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Geophysical Data Analysis: Understanding Inverse Problem Theory and Practice

Max A. Meju

Course Notes Series, No. 6
S. N. Domenico, Editor



Society of Exploration Geophysicists

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Meju, Max A., 1959—
Geophysical data analysis / Max A. Meju.
p. cm. — (Course notes series; v. 6)
Includes bibliographical references.
ISBN 1-56080-027-5 : \$25.00
1. Geophysics—Observation. 2. Geophysics—Technique.
3. Numerical analysis. 4. Inverse problems (Differential equations)—
Numerical solutions. I. Title. II. Series.
QC802.A1M45 1994
550—dc20

ISBN 0-931830-48-6 (Series)
ISBN 1-56080-027-5 (Volume)

Society of Exploration Geophysicists
P.O. Box 702740
Tulsa, Oklahoma 74170-2740

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Published 1994

Reprinted 1998, 2001

Printed in the United States of America

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Preface

Geophysical data analysis is a very practical subject and this book is intended to be a simple guide to techniques of parameter estimation and error analysis. I have placed emphasis on the reconciliation of theory and practical data to enable the reader understand how to tackle typical problems in data analysis. It is hoped that a mastery of the simple techniques described in this book will inspire confidence in the reader to consult the more classical treatment of the subject. It is pertinent to mention that this book developed out of a highly successful course of the same title given to senior undergraduate geophysics students in Leicester University since 1988 and its popularity stems from the structured learning programs and the simple effective practical approach to geophysical inversion. The course is given in the first semester to provide the students with the basic tools for quantitative analysis of geoscientific data and consists of 10 lectures and practical sessions involving the materials given in Chapters 1 to 9 in this book. Chapter 10 derives from topical issues of research interest to me and my induction courses for postgraduate students in geophysics and the industry. The contents of this book are easily digestible and require little statistical or mathematical commitment.

Max Meju
Leicester, 1994

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INTRODUCTION

1.1 Basic Concepts and Definitions.

In the geophysical and related sciences, experiments are usually performed under controlled conditions (i.e., in a systematic manner), and the outcome may be numerical values that represent our observations at fixed (or predetermined) intervals, say. These observations of some properties of the physical world are commonly referred to as the EXPERIMENTAL or OBSERVATIONAL DATA. Since such a set of data is systematically collected, there must be some way of explaining or coordinating them. To draw any inferences from these data, we need to understand the relationship between the distribution of the properties of the physical system under study (e.g, the Earth) and the observable geophysical responses. The system of equations that describe this relationship constitute the FORWARD THEORY. Inference of the properties of the physical system from observational data is the opposite procedure and we need to apply some quantitative tools collectively referred to as the INVERSE THEORY.

Inverse theory is an organised set of mathematical and statistical techniques (calculus, matrix algebra, statistical estimation and inference, etc) for retrieving useful information about a physical system (or the physical world) from controlled observations on the system. It is directly concerned with the analysis of experimental data, the fitting of mathematical models to these data by estimating the unknown parameters of the models, and optimal experimental design. Inverse theory is practiced by every scientist that analyses data relating to the physical world which in the case of geoscientists is the Earth. As a matter of fact, anyone that has fitted a line to a set of numerical data has practised inverse theory. The level of application of inverse theory may range from the simple straight-line fitting of seismic refraction data, say to the more sophisticated acoustic tomography or multi-dimensional resistivity curve matching. This course will emphasise the analysis of geoscientific data, but it should be noted that the underlying data analysis procedures are the same as those of many other specialist areas eventhough a variety of terms is used to describe the subject in the different spheres of application (e.g., optimisation theory in the mathematical sciences, tomography in the medical sciences, control theory in engineering, and decision theory in management sciences). Some of the areas in which inverse theory finds applications are itemised below.

1.1.1 Examples of problems in which inverse theory is used.

1. Curve fitting.
2. Image enhancement: digital filter design and deconvolution of seismograms.
3. Determination of earth structure and estimation of parameters of ore deposits and energy resource accumulations from geophysical observations.
4. Determination of earthquake location using wave arrival times.
5. Modelling of lithosphere's response to loading or strain rate variations in sedimentary basins.
6. Well (pump) test analysis in hydrogeology.
7. Factor analysis in geology.
8. Geochronological determinations using geomagnetic reversals data.
9. Satellite navigation.
10. Optimal control of engineering systems.
11. Medical tomography.
12. Decision making/Operational research in management and mineral economics.

However, our discussions will be limited to inverse theory and its applications in geophysical exploration of the subsurface properties of the Earth. In all the following discussions, it will be assumed that a forward theory exists for any particular problem. The types of geophysical processes or Earth-systems of particular interest to us are itemised below.

1.1.2 Geophysical Processes and Systems

Seismic or electromagnetic wave propagation through the earth and current or fluid flow in (porous) rocks are examples of geophysical processes. The Earth may be described in terms of its physical property distributions which define various physical systems that may be investigated by observing say, wave propagation in the subsurface. For ease of discussion, we will refer to the following features as constituting our geophysical systems (note that this usage may be different from the conventional approach):

1. Density distribution within the Earth.
2. Velocity distribution within the Earth.
3. Temperature distribution within the Earth.
4. Resistivity distribution within the Earth.
5. Distribution of radioactive materials within the Earth.
6. Magnetic susceptibility variations within the Earth.

1.1.3 Geophysical exploration philosophy and inverse theory

The goal of geophysical exploration is to understand or reconstruct the structure of the Earth from data recorded on, above or below the ground surface. To achieve this goal we often have to study or make observations on the various geophysical processes. Often, the recorded data may contain additive noise or are incomplete, and insufficient. However, we need to get something out of the observations and so proceed with processing the data. Inverse theory provides a formalism by which many of the questions fundamental to geophysical data processing may be entertained- e.g., the optimum sampling rate, how many more data are needed, and desired accuracies. Theoretical modelling techniques are then used as tools to improve our understanding of the relationship between the observed data (Earth's responses to some excitations which may be artificial or natural) and the various subsurface physical property changes or discontinuities that may have generated them. This search for optimum subsurface distribution of physical properties is again addressed using inverse theory. Questions pertaining to the resolving power of the data, the types of models that will reproduce the observations, and the effects of observational errors can all be attacked through inverse theory. Thus, it cannot be emphasised enough that inverse theory is of paramount importance in geophysics, especially where decisions are taken based on experimental data.

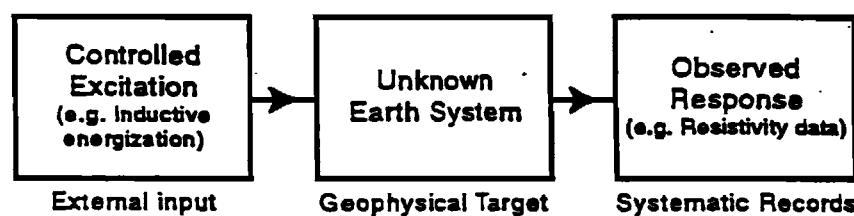
1.1.4 Types of geophysical data

Examples of data include mass and moment of inertia of the Earth, measurements of travel times of seismic waves (e.g., earthquakes and explosions), gravity anomalies, measurements of apparent resistivities of the ground, well draw-down data etc.

Geophysical data may be records of field experiments or laboratory measurements (Fig. 1.1). In field measurements, the numerical values obtained depend on density within the earth, seismic velocity, bulk and shear moduli, ground resistivity, rock permeability, magnetic susceptibility etc -which are the physical properties that characterise the Earth model. In laboratory experiments, we may generate the responses of scaled-down physical models of the earth which are useful especially in situations where the mathematical models are very complicated and difficult to work. There are other forms of data. For example, previously obtained values of some model parameters may also be classified as data and so can our quantified expectations of the form of the models of the system under consideration. However, for ease of discussion, we shall talk mostly about geophysical field measurements.

Gathering Data

Field Experiment:



Laboratory Experiment:

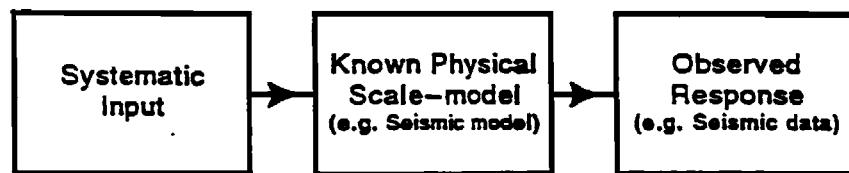


Fig. 1.1 Common methods of gathering data

When handling experimental data, it should always be borne in mind that each observation d_i can be regarded as a sample drawn from a set of equally likely events or values. If an experiment is repeated several times, the observed values under the same conditions usually vary. These variations could be due to instrumental or human error. The distribution of these samples may take the form of some probability distribution. For values referring to the same variable, we could construct a histogram and fit an expression for the **probability density function**. Note that we have employed the method of 'curve fitting' here and have thus applied inverse theory even at the datum characterisation stage. The target here is to determine the mean value $d_{\mu} = d_i$, its standard deviation, σ_i and any other statistical parameters of interest that characterise the distribution. It is good practice to estimate the data errors or uncertainties, σ as they have a bearing on the confidence to be ascribed to any estimated parameters. We will look at the effects of observational errors on the inverse solution late in the course but it will suffice to note that **each datum is a random variable whose mean value is d_i** .

1.1.5 Description or Characterisation of Geophysical Processes : Mathematical Models

Most geophysical processes can be described mathematically. As mentioned earlier, the set of equations that characterise each process or geophysical system is known as the forward theory or simply the MODEL. It is pertinent to mention here that the word "model" has various connotations in the geoscientific community. For instance, it may refer to CONCEPTUAL models as with many geologists or to PHYSICAL (laboratory-scale) and MATHEMATICAL models as is common in geophysics. In this course we will be concerned mostly with mathematical models but will make references to conceptual models where necessary.

A number of geophysical processes can be described mathematically by an integral equation of the form

$$d_i = \int_0^z K_i(z)p(z)dz \quad (1.1)$$

where d_i is the measurable or observable response of the system to an i^{th} external input or excitation (e.g., explosions or electrical current injection into the ground), $p(z)$ is a function related to some aspect of the Earth's structure or physical properties (e.g., resistivity, density or velocity as a function of depth in a laterally homogeneous Earth) referred to as the MODEL PARAMETERS, and K_i are called the DATA KERNELS.

The data kernels describe the relationship between the data and the Earth model function $p(z)$. The model parameters (e.g., velocity, resistivity, density) may be continuous functions of radius or position. For example, the travel-time t between a seismic source and receiver along a ray path L , for a continuous velocity field $v(x, z)$, is given by

$$t = \int_L \frac{1}{v(x, z)} dl \quad (1.2)$$

A mathematical description of a physical system such as above is referred to as the FORWARD THEORY. Forward theories have been developed for many geophysical processes and are routinely used to predict the data or responses that we would record over a hypothetical Earth-type structure. These data are therefore variously called THEORETICAL, SYNTHETIC or PREDICTED DATA.

1.1.6 Discretization and Linearization

In many cases of interest to us, the earth model is a continuous function of depth or radius. Consider, for example, the mass and moment of inertia of the earth. Both are related to density within the earth by the formula

$$\text{Mass} = 4\pi \int_0^R r^2 \rho(r) dr \quad (1.3a)$$

$$\text{Moment of inertia} = \frac{8\pi}{3} \int_0^R r^4 \rho(r) dr \quad (1.3b)$$

where R is the earth's radius and $\rho(r)$ corresponds to $p(z)$ in eq. (1.1), and is the density at radial distance r . Equations (1.3a & 1.3b) may be combined to give the general expression

$$d_i = \int_0^R K_i(r) \rho(r) dr \quad (1.4)$$

which is the same as eq. (1.1). This integral is easily evaluated using digital computers. This involves the use of discrete mathematics. To approximate this integral on a computer, we use a summation with $\rho(r)dr$ set to m and K_i to G_i , say, giving us the very useful computational formula

$$d_i = \sum G_{ij} m_j . \quad (1.5)$$

In this situation, we say that the theoretical problem is DISCRETIZED. It is common practice in geophysics to work with discrete numbers. For technical reasons our field or experimental observations are recorded over finite intervals (e.g., discrete frequencies or fixed bandwidth) instead of all observations in the range $[0, \infty]$ required to uniquely characterise the earth-system. Also, for computational simplicity, we often describe an otherwise continuous distribution of the Earth's physical properties $p(z)$ by a finite set of parameters, e.g., a layered structure with each layer having a specific density and thickness. This practice is referred to as PARAMETERIZATION. For convenience, in this course, we will be considering only discrete models and discrete parameters which are easier to handle than the continuous distributions. We will therefore study DISCRETE INVERSE THEORY instead of CONTINUOUS INVERSE THEORY.

Let us define some other useful terms in inverse problem theory. In discrete form, eq. (1.2) may be written as

$$t_i = \sum_{j=1}^p \frac{L_{ij}}{v_j} \quad (1.6)$$

which is the formula used in practical applications. Notice that the travel-time is not directly proportional to the model parameter v but to its inverse. The relationship is said to be non-linear in v . However, if we define the model parameter as $c = 1/v$, where c is the slowness of the seismic wave, then the problem can be stated as

$$t = \sum_{j=1}^p L_{ij} c_j \quad (1.7)$$

which is of the form $d = Gm$ and the relationship is now said to be linear. Such a transformation operation may be referred to as Linearising Parameterization. Now consider the problem of calculating the apparent resistivity that will be observed over a two-layer Earth model using the Schlumberger electrode configuration (Fig. 1.2). This is given by (see Parasnis, 1986)

$$\rho_a(L) = \rho_1 \left(1 + 2L^2 \int_0^\infty K(\lambda) J_1(\lambda L) \lambda d\lambda \right) \quad (1.8)$$

where $L = AB/2$ is the distance to each current electrode from the central point, J_1 is the Bessel function of order 1, and $K(\lambda)$ is a function of the parameters (layer

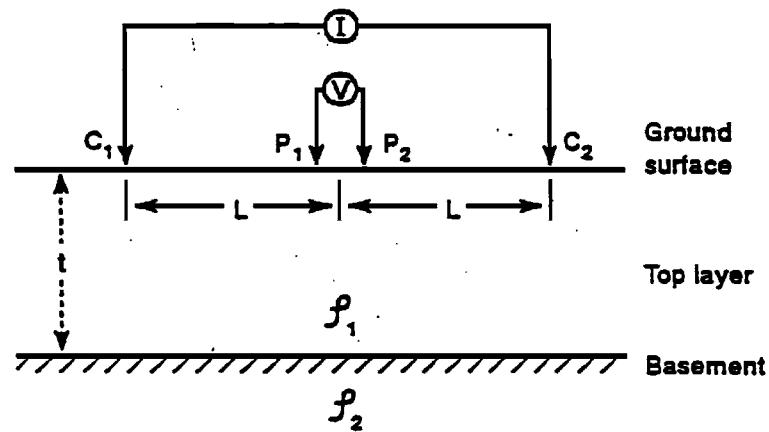


Figure 1.2 Schlumberger electrode configuration

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resistivities ρ_1, ρ_2 and top layer thickness t) of our system and the integration variable λ . $K(\lambda)$ is given by

$$K(\lambda) = \frac{-k_{1,2} \exp(-2\lambda t)}{1 + k_{1,2} \exp(-2\lambda t)}$$

where $k_{1,2} = \frac{(\rho_1 - \rho_2)}{(\rho_1 + \rho_2)}$.

It is easy to see that we cannot put eq. (1.8) in any simple form resembling $d = Gm$ as we did for eq. (1.2). The resistivity depth sounding problem is said to be **highly non-linear**. The usual method of dealing with such problems involves the derivation of linear analogues using Taylor's theorem, a procedure termed **Linearisation**.

INVERSE PROBLEMS IN GEOPHYSICS

2.1 Meaning of Inverse Problem

In order to fully understand the meaning of the term ‘inverse problem’, it is instructive to consider, first, the opposite situation dubbed the ‘forward problem’. Traditionally, the interpretation of some geophysical data (e.g., resistivity depth sounding data) involves comparison with theoretical Master curves (or nomograms). These curves are computed using certain relationships (mathematical model) assuming a particular distribution of the physical properties of the subsurface, i.e., the curves are the theoretical responses for idealised Earth-type structures. The procedure is simple :

‘Given some information on the values of the set of parameters (e.g., number of layers, their resistivities and thicknesses) for a hypothetical Earth-model, a theoretical relationship (mathematical model) is used to derive the values of some measurable quantities (e.g., apparent resistivities and phases)’.

This procedure constitutes the FORWARD APPROACH and solves our forward problem (see Fig 2.1). Note that what is generally known to many geophysicists as **‘Forward modelling by interactive computing’** is nothing but a more versatile extension of the original curve-matching technique. In interactive forward modelling the theoretical curves generated for an input model are displayed together with the field curves, say, on a interactive terminal. The model parameters are adjusted and the operations repeated until an acceptable visual fit is obtained between the field and theoretical curves.

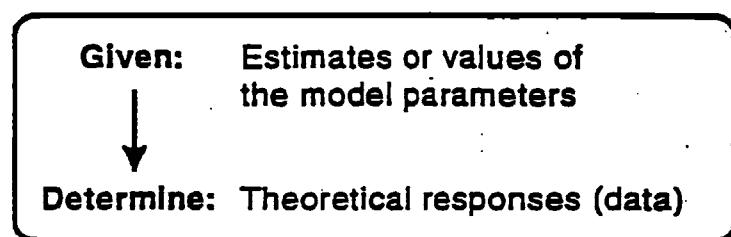
In the inverse approach, the Earth’s structure (or other useful information) is directly retrieved from the field data (Fig. 2.2). The inverse procedure is described as:

‘Given some information on the values of some measured quantities (field or experimental data), we use a theoretical relationship to derive the values of the set of parameters that explains or reproduces our field observations’.

We can illustrate the difference between the forward and inverse approach using a very simple example. Consider the temperature distribution within the Earth and assume that temperature increases linearly with depth in the Earth so that the relationship can be expressed as (e.g., Menke, 1984)

$$T(z) = a + bz \quad (2.1)$$

Forward Problem



The Forward Process

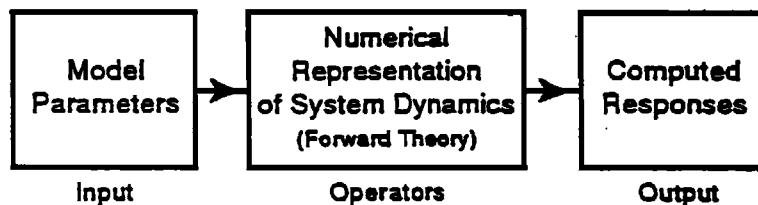
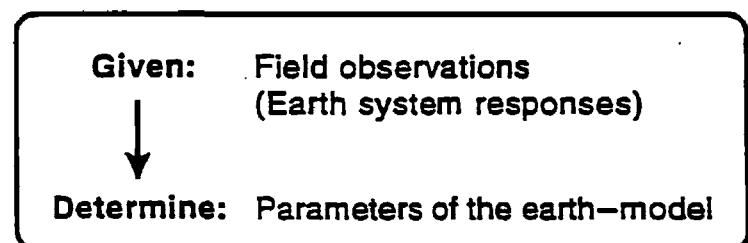


Figure 2.1

Inverse Problem



The Inversion Process

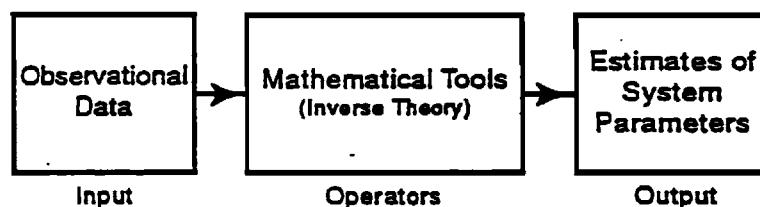


Figure 2.2

where a and b are numerical constants. Given the values of a and b (-1.5 and 0.04 respectively, say), we can calculate what the temperature T will be for any given depth value z . In calculating T at various levels, we are solving the forward problem. If, on the other hand, we measured a number of temperatures at various depths down a borehole and wish to determine a and b from our observations, then we are dealing with an inverse problem. The equation (2.1) relating T and z describes a straight line and we are thus faced with the inverse problem of fitting a straight line to the borehole data.

2.2 Sample Inverse Problems

There is a variety of inverse problems in geophysics and include the determination of earth structure from observational data, deconvolution of seismograms, earthquake location using arrival times of waves, determination of trends in time-series analysis, the determination of optimum sampling rates and other survey parameters in data acquisition problems, estimation of the resolving power of observational data, time reversals of the earth's magnetic field (an inverse problem in geochronology, *sensu stricto*) and determination of subsurface temperature distribution from borehole measurements.

3. DESCRIBING AND FORMULATING INVERSE PROBLEMS

Key Questions

A detailed description or formulation of an inverse problem will address the following nine golden questions :

1. What is the applicable parameterization- discrete or continuous ?
2. What is the nature of the geophysical data; what are the errors in the observations ?
3. Can we pose the problem mathematically and if so how well posed is it ?
4. Are there any physical constraints on the problem ?
5. What types of solution to the problem are desirable; and to what accuracy ?
Are we looking for an approximate solution, bounds of the solution or the exact solution ?
6. Is the problem linear or non-linear ?
7. Is it an overdetermined, underdetermined or even-determined problem ?
8. What is the best method of solving the problem ?
9. What are the confidence limits of the solution ?
Can it be appraised by other means ?

All the above issues will be addressed in this course.

3.1 Types of solution to inverse problems : What do we ask of a given data set ?

There is a plethora of questions that can be addressed using inverse theory. This means that depending on the problem in hand, we may have a variety of solution types. If we are analyzing geophysical time-series for instance, we may be interested in determining the optimum sampling rates or suppressing unwanted signal or simply calculating and removing a trend from time-sequential events. The desired solution in this case is the best estimated data from the processing sequence.

When interpreting data for subsurface structure, the desirable solution to our problem will be the best estimate of the subsurface physical property distributions such as layer resistivities (or the reciprocal, conductivities) and thicknesses. However, owing to the fact that some of the solutions are inherently non-unique, it may be better to seek some combined property of the subsurface (e.g., conductivity-thickness product) which are better resolved by the geophysical data in use rather than individual model parameters. We may also prefer the slowness($1/v$) to the velocity (v) of acoustic waves in the subsurface as our desired solution because of the attendant computational advantages offered by such parameterizations. In certain situations, it may be of interest to seek the non-uniqueness bounds defined by our data or a suite of extreme

models that define a particular aspect of the model or even the model space rather a single model for the subsurface. We can also seek ‘exact’ rather than ‘approximate’ solutions to problems. The parameterization involved (*i.e.*, the choice of target parameters) will often influence the way an inverse problem is posed and the solution procedure as we shall see later in the course.

3.2 Classification of inverse problems

To a large extent, the answers to some of the above questions or any other demands on a finite set of observational data will depend on the relative dimensions of the observational data and the model parameters. If the sought model consists of fewer parameters than the number of field data, then the inverse problem is said to be **OVERDETERMINED** and can be formally solved using methods based on achieving a best fit to the data. If on the other hand the sought model has more parameters than there are observational data, the inverse problem is **UNDERDETERMINED**. In this latter case, there exists an infinity of models that can satisfy the sparse data and so we must find a means of singling out one particular model out of all possible candidates. This type of problem is best attacked by constructing models whose parameters are a continuous function of position. It will be shown later that it is also possible to use the methods originally devised for overdetermined problems to obtain meaningful **‘smooth’ models** from underdetermined cases. When there are very small amounts of data and we seek a comparable number of model parameters from them, the problem is said to be **EVENLY DETERMINED** and in this case, very simple models can be constructed using **DIRECT INVERSION** schemes. The problem with this type of problem is that typical field data are rarely independent such that the problem is in effect underdetermined.

3.3 Discretization and parameterization.

For physical (or sometimes physico-chemical) reasons, we may expect the distribution of some physical property of the subsurface to be a continuous function of depth. Geophysical measurements are usually made in order to determine the subsurface properties or structure. The distribution of the physical properties can be uniquely determined if the measurements span the observational band-width $[0, \infty]$. However, this is not possible owing to technical limitations and we typically conduct our field experiments over a finite observation interval; and the outcomes are discrete numerical

values called field data which are incomplete and often inconsistent. For computational simplicity we also tend to seek the minimum set of parameters that describe our observations or the Earth's structure. The inverse problem is therefore discretised and our hypothetical Earth-model is parameterized into a finite number of parameters. Geophysical inverse theory is thus concerned with the approximation of otherwise continuous functions with a finite number of parameters. The foregoing discussion will be illustrated below using density and temperature models of the Earth.

3.4 Problem formulation

An inverse problem can be stated as: Given a set of experimental data, determine those parameters of the earth (or model) that will explain the observations. The task of formulating this problem mathematically rests on our ability to distinguish between what represents the experimental data and that which constitutes the model parameters. The process of selecting variables to represent data and model parameters may be broadly referred to as parameterization (many workers use this term for parameter selection only). We need to pose the problem in the form $d = Gm$ which is computationally manageable. For our discrete system, we have that

$$d_i = \sum_{j=1}^p G_{ij} m_j \quad (3.1)$$

The Earth can be parameterized into a number of discrete layers each with its own density (ρ_j) or seismic velocity (v_j) or electrical resistivity (ϱ_j), say. In otherwords, for the density distribution problem, instead of wanting density as a function of radius we may be interested in determining the average densities of the core and mantle. For illustration, we will consider a few examples of problem formulation next.

