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On Geophysical Inverse Problems and Constraints

P.C. Sabatier

Département de Physique Mathématique*, Université des Sciences et Techniques du Languedoc, F-34060 Montpellier Cedex, France

Abstract. Mathematical methods for linearized geophysical inverse problems are reviewed, in cases with and in cases without constraints. The role of constraints receives particular attention, both in linear convex problems and in an exactly solvable non-linear example.

Key words: Geophysical inverse problems – Constraints – Convex problems.

1. Introduction

Understanding physics proceeds through models in which a mapping, $\mathcal{M}$, is defined, from a set of "parameters", $\mathcal{C}$, to a set of "results", $\mathcal{E}$. $\mathcal{E}$ is supposed to contain the image of $\mathcal{C}$ and all the possible experimental results. In geophysics $\mathcal{C}$ is the class of "earth models", $\mathcal{M}$ is the set of "earth functionals" and $\mathcal{E}$ is the class of "earth data". Obtaining the image $e=\mathcal{M}(c)\in\mathcal{E}$ of $c\in\mathcal{C}$ is solving the *direct problem.* Obtaining all the elements $c\in\mathcal{C}$, if any, that correspond to $e\in\mathcal{E}$ is solving the *inverse problem.* Existence, uniqueness, stability, approximation and the physical description of the set of solutions are all current questions of interest. The study of geophysical inverse problems is particularly interesting for several reasons

a, The earth functional $\mathcal{M}$ is usually well-known. The questions which arise in connection with $\mathcal{M}$ come from its replacement by approximate forms rather than from essential ignorance.

b, The practical interest of inverse problems is obvious in geophysics but not always in other fields, where the definition of $\mathcal{M}$ is often questionable.

c, Most of the questions and methods appearing in connection with inverse problems appear in geophysics; of current interest are: exact methods; Monte-Carlo methods; linear methods (applied to linearized problems) and ray methods (applied to short-wave-length propagation).

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* Physique Mathématique et Théorique, Equipe de recherche associée au C.N.R.S. Ce travail a été effectué dans le cadre de la RCP 264: Problèmes Inverses

The progress in exact methods is very slow. Although their results sometimes seem very academic, one should not forget that only these methods are able to encompass global inverse problems. In recent years one notices two very remarkable analytic solutions of the geomagnetic induction problem (Bailey, 1970; Weidelt, 1972). Other recent exact studies are concerned with more schematic problems: the exact inverse problem for the phase of waves corresponding to an explosion in a spherical earth (Sabatier, 1974a), the discrete model of the inverse Love problem (Barcilon, 1976). I will not discuss exact methods further except for a remark on the effect of constraints (§ 2).

Many inverse problems of geophysics are controlled by linear partial differential equations, but the relations between parameters and data are essentially non linear. Even the gravity problem becomes linear only if one throws away constraints. Recent progress in linearized problems can be noted in the following 5 areas.

1. The physical description of the set of equivalent models is studied either by exhibiting marginal models as in the "edgehog" method (Jackson, 1973) and studies of extremals (Sabatier, 1976a, b); or by relating the "generalized solutions" of linear inverse problems to presumed stochastic properties as in the stochastic point of view in linear problems (Foster, 1961; Franklin, 1970; Jackson, 1972; Jordan and Minster, 1972).

2. Taking constraints into account, in order

a. to obtain "ideal bodies" (Parker, 1974, 1975; Sabatier, 1976b),

b. to give the general solution of the problem (Sabatier, 1976a),

c. to take into account error free measurements (Burkhard and Jackson, 1976).

3. Checking the value of approximate mappings

a. either by analyzing mathematical examples (Anderssen, 1975; Sabatier, 1974b),

or b. by analyzing global problems (Anderssen, 1975),

or c. by analyzing the convergence of iterations (Jackson, 1973; Jupp and Vozoff, 1975).

4. Analyzing the effect of errors: "method errors" due to the fact that the problem is improperly posed, "experimental errors" (i.e. those due to measurements); and obtaining "regularized solutions" in which a mixed contribution of errors give the "most probable" solution in the set of "equivalent solutions". This "regularization" has essentially been used in linear inverse problems. Two different points of view are

a. the algebraic point of view, (Lanczos, 1961; Backus and Gilbert, 1967, 1968, 1970; Backus, 1970a, b, c; Marquardt, 1963, 1970; Smith and Franklin, 1969),

b. the stochastic point of view (Foster, 1961; Franklin, 1970; Jackson, 1972; Jordan and Franklin, 1971; Jordan and Minster, 1972; Wiggins; Larner and Wisecup, 1976).

5. Using inverse methods to continue data (Ducruix et al., 1974).

Recent progress in Monte-Carlo and hedgehog methods, and in the ray methods, are to be reviewed in other lectures in this congress, so that I will not discuss them.

This paper can be considered as a survey of recent linear methods applied to

linearized inverse problems with a particular emphasis on constraints. I am convinced that a real physical problem necessarily is a constrained problem, and I would like to show that dealing with a constrained problem by methods in which the constraints are built in is not *really* more difficult than dealing with an unconstrained problem. Actually, I think that linear inverse problems with constraints are simpler, more appealing, as well as more physical than are linear inverse problems without constraints.

In § 2, we show how one or two positivity constraints completely modify the nature of an inverse problem which is controlled by a linear differential equation. This problem appears as an intermediate step in several geophysical inverse problems.

In § 3, we study some general aspects of linearized geophysical inverse problems and, in particular, the question of "linearizing" an inverse problem.

In § 4, we survey the linear methods by which the linearized inverse problems without constraints or with linear constraints have been studied. The algebraic point of view and the stochastic point of view are considered.

In § 5, we survey the linear convex methods applied to linearized inverse problems with non-negativity constraints and their fundamental applications (ideal bodies).

Concluding remarks are given in § 6.

Readers who are only interested in linear problems may skip § 2.

2. The Role of Constraints in an Exact Non-Linear Problem

In several problems of elastic wave propagation (see e.g. Aki and Ware, 1968; Sabatier, 1976a, b) one has to recover a function $Z(\tau)$ $(0<\tau<b)$ from a function of ω, $\psi(\tau, \omega)$, which is known for all real values of ω in a range of values of τ $(\tau > b)$, for which $Z(\tau)$ is known and constant. ψ and Z are everywhere interelated by the equation

$$\left[Z^2 \frac{d}{d\tau} Z^{-2} \frac{d}{d\tau} + \omega^2\right] \psi(\tau, \omega) = 0 \tag{1}$$

with the boundary condition $\psi(0, \omega) = 0$. The consistency condition,

$$\psi(\tau, \omega) = F(\omega)\, e^{i\omega t} + F^*(\omega)\, e^{-i\omega t},$$

holds for $\tau > b$ and a certain function $F(\omega)$.

Thus the inverse problem consists of recovering $Z(\tau)$ $(0 \leqq \tau \leqq b)$ from $F(\omega)$ and from $Z(b)$. We assume that $Z(\tau)$ and $Z'(\tau)$ are absolutely continuous functions (so that $Z'(b) = 0$). In addition to these smoothness assumptions two hard constraints are imposed by the physical conditions: the first one is that the impedance Z (which is simply related to the density and Lamé parameters) is *real*, and thus Z^2 is positive. The second one is that Z is constant in the range $(\tau > b)$ where the measurements are made. Now, because of the smoothness assumptions, Equation (1) is equivalent to the following one:

$$\left[\frac{d^2}{d\tau^2} + \omega^2 - V(\tau)\right] Z^{-1} \psi(\tau, \omega) = 0 \tag{2}$$

where $V(\tau)=Z\dfrac{d^2}{d\tau^2}(Z^{-1})$, so that $Z(\tau)$ is uniquely obtained from $V(\tau)$ by solving a linear 2nd order differential equation with the two conditions at $\tau=b$. Thus the inverse problem $F(\omega)\to Z(\tau)$ is equivalent to the well-known Gelfand-Levitan-Jost-Kohn inverse problem $F(\omega)\to V(\tau)$. If there were no hard constraint on Z, this problem would be strongly *underdetermined.* Determining $V(\tau)$ would then require a knowledge of $F(\omega)$ for all real ω *and* also the unknown "discrete spectrum" of the differential operator $\dfrac{d^2}{d\tau^2}-V(\tau)$, i.e. all the values of ω^2 for which (2) has a solution satisfying both the boundary condition $Z^{-1}\psi(0,\omega)=0$ and the finite norm condition $\int_0^\infty Z^{-2}\psi^2(\tau,\omega)\,d\tau<\infty$. One could arbitrarily choose a parameter for every value of the discrete spectrum (for complete discussions of this problem see for example Newton (1967) or Chadan and Sabatier (1977)). Now, because Z^2 is positive, this discrete spectrum does not exist. [*Proof:* because of the finite norm condition, $\psi(\tau)$ must go to zero as τ goes to ∞. Substituting (1) in the norm integral and integrating by parts yields the equality

$$\omega^2\int_0^\infty Z^{-2}\psi^2(\tau,\omega)\,d\tau=\int_0^\infty Z^{-2}(\psi'(\tau,\omega)]^2\,d\tau,$$

which proves that ω^2 is positive, and this is impossible because then $\psi(\tau)$ would behave asymptotically like $2\,\mathrm{Re}(F(\omega)e^{i\omega t})$ and could not go to zero]. So if the only hard constraint were $Z^2>0$, the problem would be *well posed.* Because of the other hard constraint (which implies that $V(\tau)=0$ for $\tau>b$) the problem is *overdetermined.* $F(\omega)$ must satisfy certain consistency condition (special analytic properties) that are related to the cut-off at b and, which from the physical point of view, are due to "causality".

