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Generalized Nonlinear Inverse Problems Solved Using the Least Squares Criterion

ALBERT TARANTOLA AND BERNARD VALETTE

Laboratoire de Sismologie (CNRS), Institut de Physique du Globe de Paris
Université Pierre et Marie Curie, 75230 Paris Cedex 05, France

We attempt to give a general definition of the nonlinear least squares inverse problem. First, we examine the discrete problem (finite number of data and unknowns), setting the problem in its fully nonlinear form. Second, we examine the general case where some data and/or unknowns may be functions of a continuous variable and where the form of the theoretical relationship between data and unknowns may be general (in particular, nonlinear integrodifferential equations). As particular cases of our nonlinear algorithm we find linear solutions well known in geophysics, like Jackson's (1979) solution for discrete problems or Backus and Gilbert's (1970) solution for continuous problems.

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1. INTRODUCTION

The aim of physical sciences is to discover the minimal set of parameters which completely describe physical systems and the laws relating the values of these parameters to the results of any set of measurements on the system. A coherent set of such laws is named a physical theory. To the extent that the values of the parameters can only be obtained as a results of measurements, one may equivalently consider that physical theories impose some relationships between the results of some measurements.

Theoretical relationships are often functional relationships, exactly relating the values of the parameters to the results of the measurements. Sometimes, theoretical relationships are probabilistic, as in geophysics when some property of the earth is statistically described, or as in quantum mechanics, where the probabilistic description of the results of the measurements is essential to the theory.

If, given some information on the values of the set of parameters, we try to use a theoretical relationship in order to obtain information on the values of some measurable quantities, we are solving, by definition, a 'direct (or forward) problem.' If, given some information on the values of some measured quantities, we try to use a theoretical relationship in order to obtain information on the values of the set of parameters, then we are solving an 'inverse problem.' For a direct problem the values of the parameters are 'data,' and the values of some observable quantities are 'unknowns.' For an inverse problem the data are the results of some measurements, and the unknowns are the values of parameters. We will see later that actual problems are in fact mixed problems.

One of the difficulties arising in the solution of some problems is the instability (a small change in the inputs of the problem produces a physically unacceptable large change in the outputs). This difficulty appears in direct as well as in inverse problems (see, for example, *Tikhonov* [1976]).

Inverse problems may have a more essential difficulty: nonuniqueness. There are two reasons for nonuniqueness. In some problems the nonuniqueness comes from the fact that the data are discrete; if the data were dense, the solution would be unique (see, for example, *Backus and Gilbert* [1970]). In other problems, nonuniqueness may be deeper, as, for example, in the inverse problem of obtaining the density structure of a region of the earth from the measurements of the local gravitational field: Gauss' theorem states that an infinity of different density configurations give identical gravitational fields.

The classical formulation of a problem (direct or inverse) may be stated as follows: (1) We have a certain amount of information on the values of our data set, for example, some confidence intervals. (2) We have some theoretical relationships relating data and unknowns. (3) We assume a total ignorance of the values of our unknowns; that is, the sole information must come from the data set. (4) Which are the values of the unknowns?

Such a problem may be ill posed, and the solution may be nonunique.

For maximum generality the problem should be formulated as follows:

1. We have a certain state of information on the values of our data set.

2. We have also a certain state of information on the values of our unknowns (eventually the state of null information).

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3. We have a certain state of information on the theoretical relationships relating data and unknowns.

4. Which is the final state of information on the values of the unknowns, resulting from the combination of the three preceding states of information?

Posed in terms of states of information, all problems are well posed, and the uniqueness of the final state of information may be warranted. We have given some preliminary results of such an approach [*Tarantola and Valette*, 1982] and have shown that in the particular case where the states of information can be described by Gaussian probability density functions, the least squares formalism is obtained.

The main purpose of this paper will then be to state clearly the nonlinear least squares approach to the generalized inverse problem and to give practical procedures to solve it.

For the linear problem, generalized least squares solutions are today well known. *Franklin* [1970] gave a very general solution, valid for discrete as well as for continuous problems, and *Jackson* [1979] discussed the use of a priori information to resolve nonuniqueness in geophysical discrete inverse problems.

In contrast, the nonlinear generalized least squares problem has not received much attention, and the usual way of solving such a problem is by iteration of a linearized problem, but as we will show in this paper, this procedure may give wrong solutions.

In section 2 we will study the discrete problem, and in section 3 we will deal with problems involving functions of a continuous variable. As a particular case of our solution for continuous problems we find the *Backus and Gilbert* [1970] solution. In section 4 we give some numerical illustrations of our algorithms.

2. The Discrete Problem

a. Notations

We will mainly follow the notations used by *Tarantola and Valette* [1982]. We will refer to that work as paper 1.

Let $\mathcal{S}$ be a physical system in a large sense. By large sense we mean that we consider that $\mathcal{S}$ is composed of a physical system in the usual sense plus all the measuring instruments. We say that the system $\mathcal{S}$ is 'parameterizable' if any state of $\mathcal{S}$ may be described using some functions and some discrete parameters. This means that we limit ourselves to the quantitative aspects of $\mathcal{S}$. If any state of $\mathcal{S}$ may be described using a finite set of discrete parameters, we say that $\mathcal{S}$ is a 'discrete system.' In this section of the paper we will focus our attention on such discrete systems.

Let $\mathbf{X} = \{X^1, \cdots, X^m\}$ be the finite set of parameters needed to describe the system, and let us use lowercase letters to note any particular value of the parameter set: $\mathbf{x} = \{x^1, \cdots, x^m\}$. Since in $\mathcal{S}$ we also include the measuring instruments, the parameter set contains all the data and the unknowns of the problem. Let $\mathcal{C}^m$ be the m-dimensioned space where the parameters $\mathbf{X}$ take their values; then $\mathbf{x}$ is a point of $\mathcal{C}^m$ and will be called a 'state' of $\mathcal{S}$.

Physical theories impose constraints between the possible values of the parameters. In the simplest case these constraints take a functional form

$$\begin{aligned} f^1(x^1, \cdots, x^m) &= 0 \\ &\vdots \\ f^r(x^1, \cdots, x^m) &= 0 \end{aligned} \tag{1}$$

which may be written

$$\mathbf{f}(\mathbf{x}) = 0 \tag{2}$$

for short. In most usual cases one can naturally define a partition of the set of parameters as

$$\mathbf{X} = \begin{bmatrix} X^1 \\ \vdots \\ X^m \end{bmatrix} = \begin{bmatrix} D^1 \\ \vdots \\ D^r \\ P^1 \\ \vdots \\ P^s \end{bmatrix} = \begin{bmatrix} \mathbf{D} \\ \mathbf{P} \end{bmatrix} \tag{3}$$

In such a way that equations (1) simplify to

$$\begin{aligned} d^1 &= g^1(p^1, \cdots, p^s) \\ &\vdots \\ d^r &= g^r(p^1, \cdots, p^s) \end{aligned} \tag{4}$$

or, for short,

$$\mathbf{d} = \mathbf{g}(\mathbf{p}) \tag{5}$$

In the traditional terminology for inverse problems the set $\mathbf{D}$ is named the set of data, and the set $\mathbf{P}$ is named the set of unknowns, but this terminology may be misleading. For example, in a problem of earthquake hypocenter location the left-hand side of (5) consists of the arrival times of seismic waves at stations, the coordinates of seismic stations being on the right-hand side. But the coordinates of the stations are the results of some direct measurements, in exactly the same way as the arrival times of waves; there is thus no reason for reserving the term 'data' for the arrival times (except in the particular case where uncertainties on station coordinates have to be neglected). Since we will use the traditional terminology in this paper, this remark must be kept in mind.

b. The Inputs of the Problem

Let us consider a given parameter X^α. Two possibilities arise: either X^α is a directly measurable parameter or it is not. This partition of the set of parameters $\mathbf{X}$ is certainly more intrinsic that the one based on the form of (5), as discussed in section 2*a*.

If X^α is a directly measurable parameter, and if we have measured it, we assume in this paper that the result of the measurement has a Gaussian form; that is, it may conveniently be described using the expected value ${x_0}^\alpha$, the variance, and the covariances with other measurements.

If X^α is not a directly measurable parameter (it is an unknown), we will assume, in order to solve otherwise underdetermined problems, that we have some a priori knowledge and that this knowledge may also be expressed in a Gaussian form. If the a priori knowledge about a parameter is weak, the corresponding variance will be large, or even infinite.

This a priori information may come from different sources. For example, if the parameter set is describing the properties of the earth, some a priori information may be obtained from models of planet formation. Or the a priori information for a given problem may result from a posteriori information of a

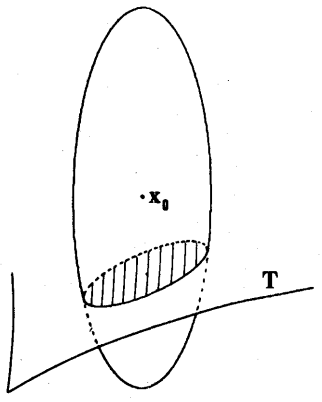

Fig. 1. Schematic illustration of the nonlinear theoretical manifold, the a priori expected point, the a priori ellipsoid of errors, and the 'induced probability' (shaded area) on the theoretical manifold.

previous inverse problem run with a different data set. More often the a priori information will simply be obtained by putting 'reasonable' error bars around a 'reasonable' central value. See *Jackson* [1979] for further discussion.

As is well known, and as we will see later, the definition of this a priori information, even with weak constraints (large variances), provides stability and uniqueness to the inversion.

In conclusion, in the least squares approach we assume that all a priori information on the parameter set (measurable as well as nonmeasurable parameters) takes the form of a vector of expected values $\mathbf{x}_0$ and a covariance matrix C_0.

When the theoretical equation (2) simplifies to (5) and the partition (3) is defined, the a priori information $(\mathbf{x}, C_0)$ takes the partitioned form:

$$\mathbf{x}_0 = \begin{bmatrix} \mathbf{d}_0 \\ \mathbf{p}_0 \end{bmatrix} \qquad C_0 = \begin{bmatrix} C_{d_0 d_0} & C_{d_0 p_0} \\ C_{p_0 d_0} & C_{p_0 p_0} \end{bmatrix} \tag{6}$$

where in most useful applications the matrix $C_{d_0 p_0} = (C_{p_0 d_0})^T$ vanishes.

c. *The Least Squares Problem*

Let $\mathbf{x}_0$ be the vector of the a priori expected values, and C_0 be the a priori covariance matrix, as defined in section 2*b*. We have assumed that the a priori information has a Gaussian form. Then $\mathbf{x}_0$ and C_0 define in the parameter space $\mathcal{C}^m$ a Gaussian probability density function

$$\rho(\mathbf{x}) = \text{const} \cdot \exp\{-\tfrac{1}{2}(\mathbf{x} - \mathbf{x}_0)^T \cdot C_0^{-1} \cdot (\mathbf{x} - \mathbf{x}_0)\} \tag{7}$$

The nonlinear theoretical equation considered in (2),

$$\mathbf{f}(\mathbf{x}) = 0 \tag{8}$$

defines in $\mathcal{C}^m$ a certain nonlinear manifold (subspace) $\mathcal{T}$. The a priori density function $\rho(\mathbf{x})$ induces on the theoretical manifold $\mathcal{T}$ a probability density function which could naturally be taken as the a posteriori density function (see Figure 1).

If (8) is linear, $\mathcal{T}$ will be a linear manifold, and it has been demonstrated in paper 1 that the induced probability density function will be Gaussian. If (8) is not linear, the induced probability density function will generally not be Gaussian.

We state then the least squares problem as the search of the point $\hat{\mathbf{x}}$ of the theoretical manifold for which the induced density of probability is maximum.