3.4.1 Density distribution within the Earth

Consider the problem of determining the average density of the core (ρ_1) and that of the mantle (ρ_2) (see Fig. 3.1) from measurements of the Earth's mass and moment of inertia. In this case, we have two data values (mass = d_1 , and moment of inertia = d_2) and two model parameters ($\rho_1 = m_1$ and $\rho_2 = m_2$). The problem can be formulated as

$$d_1 = \text{mass of earth} = \frac{4}{3}\pi c^3 \rho_1 + \frac{4}{3}\pi(a^3 - c^3)\rho_2 \quad (3.2a)$$

$$d_2 = \text{moment of inertia} = \frac{8}{15}\pi c^5 \rho_1 + \frac{8}{15}\pi(a^5 - c^5)\rho_2 \quad (3.2b)$$

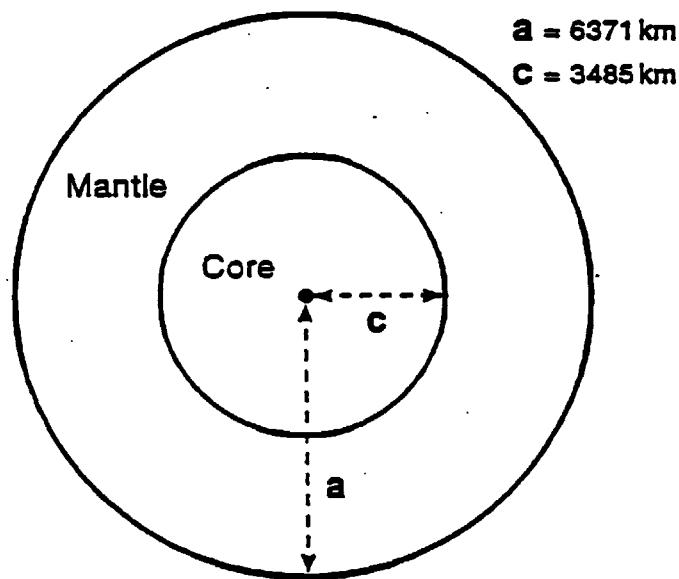


Figure 3.1 A simple parameterization of the Earth

which can be written in our favourite short-hand notation as

$$d_i = \sum_{j=1}^2 G_{ij} m_j \quad i=1,2. \quad (3.3)$$

or in component form as

$$\begin{bmatrix} d_1 \\ \dots \\ d_2 \end{bmatrix} = \begin{bmatrix} \frac{4}{3}\pi c^3 & \frac{4}{3}\pi(a^3 - c^3) \\ \dots & \dots \\ \frac{8}{15}\pi c^5 & \frac{8}{15}\pi(a^5 - c^5) \end{bmatrix} \begin{bmatrix} \rho_1 \\ \dots \\ \rho_2 \end{bmatrix}.$$

This is an even-determined system of equations and must be solved for the sought model parameters.

3.4.2 Borehole temperature measurements

Now, consider the straight line problem of fitting downhole temperature data given by eq. (2.1). Suppose that we made n temperature measurements T_i at n depths z_i and want to fit a straight line to the data. Here, $d = [T_1, T_2, \dots, T_n]^T$, and the intercept a and slope b are the two model parameters, i.e., $m = [a, b]^T$.

Now, by the forward theory the data T must satisfy the relation $T_i = a + bz_i$. So

$$T_1 = a + bz_1$$

$$T_2 = a + bz_2$$

.

.

$$T_n = a + bz_n$$

which in the matrix form $d = Gm$ is simply

$$\begin{bmatrix} T_1 \\ T_2 \\ \vdots \\ T_{n-1} \\ T_n \end{bmatrix} = \begin{bmatrix} 1 & z_1 \\ 1 & z_2 \\ \vdots & \vdots \\ 1 & z_{n-1} \\ 1 & z_n \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} \quad (3.4)$$

which is an over-determined system of equations.

3.4.3 Digital filter design in seismic deconvolution

Two signals $a(t)$ and $b(t)$ may be related by convolution with a filter $f(t)$ in the form

$$a(t) = f(t) * b(t) = \int f(\tau) b(t - \tau) d\tau. \quad (3.5)$$

A question that often crops up in signal analysis is (see Menke, 1984): **knowing $a(t)$ and $b(t)$, can $f(t)$ be determined?**

To address this issue, let us discretize the problem. If the time series is of length n and the filter is of length p , then the convolution integral of eq. (3.5) can be conveniently replaced by the computational formula

$$a_i = \Delta t \sum_{j=1}^p f_j b_{i-j+1} \quad (3.6)$$

where $b_i = 0$ if $i < 1$ or $i > n$, and Δt is the sampling interval.

Notice that equation (3.6) is linear in the unknown filter coefficients f_j and can be recast in the form $d = Gm$, where $m = f$ (the sought filter), $d = a$ (the time series data) and

$$G = \Delta t \begin{bmatrix} b_1 & 0 & 0 & 0 & 0 & \dots & \dots & 0 \\ b_2 & b_1 & 0 & 0 & 0 & & & \\ b_3 & b_2 & b_1 & 0 & 0 & & & \vdots \\ \vdots & \vdots & \vdots & b_1 & 0 & & & \vdots \\ \vdots & \vdots & \vdots & \vdots & b_1 & & & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & & & \vdots \\ b_n & b_{n-1} & b_{n-2} & b_{n-3} & \dots & \dots & \dots & b_k \end{bmatrix}$$

where $k = n - p + 1$. The above system is overdetermined, i.e., $p < n$ and can be solved for the sought filter coefficients.

We will now examine methods of solving such linear systems of equations for the sought parameter estimates.

4. SOLVING OVERDETERMINED LINEAR INVERSE PROBLEMS

4.1 Simple Linear Regression:

If an inverse problem can be represented with the explicit linear equation $d = Gm$, it is said to be LINEAR. If a perfect (or exact) relationship exists between the observations d and the model parameters m , then we can use very simple procedures to invert our measurements for m . In many practical situations, the observed data may not all lie on a straight line (see Fig. 4.1.1). If we decide to fit a line to these data, the fitted line may be some appreciable distance away from some data values. For a collection of n data pairs $\{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$, the fitted line (known as the REGRESSION line) is described by the equation

$$y = a + bx \quad (4.1)$$

and each data pair satisfies the relation

$$y_i = a + bx_i + e_i \quad (4.3)$$

where e_i is the vertical distance between the i^{th} data point and the regression line (Fig. 4.1.1). The quantity e_i is called the RESIDUAL, MISFIT or prediction ERROR. The solution to the straight line inverse problem in this case is not an exact solution since the relation $y_i = a + bx_i$ cannot be satisfied for every i and the problem is also overdetermined. This type of problem is generally solved using the LEAST SQUARES method.

In the least squares method we try to MINIMIZE the error e by determining those parameters a, b such that the sum of squares of the error (S) is minimal, i.e.,

Minimize

$$S = \sum_{i=1}^n e_i^2 = \sum_{i=1}^n (y_i - a - bx_i)^2 \quad (4.3)$$

Minimization is accomplished by differentiating S with respect to the model parameters and setting the derivatives equal to zero.

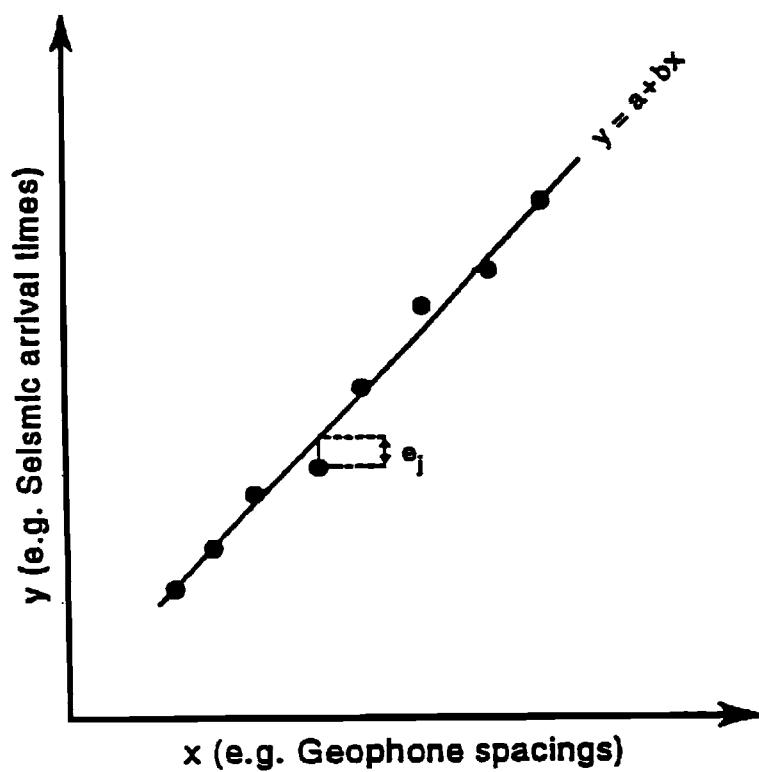
The minimization procedure

Recall that $y = (a+bx) + e$. Assuming that the experimental errors are only in the field data y_i , then equation 4.3 holds good. Next, differentiate S (in eq. 4.3) with respect to a and b and equate the result to zero, viz:

$$\frac{\partial S}{\partial a} = 2 \sum_{i=1}^n (y_i - a - bx_i)(-1) = 0$$

$$\frac{\partial S}{\partial b} = 2 \sum_{i=1}^n (y_i - a - bx_i)(-x_i) = 0$$

Figure 4.1 A simple straight-line problem



giving

$$\Sigma a + \Sigma bx_i = \Sigma y_i \quad (4.4a)$$

and

$$\left. \begin{array}{l} \Sigma ax_i + \Sigma bx_i^2 = \Sigma x_i y_i \\ \end{array} \right\} 2 \text{ simultaneous linear equations}$$

$$(4.4b)$$

whose solution for a and b is very straightforward and shown below. Re-stating these two equations, we have that

$$\Sigma y = na + (\Sigma x)b \quad (4.5a)$$

and

$$n(\Sigma xy) = n(\Sigma x)a + n(\Sigma x^2)b \quad (4.4b \times n) \quad (4.5b)$$

Next, multiply eq. (4.5a) by (Σx) so that we can subtract it from eq. (4.5b) to find b . We will find that:

$$(4.5b) \rightarrow \quad n\Sigma xy = n(\Sigma x)a + n(\Sigma x^2)b$$

$$\text{minus } (4.5a \times \Sigma x) \rightarrow \quad \underline{\underline{\Sigma x\Sigma y = n(\Sigma x)a + (\Sigma x)(\Sigma x)b}}$$

$$\text{gives } \rightarrow \quad n\Sigma xy - \Sigma x\Sigma y = [n\Sigma x^2 - (\Sigma x)(\Sigma x)]b.$$

Therefore,

$$b = \frac{n\Sigma xy - \Sigma x\Sigma y}{n\Sigma x^2 - (\Sigma x)^2} \quad \left. \right\} \text{slope of the fitted line.} \quad (4.6a)$$

Finally, find a by substituting b into equation 4.5a.

Thus,

$$a = \frac{\Sigma y - b\Sigma x}{n} = \bar{y} - b\bar{x} \quad \left. \right\} \text{intercept on the y-axis.} \quad (4.6b)$$

where \bar{y} and \bar{x} are the mean values of y and x respectively.

The formula for the least squares regression (best fitting) line is therefore

$$\hat{y} = a + bx. \quad (4.7)$$

The above concepts are used routinely in geophysical data analysis and especially when dealing with problems with one or two parameters (e.g., a simple straight-line fitting) and the technique is termed linear regression analysis or classical Least Squares fitting.

The method was originally formulated to provide a solution to the overdetermined problem but the same approach can be adopted for underdetermined problems. The solution was originally given by Gauss in 1809. When we have more than two model parameters then we require a simple extension of the above method referred to as Multiple regression analysis. However, it is possible to formulate a generalized relationship that will be applicable to any dimension of data and model parameters. This approach is commonly adopted in geophysics and the procedure uses matrix formulations instead and is aptly dubbed Generalized Least Squares or Matrix Inversion (GMI). As a prelude to GMI, we will now demonstrate an application of the classical least squares method of parameter estimation.

Example 4.1: Application of the classical least squares method in seismic refraction interpretation.

If $(x_1, t_1), (x_2, t_2), \dots, (x_n, t_n)$, represent our n observed arrival times at n geophones at distances x_i , and suppose that we can represent the head wave equation

$$t = \frac{x}{v} + T_h$$

by a linear relation of the form

$$t = a + bx \quad \left\{ \begin{array}{l} a = T_h, \\ b = 1/v \end{array} \right.$$

The errors are assumed to be in the picked arrival times t_i only. The best fit to the data with respect to minimizing the sum of the squares of the residuals, $e_i = t_i - (a + bx_i)$, is given by (see eq. 4.6)

$$b = \frac{[n \Sigma xt - (\Sigma x)(\Sigma t)]}{D} \quad (4.6 \text{ again})$$

and

$$a = \frac{(\Sigma t - b \Sigma x)}{n} = \frac{(\Sigma t \Sigma x^2 - \Sigma x \Sigma xt)}{D}$$

with the standard errors χ_b^2 and χ_a^2 being given by

$$\chi_b^2 = n \frac{\chi^2}{D} \quad (4.8a)$$

$$\chi_a^2 = \chi^2 \frac{\Sigma x^2}{D} \quad (4.8b)$$

$$\text{where } D = (n \sum x^2 - (\sum x)^2) \quad \text{and} \quad \chi^2 = \frac{1}{n-2} \sum_{i=1}^n e_i^2.$$

Note that χ^2 is estimated as the root mean square deviation of the data t_i from the calculated best line ($a + bx_i$) but with the factor $n - 2$ in the denominator since we have two model parameters (a and b) in this problem. The quantity $[n - 2]$ is referred to as the number of degrees of freedom in this problem.

Illustrative Exercise.

A table of results for seismic travel times is given below. Complete the table, determine the slope and intercept on the time-axis of the best fitting line to the data, and then compute the errors associated with the estimated parameters of the regression line.

Trace	x_i (m)	t_i (ms)	$x_i t_i$	x_i^2	bx_i	$a + bx_i$	e_i	e_i^2
1	2	5.1	10.2	4				
2	4	9.2	36.8	16				
3	6	11.9	71.4	36				
4	8	14.9	119.2	64				

Σ

Table 4.1.1. Seismic first arrivals (t_i) at four geophone positions (x_i).

Solution

The first task here is the computation of the sums $\Sigma x, \Sigma t, \Sigma xt, \Sigma x^2$. Having calculated these sums, we simply obtain b and a using equation 4.6. Next, we compute the residuals and the sum of their squares and finally calculate χ_b^2 and χ_a^2 using eq. 4.8 . For example, considering these four traces, we have that $n=4$, $\Sigma x=20$, $\Sigma t=41.1$, $\Sigma xt=237.6$, $\Sigma x^2=120$. The least squares solution for a and b is thus:

$$b = \frac{4(237.6) - 20(41.1)}{4(120) - 20^2} = 1.605; \quad \text{so that } v=623.053 \text{ m/s}$$

and

$$a = \frac{\Sigma t - b\Sigma x}{n} = \frac{41.1 - 1.605(20)}{4} = 2.25.$$

It is left to the reader to complete the exercise.

It is remarked that the above calculations can be easily done on computers using standard software packages. A simple demonstration of how the above formulations can be implemented on a computer is given in the Fortran program REGRES listed below.

```
program REGRES
c performs simple linear regression. estimates parameters
c a and b (in the problem y=ax+b) and associated errors
c based on data scatter, aerr and berr. yhat=predicted y.
c Input file contains the n data pairs: x(i),y(i)
c Author: Max A. Meju
      dimension x(200),y(200),xx(200),xy(200),yhat(200)
      character*20 infile,outfile
c initializations
      sumx=0.0
      sumxx=0.0
      sumxy=0.0
      sumy=0.0
      write(*,'(a)')' enter input filename > '
      read(*,'(a20)')infile
      open(unit=3,file=infile,status='old')
      i=1
1      read(3*,err=99)x(i),y(i)
      i=i+1
      goto 1
99    continue
      n=i-1
      close(unit=3)
      write(*,'(a)')' enter output filename > '
      read(*,'(a20)')outfile
      open(unit=3,file=outfile,status='new')
calculate required quantities xx,xy and sums
      do 10 i=1,n
      xx(i)=x(i)*x(i)
      xy(i)=x(i)*y(i)
```

```

sumx=sumx+x(i)
sumxx=sumxx+xx(i)
sumxy=sumxy+xy(i)
sumy=sumy+y(i)

10 continue
calculate the common denominator and the desired regression parameters.
den=n*sumxx-(sumx*sumx)
b=(n*sumxy-(sumx*sumy))/den
a=(sumy*sumxx-sumx*sumxy)/den
calculate root mean square errors in a,b.
sse=0.0
do 20 i=1,n
e=y(i)-a-(b*x(i))
sse=sse+(e*e)
20 continue
rmsq=sse/(n-2)
aerr=rmsq*sumxx/den
berr=n*rmsq/den
c compute best fitting line and average error
do 30 i=1,n
yhat(i)=a+b*x(i)
fmin=(a-aerr)+(b-berr)*x(i)
fmax=(a+aerr)+(b+berr)*x(i)
yherr=(abs(fmin)+abs(fmax))/2.
write(3,*)x(i),yhat(i),yherr
30 continue
close(unit=3)
stop
end

```

Fig. 4.1.2 A Fortran program for simple linear regression analysis.

4.2 Unconstrained Linear Least Squares Inversion: The Generalized Matrix Approach
As alluded to in the previous section, the least squares method of parameter estimation may be formulated in matrix notation so that the resulting algorithms can be applied

equally in the inversion of single or several data sets for one or several model parameters. This approach will be adopted in the rest of the course.

Steps involved:

Problem definition —> matrix formulation —> Least squares solution

The linear problem is posed in the generalized matrix form $d = Gm$. We now want to solve for m . For perfect data (i.e., no experimental errors),

$$m = G^{-1}d.$$

However, Gauss (1809) suggested that due to experimental errors, practical data d , would not fit the model exactly, i.e.,

$$d = Gm + e;$$

and that the best way to get a unique solution for the model parameters is to minimize the sum of squares of the residuals e . This procedure minimizes the differences between the field data and that predicted by the forward theory, the so-called euclidean distance. We therefore wish to minimize the quantity that gauges the misfit,

$$q = e^T e = \sum_{i=1}^n (d_i - \sum_j^p G_{ij} m_j)^2 \quad j=1, \dots, p. \quad (4.9)$$

As before, minimization is effected by differentiating q with respect to each of the model parameters and setting the results to zero (for a maximum or minimum). The resulting equations can then be solved for m as illustrated below.

First, we re-write eq. 4.9 as

$$q = \underbrace{(d - Gm)^T(d - Gm)}_{\text{expansion}}$$

$$\text{Therefore, } \frac{\partial q}{\partial m_j} = \frac{\partial [d^T d - d^T Gm - m^T G^T d + m^T G^T Gm]}{\partial m_j} = 0$$

or

$$-d^T G - G^T d + G^T Gm + m^T G^T G = 0$$

giving

$$2G^T Gm = 2G^T d \quad \leftarrow \text{the so-called } \textit{normal equations}$$

from which we obtain the least squares solution for the parameter estimates denoted by \hat{m} and given by

$$\hat{m} = [G^T G]^{-1} G^T d . \quad (4.10)$$

This is the unconstrained least squares solution to the inverse problem $d = Gm$. The quantity $[G^T G]^{-1} G^T$ is called the least squares Generalized Inverse and operates on the data d to recover \hat{m} . The least squares solution given above is referred to as an unbiased estimator of m in statistical parlance. It is obvious, however, that we would have to solve a set of equations to obtain \hat{m} . Some of the commonly used matrix solution methods are discussed briefly in the following section.

4.3 Obtaining Matrix Inverses and Least Squares Solutions

Notice that eq. (4.10) is of the form $x = A^{-1}y$ (the solution to the inverse problem $y = Ax$) where A^{-1} is equivalent to $[G^T G]^{-1}$ and y to $G^T d$. The main task here is to find A^{-1} , the inverse of A (called A-inverse). The method of matrix inversion to be adopted may depend on the size and degree of symmetry of A and the desired numerical robustness. For illustration, we will explore three commonly used matrix inversion methods.

4.3.1 Matrix solution of a small set of equations

4.3.1.1 Cramer's Rule

To find A^{-1} for a small set of equations, the following steps may be followed (Stroud, 1986):

- (i) evaluate the determinant of A denoted as $|A|$ or $\det(A)$
- (ii) form the matrix of cofactors of A denoted as C (the cofactor of an element is its minor together with its 'place sign')
- (iii) find the transpose of C (i.e., the adjoint of A) denoted as C^T or $\text{adj}(A)$.
- (iv) then calculate $A^{-1} = \frac{1}{|A|} \cdot C^T$

The desired solution is given by $x = \left\{ \frac{1}{|A|} \cdot C^T \right\} y$.

Example : Suppose that A and y are given as

$$A = \begin{bmatrix} 4 & 5 & 1 \\ 1 & -2 & -3 \\ 3 & -1 & -2 \end{bmatrix} \text{ and } y = \begin{bmatrix} 2 \\ 7 \\ 1 \end{bmatrix} .$$

We have that

$$|A| = 4(4-3) - 5(-2+9) + 1(-1+6) = -26$$

so that

$$C = \begin{bmatrix} c_{11} & c_{12} & c_{13} \\ c_{21} & c_{22} & c_{23} \\ c_{31} & c_{32} & c_{33} \end{bmatrix}$$

and

$$C^T = \begin{bmatrix} c_{11} & c_{21} & c_{31} \\ c_{12} & c_{22} & c_{32} \\ c_{13} & c_{23} & c_{33} \end{bmatrix} \quad \{ \text{the programmed matrix in applications; see below.}$$

$$\text{where } c_{11} = \begin{vmatrix} -2 & -3 \\ -1 & -2 \end{vmatrix} = 1; \quad c_{12} = -\begin{vmatrix} 1 & -3 \\ 3 & -2 \end{vmatrix} = -7; \quad c_{13} = \begin{vmatrix} 1 & -2 \\ 3 & -1 \end{vmatrix} = 5.$$

$$c_{21} = -\begin{vmatrix} 5 & 1 \\ -1 & -2 \end{vmatrix} = 9; \quad c_{22} = \begin{vmatrix} 4 & 1 \\ 3 & -2 \end{vmatrix} = -11; \quad c_{23} = \begin{vmatrix} 4 & 5 \\ 3 & -1 \end{vmatrix} = 19.$$

$$c_{31} = \begin{vmatrix} 5 & 1 \\ -2 & -3 \end{vmatrix} = -13; \quad c_{32} = \begin{vmatrix} 4 & 1 \\ 1 & -3 \end{vmatrix} = 13; \quad c_{33} = \begin{vmatrix} 4 & 5 \\ 1 & -2 \end{vmatrix} = -13.$$

Thus,

$$C = \begin{bmatrix} 1 & -7 & 5 \\ 9 & -11 & 19 \\ -13 & 13 & -13 \end{bmatrix}.$$

The inverse of A is given by

$$A^{-1} = \frac{1}{|A|} \cdot C^T$$

enabling us to determine the solution vector x

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \frac{1}{-26} \begin{bmatrix} 1 & 9 & -13 \\ -7 & -11 & 13 \\ 5 & 19 & -13 \end{bmatrix} \begin{bmatrix} 2 \\ 7 \\ 1 \end{bmatrix} = \frac{1}{-26} \begin{bmatrix} 52 \\ -78 \\ 130 \end{bmatrix} = \begin{bmatrix} -2 \\ 3 \\ -5 \end{bmatrix}.$$

It is easy to write a computer program to invert a 3×3 matrix. A simple Fortran program CRAMINV to effect the above solution procedure is given in Fig. 4.3.1 for

illustration and incorporates a subroutine for matrix inversion by Cramer's Rule. It is reiterated that we have to form the square matrix $A = G^T G$, and the vector $y = G^T d$ in order to solve the least squares problem using matrix inversion by Cramer's rule.

```

program CRAMINV
c simple demonstration program for matrix inversion.
c solves a linear system of equations y=Ax.
c input: (1) Matrix A, elements read row by row.
c         (2) Vector y, elements read in one line.
c output: solution vector, x.
c method: A inverted using Cramer's Rule to give another matrix,Ainv.
c         Ainv is then post-multiplied by y to give x.
c author: Max A. Meju
dimension A(3,3),Ainv(3,3),x(3),y(3)
write(*,*)' Hello there. Welcome to a 3-by-3 equations solver! '
write(*,*)'
write(*,*)' Enter elements of the A-matrix (or  $G^T G$ ), row by row'
do 10 i=1,3
  write(*,11) i
11  format(2x,' Reading Row: ',i1,' <enter row elements below>')
  read (*,*) (A(i,j),j=1,3)
10  continue
  write(*,*)'
c  read data vector y
  write(*,*)' Enter elements of y-vector ( $G^T d$ ), all in one line please'
  read (*,*) (y(i),i=1,3)
c call matrix inversion routine
  call cram3x3(A,Ainv)
c calculate the inner product Ainv*y and return as vector x.
  call inprod(Ainv,y,x,3,3)
c write out solution
  write(*,*)'
  write(*,*)' Here are the ordered elements of solution vector,x'
  write(*,*) (x(i),i=1,3)
  stop

```

end

c-----

```
subroutine cram3x3(A,Ainv)
dimension A(3,3),Ainv(3,3),Ct(3,3)
b1=(a(2,2)*a(3,3))-(a(3,2)*a(2,3))
b2=(a(2,1)*a(3,3))-(a(3,1)*a(2,3))
b3=(a(2,1)*a(3,2))-(a(3,1)*a(2,2))
```

c calculate the determinant of A.

```
det=(a(1,1)*b1)-(a(1,2)*b2)+(a(1,3)*b3)
write(*,*)' the determinant of A-matrix is: '
write(*,*)det
```

c compute the elements of C-transpose (C=Matrix of Cofactors of A)

```
Ct(1,1)=(a(2,2)*a(3,3))-(a(2,3)*a(3,2))
Ct(1,2)=-(a(1,2)*a(3,3))+(a(1,3)*a(3,2))
Ct(1,3)=(a(1,2)*a(2,3))-(a(1,3)*a(2,2))
Ct(2,1)=-(a(2,1)*a(3,3))+(a(2,3)*a(3,1))
Ct(2,2)=(a(1,1)*a(3,3))-(a(1,3)*a(3,1))
Ct(2,3)=-(a(1,1)*a(2,3))+(a(1,3)*a(2,1))
Ct(3,1)=(a(2,1)*a(3,2))-(a(2,2)*a(3,1))
Ct(3,2)=-(a(1,1)*a(3,2))+(a(1,2)*a(3,1))
Ct(3,3)=(a(1,1)*a(2,2))-(a(1,2)*a(2,1))
```

c compute A-inverse = Ct/det(A)

```
do i=1,3
  do j=1,3
    Ainv(i,j)=Ct(i,j)/det
  end do
end do
return
end
```

c-----

Subroutine Inprod(A,y,x,n,m)

c matrix by vector multiplication or inner product

```
dimension A(n,m),x(m),y(n)
```

```
do 10 i=1,n
  sum=0.0
  do 20 j=1,m
```

```

sum=sum+A(i,j)*y(j)
20 continue
x(I)=sum
10 continue
return
end

```

Fig. 4.3.1 A program for solving a small-size (3×3) system of equations using matrix inversion by Cramer's rule.

