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Some Insights into the Regularization of Ill-posed Problems

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In this paper a simple introduction to the problem of the regularization of ill-posed problems (IPP) is presented. We describe three regularization methods with simple examples which illustrate the principle that for "bad" equations it is unprofitable to carry out exact computations.

Keywords: Error vector; Regularization parameter

I INTRODUCTION

In the natural sciences ill-posed problems (IPP), as opposed to well-posed problems defined by Hadamard in 1932, appear when we consider, for example, systems described by linear equations

$$Az = u \tag{I.1}$$

in which the solutions "z" describing the direct attributes of the system possess at least one of the following properties:

(i) they are very sensitive to small changes δu and δA of vectors u and/or operators A (input data),
(ii) they are not unique,
(iii) (I.1) is not solvable for the entire space U of vectors u [1,2].

These properties are related to each other and in fact may occur as a result of the "smearing" features of the operator A which occur in many observed, indirect attributes u of the phenomenon. IPP are to be found even in the 2D case considered below [1].

The lack of stability of such systems can also be explained as a manifestation of the fact that Eq. (I.1) used to describe them is not restrictive enough [3]. For example, some components of the vector equation (I.1) are almost identical (e.g. when the determinant of the matrix A has a small value, see Section III). In fact, if the measurements were *ideal* the operator A in Eq. (I.1) could not even be inverted ($\det A = 0$) and only errors (δA) make inversion possible. But by making inversion possible in such a curious way, the above instabilities are created.

In general, when the solutions to some problem are not stable with respect to the usual information required for their unique specification, there are two ways of solving the resultant difficulty. The first, is to use **additional** information and look for solutions in a specific (compact) subset of possible solutions [1–4]. The second is to use a statistical description of the system in which small changes of usually fixed elements of the theory are treated as random quantities [5].

The choice of remedy depends on two factors: the availability of additional information and the economy of the description. For example, in the case of turbulent flow in liquid we use the second remedy, whereas in the case of prospecting for various resources we use the first method because there is additional information which if taken into account can transform IPP into problems which are well-posed, see [1–4,6].

The purpose of this paper is to illustrate the basic concepts of IPP with the help of the simplest equations. In particular, we are interested in the idea of *regularization* – a fundamental notion of the IPP approach by means of which final results are stabilized.

II REGULARIZATIONS

Because the instability of solutions to Eq. (I.1) is caused by the intrinsic indeterminate nature of the original equation, it is natural to expect that additional restrictions (properties) imposed upon possible solutions may change the situation. We therefore look for solutions with an additional *property* usually expressed by minimization of the so-called *stabilization functional*(*s*) [1,4]. With the help of this functional(s) it is possible, in many cases, to slightly change Eq. (I.1) in such a way that the solutions with the automatically acquired new property are stable with respect to small variations δA and δu of the input data if the *regularization parameter* α is in a **definite relation** R to the *error vector* $\eta = (\delta A, \delta u)$ [6,7].

Roughly speaking, the relation R between α and η expresses the practical observation that any algorithm should be accompanied by precision of measurements: it is not recommended, for example, that we make more and more subtle triangulations of a given surface without increasing the precision of measurements. All we need to do after regularization is to check whether the results obtained are stable [3; page 162]. As a regularized equation to Eq. (I.1) with a completely continuous operator A we can use, for example,

$$[A^*A + \alpha]z = A^*u, \tag{II.1}$$

[6; page 48].

In Sections III and IV we can see how the idea of regularization works in the case of a 2D linear equations (I.1) using (II.1) and simplified equations.

In Section V a regularization parameter α is related to the inverse power of "the time" s, see [2,8]. In this case instead of the regularized Eq. (II.1) we use the "gradient equation" (a relaxation method) which in the continuous case yields

$$\mathrm{d}z/\mathrm{d}s = -A^*(Az - u), \tag{II.2}$$

see [2,8]. In the discrete case

$$z_{i+1} = z_i + \theta A^*(Az_i - u), \tag{II.3}$$

see also [8]. It can be shown that, for a broad class of operators A, the asymptotes of Eqs. (II.2) and (II.3) tend to stationary solutions which can be identified with solutions to the original Eq. (I.1), see [2,9]. It turns out that in the case of imprecise input data (A, u) **and IPP (I.1)** the scenario of a typical evolution (II.2) is as follows: at the beginning of the evolution it looks as if the system tends to a solution of the ideal equation (I.1) ($\eta = 0$) which is the closest solution to the initial vector $V(0)$. This picture gradually changes and for large enough s the system tends eventually to the unique, unstable solution to Eq. (I.1) ($\eta \neq 0$). To stop this, a large but finite s has to be chosen in relation to the error vector η. We illustrate this in Section V.