Although I have not been able to prove it completely as yet, I am convinced that the two hard constraints above are essential pieces to obtain uniqueness theorems in the inverse normal modes problem (notice that the partial wave differential equations are similar to the ones given in Sabatier (1974a) and therefore can be reduced to the form (1)).

3. General Aspects of Linear Geophysical Inverse Problems

A linear inverse problem is a problem in which,

a. the set $\mathscr{C}$ of earth models and the set $\mathscr{E}$ of data are linear spaces and

b. $\mathscr{M}$ is a linear mapping.

No geophysical inverse problem is linear. Two steps are generally necessary for linearizing a geophysical inverse problem

a. The sets $\mathscr{C}$ and $\mathscr{E}$ must be made into linear spaces by throwing away constraints. This is enough to linearize some important problems – e.g. the gravity problem and the geomagnetism problem.

b. The mapping $\mathcal{M}$ must be replaced by a linear mapping $\mathcal{M}_0$. Usually this can be done as follows. One knows a model m_0 which gives a (good or bad) fit $\mathcal{M}m_0$ of the data, and that $\mathcal{M}$ is differentiable in the neighborhood of m_0 (i.e. that

$$\Delta = \mathcal{M}(m_0+m) - \mathcal{M}(m_0) = \mathcal{M}_0(m) + r_0(m) \tag{3}$$

where $\mathcal{M}_0$ is linear and the norm in $\mathcal{E}$ of $r_0(m)$ is infinitesimally small compared to $\|m\|_{\mathcal{C}}$ when $\|m\|_{\mathcal{C}} \to 0$). "Linearizing" means replacing $\mathcal{M}$ by $\mathcal{M}_0$, Δ being the difference between the data and the "fit" $\mathcal{M}m_0$. If the sets $\mathcal{E}$ and $\mathcal{C}$ are defined (or redefined) in such a way that a linear operator $\mathcal{N}$ does exist, which solves equations $\mathcal{N}\mathcal{M}_0 x = x$, linearizing is justified whenever an algorithm like

$$m_1 = \mathcal{N}(\Delta); \ldots; m_{i+1} = \mathcal{N}(\Delta - r_0(m_i)) \tag{4}$$

is well-defined and converges towards a solution of $\mathcal{M}_0(m) = \Delta - r_0(m)$ which is close enough to the linear term m_1. A sufficient condition for this is that both $r_0(m)$ be lipschitzian with its Lipschitz constant l satisfying the inequality (Sabatier, 1974a)

$$lN < 1 \tag{5}$$

where N is the norm of $\mathcal{N}$. In this case, the exact solution m_∞ which is obtained from (4) is in one-to-one correspondence with m_1, and the "linearized problem" is a good "image" of the "exact problem". The value of (lN) is a measure of the quality of the approximation.

Now we meet 3 cases in geophysical inverse problems:

A. "Problems Using Continuous Data"

We mean problems in which a first step has been to construct a continuous function interpolating the data. The ambiguities that are associated with this step are separately studied and we then assume that the interpolating function is the data. This often has important consequences: $\mathcal{M}$ is in most cases a bijective mapping, and at least twice differentiable. $\mathcal{N}$ is unique (it is in many cases obtained from the Green's function of a simpler problem – see e.g. Knopoff 1961, 1962). Because of the double differentiability, $r_0(m)$ is $O(\|m\|^2)$. Thus, if Δ is small enough, the sequence (m_i) is contained in a ball in which l itself is $O(\|m\|)$. The convergence factor (5) is itself $O(\|m_1\|)$ or $O(N\|\Delta\|)$ and the linear approximation is good whenever $\|\Delta\|$ is small enough – not a surprising result.

B. "Problems Using Finite Sets of Data"

Here, there are many matrices $\mathcal{N}$ solving $\mathcal{N}\mathcal{M}x = x$. They are called the generalized inverses of $\mathcal{M}$. The radius of the ball in which the algorithm (4) converges depends on the norm N of $\mathcal{N}$. If N is large only excellent fits m_0 enable one to linearize the problem in their neighbourhoods.

There was recently some criticism of linearizing techniques (see e.g. Sabatier, 1974a; Anderssen, 1975), concluding that their validity should be carefully

checked in every case. This can be done by trying to obtain exact solutions from the most "marginal" solutions which are still admissible on physical grounds, those for which N is the largest. One has good justification for studying marginal solutions (see below in §4 the edgehog method and in §5 the extremals).

C. Problems in Which There May be Several "Branches" of Solutions

In non linear problem, either "bifurcations" or strong "discontinuities" can lead to separated branches of solutions. They probably exist in geophysics. Take for instance the "approximate" inversion techniques obtained by ray methods in travel time inversions. Well-known results [Gerver and Markushevish, 1966, 1967], clearly show the various contributions of the low velocity lids: $X(p)$ being the epicentral distance, p the ray parameter, T the travel time, $t(p)=T(p)-pX(p)$ one obtains:

$$\frac{dt}{dp}=-X(p)-\sum_k \sigma_k \delta(p-p_k) \tag{6}$$

where the jumps σ_k correspond to the unknown low-velocity ranges, p_k the velocity lids. Clearly no linear model can represent the whole contribution and $\delta(p-p_k)$ is the Dirac distribution. On the other hand, linearizing is still useful in the neighborhood of a given model (Kennet, 1976).

4. Linear Inverse Problems

So as to be both simple and sufficiently general, we shall assume in the following that the space $\mathscr{C}$ of "earth models" is the Hilbert space $L_2(\Omega)$, where Ω is a finite interval in $\mathbb{R}$ and that the mapping of $\mathscr{C}$ into $\mathscr{E}$ is made of M linear functionals, the "earth functionals", whose kernels $G_i(r)$ belong to $L_2(\Omega)$. Thus, the equations

$$\int_\Omega G_i(r)\, m(r)\, dr = g_i(m) \qquad (i=1, \ldots, M) \tag{7}$$

should be satisfied by the model $m(r)$, with $g_i(m)$ equal (or approximately equal) to the data e_i to within an estimated error. If we make a partition of Ω into N subdomains $\Omega_1, \ldots, \Omega_N$ such that $\sum_i \Omega_i = \Omega$ and $\mathrm{Sup}(\mathrm{mes}\,\Omega)=h$, we can "discretize" the Equation (7) by deciding to only consider models m of a special form. For instance consider only those models which are constant in each subdomain. Thus, with obvious notations, (7) is reduced to a vectorial equation:

$$(\mathbf{G}\,\mathbf{m})_i = \sum_{k=1}^{N} G_{ik} m_k = g_i(\mathbf{m}). \tag{8}$$

We call this transformation an N-discretization of step-size h. When $N\to\infty$, $h\to 0$, the class of solutions thus obtained is large enough for all physicists needs.

The linear inverse problem consists of obtaining all the information we can concerning $m(r)$ from a knowledge of the M data $e_1, \ldots, e_M$, and the estimated errors. This information can be described either by algebraic means (algebraic point of view, or A.P.V.) or by reference to statistics (stochastic point of view, or S.P.V.).

The information is equivalent, only the point of view is modified, as we shall easily see in the formulas.

4.1. A.P.V.: Backus-Gilbert Kernels

We sketch the now classical Backus and Gilbert method (Backus and Gilbert, 1967, 1968, 1970; Backus, 1970a, b, c), which both gives an average solution and a simple representation of the set of equivalent solutions of (7). Clearly (7) has a solution if we can construct a kernel $A(r_0, r)$ such that:

(i) for any r_0 in R and any earth model $m(r)$ in the class $\mathscr{C}$ studied

$$m(r_0) = \int_{\Omega} A(r_0, r)\, m(r)\, dr \tag{9}$$

and (ii)

$$A(r_0, r) = \sum_{i=1}^{M} a_i(r_0)\, G_i(r). \tag{10}$$

The solution is then

$$m(r) = \sum_i e_i\, a_i(r). \tag{11}$$

Unfortunately, (unless we take for $\mathscr{C}$ M-dimensional sets), the solution of (7) is not unique, and it is not possible to construct a kernel that satisfies (9) for any m, r, r_0. But it is often possible to construct "approximate" kernels $A(r_0, r)$, viz. linear combinations of the $G_i(r)$'s which "look" in some sense "like" $\delta(r_0 - r)$.

More precisely, one selects, among the linear combinations of the $G_i(r)$'s, the one which has, in the Backus-Gilbert terminology, the best "δ-ness". Usually, $A(r_0, r)$ appears as a peaked function, whose width is a measure of the "δ-ness". Thus (11) gives an average solution of (7), and the δ-ness gives an appraisal of the deviation from each other of equivalent models. This deviation can be visualized in another way. The non-uniqueness means that there exist functions $m(r)$ which average to zero over all but small length scales and represent the deviations between acceptable models. Thus there will be some smallest length l_0 such that the acceptable models have approximately the same average over an interval of length l_0 at r. l_0 is called the "resolving length" at r.

Backus and Gilbert used mainly two ways of constructing averaging kernels. The first one consists of minimizing $\int_{\Omega} (r - r_0)^2 [A(r_0, r)]^2\, dr$ over all the combinations (10). This has the interest of giving functions with very small tails outside the "δ-like" peak. The second one consists of using the orthogonal projection operator of $\mathscr{C}$ into the space spanned by the $[G_i(r)]$. This kernel often has a smaller width than the former one, but produces large oscillating tails. The model it yields is the solution of (7) which has the least norm in $L_2(\Omega)$.