In order to find this maximum we must minimize the argument of the exponential in (7). The problem is thus equivalent to searching for the point $\hat{\mathbf{x}}$ verifying the set of equations

$$\mathbf{f}(\hat{\mathbf{x}}) = 0 \tag{9}$$

$$s(\hat{\mathbf{x}}) = (\hat{\mathbf{x}} - \mathbf{x}_0)^T \cdot C_0^{-1} \cdot (\hat{\mathbf{x}} - \mathbf{x}_0) \quad \text{minimum over } \mathcal{T} \tag{10}$$

Equations (9) and (10) are our definition of the least squares problem.

We have assumed that the a priori information has a Gaussian form. If this is not the case and if we assume that the probabilistic distributions under consideration have an expected value and a covariance matrix, it is usual to employ the least squares criterion to define a 'least squares estimator' and to prove that this estimator has some properties (variance minimum, $\cdots$). See, for example, *Rao* [1973].

In fact, if the probabilistic distributions under consideration are clearly not Gaussian (long tailed, asymmetric, multimoded, laterally bounded, etc.), it is well known that the least squares criterion gives unacceptable results. For such cases the general techniques described in paper 1 should be used.

Equation (10) makes sense only if C_0 is regular. A covariance matrix becomes singular if there are null variances or if there are perfect correlations between parameters. In these cases the multidimensional ellipsoid representing C_0 degenerates into an ellipsoid of lower dimension. It is always possible to restrict the definition of the a priori probability density function to the corresponding subspace. We will see later that the algorithms leading to the solution of (9) and (10) are well defined even if C_0 is singular.

If a point $\hat{\mathbf{x}}$ verifies the set of equations (9) and (10), then it must verify the set

$$\mathbf{f}(\hat{\mathbf{x}}) = 0 \tag{11}$$

$$s(\hat{\mathbf{x}}) \text{ stationary over } \mathcal{T} \tag{12}$$

As is well known in all problems of searching for minima, the set of equations (11) and (12) may contain, in addition to the solution of (9) and (10), local minima, saddle points, maxima, etc. We will discuss this point later.

We show in the appendix that (11) and (12) are equivalent to the implicit equation

$$\hat{\mathbf{x}} = \mathbf{x}_0 + C_0 \cdot F^T \cdot (F \cdot C_0 \cdot F^T)^{-1} \cdot \{F \cdot (\hat{\mathbf{x}} - \mathbf{x}_0) - \mathbf{f}(\hat{\mathbf{x}})\} \tag{13}$$

where F is the matrix of partial derivatives:

$$F^{ik} = \partial f^i / \partial x^k \tag{14}$$

taken at the point $\hat{\mathbf{x}}$.

Equation (13) must of course be solved using an iterative procedure. If we assume that the elements F^{ik} of the matrix F are continuous functions of $\mathbf{x}$, the simplest procedure is obtained using a fixed point method:

$$\hat{\mathbf{x}}_{k+1} = \mathbf{x}_0 + C_0 \cdot F_k^T \cdot (F_k \cdot C_0 \cdot F_k^T)^{-1} \cdot \{F_k \cdot (\hat{\mathbf{x}}_k - \mathbf{x}_0) - \mathbf{f}(\hat{\mathbf{x}}_k)\} \tag{15}$$

where the derivatives are taken at the current point $\hat{\mathbf{x}}_k$.

In the rest of this paper the algorithm defined by (15) will be called the algorithm of total inversion (T.I.).

The iterative process (15) must be started at an arbitrary point $\hat{\mathbf{x}}_0$. A reasonable (although not obligatory) choice is to take the a priori point $\mathbf{x}_0$ as the starting point, that is, $\hat{\mathbf{x}}_0 = \mathbf{x}_0$.

If s has only one stationary point over $\mathcal{T}$, then it is easy to see that at this point, s is necessarily a minimum and that the T.I. algorithm converges always to the point $\hat{\mathbf{x}}$ which minimizes s (independently of the chosen starting point $\hat{\mathbf{x}}_0$). If we are not sure that s has only one stationary point, then we must check the possible existence of secondary minima or other stationary points (for instance, by starting the iterative procedure at different starting points $\hat{\mathbf{x}}_0 \neq \mathbf{x}_0$).

The total inversion algorithm is, in fact, some kind of generalization of Newton's algorithm for the search of the zeros of a nonlinear function $f(x)$. As is the case for Newton's algorithm, the total inversion algorithm will only converge in those problems where the nonlinearity is not too severe.

In ordinary iterative procedures for inverse problems, iterations are stopped when two successive solutions are close enough. In the total inversion algorithm we may also use this criterion, but because the solution $\hat{\mathbf{x}}$ must verify $\mathbf{f}(\hat{\mathbf{x}}) = 0$ and because $\mathbf{f}(\hat{\mathbf{x}}_k)$ is computed at each iteration, we can alternatively choose to stop the iterative procedure when the values $\mathbf{f}(\hat{\mathbf{x}}_k)$ are close enough to zero.

In order to give meaning to (13) and (15) we must assume that all the matrices of the type $F \cdot C_0 \cdot F^T$ are nonsingular. This is true in a great variety of circumstances. For example, from a practical point of view, a useful set of sufficient (although not necessary) conditions will be (1) that C_0 has neither null variances nor perfect correlations and (2) that theoretical equations (2) take the explicit form (5).

By hypothesis 1, C_0 is a positive definite matrix. By hypothesis 2 the matrix F takes the partitioned form

$$F = [I \quad -G] \tag{16}$$

where I is the identity matrix and G is a matrix of partial derivatives. Then F has a maximum rank, and $F \cdot C_0 \cdot F^T$ is then positive definite and thus regular.

In fact, the matrix $F \cdot C_0 \cdot F^T$ will only be singular in some very pathological cases. Nevertheless, in actual problems the matrix $F \cdot C_0 \cdot F^T$ may be numerically singular. This point will be discussed in section 2*d*.

In the iteration of algorithm (15) we must compute the vector $\mathbf{V} = F_k \cdot (\hat{\mathbf{x}}_k - \mathbf{x}_0) - \mathbf{f}(\hat{\mathbf{x}}_k)$. We must also compute the matrix $M = (F_k \cdot C_0 \cdot F_k^T)$ and then compute the vector $\mathbf{V}' = M^{-1} \cdot \mathbf{V}$. It is well known in numerical analysis that the computation of the vector $\mathbf{V}'$ does not require the effective inversion of the matrix M. This in an important point when the dimension of M is large, because the inversion is very time consuming.

d. Case $\mathbf{d} = \mathbf{g}(\mathbf{p})$

Let us assume that the parameters $\mathbf{X}$ may be divided into the data set $\mathbf{D}$ and the parameter set $\mathbf{P}$ in such a way that the theoretical equation $\mathbf{f}(\mathbf{x}) = 0$ simplifies to

$$\mathbf{f}(\mathbf{x}) = \mathbf{d} - \mathbf{g}(\mathbf{p}) = 0 \tag{17}$$

The matrix F defined by (14) takes then the partitioned form

$$F = [I \quad -G] \tag{18}$$

where G is the matrix of partial derivatives.

$$G^{i\alpha} = \partial g^i / \partial p^\alpha \tag{19}$$

Using (6), (17), and (18), the solution (15) gives the corresponding algorithms allowing the computation of $\hat{\mathbf{d}}$ and $\hat{\mathbf{p}}$. As is shown in the appendix, we obtain easily

$$\begin{aligned}\hat{\mathbf{p}}_{k+1} = \mathbf{p}_0 &+ [C_{p_0p_0} \cdot G_k^T - C_{p_0d_0}] \\ &\cdot [C_{d_0d_0} - C_{d_0p_0} G_k^T - G_k \cdot C_{p_0d_0} + G_k \cdot C_{p_0p_0} \cdot G_k^T]^{-1} \\ &\cdot \{\mathbf{d}_0 - \mathbf{g}(\hat{\mathbf{p}}_k) + G_k \cdot (\hat{\mathbf{p}}_k - \mathbf{p}_0)\}\end{aligned} \tag{20}$$

The corresponding algorithm for $\hat{\mathbf{d}}_{k+1}$ may then be written (see appendix) as

$$\hat{\mathbf{d}}_{k+1} = \mathbf{g}(\hat{\mathbf{p}}_k) + G_k \cdot (\hat{\mathbf{p}}_{k+1} - \hat{\mathbf{p}}_k) \tag{21}$$

Formula (20) generalizes to the nonlinear case the solution of *Franklin* [1970] for the linear problem.

Uncertainties in $\mathbf{d}_0$ are often independent of uncertainties in $\mathbf{p}_0$. Correspondingly,

$$C_{d_0p_0} = (C_{p_0d_0})^T = 0 \tag{22}$$

In that case, (20) becomes simpler and may be written in three different ways (see appendix):

$$\begin{aligned}\hat{\mathbf{p}}_{k+1} = \mathbf{p}_0 &+ C_{p_0p_0} \cdot G_k^T \cdot (C_{d_0d_0} + G_k \cdot C_{p_0p_0} \cdot G_k^T)^{-1} \\ &\cdot [\mathbf{d}_0 - \mathbf{g}(\hat{\mathbf{p}}_k) + G_k \cdot (\hat{\mathbf{p}}_k - \mathbf{p}_0)]\end{aligned} \tag{23}$$

$$\begin{aligned}\hat{\mathbf{p}}_{k+1} = \mathbf{p}_0 &+ (G_k^T \cdot C_{d_0d_0}^{-1} \cdot G_k + C_{p_0p_0}^{-1})^{-1} \cdot G_k^T \cdot C_{d_0d_0}^{-1} \\ &\cdot [\mathbf{d}_0 - \mathbf{g}(\hat{\mathbf{p}}_k) + G_k \cdot (\hat{\mathbf{p}}_k - \mathbf{p}_0)]\end{aligned} \tag{24}$$

$$\begin{aligned}\hat{\mathbf{p}}_{k+1} = \hat{\mathbf{p}}_k &+ (G_k^T \cdot C_{d_0d_0}^{-1} \cdot G_k + C_{p_0p_0}^{-1})^{-1} \cdot \{G_k^T \cdot C_{d_0d_0}^{-1} \\ &\cdot [\mathbf{d}_0 - \mathbf{g}(\hat{\mathbf{p}}_k)] - C_{p_0p_0}^{-1} \cdot (\hat{\mathbf{p}}_k - \mathbf{p}_0)\}\end{aligned} \tag{25}$$

For different configurations of matrices $C_{d_0d_0}$, $C_{p_0p_0}$, and G, these three algorithms, although mathematically equivalent, may be very different in time consumption.

It is easy to see that if the matrices $C_{d_0d_0}$ and $C_{p_0p_0}$ are regular, all the inverse matrices in (23)–(25) are also regular.

It may happen in actual problems that although mathematically regular, the algorithm may become numerically singular or unstable. This will always mean that the a priori information does not constrain the solution enough. A reduction of the variances in $C_{p_0p_0}$ will stabilize the solution, in the same way that dropping 'small eigenvalues' stablizes the solution of *Wiggins* [1972], which is based on the Lancsöz decomposition. But we must emphasize that since variances in $C_{p_0p_0}$ describe our a priori knowledge on parameters, reducing these variances in order to stabilize the solution means that we are introducing a priori information that, in fact, we do not possess. This fact may be hidden in formalisms where the a priori information on parameters is not explicitly stated.

Nevertheless, in most actual geophysical problems, variances in $C_{p_0p_0}$ representing the actual a priori knowledge (confidence in $\mathbf{p}_0$) allow a stable inversion of the data set, even when the number of parameters is, by many orders of magnitude, larger than the number of data (see section 2*f* for the measure of the extent to which the data set resolves the value of a given parameter).