For regularized Eqs. (II.1)–(II.3), the stabilization functional mentioned at the beginning of this section is the Euclidean norm of vector z, Section V. In other words, by means of regularizations Eqs. (II.1)–(II.3) we can get an approximated solution to Eq. (I.1) whose norm is minimalized with respect to errors.

III THE 2D LINEAR SYSTEM

Following [1] we consider the ill-posed problem described by a system of two linear equations:

$$\begin{aligned} z_1 + z_2 &= 1, \\ (1+\mu)z_1 + z_2 &= 1 + \delta, \end{aligned} \tag{III.1}$$

which can give arbitrary values of z_1 and z_2 for any small δ and μ:

$$z_1 = \delta/\mu, \quad z_2 = 1 - \delta/\mu. \tag{III.2}$$

The above instability is a consequence of the fact that for $\mu = \delta = 0$ (III.1) is reduced to one equation only. Using the regularized equation (II.1) with matrix

$$A = \begin{pmatrix} 1 & 1 \\ 1+\mu & 1 \end{pmatrix} \tag{III.3}$$

we obtain, for example

$$z_1 = (\mu\delta + [1 + (1+\mu)(1+\delta)]\alpha)/(\mu^2 + 2\alpha + \alpha^2 + [1 + (1+\mu)^2]\alpha) \tag{III.4}$$

with α as the regularization parameter and the *error vector* $\eta = (\mu, \delta)$ characterizing the accuracy of the input data. We see that z_1 is stable with respect to small changes of the error vector η if that vector is in an appropriate relation R with α. This relation is the following

$$|n| \ll \alpha. \tag{III.5}$$

Taking into account (III.5) we do in fact get from (III.4)

$$\begin{aligned} z_1 &\cong ([1+(1+\mu)(1+\delta)]\alpha)/(2\alpha+\alpha^2+[1+(1+\mu)^2]\alpha) \\ &\cong 2/(4+\alpha), \end{aligned} \tag{III.6}$$

where in order to obtain the last equality the absolute smallness of η was also taken into account. The required stability of formula (III.4) with respect to the error vector η is realized here by the fact that (III.6) which does not depend on η is close to (III.4). Of course, in order not to be too far from the original Eq. (I.1) or (III.1) we have to assume that α is small, in which case we get a final value for $z_1 \cong 1/2$. In this case, from the first Eq. (III.1), we get

$$z_1 \cong z_2 \cong \tfrac{1}{2}. \tag{III.7}$$

These results can be obtained directly from (III.1) and (III.2) by initially narrowing down the set of possible solutions by some ad hoc assumption like a demand that the norm of the required solution is minimal or a demand for symmetry. In the first case we would have to minimize

$$|z|^2 = (\delta/\mu)^2 + (1-\delta/\mu)^2 \tag{III.8}$$

while in the second case symmetry could be understood as the equality

$$z_1 = z_2 \tag{III.9}$$

resulting from the symmetrical shape of the exact equation (III.1).

IV THE SIMPLIFIED REGULARIZATION

The regularization (II.1) of the original Eq. (I.1) in the case of operator $A^* = A > 0$ can be substituted by a *simplified* regularization

$$(\alpha I + A)z = u \tag{IV.1}$$

considered in [7, pages 84–89] for closed operators A. This method of regularization is particularly recommended when the Gauss transformation: $A \Rightarrow A^*A$, disturbs the original structure of the operator A, for example, transforms the diagonal plus lower triangular operator into a diagonal plus upper triangular operator. We consider regularization (IV.1) for the original equation

$$\begin{aligned} z_1 + \mu z_2 &= 1, \\ \mu z_1 &= 0 \end{aligned} \tag{IV.2}$$

with error vector $\eta = (\mu, 0)$. Without regularization, the solution to (IV.2) is

$$z_1 = 0, \quad z_2 = 1/\mu. \tag{IV.3}$$

With simplified regularization (IV.1) (in fact, the corresponding matrix A is only approximately positive) we get

$$z_1 = \alpha/[\alpha(\alpha+1) - \mu^2], \quad z_2 = \mu/[\mu^2 - \alpha(1+\alpha)]. \tag{IV.4}$$