4.2. A.P.V.: The Least-Norm Solution

For the sake of simplicity, let us consider the discretized Equation (8), with $N > M$. Let $R(\mathbf{G})$ be the image of $\mathbf{G}$, i.e. the space spanned by its N column vectors (its dimensionality clearly is the rank $p \leqq M$ of $\mathbf{G}$). Let $\mathbf{G}^*$ be the adjoint matrix of $\mathbf{G}$ (its transposed matrix in our case of real matrices). Clearly, the ortho-projector P on the space spanned by the $G_i(r)$'s is nothing but the ortho-projector onto $R(\mathbf{G}^*)$, say $P_{R(\mathbf{G}^*)}$ (the properties of an ortho-projector are $P^2 = P = P^*$). Now, let $n(\mathbf{G})$ be the null-space of $\mathbf{G}$. Since, for any vector $\mathbf{q}$ of $\mathbb{R}_M$, one obviously has the following equality between scalar products,

$$\langle \mathbf{G}\,\mathbf{m}, \mathbf{q} \rangle = \langle \mathbf{m}, \mathbf{G}^*\,\mathbf{q} \rangle = \langle \mathbf{G}\,P_{R(\mathbf{G}^*)}\,\mathbf{m}, \mathbf{q} \rangle,$$

it follows that the orthogonal complement in $\mathbb{R}_N$ of $P_{R(\mathbf{G}^*)}\mathbf{m}$ to $\mathbf{m}$ belongs to $n(\mathbf{G})$, and, for any $\mathbf{m}$

$$\left.\begin{aligned} &\mathbf{m} = P_{R(\mathbf{G}^*)}\,\mathbf{m} + \mathbf{m}_\perp \\ &\|m\|^2 = \|P_{R(\mathbf{G}^*)}\,\mathbf{m}\|^2 + \|\mathbf{m}_\perp\|^2. \end{aligned}\right\} \tag{13}$$

Thus using $P_{R(G^*)}$ for $\int_\Omega A(r_0, r)\,\mathrm{dr}.$ yields the solution of (7) which has the least norm:

$$m_a(r) = \sum_{i,j} P_{ij}\, e_i\, G_j(r). \tag{14}$$

4.3. A.P.V.: Generalized Inverse

Let $\mathbf{G}$ be an $M \times N$ matrix of arbitrary rank. A generalized inverse of $\mathbf{G}$ is an $N \times M$ matrix $\mathbf{G}^-$ such that $\mathbf{x} = \mathbf{G}^-\,\mathbf{y}$ is a solution of $\mathbf{G}\,\mathbf{x} = \mathbf{y}$ for any $\mathbf{y}$ in the range of $\mathfrak{G}$ (see f.e. Rao and Mitra, 1971, p. 20; Smith and Franklin 1969). For $N > M$ there is usually an infinity of generalized inverses. All them satisfy the necessary and sufficient condition:

$$\mathbf{G}^- \text{ exists} \Leftrightarrow \mathbf{G}\,\mathbf{G}^-\,\mathbf{G} = \mathbf{G}. \tag{15}$$

Among these generalized inverses one is particularly interesting, the Moore-Penrose inverse, $\mathbf{G}_{MP}$ which is such that

$$\mathbf{G}\,\mathbf{G}_{MP}^- = P_{R(\mathbf{G})}$$

and

$$\mathbf{G}_{MP}^-\,\mathbf{G} = P_{R(\mathbf{G}^*)}. \tag{16}$$

One can derive it, for instance, by noticing that it follows from (16) that

$$\mathbf{G}_{MP}^- = \mathbf{G}^*(\mathbf{G}\,\mathbf{G}^*)_{MP}^-. \tag{17}$$

If $\mathbf{G}$ has rank M, $\mathbf{G}\,\mathbf{G}^*$ is positive definite and $(\mathbf{G}\,\mathbf{G}^*)_{MP}^- = (\mathbf{G}\,\mathbf{G}^*)^{-1}$. Otherwise (rank $K \ll M$), $\mathbf{G}\,\mathbf{G}^*$ can be diagonalized by an orthogonal transformation $\mathbf{U}$:

$$\mathbf{G}\,\mathbf{G}^* = \mathbf{U}\,\Lambda\,\mathbf{U}^*. \tag{18}$$

Here $\Lambda_{ij}=\lambda_i^2\,\delta_{ij}$ $(i=1, 2, \ldots, M)$, and we assume in the following that the λ_i^2 are ordered by decreasing magnitude, so that $\lambda_i \neq 0$ for $i \leqq K$, and $\lambda_i=0$ for $i>K$. The desired generalized inverse is then simply obtained by dropping the parts of Λ that correspond to the zero eigenvalues (see Penrose, 1955; Lanczos, 1961; Wiggins, 1972; Jackson, 1972). This is possible because (Lanczos, 1961) the columns of $\mathbf{U}$ (or the rows of $\mathbf{U}^*$) beyond the label K have no effect on the result. What remains is that

$$\mathbf{G}\,\mathbf{G}^*=\mathbf{U}_K\,\Lambda_K\,\mathbf{U}_{K^*}, \tag{19}$$

where $\mathbf{U}_K$ is the semi orthogonal $M \times K$ matrix which is formed out of the column vectors $\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_K$ and Λ_K is the square diagonal $K \times K$ matrix containing only the non-zero eigenvalues. Thus the model given by the Moore Penrose inverse is simply

$$\mathbf{m}_{MP}=\mathbf{G}^*\,\mathbf{U}_K\,\Lambda_K^{-1}\,\mathbf{U}_K^*\mathbf{g}. \tag{20}$$

For a consistent system m_{MP} is the least-norm model $\mathbf{m}_a$. For an inconsistent system, the formula (20) is still defined and it is possible to show that it yields the so-called "least square solution".

4.4. A.P.V.: The Errors

For a consistent system $(N \geqq M,\ K=M)$, (20) gives an exact solution of the problem. Now, assume that the g_i's are known up to possible errors $(|g_i-e_i| \leqq \Delta e_i)$. Then, since $\mathbf{U}_K^*$ is an isometric transformation, a small error Δe on $\mathbf{g}$ gives an error Δf of the same norm on $\mathbf{U}_K^*\mathbf{g}$, but the component Δf_i along the i-th principal axis of $\mathbf{G}\,\mathbf{G}^*$ is then divided by λ_i. If λ_i is very small, a very large error can result. The matrix is called "ill-conditionned". The trouble is that these large model errors corresponding to small data errors may be irrelevant if you go back to the unlinearized problem (see §3 above). Thus one is led to limit the variations of $\mathbf{m}$ which are allowed when $\mathbf{g}$ is modified. The way this is done can be understood in two ways.

a. Geometrical. Since the ill-conditionning means that a number of equations are almost linear combinations of one another, we can try ordering the equations in such a way that the vector defined on the left hand side makes a smaller and smaller angle with the space generated by the previous equations and stopping the system when a certain minimum angle is reached. The remaining equations can be considered as simple consistency conditions *in the range of errors* (see Figs. 1, 2, 3).

b. Algebraic. The Lanczos decomposition of a real matrix $\mathbf{G}$ is

$$\mathbf{G}=\mathbf{U}\mathbf{S}\mathbf{V}^T \tag{21}$$

where the $M \times M$ matrix $\mathbf{U}$ and the $N \times N$ matrix $\mathbf{V}$ are orthogonal $(\mathbf{U}^T\mathbf{U}=\mathbf{I}_M$, $\mathbf{V}^T\mathbf{V}=\mathbf{I}_N)$, the $M \times N$ matrix $\mathbf{S}$ is diagonal, with elements

$$|s_1| \geqq |s_2| \geqq \cdots \geqq |s_K|>0, \qquad s_{K+1}=\cdots=s_N=0.$$

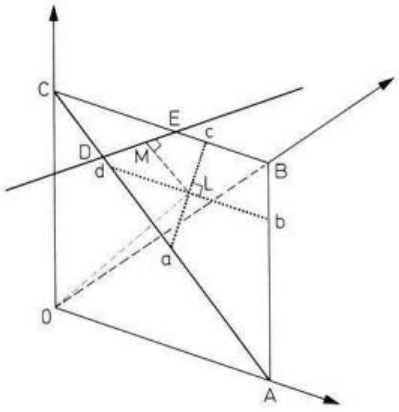

Fig. 1. *No error* (perspective). The whole plane ABC is the set of solutions of the problem $\mathbf{u} \cdot \mathbf{m} = u$. This set reduces to the triangle ABC if positivity constraints are added. The least norm solution is L. The quadrangle a, b, c, d gives an example of edgehogged set as obtained in §5.7.