The case where the a priori constraints on parameters are infinitely weak is obtained using a covariance matrix $C_{p_0p_0}$ of the form $C_{p_0p_0} = \sigma^2 \cdot I$ in the limit where $\sigma^2 \to \infty$. Two particular cases give simple solutions. For obvious reasons a problem where the matrix $G_k^T \cdot G_k$ is regular will be named purely overdetermined, whereas a problem where the matrix $G_k \cdot G_k^T$ is regular will be named purely underdetermined.

For a purely overdetermined problem the limit $\sigma^2 \to \infty$ gives, using (25),

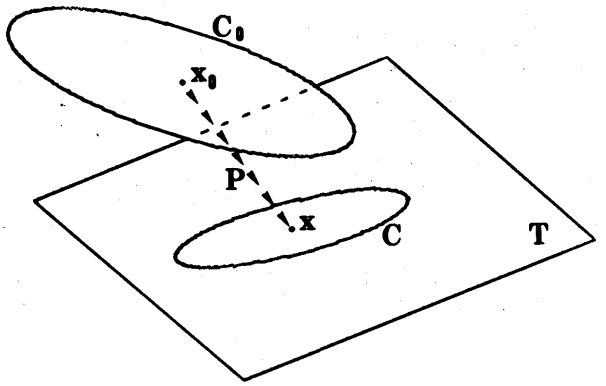

Fig. 2. The projector $P = I - C_0 \cdot F^T(F \cdot C_0 \cdot F^T)^{-1} \cdot F$ is the orthogonal (relative to C_0^{-1}) projector over the linear theoretical variety. It projects the a priori vector $\mathbf{x}_0$ as well as the a priori covariance tensor C_0, giving $\hat{\mathbf{x}}$ and C, respectively.

$$\hat{\mathbf{p}}_{k+1} = \hat{\mathbf{p}}_k + (G_k^T \cdot C_{d_0d_0}^{-1} \cdot G_k)^{-1} \cdot G_k^T \cdot C_{d_0d_0}^{-1} \cdot \{\mathbf{d}_0 - \mathbf{g}(\hat{\mathbf{p}}_k)\} \quad (26)$$

which corresponds to the solution of the classical nonlinear least squares problem.

For a purely underdetermined problem the limit $\sigma^2 \to \infty$ gives, using (23),

$$\hat{\mathbf{p}}_{k+1} = \mathbf{p}_0 + G_k^T \cdot (G_k \cdot G_k^T)^{-1} \cdot \{\mathbf{d}_0 - \mathbf{g}(\hat{\mathbf{p}}_k) - G_k \cdot (\mathbf{p}_0 - \mathbf{p}_k)\} \quad (27)$$

Equation (26) shows that the solution of a purely overdetermined problem is independent of the a priori value $\mathbf{p}_0$.

Equation (27) shows that the solution of a purely underdetermined problem is independent of the values of observational errors $C_{d_0d_0}$. If in the limit $k \to \infty$ we left-multiply (27) by G, we see that the solution $\hat{\mathbf{p}} = \hat{\mathbf{p}}_\infty$ of a purely underdetermined problem fits exactly the observed values of data: $\hat{\mathbf{d}} = \mathbf{g}(\hat{\mathbf{p}}) = \mathbf{d}_0$.

e. Linear Problem

By linear problem we mean that the general equations $\mathbf{f}(\mathbf{x}) = 0$ take the linear form

$$\mathbf{f}(\mathbf{x}) = F \cdot \mathbf{x} = 0 \quad (28)$$

where F is a matrix of perfectly known elements (if some of the elements are not perfectly known, they must be considered as parameters, and then the problem is not linear).

Using (28), (13) simplifies to the explicit solution

$$\hat{\mathbf{x}} = \mathbf{x}_0 - C_0 \cdot F^T \cdot (F \cdot C_0 \cdot F^T)^{-1} \cdot F \cdot \mathbf{x}_0 \quad (29)$$

As was pointed out in section 2*c*, if the probability density function describing the a priori information is Gaussian, the a posteriori density function will also be Gaussian; thus solution (29) will be the expected value. The a posteriori covariance matrix may also be computed, leading to (see appendix)

$$C = C_0 - C_0 \cdot F^T \cdot (F \cdot C_0 \cdot F^T)^{-1} \cdot F \cdot C_0 \quad (30)$$

If we define the linear operators

$$Q = C_0 \cdot F^T \cdot (F \cdot C_0 \cdot F^T)^{-1} \cdot F \qquad P = I - Q \quad (31)$$

it may easily be shown that they have the following properties:

$$P + Q = I \qquad P \cdot Q = Q \cdot P = 0$$
$$P^2 = P \qquad Q^2 = Q \quad (32)$$
$$P \cdot C_0 = C_0 \cdot P^T \qquad Q \cdot C_0 = C_0 \cdot Q^T$$

which imply that P and Q are projectors and that they are orthogonal relative to C_0^{-1}.

Equations (29) and (30) then take the beautiful form

$$\hat{\mathbf{x}} = P \cdot \mathbf{x}_0 \quad (33)$$

$$C = P \cdot C_0 \quad (34)$$

These equations show that the same projector P projects the a priori value $\mathbf{x}_0$ to give the a posteriori value $\mathbf{x}$ and projects the a priori covariance matrix C_0 to give the a posteriori covariance matrix C (see Figure 2).

Equations (33) and (34) have been obtained in paper 1 for a Gaussian problem, without the use of the least squares criterion.

Let us now turn to the usual linear problem where the set of parameters $\mathbf{X}$ is divided into the data set $\mathbf{D}$ and the parameter set $\mathbf{P}$ and where the theoretical equation (28) simplifies to

$$F \cdot \mathbf{x} = [I \quad -G] \cdot \begin{bmatrix} \mathbf{d} \\ \mathbf{p} \end{bmatrix} = \mathbf{d} - G \cdot \mathbf{p} = 0 \quad (35)$$

that is,

$$\mathbf{d} = G \cdot \mathbf{p} \quad (36)$$

where G is a matrix of perfectly known elements.

Using (35) and equations (6), the solution of this problem is readily obtained from (33) and (34). For the parameter components, (33) gives

$$\hat{\mathbf{p}} = \mathbf{p}_0 + (C_{p_0p_0} \cdot G^T - C_{p_0d_0}) \cdot (C_{d_0d_0} - C_{d_0p_0} \cdot G^T - G \cdot C_{p_0d_0} + G \cdot C_{p_0p_0} \cdot G^T)^{-1} \cdot (\mathbf{d}_0 - G \cdot \mathbf{p}_0) \quad (37)$$

For the data components the expression obtained from (33) can be put in the form (see appendix for details)

$$\hat{\mathbf{d}} = G \cdot \hat{\mathbf{p}} \quad (38)$$

where $\hat{\mathbf{p}}$ is the solution (37). This simply means that the least squares solution exactly verifies the theoretical equation.

Equation (34) gives, for the parameter components of the a posteriori covariance matrix,

$$C_{\hat{p}\hat{p}} = C_{p_0p_0} - (C_{p_0p_0} \cdot G^T - C_{p_0d_0}) \cdot (C_{d_0d_0} - C_{d_0p_0} \cdot G^T - G \cdot C_{p_0d_0} + G \cdot C_{p_0p_0} \cdot G^T)^{-1} \cdot (G \cdot C_{p_0p_0} - C_{d_0p_0}) \quad (39)$$

while the other components may be put in the form (see appendix)

$$C_{\hat{d}\hat{p}} = G \cdot C_{\hat{p}\hat{p}}$$
$$C_{\hat{p}\hat{d}} = C_{\hat{p}\hat{p}} \cdot G^T \quad (40)$$
$$C_{\hat{d}\hat{d}} = G \cdot C_{\hat{p}\hat{p}} \cdot G^T$$

in accordance with (38).

In the particular case $\mathbf{p}_0 = \mathbf{0}$, (37) and (39) coincide with the solution of *Franklin* [1970].

If uncertainties in $\mathbf{d}_0$ are uncorrelated with uncertainties in $\mathbf{p}_0$, then $C_{d_0p_0} = (C_{p_0d_0})^T = 0$, and (37) simplifies to

$$\hat{\mathbf{p}} = \mathbf{p}_0 + C_{p_0p_0} \cdot G^T \cdot (C_{d_0d_0} + G \cdot C_{p_0p_0} \cdot G^T)^{-1} \cdot (\mathbf{d}_0 - G \cdot \mathbf{p}_0) \quad (41)$$

while the a posteriori covariance matrix becomes

$$C_{\hat{p}\hat{p}} = C_{p_0p_0} - C_{p_0p_0} \cdot G^T \cdot (C_{d_0d_0} + G \cdot C_{p_0p_0} \cdot G^T)^{-1} \cdot G \cdot C_{p_0p_0} \quad (42)$$

Using matricial identities, (41) and (42) may be written in a different form (see appendix):

$$\hat{\mathbf{p}} = \mathbf{p}_0 + (G^T \cdot {C_{d_0d_0}}^{-1} \cdot G + {C_{p_0p_0}}^{-1})^{-1} \cdot G^T \cdot {C_{d_0d_0}}^{-1} \cdot (\mathbf{d}_0 - G \cdot \mathbf{p}_0) \quad (43)$$

$$C_{\hat{p}\hat{p}} = (G^T \cdot {C_{d_0d_0}}^{-1} \cdot G + {C_{p_0p_0}}^{-1})^{-1} \quad (44)$$

Equations (41) and (42) coincide with the solution given by *Jackson* [1979].

The case where the a priori constraints on parameters are infinitely weak has been discussed in section 2*d*. For a purely underdetermined problem we obtain, using (41),

$$\hat{\mathbf{p}} = \mathbf{p}_0 + G^T \cdot (G \cdot G^T)^{-1} \cdot (\mathbf{d}_0 - G \cdot \mathbf{p}_0) \quad (45)$$

and, using (42),

$$C_{\hat{p}\hat{p}} = \sigma^2\{I - G^T \cdot (G \cdot G^T)^{-1} \cdot G\} \quad (46)$$

For a purely overdetermined problem we obtain, using (43),

$$\hat{\mathbf{p}} = (G^T \cdot {C_{d_0d_0}}^{-1} \cdot G)^{-1} \cdot G^T \cdot {C_{d_0d_0}}^{-1} \cdot \mathbf{d}_0 \quad (47)$$

and, using (44),

$$C_{\hat{p}\hat{p}} = (G^T \cdot {C_{d_0d_0}}^{-1} \cdot G)^{-1} \quad (48)$$

Equation (45) shows that the solution of a purely underdetermined problem is independent of $C_{d_0d_0}$ and fits exactly the observed values of the data ($\hat{\mathbf{d}} = G \cdot \hat{\mathbf{p}} = \mathbf{d}_0$).

Equation (47) shows that the solution of a purely overdetermined problem is independent of $\mathbf{p}_0$. This solution is well known and is traditionally called the 'normal solution.'

Of course, if G is a square matrix and if it is regular, then (45) and (47) reduce to the Kramer solution: $\hat{\mathbf{p}} = G^{-1} \cdot \mathbf{d}_0$.

f. Remarks

1. The usual approach to solving the nonlinear problem is through iteration of a linearized problem. If the data set **D** overdetermines the problem sufficiently so that all a priori information on the parameter set **P** can be neglected, then the iteration of a linearized problem always leads to the correct solution. If the data set does not overdetermine the problem, there is a common mistake which leads to a wrong solution. Let us examine this problem in some detail in the usual case where $C_{d_0p_0} = (C_{p_0d_0})^T = 0$.