Note that a slight modification of the above strategy is required for a 2×2 matrix. It is obvious that we cannot calculate C for such a matrix using the method described above for the 3×3 matrix. In general, for a square matrix A , if there is another matrix F such that the matrix product $AF = I$, then $F = A^{-1}$ and is given by

$$F = \frac{1}{\det(A)} \cdot B$$

providing that it exists, i.e., $\det(A) \neq 0$. The matrix B plays the role of C in this case. Let us see how easily B can be determined. Given the matrix

$$A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

we have that $\det(A) = ad - bc$. Now the matrix product

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix} = \begin{bmatrix} (ad-bc) & 0 \\ 0 & (ad-bc) \end{bmatrix} = \det(A) \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

It is obvious that dividing this product by $\det(A)$ will yield I . The desired matrix, B is therefore the post-multiplying matrix on the left-hand side of the above matrix equations, i.e.,

$$B = \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}.$$

For purposes of illustration, let us try and solve the problem $d = Gm$ where $d = \begin{bmatrix} 4 \\ 14 \end{bmatrix}$

$$\text{and } G = \begin{bmatrix} 8 & 10 \\ 2 & -4 \end{bmatrix}.$$

We could elect to find the exact solution $m = G^{-1}d$ or the least squares solution $m = [G^T G]^{-1} G^T d$ since both approaches will lead to the same result for this problem. For the former approach, we have that $G^{-1} = (1/\det(G)) \cdot B$ where

$$\det(G) = (-32 - 20) = -52 \text{ and } B = \begin{bmatrix} -4 & -10 \\ -2 & 8 \end{bmatrix} \equiv C^T$$

so that

$$m = \frac{1}{-52} \begin{bmatrix} -4 & -10 \\ -2 & 8 \end{bmatrix} \begin{bmatrix} 4 \\ 14 \end{bmatrix} = \frac{1}{-52} \begin{bmatrix} 156 \\ -104 \end{bmatrix} = \begin{bmatrix} 3 \\ -2 \end{bmatrix}.$$

Using the least squares approach, let us define

$$y = G^T d = \begin{bmatrix} 8 & 2 \\ 10 & -4 \end{bmatrix} \begin{bmatrix} 4 \\ 14 \end{bmatrix} = \begin{bmatrix} 60 \\ -16 \end{bmatrix}$$

and

$$A = G^T G = \begin{bmatrix} 8 & 2 \\ 10 & -4 \end{bmatrix} \begin{bmatrix} 8 & 10 \\ 2 & -4 \end{bmatrix} = \begin{bmatrix} 68 & 72 \\ 72 & 116 \end{bmatrix}.$$

We have that

$$\det(A) = (68 \times 116) - (72 \times 72) = 2704 \text{ and } B = \begin{bmatrix} 116 & -72 \\ -72 & 68 \end{bmatrix}$$

yielding the estimates

$$m = \frac{1}{2704} \begin{bmatrix} 116 & -72 \\ -72 & 68 \end{bmatrix} \begin{bmatrix} 60 \\ -16 \end{bmatrix} = \frac{1}{2704} \begin{bmatrix} 8112 \\ -5408 \end{bmatrix} = \begin{bmatrix} 3 \\ -2 \end{bmatrix}.$$

4.3.2 Matrix solution of a large set of equations

4.3.2.1 Gauss Elimination Method

Gauss elimination method proceeds in three steps: initialization, forward reduction by elimination and backward substitution. We will illustrate these operational steps using the problem $y = Ax$ where

$$y = \begin{bmatrix} 2 \\ 7 \\ 1 \end{bmatrix} \text{ and } A = \begin{bmatrix} 4 & 5 & 1 \\ 1 & -2 & -3 \\ 3 & -1 & -2 \end{bmatrix}.$$

Step 1: Initialization.

The solution process is initialized by forming the partitioned or augmented matrix

$$A_{\star}^{(0)} = [A : y] = \left[\begin{array}{ccc|c} 4 & 5 & 1 & 2 \\ 1 & -2 & -3 & 7 \\ 3 & -1 & -2 & 1 \end{array} \right]$$

that is,

$$\left. \begin{aligned} a_{ij}^{(0)} &= a_{ij} & j=1, \dots, p \\ a_{ij}^{(0)} &= y_i & j=p+1 \end{aligned} \right\} i=1, 2, \dots, n$$

noting, however, that $p=n$ here.

Step 2: Elimination.

Successive forward reduction of the above partitioned matrix is effected at this stage. We want reduce the coefficients of A_{\star} such that for the original coefficient matrix part, the diagonal element $a(i, i)$ is unity and the subdiagonal element $a(i, i-m)$ is zero. When this operation is complete, the system is said to be triangularized. To triangularize A_{\star} , divide the i^{th} row by the element $a(i, i)$ giving the equivalent row vector $r^{(i)}$; then for each of the successive rows (i.e., row L , $L=i+1$ to n) multiply the elements of $r^{(i)}$ by the constant factor $a(L, i)$ and subtract the result from the L^{th} row of A_{\star} . Note that the elements of the i^{th} row of A_{\star} are not modified at this level of operations but the rest are. These operations are repeated with the next row $i+1$ furnishing the required $r^{(i+1)}$, and so on. The procedure will become clear when we tackle the above sample problem.

Starting from row 1, $r^{(1)} = [1, 1.25, 0.25 : 0.5]$ and the multiplicative factors are given by $a(2, 1) = 1$ for row 2 and $a(3, 1) = 3$ for row 3 leading to

$$A_{\star} = \left[\begin{array}{ccc|c} 4 & 5 & 1 & 2 \\ 0 & -3.25 & -3.25 & 6.5 \\ 0 & -4.75 & -2.75 & -0.5 \end{array} \right].$$

Next, repeat the operations using row 2, viz; divide row 2 by -3.25 yielding $r^{(2)}$, and subtract $-4.75 \times r^{(2)}$ from row 3 to give

$$A_r = \begin{bmatrix} 4 & 5 & 1 & \vdots & 2 \\ 0 & -3.25 & -3.25 & \vdots & 6.5 \\ 0 & 0 & 2 & \vdots & -10 \end{bmatrix}.$$

This completes the triangularization process for the chosen example and the solution for x can now be found by backward substitution (working up from the last row) as shown next.

Step 3: Back-substitution.

Starting from the last row of the reduced partitioned matrix, we have that $2x_3 = -10$ or $x_3 = -5$. Substituting this back into the second row gives $(3.25 \times 5) - 3.25 x_2 = 6.5$ or $x_2 = 3$. Finally, for the first row, we have that $4x_1 + 5x_2 + x_3 = 2$ or $x_1 = -2$.

The solution is therefore

$$x = \begin{bmatrix} -2 \\ 3 \\ -5 \end{bmatrix}.$$

Notice that the elimination operation can be described by the formula

$$a_{ij} = a_{ij} - a_{kj} \left(\frac{a_{ik}}{a_{kk}} \right) \left\{ \begin{array}{l} j=n+1, n, n-1, \dots, k \\ i=k+1, k+2, \dots, n \end{array} \right. \left\{ \begin{array}{l} k=1, 2, \dots, n-1 \\ a_{kk} \neq 0 \end{array} \right.$$

and the back-substitution by

$$x_n = \frac{a_{n,n+1}}{a_{nn}}$$

$$x_k = \frac{a_{i,n+1} - \sum_{j=i+1}^n a_{ij}x_j}{a_{ii}} \quad i=n-1, n-2, \dots, 1.$$

Note that the whole solution process requires about $n^3/3$ multiplications, $n^3/3$ additions and about $n^2/2$ divisions.

4.3.2.2 Gauss-Jordan Method

This is an extension of the Gauss elimination method and consists of three operations (1) initialization, (2) normalization and (3) forward and backward reduction by elimination. The initialization process is as for the Gauss elimination method. In normalization, a permanent change is made to the partitioned matrix by scaling each

row by its pivot element a_{ii} . The coefficient matrix part of the partitioned matrix is then reduced to an identity matrix by eliminating the offdiagonal elements of each row and column. The solution is given by the augmenting segment of the final partitioned matrix, i.e., the column corresponding to y in the initial matrix.

Using the previous example, we have that

$$A_*^{(0)} = [A : y] = \begin{bmatrix} 4 & 5 & 1 & \vdots & 2 \\ 1 & -2 & -3 & \vdots & 7 \\ 3 & -1 & -2 & \vdots & 1 \end{bmatrix}.$$

Next, normalize (or divide each element of) *row 1* by 4 to give $r^{(1)}$; subtract $a_{21} \times r^{(1)}$ from *row 2* and $a_{31} \times r^{(1)}$ from *row 3* to give

$$A_* = \begin{bmatrix} 1 & 1.25 & .25 & \vdots & .5 \\ 0 & -3.25 & -3.25 & \vdots & 6.5 \\ 0 & -4.75 & -2.75 & \vdots & -0.5 \end{bmatrix}.$$

Similarly, divide *row 2* by -3.25 to give $r^{(2)}$ and subtract $-4.75 \times r^{(2)}$ from *row 3* (forward reduction). We also subtract $1.25 \times r^{(2)}$ from *row 1* (backward reduction) yielding

$$A_* = \begin{bmatrix} 1 & 0 & -1 & \vdots & 3 \\ 0 & 1 & 1 & \vdots & -2 \\ 0 & 0 & 2 & \vdots & -10 \end{bmatrix}.$$

In the same fashion, normalize *row 3* by 2. Finally, subtract $1 \times r^{(3)}$ from *row 2* and $-1 \times r^{(3)}$ from *row 1* (backward reduction) to give the desired partitioned matrix

$$A_* = \begin{bmatrix} 1 & 0 & 0 & \vdots & -2 \\ 0 & 1 & 0 & \vdots & 3 \\ 0 & 0 & 1 & \vdots & -5 \end{bmatrix}$$

whose last column is the solution vector x . It is obvious that if the determinant of A is zero or if the pivot element a_{ii} is zero, then the above operations are not possible. This is also true for the Gauss elimination method discussed in the previous section. What is done in many practical solution schemes is to interchange rows or columns of A_* if the pivot elements are found to be zero or to use the largest coefficient in a row or column as pivot elements but such operations require a very good book-keeping system for the interchanges in order to reconstruct the correct solution.

4.3.2.3 LU (or Triangular) Decomposition Method

A square matrix A , can be written as a product of two other matrices L and U , i.e.,

$$A = LU = \begin{bmatrix} L_{11} & 0 & 0 \\ L_{21} & L_{22} & 0 \\ L_{31} & L_{32} & L_{33} \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}$$

$$= \begin{bmatrix} L_{11}u_{11} & L_{11}u_{12} & L_{11}u_{13} \\ L_{21}u_{11} & L_{21}u_{12} + L_{22}u_{22} & L_{21}u_{13} + L_{22}u_{23} \\ L_{31}u_{11} & L_{31}u_{12} + L_{32}u_{22} & L_{31}u_{13} + L_{32}u_{23} + L_{33}u_{33} \end{bmatrix}$$

where L is a lower-triangular matrix (i.e., has no non-zero element above the main diagonal) and U is an upper-triangular matrix (with no non-zero element below the main diagonal). Notice that both the elements u_{ii} and L_{ii} are contained in the main diagonal. Specifying either L_{ii} or u_{ii} allows us to determine the other elements of U and L . For example, let $u_{11} = u_{22} = \dots = 1$ (or alternatively, put $L_{11} = L_{22} = 1$) as in common practice, then

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = LU$$

$$= \begin{bmatrix} L_{11} & L_{11}u_{12} & L_{11}u_{13} \\ L_{21} & L_{21}u_{12} + L_{22}u_{22} & L_{21}u_{13} + L_{22}u_{23} \\ L_{31} & L_{31}u_{12} + L_{32}u_{22} & L_{31}u_{13} + L_{32}u_{23} + L_{33}u_{33} \end{bmatrix}$$

enabling the values of L_{ij} and u_{ij} to be easily determined. The procedure is simple. Starting from location a_{ii} ($i=1$), we work first down the i^{th} column and then along the i^{th} row finding the values of the system components L_{ij} and u_{ij} by comparison with the given coefficients of A . This in essence is Crout's algorithm for determining L and U . Having decomposed A , how do we proceed to solve the problem $Ax=y$? We note that the equation $A = LU$ implies that $Ax = LUx$ and therefore $Ax = L(Ux) = y$. We

therefore put $Ux = c$ and solve $Lc = y$ to obtain c . Finally, we solve $Ux = c$ to obtain x . Let us demonstrate how the method works by solving the problem $Ax=y$ where

$$A = \begin{bmatrix} 4 & 5 & 1 \\ 1 & -2 & -3 \\ 3 & -1 & -2 \end{bmatrix} \text{ and } y = \begin{bmatrix} 2 \\ 7 \\ 1 \end{bmatrix}.$$

Now, let $u_{11} = u_{22} = \dots = 1$ in the equation $A=LU$ so that

$$A = \begin{bmatrix} L_{11} & L_{11}u_{12} & L_{11}u_{13} \\ L_{21} & L_{21}u_{12} + L_{22} & L_{21}u_{13} + L_{22}u_{23} \\ L_{31} & L_{31}u_{12} + L_{32} & L_{31}u_{13} + L_{32}u_{23} + L_{33} \end{bmatrix} = \begin{bmatrix} 4 & 5 & 1 \\ 1 & -2 & -3 \\ 3 & -1 & -2 \end{bmatrix}.$$

From the first column of A (starting at location a_{11}), we notice that $L_{11}=4$, $L_{21}=1$ and $L_{31}=3$; and so for the rest of the first row (i.e., positions a_{12} and a_{13}) we have that $u_{12}=5/4=1.25$, $u_{13}=1/4=0.25$. Using these values and proceeding down the second column from location a_{22} , we find that $L_{22}=-3.25$ and $L_{32}=-4.75$. Working along the rest of the second row, we obtain $u_{23}=1$. Finally, from the third column, we have that $L_{33}=2$. The decomposition is therefore,

$$A = LU = \begin{bmatrix} 4 & 0 & 0 \\ 1 & -3.25 & 0 \\ 3 & -4.75 & 2 \end{bmatrix} \begin{bmatrix} 1 & 1.25 & 0.25 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{bmatrix}.$$

Let us now proceed to determine the solution. We have that

$$Lc = \begin{bmatrix} 4 & 0 & 0 \\ 1 & -3.25 & 0 \\ 3 & -4.75 & 2 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} = \begin{bmatrix} 2 \\ 7 \\ 1 \end{bmatrix}.$$

Working from the top (forward substitution), we have that $4c_1 = 2$ or $c_1 = 0.5$. From the next row, we obtain $c_2 = -2$. The last unknown is then determined as $c_3 = -5$. Using these values determined for c , we solve for x in the system $Ux=c$, i.e.,

$$Ux = \begin{bmatrix} 1 & 1.25 & 0.25 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} .5 \\ -2 \\ -5 \end{bmatrix}.$$

By back-substitution (starting from the bottom), we find that $x_3 = -5$, $x_2 = 3$ and $x_1 = -2$ which agrees with the results obtained using the other methods of solution.

It is possible to develop a computational formula for the above *LU* decomposition operations. Recall that the first thing we did during the decomposition of A was to set $u_{ii} = 1$, for $i = 1$ to n . We then found the values of L_{i1} (elements of the first column, $i = 1, \dots, n$) as $L_{i1} = a_{i1}$ and the corresponding row elements as $u_{1j} = a_{1j}/L_{11}$. These, and subsequent column and row manipulations, are described by the formula

$$L_{ij} = a_{ij} - \sum_{k=1}^{j-1} L_{ik} u_{kj}$$

for each $i = 1, \dots, n$ and

$$u_{ij} = \frac{1}{L_{ii}} \left(a_{ij} - \sum_{k=1}^{i-1} L_{ik} u_{kj} \right) \quad j = i+1, \dots, n.$$

where the summation terms are set equal to zero in the first column and row manipulations. Note that the scheme breaks down when the determinant of A (or L_{ii}) is zero. To prevent any undesirable effects in *LU* decompositions, it is thus important to employ a partial pivoting technique in which rows are interchanged. This is an effective stabilization measure and is described in most standard texts.

4.3.2.4 Generalized matrix inversion

Although it is rewarding to understand the various ways of solving a linear problem, quite often we seek a general strategy for solving such problems. The main task in the development of a general purpose linear solution package is finding a single routine for inverting the given matrix A or $G^T G$. Fortunately, there are many published routines in the literature that can accomplish this task (see e.g., Press et al., 1986) making program development easy; we simply provide a control unit or driver program for the available subroutines. For illustration, an inversion program LINPACK incorporating a generalized matrix inversion routine is given in Fig. 4.3.2.

program LINPACK

- c A simple demonstration of the amalgamation of existing subroutines
- c and a driver unit forming a general purpose linear inversion package.
- c n= no. data(max=20); m= no. parameters(max=10).

c Data entered on-line or read from diskfile containing n lines of field data (d)
c followed by m rows of the design matrix components (G).
c Author: Max A. Meju
c-----
dimension d(20),Gt(10,20),G(20,10),Gtd(10),xm(10)
dimension A(10,10),wksp1(10),wksp2(10)
character*1 ans,infile*20
c
write(*,*) ' Enter no. of rows & columns in G: NROW,NCOL'
read(*,*)n,m
write(*,'(A,\$)')' Are your data stored in a file ? Y:N '
read(*,'(A)')ans
if(ans.eq.'Y'.or.ans.eq.'y')then
write(*,*)' Enter INPUT filename '
read(*,'(A20)')infile
open(unit=3,file=infile,status='old')
ichan=3
else
ichan=5
write(*,*) ' Now enter Field data d, one at a time'
endif
do 10 i=1,n
read(ichan,*) d(i)
10 continue
if(ans.ne.'Y'.or.ans.ne.'y')then
write(*,*)' Now enter G-matrix row by row'
endif
do 20 i=1,n
read(ichan,*)(G(i,j),j=1,m)
20 continue
if(ichan.EQ.3)then
close(unit=3,status='keep')
endif
c next form G-transpose, get Gt*d, GtG=A, and A-inverse
do 30 i=1,n
do 40 j=1,m

```

        Gt(j,i)=G(i,j)
40    continue
30    continue
      call inprod(10,20,m,n,Gt,d,Gtd)
      call mxprod(10,20,m,n,Gt,G,A)
call generalized matrix inversion routine
      CALL INVERT(10,m,A,wksp1,wksp2)
c finally, calculate solution vector, xm
      call inprod(10,20,m,n,A,Gtd,xm)
c compute errors and print results
      do 50 i=1,m
         write(*,*)xm(i)
50    continue
      stop
      end

c-----
      subroutine INPROD(mm,nn,m,n,A,x,y)
      dimension x(nn),y(nn),A(mm,nn)
c matrix A multiplied by vector x, returns vector y
      do 30 i=1,m
         sum=0.0
         do 40 j=1,n
            sum=x(j)*A(i,j)+sum
40      continue
         y(i)=sum
30      continue
      return
      end

c-----
      subroutine MXPROD(mm,nn,m,n,A,B,C)
c matrix multiplication: A*B=C
      dimension A(mm,nn),B(nn,mm),C(mm,mm)
      do 10 i=1,m
         do 20 j=1,m
            sum=0.0
            do 30 k=1,n

```

```
        sum=sum+A(i,k)*B(k,j)
30    continue
      C(i,j)=sum
20    continue
10    continue
      return
      end
c-----
C-----  
SUBROUTINE INVERT (NN,N,A,B,C)  
C INVERSION OF NONSYMMETRIC MATRIX A  
DIMENSION A(NN,NN),B(NN),C(NN)  
C N=SIZE OF GIVEN MATRIX,N>1  
C B AND C ARE WORKING SPACE VECTORS  
c adapted from Akin, J.E., 1986: Finite Element Analysis for  
c undergraduates, Academic Press, p.20.  
N1=N-1  
A(1,1)=1./A(1,1)  
DO 11 M=1,N1  
  K=M+1  
1  DO 3 I=1,M  
    SUM=0.0  
    DO 2 J=1,M  
2  SUM=SUM+A(I,J)*A(J,K)  
3  B(I)=SUM  
  D=0.0  
  DO 4 I=1,M  
4  D=D+A(K,I)*B(I)  
  D= -D + A(K,K)  
  A(K,K) = 1./D  
  DO 5 I=1,M  
5  A(I,K)=-B(I)*A(K,K)  
  DO 7 J=1,M  
    SUM=0.0  
    DO 6 I=1,M  
6  SUM=SUM+A(K,I)*A(I,J)  
7  C(J)=SUM
```

```

DO 8 J=1,M
8   A(K,J)=-C(J)*A(K,K)
DO 10 I=1,M
DO 9 J=1,M
9   A(I,J)=A(I,J)-B(I)*A(K,J)
10  CONTINUE
11  CONTINUE
      RETURN
END

```

Fig. 4.3.2. A linear inversion package incorporating pre-existing routines.

It was mooted previously that the Gauss methods and LU decomposition technique require additional stabilization measures to be effective in general terms. What was not mentioned then is that these algorithms do not furnish us with diagnostic information about the cause of any undesirable effects. A more illuminating and robust matrix inversion technique is furnished by the singular value decomposition method. For example, singular problems can sometimes be turned into non-singular ones by this method without any added sophistication unlike the other solution methods (see Press et al., 1986, p.20). As we shall see later on, it also allows us to pin-point what the problem is and is thus the favoured approach in least squares inversion of geophysical data.

4.3.2.5 The singular value decomposition (*SVD*) of a matrix

An $n \times n$ or $n \times p$ matrix G , say, can be factored into a product of three other matrices :

$$G = U\Lambda V^T \quad (4.11)$$

where for n data and p parameters, $U_{(n \times p)}$ and $V_{(p \times p)}$ are respectively the data space and parameter space eigenvectors, and Λ is a $p \times p$ diagonal matrix containing at most r non-zero eigenvalues of G , with $r \leq p$. These diagonal entries in Λ ($\lambda_1, \lambda_2, \dots, \lambda_p$) are called the singular values of G . This factorisation is known as the singular value (or spectral) decomposition *SVD* of G (Lanczos, 1961). If the eigenvalues of a matrix are small, the matrix is said to be **ILL-CONDITIONED**. The SVD method is

very popular with geophysical data analysts because it is mathematically robust and numerically stable and also provides other vital information on the state of the model and data thus enabling model resolution and covariance studies.

Application of SVD to Generalized Matrix Inversion

The least squares solution to the inverse problem of the form $d = Gm$ is given by

$$\hat{m} = (G^T G)^{-1} G^T d$$

where the quantity $[(G^T G)^{-1} G^T]$ operates on d to recover \hat{m} . This operator, the least squares generalized inverse, is akin to the G^{-1} (G-inverse) for perfect data (described above). The SVD technique is commonly used in geophysics for solving the NORMAL EQUATIONS for the least squares estimates \hat{m} .

Let us know express the above inversion formula in terms of the SVD of G . We have that $G^T = V \Lambda U^T$. Thus,

$$G^T G = V \Lambda U^T \cdot U \Lambda V^T = V \Lambda^2 V^T$$

since $U^T U = I$. The inverse of this matrix is simply $(G^T G)^{-1} = V \Lambda^{-2} V^T$. The generalized inverse is then given by

$$(G^T G)^{-1} G^T = V \Lambda^{-2} V^T \cdot V \Lambda U^T = V \Lambda^{-1} U^T$$

since $V^T V = I$.

Note that the generalized inverse may also be derived in the following simple fashion:

$$(G^T G)^{-1} = G^{-1} (G^T)^{-1} = V \Lambda^{-1} U^T \cdot U \Lambda^{-1} V^T = V \Lambda^{-2} V^T$$

so that

$$(G^T G)^{-1} G^T = G^{-1} (G^T)^{-1} G^T \cong G^{-1} = V \Lambda^{-1} U^T.$$

In any case, the least squares solution is given by

$$\boxed{\hat{m} = (G^T G)^{-1} G^T d = V \Lambda^{-1} U^T d} \text{ or simply } \boxed{\hat{m} = \left(\frac{V}{\Lambda} \right) \times (U^T d)} \quad (4.12)$$

↑ ↑ ↑
vector matrix vector

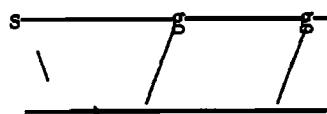
Equation (4.12) is programmed in routine applications. A comprehensive linear inversion program SVDINV (see Meju, 1994a) using the SVD method is given in Appendix A and will be used for demonstrating various techniques of parameter estimation and uncertainty analysis.