The set of solutions of $\mathbf{u} \cdot \mathbf{m} = u$, $\mathbf{v} \cdot \mathbf{m} = v$ is the straight line DE (unconstrained) or the segment DE (constrained) and M is the least norm solution

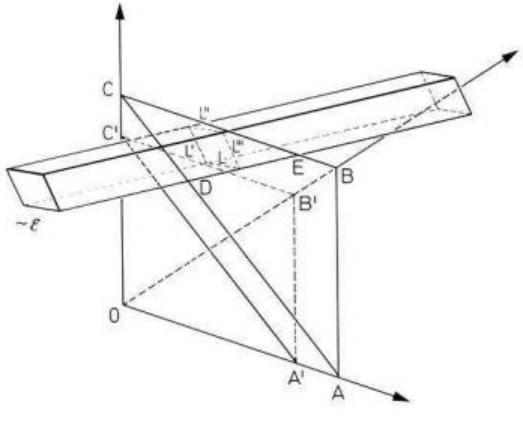

Fig. 2. *Errors, well conditioned* (perspective). The set of solutions of $\mathbf{u} \cdot \mathbf{m} = u \pm \varepsilon$, $\mathbf{v} \cdot \mathbf{m} = v \pm \varepsilon$ with a large angle **u**, **v**, is a tube (unconstrained) or its restriction to the positive cone (constrained)

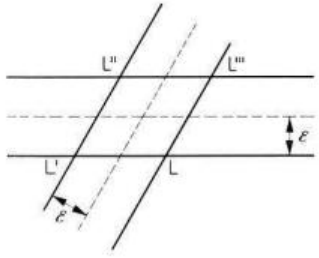

Fig. 3. *Errors, "well conditioned"* (cross section). The section is normal to DE of Figure 2

(Notice that $\mathbf{G}^{-}_{MP}$, according to the analysis above, is equal to $\mathbf{V}_K \mathbf{S}_K^{-1} \mathbf{U}_K^T$ or to $\mathbf{V}\mathbf{S}^{-}\mathbf{U}^T$, with $s_j^{-} = (s_j)^{-1}$ for $|s_j| > 0$, 0 for $s_j = 0$).

Now suppose the model **m** receives a small perturbation $\boldsymbol{\delta}\mathbf{m}$. $V^T \boldsymbol{\delta}\mathbf{m}$ has the same norm, and is related to the results by the equation

$$\delta_r \equiv \mathbf{U}^T \boldsymbol{\delta}\mathbf{g} = \mathbf{S}\mathbf{V}^T \boldsymbol{\delta}\mathbf{m} \equiv (\mathbf{s}/s_1)\, \boldsymbol{\delta}\mathbf{p} \equiv \mathbf{k}\, \boldsymbol{\delta}\mathbf{p} \tag{22}$$

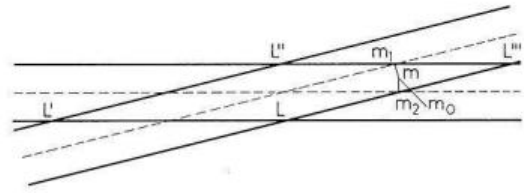

Fig. 4. *Errors "ill conditionned"* (cross section). The set of solutions of $\mathbf{u}\cdot\mathbf{m}=u\pm\varepsilon$, $\mathbf{v}\cdot\mathbf{m}=v\pm\varepsilon$, with small angle $\mathbf{u}$, $\mathbf{v}$, is a tube with a very large section. The Marquardt's solution m is so that $(mm_1)^2+(mm_2)^2+\mu^{-2}(mm_0)^2$ minimum

where the identities introduce new notation. Clearly the parameters of $\boldsymbol{\delta}\mathbf{m}$ that correspond to components of $\boldsymbol{\delta}\mathbf{p}$, such that the relevant eigenvalues are relatively small, have a relatively small effect the "results" (notice $\|\boldsymbol{\delta}\mathbf{r}\|=\|\boldsymbol{\delta}\mathbf{g}\|$). They are "*unimportant*". If the relevant eigenvalue is zero, they do not perturb the "result" at all. They are then "*irrelevant*". In inversion methods, one starts with an "initial" model $\mathbf{m}_0$ giving a fit $\mathbf{g}_0$, and $\boldsymbol{\delta}\mathbf{g}$ is primarily the shift of $\mathbf{g}$ from $\mathbf{g}_0$, and secondarily can be used to study errors ($\boldsymbol{\delta}\mathbf{e}$). By truncating at rank K as above, one suppresses the (infinite) effect of errors on "irrelevant" parameters. It remains to damp or to drop the effect on "unimportant" parameters. There are two current methods. In the *truncation method* (Hanson, 1971; Madden, 1972; Osborne, 1972; Varah, 1973), a "threshold" μ is chosen for the admissible values of k_i, and the values below μ. Clearly this approach is close to the geometrical one quoted above. In the Marquardt (1963) method, one minimizes

$$\|\boldsymbol{\delta}\mathbf{g}-\mathbf{G}\boldsymbol{\delta}\mathbf{m}\|^2+v^2\|\boldsymbol{\delta}\mathbf{m}\|^2, \tag{23}$$

where the "Marquardt parameter" v controls the size of $\boldsymbol{\delta}\mathbf{m}$. Both methods belong to a larger class of methods in which the parameters are controlled by replacing (22) by formulas of the type (θ being the well known Heaviside function)

$$\delta p_i=\theta(K-i)\,t_i\,\delta r_i/k_i. \tag{24}$$

Here t_i is, for instance, equal to $\theta(k_i-\mu)$ in the truncation method, and to $k_i^2[k_i^2+v^2/s_1^2]^{-1}$ in the Marquardt method (see Fig. 4). Thus the algebraic methods are able to deal with ill-conditionned problems, but clearly the "physical" justification of a precise damping is obscure and it is time to recall Lanczos remark (1961, p. 132), "*a lack of information cannot be remedied by any mathematical trickery*".

4.5. Stochastic Point of View

The stochastic point of view enables one to put a statistical content into the methods which deal with the errors. Physically, this means that if one trusts a certain statistical interpretation of errors, and ergodicity, the solutions can be classed according to ones degree of confidence. Fundamentally, one replaces the equation $\mathbf{G}\boldsymbol{\delta}\mathbf{m}-\boldsymbol{\delta}\mathbf{e}=\boldsymbol{\delta}\mathbf{g}$ by the equation:

$$\mathbf{G}\,\mathbf{p}_s+\mathbf{p}_n=\mathbf{p}_d \tag{25}$$

where $\mathbf{p}_s$ is a stochastic process describing the "signal", or "earth model", (and defined on the earth model space, $\mathbb{R}_N$, or L_2 in the continuous problem). $\mathbf{p}_n$ is the "noise process", describing errors on the data, $\mathbf{p}_d$ is the "data process". Both are defined on $\mathbb{R}_M$.

This way of looking at linear inverse problems is not very recent. Foster (1961) used the Wiener-Kolmogorov smoothing theory to determine the "optimum estimate" of the "signal" $\delta\mathbf{m}$ (our notation), and obtained a formula of the form appearing below. Twomey (1963), Strand and Westwater (1968) minimized $(\mathbf{G}\delta\mathbf{m}-\delta\mathbf{g})$ over a statistical ensemble, with similar results. Marquardt (1970) took into account the statistical distribution of errors to justify damping methods and obtained improved methods (e.g. "ridge regression"). Meanwhile, Backus and Gilbert (1970) took into account error statistics in a careful study of the various error terms (see the item on trade-off curves below). The same year, a very complete paper of Franklin on "well posed stochastic extensions of ill posed linear problems" gave a nice analysis of the question. Both papers were well adapted to the needs of geophysicists and have had many continuations (e.g. Jordan and Franklin, 1971; Jordan and Minster, 1972; Wiggins, 1972; Jackson, 1972, 1973). Stochastic processes appearing in Equation (25) are defined on real Hilbert spaces. A linear random process $\mathbf{p}_x$, which is defined on the real Hilbert space $\mathscr{H}$, is a linear functional mapping $\mathscr{H}$ into $\mathbb{R}$. Thus, it maps each element $\mathbf{h}$ of $\mathscr{H}$ into the random variable $\mathbf{p}_x\mathbf{h}$, whose mean $m_x(\mathbf{h})$ is equal to the expectation $E[\mathbf{p}_x\mathbf{h}]$. We can remove bias by subtracting from the processes their expectations, which are supposed to be known. Let us assume that this has been done from the beginning, so that $E[\mathbf{p}_x\mathbf{h}]=0$. The variance $\sigma_x^2(\mathbf{h})$ of $\mathbf{p}_x\mathbf{h}$ is the expectation of $(\mathbf{p}_x\mathbf{h})^2$, and thus is a positive quadratic form, which can be written as $\mathbf{h}\mathbf{C}_{xx}\mathbf{h}$, where $\mathbf{C}_{xx}$ is the autocorrelation of the process $\mathbf{p}_x$. Analogously, for 2 processes, $\mathbf{p}_x$ and $\mathbf{p}_y$, respectively defined over $\mathscr{H}$ and $\mathscr{K}$, there exists a linear mapping $\mathbf{C}_{xy}$ from $\mathscr{K}$ to $\mathscr{H}$. It is called the cross-correlation operator of $\mathbf{p}_x$ and $\mathbf{p}_y$, and is such that for any $\mathbf{h}$ of $\mathscr{H}$ any $\mathbf{k}$ of $\mathscr{K}$, the expectation of $(\mathbf{p}_x\mathbf{h})(\mathbf{p}_y\mathbf{k})$ is $\mathbf{h}\mathbf{C}_{xy}\mathbf{k}$ (evidently $\mathbf{C}_{xy}=\mathbf{C}_{yx}$). The process $\bar{\mathbf{p}}_s$ is said to be the best linear estimate of $\mathbf{p}_s$ if it minimizes the variance

$$\varepsilon^2(\mathbf{m})=E\{[(\mathbf{p}_s-\bar{\mathbf{p}}_s)\mathbf{m}]^2\} \quad \text{for all } \mathbf{m}\in\mathscr{C}.$$