Our solution to the nonlinear problem was (equation (25))

$$\hat{\mathbf{p}}_{k+1} = \hat{\mathbf{p}}_k + (G_k^T \cdot {C_{d_0d_0}}^{-1} \cdot G_k + {C_{p_0p_0}}^{-1})^{-1} \cdot \{G_k^T \cdot {C_{d_0d_0}}^{-1} \cdot [\mathbf{d}_0 - \mathbf{g}(\hat{\mathbf{p}}_k)] + {C_{p_0p_0}}^{-1} \cdot [\mathbf{p}_0 - \hat{\mathbf{p}}_k]\} \quad (49)$$

which has been shown to be equivalent to

$$\hat{\mathbf{p}}_{k+1} = \mathbf{p}_0 + (G_k^T \cdot {C_{d_0d_0}}^{-1} \cdot G_k + {C_{p_0p_0}}^{-1})^{-1} \cdot G_k^T \cdot {C_{d_0d_0}}^{-1} \cdot \{\mathbf{d}_0 - \mathbf{g}(\hat{\mathbf{p}}_k) + G \cdot (\hat{\mathbf{p}}_k - \mathbf{p}_0)\} \quad (50)$$

The solution to the linear problem was (equation (43))

$$\hat{\mathbf{p}} = \mathbf{p}_0 + (G^T \cdot {C_{d_0d_0}}^{-1} \cdot G + {C_{p_0p_0}}^{-1})^{-1} \cdot G^T \cdot {C_{d_0d_0}}^{-1} \cdot (\mathbf{d}_0 - G \cdot \mathbf{p}_0) \quad (51)$$

If we want our approach to be consistent, we must force the general (nonlinear) solution to give the linear solution as a particular case. It is easy to see that for a linear problem the algorithm (50) reduces to (51).

Let us show that this is not the case in the usual approach. Linearizing a problem means replacing the nonlinear equation $\mathbf{d} = \mathbf{g}(\mathbf{p})$ by its first-order development around a point $\hat{\mathbf{p}}_k$:

$$\mathbf{d} = \mathbf{g}(\hat{\mathbf{p}}_k) + G_k \cdot (\mathbf{p} - \hat{\mathbf{p}}_k) \quad (52)$$

If we call the values

$$\Delta\hat{\mathbf{d}}_k = \mathbf{d}_0 - \mathbf{g}(\hat{\mathbf{p}}_k) \quad (53)$$

'residuals' and we call the values

$$\Delta\hat{\mathbf{p}}_{k+1} = \hat{\mathbf{p}}_{k+1} - \hat{\mathbf{p}}_k \quad (54)$$

'corrections', then the linearized least squares problem consists of the search for the values $\Delta\mathbf{p}_{k+1}$ minimizing the sum

$$s = (G_k \cdot \Delta\hat{\mathbf{p}}_{k+1} - \Delta\hat{\mathbf{d}}_k)^T \cdot {C_{d_0d_0}}^{-1} \cdot (G_k \cdot \Delta\hat{\mathbf{p}}_{k+1} - \Delta\hat{\mathbf{d}}_k) \quad (55)$$

if the problem is overdetermined enough. For an underdetermined problem it is usually required that each successive correction $\Delta\hat{\mathbf{p}}_{k+1}$ be as small as possible, and the sum (55) is replaced by

$$s' = s + (\Delta\hat{\mathbf{p}}_{k+1})^T \cdot {C_{p_0p_0}}^{-1} \cdot (\Delta\hat{\mathbf{p}}_{k+1}) \quad (56)$$

The corresponding solution is then easily found to be

$$\Delta\hat{\mathbf{p}}_{k+1} = (G_k^T \cdot {C_{d_0d_0}}^{-1} \cdot G_k + {C_{p_0p_0}}^{-1})^{-1} \cdot G_k^T \cdot {C_{d_0d_0}}^{-1} \cdot \Delta\hat{\mathbf{d}}_k \quad (57)$$

Using (53) and (54) we see that (57) leads to the algorithm

$$\hat{\mathbf{p}}_{k+1} = \hat{\mathbf{p}}_k + (G_k^T \cdot {C_{d_0d_0}}^{-1} \cdot G_k + {C_{p_0p_0}}^{-1})^{-1} \cdot G_k^T \cdot {C_{d_0d_0}}^{-1} \cdot \{\mathbf{d}_0 - \mathbf{g}(\hat{\mathbf{p}}_k)\} \quad (58)$$

By comparison of (58) with (49) we see that in (58) the term ${C_{p_0p_0}}^{-1} \cdot [\mathbf{p}_0 - \hat{\mathbf{p}}_k]$ is missing. Thus the linear solution (51) cannot be obtained as a particular case of (58), which clearly means that (58) is wrong.

The mistake is to require each successive partial correction $\hat{\mathbf{p}}_{k+1} - \hat{\mathbf{p}}_k$ to be as small as possible. The right condition is, in fact, to require each successive total correction $\hat{\mathbf{p}}_{k+1} - \mathbf{p}_0$ to be as small as possible. It is then easy to see that the right equation (49) is obtained.

In any case the fully nonlinear approach developed in sections 2*c* and 2*d* is simpler and more natural than the approach consisting of the linearization of a nonlinear theory.

2. We have only been able to define the a posteriori covariance matrix for the linear case. For a strongly nonlinear problem the a posteriori errors may be far from Gaussian, and even if the covariance matrix could be computed, it would not be of great interest. If the nonlinearity is weak, then the a posteriori covariance matrix can be approximately computed using the formula obtained for the linear case.

3. Let us recall the formula (30) giving the a posteriori covariance matrix for a linear problem:

$$C = C_0 - C_0 \cdot F^T \cdot (F \cdot C_0 \cdot F^T)^{-1} \cdot F \cdot C_0 \quad (59)$$

Since the second right-hand term is clearly positive semidefinite, its diagonal terms are not negative, so the a posteriori variances are small or equal to the a priori ones. Further-

more, a parameter will be completely unresolved if it does not appear, in fact, in the equations $\mathbf{f}(\mathbf{x}) = 0$ and if no correlation is introduced by the a priori covariances between this parameter and other parameters. The corresponding column of F will then be null, and the corresponding row of C_0 will only have one nonnull element, the diagonal one. It is then easy to see that the corresponding diagonal term of the second right-hand term of (59) will be null. This implies that the a posteriori variance will equal the a priori one.

We have thus demonstrated that in the total inversion approach, the variances have the following properties:

In general,

$$\text{(a posteriori variance)} \leq \text{(a priori variance)}$$

For a nonresolved parameter,

$$\text{(a posteriori variance)} = \text{(a priori variance)}$$

The more the a posteriori variance differs from the a priori variance, the more we have increased the amount of knowledge on the value of the parameter.

We see thus that in the total inversion approach, the classical analysis of variance contains the analysis of resolution.

4. In this paper we have assumed that our theory allows an exact computation of the direct problem. Sometimes our theories contain some approximations and allow only an approximate computation of the values of the data. Let C_T be the covariance matrix of theoretical errors. In paper 1 we have demonstrated that to take into account these theoretical errors we must simply replace $C_{d_0 d_0}$ by $C_{d_0 d_0} + C_T$ in all formulas of sections 2*d* and 2*e*.

3. The Continuous Problem

a. Notations

In this section we will formally extend the results of section 2 to the case where some of the data and/or unknows are functions of a continuous variable.

Let us start with one linear problem involving only one data function and one unknown function:

$$d(s) = \int g(s, r) \cdot p(r)\, dr \tag{60}$$

In order to have compact notations, (60) is usually written in vectorial notation:

$$\mathbf{d} = G \cdot \mathbf{p} \tag{61}$$

where, as is easily seen from (60), G is a linear operator. The function $g(s, r)$ is then called the kernel of G.

In some problems, instead of having two functions $d(s)$ and $p(r)$ we may have one function and one discrete vector. For example, in a problem with discrete data, (60) becomes

$$d^i = \int g(s^i, r) \cdot p(r)\, dr \tag{62}$$

while (61) keeps the same form.

We will admit that the linear operator G may be of the most general form. In particular, we accept for G differential operators.

It must be pointed out that if we accept distributions as kernels, the differential equation

$$d(s) = (dp(r)/dr)_{r=s} \tag{63}$$

may be written as

$$d(s) = \int [-\delta'(s - r)] \cdot p(r)\, dr \tag{64}$$

where δ' is the derivative of the Dirac distribution. With this convention, (60) may represent integral as well as differential equations.

A slightly more general equation than (61) is

$$F^1 \cdot \mathbf{x}^1 = F^2 \cdot \mathbf{x}^2 \tag{65}$$

where F^1 and F^2 are linear operators and $\mathbf{x}^1$ and $\mathbf{x}^2$ are continuous or discrete vectors. In actual problems in geophysics we must deal with more than one data vector (for example, some seismograms or magnetic records) and with more than one parameter vector (for example, some functions describing the earth). Let us write $\mathbf{x}^1, \cdots, \mathbf{x}^m$ for all the continuous or discrete vectors we need to describe our system. A general linear relationship between these vectors is written as

$$\begin{aligned} F^{11}\mathbf{x}^1 + \cdots + F^{1m}\mathbf{x}^m &= 0 \\ \vdots \qquad\quad \vdots \qquad\quad \vdots \qquad\quad &\vdots \\ F^{r1}\mathbf{x}^1 + \cdots + F^{rm}\mathbf{x}^m &= 0 \end{aligned} \tag{66}$$

Let us define

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}^1 \\ \vdots \\ \mathbf{X}^m \end{bmatrix} \tag{67}$$

If $\mathbf{X}^j$ belongs to a Hilbert space H^j, the vector $\mathbf{X}$ belongs to the real Hilbert space $H = H^1 \times \cdots \times H^m$. If we also define the linear operator

$$F = \begin{bmatrix} F^{11} & \cdots & F^{1m} \\ \vdots & & \vdots \\ F^{r1} & \cdots & F^{rm} \end{bmatrix} \tag{68}$$

then the linear equations (66) are simply written as

$$F \cdot \mathbf{x} = 0 \tag{69}$$

Since we also want to deal with nonlinear problems, we must consider a general nonlinear relationship of the form

$$\mathbf{f}(\mathbf{x}) = 0 \tag{70}$$

where $\mathbf{f}$ is any nonlinear integrodifferential operator acting on $\mathbf{x}$. We will later assume that $\mathbf{f}$ is differentiable. Its derivative is, by definition, a linear operator and will have the form (68).

b. Results of Measurements and a Priori Information on Parameters

Let $\mathbf{X}^i$ be one of the elements of $\mathbf{X}$. If $\mathbf{X}^i$ is a discrete vector, as was discussed in section 2*b*, we use a vector of expected values and a covariance matrix to describe the results of our measurements, as well as the a priori information on nondirectly measurable parameters.

If $\mathbf{X}$ is a continuous vector, that is, a function $s \rightarrow X(s)$ of a continuous variable s, we must use the concepts of the theory of random functions. A random function is defined as a function which, for each value of the variable, is a random variable. The expected value $X_0(s)$ of the random function is defined as the (nonrandom) function whose value at each point s equals the expected value of the random variable $X(s)$. The covariance function $C_0(s, s')$ is defined as the two-variable (nonrandom) function whose value at the point (s, s') equals the covariance between the random variables at

the points s and s'. It is well known (see, for example, *Pugachev* [1965]) that covariance functions have almost all the properties of covariance matrices: they are symmetric, positive semidefinite, etc.

Covariance matrices and covariance functions naturally define linear operators which are named covariance operators.

For the sake of generality we will not assume that errors between two vectors $\mathbf{X}^j$ and $\mathbf{X}^k$ must be uncorrelated; we will thus also consider cross-covariance operators C^{jk}. To make our notations compact, we will define the matrix of covariance operators as

$$C_0 = \begin{bmatrix} C^{11} & \cdots & C^{1m} \\ \vdots & & \vdots \\ C^{m1} & \cdots & C^{mm} \end{bmatrix} \tag{71}$$

We will assume that C_0 is a positive definite operator.

