{1}{\lambda_i}(u_i, y)u_i. \tag{9.16}$$

If we assume that the eigenfunctions of L are closed in X, then formally we can write

$$x = \sum_{i=1}^{\infty} \frac{1}{\lambda_i}(u_i, y)u_i \tag{9.17}$$

and

$$\|x - x_n\|^2 \leq \sum_{i=n+1}^{\infty} \frac{1}{\lambda_i^2}(u_i, y)^2. \tag{9.18}$$

Whether (9.17) actually defines a convergent series depends on y as well as on the distribution of the eigenvalues of L. If the series does converge, then (9.18) apparently indicates that we can get arbitrarily high accuracy by making n sufficiently large. Furthermore, since the computation of x_n by (9.16) seems to be a well-conditioned numerical process one might think that this gives us a way of solving ill-posed problems with no difficulty whatsoever! Such a conclusion ought to look very suspicious and there is indeed a flaw in our reasoning. The eigenvalues and eigenfunctions of L are generally not known and must be computed numerically. This means that the eigenvalues of small magnitude and their associated eigenvectors will have large relative errors, making it difficult to evaluate (9.16) accurately. Therefore, one must try and keep n as small as possible within the constraints of accuracy requirements.

Eigenfunction expansions for ill-posed problems (specifically the Fredholm equation of the first kind) were suggested in (Baker *et al.*, 1964). More recent treatments advocate the more general singular function expansions. If $\{\lambda_i, u_i, v_i\}$ satisfy

$$Lu_i = \lambda_i v_i, \quad L^* v_i = \lambda_i u_i \tag{9.19}$$

where L^* denotes the adjoint of L, then the λ_i are called the singular values and u_i, v_i the singular functions of L. If we modify Galerkin's

method so that x_n is a linear combination of the u_i, but $Lx_n - y$ is made orthogonal to span$\{v_i\}$, then the above analysis goes through in essentially the same way.

Of course it is not necessary to use eigenfunctions or singular functions in the expansion; any set closed in X will do. The major advantage of the eigenfunction expansion is that the analysis of the conditioning of (9.14) and error bounds, such as (9.18), are easy to obtain.

Also, as an alternative to Galerkin's method we can use a least-squares technique, leading to a system of the form (9.14) with $a_{ij} = (L\varphi_{ni}, L\varphi_{nj})$ and $b_i = (L\varphi_{ni}, y)$. A considerable amount of work on the use of least-squares methods in this setting has been done (see Kammerer and Nashed, 1972). Another avenue of approach uses the fact that ill-posed problems arise primarily in connection with the "unravelling" of experimental observations as indicated at the beginning of this chapter. Since the observational errors often have known probability distributions it is possible to satisfy (9.3) subject to certain statistical requirements. This idea is explored in (Strand and Westwater, 1968).

Finally, we caution the reader not to take our rather descriptive treatment of the subject as an indication that there are no theoretical treatments of ill-posed problems. (Although it seems fair to say that there exists no unified theory at the present.) The already mentioned work of Kammerer and Nashed and the contributions of Wahba [see for example, (Wahba, 1973)] use sophisticated function-analytic methods to explore these questions. The regularization methods have been studied extensively in Russia; a large number of papers on the topic can be found in the Russian literature, particularly in the U.S.S.R. journal *Computational Mathematics and Mathematical Physics*.

Attempts were made to solve ill-posed problems long before the modern mathematical methods of regularization were developed. Brilliant intuitions led scientists to acceptable results in solving inverse problems which included relatively simple models with small numbers of parameters. But intuitive methods are only possible when the precision of the input data is not high. Present experimental equipment involving very precise measurements and powerful computers have made necessary a technology for solving inverse problems.

Nowadays, there is the theory of the regularization of ill-posed problems, and this allow us to find effective numerical algorithms for a wide range of inverse problems. The fundamental point in this theory is the concept of a regularizing algorithm. This is defined as an operator (or a rule) R which establishes a relationship between each pair (u_δ, δ) and an element $z_\delta \in Z$ such that $z_\delta \xrightarrow{z} \bar{z}$ as $\delta \to 0$. Regularizing algorithms were developed for many ill-posed problems and implemented on computers. This allowed us to formulate a new approach to the automated processing of experimental data and to create automated packages for data processing in geophysics, plasma physics, astrophysics, spectrometry, etc. The modern methods of the theory of regularization has promoted considerable progress in solving the problems of synthesis of antennas, optical elements for laser light focusing, and optical coatings. Regularizing algorithms also provide a basis for the modern methods for reconstructing images in medical and industrial tomography and pattern recognition.