Franklin (1970), assuming that the autocorrelation $\mathbf{C}_{dd}$ of the data is positive definite, was able to prove that $\bar{\mathbf{p}}_s$ is equal to $\mathbf{C}_{sd}(\mathbf{C}_{dd})^{-1}\mathbf{p}_d$. Besides, with the reasonably simple assumption that the signal and noise processes are uncorrelated, he calculated $\mathbf{C}_{sd}$ and $\mathbf{C}_{dd}$ in terms of $\mathbf{C}_{ss}$ and $\mathbf{C}_{nn}$, thus obtaining, as a best estimation, the inversion formula:

$$\delta\bar{\mathbf{m}}=\mathbf{C}_{ss}\mathbf{G}^*(\mathbf{G}\mathbf{C}_{ss}\mathbf{G}^*+\mathbf{C}_{nn})^{-1}\delta\bar{\mathbf{g}}. \tag{26}$$

4.6. Relations between Stochastic and Algebraic Points of View

a. If $\mathbf{C}_{nn}$ is zero, (26) defines a generalized inverse since it satisfies (15). By requiring $\|\mathbf{C}_{nn}\|$ to be small enough, one obtains a solution which is arbitrarily close to the one given by the generalized inverse.

b. The effect of non vanishing noise is to avoid the difficulties due to eigenvalues which are too small. One sees it easily in the case where $\mathbf{C}_{nn}$ is diagonal (data errors uncorrelated, with non zero variance). To be still more simple, assume that $\mathbf{p}_n$ and $\mathbf{p}_s$ are white, so that

$$\delta\bar{\mathbf{m}} = \mathbf{G}^*(\mathbf{G}\mathbf{G}^* + \sigma^2 \mathbf{I}_M)^{-1}\,\delta\mathbf{g}. \tag{27}$$

Then to the eigenvalues of $\mathbf{G}\mathbf{G}^*$ is added a constant σ^2 and the problem is regularized as in Marquardt's method. Solving $\mathbf{G}\delta\mathbf{m} - \delta\mathbf{e} = \delta\mathbf{g}$ in such a way that $\|\delta\mathbf{e}\|^2 + \sigma^2\|\delta\mathbf{m}\|^2$ be minimum would yield the same result and can be used by itself to define the regularization (Marquardt, 1963, 1970; Burkhard and Jackson, 1976). It remains to give an interpretation of $\mathbf{C}_{ss}$, which is arbitrary up to this point. Changing the vector basis so as to diagonalize $\mathbf{C}_{ss}$, and ordering the eigenvectors by decreasing smoothness, one can easily show (Jordan and Minster, 1972) that the eigenvalues (i.e. the variances), give rise to weight factors in expansions of $\delta\bar{\mathbf{m}}$ in terms of this basis. $\mathbf{C}_{ss}$ thus appears as a smoothing operator (Jordan, 1972).

c. Comparing Equations (26) and (9), we see that the rows of $\mathbf{C}_{ss}\,\mathbf{G}^*(\mathbf{G}\mathbf{C}_{ss}\mathbf{G}^*)^{-1}$ in the discrete problem play the same role as the Backus and Gilbert resolving kernels (Wiggins, 1972; Jackson, 1972). The smoothing or roughing effect of $\mathbf{C}_{ss}$ has therein an obvious geometrical interpretation (the δ function is the roughest of all possible kernels).

4.7. Trade-Off Curves

The Backus-Gilbert theory of linear estimation (1970) suggests that when noise is present, there exists a trade-off between the *ability to resolve detail* and the *reliability* of the estimate. Again we study the equation $\mathbf{G}\delta\mathbf{m} - \delta\mathbf{e} = \delta\mathbf{g}$, where δe is the noise in experimental results. We look for a best estimate $\overline{\delta\mathbf{m}}$ of the form $\overline{\delta\mathbf{m}} = \mathbf{C}^*_{ss}\mathbf{G}^*\mathbf{b}$, where $\mathbf{b}$ is to be determined. For any choice of $\mathbf{b}$, there is an *error of estimation*:

$$\varepsilon_1^2(\mathbf{b}) = (\delta\bar{\mathbf{m}} - \mathbf{C}^*_{ss}\mathbf{G}^*\mathbf{b})\,\mathbf{C}_{ss}^{-1}(\delta\bar{\mathbf{m}} - \mathbf{C}^*_{ss}\mathbf{G}^*\mathbf{b}). \tag{28}$$

There is a noise error, equal by definition to the variance of the projection of $\mathbf{p}_n$ onto $\mathbf{b}$

$$\varepsilon_2^2(\mathbf{b}) = \mathbf{b}\,\mathbf{C}_{nn}\,\mathbf{b}. \tag{29}$$

A weighted combination of these two errors is

$$\varepsilon^2(\theta, \mathbf{b}) = \varepsilon_1^2(\mathbf{b})\cos\theta + \varepsilon_2^2(\mathbf{b})\sin\theta.$$

Now, suppose we define $\mathbf{b}(\theta)$ so as to minimize $\varepsilon^2(\theta, \mathbf{b})$ over all the possible $\mathbf{b}$ and draw the graph of $\varepsilon_2^2(\theta, \mathbf{b}(\theta))$ vs $\varepsilon_1^2(\theta, \mathbf{b}(\theta))$. This graph is convex towards the origin and the point which is the closest to 0 is obtained for $\theta \sim \pi/4$, and corresponds to an inversion formula of the stochastic form. The two extreme points of the graph correspond respectively to a generalized inverse and to $\mathbf{b} = 0$.

4.8. Marginal Solutions and the Edgehog Method

Refinements of inversion formulas which yield the "best choice" of a solution must not make us forget Lanczös remark. It is essential to get an appraisal of the extent of the set of solutions and to class them according to some criteria, for instance the rms residual, $r \equiv M^{-\frac{1}{2}} \|\mathbf{g} - \mathbf{G}\mathbf{m}\|$, and the smoothness criterion $s \equiv N^{-\frac{1}{2}} \|m\|$, where the ordinary euclidian norms are meant (These criteria both appear in Equation (23) and, eventually, in stochastic inverses). Thus marginal solutions are those for which r and s are large. Extreme admissible solutions, or edge solutions, are those for which they reach a value (e.g. 1) beyond which the physicist decides to have no confidence at all in the models. Constructing the edge solutions, and using them to appraise the extent of solutions and to check linearization validity, is the "edgehog" method (Jackson, 1973). The limitations of this very interesting approach obviously reside in the arbitrariness of the constraints which have been imposed.

4.9. Linear Constraints

When direct physical measurements have been made (for example if one digs a hole), there are linear constraints on the admissible models. Complications which result from these additional equations can be disentangled by some linear algebra. (Burkhard and Jackson, 1976).

4.10. Applications

Most of the papers that have been quoted for the theoretical content also contain application. Among other recent applications are Gilbert et al. (1974), Johnson and Gilbert, (1974), Green, (1975), Crosson, (1976), Wiggins et al. (1976).

5. Lateral Constraints in Linear Inverse Problems

5.1. Fundamental Equations

We study the linear problem

$$\int_{\Omega} G_i(x) f^{(r)}(\mathbf{x}) \, d\mathbf{x} = m_i \quad i = 1, 2, \ldots, M; \qquad r = 1, 2, \ldots, R \tag{30}$$

with the non-negativity constraints

$$f^{(r)}(x) \geqq 0 \tag{31}$$

and, in most cases, the uniform bound $f^{(r)}(x) \leqq C$. Actually, as we can see n examples, linear inverse problems with lateral constraints can always be reduced

to this canonical form (30, 31). For example, if we study the problem which is made up of Equation (30) and the constraints $0 \leqq f^{(r)}(\mathbf{x}) \leqq g(\mathbf{x})$, we can replace it, using slack parameters, by the following system:

$$\begin{aligned} &\int_{\Omega} G_i(\mathbf{x}) f^{(r)}(\mathbf{x})\, d\mathbf{x} = m_i \quad i=1,\ldots,M, \qquad r=1,\ldots,R \\ &f^{(r)}(\mathbf{x}) + f^{(r+R)}(\mathbf{x}) = g(\mathbf{x}) \\ &f^{(r)}(\mathbf{x}) \geqq 0 \qquad r=1,\ldots,2R \end{aligned} \tag{32}$$

which is obviously in the canonical form. For constraints like $g(\mathbf{x}) \leqq f^{(r)}(\mathbf{x}) \leqq h(\mathbf{x})$, it suffices to consider the functions $(f^{(r)}(\mathbf{x}) - g(\mathbf{x}))$, and to use the reduction which is given above. Proximity constraints, like $|f^{(r)}(\mathbf{x}) - f_0^{(r)}(\mathbf{x})| \leqq \Delta(\mathbf{x})$, can be reduced in the same way.