Matrix C_0 and vector

$$\mathbf{x}_0 = \begin{bmatrix} (\mathbf{x}^1)_0 \\ \vdots \\ (\mathbf{x}^m)_0 \end{bmatrix} \tag{72}$$

display the results of measurements, the a priori information, and our confidence in these a priori estimators.

c. *The General Nonlinear Least Squares Problem*

Let a system be described through a set $\mathbf{X}$ of continuous and/or discrete vectors. Let $\mathbf{x}_0$ be the a priori value of $\mathbf{X}$, and let C_0 be the corresponding covariance operator. Let a physical theory impose a nonlinear relationship of the form

$$\mathbf{f}(\mathbf{x}) = 0 \tag{73}$$

on the possible values of $\mathbf{X}$, where $\mathbf{f}$ is any nonlinear differentiable operator acting on $\mathbf{X}$. There is no reason for $\mathbf{x}_0$ to verify (73). Since C_0 is a positive definite operator, its inverse C_0^{-1} can be defined, and the least squares problem may then be stated as the search for the point $\hat{\mathbf{x}}$ minimizing

$$s(\mathbf{x}) = [(\hat{\mathbf{x}} - \mathbf{x}_0), C_0^{-1}(\hat{\mathbf{x}} - \mathbf{x}_0)] \tag{74}$$

among the points verifying (73), where [,] represents the scalar product of H.

The problem defined by (73) and (74) is formally the same problem as the one defined in section 2*c*, so the solution given by (13) can be formally extended to give the solution of the present, more general problem. The solution of (73) and (74) will then verify

$$\hat{\mathbf{x}} = \mathbf{x}_0 + C_0 \cdot F^* \cdot (F \cdot C_0 \cdot F^*)^{-1} \cdot \{F \cdot (\hat{\mathbf{x}} - \mathbf{x}_0) - f(\hat{\mathbf{x}})\} \tag{75}$$

where the linear operator F is the derivative of the nonlinear operator $\mathbf{f}$ (having structure identical with that of the operator defined in (68)) and where F^* is its adjoint.

The solution of (75) may be obtained using a fixed point method:

$$\hat{\mathbf{x}}_{k+1} = \mathbf{x}_0 + C_0 \cdot F_k^* \cdot (F_k \cdot C_0 \cdot F_k^*)^{-1} \cdot \{F_k \cdot (\hat{\mathbf{x}}_k - \mathbf{x}_0) - f(\hat{\mathbf{x}}_k)\} \tag{76}$$

d. *Remarks*

1. If the problem is discrete, the linear operator C_0 is a matrix, and its inverse C_0^{-1} can act on any vector $(\hat{\mathbf{x}} - \mathbf{x}_0)$, so (74) has always a sense. If the problem involves some functions of a continuous variable, the operator C_0 is not necessarily surjective (the image of C_0 is not the entire Hilbert space). To give a meaning to (74), we must assume that $(\mathbf{x} - \mathbf{x}_0)$ belongs to the image of C_0. It is easy to see from (75) that the solution furnished by the algorithm (76) verifies this constraint. From a practical point of view, this means that the definition of C_0 defines also the space of possible solutions. For example, covariance operators are, in general, smoothing operators; if this is the case, then the difference between the computed solution and the a priori point, $(\hat{\mathbf{x}} - \mathbf{x}_0)$, will be smooth (see section 3*f*).

2. Since (75) is a transcription of (13), the particular cases studied in sections 3*d* and 3*e* are automatically generalized to the case where some of the vectors are continuous, and they do not have to be studied here.

e. *The Backus and Gilbert Problem*

Backus and Gilbert [1970] have examined the problem of the inversion of a finite set of discrete data, d^i, when the unknown is a function $p(r)$.

We will first state the problem in a general way and later make the particular Backus and Gilbert assumptions. If a problem involves a discrete vector $\mathbf{d}$ and a continuous vector $\mathbf{p}$, the vector $\mathbf{x}$ defined in (67) takes the form

$$\mathbf{x} = \begin{bmatrix} \mathbf{d} \\ \mathbf{p} \end{bmatrix} \tag{77}$$

We will assume that the theoretical equation is nonlinear and takes the explicit form

$$\mathbf{f}(\mathbf{x}) = \mathbf{d} - \mathbf{g}(\mathbf{p}) = 0 \tag{78}$$

With our assumptions, $\mathbf{g}$ is a vector of ordinary nonlinear functionals

$$d^i = g^i[p(r)] \tag{79}$$

The results of the measurements will be described by the discrete vector of expected values $\mathbf{d}_0$ and the covariance matrix $C_{d_0 d_0}$. If we have some a priori knowledge on the function $p(r)$, let us describe it using the expected value $p_0(r)$ and the covariance function $C_{p_0 p_0}(r, r')$. If we assume null covariances between $\mathbf{d}_0$ and $\mathbf{p}_0$, the covariance operator defined by (71) takes the form

$$C_0 = \begin{bmatrix} C_{d_0 d_0} & 0 \\ 0 & C_{p_0 p_0} \end{bmatrix} \tag{80}$$

With these hypotheses the general algorithm (76) leads to the equivalent of (23):

$$\mathbf{p}_{k+1} = \mathbf{p}_0 + C_{p_0 p_0} \cdot G_k^* \cdot (C_{d_0 d_0} + G_k \cdot C_{p_0 p_0} \cdot G_k^*)^{-1} \cdot \{\mathbf{d}_0 - \mathbf{g}(\hat{\mathbf{p}}_k) + G_k \cdot (\hat{\mathbf{p}}_k - \mathbf{p}_0)\} \tag{81}$$

Explicitly,

$$\hat{p}_{k+1}(r) = p_0(r) + \int dr' \sum_i \sum_j C_{p_0 p_0}(r, r') \cdot G_k^i(r') \cdot (S^{-1})^{ij} \cdot \{d_0^j - g^j(\hat{\mathbf{p}}_k) + \int dr'' \cdot G_k^j(r'') \cdot [\hat{p}_k(r) - p_0(r)]\} \tag{82}$$

where the matrix S_k is given by

$$S_k^{ij} = (C_{d_0 d_0})^{ij} + \int dr' \int dr'' \, G_k^i(r') \cdot C_{p_0 p_0}(r', r'') \cdot G_k^j(r'') \tag{83}$$

and $G_k^i(r)$ is the derivative of the nonlinear functional $g^i(\mathbf{p})$ taken at $\mathbf{p} = \hat{\mathbf{p}}_k$.

For a linear problem, (79) becomes

$$d^i = \int dr \cdot G^i(r) \cdot p(r) \tag{84}$$

Equation (81) then gives the explicit solution

$$\hat{\mathbf{p}} = \mathbf{p}_0 + C_{p_0p_0} \cdot G^* \cdot (C_{d_0d_0} + G \cdot C_{p_0p_0} \cdot G^*)^{-1} \cdot \{\mathbf{d}_0 - G \cdot \mathbf{p}_0\} \tag{85}$$

Explicitly,

$$\hat{p}(r) = p_0(r) + \int dr' \sum_i \sum_j C_{p_0p_0}(r, r') \cdot G^i(r') \cdot (S^{-1})^{ij} \cdot \left\{ d_0^j - \int dr'' \cdot G^j(r'') \cdot p_0(r'') \right\} \tag{86}$$

where the matrix S is given by

$$S^{ij} = (C_{d_0d_0})^{ij} + \int dr' \int dr'' \, G^i(r') \cdot C_{p_0p_0}(r', r'') \cdot G^j(r'') \tag{87}$$

In this linear case we can compute exactly the a posteriori covariance function of $\hat{p}(r)$. By analogy with (43) we have

$$C_{\hat{p}\hat{p}} = C_{p_0p_0} - C_{p_0p_0} \cdot G^* \cdot (C_{d_0d_0} + G \cdot C_{p_0p_0} \cdot G^*)^{-1} \cdot G \cdot C_{p_0p_0} \tag{88}$$

Explicitly,

$$C_{\hat{p}\hat{p}}(r, r') = C_{p_0p_0}(r, r') - A(r, r') \tag{89}$$

where

$$A(r, r') = \int dr'' \sum_i \sum_j \int dr''' \cdot C_{p_0p_0}(r, r'') \cdot G^i(r'') \cdot (S^{-1})^{ij} \cdot G^j(r''') \cdot C_{p_0p_0}(r''', r') \tag{90}$$

The closer the function $A(r, r')$ approaches the function $C_{p_0p_0}(r, r')$, the closer the a posteriori covariance function approaches zero, that is, the better the data set resolves the function $p(r)$.

In order to obtain the Backus and Gilbert solution of the problem we must consider the particular case where the data are assumed to be error free.

$$C_{d_0d_0} = 0 \tag{91}$$

and the confidence we have in our a priori information $p_0(r)$ tends to vanish; that is, the a priori covariance function $C_{p_0p_0}(r, r')$ has infinite variances and null covariances:

$$C_{p_0p_0}(r, r') = k \cdot \delta(r - r') \tag{92}$$

where δ is the Dirac distribution and k is a constant. The linear operator whose kernel is given by (92) is proportional to the identity operator

$$C_{p_0p_0} = k \cdot I \tag{93}$$

Using (91) and (93), (85) and (88) become

$$\hat{\mathbf{p}} = \mathbf{p}_0 + G^*(G \cdot G^*)^{-1} \cdot (\mathbf{d}_0 - G \cdot \mathbf{p}_0) \tag{94}$$

$$C_{pp} = k \cdot [I - G^* \cdot (G \cdot G^*)^{-1} G] \tag{95}$$

Explicitly,

$$\hat{p}(r) = p_0(r) + \sum_i \sum_j G^i(r) \cdot (S^{-1})^{ij} \cdot \left\{ d_0^j - \int dr' \cdot G^j(r') \cdot p_0(r') \right\} \tag{96}$$

$$C_{\hat{p}\hat{p}}(r, r') = k \cdot [\delta(r - r') - A(r, r')] \tag{97}$$

where

$$S^{ij} = \int dr \cdot G^i(r) \cdot G^j(r) \tag{98}$$

$$A(r, r') = \sum_i \sum_j G^i(r) \cdot (S^{-1})^{ij} \cdot G^j(r') \tag{99}$$

By left-multiplying (94) by G, we see that our solution exactly fits the observed data set ($\hat{\mathbf{d}} = G \cdot \hat{\mathbf{p}} = \mathbf{d}_0$).

If we put $p_0(r) \equiv 0$ in (96), we obtain the Backus and Gilbert solution of the problem. Let us explain the existence of $\mathbf{p}_0(r)$ in (94) from the Backus and Gilbert point of view. With our notations their solution is written as

$$\hat{\mathbf{p}}_{BG} = G^* \cdot (G \cdot G^*)^{-1} \cdot \mathbf{d}_0 \tag{100}$$

Backus and Gilbert argue that we can add to (100) any function $p'(r)$ which has no effect on the values of computed data, that is, such that

$$\int dr \cdot G^i(r) \cdot p'(r) = 0 \tag{101}$$

that is,

$$G \cdot \mathbf{p}' = 0 \tag{102}$$

Our solution (94) differs from (100) by the additive term

$$\mathbf{p}' = \mathbf{p}_0 - G^* \cdot (G \cdot G^*)^{-1} \cdot G \cdot \mathbf{p}_0 \tag{103}$$

By left-multiplying this term by G we see that the addition of $\mathbf{p}'$ to $\hat{\mathbf{p}}_{BG}$ has no effect on the values of computed data, so the solution (94) verifies the Backus and Gilbert requirements. From our point of view, the Backus and Gilbert solution corresponds to the particular choice $\mathbf{p}_0 \equiv 0$.

The function (99) is named the 'resolving kernel' in the Backus and Gilbert paper, and they show that the closer $A(r, r')$ approaches a Dirac function $\delta(r - r')$, the better the solution is resolved by the data set. Equation (97) gives the probabilistic interpretation of their 'δ-ness' criterion: If $A(r, r')$ approaches $\delta(r - r')$, the a posteriori covariance function $C_{\hat{p}\hat{p}}(r, r')$ tends to vanish; that is, the solution tends to be perfectly resolved. Equation (89) shows the generalization of the δ-ness criterion to the case where the a priori information is used.