4.4 Sample Applications of Unconstrained Inversion

We will apply eq. (4.10) to three simple cases to illustrate its usefulness:- (i) a simple seismic refraction straight line problem, (ii) determination of the average density of the Earth, and (iii) a simple delay-time seismic experiment (basic time-term analysis).

Example 4.4.1 : The straight line problem : Interpretation of seismic refraction data.
Given the following seismic refraction travel-time data (see Table 4.1.1),

x_i (m)	t_i (msec)
2	5.1
4	9.2
6	11.9
8	14.9



determine the wave velocity in the subsurface. Compare your result with that obtained graphically.

Solution:

Recall that the equation of a straight line is given by $y=a+bx$. In the notation used in this section, this can be re-written as

$$d_i = m_1 + m_2 x_i;$$

so that the matrix equation $\mathbf{d}=\mathbf{G}\mathbf{m}$ is of the form

$$\begin{bmatrix} d_1 \\ d_2 \\ \vdots \\ d_n \end{bmatrix} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \end{bmatrix}$$

We need the matrix products $\mathbf{G}^T \mathbf{G}$ and $\mathbf{G}^T \mathbf{d}$ to determine $\hat{\mathbf{m}}$. These are given by

$$G^T G = \begin{bmatrix} 1 & 1 & \dots & 1 \\ x_1 & x_2 & \dots & x_n \end{bmatrix} \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} = \begin{bmatrix} n & \Sigma x_i \\ \dots & \dots \\ \Sigma x_i & \Sigma x_i^2 \end{bmatrix}$$

and

$$G^T d = \begin{bmatrix} 1 & 1 & \dots & 1 \\ x_1 & x_2 & \dots & x_n \end{bmatrix} \begin{bmatrix} d_1 \\ d_2 \\ \vdots \\ d_n \end{bmatrix} = \begin{bmatrix} \Sigma d_i \\ \Sigma x_i d_i \end{bmatrix}$$

Thus the least squares solution is given by

$$\hat{m} = [G^T G]^{-1} G^T d = \begin{bmatrix} n & \Sigma x_i \\ \Sigma x_i & \Sigma x_i^2 \end{bmatrix}^{-1} \begin{bmatrix} \Sigma d_i \\ \Sigma x_i d_i \end{bmatrix}$$

How do we obtain $[G^T G]^{-1}$?

In this case, we are dealing with a 2×2 matrix since Σx , Σx^2 , and n are just single numbers. We may therefore use the procedure outlined in Section 4.3.1 to obtain the inverse of $G^T G$ as

$$[G^T G]^{-1} = \frac{1}{|G^T G|} \cdot B$$

where

$$|G^T G| = n\Sigma x^2 - \Sigma x \Sigma x$$

and

$$B = \begin{bmatrix} \Sigma x^2 & -\Sigma x \\ -\Sigma x & n \end{bmatrix}$$

Thus,

$$\begin{bmatrix} m_1 \\ m_2 \end{bmatrix} = \frac{1}{n\Sigma x^2 - (\Sigma x)^2} \begin{bmatrix} \Sigma x^2 & -\Sigma x \\ -\Sigma x & n \end{bmatrix} \begin{bmatrix} \Sigma d \\ \Sigma x d \end{bmatrix}$$

or simply (if we replace d in $G^T d$ with t)

$$m_1 = \frac{\Sigma t \Sigma x^2 - \Sigma x \Sigma xt}{n \Sigma x^2 - (\Sigma x)^2}; \text{ and } m_2 = \frac{n \Sigma xt - \Sigma x \Sigma t}{n \Sigma x^2 - (\Sigma x)^2}.$$

Notice that the above solution is exactly the same as that of eq. 4.6 (Section 4.1). Therefore from Table 4.1.1, $n=4$, $\Sigma x=20$, $\Sigma t=41.1$, $\Sigma xt=237.6$ and $\Sigma x^2=120$; and we find that $m_1=2.25$ and $m_2=1.605$. Thus, $v = \frac{1}{m_2} = 623.053 \text{ m/s}$.

Example 4.4.2 : Determination of the average density of the Earth

Given that the earth's mass and moment of inertia are both related to the density distribution within it, can we estimate the average density of the earth from measurements of its total mass and moment of inertia? This inverse problem (adapted from K.A.Whaler, 1986, unpublished) is overdetermined since there are two measured data and we seek only one model parameter.

Preliminaries:

Our elementary forward theory tells us that

$$\text{mass of earth, } M = \frac{4}{3}\pi R^3 \bar{\rho}$$

and

$$\text{moment of inertia, } I = \frac{2}{5}MR^2 = \frac{8}{15}\pi R^5 \bar{\rho}$$

where M and I are measurable quantities (which serve as our data in this inverse problem). Let us introduce a useful practical concept at this juncture. Notice from the above forward relations that the two types of data differ in magnitude by a factor of about R^2 . Since we are trying to retrieve a common parameter, $\bar{\rho}$ from the joint measurements, M and I , it is desirable to normalize them to a common-scale by scaling the measurement of the moment of inertia by R^2 , say. Our working equations would then look like

$$d_1 = \frac{4}{3}\pi R^3 \bar{\rho} \quad \text{and} \quad d_2 = \frac{\frac{8}{15}\pi R^5 \bar{\rho}}{R^2} = \frac{8}{15}\pi R^3 \bar{\rho}.$$

Let us now define the interpretive data for this illustrative exercise. We will use the data given in Lambeck (1980, Table 2.5) as our field measurements, namely:

$R=6.371 \times 10^6$ m, the mean radius of the earth; $M=5.974 \times 10^{24}$ kg; and for simplicity we will assume that $I/MR^2=0.33$. Thus, our chosen set of data consists of

$$d_1 = \text{Mass of the Earth} = 5.9740 \times 10^{24} \text{ kg}$$

and

$$d_2 = \frac{\text{moment of inertia}}{R^2} = 1.97142 \times 10^{24} \text{ kg} .$$

This completes the data preparation operations and we may now proceed to solve the inverse problem.

Solution:

First, form $d=Gm$

$$\begin{pmatrix} 5.9740 \times 10^{24} \\ 1.97142 \times 10^{24} \end{pmatrix} = \begin{pmatrix} \frac{4}{3}\pi R^3 \\ \frac{8}{15}\pi R^3 \end{pmatrix}(\bar{\rho}) = K \begin{pmatrix} 5 \\ 2 \end{pmatrix} \bar{\rho} .$$

$\overset{\uparrow}{d} \quad \overset{\uparrow}{G} \quad \overset{\uparrow}{m} \quad \overset{\uparrow}{\overbrace{Gm}}$

$$\text{where } K = \frac{4}{15}\pi R^3 = 2.166414 \times 10^{20} \text{ m}^3.$$

Next form $G^T G$ and find the generalised inverse $(G^T G)^{-1}$

$$G^T G = K^2 [5 \ 2] \begin{bmatrix} 5 \\ 2 \end{bmatrix} = K^2(25+4) = 29K^2 \leftarrow \text{just a number.}$$

Notice that $G^T G$ is just a number here and so its inverse is simply

$$(G^T G)^{-1} = \frac{1}{29K^2} .$$

Now, obtain $G^T d$ as

$$G^T d = K[5 \ 2] \begin{bmatrix} 5.9740 \times 10^{24} \\ 1.97142 \times 10^{24} \end{bmatrix} = K \times 33.813 \times 10^{24} \leftarrow \text{just a number.}$$

Finally, obtain the least squares solution for the average density $\bar{\rho}=\hat{m} = (G^T G)^{-1} G^T d$. This is simply

$$\bar{\rho} = \left(\frac{1}{29 \times K^2} \right) (K \times 33.813 \times 10^{24}) = 5382 \text{ kgm}^{-3}.$$

Example 4.4.3 : A simplified seismic refraction time-term analysis.

Consider the refraction seismology delay-time experiment in which two shots S_1 and S_2 , are recorded at three receiver positions R_1 , R_2 and R_3 as illustrated in Fig. 4.4.3.1. The subsurface structure consists of two layers of velocity v_0 and v_1 (where $v_1 > v_0$). The travel-time between a shot and a receiver on the surface t_{ij} is given by

$$t_{ij} = \frac{x_{ij}}{v_1} + \delta_i + \gamma_j \quad \longleftrightarrow \text{forward model}$$

where x_{ij} is the horizontal distance between shot and receiver positions and δ_i and γ_j are the delay times associated with the i^{th} shot and the j^{th} receiver positions.

For a particular experiment, the following results were obtained (Hatton, Worthington and Makin, 1986).

(i, j)	(t_{ij})	(x_{ij})
1,1	2.323	6.000
1,2	2.543	6.708
1,3	2.857	8.485
2,1	2.640	7.616
2,2	2.529	7.000
2,3	2.553	7.616

Table 4.4.3.1 Seismic travel-time data.

It is required to obtain the velocity v_1 and the delay parameters δ and γ from these travel-time data. Formulate and solve this problem using the generalised matrix inversion method.

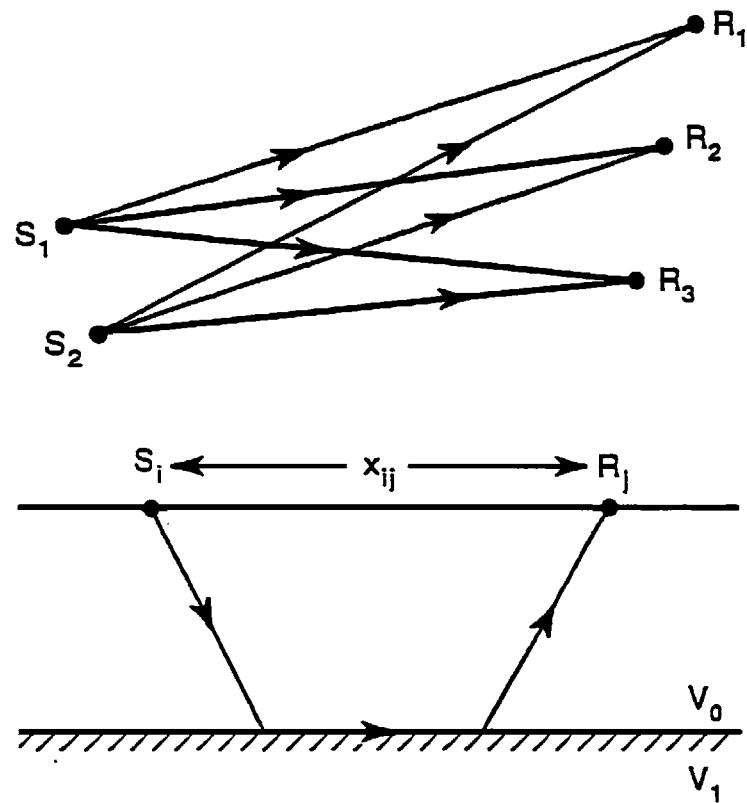


Fig. 4.4.3.1 A simple delay-time experiment (after Hatton et al., 1986)

A suggested solution process:

According to this model, for each shot S_i , the observation at the three recording positions R_j must satisfy $t_{ij} = \frac{x_{ij}}{v_1} + \delta_i + \gamma_j$. Thus,

$$t_{i1} = \frac{x_{i1}}{v_1} + \delta_i + \gamma_1$$

$$t_{i2} = \frac{x_{i2}}{v_1} + \delta_i + \gamma_2$$

$$t_{i3} = \frac{x_{i3}}{v_1} + \delta_i + \gamma_3.$$

Consequently, for the two shots S_1 and S_2 the model parameters of the problem are $\delta_1, \delta_2, \gamma_1, \gamma_2, \gamma_3$, and $\frac{1}{v_1}$ (or v_1) and the matrix formulation of the problem is simply

$$\begin{bmatrix} t_{11} \\ t_{12} \\ t_{13} \\ t_{21} \\ t_{22} \\ t_{23} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 1 & 0 & 0 & x_{11} \\ 1 & 0 & 0 & 1 & 0 & x_{12} \\ 1 & 0 & 0 & 0 & 1 & x_{13} \\ 0 & 1 & 1 & 0 & 0 & x_{21} \\ 0 & 1 & 0 & 1 & 0 & x_{22} \\ 0 & 1 & 0 & 0 & 1 & x_{23} \end{bmatrix} \begin{bmatrix} \delta_1 \\ \delta_2 \\ \gamma_1 \\ \gamma_2 \\ \gamma_3 \\ 1/v_1 \end{bmatrix} \quad (4.13)$$

$d \qquad \qquad G \qquad \qquad m$

Note that x_{ij} appear only in the design matrix (kernel) since they describe the geometry of the experiment and are not considered as data in the equation $d=Gb$.

Now proceed to solve the problem:

first, calculate the SVD of G ,

next, find $\frac{V}{\Lambda} = VQI$, find $U^T d$ and then obtain m as $VQI * U^T d$.

The results of the decomposition of G are summarised in Fig. 4.4.3.2. below.

Singular Values, Λ ($\lambda_i = q_i$)

17.97092

1.732372

0.1539608

6.7762068E-07 $\leftarrow \lambda_4$ near-zero; will cause problems when inverted

1.420821

1.414207

U-tranpose matrix (U^T)

-0.3373460	-0.3764554	-0.4749875	-0.4267564	-0.3927588	-0.4271839
0.4197269	0.4190062	0.4152228	-0.3976767	-0.3971975	-0.3999271
-0.5317655	-0.00106414	0.4531686	0.4847122	-0.04687573	-0.5241370
0.2695436	-0.5769362	0.3073922	-0.2695442	0.5769363	-0.3073921
-0.3377683	-0.3011901	0.5493414	-0.3341068	-0.3062310	0.5366699
0.4904181	-0.5090613	0.01867663	0.4904131	-0.5090622	0.018678255

 V -matrix divided by Λ ($V/\Lambda = VQI$).

-0.0036809710	0.4178268	-3.360666	659978.2	-0.044392757	0.000016756792
-0.0038603232	-0.3981171	-3.640744	659976.2	-0.051352862	0.000016076374
-0.0023659754	0.00734722	-1.985073	-659977.9	-0.3328176	0.4904165
-0.002381803	0.00726665	-2.022428	-659974.2	-0.3008910	-0.5090644
-0.002793490	0.00509664	-2.993924	-659975.8	0.5379646	0.018677600
-0.055216759	-0.00090729	0.8023227	-0.1106218	0.0065730996	-0.0000021703945

Fig. 4.4.3.2 Results of SVD calculations.

The least squares estimates of the sought parameters are:

$$\delta_1 = -532.811, \delta_2 = -532.89, \gamma_1 = 533.63, \gamma_2 = 533.68, \gamma_3 = 533.55, \frac{1}{v} = 0.250$$

Notice that all but the slowness parameter estimates are unrealistic. The correct estimated values of the model parameters are (cf. Hatton et al., 1986) :

$$\delta_1 = 0.433, \delta_2 = 0.346, \gamma_1 = 0.391, \gamma_2 = 0.433, \gamma_3 = 0.304, \frac{1}{v} = 0.250$$

So what was the problem in our present calculations ? A glance at the values of the singular values (λ) will reveal that the value corresponding to fourth parameter of the problem is near-zero (6.7762068E-07) and that the elements of the corresponding column of the matrix VQI have almost constant values ($\approx \pm 659978$). The value of λ_4 is most probably an artifact of the computer used (round-off error !). This highlights

one of the problems faced during numerical matrix inversion - small eigenvalues cause a great deal of problem and the corresponding parameter and columns or rows of associated matrices should be deleted from the interpretation process or some form of problem regularisation measure introduced. This subject will be explored in detail in Section 5.

It is also obvious from these results that only the velocity can be accurately determined. The delay times may not be uniquely determined using the unconstrained solution process required by our original problem formulation (eq. 4.13). This is so because an alteration of the value of δ followed by a compensating adjustment in the values of γ will leave the system of equations (4.13) unaffected (see Hatton et al., 1986). However, it is comforting to know that the remedy to this problem is simply to specify *a priori* the value of one of the delay times. This helps constrain the least squares solution process by acting more or less like a 'path-finder' enabling the rest to be safely found ! The subject of constrained inversion will be examined in the following discussions but first, let us find out how much we have learnt so far in the form of an exercise.

4.5 PROBLEM SESSION

- 4.5.1 Given the following borehole temperature data, find the slope and intercept on the z-axis and hence predict the temperature at a depth of 390m.

Depth, z (m)	Temp, $t(^{\circ}\text{C})$
30	25.0
70	26.2
180	29.7
250	34.3
300	35.5

5. CONSTRAINED LINEAR LEAST SQUARES INVERSION

In many geophysical problems it is possible to generate a set of completely different solutions that adequately explains the experimental data, especially where measurement errors are present. Ultimately, one solution has to be selected as the 'best' or most feasible answer to the problem. To do this we have to add to the problem some information not contained in the original equation $d = Gm$. This extra information is referred to as *a priori* information and serves to constrain our solutions so as to satisfy any of our quantified expectations of the model parameters. A priori information can take several forms. It may represent previously obtained geophysical, borehole or geological data or may simply be dictated by the physics of the problem. Consequently, constrained inversion takes many forms.

5.1 Inversion with prior information

We can incorporate previously obtained information about the sought model parameters in our problem formulation. This external information could be in the form of results from previous experiments or quantified expectations dictated by the physics of the problem. Generally, these external data help to single out a unique solution from among all equivalent ones (and it may be noted that our initial definition of what may be termed 'data' has now been revised to include prior parameter estimates). The solution process is said to be constrained. The procedure is simple. The constraining equations (data) are arranged to form an expression of the form

$$Dm = h$$

where D is a matrix (with all the off-diagonal elements equal to zero) that operates on the model parameters m to yield or preserve the *a priori* values of m that are contained in the vector h . The equation $Dm = h$ means that we are employing linear equality constraints that are to be satisfied exactly. The mathematical development is straightforward. We wish to bias m , towards h .

We simply *minimize*

$$\phi = (d - Gm)^T(d - Gm) + \beta^2(Dm - h)^T(Dm - h). \quad (5.1)$$

Setting to zero the derivatives of ϕ with respect to the model parameters m we find that

$$2G^T Gm - 2G^T d + 2\beta^2 D^T Dm - 2\beta^2 D^T h = 0$$

giving

$$(G^T G + \beta^2 D^T D)m = G^T d + \beta^2 D^T h \quad \leftarrow \text{Normal equations}$$

or if D is the identity matrix

$$(G^T G + \beta^2 I) \mathbf{m} = (G^T d + \beta^2 h) \quad \longleftrightarrow \text{Normal equations}$$

from which we obtain the constrained solution

$$\hat{\mathbf{m}}_c = (G^T G + \beta^2 I)^{-1} (G^T d + \beta^2 h) \quad (5.2)$$

This is the constrained linear inversion formula. The method is also referred to as the biased linear estimation technique. Its main advantage is that it helps single out a unique solution out of the infinitely many plausible solutions to an overdetermined problem in the presence of observational errors or uncertainties. However, this procedure should only be used when it is reasonably justified since it may produce undesirable effects when h is unrealistic (see Twomey, 1977).

5.1.1 Implementation.

The constraints are implemented by arranging the constraining equations as rows in the original data equation $d=Gm$. The auxiliary parameter β is chosen by trial and error. β is called an undetermined or Lagrange multiplier. This solution process may thus be referred to as a Lagrange multiplier method.

5.1.2 Formulating constraining equations

The equation $Dm=h$ is generally of the form

$$\begin{bmatrix} 1 & & \\ & \ddots & \\ & & 1 \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \\ \vdots \\ m_p \end{bmatrix} = \begin{bmatrix} h_1 \\ h_2 \\ \vdots \\ h_p \end{bmatrix} \quad (5.3)$$

However, the structure can be modified as required. For example, if only one parameter value is known, we do not need the full set-up above. We simply require

$$\begin{bmatrix} 1 & 0 & \dots & 0 \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \\ \vdots \\ m_p \end{bmatrix} = [h_{\text{known}}] \longleftrightarrow \text{just a number, not a vector.} \quad (5.4)$$

If, on the other hand, we know the first and fourth parameter values for a four-parameter problem say, the full constraining equations will be

$$\begin{bmatrix} 1 & 0 & 0 & 1 \\ & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \\ m_3 \\ m_4 \end{bmatrix} = \begin{bmatrix} h_1 \\ 0 \\ 0 \\ h_4 \end{bmatrix} \quad (5.5)$$

but in practice only the first and fourth rows of the constraining equations are really necessary. The appropriate equations are then appended onto the initial equation $Gm=d$. Operationally, we only need to add the extra rows of *a priori* data onto G and d , e.g., for the case represented by eq. 5.4 we simply add the row [1 0 ... 0] onto the bottom of the G matrix and the known value of a parameter [h_{known}] onto the bottom of the actual field data d . Where desired, both D and h are premultiplied by β (usually chosen to be less than or equal to unity). The constrained solution is obtained using the procedures outlined in Section 4.

5.1.3 Sample Applications of Constrained Inversion

Examples of applications of constrained inversion with prior data are given below to facilitate a practical understanding of all the concepts highlighted in the preceding discussions.

Example 5.1.1: Constrained fitting of a straight line to seismic refraction data
 Suppose that we are interested in fitting a straight line $d_i = m_1 + m_2 x_i$ (or in collective form $d = Gm$ (where $m = [m_1, m_2]^T$) to seismic refraction first arrivals represented by the data pairs $(\{x_i, t_i\}, i=1, n)$. Now let us assume that we have prior information or reason to believe that the fitted line must pass through a particular point with coordinates (x_c, t_c) , say the origin. We can constrain the least squares solution process to satisfy this *a priori* information or assumption. The procedure is illustrated below.

For the straight line problem, we have two model parameters - the intercept m_1 and slope m_2 . Suppose that we want the line to pass through (x_c, t_c) . That is, we have one constraint (note that you may impose a number of constraints) on the problem. The constraining equation $Dm=h$ will therefore be of the form

$$[1 \ x_c] \begin{bmatrix} m_1 \\ m_2 \end{bmatrix} = [t_c]$$

$\overset{\uparrow}{D}$ $\overset{\uparrow}{m}$ $\overset{\uparrow}{h}$

This equation is then appended onto the original data equations $d=Gm$ and the whole system solved for the constrained least squares solution (the desirable regression line). Note that this additional row of extraneous (constraining) data would mean that our original expressions for $G^T G$ and $G^T d$ in the unconstrained inverse problem (Example 4.2) will need to be modified somewhat to:

$$(G^T G + \beta^2 I) = \begin{bmatrix} n & \sum x_i : 1 \\ \sum x_i & \sum x_i^2 : x_c \\ \dots & \dots \\ 1 & x_c : 0 \end{bmatrix} \quad \text{← augmenting equations}$$

and

$$(G^T d + \beta^2 h) = \begin{bmatrix} \sum t_i \\ \sum x_i t_i \\ \dots \\ t_c \end{bmatrix} \quad \text{← augmenting equation}$$

where we have assigned a value of unity to β .

The constrained least squares solution for the straight line through (x_c, t_c) is therefore

$$\hat{m}_c = \begin{bmatrix} m_1 \\ m_2 \\ \beta \end{bmatrix} = \begin{bmatrix} n & \sum x_i & 1 \\ \sum x_i & \sum x_i^2 & x_c \\ 1 & x_c & 0 \end{bmatrix}^{-1} \begin{bmatrix} \sum t_i \\ \sum x_i t_i \\ t_c \end{bmatrix}$$

Illustrative Exercise.

Using the data given in Table 4.1.1, obtain the parameters of the best-fitting line that passes through the point $(x_c=8, y_c=14.9)$.