5.2. *Description of the Set of Solutions*

Problems like (30) and (31) are not linear problems but convex problems. In the following, for the sake of simplicity, we assume that $R=1$ and drop the superscript. The "convex" property means that if $f_1(\mathbf{x})$ and $f_2(\mathbf{x})$ are solutions of (30) and (31), then, for any $0 \leqq \lambda \leqq 1$, $\lambda f_1(\mathbf{x}) + (1-\lambda) f_2(\mathbf{x})$ is a solution. A simple example of a convex set is a triangle. Now it is clear that everybody labels a triangle by naming its 3 vertices. But what is a vertex? Let us identify a point with its coordinates. A vertex f clearly is a point of the triangle which cannot be equal to a convex combination $\lambda f_1 + (1-\lambda) f_2$ of two other points of the triangle with $0 < \lambda < 1$ unless $f_1 = f_2 = f$. This is called an "extremal point" of a convex set. One sees that every point f in a triangle is a linear convex combination of its extremals: if f_1, f_2, f_3 are the 3 vertices,

$$\begin{aligned} &f = \lambda_1 f_1 + \lambda_2 f_2 + \lambda_3 f_3 \\ &\lambda_1 + \lambda_2 + \lambda_3 = 1 \qquad \lambda_1, \lambda_2, \lambda_3 \geqq 0. \end{aligned} \tag{33}$$

Remarkably, this property is much more general: any convex compact set can be completely described as the set of all convex linear combinations of its extremals (the Krein-Milman theorem). For unbounded sets in $\mathbb{R}_N$ there are analogous results taking into account extremal directions.

Describing the set of solutions of (30) and (31) thus involves 2 steps, checking that the above theorems apply, and finding the extremals. Take for instance the following simple problem:

$$\int_0^1 f(x)\, dx = 1; \qquad \int_0^1 x f(x)\, dx = v \tag{34}$$

where the non negative function $f(x)$ is sought in the class of integrable functions. The extremals of (34) are the generalized functions:

$$\left.\begin{aligned} \delta_{a,b}(x) = \frac{b-v}{b-a}\delta(x-a) + \frac{v-a}{b-a}\delta(x-b) \\ 0 \leqq a < v \qquad v < b \leqq 1 \end{aligned}\right\} \text{ and } \quad \delta(x-v). \tag{35}$$

It is not difficult (Sabatier, 1976a) to directly identify the set of solutions of (34) with the set of linear combinations of $\delta_{a,b}(x)$, so that the general solution is

$$f(x)=\iint_{\substack{a=0,b=v\\ a=v,b=1}}\lambda(a,b)\left[\frac{b-v}{b-a}\delta(x-a)+\frac{v-a}{b-a}\delta(x-b)\right]da\,db \tag{36}$$

where $\lambda(a,b)$ is arbitrarily chosen except for the conditions

$$\lambda(a,b)\geqq 0;\qquad \iint_{\substack{a=0,b=v\\ a=v,b=1}}\lambda(a,b)\,da\,db=1. \tag{37}$$

We notice that the extremals are made up of two δ-functions which are situated in 2 well-defined simple intervals. In the general case, for M continuous kernels $G_i(\mathbf{x})$, extremals are combinations of M δ-functions, but these δ-functions are not any longer situated in M simple intervals. However, if the functions $G_i(\mathbf{x})$ are nice enough, (e.g. gravity problem), the sets in which the δ functions move are still made up of a finite number of intervals.

Describing the set of solutions by means of its extremals is a complete "description" from the mathematical point of view, but, as we have seen in §4, many physicists first want to get a "best solution", for whatever meaning the word "best" has there. Clearly, this leads one to look for the solution for which a certain functional is minimum. If this functional is linear, one obtains the following standard form of the problem:

Find $f(x)\geqq 0$, and $\operatorname{Min} z$, such that

$$\begin{cases}\int_{\Omega} G_i(\mathbf{x})\,f(\mathbf{x})\,d\mathbf{x}=m_i \qquad i=1,2,\ldots,M\\ \int_{\Omega} C(\mathbf{x})\,f(\mathbf{x})\,d\mathbf{x}=z.\end{cases} \tag{38}$$

This form is obviously obtained if one seeks the model $f(\mathbf{x})$ of minimum norm $\int_{\Omega} w(\mathbf{x})\,f(\mathbf{x})\,d\mathbf{x}$, where $w(\mathbf{x})$ is a (non-negative) weight function. It is also obtained if one wants to minimize the distance

$$\operatorname*{Sup}_{x\in\Omega}|w(\mathbf{x})(f(\mathbf{x})-f^{(0)}(\mathbf{x}))|,$$

where $f^{(0)}(\mathbf{x})$ is an "initial" model. One has then to find non negative $f(\mathbf{x})$, $g(\mathbf{x})$, $h(\mathbf{x})$, α, and one has to find $\operatorname{Min} z$ (over all possible functions and parameters) such that

$$\left.\begin{aligned} &w(\mathbf{x})(f(\mathbf{x})-f^{(0)}(\mathbf{x}))+g(\mathbf{x})=\alpha\\ &w(\mathbf{x})(f(\mathbf{x})-f^{(0)}(\mathbf{x}))-h(\mathbf{x})=\alpha\end{aligned}\right\} \tag{39}$$

$$\int_{\Omega} G_i(\mathbf{x})\,f(\mathbf{x})\,d\mathbf{x}=m_i;\qquad z=\alpha.$$

Intermediate criteria in which a certain linear convex combination

$[\lambda\int_{\Omega} w(\mathbf{x})\,f(\mathbf{x})\,d\mathbf{x}+(1-\lambda)\operatorname{Sup}|\ |]$, is minimized, can also be dealt with.

Needless to say, one could also decide to minimize a quadratic form, but the semi linear character of the problem would disappear.

The absolute effect of experimental errors is studied in equations which can be reduced to the forms (30–31) or (38). Indeed, one simply has to replace (30) by

$$\left|\int_{\Omega} G_i(\mathbf{x})\, f(\mathbf{x})\, d\mathbf{x} - m_i\right| < \Delta_i,$$

or equivalently by

$$\left.\begin{aligned} \int_{\Omega} G_i(\mathbf{x})\, f(\mathbf{x})\, d\mathbf{x} - \gamma_i &= m_i - \Delta_i \\ \int_{\Omega} G_i(\mathbf{x})\, f(\mathbf{x})\, d\mathbf{x} + \delta_i &= m_i + \Delta_i \end{aligned}\right\} \qquad \text{(30 bis)}$$

where the slack variables γ_i and δ_i have to be non-negative.

In any case, because of the infinity of extremals, it is difficult to study this problem, and we had better to discretize it.

5.3. *Discretization*

With a discretization of step-size h, and obvious notations, the Equations (38) are replaced by

$$\sum_{k=1}^{N} G_{ik} f_k = m_i \qquad i = 1, \ldots, M \qquad \text{(40a)}$$

$$\sum_{k=1}^{N} C_k f_k = \alpha. \qquad \text{(40b)}$$

The problem itself is unchanged. Simply, you are now looking for its solutions in a special class (see §4). The extremals of the set of solutions of (40a) are vectors $\{f_n\}$ with *at most* M components different from zero. Clearly, when h goes to zero, each extremal looks more and more like a set of M δ-functions. Suppose the functions $G_i(x)$ are such that the δ functions in almost all the limit extremals can be uniquely identified for all step-sizes smaller than a given h, and that for all smaller step sizes you can also identify the sets of intervals for which these δ functions will have their support. In this case going beyond h only refine the end points of each interval, and the "δ-ness" of the extremal components. At this point, nothing but trivial additional information can be obtained by still reducing h. One can say we have "saturated" our ability to obtain information from the result – clearly this fact justifies the studies of this kind of problem with finite discretization steps. Besides, the Krein-Milman theorem fully applies to the set of solutions obtained in a discretized problem, so that its extremals and extremal directions again completely characterize it. However in real computations on experimental results this step size is usually too small to have a direct practical application. In artificial examples the methods works. In other words, in real examples it is hopeless to try to describe *all* possible solutions.

For a given discretization, all the extremals of (40a) can be obtained through *finite* algorithms described under the general label "linear programming". There are ways to manage this research and reduce the step size of discretization, by using the preliminary information of a Backus Gilbert method

to save time, the approach to saturation being recognized by a characteristic evolution of most extremals (Sabatier, 1976a). But obtaining all extremals is in real problems *much too complicated*, even with $N \sim M$, because there are just too many. Fortunately, the geophysicist is already happy if he can recognize his "best" solution, appraise the errors and the spread of possible solutions. As we see now, all these "theoretical measurements" are easily done.