We have then shown that our solution contains the Backus and Gilbert solution and that we generalize this solution to the case where the data may have a general Gaussian error distribution, where we may take into account a priori assumptions on the unknown function and where the theoretical relationship between the data and the unknown function is nonlinear.

4. Three Numerical Illustrations

In this section we examine three problems that cannot naturally be solved using traditional approaches. These three problems are as follows.

1. The computation of a regional stress tensor from the measurements of the strike and dip of faults and the direction and sense of striae on these faults. This is a discrete

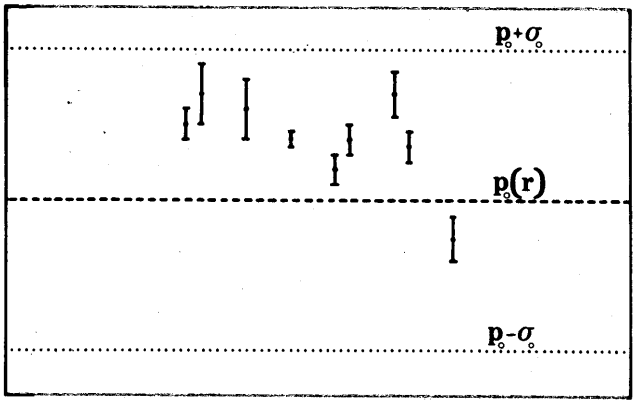

Fig. 3. Data used for the problem of estimation of a curve, given some of its points, and error bars. We also show the a priori value $p_0(r)$ and its a priori error bar.

problem, and its interest arises from the fact that the theoretical nonlinear equations do not take the form $\mathbf{d} = \mathbf{g}(\mathbf{p})$ but the more general form $\mathbf{f}(\mathbf{x}) = 0$.

2. The estimation of a curve given some of its points, or given the values of its derivative at some points. This is a linear and highly underdetermined problem. We will show that we can naturally solve it using the a priori hypothesis that the corresponding curve is smooth.

3. The solution of a gravimetric nonlinear problem with an unknown function and a discrete set of data.

a. Computation of a Regional Stress Tensor

To describe the orientation of a fault plane and striae, we use three angles: strike (d), dip (p), and slip (i). The components of the unit normal, $\mathbf{n}$, and unit striae, $\mathbf{s}$, are then easily computed as functions of d, p, and i. Let T be the regional deviatoric stress tensor. It is shown by *Angelier et al.* [1982] that if we assume that slickenslides on faults are caused by the existence of a regional stress tensor T, then on each fault we must have

$$\mathbf{s} \cdot T \cdot \mathbf{n} - [\|T \cdot \mathbf{n}\|^2 - (\mathbf{n} \cdot T \cdot \mathbf{n})^2]^{1/2} = 0 \qquad (104)$$

We see then that each set of three measured quantities (d, p, i) leads to one theoretical nonlinear equation of the form $\mathbf{f}(\mathbf{x}) = 0$. Algorithms which assume that the theoretical equations have the form $\mathbf{d} = \mathbf{g}(\mathbf{p})$, where $\mathbf{d}$ is the data set, cannot solve this problem in a natural way. See the paper by Angelier et al. for more details and numerical results.

b. Estimation of a Curve Given Some Points

This is a very common problem in all branches of physics. Let d be a quantity that physically depends on a quantity r; that is, we assume that d and r are functionally related:

$$d = p(r) \qquad (105)$$

Let us assume that we have measured the value of d for some values of r and that we have obtained the results shown in Figure 3. Our aim is to give a 'reasonable' expression for $p(r)$ that fits the experimental points 'reasonably well.'

Our unknown is the function $p(r)$, and our data are the points d^i. The theoretical equation is

$$d^i = p(r^i) \qquad (106)$$

which can also be written as

$$d^i = \int \delta(r - r^i) \cdot p(r)\, dr \qquad (107)$$

Equation (107) shows that our problem is linear with kernel

$$G^i(r) = \delta(r^i - r) \qquad (108)$$

The a priori information on the problem is as follows: (1) The results of the measurements are described using the observed values d_0^i of Figure 3 and their standard deviations σ_0^i. (2) Since the problem is highly underdetermined, we must use some kind of a priori information. Let us assume that we have some reasons to force the solution $p(r)$ to be not too far from $p_0(r)$. Let σ be the confidence we have on this a priori value. This means that we expect the dispersion of $p(r)$ around $p_0(r)$ to be of the order of σ. Finally, we will introduce the assumption that $p(r)$ is smooth. Since $p_0(r)$ is smooth by definition, the simplest way to impose the smoothness of $p(r)$ is to impose that if, at a given point r, the value of $p(r)$ has a deviation $p(r) - p_0(r)$ of given sign and magnitude, we want, at a neighboring point r', the deviation $p(r') - p_0(r')$ to have the same sign and similar magnitude. In other words, we want to impose a priori nonnull covariances between points r and r'. Many choices of covariance functions may correspond to the physics of each problem. Let us take here a covariance function of the form

$$C_{p_0p_0}(r, r') = \sigma^2 \exp\left\{-\frac{1}{2}\frac{(r - r')^2}{\Delta^2}\right\} \qquad (109)$$

which means that the variance at the point r, $C_{p_0p_0}(r, r)$, equals σ and that the correlation length between errors is Δ.

Since we have precisely defined the a priori values $\mathbf{d}_0$, $C_{d_0d_0}$, $\mathbf{p}_0$, and $C_{p_0p_0}$ and the theoretical equation (107), the solution of our problem is readily obtained from (86). Using (108), (86) gives

$$\hat{p}(r) = p_0(r) + \sum_i \sum_j C_{p_0p_0}(r, r^i) \cdot (S^{-1})^{ij} \cdot [d_0^j - p_0(r^j)] \qquad (110)$$

where

$$S^{ij} = (C_{d_0d_0})^{ij} + C_{p_0p_0}(r^i, r^j) \qquad (111)$$

The a posteriori covariance function is obtained from (89):

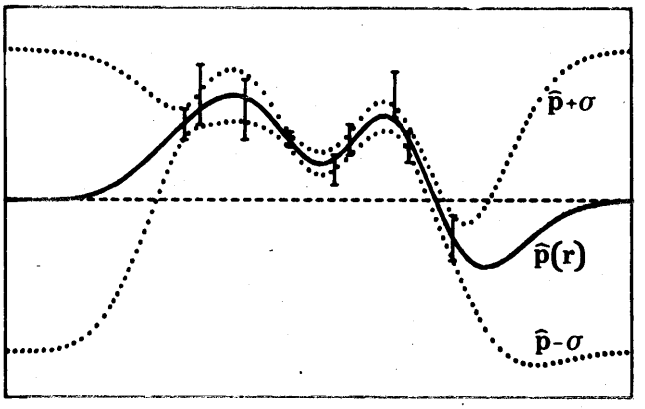

Fig. 4. Solution obtained using our algorithm (solid curve). We also show the standard error at each point $[C_{\hat{p}\hat{p}}(r, r)]^{1/2}$. Note that far from the data the standard error tends to equal the a priori standard error.

$$C_{\hat{p}\hat{p}}(r, r') = C_{p_0p_0}(r, r') - \sum_i \sum_j C_{p_0p_0}(r, r^j) \cdot (S^{-1})^{ij} \cdot C_{p_0p_0}(r^i, r') \quad (112)$$

In Figure 4 we show the solution $\hat{p}(r)$ given by (110), and we also show the a posteriori standard deviation $[C_{\hat{p}\hat{p}}(r, r)]^{1/2}$.

Figure 5 shows the covariance function $C_{\hat{p}\hat{p}}(r, r')$ for a particular value of r'.

If instead of giving the value of the function at some points we give the value of its derivative, the problem is very similar. Equations (106), (107), and (108) should be written as

$$d^i = p'(r^i) \quad (113)$$

$$d^i = \int (-\delta'(r^i - r)) \cdot p(r)\, dr \quad (114)$$

$$G^i(r) = -\delta'(r^i - r) \quad (115)$$

respectively, where δ' is the derivative of the Dirac distribution.

Equations (110), (111), and (112) then become

$$\hat{p}(r) = p_0(r) + \sum_i \sum_j \left(\frac{\partial C_{p_0p_0}(r, r')}{\partial r'}\right)_{r'=r^i} \cdot (S^{-1})^{ij} \cdot [d_0^j - p_0'(r^i)] \quad (116)$$

$$S^{ij} = (C_{d_0d_0})^{ij} + \left(\frac{\partial^2 C_{p_0p_0}(r, r')}{\partial r\, \partial r'}\right)_{r=r^i, r'=r^j} \quad (117)$$

$$C_{\hat{p}\hat{p}}(r, r') = C_{p_0p_0}(r, r') - \sum_i \sum_j \left(\frac{\partial^2 C_{p_0p_0}(r, r'')}{\partial r''}\right)_{r''=r^i} \cdot (S^{-1})^{ij} \cdot \left(\frac{\partial^2 C_{p_0p_0}(r''', r')}{\partial r'''}\right)_{r'''=r^j} \quad (118)$$

respectively.

The curve $\hat{p}(r)$ is a smooth curve whose derivative at the points r^j approaches d_0^j.

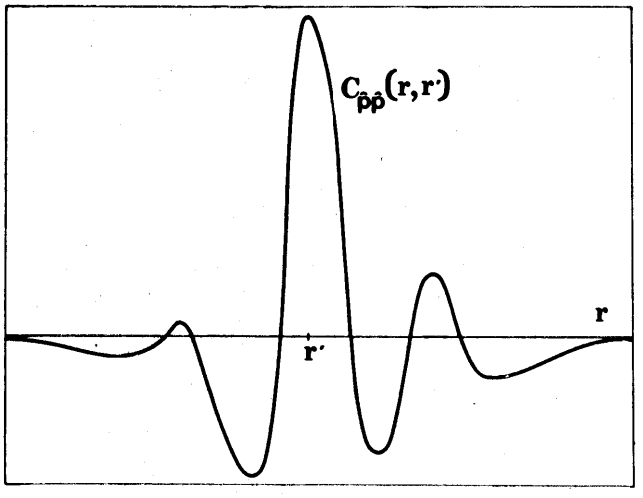

Fig. 5. The covariance curve $C_{\hat{p}\hat{p}}(r, r')$ computed at an arbitrary point r'. This curve generalizes the 'resolving kernel' of *Backus and Gilbert* [1970].

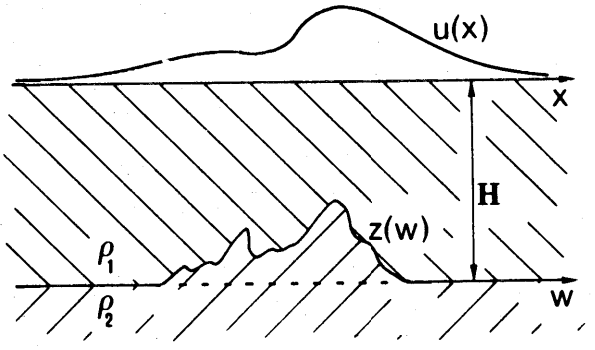

Fig. 6. The gravitational inverse problem of obtaining the shape of a frontier between two media of different density, using as data the anomaly at the surface.

c. *Nonlinear Problem With Discrete Data and a Function as Unknown*

Our last example has been borrowed from *Tikhonov* [1976], who shows it as an example of an ill-posed nonlinear problem.

Let us assume a layer of uniform density over a half space of uniform but different density. If between two points a and b the interface is not planar but has a shape $z(w)$ (see Figure 6), the vertical component of gravity and the free surface will have an anomaly $u(x)$. Assuming a two-dimensional problem, it may be shown that

$$u(x) = \int_a^b \log \frac{(x - w)^2 + H^2}{(x - w)^2 + [H - z(w)]^2}\, dw \quad (119)$$

We want to solve the inverse problem of estimating the function $z(w)$ from a finite set of measurements of the anomaly

$$d_0^i = u(x^i) \quad (120)$$

The general solution of the problem is given by (81) or (82). Let us explain the computation of the kernel $G_k^i(w)$ of the nonlinear functional (119).