Solution procedure :

The main task here is to determine the inverse of the 3×3 matrix $(G^T G + \beta^2 I)$. This can be done using the procedure outlined in Section 4.3.1. The elements of the matrix of cofactors of $(G^T G + \beta^2 I)$ are:

$$c_{11} = \left| \begin{matrix} \Sigma x^2 & x_c \\ x_c & 0 \end{matrix} \right| = -x_c^2 ; \quad c_{12} = - \left| \begin{matrix} \Sigma x & x_c \\ 1 & 0 \end{matrix} \right| = x_c ; \quad c_{13} = \left| \begin{matrix} \Sigma x & \Sigma x^2 \\ 1 & x_c \end{matrix} \right| = x_c \Sigma x - \Sigma x^2 ;$$

$$c_{21} = - \left| \begin{matrix} \Sigma x & 1 \\ x_c & 0 \end{matrix} \right| = x_c ; \quad c_{22} = \left| \begin{matrix} n & 1 \\ 1 & 0 \end{matrix} \right| = -1 ; \quad c_{23} = - \left| \begin{matrix} n & \Sigma x \\ 1 & x_c \end{matrix} \right| = \Sigma x - nx_c ;$$

$$c_{31} = \left| \begin{matrix} \Sigma x & 1 \\ \Sigma x^2 & x_c \end{matrix} \right| = x_c \Sigma x - \Sigma x^2 ; \quad c_{32} = - \left| \begin{matrix} n & 1 \\ \Sigma x & x_c \end{matrix} \right| = \Sigma x - nx_c ; \quad c_{33} = \left| \begin{matrix} n & \Sigma x \\ \Sigma x & \Sigma x^2 \end{matrix} \right| = n \Sigma x^2 - (\Sigma x)^2 .$$

Therefore,

$$C = \begin{bmatrix} -x_c^2 & x_c & (x_c \Sigma x - \Sigma x^2) \\ x_c & -1 & (\Sigma x - nx_c) \\ (x_c \Sigma x - \Sigma x^2) & \Sigma x - nx_c & n \Sigma x^2 - (\Sigma x)^2 \end{bmatrix}$$

Notice that

$$C^T \equiv C .$$

We then obtain the required determinant as

$$\begin{aligned} \det(G^T G + \beta^2 I) &= |G^T G + \beta^2 I| = n(\Sigma x^2 \cdot 0 - x_c^2) - \Sigma x(0 - x_c) + 1.(x_c \Sigma x - \Sigma x^2) \\ &= 2x_c \Sigma x - \Sigma x^2 - nx_c^2 . \end{aligned}$$

so that the constrained least squares solution is given by

$$m_c = \begin{bmatrix} m_1 \\ m_2 \\ \beta \end{bmatrix} = \frac{1}{2x_c \Sigma x - \Sigma x^2 - nx_c^2} [C^T] \begin{bmatrix} \Sigma t \\ \Sigma xt \\ t_c \end{bmatrix}$$

We can now determine the values of m that will satisfy the constraint ($x_c = 8, t_c = 14.9$) . Using the data from Table 4.1.1, we have that

$$(G^T d + \beta^2 h) = \begin{bmatrix} 41.1 \\ 237.6 \\ 14.9 \end{bmatrix}$$

$$|G^T G + \beta^2 I| = 2(8 \times 20) - 120 - (4 \times 64) = -56$$

$$C^T = \begin{bmatrix} -64 & 8 & 40 \\ 8 & -1 & -12 \\ 40 & -12 & 80 \end{bmatrix}$$

Therefore,

$$\begin{bmatrix} m_1 \\ m_2 \\ \beta \end{bmatrix} = \frac{1}{-56} \begin{bmatrix} -64 & 8 & 40 \\ 8 & -1 & -12 \\ 40 & -12 & 80 \end{bmatrix} \begin{bmatrix} 41.1 \\ 237.6 \\ 14.9 \end{bmatrix}.$$

So the slope of the best-fitting line passing through the point (x_c, t_c) is

$$m_2 = \frac{-87.6}{-56} = 1.564285714 ; (v = 1/m_2 = 639.27 \text{ m/s})$$

with the intercept on the time-axis given by :

$$m_1 = \frac{-133.6}{-56} = 2.385714286 .$$

Finally, test the solution for consistency using the relation $\hat{t} = m_1 + m_2 \hat{x}$. We have that

$$\hat{t}_{x=8} = 2.385714286 + (1.564285714 \times 8) = 14.9$$

which means that our estimates for the model parameters m satisfy the constraints. These results can be verified using the inversion programs **Craminv**, **Linpack** or **Svdinv**. Note that **Craminv** can be used to solve this problem; we have to input $(G^T d + \beta h)$ as the y -vector and the matrix $(G^T G + \beta I)$ as the A -matrix, i.e.,

$$A = \begin{bmatrix} n & \Sigma x_i & 1 \\ \Sigma x_i & \Sigma x_i^2 & x_c \\ 1 & x_c & 0 \end{bmatrix} = \begin{bmatrix} 4 & 20 & 1 \\ 20 & 120 & 8 \\ 1 & 8 & 0 \end{bmatrix}.$$

This will yield the solution: $m_1 = 2.385714; m_2 = 1.564286; \beta = .2714308$.

Example 5.1.2 : Constrained seismic refraction time-term analysis. (of Example 4.4.3)

Consider the refraction seismology delay-time problem of Example 4.4.3. Let us constrain the problem by specifying one of the delay-time and see if a unique solution can be obtained for all six parameters of the inverse problem. Assuming that we know the value of δ_1 , how would we formulate and solve the constrained problem for the six parameters ?

Firstly, the required constraining equation is similar to eq. 5.4 and given by

$$[\delta_1] = [1 \ 0 \ 0 \ 0 \ 0 \ 0] \begin{bmatrix} \delta_1 \\ \delta_2 \\ \gamma_1 \\ \gamma_2 \\ \gamma_3 \\ 1/v_1 \end{bmatrix}$$

↑
0.433

The structure of the augmented G and d is shown in Fig. 5.1.1 while the results of the application of the SVD method to the system of equations are given in Fig. 5.1.2. Note here that $\beta = 1$.

G -matrix plus bottom row of constraint D	d plus one constraining datum σ_1
1,0,1,0,0,6.	2.323
1,0,0,1,0,6.708	2.543
1,0,0,0,1,8.485	2.857
0,1,1,0,0,7.616	2.640
0,1,0,1,0,7.0	2.529
0,1,0,0,1,7.616	2.553
1,0,0,0,0,0 $\leftarrow \beta D$	0.433 $\leftarrow \beta h$

Fig. 5.1.1 Input data structure. Note that $\beta=1$ in this example.

Singular values, Λ ($\lambda_i = q_i$)

17.97105

1.898747

0.6343145

0.098960817 $\leftarrow \lambda_4$ now better conditioned

1.421898

1.414207

U-transpose matrix (U^T)

-0.3373508	-0.3764591	-0.4749891	-0.4267474	-0.3927506	-0.4271749	-0.0036922784
0.3908712	0.3841310	0.3553412	-0.3553166	-0.3503931	-0.3689544	0.4338698
0.0977789	0.1944664	0.2359648	-0.06169433	-0.1618290	-0.2929147	-0.8838264
-0.5554522	-0.03372441	0.4192865	0.50200870	-0.02007838	-0.4823709	0.1715710
-0.3197534	-0.28229870	0.5672691	-0.35033420	-0.3229672	0.5177553	-0.034040175
0.4903344	-0.5091351	0.0188053	0.4903353	-0.5091333	0.0188096	0.000004396

V-matrix divided by Λ ($V/\Lambda = VQI$)

-0.00369238	0.4338701	-0.8838334	0.1715780	-0.034040730	0.000004515
-0.00386020	-0.2980839	-1.2835310	-0.044986647	-0.076933742	0.00000761725
-0.00236593	0.0098617	0.0896802	-5.45729400	-0.33143010	0.4903358000
-0.00238176	0.0093580	0.08111537	-5.49373700	-0.2993690	-0.509135700
-0.00279343	-0.003776	-0.1415401	-6.44167400	0.5366624	0.018807005
-0.05521560	-0.0088096	0.1486551	0.7883733	0.007619273	0.00000076958

Fig. 5.1.2 SVD results for the constrained problem.

The calculated least squares estimates are :

$$\delta_1=0.433, \delta_2=0.346, \gamma_1=0.391, \gamma_2=0.433, \gamma_3=0.304, \frac{1}{v_1}=0.250$$

Notice that all the parameters have been accurately estimated this time. Notice also that the singular value corresponding to the fourth parameter is no longer close to zero (0.098960817).

One question that readily comes to mind is: can the solution process be stabilized or what may be done if no prior estimate of one of the delay-times is available ?

The answer to this question can be found in the next section.

5.2 Inversion with Smoothness Measures .

A very effective way of inverting a finite collection of inexact data is to impose the constraint that the desired solution be smooth. This measure may be based on the physics of the problem or on purely geological considerations. For instance, consider trying to invert the seismic data for the delay-times as in Example 5.1.2 but without

any known estimates of a delay-time. It may be wondered whether the exact solution can be found by any means other than that discussed in Section 5.1 and we also saw how unstable the solution process can be for problems with very small singular values. The simplest and cheapest remedy for such problems or a prescription for indeterminacy, or non-uniqueness in inversion is given below:

If in doubt SMOOTH ← remedy for non-uniqueness

Note that the solution obtained with smoothness constraints is a conservative estimate of the actual model and is the best that one could hope for in the absence of reliable *a priori* information.

5.2.1 Problem formulation:

Let us now examine how a problem can be formulated to yield a smooth solution. If it is desired that the model parameters vary slowly with position, say, then we may choose to minimize the difference between physically adjacent parameters $(m_1 - m_2)$, $(m_2 - m_3), \dots, (m_{p-1} - m_p)$. These first differences can be written as constraining equations in the form $Dm = h$, viz:

$$\begin{bmatrix} 1 & -1 & & & \\ & 1 & -1 & & \\ & & \ddots & & \\ & & & 1 & -1 \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \\ \vdots \\ m_p \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix} \quad (5.6a)$$

$\uparrow \qquad \uparrow \qquad \uparrow$

$D \qquad m \qquad h$

where D is the difference operator known here as the **smoothness matrix** and Dm is the **smoothness** or **FLATNESS** of the solution vector m . Note that D is of dimension $l \times p$ since there are $l = (p-1)$ first differences between the p parameters and h is of dimension $l \times 1$. A detailed treatment of such constraints can be found in the excellent text by Twomey (1977, Chap. 6).

If the model parameters do not vary smoothly with position, then the use of constraining equations of the form (cf. eq. 5.3)

$$\begin{bmatrix} 1 & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \\ \vdots \\ m_p \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \quad (5.6b)$$

$\uparrow \quad \uparrow \quad \uparrow$
 $D \quad m \quad h$

is recommended. In this case, D is the identity matrix of dimension $p \times p$ and h is of dimension $p \times 1$. It is interesting to note that it is then a form of biased estimation with non-informative *a priori* information. The operation effectively damps the length of the solution (by forcing it into conformity with h) leading to a stable inversion process. To gauge the smoothness of our solution, we use a quadratic measure $q_2(m)$ given by

$$q_2(m) = (Dm - h)^T(Dm - h) = m^T D^T D m$$

Let us define another matrix, $H = D^T D$ for the sake of notational simplicity.

We state the constrained problem as: From the incomplete, insufficient and inconsistent field data, find, amongst all possible solutions with residuals $q_1 = |d - Gm|^2$, the smoothest as judged by the measure $q_2(m)$.

Mathematically, the above statement is equivalent to: minimize $q_2 = m^T H m$ under the condition $|d - Gm|^2 = q_1$ or more generally $|d - Gm|^2 \leq q_T$ where q_T is the maximum tolerable residuals or misfit.

The constrained problem requires that we minimize $\|d - Gm\|^2$ and $q_2(m)$ together, i.e., minimize

$$\phi = (d - Gm)^T(d - Gm) + \beta^2(m^T D^T D m) \quad (5.6c)$$

5.2.2 Problem solution

It is obvious that we will use the method of Lagrange multipliers as before, where β is largely undetermined (i.e., $0 \leq \beta \leq \infty$). Minimization requires that for all j

$$\frac{\partial(d^T d - m^T G^T d - d^T Gm + m^T G^T Gm + \beta^2 m^T H m)}{\partial m_j} = 0$$

so that

$$(G^T G + \beta^2 H)m = G^T d \quad \longleftrightarrow \text{The Normal Equations}$$

from which we obtain the smoothest solution

$$\mathbf{m}_s = (\mathbf{G}^T \mathbf{G} + \beta^2 \mathbf{H})^{-1} \mathbf{G}^T \mathbf{d} \quad (5.7)$$

if \mathbf{D} is a first difference operator or simply

$$\mathbf{m}_s = (\mathbf{G}^T \mathbf{G} + \beta^2 \mathbf{I})^{-1} \mathbf{G}^T \mathbf{d} \quad (5.8)$$

if $\mathbf{D} = \mathbf{I}$. The above solutions are biased linear estimators, *sensu stricto* (Meju, 1994d). Equation 5.8 is popularly known as the Damped Least Squares solution and is mathematically equivalent to adding a positive constant bias to the eigenvalues of the design matrix to improve its condition before inversion- the well-known Marquardt(1970) method. Let us explain this latter approach in more detail for the sake of clarity. Recall that the unconstrained least squares solution is given in terms of the SVD of \mathbf{G} as

$$\hat{\mathbf{m}} = (\mathbf{G}^T \mathbf{G})^{-1} \mathbf{G}^T \mathbf{d} = \mathbf{V} \Lambda^{-1} \mathbf{U}^T \mathbf{d} \text{ or simply } \hat{\mathbf{m}} = \left(\frac{\mathbf{V}}{\Lambda} \right) \times (\mathbf{U}^T \mathbf{d}) \quad (4.12)$$

To damp the absolute values of the parameter estimates, we simply add a small bias, β to the eigenvalues, i.e., the diagonal matrix Λ^{-1} is replaced operationally by the damped variant

$$\Lambda_D^{-1} = \frac{\Lambda}{(\Lambda + \beta)^2} \quad (5.9)$$

yielding the constrained inversion computational formula

$$\mathbf{m}_D = (\mathbf{G}^T \mathbf{G} + \beta \mathbf{I})^{-1} \mathbf{G}^T \mathbf{d} = \mathbf{V} \Lambda_D^{-1} \mathbf{U}^T \mathbf{d} \text{ or simply } \mathbf{m}_D = (\mathbf{V} \Lambda_D^{-1}) \times (\mathbf{U}^T \mathbf{d}) \quad (5.10)$$

It should be noted that we have not appended any zeros to the data vector \mathbf{d} as in the former approach. There is thus a subtle difference between the two schemes and they do not yield the same results and we shall see later; the former method is also more flexible as we do not need to augment all the diagonal elements of $\mathbf{G}^T \mathbf{G}$ to obtain a reliable solution.

5.2.3 Geometrical interpretation of inversion with smoothness measures

The quadratic factor β and the measures q_2 and q_1 are the essential ingredients in the generation of smooth models as illustrated in the following interpretative analysis

Geometrical interpretation of constrained inversion

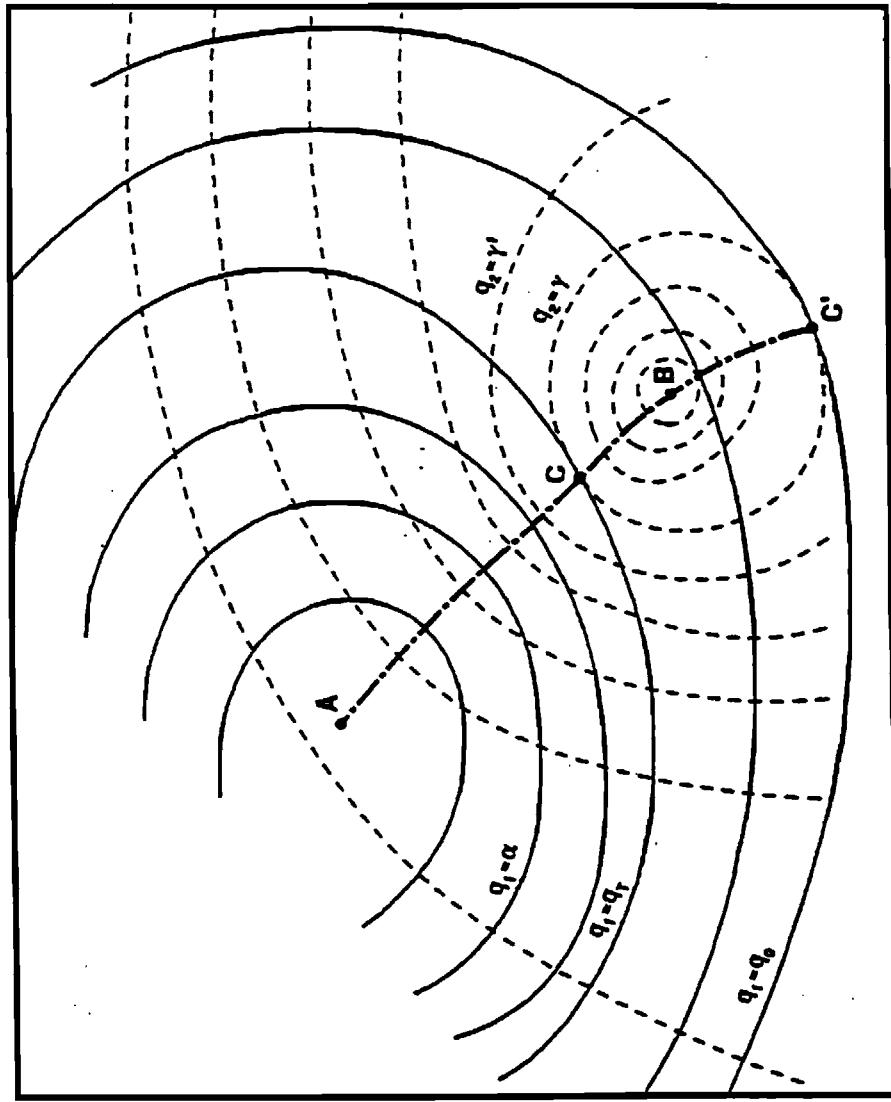


Fig. 5.2.1 A 2-D simplification of solution trajectory in function space
(after Twomey, 1977)

(adapted from Twomey, 1977, Chap. 6) aimed at providing a clearer understanding of the constrained inversion process, and especially those aspects that may have practical implications. Notice that eq. (5.6c) may be written as

$$\phi = q_1 + \beta^2 q_2 .$$

The measure q_2 is zero only when $m_1=m_2=\dots=m_p=0$, (see eqs. 5.6a and 5.6b) or when $m_1=m_2=\dots=m_p$ and D is a first difference operator such that $Dm=h=0$ (eq. 5.6a). In these idealized conditions, q_2 is said to have an absolute minimum and for ease of discussion, its location will be denoted by B in Fig. 5.2.1. Similarly, q_1 attains a minimum at some other point in function space denoted by A in this figure. If eq. (5.6c) is minimized, the solution travels from B to A as β is varied from an infinitely large value to zero, say. Since the quantities q_1 and q_2 can be computed for the solution obtained for any particular value of β , the travel path of the smooth solutions can be monitored as β is varied. Such a solution trajectory is illustrated in Fig. 5.2.1. The contours in this figure are the l -dimensional hypersurfaces of constant q_1 and q_2 . If the inverse problem is posed as the search for the solution satisfying the constraints $q_1=q_T$ and $q_2=\gamma$ in this figure, say, it is clear that the desired point where the $q_1=q_T$ and $q_2=\gamma$ contours touch, C is located some distance away from the minima A and B. To get to this point from B requires a suitable choice of the quadratic factor β ; one can easily overshoot the point C (thus missing the desired solution) by using coarse steps in (or unrealistic values of) β . Also, if we specified a large threshold misfit, say $q_1 = q_0$, we may obtain the undesirable solution C' which also satisfies the smoothness constraint. Thus, a suitable choice of β and an appropriate misfit criterion are a *sine qua non* for the constrained inversion process, especially when dealing with ill-posed linear problems. In routine inversion, an acceptable solution will have the minimum combined measure $q=(q_1+\beta q_2)$. However, since β is undetermined, it is good practice to find all acceptable solutions and make a selection from among them on a basis other than a statistical one (see also Meyer, 1977, p.400).

5.2.4 Sample Applications of smoothness constraints

5.2.4.1 Seismic Refraction Time-Term analysis

The delay-time data used in the previous refraction seismology exercises have been inverted using the two types of smoothness constraints represented by equations 5.6a and 5.6b for various values of β . The typical data structure for inversion with β -

weighted first-difference operators is illustrated in Figure 5.2.2. Notice that we have incorporated $p-2$ constraints instead of $p-1$ as defined in eq. 5.6a. The assumption here is that the delay parameters are slowly varying spatially and the well-determined slowness parameter is left unconstrained.

<i>G</i> -matrix (augmented with $p-2$ rows of constraint βD)	<i>d</i> -vector (augmented with zeros)
1,0,1,0,0,6.	2.323
1,0,0,1,0,6.708	2.543
1,0,0,0,1,8.485	2.857
0,1,1,0,0,7.616	2.64
0,1,0,1,0,7.0	2.529
0,1,0,0,1,7.616	2.553
0.01,-0.01,0,0,0,0 ←	0.0 ←
0,0.01,-0.01,0,0,0, ↑	0.0 ↑
0,0,0.01,-0.01,0,0 βD ↓	0.0 βh ↓
0,0,0,0,0.01,-0.01 ←	0.0 ←

Fig. 5.2.2 Input data structure with first-difference operator for $\beta=0.01$.

The actual results obtained with δ_1 specified is re-stated below for comparison

$$\delta_1=0.433, \delta_2=0.346, \gamma_1=0.391, \gamma_2=0.434, \gamma_3=0.304, \frac{1}{v_1}=0.250 \quad (5.11a)$$

and constitutes our target solution.

The results obtained on appending a β -weighted $p \times p$ identity matrix (eq. 5.6b) onto the bottom of the *G*-matrix are summarised in Table 5.2.1 for a range of values of β . It can be appreciated from this table that the results for $\beta=0.0000055$ agree with those derived from inversion using a known value of a δ -parameter (see eq. 5.11a). However, while the correct solution may be obtained using this method for some value of β , selecting this solution on the basis of the computed residuals may not be a straightforward task since the solution with the least residuals may not be the correct one as shown in Table 5.2.1 and there may be more than one solution with the same residuals.

β	Solution							SSE_d	SSE_{d+h}
1.0	.088	-.0016	.065	.091	-.070	.344		2.37232e-02	1.67160e-01
0.1	.382	.286	.250	.291	.128	.279		1.27660e-03	5.96765e-03
0.01	.501	.414	.320	.363	.232	.250		2.61112e-07	7.75681e-05
0.001	.503	.416	.321	.364	.234	.250		5.91967e-09	7.84060e-07
0.0001	.502	.416	.321	.364	.234	.250		5.87437e-09	1.36563e-08
0.00001	.481	.393	.343	.386	.256	.250		5.88756e-09	5.96562e-09
0.000006	.441	.355	.382	.425	.295	.250		5.89796e-09	5.92665e-09
0.0000056	.434	.347	.389	.432	.302	.250		5.89807e-09	5.92321e-09
0.0000055	.433	.346	.391	.434	.304	.250		5.87994e-09	5.90422e-09
0.0000054	.428	.341	.395	.438	.308	.250		5.87966e-09	5.90316e-09
0.000005	.419	.332	.405	.448	.318	.250		5.87778e-09	5.89812e-09
0.000004	.362	.276	.461	.504	.374	.250		5.89932e-09	5.91334e-09
0.000001	-1.72	-1.81	2.55	2.59	2.46	.250		5.89733e-09	5.92285e-09

Table 5.2.1 Variation in smooth solutions with β for $D = I$. The parameter estimates are given in columns 2 - 7. SSE_d is the sum of squared errors corresponding to the observational data while SSE_{d+h} is the combined residuals due to the actual and *a priori* data. The acceptable parameter estimates are shown in bold print while the solution with the minimum residuals is marked by an arrow.

It would be desirable to be able to know when the correct estimates have been found. Is there any solution to this choice problem? It is clear from Table 5.2.1 that the slowness ($1/v$) parameter is well determined in most cases. It may thus be useful to allow such a parameter to "float freely" while the variations between the rest are smoothed by a p -2 first-difference operator. The results of such an approach are summarised in Table 5.2.2. It is obvious from this table that very good estimates of the true parameters can be obtained for this data set for $0.0000110 \leq \beta \leq 0.0000114$ using this technique. Notice also from Table 5.2.2 that the improved behaviour of the residuals of the combined actual and *a priori* data set may be used to select an optimal set of values for the sought parameters: in this case, the solution with the minimum value of SSE_{d+h} is in accord with that derived using a known value of a delay parameter. As in the previous comparable case, the stability of the solution process over a wide range of β is apparent.

β	Solution						SSE_d	SSE_{d+h}
1.0	.560	.516	.516	.528	.490	.211	5.78974e-03	9.36119e-03
0.1	.459	.373	.373	.415	.288	.249	4.91896e-06	2.57990e-04
0.01	.455	.368	.368	.411	.281	.249	6.43308e-09	2.63539e-06
0.001	.455	.368	.368	.411	.281	.250	5.89409e-09	3.21941e-08
0.0001	.455	.368	.369	.412	.282	.250	5.90245e-09	6.16546e-09
0.00005	.454	.367	.370	.413	.283	.250	5.89637e-09	5.96213e-09
0.000025	.451	.364	.373	.416	.286	.250	5.90745e-09	5.92394e-09
0.0000114	.433	.346	.390	.433	.303	.250	5.89733e-09	5.90100e-09
0.0000111	.433	.346	.391	.434	.304	.250	5.87488e-09	5.87837e-09 ←
0.00001105	.432	.345	.391	.434	.304	.250	5.87983e-09	5.88330e-09
0.0000110	.432	.346	.391	.434	.304	.250	5.89847e-09	5.90019e-09
0.000010	.429	.342	.395	.438	.308	.250	5.90711e-09	5.91002e-09
0.000005	.346	.259	.478	.521	.391	.250	5.91007e-09	5.91193e-09
0.000001	-2.29	-2.38	3.11	3.16	3.03	.250	5.94508e-09	5.97523e-09
0.0000001	-180.3	-180.4	181.1	181.1	181.0	.250	1.58823e-07	1.60129e-07

Table 5.2.2 Variation in smooth solutions with damping factor using a $p=2$ first-difference operator. The velocity parameter was unconstrained in these calculations and the solution with the smallest residuals is marked by an arrow.

An examination of the solutions derived for various values of β with the conventional Marquardt-type damping in which β is added directly to the singular values of the problem (eq. 5.10) failed to reproduce the correct values of the parameters over the range of values of β used in the tests. In fact the best estimates from this technique were

$$\delta_1=0.481, \delta_2=0.394, \gamma_1=0.342, \gamma_2=0.386, \gamma_3=0.255, \frac{1}{v_1}=0.250. \quad (5.11b)$$

It would thus appear that we may not recover the true solution via this avenue. All the above calculations were performed using the computer program SVDINV (listed in Appendix A).

6. ERROR ANALYSIS IN LINEAR INVERSION

One question that is fundamental to geophysical data analysis is, how representative of the real geophysical system is our reconstructed least squares model or how accurate is our solution to the given problem? Recall that our initial assumption was that the experimental data contain errors (which is why we cannot fit them exactly). One may therefore be interested in how the experimental errors translate into errors in the model estimates. The answers obviously come from statistics. Inverse theory not only provides us with estimate of the relevant parameters but also furnishes a plethora of related information that enable us to gauge the “goodness” of the least squares solution to the inverse problem. Some of such “auxiliary parameters” are described following a discussion of how to incorporate available observational errors directly in the inversion process.