5.4. *Theoretical Measurements of the Set*

We give here several examples, some of them are not in Sabatier (1976a, b), and all of which reduce to the standard forms. Thus they can be solved by "linear programming". Let us notice at this point, for the reader who is not familiar with these techniques, that the solution of (40) is a *particular extremal* of (40a). It is obtained rapidly by well-known algorithms. Experience shows that, with modern programs, the computation time depends essentially on M. Admittedly, slack variables increase M, but it usually is possible to "reduce" their number in the algorithms that are used for computations. For the sake of clarity, we do not present these algorithms here and keep the standard form (39). We now proceed with examples:

a. "*Best fit*". Determining the solution $f_1(x)$ which is the closest to an initial function $f^{(0)}(x)$ (not necessarily satisfying the constraints), for a certain weighted absolute norm, means minimizing $\mathrm{Sup}\,|w(x)(f(x)-f^{(0)}(x)|$. Discretizing (39) readily yields equations that are solvable by "linear programming". That the solution is an extremal means that, out of the $3N$ numbers f_n, g_n, h_n, only $2N+M$ are $\neq 0$. Thus the best fit $\{\bar{f}_n\}$ reaches one of the values 0 or $(f_n^{(0)}+\alpha)$ or $(f_n^{(0)}-\alpha)$ for $N-M$ values of n. Min α is the desired smallest distance.

b. Incidence of Absolute Errors. It can be studied by everywhere replacing Equation (30) by the Equation (30 bis) (in § 5.2) (minimizing, if any, will be done also over these additional slack variables). The effect of the errors on the set of extremals (Sabatier, 1976a) is usually small (displacements and progressive deformation); introducing constraints is usually a regularization factor (see Fig. 4). In certain cases only, the problems with non vanishing errors lead to sets of extremals, and thus sets of solutions, that really differ from those without errors. Because of this there can result instabilities in solutions defined through certain rules (e.g. a defined weighted average of extremals). Other instabilities can come from ill-conditioning of the matrix $\{G_{ik}\}$, certain equations being almost linearly dependent on the others. One can regularize the system by truncation (this is understood and done as in § 4.4, geometrical and algebraic points of view). One can also obtain a regularized solution by minimizing

$$\operatorname*{Sup}_{\substack{i=1,\ldots,M \\ \mathbf{x}\in\Omega}} \left\{ w_i \left| m_i - \int_{\Omega} G_i(\mathbf{x}) f(\mathbf{x})\, d\mathbf{x} \right|,\ v^2 \bar{w}(\mathbf{x}) |f(\mathbf{x}) - f^{(0)}(\mathbf{x})| \right\}: \tag{41}$$

The weights w_i can be chosen as a function of the error margin and the weight function $\bar{w}(\mathbf{x})$ as a function of the a priori confidence in the "a priori model $f^{(0)}(x)$. v^2 is a convenient control of the regularisation. This corresponds

in our linear convex problem to the Marquardt method of § 4.4 (L^2 norms can be treated by convex programming but not quite so simply). The discretized problem reads: find non-negative numbers $\{f_k\}$, $\{\alpha_i\}$, $\{\beta_i\}$, $\{\gamma_i\}$, $\{\delta_i\}$, α, and Min z such that $z=\alpha$ and

$$w_i\left[\sum_{k=1}^{N} G_{ik} f_k - m_i\right] - \alpha_i = -\alpha \qquad i=1, \ldots, M$$

$$w_i\left[\sum_{k=1}^{N} G_{ik} f_k - m_i\right] + \beta_i = \alpha$$

$$v^2 \bar{w}_n [f_n - f_n^{(0)}] - \gamma_n = -\alpha$$

$$v^2 \bar{w}_n [f_n - f_n^{(0)}] + \delta_n = \alpha.$$

Notice finally that when errors are taken into account, one can consider the analysis as "saturated" as soon as the gain of information when h is decreased goes neatly under the threshold of errors.

c. Stability is sometimes meant by experimentalists to be the absence of strong oscillations in the interpolation, due to the model, between experimental points. Suppose measurements are made at integer points i on a line and $G_i(\mathbf{x})$ is the value for $h=i$ of a continuous function $G(h, \mathbf{x})$. Then, a measure of this "statility" is

$$\operatorname*{Sup}_{i,\, \lambda \in (0,1)} \left| \int_{\Omega} G_{\lambda i + (1-\lambda)(i+1)}(\mathbf{x}) f(\mathbf{x})\, d\mathbf{x} - \lambda m_i - (1-\lambda) m_{i+1} \right|$$

where λ can be separately discretized. This can be taken into account to select a model. If measurements are on a surface, the same is done with a triangular covering between measurements.

d. Moments. Linear measurements of the set, e.g. $X(f)=\int_{\Omega} \alpha(\mathbf{x}) f(\mathbf{x})\, d\mathbf{x}$, can be called "moments". All points $Z(f)$ whose coordinates are moments (e.g. $X(f)$ and $Y(f)$) belong to a convex set (here in the plane X, Y). The diagrams which are thus obtained often give a fairly good idea of the uncertainties. Plane diagrams are the simplest, but vectorial diagrams, or three dimensional diagrams, can be obtained in the same way (Sabatier, 1976b). Diagrams of obvious physical interest are obtained from the mass $\int_{\Omega} f(\mathbf{x})\, d\mathbf{x}$ and the "first" moments $\int_{\Omega} \mathbf{x} f(\mathbf{x})\, d\mathbf{x}$. They show the uncertainty on the center-of-mass of the models.

e. "*Edgehog with Hard Constraints*". Since, in real cases, it is hopeless to obtain all the extremals, we can limit our study to obtaining a set of particular interest for the problem we consider, and which already gives an idea of the set of solutions. One can imagine many methods (drawing orthogonal directions through the "best" solution, etc. ...). Here we only suggest a curious method which is particularly simple (i) when the Moore Penrose inverse solution f^{MP} (or the Backus Gilbert solution) has been obtained and turns out to be non negative; (ii) for a discretization with N not very much larger that M and already close to saturation. Then the general solution of the unconstrained problem is

$f = f^{MP} + \sum_{1}^{N-M} \mu_j \phi_j$, where $\phi_1, \ldots, \phi_{N-M}$, are $N-M$ orthonormal vectors spanning the orthogonal complement in $\mathbb{R}_N$ of the image $R(\mathbf{G}^*)$ of $\mathbf{G}^*$. Successively considering the solutions of the particular form $f - f^{(0)} = \lambda_i \phi_i$, we can determine the non negative values λ_i^s and $-\lambda_i^I$ such that f is non negative for $\lambda_i \in (-\lambda_i^I, \lambda_i^s)$. The $2(N-M)$ values of f thus obtained belong to the boundary set of solutions (although they are not necessarily extremal points – see Fig. 1, the quadrangle abcd). They define an "edgehogged" subset of the convex set of solutions.

5.5. *Ideal Bodies*

In convex problems, it is sound to look for all kinds of "extreme" solutions. Among them, Parker's ideal body (Parker, 1974) is the one whose supremum is the smallest of all supremums of all solutions of the problem. Thus we have to find non negative functions $f(\mathbf{x})$(or f_k) and $\phi(\mathbf{x})$(or ϕ_k), and Min α such that

$$\begin{aligned} &\int_{\Omega} G_i(\mathbf{x}) f(\mathbf{x})\, dx \left(\text{or } \sum_{k=1}^{N} G_{ik} f_k \right) = m_i \\ &f(\mathbf{x}) + \phi(\mathbf{x}) \,(\text{or } f_k + \phi_k) = \alpha. \end{aligned} \tag{4.2}$$

Here the discretized forms are in the parentheses. In the discretized problems there are $(2N+1)$ unknowns (including α), and $N+M$ equations. Necessarily $N-M+1$ unknowns are zero. α cannot vanish unless the problem is trivial. Thus $(N-M+1)$ zeros are to be taken among the f_k's or the ϕ_k's. In other words, f_k has to be either 0 or α except on $(M-1)$ domains Ω_k. When the discretization step goes to zero, one sees that the function $f(\mathbf{x})$ takes only two values, 0 or α, except on a set of zero measure. It remains to prove that there exists a limit form and to study its uniqueness. It has been proved by Sabatier (1976b) that there exist limit forms, but that the ideal body is unique only with stronger assumptions on the G_i's. These assumptions are verified in the case of gravity functionals. Hence Parker's ideal body exists, is unique, and can be constructed by linear programming for an arbitrary set of gravity measurements.

5.6. *The Stochastic Point of View*

The statistical distribution of errors induces a statistical distribution of *sets* of solutions which is easy to describe as long as deformations are not too strong (Sabatier, 1976b).

The stochastic point of view may be studied in the presence of lateral constraints by considering a signal process with values in the positive cone of $\mathbb{R}_N$ instead of $\mathbb{R}_N$. If this is not done, one takes into account in $\mathbf{p}_s$ unphysical models, and certain correlation matrices in (26) may lead to them. If it was done the estimation thus obtained, and its dispersion would be more physical, since it would take a priori information into better account. More refined a priori information can also be easily introduced with the help of information theory (E.T. Jaynes, 1957). Arguments saying that best estimations automatically produce formulas like (26), and thus Marquardt's regularization, are not quite correct, since they depend on some arbitrary statistical assumptions. With others, it is probably

possible to justify other kinds of regularizations. In any case, introducing a priori constraints in an estimation is probably not difficult. During the colloquium, Professor Jackson kindly pointed out to us that in the one-dimensional case, if we assume that the random variable x is constrained to lie in $(0, T)$, and a measurement is made, which is contaminated by a random gaussian error of variance σ^2, then the probability density function $p(x)$ of x conditional on the estimate $\hat{x}$ is given by:

$$p(x)=\begin{cases} g(x-\hat{x}, \sigma) \Big/ \int_0^T g(x-\hat{x}, \sigma) & \text{for } x \in (0, T) \\ 0 & \text{for } x \notin (0, T). \end{cases}$$

One has made the assumption that the a priori density of x is uniform on $(0, T)$, and $g(r, \sigma)$ is $\exp[-\frac{1}{2}r^2/\sigma^2]$. Thus, if acceptability conditions are defined by a lower bound on p, either the hard constraints are weaker than the lower bound and then the acceptability conditions are "attracted" towards the hard constraints, or the hard constraints are much stronger and one can forget about statistics. The effect is probably qualitatively similar in multidimensional problems. Taking into account constraints in the statistics obviously is necessary when there are choices of $\mathbf{C}_{ss}$ for which the formula (26) yields models violating the constraints.

5.7. *Applications*

Theoretical results in the linear problems with lateral constraints are recent, and applications are still more recent. We recall papers on ideal bodies by Parker (1974, 1975), on the method described here and its theoretical applications by Sabatier (1976) ab. We quote for practical applications Safon Vasseur and Cuer (1976c).