Equation (119) defines a nonlinear operator which may be written as

$$\mathbf{u} = \mathbf{g}(\mathbf{z}) \quad (121)$$

Let $\boldsymbol{\varepsilon}$ be a function of w. It can be shown that in the limit when $\boldsymbol{\varepsilon} \to 0$, the operator which associates to $\boldsymbol{\varepsilon}$, the function

$$\mathbf{g}(\mathbf{z}_k + \boldsymbol{\varepsilon}) - \mathbf{g}(\mathbf{z}_k) \quad (122)$$

is a linear operator. It is by definition the derivative of $\mathbf{g}(\mathbf{z})$ at the point $\mathbf{z}_k$. If we note $G_k^i(w)$, the kernel of the derivative, we have then

$$\int_a^b G_k^i(w)\, \varepsilon(w)\, dw = \int_a^b \left\{ \log \left(\frac{(x^i - w)^2 + H^2}{(x^i - w)^2 + \{H - [z_k(w) + \varepsilon(w)]\}^2} \right) - \log \left(\frac{(x^i - w)^2 + H^2}{(x^i - w)^2 + [H - z_k(w)]^2} \right) \right\} dw \quad (123)$$

in the limit $\boldsymbol{\varepsilon} \to 0$. The computation of the limit on the right-hand side is carried out formally in exactly the same way as

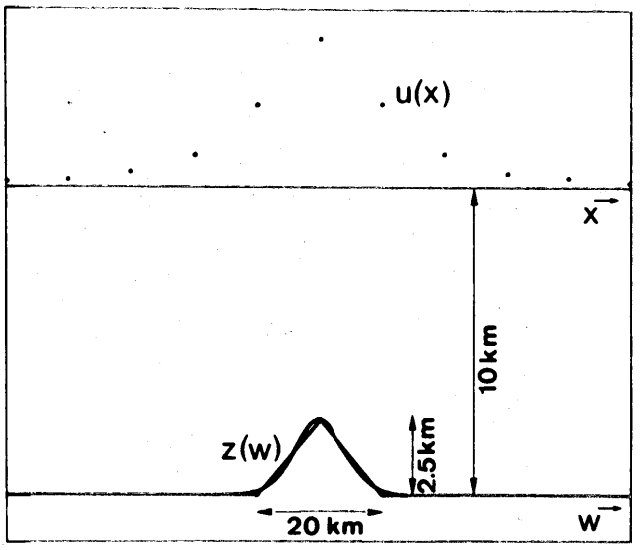

Fig. 7. Synthetic data (top) generated from a 'true model' (triangle at bottom). The smooth curve near the triangle corresponds to the results of the inversion of the synthetic data (which have been contaminated with errors, as shown in Table 1).

for the computation of the classical derivative of the expression

$$\log \frac{(x^i - w)^2 + H^2}{(x^i - w)^2 + (H - z)^2} \tag{124}$$

with respect to the variable z. We obtain then

$$G_k^i(w) = \frac{2(H - z(w))}{(x^i - w)^2 + [H - z(w)]^2} \tag{125}$$

We have generated a set of synthetic data as described in Figure 7 and Table 1. This data set has been contaminated with arbitrary errors, and it has then been inverted in order to evaluate $z(w)$. The following assumptions have been made:

1. The standard error of the data is 0.10 units ($C_{d_0 d_0} = 0.01 \cdot I$).
2. The a priori estimate of $z(w)$ is $z_0(w) \equiv 0$ with an error bar of 5 km.
3. We do not want any oscillations of the solution with wavelength shorter than 1 km.

From assumptions 2 and 3 it follows that an adequate a priori covariance function may be

$$C_{p_0 p_0}(w, w') = \sigma^2 \exp\left\{ -\frac{1}{2} \frac{(w - w')^2}{\Delta^2} \right\} \tag{126}$$

with $\sigma = 5$ km and $\Delta = 1$ km.

The result is obtained by application of the algorithm (82):

$$\hat{z}_{k+1}(w) = \int dw' \sum_i \sum_j C_{p_0 p_0}(w, w') \cdot G_k^i(w') \cdot (S^{-1})^{ij} \cdot \left\{ d_0^j - g^j(\hat{z}_k) + \int dw'' G_k^j(w'') \cdot z_k(w'') \right\} \tag{127}$$

and is shown in Figure 7.

The number of iterations needed depends strongly on the starting point. For the starting point $\hat{z}_0(w) \equiv z_0(w) \equiv 0$ an accuracy of a few percent is obtained in two iterations. Figure 8 shows the results of the first two iterations for a remote starting point. The final result is independent of the starting point $\hat{z}_0(w)$ (but of course depends on the a priori point $z_0(w)$, which has always been taken as null in this example.

The result of the inversion looks similar to the true value of Figure 8, but the sharp slope discontinuities of the true solution have been smoothed.

The integrations involved in the algorithm (82) have been numerically performed using a grid of 100 points. The reduction of the number of points to 50 does not alter the solution significantly.

5. Conclusion

We have shown that the least squares problem admits a general definition, valid for discrete as well as for continuous problems, for overdetermined as well as for underdetermined problems and for linear as well as for nonlinear problems. We have shown that the use of the concept of an a priori covariance matrix (or function) allows one to obtain stable solutions for otherwise unstable problems, or smooth solutions when required. Our general solution (76) solves the simpler problems of least squares adjustments, as well as problems involving any number of integrodifferential equations. The convergence of the algorithm will only be ensured if the nonlinearity is not too strong.

Appendix

Let us first demonstrate the equivalence of (13) and (11) and (12).

We will call $\mathcal{T}$ the nonlinear manifold defined by the equation $\mathbf{f}(\mathbf{x}) = 0$ (the theoretical manifold). We assume $\mathbf{f}$ to be differentiable. The matrix of partial (Fréchet) derivatives,

$$F^{ik} = \partial f^i / \partial x^k \tag{A1}$$

defines a linear application which is named the tangent linear application. We will assume F to be of maximum rank. Let S be the tangent linear application of s:

$$S^k = \partial s / \partial x^k \tag{A2}$$

Let $\hat{\mathbf{x}}$ be a solution of (11) and (12). Then s is stationary at $\hat{\mathbf{x}}$; that is, the tangent linear application S is null over the tangent linear manifold to $\mathcal{T}$ at $\hat{\mathbf{x}}$. We easily obtain

$$S = 2(\hat{\mathbf{x}} - \mathbf{x}_0)^T \cdot C_0^{-1} \tag{A3}$$

Since a vector $\mathbf{V}$ belongs to the tangent linear manifold to $\mathcal{T}$ at $\hat{\mathbf{x}}$ if and only if $F \cdot \mathbf{V} = 0$, (11) and (12) are equivalent to

TABLE 1. Values of Data Used for the Gravitational Problem

Error Free Values of Data	Values of Data Contaminated With Errors
0.181	0.200
0.280	0.250
0.487	0.500
1.023	1.000
2.676	2.650
4.770	4.800
2.676	2.700
1.023	1.050
0.487	0.450
0.280	0.300
0.181	0.150

$$\mathbf{f}(\hat{\mathbf{x}}) = 0 \tag{A4}$$

$$F \cdot \mathbf{v} = 0 \Rightarrow (\hat{\mathbf{x}} - \mathbf{x}_0)^T \cdot C_0^{-1} \cdot \mathbf{v} = 0 \tag{A5}$$

Since F is of maximum rank, (A5) implies the existence of a vector of Lagrange parameters, L, such that $(\hat{\mathbf{x}} - \mathbf{x}_0)^T \cdot C_0^{-1} = \mathbf{L}^T \cdot F$. Equations (A4) and (A5) are then equivalent to

$$\mathbf{f}(\hat{\mathbf{x}}) = 0 \tag{A6}$$

$$\exists\, \mathbf{L} : (\hat{\mathbf{x}} - \mathbf{x}_0) = C_0 \cdot F^T \cdot \mathbf{L} \tag{A7}$$

By left-multiplying (A7) by F we obtain

$$F \cdot (\hat{\mathbf{x}} - \mathbf{x}_0) = (F \cdot C_0 \cdot F^T) \cdot \mathbf{L} \tag{A8}$$

and since C_0 is positive definite and F is of maximum rank,

$$\mathbf{L} = (F \cdot C_0 \cdot F^T)^{-1} \cdot F \cdot (\hat{\mathbf{x}} - \mathbf{x}_0) \tag{A9}$$

Equations (A6) and (A7) are then equivalent to the set of equations

$$\mathbf{f}(\hat{\mathbf{x}}) = 0 \tag{A10}$$

$$(\hat{\mathbf{x}} - \mathbf{x}_0) = C_0 \cdot F^T \cdot (F \cdot C_0 \cdot F^T)^{-1} \cdot F \cdot (\hat{\mathbf{x}} - \mathbf{x}_0) \tag{A11}$$

which are equivalent to the single equation

$$(\hat{\mathbf{x}} - \mathbf{x}_0) = C_0 \cdot F^T \cdot (F \cdot C_0 \cdot F^T)^{-1} \cdot \{F \cdot (\hat{\mathbf{x}} - \mathbf{x}_0) - \mathbf{f}(\hat{\mathbf{x}})\} \tag{A12}$$

It is obvious that (A10) and (A11) imply (A12). The reciprocal is easily demonstrated by left-multiplying (A12) by F.

Let us now turn to the demonstration of equations (20) and (21).

Using (6), (17), and (18), we successively obtain

$$F_k \cdot (\mathbf{x}_k - \mathbf{x}_0) - \mathbf{f}(\mathbf{x}_k) = [I \quad -G_k] \cdot \begin{bmatrix} \hat{\mathbf{d}}_k - \mathbf{d}_0 \\ \hat{\mathbf{p}}_k - \mathbf{p}_0 \end{bmatrix} - [\hat{\mathbf{d}}_k - \mathbf{g}(\hat{\mathbf{p}}_k)]$$
$$= -\{\mathbf{d}_0 - \mathbf{g}(\hat{\mathbf{p}}_k) + G_k \cdot (\hat{\mathbf{p}}_k - \mathbf{p}_0)\} \tag{A13}$$

$$C_0 \cdot F_k^T = \begin{bmatrix} C_{d_0d_0} & C_{d_0p_0} \\ C_{p_0d_0} & C_{p_0p_0} \end{bmatrix} \cdot \begin{bmatrix} I \\ -G_k^T \end{bmatrix} = \begin{bmatrix} C_{d_0d_0} - C_{d_0p_0} \cdot G_k^T \\ C_{p_0d_0} - C_{p_0p_0} \cdot G_k^T \end{bmatrix} \tag{A14}$$

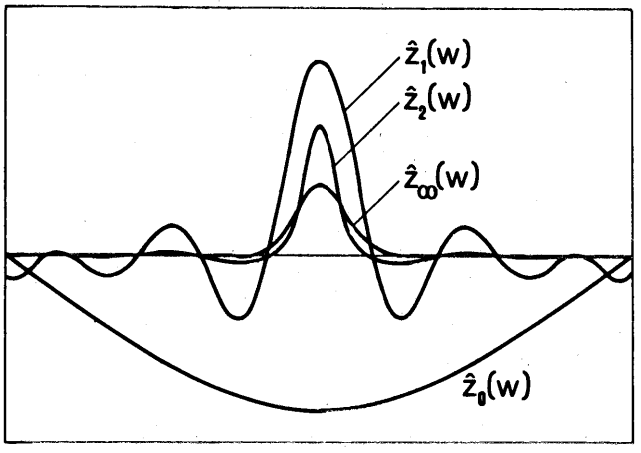

Fig. 8. The problem is nonlinear, and this figure illustrates the convergence of the algorithm when the 'starting point' is far from the 'true solution.' The final solution is rigorously independent of the starting point.