6.1 Elaborate Treatment of Observational Errors in Inversion

It may be appreciated from our treatment of inversion so far that the process involves finding a solution that minimizes a suitably chosen quantity- the squared distance between our solution and the given data. Our desire should be that the solution be both numerically and statistically stable. Statistical stability is important because of the differencing uncertainties associated with our observations. If observational errors are available, we can incorporate them directly in the problem formulation to obtain a more acceptable weighted solution. Thus, assuming that the n standard data errors, σ_i are Gaussian with zero mean and are statistically independent, we can define an $n \times n$ diagonal weighting matrix, W as

$$W = \text{diag}[\frac{1}{\sigma_1}, \frac{1}{\sigma_2}, \frac{1}{\sigma_3}, \dots, \frac{1}{\sigma_n}] = \sigma^{-1}I.$$

We can then re-state the constrained inversion problem of Section 5.2, for example, as:
minimize

$$q = (Wd - WGm)^T(Wd - WGm) + \beta^2(m^T D^T D m)$$

where the weighting (or scaling) of each datum by its associated observational error ensures that undue importance is not given to poorly estimated (i.e., noisy) data. This is a somewhat more robust formulation and the solution is identically,

$$m_s = ((WG)^T WG + \beta^2 H)^{-1} (WG)^T W d \quad (6.1a)$$

or simply

$$m_s = ((WG)^T WG + \beta^2 I)^{-1} (WG)^T W d \quad (6.1b)$$

if $D = I$. Notice that β is just a single number in the above formulation. If we are interested in retaining specified values of the parameters, i.e., biased estimation *proper* (Section 5.1), a recommended elegant approach is to define a diagonal matrix of undetermined multipliers β and re-state the problem as *minimize*

$$q = (Wd - WGm)^T (Wd - WGm) + \beta(Dm - h)^T \beta^T (Dm - h).$$

The solution to this problem is

$$m_b = ((WG)^T WG + D^T BD)^{-1} [(WG)^T W d + BD^T h] \quad (6.2)$$

where $B = \beta^T \beta$. The diagonal elements of β are assigned a constant positive value for those parameters specified *a priori* and the rest are set to nought. The somewhat identical role of the matrices W and β is obvious and we shall examine the statistical implications later. Notice that if we define another matrix $E = W^T W$, then eq. 6.2 may be expressed in another enlightening form

$$m_b = (G^T EG + D^T BD)^{-1} [G^T Ed + D^T Bh] \quad (6.3)$$

which in every respect is equivalent to the so-called **Bayesian Estimator** (see e.g., Jackson and Matsu'ura, 1985; Duijndam, 1988).

6.2 Assessing the Quality of a Solution

6.2.1 Goodness-of-fit

This is the commonly used model acceptance criterion. Assuming that our data d_i are normally distributed about their expected values and with known uncertainties σ_i (the experimental errors), we can assess the fit between the observed and predicted data by calculating the statistical parameter q defined by

$$q = \sum_{i=1}^n \frac{(d_i^{obs} - G_{ij} m_j)^2}{\sigma_i^2} \quad j = 1, p$$

or simply

$$q = \sum_{i=1}^n \|Wd^{obs} - WGm\|^2 \text{ for a weighted solution.}$$

For n independent observations and p independent parameters, q is distributed as χ^2 (Chi-square) with $(n-p)$ degrees of freedom.

In geophysical inversion, we reject or accept a solution to the problem being considered based on the value of q . The expected value of q is n (from Chi-square statistics) but in practice a model with $n-p < q \lesssim n+\sqrt{2n}$ is acceptable. However, if $q \ll n$, the model is said to over-fit the observed data and if $q \gg n$, the model under-fits the data. Over-fitting may lead to solutions that contain artifacts of the computer!

If experimental errors are not available, an unbiased estimate of σ^2 is given by

$$\sigma^2 = \frac{(d^T d - m^T G^T G m)}{n-p} \equiv \frac{\text{sum of squares of residuals}}{n-p}.$$

Another measure of goodness of a solution is the Root Mean Square (rms) error given by

$$\text{rms} = \frac{1}{n} \sum_{i=1}^n \frac{(d_i^{obs} - G_{ij}m_j)^2}{\sigma^2}$$

or simply

$$\text{rms} = \frac{1}{n} \sum_{i=1}^n \|Wd_i^{obs} - WGm\|^2 \text{ for a weighted solution.}$$

Obviously one should not aim for solutions with $1.0 \ll \text{rms} \gg 1.0$. Note that the number of degrees of freedom for a constrained solution with l independent constraint equations is $\{n - p + l\}$ and we should substitute this quantity for $n - p$ in the above formulations where appropriate.

6.2.2 Parameter Resolution Matrix

For a linear system, we can assess the quality of the model derived from a given data set by examining the parameter resolution matrix (Jackson, 1972). We will show how it is derived for the unbiased least squares solution and then apply the same strategy to the cases where we have constrained the solution process.

Case 1: Unconstrained solution

Recall that the unconstrained least squares solution is $m = \{(G^T G)^{-1} G^T\} d$ which in terms of SVD is simply $m = \{V \Lambda^{-1} U^T\} d$. Let us denote the quantity in braces as H .

The matrix H is the generalized inverse used in the estimation and post-multiplying it by the applicable design matrix (or data kernel) gives the resolution matrix R , i.e.,

$$R = HG = (G^T G)^{-1} G^T \cdot G = I \quad (6.3a)$$

In terms of the SVD of G ,

$$R = \{V\Lambda^{-1}U^T\}\{U\Lambda V^T\} = VV^T.$$

R is of dimension $p \times r$ (where r is the number of non-zero eigenvalues of the problem). If $R = I$ (identity matrix), i.e., $r=p$, then each model parameter is uniquely determined. The deviation of the rows of R from those of the identity matrix, I , is generally assumed to be a measure of the lack of resolution for the corresponding model parameters.

Case 2 : The Marquardt damped solution

For the damped least squares solution given by eq. 5.10, we have that

$$R = (G^T G + \beta I)^{-1} G^T \cdot G = I + \left(\frac{G^T G}{\beta I}\right) \quad (6.3b)$$

which, in terms of the SVD of G , is simply

$$R = V\Lambda_D^{-2}V^T \cdot V\Lambda^2 V^T = \frac{V\Lambda^2 V^T}{(\Lambda + \beta I)^2}.$$

It is obvious that the damped solution obtained by simply adding a constant bias to the eigenvalues of a problem does not have a perfect resolution.

Case 3: Inversion with *a priori* data

The constrained inversion formula represented by eq. 5.2, may be written as

$$\hat{m}_c = \{(G^T G + \beta^2 D^T D)^{-1} G^T\} \cdot d + \{(G^T G + \beta^2 D^T D)^{-1} \beta D^T\} \cdot \beta h$$

and hence the parameter resolution matrix may be calculated as

$$R = (G^T G + \beta^2 D^T D)^{-1} G^T \cdot G + (G^T G + \beta^2 D^T D)^{-1} \beta D^T \cdot \beta D$$

$$= (G^T G + \beta^2 D^T D)^{-1} (G^T G + \beta^2 D^T D) = I \quad (6.3c)$$

which in terms of SVD of the augmented (or partitioned) design matrix G_* , defined as

$$G_* = \begin{bmatrix} G \\ \beta D \end{bmatrix}$$

is simply $V_* V_*^T$. Thus the constrained solution incorporating *a priori* parameter estimates has perfect resolution. It is may be noted that the constrained solution obtained by augmenting the matrix G with the identity matrix D and the data vector d with the null vector h (i.e., eq. 5.8) also has perfect resolution since the null vector is some kind of fictitious *a priori* data eventhough the inversion formula is mathematically equivalent to the popular Marquardt formula represented by eq. 5.10.

It is remarked here that the resolution matrix is only an experimental design guide. It is always an identity matrix for cases 1 and 3. It has nothing to do with the actual field observations and its utility in parameter error analysis has often been over-stated in the geophysical inversion literature. A perfect resolution does not imply in every respect an accurate or reliable model. To illustrate, the calculated values of R for the refraction seismology delay-time problem of Examples 4.4.3 and 5.1.2 are shown in Tables 6.2.2.1 and 6.2.2.2 respectively.

col.1	col.2	col.3	col.4	col.5	col.6
.9999997	7.14512E-08	1.82836E-08	1.75506E-08	2.93858E-08	-1.18523E-08
7.14512E-08	1.00000	3.67795E-08	3.40229E-08	2.22605E-08	-7.54078E-08
1.82836E-08	3.67795E-08	1.00000	-1.38533E-08	1.32156E-07	-9.01755E-09
1.75506E-08	3.40229E-08	-1.3853E-08	1.000000	1.12674E-07	1.25385E-08
2.93858E-08	2.22605E-08	1.32156E-07	1.12674E-07	.9999999	-9.54640E-09
-1.1852E-08	-7.5408E-08	-9.0176E-09	-1.25385E-08	-9.54640E-09	.9999999

Table 6.2.2.1. Resolution matrix, R for an unconstrained six-parameter problem. The i^{th} column elements relate to the i^{th} parameter. The degree of correlation between the various parameters can be gleaned from the rows of the matrix. Notice that R is delta-like suggesting perfect resolution.

col.1	col.2	col.3	col.4	col.5	col.6
1.000000	4.10187E-08	-2.0286E-09	-7.94157E-09	-4.34869E-09	-6.02772E-09
4.10187E-08	1.000000	-1.6353E-08	-5.59144E-09	-9.41843E-09	-9.81052E-08
-2.0286E-09	-1.6353E-08	1.000000	-3.89008E-08	-1.34107E-07	1.57051E-08
-7.9416E-09	-5.5914E-09	-3.8901E-08	1.000000	-9.6212E-08	4.16797E-09
-4.3487E-09	-9.4184E-09	-1.3411E-07	-9.6212E-08	1.000000	1.50810E-08
-6.0277E-09	-9.8105E-08	1.57051E-08	4.16797E-09	1.50810E-08	1.000000

Table 6.2.2.2. Resolution matrix, R for a constrained six-parameter problem.
Notice in this case that R is also delta-like suggesting perfect resolution.

It is obvious that even the unconstrained problem which we know not to be determined by the practical data has a perfect resolution. The calculated R for an optimal damped solution (i.e., augmented singular values) for the seismic delay-time problem is given in Table 6.2.2.3 for the sake of completeness. Notice in this case that R is not an identity

col.1	col.2	col.3	col.4	col.5	col.6
7.99918E-01	-2.00064E-01	1.99958E-01	1.99957E-01	1.99939E-01	1.65436E-05
-2.00064E-01	7.99907E-01	1.99955E-01	1.99954E-01	1.99935E-01	1.78145E-05
1.99958E-01	1.99955E-01	7.99956E-01	-2.00016E-01	-2.00027E-01	9.78324E-06
1.99957E-01	1.99954E-01	-2.00016E-01	7.99955E-01	-2.00027E-01	9.94825E-06
1.99939E-01	1.99935E-01	-2.00027E-01	-2.00027E-01	7.99929E-01	1.44205E-05
1.65436E-05	1.78145E-05	9.78324E-06	9.94825E-06	1.44205E-05	9.99994E-01

Table 6.2.2.3 Resolution matrix for an optimal damped solution for $\beta = 0.00001$.
Notice that the diagonal elements corresponding to the first five parameters have values of about 0.8 while the sixth parameter has a diagonal element of 1.0 so that $R \neq I$. The velocity parameter is thus the only parameter that may have been well determined in this inversion.

matrix which is in accord with our derivation in Section 6.2.2. The information provided by R here is that the slowness (and by implication the velocity) parameter may have been well determined. As we saw for the unconstrained inversion problem, a delta-like

R does not guarantee a meaningful solution. A cautious use of R would thus seem appropriate when dealing with practical data. For instance, it may be said that providing that the generalized inverse used in the calculations exists, then the true solution may be found if $R = I$; a lack of perfect resolution would therefore suggest that the true solution may not be found.

6.3 Errors/Bounds on the Parameter Estimates

An important aspect of geophysical data analysis (or interpretation) is the determination of bounds (or confidence limits) on the various model parameters that are consistent with the experimental data and their associated errors.

6.3.1 Parameter Covariance matrix

The simplest form of model error estimation is the determination of the limits of the parameters from the Covariance matrix, $Cov(m)$. The Covariance matrix depends on the covariance of the experimental errors and the way in which we map the data errors into parameter errors (Menke, 1984). For illustration, let us express the estimated least squares solution as

$$m^{est} = (G^T G)^{-1} G^T d = Ld$$

where L is the generalized inverse used in the inversion. The above expression shows that m^{est} is a linear transformation of d . The mathematical expectation (E) value of m^{est} is

$$E(m^{est}) = E(Ld) = LE(d)$$

If the experimental data are uncorrelated and of equal variance σ^2 , then (by Law of propagation of errors)

$$Cov(m^{est}) = L[Cov(d)]L^T$$

$$Cov(m^{est}) = \{(G^T G)^{-1} G^T\} [\sigma^2 I] \{(G^T G)^{-1} G^T\}^T = \sigma^2 (G^T G)^{-1} \quad (6.4a)$$

since $\{(G^T G)^{-1} G^T\}^T = G(G^T G)^{-1}$.

For the Marquardt-type damped least squares solution,

$$\mathbf{m}^{est} = (\mathbf{G}^T \mathbf{G} + \beta \mathbf{I})^{-1} \mathbf{G}^T \mathbf{d} = \mathbf{Ld}$$

and the covariance matrix is given by

$$\begin{aligned} Cov(\mathbf{m}^{est}) &= (\mathbf{G}^T \mathbf{G} + \beta \mathbf{I})^{-1} \mathbf{G}^T [\sigma^2 \mathbf{I}] \mathbf{G} (\mathbf{G}^T \mathbf{G} + \beta \mathbf{I})^{-1} \\ &= \sigma^2 (\mathbf{G}^T \mathbf{G} + \beta \mathbf{I})^{-1} \mathbf{G}^T \mathbf{G} (\mathbf{G}^T \mathbf{G} + \beta \mathbf{I})^{-1}. \end{aligned} \quad (6.4b)$$

Using a similar argument, the covariance matrix for the solution incorporating *a priori* information is identically

$$\begin{aligned} Cov(\mathbf{m}^{est}) &= (\mathbf{G}^T \mathbf{G} + \beta^2 \mathbf{D}^T \mathbf{D})^{-1} \mathbf{G}^T [\sigma^2 \mathbf{I}] \mathbf{G} (\mathbf{G}^T \mathbf{G} + \beta^2 \mathbf{D}^T \mathbf{D})^{-1} \\ &\quad + (\mathbf{G}^T \mathbf{G} + \beta^2 \mathbf{D}^T \mathbf{D})^{-1} \beta \mathbf{D}^T [\beta^2 \mathbf{I}]^{-1} \beta \mathbf{D} (\mathbf{G}^T \mathbf{G} + \beta^2 \mathbf{D}^T \mathbf{D})^{-1} \end{aligned}$$

giving

$$Cov(\mathbf{m}^{est}) = (\mathbf{G}^T \mathbf{G} + \beta^2 \mathbf{D}^T \mathbf{D})^{-1} \{\sigma^2 \mathbf{G}^T \mathbf{G} + \mathbf{D}^T \mathbf{D}\} (\mathbf{G}^T \mathbf{G} + \beta^2 \mathbf{D}^T \mathbf{D})^{-1}. \quad (6.4c)$$

Note, however, that if the elaborate treatment of data errors described in Section 6.1 was effected (see eq. 6.2 & 6.3), then

$$\begin{aligned} Cov(\mathbf{m}^{est}) &= (\mathbf{G}^T \mathbf{E} \mathbf{G} + \mathbf{D}^T \mathbf{B} \mathbf{D})^{-1} (\mathbf{W} \mathbf{G})^T \{ \mathbf{E} [\sigma^2 \mathbf{I}] \} \mathbf{W} \mathbf{G} (\mathbf{G}^T \mathbf{E} \mathbf{G} + \mathbf{D}^T \mathbf{B} \mathbf{D})^{-1} \\ &\quad + (\mathbf{G}^T \mathbf{E} \mathbf{G} + \mathbf{D}^T \mathbf{B} \mathbf{D})^{-1} (\beta \mathbf{D})^T \{ \mathbf{B} [\mathbf{B}]^{-1} \} \beta \mathbf{D} (\mathbf{G}^T \mathbf{E} \mathbf{G} + \mathbf{D}^T \mathbf{B} \mathbf{D})^{-1} \end{aligned}$$

or simply,

$$\begin{aligned} Cov(\mathbf{m}^{est}) &= (\mathbf{G}^T \mathbf{E} \mathbf{G} + \mathbf{D}^T \mathbf{B} \mathbf{D})^{-1} \{ \mathbf{G}^T \mathbf{E} \mathbf{G} + \mathbf{D}^T \mathbf{B} \mathbf{D} \} (\mathbf{G}^T \mathbf{E} \mathbf{G} + \mathbf{D}^T \mathbf{B} \mathbf{D})^{-1} \\ &= (\mathbf{G}^T \mathbf{E} \mathbf{G} + \mathbf{D}^T \mathbf{B} \mathbf{D})^{-1}. \end{aligned} \quad (6.4d)$$

where the symbols are as previously defined and the covariance matrices of the actual and *a priori* data in this standardized framework are identity matrices.

Having derived working expressions for the covariance matrices, let us try and see what they represent. $Cov(\mathbf{m})$ is a parameter-by-parameter matrix whose i^{th} diagonal element is the statistical variance of the i^{th} parameter m_i , and whose off-diagonal

elements, the covariances, indicate the correlations between the model parameters. Large off-diagonal elements Cov_{ij} mean that the i^{th} and j^{th} model parameters are highly correlated. The square roots of the diagonal elements of $Cov(\mathbf{m})$ are generally referred to as the standard deviations of the least squares parameter estimates and may be used to estimate the bounds of the model parameters. Notice that eq. 6.4c reduces to eq. 6.4a when $\beta=0$ but yields smaller values when $\beta \neq 0$. Note also that the variances and covariances of parameters constrained to be equal to fixed values in biased estimation are effectively zero while the corresponding quantities for the free (i.e., unconstrained) parameters in the problem is reduced.

6.3.2 Extreme parameter sets : Extremal inversion.

We may elect to determine a solution with the maximum tolerable sum of squared residuals. One method of extremal inversion is the Most Squares Method of Jackson (1976) in which a value is determined for each parameter which is maximum (or minimum) under the constraint that the misfit of the observed and calculated data is equal to some specified value. The essential feature of the method is that it produces a class of models which defines a zone within which the true solution, if it exists, may be found. The mathematical formulation of this extremal inversion problem is straightforward. We state the problem as follows:

Given an optimal least squares solution to an inverse problem, \mathbf{m} with residuals q_{LS} , find (on account of the observational uncertainties) other solutions which fit the data to a specified threshold residual q_T ; or equivalently, extremize the linear objective function $\mathbf{m}^T b$ under the constraint

$$| \mathbf{d} - \mathbf{Gm} |^2 = q_T \quad (6.5)$$

where the function b is a vector of zeros with the k^{th} element (to be maximized) set equal to unity; i.e., $b^T = [0, \dots, 0, 1^k, 0, \dots, 0]$ and \mathbf{m} is the vector of model parameters. This search for extreme solutions can be effected simply by minimizing the function

$$\mathcal{L} = \mathbf{m}^T b + \frac{1}{2\mu} \{ (\mathbf{d} - \mathbf{Gm})^T (\mathbf{d} - \mathbf{Gm}) - q_T \} \quad (6.6)$$

where we have introduced the Lagrange multiplier $1/2\mu$. At the extremum, we have that

$$\frac{\partial}{\partial \mathbf{m}} \left(\mathbf{m}^T b + \frac{1}{2\mu} \{ \mathbf{m}^T \mathbf{G}^T \mathbf{Gm} - 2\mathbf{m}^T \mathbf{G}^T \mathbf{d} + \mathbf{d}^T \mathbf{d} - q_T \} \right) = 0 \quad (6.7)$$

or

$$G^T G m = G^T d - \mu b$$

from which we obtain the most squares solution

$$m_{ms} = [G^T G]^{-1} [G^T d - \mu b] \quad (6.8)$$

Thus the value of $\mu = 0$ corresponds to the unconstrained least squares solution. However, since eq. 6.8 must satisfy eq. 6.5, we have that

$$\begin{aligned} q_T &= d^T d - d^T G m - m^T G^T d + m^T G^T G m \\ &= d^T d - d^T G (G^T G)^{-1} (G^T d - \mu b) - (d^T G - \mu b^T) (G^T G)^{-1} G^T d \\ &\quad + (d^T G - \mu b^T) (G^T G)^{-1} G^T G (G^T G)^{-1} (G^T d - \mu b) \end{aligned}$$

which simplifies to

$$q_T = d^T d - d^T G [G^T G]^{-1} G^T d + \mu^2 b^T [G^T G]^{-1} b$$

so that

$$\mu = \left(\frac{q_T - d^T d + d^T G [G^T G]^{-1} G^T d}{b^T [G^T G]^{-1} b} \right)^{1/2} = \pm \left(\frac{q_T - q_{LS}}{b^T [G^T G]^{-1} b} \right)^{1/2} \quad (6.9)$$

where $q_{LS} = (d^T d - d^T G [G^T G]^{-1} G^T d)$ is the sum of squared residuals of the optimal least squares solution. Since there are two solutions for μ for each model parameter, there will be $2p$ solutions (for the p parameters) whenever $q_T > q_{LS}$. Note that setting all the elements of the parameter projection vector b to unity (i.e., $b = [1, 1, \dots, 1]^T$) will yield two (i.e., *plus* and *minus*) solutions that may be interpreted as the upper and lower solution envelopes of our least squares solution. If the errors on the data are assumed univariate and uncorrelated, it is expected that q_T will have a value close to the number of the data, i.e., $q_T \approx n$.

We can compare directly the most squares and least squares solutions. Equation 6.8 can be written as

$$m_{ms} = (G^T G)^{-1} G^T d - \mu (G^T G)^{-1} b$$

$$= m_{LS} \pm \left(\frac{q_T - q_{LS}}{b^T(G^T G)^{-1} b} \right)^{1/2} (G^T G)^{-1} b \quad (6.10)$$

where m_{LS} is the least squares solution. The most squares solution envelope may thus be interpreted as the confidence limits of the least squares solution.

As we saw in Section 4 (Ex. 4.4.3), the unconstrained least squares solution process is unstable in certain situations. The same problem may plague the most squares method (Eq. 6.10) if the matrix $G^T G$ is ill-conditioned. Meju (1994d) suggests that a bound could be placed on the size of the solutions as in the conventional inversion employing smoothness constraints. The constrained problem is defined simply as:

Given an optimal least squares solution to an inverse problem, m with residuals q_{LS} , find (on account of the observational uncertainties) the smoothest solutions (as gauged by the measure $m^T D^T D m$) which fit the data to a specified threshold residual q_T .

Note in this case that there are two types of data under consideration: the actual experimental data and the extraneous constraining data. The threshold residual is therefore conveniently defined as

$$q_T = |d - Gm|^2 + \beta^2 m^T D^T D m \quad (6.11)$$

and the objective function is stated as:

$$\mathcal{L} = m^T b + \frac{1}{2\mu} \{(d - Gm)^T(d - Gm) + \beta^2 m^T D^T D m - q_T\} \quad (6.12)$$

so that

$$\frac{\partial}{\partial m} \left(m^T b + \frac{1}{2\mu} \{m^T G^T G m - 2m^T G^T d + d^T d + \beta^2 m^T D^T D m - q_T\} \right) = 0$$

or

$$[G^T G + \beta^2 D^T D]m = G^T d - \mu b \quad (6.13)$$

from which we obtain the damped most squares solution

$$m_{dms} = [G^T G + \beta^2 H]^{-1}[G^T d - \mu b] \quad (6.14)$$

where $H = D^T D$. Now, equation 6.14 must satisfy eq. (6.11). Therefore,

$$\begin{aligned} q_T &= d^T d - d^T G m - m^T G^T d + m^T G^T G m + \beta^2 m^T H m \\ &= d^T d - d^T G m - m^T G^T d + m^T \{G^T G + \beta^2 H\} m \\ &= d^T d - d^T G (G^T G + \beta^2 H)^{-1} (G^T d - \mu b) - (d^T G - \mu b^T) (G^T G + \beta^2 H)^{-1} G^T d \\ &\quad + (d^T G - \mu b^T) (G^T G + \beta^2 H)^{-1} \{G^T G + \beta^2 H\} (G^T G + \beta^2 H)^{-1} (G^T d - \mu b) \end{aligned}$$

which simplifies to

$$q_T = d^T d - d^T G (G^T G + \beta^2 H)^{-1} G^T d + \mu b^T (G^T G + \beta^2 H)^{-1} \mu b$$

so that

$$\mu = \pm \left(\frac{q_T - q_{LS}}{b^T [G^T G + \beta^2 H]^{-1} b} \right)^{1/2} : \quad (6.15)$$

where $q_{LS} = d^T d - d^T G (G^T G + \beta^2 H)^{-1} G^T d$. If $D = I$, then $H = I$. Equation (6.14) is a stable inversion formula and the operation is equivalent to adding a positive constant bias to the main diagonal of the matrix $G^T G$. β may be chosen to be a small number much less than unity ($\ll 1$) and the expected value of q_T is $n-l$, where there are l constraints in the problem.