6. Concluding Remarks

Introducing lateral constraints leads us to problems in which linear combinations are replaced by linear convex combinations. From the purely mathematical point of view, the increased complication is balanced by the fact that most constrained problems are bounded.

From the computational point of view, the algorithms which are used in the constrained cases (linear programming) are as efficient and well-known as the others. Regularization is easy in both kinds of problems, and is not so often necessary in constrained problems. The stochastic point of view has not been very much studied as yet in the constrained problems but we do not think it is much more complicated than in the others. Clearly, if the constraints are very far from the solutions of interest, there is no essential need for the approach of § 5. But if they are close to the solutions, the geophysicist should not be afraid to use inversion techniques which definitely take the constraints into account, and which are more general, although not more difficult, than the ones with which he usually deals.

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References

Aki, K., Ware, J.A.: Continuous and discrete inverse-scattering problems in a stratified elastic medium. J. Acoust. Soc. Am. **45**, 911–921, 1969

Anderssen, R.S.: On the linearisation of geophysical inversion problems. Preprint Computer Centre, Australian National University 1975a

Anderssen, R.S.: On the inversion of global electromagnetic induction data. Phys. Earth Planet. Interiors (Netherlands) **10**, 292–298, 1975b

Backus, G.E., Gilbert, F.J.: Numerical applications of a formalism for geophysical Inverse Problems. Geophys. J.R. Astr. Soc. **13**, 247–276, 1967

Backus, G., Gilbert, F.: The resolving power of gross earth data. Geophys. J.R. Astr. Soc. **16**, 169–205, 1968

Backus, G., Gilbert, F.: Uniqueness in the inversion of inaccurate gross earth data. Phil. Trans. Roy. Soc. London **266**, 123–192, 1970

Backus, G.: Inference from inadequate and inaccurate data, I. Proceedings of the National Academy of Sci. **65**, 1, 1–7, 1970

Backus, G.: Inference from inadequate and inaccurate data, II. Proceedings of the National Academy of Sciences **65**, 2, 281–287, 1970b

Backus, G.: Inference from inadequate and inaccurate data, III. Proceedings of the National Academy of Sciences **67**, 1, 282–289, 1970c

Bailey, R.C.: Inversion of the geomagnetic induction problem. Proc. Roy. Soc., London **A 315**, 185–194, 1970

Barcilon, V.: A discrete model of the inverse Love wave problem. Geophys. J.R. Astr. Soc. **44**, 61–76, 1976

Burkhard, N., Jackson, D.D.: Application of stabilized linear inverse theory to gravity data. J. Geophys. Res. **81**, 8, 1513–1518, 1976

Chadan, K., Sabatier, P.C.: Inverse problems of quantum scattering theory. To be published by Springer Berlin-Heidelberg-New York: 1977

Crosson, R.S.: Crustal structure modeling of earthquake data I – Simultaneous least squares estimation of hypocenter and velocity parameters. J. Geophys. Res. **81**, 17, 3036–3046, 1976

Ducruix, J., LeMouel, J.L., Courtillot, V.: Continuation of three-dimensional potential fields measured on an uneven surface. Geophys. J.R. Astr. Soc. **38**, 299–314, 1974

Foster, M.: An application of the Wiener-Kolmogorov smoothing theory to matrix inversion. J. Soc. Indust. Appl. Math. **9**, 3, 387–392, 1961

Franklin, J.N.: Well-posed stochastic extensions of ill-posed linear problems. J. Math. Anal. and Applications **31**, 682–716, 1970

Gilbert, F., Dziewonski, A., Brune, J.: An informative solution to a seismological inverse problem. Proc. Natl. Acad. Sci. USA **70**, 1410–1413, 1973

Gerver, M., Markushevich, V.: Determination of a seismic wave velocity from the traveltime curve. Geophys. J.R. Astr. Soc. **11**, 165–173, 1966

Gerver, M.L., Markushevich, V.M.: On the characteristic properties of travel-time curves. Geophys. J.R. Astr. Soc. **13**, 241–146, 1967

Green, W.R.: Inversion of gravity profiles by use of a Backus-Gilbert approach. Geophysics **40**, 5, 763–772, 1975

Hanson, R.J.: A numerical method for solving Fredholm integral equations of the first kind using singular values. Siam Y. Num. An. **8**, 616–622, 1971

Jackson, D.D.: Interpretation of inaccurate, insufficient and inconsistent data. Geophys. J. R. Astr. Soc. **28**, 97–110, 1972

Jackson, D.D.: Marginal solutions to quasi-linear inverse problems in geophysics: the Edgehog method. Geophys. J.R. Astr. Soc. **35**, 121–135, 1973

Jaynes, E.T.: Information theory and statistical mechanics. Phys. Rev. **106**, 620–630, 1957

Johnson, L.E., Gilbert, F.: Inversion and inference for teleseismic ray data. Institute of Geophysics and Planetary Physics, University of California, San Diego, 1971

Jordan, T.H., Franklin, J.N.: Optimal solutions to a linear inverse problem in geophysics. Proceedings of the National Academy of Sciences. **68**, 2, 291–293, 1971

Jordan, T.H., Minster, J.B.: Application of a stochastic inverse to the geophysical inverse problem. Contribution no: 2036, Geological and Planetary Sci., California Institute of Technology, Pasadena, California

Jupp, D.L.B., Vozoff, K.: Stable iterative methods for the inversion of geophysical data. Geophys. J.R. Astr. Soc. **42**, 957–976, 1975

Kennett, B.L.N.: A comparison of travel-time inversions. Geophys. J.R. Astr. Soc. **44**, 517–536, 1976

Knopoff, L.: Green's function for eigenvalue problems and the inversion of Love wave dispersion data. Geophys. J.R. Astr. Soc. 161–173, 1961

Knopoff, L.: Higher order Born Approximations for the inversion of Love wave dispersion. Geophys. J.R. Astr. Soc. **7**, 2, 149–157, 1962

Lanczos, C.: Linear differential operators. New York: Van Nostrand 1961

Marquardt, D.W.: An algorithm for least-squares estimation of nonlinear parameters. J. Soc. Ind. Appl. Math. **11**, 431–441, 1963

Marquardt, D.W.: Generalized inverses, ridge regression, biased linear estimation, and nonlinear estimation. Technometrics **12**, 3, 591–612, 1970

Osborne, M.R.: A class of methods for minimizing a sum of squares. Aust. Com. J. **4**, 164–169, 1972

Parker, R.L.: The inverse problem of electrical conductivity in the mantle. Geophys. J.R. Astr. Soc. **22**, 121–138, 1970

Parker, R.L.: Best bounds on density and depth from gravity data. Geophysics **39**, 5, 644–649, 1974

Parker, R.L.: The theory of ideal bodies for gravity interpretation. Geophys. J.R. Astr. Soc. **42**, 315–334, 1975

Penrose, R.: A generalized inverse for matrices. Proc. Cambridge Phil. Soc. **51**, 406–413, 1955

Rao, C.R., Mitra, S.K.: Generalized inverse of matrices and its applications. New York: Wiley & Sons 1971

Sabatier, P.C.: Comparative evolution of the inverse problems. Mathematics of Profile Inversion NASA TMX 62, 1972

Sabatier, P.C.: Problème direct et inverse de diffraction d'une onde élastique par une zone perturbée sphérique. I et Compléments. C.R. Acad. Sci. Paris **278**, 545–547 and 603–606, 1974a

Sabatier, P.C.: Remarks on approximate methods in geophysical inverse problems. Proc. Roy. Soc., London **A337**, 49–71, 1974b

Sabatier, P.C.: Positivity constraints in linear inverse problems I general theory. Preprint Montpellier PM/75/18, to be published in Geophys. J.R. Astr. Soc. 1976a (accepted for publ.)

Sabatier, P.C.: Positivity constraints in linear inverse problems II. Applications. Preprint Montpellier PM/75/18 to be published in Geophys. J.R. Astr. Soc. 1976b (accepted for publ.)

Safon, C., Vasseur, G., Cuer, M.: Some applications of linear programming to the inverse gravity problem. (submitted for publication in Geophysics 1976)

Smith, M.L., Franklin, J.N.: Geophysical application of generalized inverse theory. J. Geophys. Res. **74**, 10, 2783–2785, 1969

Strand, O.N., Westwater, E.R.:

(a) Minimum rms estimation of the numerical solution of a Fredholm integral equation of the 1st kind. Siam Y. Num. An. **5**, 287–295, 1968

(b) Statistical estimation of the numerical solution of a Fredholm integral equation of the 1st kind. J. Ass. Comp. Mech. **15**, 100–114, 1968

Twomey, S.: The application of numerical filtering to the solution of integral equations encountered in indirect sensing measurements. J. Franklin Inst. **279**, 95–109, 1965

Varah, J.H.: On the numerical solution of ill-conditionned linear systems with applications to ill-posed problems. Siam J. Num. Anal. **10**, 257–287, 1973

Weidelt, P.: The inverse problem of geomagnetic induction. Z. Geophys **38**, 257–289, 1972

Wiggins, R.A.: The general linear inverse problems: implication of surface waves and free oscillations for earth structure. Rev. Geophys. Space Phys. **10**, 251–285, 1972

Wiggins, R.A., Larner, K.L., Wisecup, R.D.: Residual statics analysis as a general linear inverse problem. Preprint Western Geoph. C^0 Houston 1976

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