For restriction (III.5) and the small regularization parameter α we get the approximated solution

$$z_1 \cong 1, \quad z_2 \cong 0. \tag{IV.5}$$

We would obtain a similar result for the regularization (II.1) albeit with more complicated formulas.

V THE GRADIENT REGULARIZATION

In this section we examine how the gradient method (II.2) works. We have

$$\dot{z} = -A^*(Az - \mu). \tag{V.1}$$

The matrix A for (IV.2) can be decomposed into two parts:

$$A = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \mu \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \equiv P + \mu W. \tag{V.2}$$

The first is a projector $P = P^2$ upon the first component of vector z, the second can be treated as a small perturbation μW which affects the "evolution" of (V.1) only for large "times" s. So if times s which are not extremely large are taken into account, we can put

$$A \cong P \tag{V.3}$$

into (V.1) and consider the simplified equation

$$\dot{z} = -P(z - u) \tag{V.4}$$

with vector $u = (1, 0)$. Hence

$$z_1 = 1 - \mathrm{e}^{-s} + z_1(0)\mathrm{e}^{-s}, \quad z_2 = z_2(0). \tag{V.5}$$

For a large enough s, $z_1 \cong 1$ as in the regularized case (IV.5). We get the second regularized result (IV.5) if we put initial vector $z(0) = 0$. This is not an accidential choice but a result of interpretation of the asymtotes of the gradient method, see the comment after (V.15). It is interesting to note that the expected unstable result (IV.3) does not occur when $s \Rightarrow \infty$ because of the simplification (V.3).

The indeterminate nature of the second component of the asymptote of vector z in (V.5) is a specific feature of the gradient method in the case of (ii), see the beginning of the paper. It can be avoided if we use a double regularization with s and α as regularizing parameters. In this case, instead of (V.3),

$$A \cong \alpha I + P. \tag{V.6}$$

At the end of this section we give an exact description of solutions to Eqs. (V.1) and (V.2) to show how the unstable (exact) and stable (regularized) solutions of Eq. (IV.2) are obtained. To do this we use general formulas describing s-dependence of solutions of Eq. (V.1) with the help of the eigenvectors $\phi^{(i)}$

$$A^* A\phi^{(i)} = E_i\phi^{(i)} \tag{V.7}$$

where eigenvalues $E_{(i)}$ are positive numbers. They are

$$z(s) = \sum_i (\phi^{(i)}, z(0)) \exp(-E_i s)\phi^{(i)} + \sum_i \int_0^s (\phi^{(i)}, A^* u) \exp(E_i(\tau - s))\phi^{(i)} \mathrm{d}\tau. \tag{V.8}$$

In the case (V.2)

$$E_i = [2\mu^2 + 1 - (-1)^i (4\mu^2 + 1)^{1/2}]/2$$

for $i = 1, 2$ and the orthonormal eigenvectors

$$\phi^{(i)} = \{1 + [\mu/(E_i - \mu^2)]^2\}^{-1/2} \begin{pmatrix} 1 \\ \mu/(E_i - \mu^2) \end{pmatrix} \tag{V.9}$$

and vector

$$A^* u = \begin{pmatrix} 1 \\ \mu \end{pmatrix}.$$

From (V.8)

$$z(s) = \sum(\phi^{(i)}), z(0)) \exp(-E_i s)\phi^{(i)} + \sum(\phi^{(i)}, A^* u) E_i^{-1} (1 - \mathrm{e}^{-E_i s})\phi^{(i)} \tag{V.10}$$

and because eigenvalues E_{i}, for $\mu \neq 0$, are positive numbers from (V.9) and (V.12) we can conclude that

$$z(\infty) = (E_1 - E_2)^{-1} \hat{\phi}^{(1)} + (E_2 - E_1)^{-1} \hat{\phi}(2), \tag{V.11}$$