Note that we can also formulate the problem to preserve any *a priori* parameter estimates as in Section 5.1. In this case the constrained most squares solution is

$$m_{cms} = [G^T G + \beta^2 H]^{-1} [G^T d + \beta^2 h - \mu b] \quad (6.16)$$

where $H = D^T D$ (cf. Eq. 5.2) and must satisfy the condition:

$$\begin{aligned} q_T &= |d - G m|^2 + |D m - h|^2 \\ &= d^T d + \beta^2 h^T h - (d^T G + \beta^2 h^T D) m - m^T (G^T d + \beta^2 D^T h) + m^T (G^T G + \beta^2 D^T D) m . \end{aligned} \quad (6.17)$$

Using eq. (6.16) in the place of m in eq. (6.17), we have that

$$q_T = d^T d + \beta^2 h^T h - (d^T G + \beta^2 h^T D)(G^T G + \beta^2 H)^{-1} (G^T d + \beta^2 D^T h) \\ + \mu b^T (G^T G + \beta^2 H)^{-1} \mu b$$

giving

$$\mu = \pm \left(\frac{q_T - q_{LS}}{b^T [G^T G + \beta^2 H]^{-1} b} \right)^{1/2} \quad (6.18)$$

where $q_{LS} = d^T d + \beta^2 h^T h - (d^T G + \beta^2 h^T D)(G^T G + \beta^2 H)^{-1} (G^T d + \beta^2 D^T h)$.

The threshold residual may be set to a value close to $n-l$ for a problem with l constraints.

6.4 Example of inversion and detailed error analysis: a recommended practice

As an illustration of a good inversion practice, let us analyse a simple linear problem (see also, Meju 1994c).

Problem: Given the following $\{x, y\}$ data pairs (Jackson, 1976) for a straight-line inverse problem:

x	y
-1.000000	-1.124600
-8.000000E-01	7.080000E-02
-6.000000E-01	-9.942000E-01
-4.000000E-01	-7.038000E-01
-2.000000E-01	9.637000E-01
0.000000E+00	5.810000E-02
2.000000E-01	-7.820000E-02
4.000000E-01	-1.069000E-01
6.000000E-01	-9.231000E-01
8.000000E-01	-7.819000E-01
1.000000	-4.250000E-02

determine the least solution for the slope and intercept, compute the residuals, the resolution and covariance matrices and the bounding models.

Solution: There are two model parameters in this problem: m_1 (intercept) and m_2 (slope). Using the procedure outlined for fitting straight lines to x, y data pairs, we will obtain the following unconstrained least squares estimates:

$$m_1 = -3.329636E-01, \quad m_2 = 1.074954E-01.$$

The computed data misfit, $q = |d - Gm|^2 = 3.898074$.

The resolution information is simply:

$$\begin{bmatrix} 1.000000 & -1.594859E-15 \end{bmatrix} \leftarrow \text{row}_1 \text{ of } R$$
$$\begin{bmatrix} -1.594859E-15 & 1.000000 \end{bmatrix} \leftarrow \text{row}_2$$

To calculate $Cov(m)$, we will assume that the experimental errors in the data are Gaussian, statistically independent, of zero mean, and of unit variance.

The resulting covariance information is simply:

$$\begin{bmatrix} 9.090909E-02 & -3.624680E-16 \end{bmatrix} \leftarrow \text{row}_1 \text{ of } Cov(m)$$
$$\begin{bmatrix} -1.449872E-16 & 2.272727E-01 \end{bmatrix} \leftarrow \text{row}_2$$

The square roots of the diagonal elements of $Cov(m)$ are the standard deviations of the estimates, viz:

$$\sigma_{m_1} = \pm 3.015113E-01, \quad \sigma_{m_2} = \pm 4.767313E-01.$$

The most-squares extreme parameter sets are:

(a) plus solutions (μ positive)

$$\begin{bmatrix} 4.705472E-01 & 1.074954E-01 \end{bmatrix} \leftarrow m_1 \text{ extremized using } b = [1, 0]^T$$
$$\begin{bmatrix} -3.329636E-01 & 1.377958 \end{bmatrix} \leftarrow m_2 \text{ extremized using } b = [0, 1]^T$$

(b) minus solutions (μ negative)

$$\begin{bmatrix} -1.136474 & 1.074954E-01 \end{bmatrix} \leftarrow m_1 \text{ extremized using } b = [1, 0]^T$$
$$\begin{bmatrix} -3.329636E-01 & -1.162967 \end{bmatrix} \leftarrow m_2 \text{ extremized using } b = [0, 1]^T$$

The most-squares solution envelopes are:

(a) plus solution

$$\begin{bmatrix} 9.653091E-02 & 1.181232 \end{bmatrix} \leftarrow \text{upper envelope: } m \text{ extremized using } b = [1, 1]^T$$

(b) minus solution

$$\begin{bmatrix} -7.624581E-01 & -9.662411E-01 \end{bmatrix} \leftarrow \text{lower envelope}$$

The threshold residual, q_T was set to 11 (i.e., n) in these calculations. Notice that the range of parameters provided by the most-squares method for the data are greater than that indicated by the standard deviations of the least squares estimates. All the above results were obtained using the inversion program SVDINV (which incorporates the subroutine MOSTSQ) and are in good agreement with those given in Jackson(1976). This concludes our discussion of linear inversion theory and practice.

7.1 Characterization of nonlinearity

In most of the interesting inverse problems in geophysics the data are related to the model parameters in a nonlinear way (i.e., not in the explicit form $d=Gm$). Recall that even the simple refraction delay-time problem examined under Chapters 4 and 5 is actually non-linear since the travel paths of seismic waves through a layered medium are proportional to the path length in the layer but inversely proportional to the velocity, i.e.,

$$t_i = \sum_{j=1}^p \frac{L_{ij}}{v_j} = \sum_{j=1}^p L_{ij} c_j \quad (7.1)$$

where t_i is the total travel time for the i^{th} ray, L_{ij} is the i^{th} ray path in the j^{th} layer and v_j is the velocity in the j^{th} layer. The model parameters are inversely, rather than linearly, related to the travel time data; and we had to use the slowness ($c = \frac{1}{v}$) instead of v as the parameter of the linear problems of the previous sections. It may be remarked here that the way that a given problem is posed may sometimes determine whether it is in effect linear or not. For instance, if we are interested in a gravity or magnetic model where the model parameters are the anomalous density or susceptibility in cells of fixed position, then such a problem may be considered as being effectively linear. Another set of problems that may be easily manipulated are those in which the forward theory involves simple exponential functions. For instance, in carbon dating (using radioactive decay data for Carbon-14), the forward theory states that the fraction f of an original amount of Carbon-14 remaining after time t has elapsed is given by

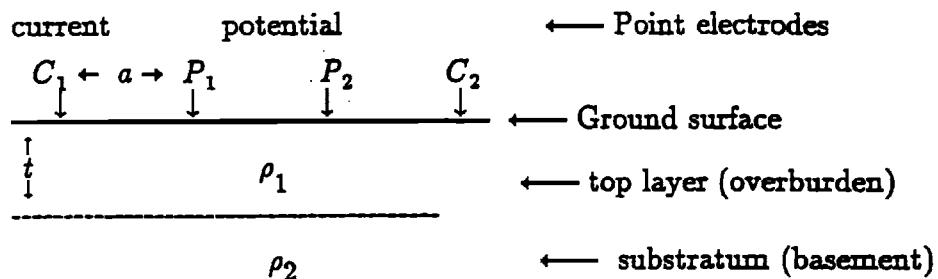
$$f = 1.0e^{mt} \quad (7.2)$$

where m is the unknown parameter. Now, from experimental and theoretical studies, it is known that a linear relationship exists between t and $\log f$. Taking the logarithm of both sides of Eq. (7.2), we have that

$$d = \log f = mt \quad (7.3)$$

which describes the equation of a straight line. The desired parameter may then be

estimated using the linear methods of the previous sections. On a different level, consider the case where we are interested in investigating the resistivity structure of a 2-layer Earth using the popular Wenner electrode configuration illustrated below.



Wenner electrode array.

The forward theory states that the apparent resistivity ρ_a observable on the surface of the above hypothetical Earth-model is given by:

$$\rho_a = \rho_1 \left\{ 1 + 4 \sum_{n=1}^{\infty} \frac{k^n}{\sqrt{[1+(\frac{2nt}{a})^2]}} - 2 \sum_{n=1}^{\infty} \frac{k^n}{\sqrt{[1+(\frac{nt}{a})^2]}} \right\} \quad (7.4)$$

$$\text{where } k = \left(\frac{\rho_2 - \rho_1}{\rho_2 + \rho_1} \right)$$

is the reflection coefficient at the interface between the top layer and the basement. An examination of equations (7.1)-(7.4) will reveal that we cannot perform a simple linearizing parameterization for the resistivity inverse problem. In other words, it is very difficult to put this expression in a form resembling $d=Gm$ as we did in the seismic and radioactive decay examples. To illustrate this point, let us re-define our model parameter and our data kernel as

$$m = k = \frac{(\rho_2 - \rho_1)}{(\rho_2 + \rho_1)}$$

and

$$G_{an} = \frac{4}{\sqrt{[1+(2nt/a)^2]}} - \frac{2}{\sqrt{[1+(nt/a)^2]}} .$$

We can then re-express the data-model parameter relationship as

$$\rho_a = \rho_1 + \sum_{n=1}^{\infty} G_{an} m^n \quad (7.4b)$$

leaving us with an infinite power series. It is obvious that even such transformations may not reduce the inherent non-linearity in the inverse problem of resistivity depth-sounding. However, theory and experiment both suggest that apparent resistivity data exhibit a log-normal distribution and we may be tempted to consider the logarithm of the parameters of the resistivity model instead of the original data themselves – a common practice in resistivity inversion. Now, let us re-write equation (7.4) in terms of k , $\frac{a}{t}$ and $\frac{\rho_a}{\rho_1}$; we have that

$$\frac{\rho_a}{\rho_1} = 1 + 4 \sum_{n=1}^{\infty} \frac{k^n}{\sqrt{[1+4n^2(\frac{a}{t})^2]}} - 2 \sum_{n=1}^{\infty} \frac{k^n}{\sqrt{[1+n^2(\frac{a}{t})^2]}} \quad . \quad (7.5)$$

Notice that the system is still non-linear. If we consider the data pair $(\frac{a}{t}, \frac{\rho_a}{\rho_1})$, in a logarithmic coordinate system the point will be defined by $(\{\log a - \log t\}, \{\log \rho_a - \log \rho_1\})$. Since the unknown parameters t and ρ_1 are constants, so will their logarithms. It follows that simply plotting $\{\log \rho_a\}$ versus $\{\log a\}$ will result only in a shift of a constant distance $\{\log \rho_1\}$ vertically and $\{\log t\}$ horizontally with the shape of the curve unaffected. [Theoretical curves computed for various values of t and ρ may then be directly compared on logarithmic scales with our transformed field curves. This is the basis of Logarithmic Curve Matching in resistivity interpretation.] It may be comforting to think that we have reduced the inherent non-linearity by considering the logarithms of the ρ_a and the model parameters, but in actual fact the problem is still not in the form $d = Gm$. The question thus arises: given that some nonlinear problems are not amenable to simple linearizing transformations, can a general procedure be formulated for attacking them so that the well-understood linear inversion methods may be used in estimating the unknown model parameters? Part of the answer to this question comes from elementary calculus as we shall soon see.

The general form of these non-linear problems is :

$$d_i = f_i(m_1, m_2, \dots, m_p) = f_i(m); \quad i=1, n \quad (7.6)$$

where f is the forward functional that allows us to calculate the theoretical responses for a given set of model parameters, m and experimental geometry. Our two-fold target is to reduce them firstly into forms that can be handled by the data fitting and model

parameter estimation methods developed for linear problems and to find approximate meaningful solutions to the problems. The first part of the above strategy is called **linearization** while the second part is termed **model identification and appraisal**.

7.2 A General Strategy for Handling Non-linear Problems

Gauss suggested that non-linear problems can be solved in successive approximations using the linear least squares method. This involves the conversion the non-linear problem into an approximate linear form by expanding the functional $f(m)$ in Taylor series about an initial guess of the what the values the model parameters might be. This is the standard strategy adopted in geophysical inversion.

7.2.1 The initial model and linearization

Most non-linear inversion schemes require as a starting point, the provision of some approximate (assumed or inferred) values of the desired model parameters, which we shall simply call m^0 . m^0 is variously referred to as the **first guess**, **initial model** or **starting model**). This starting model may be based on *a priori* information (e.g., previous results) or may be simply an intelligent guess and often spells the difference between success and failure in finding a meaningful solution, or between rapid and slow convergence to the solution. From the forward theory the theoretical responses corresponding to m^0 for the p model parameters are :

$$d_i^0 = f_i(m_1^0, m_2^0, m_3^0, \dots, m_p^0)$$

or simply

$$d^0 = f(m^0). \quad (7.7)$$

Next, assume that $f(m)$ is linear around m^0 such that a small perturbation of the model responses about m^0 can be expressed using **Taylor's theorem** as

$$f(m) = f_i(m_1^0 + \delta m_1, m_2^0 + \delta m_2, m_3^0 + \delta m_3, \dots, m_p^0 + \delta m_p)$$

$$= f_i(m^0) + \frac{\partial f_i}{\partial m_1} \delta m_1 + \frac{\partial f_i}{\partial m_2} \delta m_2 + \frac{\partial f_i}{\partial m_3} \delta m_3 + \dots + \frac{\partial f_i}{\partial m_p} \delta m_p + \text{higher order terms}$$

i.e., the function $d=f(m)$ is expanded about the point (m_1^0, \dots, m_p^0) in parameter space.

Writing the above Taylor series expansion in short-hand form, we have that

$$f(\mathbf{m}) = f(\mathbf{m}^0) + \left\{ \sum_{j=1}^p \frac{\partial f_i(\mathbf{m}^0)}{\partial m_j} \Big|_{\mathbf{m}=\mathbf{m}^0} \delta m_j \right\} + O(\|\delta \mathbf{m}\|^2) \quad (7.8)$$

where we have neglected the higher order terms, an approximation that is valid only if the series converges (i.e., δm_j are small, for all j).

In any case, the observational data d that we wish to invert for \mathbf{m} are typically associated with observational errors and the relationship between d and \mathbf{m} needs to take account of these additive noise e . Thus in practical situations we have that

$$\mathbf{d} = f(\mathbf{m}) + \mathbf{e} \quad (7.9)$$

and this equation will constitute our working model.

To estimate a meaningful \mathbf{m} , we therefore need to minimize this error as best as possible. From eq.(7.9), it follows that $e = d - f(\mathbf{m})$. Now, using eq.(7.8), we have that

$$\mathbf{d} - f(\mathbf{m}) = \mathbf{d} - f(\mathbf{m}^0) - \left\{ \sum_{j=1}^p \frac{\partial f_i(\mathbf{m}^0)}{\partial m_j} \Big|_{\mathbf{m}=\mathbf{m}^0} \delta m_j \right\} \quad (7.10)$$

where we have neglected terms of order higher than one. For notational simplicity, let us define the vector $\mathbf{y} = \mathbf{d} - f(\mathbf{m}^0)$ representing the differences between the actual field data and those calculated for our initial model, and denote the quantities $\partial f_{ij}/\partial m_j$ and $\delta \mathbf{m}$ as A and \mathbf{x} . We can then re-state eq. (7.10) as

$$\mathbf{d} - f(\mathbf{m}) = \mathbf{y} - A\mathbf{x}$$

and eq. (7.9) may simply be stated as

$$\mathbf{e} = \mathbf{y} - A\mathbf{x} \quad (7.11)$$

which is now in the desirable linear form if \mathbf{y} , A and \mathbf{x} are respectively likened to d , G and \mathbf{m} for linear problems. Note that A is the matrix of the partial derivatives of f with respect to each of the model parameters m_j . Thus each j^{th} column of A will contain the partials with respect to the j^{th} parameter. The size of this matrix will be $(n \times p)$ for n experimental data and p model parameters. The matrix is also called the Jacobian matrix. The vector \mathbf{x} contains the unknown corrections to be determined and applied to \mathbf{m}^0 so as to minimize e .

7.3 Unconstrained non-linear inversion

7.3.1 Problem formulation

We are now in a position to formulate our inverse problem. To reiterate, in this case, we will be searching for corrections or perturbations to our initial model. Since we typically collect more data than there are model parameters, the problem is overdetermined. As before, the least squares method will be adopted in such minimization problems because of its mathematical robustness when dealing with band-limited, noisy data. Let e be the residual error associated with our predictions (since our model will not fit the field data exactly). We wish to minimize the objective function

$$q = e^T e = (d - f(m))^T (d - f(m)). \quad (7.12)$$

Using the results from the previous section, we can re-write the problem as

minimize

$$q = e^T e = (y - Ax)^T (y - Ax). \quad (7.13)$$

7.3.2 Problem solution: The Gauss-Newton method.

As in the linear case minimization is effected by setting to zero the derivatives of q with respect to each of the desired parameters perturbations x_j , i.e.,

$$\frac{\partial q}{\partial x_j} = \frac{\partial(y^T y - x^T A^T y - y^T A x + x^T A^T A x)}{\partial x_j} = 0$$

giving

$$-A^T y - y^T A + A^T A x + x^T A^T A = 0$$

or

$$2A^T A x - 2A^T y = 0$$

from which we obtain our least squares solution for the parameter perturbations

$$x = (A^T A)^{-1} A^T y \quad (7.14)$$

This perturbation ($x = \delta m$) is then applied to our starting model m^0 to yield a better estimate of the solution to our problem:

$$m^1 = m^0 + x \quad (7.15)$$

However, the new model m^1 may not fit our data adequately such that we may need to repeat the procedure using m^1 as the new starting model. The successive application of this procedure is described as **unconstrained iterative least squares fitting** (or the **Gauss-Newton Method**). The iterative formula would then be

$$m^{k+1} = m^k + (A^T A)^{-1} A^T y \quad (7.16)$$

where the Jacobian matrix A is evaluated at m^k . Let us now consider an idealized problem to illustrate this method of iterative solution.

7.3.3 Example of iterative application of Newton's method

For a single parameter problem, given an equation of the form $f(m) = m^4 + m - 1 = 0$, find the solution to this equation near the region $m = 1$ and correct to two places of decimal.

Solution procedure:

If we were not told to search for the solution in the region $m = 1$, it is instructive to tabulate and plot the function graphically so as to know approximately (or guess) where the solution might be. A table of the function would look like

m	-2	-1	0	1	2	←x-axis
$f(m)$	17	1	-1	-1	13	←y-axis

Table 7.3.3.1 Tabulated values of $f(m)=0$.

An x-y plot would show that the curve cuts the $f(m)=0$ (i.e. y-) axis between $m=1$ and $m=2$ and also between 0 and -1 on the m - (or x-) axis.

Now, assuming that we know that there is a solution near $m=m^0$, expanding $f(m)$ about m^0 as in eq. (7.8) gives

$$\begin{aligned} f(m) &= f(m^0 + \delta m) = f(m^0) + \frac{\partial f(m^0)}{\partial m} \delta m + O(\|\delta m\|^2) \\ &\approx f(m^0) + \frac{\partial f(m^0)}{\partial m} \delta m. \end{aligned}$$

Now, from the problem statement

$$f(m^0) + \frac{\partial f(m^0)}{\partial m} \delta m = f(m^0) + f'(m^0) \delta m = 0$$

so that

$$\delta m = -\frac{f(m^0)}{f'(m^0)}$$

which is the solution to be applied iteratively to m^0 until a stable solution of the desired accuracy is obtained. Notice that we are actually solving a problem of the form $y=Ax$ for x . Its solution for x is the same as that given by eq. (7.14) and will therefore suffice to illustrate the iterative process. In the above formulation, $d=0$ by implication. This digression aside, the next step is to update the solution thus: $m^1=m^0+\delta m$.

Using m^1 as the new guess solution, a new δm is found (after evaluating a new partial derivative with respect to m^1 , i.e., $f'(m^1)$) and added onto m^1 giving m^2 .

The process is repeated until the desired solution is found. Let us complete the exercise.

Required Steps: $m^0=1$, $f'(m^0)=4m^3-1$

and so,

$$m^1 = 1 + \left(-\frac{f(1)}{f'(1)}\right) = 1 + \frac{1}{3} = 1 + 0.3333 = 1.3333$$

$$m^2 = 1.3333 + \left(-\frac{f(1.3333)}{f'(1.3333)}\right) = 1.3333 - \left(\frac{(1.333)^4 - (1.3333) - 1}{4(1.3333)^3 - 1}\right) \leftarrow \begin{array}{l} \text{predicted response} \\ \text{partial derivative} \end{array}$$

$$= 1.3333 - 0.0973 = 1.236 \leftarrow \begin{array}{l} \text{not good enough (since second decimal place} \\ \text{is still non-zero in } \delta m, \text{ so obtain next iterate).} \end{array}$$

$$m^3 = 1.236 + \left(-\frac{f(1.236)}{f'(1.236)}\right) = 1.236 - 0.0141$$

$$= 1.2214 \text{ (second decimal place still changing, so obtain next iterate).}$$

Using m^3 as the initial model, we have that

$$\delta m = \left(-\frac{f(1.2214)}{f'(1.2214)}\right) = -0.006 \text{ (second decimal place is zero in } \delta m, \text{ so stop).}$$

Therefore, the desired solution is 1.22 .

7.3.4 Problem session

Find a solution for m correct to two places of decimal of $f(m) = m^3 - 8m + 6 = 0$ near $m=2$.

7.3.5 Limitations of the Gauss-Newton method

Considering the assumptions and approximations made in order to derive the above algorithm, one question that comes to mind is : Will this unconstrained iterative procedure always solve our non-linear problem ? The main drawbacks of this technique is that a good approximation to the actual model (i.e., a good first guess) is required for the procedure to converge and that the matrix $A^T A$ may be singular or near-singular producing undesirable effects. The latter results when $A^T A$ is ill-conditioned (i.e., the eigenvalues are very small or near-zero). As we saw in Section 4, the calculated solution becomes so large as not to be physically realizable when the eigenvalues are very small. The solution, in this case, is said to 'over-shoot the linear range'. Thus in practice it is necessary to correct m^k by only a fraction of x with the attendant decrease in rate of convergence. Note also that even if $A^T A$ is non-singular, the solution may still diverge or converge very slowly.

7.3.6. The Steepest - Descent (or gradient) method

The method of Steepest descent is a simple *gradient* method. In this method, the initial model is corrected in the direction of the negative gradient of the objective function q , i.e.,

$$x = -k \left\{ \frac{\partial q}{\partial m} \right\} \quad (7.17)$$

where k is a suitably defined constant. Recall that

$$q = (d - f(m))^T (d - f(m)) = |d - f(m)|^2.$$

Thus,

$$\frac{\partial q}{\partial m} = -2(d - f(m)) \cdot \frac{\partial f(m)}{\partial m} \equiv -2A^T(d - f(m)) \quad (7.18)$$

so that the parameter corrections are given (using eq. 7.17) as

$$\begin{aligned}
 x &= -k \left\{ -2A^T(d - f(m)) \right\} = 2kA^T(d - f(m)) \\
 &= [2k]A^Ty .
 \end{aligned} \tag{7.19}$$

It is obvious that replacing the constant factor $[2k]$ in eq. (7.19) with $[A^TA]^{-1}$ will lead to the Gauss-Newton solution given by eq. (7.14). The value of k determines the step-size of the corrections. Notice that eq. (7.19) does not contain any inverse matrix. The scheme does not diverge and this is an advantage over the Gauss-Newton method provided k is small enough. It has good initial convergence characteristics.

7.3.7 Drawback of the Steepest Descent method

A major shortcoming of the method of Steepest-descent is that the rate of convergence decreases as the least squares solution is approached unlike the Gauss-Newton method. It is often inefficient, requiring a large number of steps and is therefore not recommended for practical inversion applications.

7.3.8 Are there any remedies for instability and non-convergence ?

To prevent unbounded solution growth when A^TA is ill-conditioned, Levenberg (1944) suggested a method of 'Damped least squares' to damp the absolute values of the parameter perturbations during successive applications of Taylor's approximations. Levenberg suggested that arbitrary positive weights be added to the main diagonal of A^TA and also showed that the directional derivative of the residual sum of squares q has a minimum when the weights are equal. This idea was later used by Marquardt (1963, 1970) to develop a very useful non-linear algorithm. This technique is called Ridge Regression or the Marquardt-Levenberg method and is the most popular inversion procedure within the geophysical community. It is essentially an interpolation between the Gauss-Newton and Steepest-descent methods and successfully combines their useful properties in the hybrid scheme.

7.4. Constrained Inversion: Ridge Regression or the Marquardt-Levenberg Method

The underlying philosophy here is that the parameter changes x_i may over-shoot the linear range (for a non-linear problem) if their absolute values are left unchecked. A bound is therefore placed on the size of the perturbations thereby constraining the step-length of the solutions. Operationally, in ridge regression we minimize both the residual $e = \|y - Ax\|$ and the size of x .

7.4.1 Statement of the minimization problem

Minimize the objective function

$$\phi = q_1 + \beta q_2 = e^T e + \beta(x^T x - L_0^2) \quad (7.20)$$

where we are minimizing some combination ϕ of the prediction error and solution length and we have placed a bound L_0^2 on the energy of the parameter changes; and β is an undetermined (Lagrange) multiplier that determines the relative importance that will be given to q_1 and q_2 . Here, β is referred to as the **damping factor**. Note therefore that ridge regression is essentially a constrained non-linear least squares method. If a value close to zero is assigned to β , the solution approximates the Gauss-Newton solution.

7.4.2 Problem solution

Minimization of eq. (7.20) is effected in the same manner as for the unconstrained least squares method. The procedure is simple :

differentiate ϕ with respect to x , equate result to zero and solve for x

$$\frac{\partial \phi}{\partial x} = \frac{\partial \{(y - Ax)^T(y - Ax) + \beta(x^T x - L_0^2)\}}{\partial x} = 0 \quad (7.21)$$

Hint:

expand the terms in the numerator of eq. 7.21 and then carry out the differentiation .