$$F_k \cdot C_0 \cdot F_k^T = C_{d_0d_0} - C_{d_0p_0} \cdot G_k^T - G_k \cdot C_{p_0d_0} + G_k \cdot C_{p_0p_0} \cdot G_k^T \tag{A15}$$

then (15) gives

$$\begin{bmatrix} \hat{\mathbf{d}}_{k+1} \\ \hat{\mathbf{p}}_{k+1} \end{bmatrix} = \begin{bmatrix} \mathbf{d}_0 \\ \mathbf{p}_0 \end{bmatrix} + \begin{bmatrix} C_{d_0p_0} \cdot G_k^T - C_{d_0d_0} \\ C_{p_0p_0} \cdot G_k^T - C_{p_0d_0} \end{bmatrix} \cdot [C_{d_0d_0} - C_{d_0p_0} \cdot G_k^T - G_k \cdot C_{p_0d_0} + G_k \cdot C_{p_0p_0} \cdot G_k^T]^{-1} \cdot [\mathbf{d}_0 - \mathbf{g}(\hat{\mathbf{p}}_k) + G_k \cdot (\hat{\mathbf{p}}_k - \mathbf{p}_0)] \tag{A16}$$

The solution for $\hat{\mathbf{p}}_{k+1}$ coincides with (20). To obtain (21), we must first demonstrate a matricial identity. From the trivial equality

$$(C_{d_0d_0} - C_{d_0p_0} \cdot G^T) = (C_{d_0d_0} - C_{d_0p_0} \cdot G^T - G \cdot C_{p_0d_0} + G \cdot C_{p_0p_0} \cdot G^T) - G \cdot (C_{p_0p_0} \cdot G^T - C_{p_0d_0}) \tag{A17}$$

we deduce, by right-multiplication with the appropriate matrix,

$$(C_{d_0d_0} - C_{d_0p_0} \cdot G^T) \cdot (C_{d_0d_0} - C_{d_0p_0} \cdot G^T - G \cdot C_{p_0d_0} + G \cdot C_{p_0p_0} \cdot G^T)^{-1} = I - G \cdot (C_{p_0p_0} \cdot G^T - C_{p_0d_0}) \cdot (C_{d_0d_0} - C_{d_0p_0} \cdot G^T - G \cdot C_{p_0d_0} + G \cdot C_{p_0p_0} \cdot G^T)^{-1} \tag{A18}$$

Using (A18), the solution for $\hat{\mathbf{d}}_{k+1}$, as given by (A16), may be written as

$$\hat{\mathbf{d}}_{k+1} = \mathbf{d}_0 - [I - G_k \cdot (C_{p_0p_0} \cdot G_k^T - C_{p_0d_0}) \cdot (C_{d_0d_0} - C_{d_0p_0} \cdot G_k^T - G_k \cdot C_{p_0d_0} + G_k \cdot C_{p_0p_0} \cdot G_k^T)^{-1}] \cdot [\mathbf{d}_0 - \mathbf{g}(\hat{\mathbf{p}}_k) + G_k \cdot (\hat{\mathbf{p}}_k - \mathbf{p}_0)]$$
$$= \mathbf{g}(\hat{\mathbf{p}}_k) - G_k \cdot \hat{\mathbf{p}}_k + G_k \cdot \hat{\mathbf{p}}_{k+1} \tag{A19}$$

which demonstrates (21).

To demonstrate (24) and (25), we will use the matricial identities

$$C_{p_0p_0} \cdot G^T \cdot (C_{d_0d_0} + G \cdot C_{p_0p_0} \cdot G^T)^{-1} = (G^T \cdot C_{d_0d_0}^{-1} \cdot G + C_{p_0p_0})^{-1} \cdot G^T \cdot C_{d_0d_0}^{-1} \tag{A20}$$

$$(G^T \cdot C_{d_0d_0}^{-1} \cdot G + C_{p_0p_0}^{-1})^{-1} = C_{p_0p_0} - C_{p_0p_0} \cdot G^T \cdot (C_{d_0d_0} + G \cdot C_{p_0p_0} \cdot G^T)^{-1} \cdot G \cdot C_{p_0p_0} \tag{A21}$$

which have been demonstrated in paper 1.

Equation (24) is deduced from (23) using (A20). It is obvious that (23) can be written as

$$\hat{\mathbf{p}}_{k+1} = \hat{\mathbf{p}}_k + C_{p_0p_0} G_k^T \cdot (C_{d_0d_0} + G_k \cdot C_{p_0p_0} \cdot G_k^T)^{-1} \cdot [\mathbf{d}_0 - \mathbf{g}(\hat{\mathbf{p}}_k)] - [C_{p_0p_0} - C_{p_0p_0} \cdot G_k^T \cdot (C_{d_0d_0} + G_k \cdot C_{p_0p_0} \cdot G_k^T)^{-1} \cdot G_k \cdot C_{p_0p_0}] \cdot C_{p_0p_0}^{-1} \cdot (\hat{\mathbf{p}}_k - \mathbf{p}_0) \tag{A22}$$

Equation (25) is deduced from (A22) using (A20) and (A21).

A proper derivation of (30) has been made in paper 1, where C is obtained as the covariance matrix of the a posteriori probability density function. A formal derivation of (30) is obtained if we consider (29) as a relation between random variables. By definition of covariance matrix,

$$C = E\{[\hat{\mathbf{x}} - E(\hat{\mathbf{x}})][\hat{\mathbf{x}} - E(\hat{\mathbf{x}})]^T\} \tag{A23}$$

where E stands for mathematical expectation. Using the notations of (31), (32), and (33), we successively obtain

$$\begin{aligned} C &= E\{[P\mathbf{x}_0 - E(P\mathbf{x}_0)][P\mathbf{x}_0 - E(P\mathbf{x}_0)]^T\} \\ &= P \cdot E\{[\mathbf{x}_0 - E(\mathbf{x}_0)][\mathbf{x}_0 - E(\mathbf{x}_0)]^T\}P^T \\ &= P \cdot C_0 \cdot P^T = P^2 \cdot C_0 = P \cdot C_0 \end{aligned} \tag{A24}$$

which demonstrates (34) and (30).

The proof of (37) and (38) is a particular case of that of (20) and (21). Using (6), (35), and (36), (33) becomes

$$\begin{aligned} \begin{bmatrix} \hat{\mathbf{d}} \\ \hat{\mathbf{p}} \end{bmatrix} &= \begin{bmatrix} \hat{\mathbf{d}}_0 \\ \mathbf{p}_0 \end{bmatrix} + \begin{bmatrix} C_{d_0p_0} \cdot G^T - C_{d_0d_0} \\ C_{p_0p_0} \cdot G^T - C_{p_0d_0} \end{bmatrix} \\ &\cdot [C_{d_0d_0} - C_{d_0p_0} \cdot G^T - G \cdot C_{p_0d_0} \\ &+ G \cdot C_{p_0p_0} \cdot G^T]^{-1} [\mathbf{d}_0 - G \cdot \mathbf{p}_0] \end{aligned} \tag{A25}$$

The solution for $\hat{\mathbf{p}}$ coincides with (37). Using (A18), the solution for $\hat{\mathbf{d}}$ may be written as

$$\begin{aligned} \hat{\mathbf{d}} &= \mathbf{d}_0 - [I - G \cdot (C_{p_0p_0} \cdot G^T - C_{p_0d_0}) \cdot (C_{d_0d_0} - C_{d_0p_0} \cdot G^T \\ &\quad - G \cdot C_{p_0d_0} + G \cdot C_{p_0p_0} \cdot G^T)^{-1} \\ &\quad \cdot (\mathbf{d}_0 - G \cdot \mathbf{p}_0) = G \cdot \hat{\mathbf{p}} \end{aligned} \tag{A26}$$

which demonstrates (38).

Using (6) and (35), (34) becomes

$$\begin{aligned} \begin{bmatrix} C_{\hat{\mathbf{d}}\hat{\mathbf{d}}} & C_{\hat{\mathbf{d}}\hat{\mathbf{p}}} \\ C_{\hat{\mathbf{p}}\hat{\mathbf{d}}} & C_{\hat{\mathbf{p}}\hat{\mathbf{p}}} \end{bmatrix} &= \begin{bmatrix} C_{d_0d_0} & C_{d_0p_0} \\ C_{p_0d_0} & C_{p_0p_0} \end{bmatrix} - \begin{bmatrix} C_{d_0d_0} - C_{d_0p_0} \cdot G^T \\ C_{p_0d_0} - C_{p_0p_0} \cdot G^T \end{bmatrix} \\ &\cdot [C_{d_0d_0} - C_{d_0p_0} \cdot G^T - G \cdot C_{p_0d_0} + G \cdot C_{p_0p_0} \cdot G^T]^{-1} \\ &\cdot [C_{d_0d_0} - G \cdot C_{p_0d_0} \qquad C_{d_0p_0} - G \cdot C_{p_0p_0}] \end{aligned} \tag{A27}$$

For $C_{\hat{\mathbf{p}}\hat{\mathbf{p}}}$ we directly obtain from (A27) the expression (39). For $C_{\hat{\mathbf{d}}\hat{\mathbf{p}}}$ we obtain successively

$$\begin{aligned} C_{\hat{\mathbf{d}}\hat{\mathbf{p}}} &= C_{d_0p_0} - (C_{d_0d_0} - C_{d_0p_0} \cdot G^T)[\ \ ]^{-1}(C_{d_0p_0} - G \cdot C_{p_0p_0}) \\ &= C_{d_0p_0} - [I - G \cdot (C_{p_0p_0} \cdot G^T - C_{p_0d_0})[\ \ ]^{-1}] \\ &\quad \cdot (C_{d_0p_0} - G \cdot C_{p_0p_0}) = G \cdot C_{\hat{\mathbf{p}}\hat{\mathbf{p}}} \end{aligned} \tag{A28}$$

where we have used (A18). For $C_{\hat{\mathbf{d}}\hat{\mathbf{d}}}$ we obtain successively from (A27), using (A18),

$$\begin{aligned} C_{\hat{\mathbf{d}}\hat{\mathbf{d}}} &= C_{d_0d_0} - (C_{d_0d_0} - C_{d_0p_0} \cdot G^T)[\ \ ]^{-1}(C_{d_0d_0} - G \cdot C_{p_0d_0}) \\ &= C_{d_0d_0} - [I - G \cdot (C_{p_0p_0} \cdot G^T - C_{p_0d_0})[\ \ ]^{-1}] \\ &\quad \cdot (C_{d_0d_0} - G \cdot C_{p_0d_0}) \\ &= G \cdot C_{p_0d_0} + G \cdot (C_{p_0p_0} \cdot G^T - C_{p_0d_0})[\ \ ]^{-1} \\ &\quad \cdot (C_{d_0d_0} - G \cdot C_{p_0d_0}) \\ &= G \cdot C_{p_0d_0} + G \cdot (C_{p_0p_0} \cdot G^T - C_{p_0d_0})[I - [\ \ ]^{-1} \\ &\quad \cdot (G \cdot C_{p_0p_0} - C_{d_0p_0}) \cdot G^T] \\ &= G \cdot C_{p_0p_0} \cdot G^T - G \cdot (C_{p_0p_0} \cdot G^T - C_{p_0d_0})[\ \ ]^{-1} \\ &\quad \cdot (G \cdot C_{p_0p_0} - C_{d_0p_0}) \cdot G^T \\ &= G \cdot C_{pp} \cdot G^T \end{aligned} \tag{A29}$$

Equations (A28) and (A29) demonstrate (40).

Equations (43) and (44) are obtained from (41) and (42) using (A20) and (A21).

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