where orthogonal vectors $\hat{\phi}^{(i)}$ are defined as in (V.9) but without a normalizing term. Hence, taking into account that

$$E_1 + E_2 = 2\mu^2 + 1, \quad E_1 E_2 = \mu^4, \tag{V.12}$$

we get (IV.3), a result which illustrates the theorem that solutions of Eq. (II.2) asymptotically tend to solutions of the original Eq. (I.1). To get, via the gradient method, stable solutions (IV.5) of the regularized Eq. (IV.1) we have to choose a finite s in appropriate relation to μ. Taking into account that for small values of μ,

$$E_1 \cong 1 \text{ and } E_2 \cong \mu^4 \tag{V.13}$$

and

$$\phi^{(1)} = \begin{pmatrix} 1 \\ \mu \end{pmatrix}, \quad \phi^{(2)} = \begin{pmatrix} \mu \\ -1 - \mu^2 \end{pmatrix},$$

we get from (V.8)

$$\begin{aligned} z(s) \cong & \{[z_1(0) + \mu z_2(0)]\mathrm{e}^{-s} + (1 + \mu^2)(1 - \mathrm{e}^{-s})\}\begin{pmatrix} 1 \\ \mu \end{pmatrix} \\ & + \{[\mu z_1(0) - z_2(0)]\mathrm{e}^{-s\mu^4} - \mu^3\mu^{-4}(1 - \mathrm{e}^{-s\mu^4})\}\begin{pmatrix} \mu \\ -1 \end{pmatrix}. \end{aligned} \tag{V.14}$$

Now it is easy to see how the regularized solution (IV.5) emerges from (V.14). We have to assume that large but finite s satisfies relations:

$$\begin{aligned} & s \gg 1, \\ & s\mu^4 \cong 0 \end{aligned} \tag{V.15}$$

and

$$s\mu^3 \cong 0.$$

Of course, we assume that $\mu \cong 0$. Ignoring as before the $z(0)$-dependent term we get (IV.5). In fact this point can be justified in a deeper sense: The reader is reminded that solutions to Eq. (IV.2), since they are solutions to IPP, are not unique (for the ideal case $\mu = 0$). In this case the gradient method chooses the closest solution of (IV.2) to the initial vector $z(0)$, see [2,10]. The choice

$$z(0) = 0 \tag{V.16}$$

is equivalent to a choice of solution with minimal norm (normal solution).

Choosing $s = b\mu^{-4}$ we see that s is large and the first relation of (V.15) is satisfied for small parameters b and μ, appropriately related to each other. The second relation of (V.15) is automatically satisfied for a small b because $s\mu^4 = b$. From the third relation of (V.15) we obtain $b \ll \mu$ because $s\mu^3 = b/\mu$. Hence we get a typical relation between the parameter s^{-1} related to a regularization parameter α, see [2], and the error parameter μ

$$s^{-1} \gg \mu^4 \tag{V.17}$$

a characteristic phenomenon when dealing with IPPS.

VI FINAL REMARKS

In mathematical descriptions of certain domains of Nature, we often encounter a critical situation in which notions and algorithms previously checked out many times cease to work. These symptoms are divergences or instabilities which make calculations difficult or impossible. In such cases we talk about IPPS discussed above, or about non-computability as in the case of the eigenvalue problem for unbounded self-adjoint operators in Hilbert space [11], or about non-uniform convergence or even complete divergence of the perturbation series [12], and so on. In all these cases remedies have been found in the form of certain modifications of the previous notions which are equivalent to extensions or reductions (or both) of the spaces in which equations were previously considered. Irrespective of whether an extension is treated as a source of trouble [1–4,7–9] or a device making possible certain transformations [5,9,10], we have to use additional conditions to pick out physical solutions. These additional conditions differ from the classical ones (initial, boundary) in that they are usually of a qualitative nature and take into account the specific properties of required solutions like normality [1–4], the zeroth order essentiality [12], symmetry [10], interpretation [11] and so on [13]. A practical realization of the above program can be executed by means of a regularization method substituting Eq. (I.1) by Eqs. (II.1) or (II.2) and (II.3) or (IV.1). In this way the experience and knowledge of the scientist or engineer can compensate for technical (computational, measurement) imperfection.

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