We will then find that

$$2A^T A x - 2A^T y - 2\beta x = 0$$

or

$$(A^T A + \beta I)x = A^T y \quad \leftarrow \text{the normal equations}$$

from which we obtain the ridge regression or constrained or damped least squares solution for the parameter perturbations

$$x_r = [A^T A + \beta I]^{-1} A^T y . \quad (7.22)$$

The solution x_r is then used in an iterative process to fit our data. If our starting model is m^0 , non-linearity is dealt with using the iterative formula

$$m^{k+1} = m^k + [A^T A + \beta I]^{-1} A^T y \quad (7.23)$$

where A is evaluated at m^k and $m^k = [m^0 + x_r^k + x_r^{k-1} + x_r^{k-2} + x_r^{k-3} + \dots + x_r^1]$ for $k+1$ iterations.

A comparison of equations (7.16) and (7.23) will reveal that the latter is an effective way of dealing with singularities in $A^T A$. Ridge regression is in effect a hybrid technique in the sense that it combines the steepest descent and the Gauss-Newton methods. The steepest descent method dominates when the starting model is far from the solution to the problem while the least squares method becomes dominant as the solution is approached. Marquardt(1970) showed that ridge regression is similar in character to generalized inversion, and that $(A^T A + \beta I)^{-1} A^T$ approaches the generalized inverse of Penrose (1955) as $\beta \rightarrow \infty$, and interpreted the matrix βI as the covariance matrix of a set *a priori* data.

7.4.3 Application of SVD in non-linear inversion

The least squares solution given by eq. 7.14 can be written in terms of SVD as

$$x = [A^T A]^{-1} A^T y = [V \Lambda^{-2} V^T] V \Lambda U^T y = V \Lambda^{-1} U^T y \quad (7.24)$$

where we have assumed that $r=p$ and that the inverse of $A^T A$ (i.e., $V \Lambda^{-2} V^T$) exists. In ridge regression, we replace the $1/\lambda_j$ in the Λ^{-1} matrix by the element

$$\lambda_{r,j}^{-1} = \frac{\lambda_j}{(\lambda_j^2 + \beta)} \quad (7.25)$$

so that the ridge regression estimate, in terms of SVD is formally

$$x_r = V \Lambda_r^{-1} U^T y \quad (7.26)$$

where Λ_r^{-1} is related to Λ^{-1} by the transform (7.25). The advantages of using these transformed variables are obvious : when λ_j is much larger than β , the quantity $(\lambda_j + \beta)$ differs very little from λ_j ; and when λ_j is close to zero, the addition of a positive bias β will ensure that $A^T A$ will not be so close to singularity.

7.4.4 Determination of damping factors in ridge regression

For automated inversion, the common practice is to set β first to a large positive value thus taking advantage of the good initial convergence properties of the steepest descent method and thereafter β is multiplied by a factor less than unity after each iteration so that the linear least squares method predominates near the solution. A variant of this procedure (Johansen, 1977) assumes as β the smallest eigenvalue of $A^T A$ matrix and if divergence occurs, it is replaced by the next largest eigenvalue until the solution is obtained. A more sophisticated method of damping has been developed by Meju (1988, 1992) and is in effect a hybrid of the two methods highlighted above. The damping factors are determined empirically – from what might be likened to approximate derivatives of a Lagrangian function (see Herskovits, 1986) – and used in a minimization sub-problem at each iteration. The procedure for estimating the damping factors is illustrated graphically in Fig. 7.1. Operationally, the largest and smallest eigenvalues of the problem are multiplied by 10. and 0.1 respectively giving λ_l and λ_s , that are used to determine the coefficients of a parabola from which ten samples of the auxiliary factors λ_k are obtained using the formula (Meju, 1992)

$$\lambda_k = (\{100\lambda_s - \lambda_l\} + \{\lambda_l - \lambda_s\}k^2)/99., \quad k = 1, \dots, 10. \quad (7.27)$$

The factors λ_k are squared to give the damping factors β_k required in a line search procedure based on equation (7.23). This technique involves coarse steps in β in the region of β_l , but the steps become finer towards β_s (see Fig. 7.1). The damping factor is set initially to the largest value β_{10} so that the characteristics of the steepest descent method dominates and then successively smaller values of β_k are used thus enabling the least squares method to be dominant at the later stages of the line search procedure. The solution before divergence is returned as the next iterate in the main calling program. However, if no divergence occurs during this intermediate search for an optimal solution, a value of zero is assigned to β yielding the unconstrained least squares estimate.

7.4.5 Ridge regression in practice

It will be assumed here that our field data have associated errors. These errors are then used to define a weighting matrix W as before. An effective ridge regression algorithm that uses a 1-D line search procedure is given below to illustrate how the method may be implemented in practical applications. The algorithm is simply (Meju, 1992):

Determination of damping factor

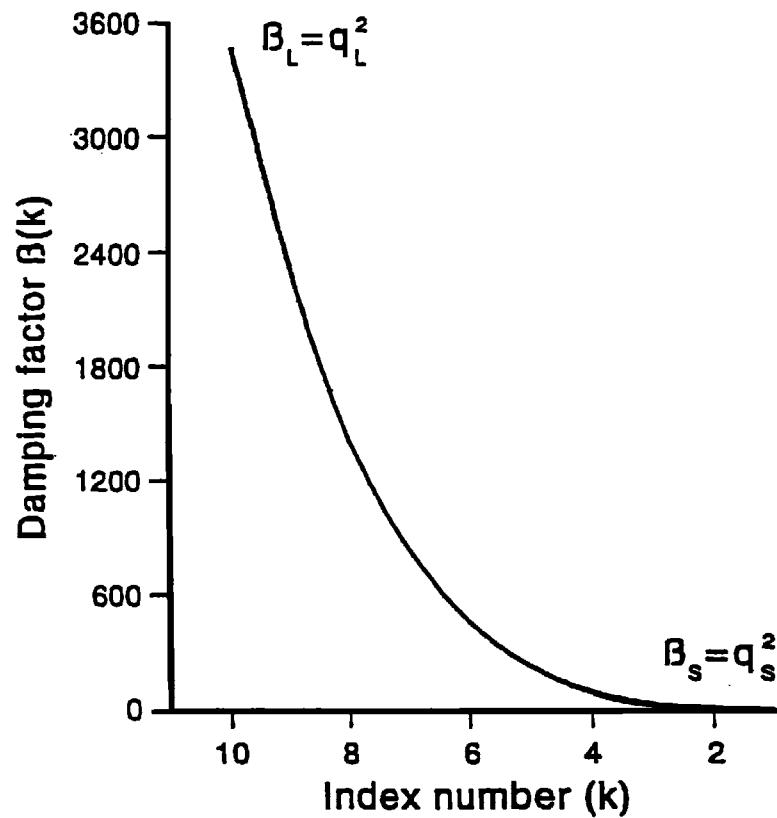


Figure 7.1

Step 1. Select a starting model, m_0 .

Step 2. Calculate

$$(W\mathbf{y}) = Wd - Wf(m_0)$$

and

$$q_1^0 = \sum_{i=1}^n (W\mathbf{y})_i^2$$

Step 3. If the computed responses fit the experimental data d , or other stopping criteria met (e.g., $q_1^0 \geq q_T$), STOP.

Step 4. Obtain the weighted partial derivatives, $(WA) = A_*$.

Step 5. Calculate the SVD of A_* .

Step 6. Obtain the most feasible solution using a line-search procedure in a ridge regression sub-program.

(a) calculate damping factors for the line search procedure

$$\lambda_k = (\{100\lambda_s - \lambda_l\} + \{\lambda_l - \lambda_s\}k^2)/99., \quad (7.27)$$

and hence

$$\beta_k = \lambda_k^2, \quad k=1, \dots, 10.$$

where λ_s and λ_l are the smallest and largest singular values of A_* multiplied respectively by 0.1 and 10.

(b) set $\beta_0 = 0.0$

(c) perform line search with ridge regression

Loop ($j=1$ to 11 and $k=11-j$)

$$\text{Get } \text{diag}[\Lambda]_i^{-1} = \text{diag}[\Lambda]_i / (\text{diag}[\Lambda]_i^2 + \beta_k), \quad i=1, p$$

$$\text{Calculate } m_j = m_0 + V\Lambda^{-1}U^T y_*$$

$$\text{Compute } q_1^j = \sum_{i=1}^n |Wd - Wf(m_j)|^2$$

If ($q_1^j > q_1^{j-1}$)

set optimal solution to m_{j-1} and quit

else

set optimal solution to m_j

End Loop

Step 7. Set the optimum model from step 6 as the new iterate (i.e., m_0).

Step 8. Goto Step 2.

The above ridge regression procedure has been found to be very effective in resistivity data inversion (e.g., Meju, 1992; Meju and Hutton, 1992.). Notice that the computational requirement at Step 6 is minimal once the factorisation of A_s has been done. The interested reader may note that Herskovits (1986) provides a very rigorous analysis of a two-stage minimization algorithm in which a somewhat analogous line-search procedure assures the global convergence of the scheme and the feasibility of the iterates. However, as shown for linear problems, the results from Marquardt inversion may be a smoothed version of the truth. The question then arises: **Can a unique solution be determined for a nonlinear problem?** We will now examine some ways of addressing the problem of non-uniqueness in nonlinear inversion.

A Generalized Approach

In interpreting a scanty set of inexact data, conventional wisdom is to seek models that are in agreement with *a priori* data derived from say, previous geophysical studies, borehole or geological data. These extraneous information help single out a plausible solution from amongst all possible ones admitted by the inexact practical data. In Chapter 5, we saw how the use of *a priori* data in linear inversion helps resolve the problem of non-uniqueness. Unfortunately, while the solution to the linear inverse problem incorporating *a priori* information is well known (see e.g., Jackson, 1979), there is no unequivocal technique as yet for resolving non-uniqueness in nonlinear inversion. A naive approach to using *a priori* information in nonlinear inversion involves holding constant the values of some of the sought parameters within an iterative inversion scheme. The formal approach is to incorporate the *a priori* data directly in the problem formulation. Much of the published formal treatment of *a priori* information in nonlinear inversion adopt a probabilistic approach (e.g., Gol'tsman, 1971, 1975; Tarantola & Valette, 1982; Jackson & Matsu'ura, 1985; Pous et al., 1987; Duijndam, 1988) which, it may be argued, best characterises the huge variability in practical geophysical measurements (Meju, 1994d). We will adopt the same approach as in our treatment of linear inversion since it involves simple matrix algebra and minimal statistical commitment. Following Meju (1994d), the problem of inversion with *a priori* information will be addressed within a unifying framework of biased estimation with emphasis on simplicity and effective practical procedures. In this approach a distinction is made between starting models and *a priori* information for clarity. We shall aim to make the inversion scheme flexible enough to allow for the construction of a variety of least squares solutions using either reliable or diffuse *a priori* data thus making it a useful practical tool for exploiting particular geophysical situations. To achieve this objective, we will need to consider several forms of *a priori* constraints or solution simplicity measures and take the observational errors into account. Finally, we will show the relationships between the ensuing algorithms and various classical inversion algorithms. This strategy, it is hoped will enable us to analyse and understand the more rigorous algorithms for non-linear inversion (e.g., Tarantola & Valette, 1982).

8.1 Underlying Philosophy

The biased estimation philosophy is simple and the undergirding principles are similar to those described in Chapter 5. In some practical inverse problems, we may have some

idea about the form of the solution, the range of possible values that the sought parameters might assume, or have reliable prior estimates of some of the parameters of the problem. Our goal in biased estimation is to retain, where available, any reliable prior estimates or desirable structural forms in the final solution to an inverse problem. However, in cases where there are no realistic prior estimates or structural form of the solution and we can only make an intelligent guess as to what they might be, it is desired that the solution process be stable and that the final solution be independent of the initial guess. It is thus imperative that we must distinguish between *a priori* information, h and initial (or starting) models, m^0 in this approach. The components of the starting model may include the reliable *a priori* estimates towards which we wish to bias the final solution, but this is not obligatory.

We also strive to maintain statistical stability in our solution process. Thus, owing to the nature of practical data and if we assume that the standard errors σ associated with our n observational data, d are statistically independent, an $n \times n$ diagonal weighting matrix $W = \sigma^{-2} I$ may be defined and used for scaling our data equations so that undue importance is not given to poorly estimated data especially when our *a priori* assumptions are not very accurate or reliable. This scaling operation can also be interpreted as a process of normalization or standardization (as the data equations are thus rendered dimensionless and uncorrelated).

8.2 Non-linear Inversion with *a priori* information

In order to retain the desired *a priori* estimates h of the p sought model parameters in the final solution to an inverse problem involving our band-limited observational data, the necessary constraining equations may be developed in the form $Dm = h$. In this case, $D_{p \times p}$ is an identity matrix that operates on the p parameter, m to yield or preserve the *a priori* data contained in the vector h , i.e.,

$$Dm = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \\ \vdots \\ m_p \end{bmatrix} = \begin{bmatrix} h_1 \\ h_2 \\ \vdots \\ h_p \end{bmatrix}. \quad (8.1a)$$

Alternatively, if we are interested in retaining a particular form of the solution that is in accord with the physics of the problem, say, we can also develop the appropriate constraints as in eq. (8.1a). For example, if we desire that the model parameters vary

smoothly with position, then we need to minimize the differences between physically adjacent parameters using the constraints

$$Dm = \begin{bmatrix} 1 & -1 & & & \\ & 1 & -1 & & \\ & & \ddots & & \\ & & & 1 & -1 \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \\ \vdots \\ m_p \end{bmatrix} = \begin{bmatrix} h_1 \\ h_2 \\ \vdots \\ h_l \end{bmatrix} \quad (8.1b)$$

where $l = p-1$, and the $l \times p$ matrix D is a first difference operator. Such smoothness (or derivative regularization) measures appear to have been introduced in data inversion by Twomey (1963, 1977) and Tikhonov (e.g., Tikhonov, 1963; Tikhonov & Glasko, 1965, 1975; Tikhonov & Arsenin, 1977) and may be called Twomey-Tikhonov smoothness measures. Note that other regularization measures can be developed but the two defined above will suffice in this course.

8.2.1 Retention of known parameter values in the solution

8.2.1.1 Problem formulation

Our goal here is to bias m towards h . We simply state the problem as: "Given a finite collection of inexact observational data, find the solution amongst all the equivalent ones (on account of data and model errors), that explains the observations and satisfies the available reliable estimates of the model parameters". Mathematically, the above statement is equivalent to minimizing the prediction error $e^T e$ and the departure of the solution from the specified constraints as discussed for linear problems. The mathematical development involving an elaborate treatment of the data errors is straightforward. If reliable estimates of m are given in h , then we simply minimize the Lagrangean function (Meju, 1994d)

$$\mathcal{L} = (Wd - Wf(m))^T (Wd - Wf(m)) + (\beta[Dm - h])^T (\beta[Dm - h]) \quad (8.2)$$

where β is a diagonal matrix of Langrange multipliers that enables us to pick out those parameters that should be forced into conformity with the prior estimates leaving the rest unconstrained. The diagonal elements corresponding to the prior data are assigned a constant value greater than zero while those corresponding to the free parameters are zero and may not be considered in the interpretation process (Meju, 1994d). The most applicable constraints for this kind of problem are given by eq. (8.1a). If $f(m)$ is continuous and differentiable, expanding it about an initial model m^0 using

Taylor's theorem gives the linearized approximation of eq. (8.2), i.e.,

$$\mathcal{L} = (\mathbf{W}\mathbf{y} - \mathbf{W}\mathbf{A}\mathbf{x})^T (\mathbf{W}\mathbf{y} - \mathbf{W}\mathbf{A}\mathbf{x}) + \{[\mathbf{D}(\mathbf{m}^0 + \mathbf{x}) - \mathbf{h}]^T \boldsymbol{\beta}^T \boldsymbol{\beta} [\mathbf{D}(\mathbf{m}^0 + \mathbf{x}) - \mathbf{h}]\} \quad (8.3)$$

where $\mathbf{y}_i = d_i - f_i(\mathbf{m}^0)$, A is the $n \times p$ matrix with elements $A_{ij} = \frac{\partial f_i(\mathbf{m}^0)}{\partial m_j}$, and we have used the approximation $\mathbf{x} = \mathbf{m} - \mathbf{m}^0$.

8.2.1.2 Problem solution

Minimization is effected by setting the derivatives of \mathcal{L} with respect to \mathbf{x} to zero as usual. **HINT:** It is always helpful to expand equation (8.3) before differentiation. Thus, dropping the \mathbf{W} term and defining the matrix $B = \boldsymbol{\beta}^T \boldsymbol{\beta}$ for notational simplicity, we have that

$$\begin{aligned} \mathcal{L} = & (\mathbf{y}^T \mathbf{y} - \mathbf{y}^T \mathbf{A} \mathbf{x} - \mathbf{x}^T \mathbf{A}^T \mathbf{y} + \mathbf{x}^T \mathbf{A}^T \mathbf{A} \mathbf{x}) + B \{ \mathbf{m}^{0T} \mathbf{D}^T \mathbf{D} \mathbf{m}^0 + \mathbf{m}^{0T} \mathbf{D}^T \mathbf{D} \mathbf{x} \\ & - \mathbf{m}^{0T} \mathbf{D}^T \mathbf{h} + \mathbf{x}^T \mathbf{D}^T \mathbf{D} \mathbf{m}^0 + \mathbf{x}^T \mathbf{D}^T \mathbf{D} \mathbf{x} - \mathbf{x}^T \mathbf{D}^T \mathbf{h} - \mathbf{h}^T \mathbf{D} \mathbf{m}^0 - \mathbf{h}^T \mathbf{D} \mathbf{x} + \mathbf{h}^T \mathbf{h} \}. \end{aligned} \quad (8.4)$$

We can now carry out a simple differentiation without the risk of forgetting some terms. At the minimum, we have that

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \mathbf{x}} = & -\mathbf{y}^T \mathbf{A} - \mathbf{A}^T \mathbf{y} + \mathbf{A}^T \mathbf{A} \mathbf{x} + \mathbf{x}^T \mathbf{A}^T \mathbf{A} + \mathbf{m}^{0T} \mathbf{D}^T \mathbf{B} \mathbf{D} + \mathbf{D}^T \mathbf{B} \mathbf{D} \mathbf{m}^0 + \mathbf{D}^T \mathbf{B} \mathbf{D} \mathbf{x} \\ & + \mathbf{x}^T \mathbf{D}^T \mathbf{B} \mathbf{D} - \mathbf{D}^T \mathbf{B} \mathbf{h} - \mathbf{h}^T \mathbf{B} \mathbf{D} = 0. \end{aligned} \quad (8.5)$$

That is,

$$-2\mathbf{A}^T \mathbf{y} + 2\mathbf{A}^T \mathbf{A} \mathbf{x} + 2\mathbf{D}^T \mathbf{B} \mathbf{D} \mathbf{m}^0 + 2\mathbf{D}^T \mathbf{B} \mathbf{D} \mathbf{x} - 2\mathbf{D}^T \mathbf{B} \mathbf{h} = 0 \quad (8.6)$$

yielding the normal equations

$$\mathbf{A}^T \mathbf{A} \mathbf{x} + \mathbf{D}^T \mathbf{B} \mathbf{D} \mathbf{x} = \mathbf{A}^T \mathbf{y} + \mathbf{D}^T \mathbf{B} \mathbf{h} - \mathbf{D}^T \mathbf{B} \mathbf{D} \mathbf{m}^0 \quad (8.7)$$

whose biased solution (with the \mathbf{W} term reinstated) for the parameter corrections to be applied to \mathbf{m}^0 is

$$\mathbf{x} = [(\mathbf{W}\mathbf{A})^T \mathbf{W}\mathbf{A} + \mathbf{B}]^{-1} [(\mathbf{W}\mathbf{A})^T \mathbf{W}\mathbf{y} + \mathbf{B}\{\mathbf{h} - \mathbf{m}^0\}] \quad (8.8)$$

since $D=I$ (eq. 8.1a) and $BI=B$.

Nonlinearity is dealt with using an iterative formula of the form

$$\mathbf{m}^{k+1} = \mathbf{m}^k + [(WA)^T WA + B]^{-1} [(WA)^T Wy + B\{\mathbf{h} - \mathbf{m}^k\}] \quad (8.9)$$

where the Jacobian matrix A and the data misfit vector y are evaluated at \mathbf{m}^k and the iteration is begun at $k=0$. The term $B\{\mathbf{h}-\mathbf{m}^k\}$ on the right-hand side of eq. (8.9) helps to force the solution into conformity with the specified *a priori* parameter estimates and this inversion formula is dubbed the **maximum-bias algorithm** by Meju (1994d).

If the *a priori* information is diffuse (or unreliable), then it may be desirable to set the constraints equal to zero, i.e., $\mathbf{h} = [0, 0, \dots, 0]^T$, and all the elements of β are set equal to a constant value ($0 < \beta < 1$) so that all the parameters have equal importance. In this case, β may be conveniently replaced by the single undetermined multiplier β . We then have that

$$\mathcal{L} = (Wd - Wf(\mathbf{m}))^T (Wd - Wf(\mathbf{m})) + \beta^2 \mathbf{m}^T D^T D \mathbf{m} \quad (8.10a)$$

which can be approximated by the linearized system

$$\mathcal{L} = (Wy - WAx)^T (Wy - WAx) + \{\beta^2 (\mathbf{m}^0 + \mathbf{x})^T D^T D (\mathbf{m}^0 + \mathbf{x})\}. \quad (8.10b)$$

The solution for the parameter corrections is simply

$$\mathbf{x}_* = [(WA)^T WA + \beta^2 I]^{-1} [(WA)^T Wy - \beta^2 \mathbf{m}^0] \quad (8.11)$$

and the iteration formula is identically

$$\mathbf{m}^{k+1} = \mathbf{m}^k + [(WA)^T WA + \beta^2 I]^{-1} [(WA)^T Wy - \beta^2 \mathbf{m}^k] \quad (8.12)$$

since $D=I$. Here, $\beta^2 I$ serves to control the step-size of the solution while $\beta^2 \mathbf{m}^k$ helps reduce its bias towards the null vector \mathbf{h} and we may refer to the procedure as inversion with smoothness constraint or the **minimum-bias algorithm**.

8.2.2 Retention of known form of the solution

Let us now turn to the situation where the bias in the solution is dictated by physical arguments, say. In the case where h contains our specified differences between adjacent parameters (e.g., a fixed-step model) and the applicable constraints are given by eq. (8.2). Here, all the parameters have equal importance and we need use only a single undetermined multiplier β . That is, we need to minimize the function

$$\mathcal{L} = (\mathbf{Wd} - \mathbf{Wf}(m))^T (\mathbf{Wd} - \mathbf{Wf}(m)) + \beta^2 (\mathbf{Dm} - h)^T (\mathbf{Dm} - h) \quad (8.13)$$

and the solution for the x that will lead to the minimization of the function \mathcal{L} is identically

$$x = [(WA)^T WA + \beta^2 H]^{-1} [(WA)^T Wy + \beta^2 D^T \{h - Dm^0\}] . \quad (8.14)$$

where the matrix $H = D^T D$.

In many practical situations where there are gradational changes in physical properties in the subsurface say, we may be interested in obtaining the smoothest solution with minimized differences between adjacent parameters. For instance, for physical reasons one can argue that there are no sharp discontinuities in resistivity in the subsurface and elect to invert the observational data for smooth models (e.g., Constable et al., 1987; Meju and Hutton, 1992). In such cases, we do not really have any quantifiable estimates of h then conventional wisdom dictates that we set the elements of h in eq. (8.2) equal to zero and the applicable constraints are given by eq. (8.1b). The problem is thus defined as the search for the smoothest model (as gauged by the smoothness measure $\beta^2 m^T D^T Dm$) that will explain the given experimental data. Mathematically, we minimize the function

$$\mathcal{L} = (\mathbf{Wd} - \mathbf{Wf}(m))^T (\mathbf{Wd} - \mathbf{Wf}(m)) + \beta^2 m^T D^T Dm \quad (8.15)$$

whose solution for the parameter corrections is (Meju 1994d)

$$x_s = [(WA)^T WA + \beta^2 H]^{-1} [(WA)^T Wy - \beta^2 Hm^0] . \quad (8.16)$$

In this case, the term $\beta^2 H$ serves to regularize (Tikhonov, 1963) the solution process while the term $-\beta^2 Hm^0$ helps control the solution's departure from the stipulated form

(i.e. $\mathbf{h} = [0, \dots, 0]^T$).

8.2.3 Consistency analysis of non-linear solutions

A good practice in non-linear formulations is to ascertain that the solution process will yield the linear solution if the problem is sufficiently linear, i.e., that the formulations are consistent with the well understood linear analogues (Meju, 1994d). Recall that in linear inversion the sought model parameters were directly retrieved from the data. In non-linear estimation, we may also solve explicitly for the sought parameters instead of the usual parameter corrections and the solution thus obtained should reduce to the linear solution if the problem tackled is near-linear. This approach is also useful when calculating parameter covariances in non-linear estimation as shown later. To achieve this goal, we simply go back to the appropriate normal equations, replace \mathbf{x} with the quantity $(\mathbf{m} - \mathbf{m}^0)$ and then solve directly for \mathbf{m} .

Taking the data errors into account, for the unconstrained (Gauss-Newton) solution we have that

$$((\mathbf{W}\mathbf{A})^T \mathbf{W}\mathbf{A})(\mathbf{m} - \mathbf{m}^0) = (\mathbf{W}\mathbf{A})^T \mathbf{W}\mathbf{y}$$

giving the unbiased estimate

$$\mathbf{m} = ((\mathbf{W}\mathbf{A})^T \mathbf{W}\mathbf{A})^{-1} (\mathbf{W}\mathbf{A})^T \{\hat{\mathbf{d}}\} \quad (8.17)$$

where $\{\hat{\mathbf{d}}\} = \{\mathbf{W}\mathbf{y} + \mathbf{W}\mathbf{A}\mathbf{m}^0\}$ is a kind of data and the algorithm can be forced to give our unconstrained linear least squares solution if the problem is linear.

The normal equations for maximum-bias estimator (eq. 8.7) may be written as

$$\mathbf{A}^T \mathbf{E} \mathbf{A} \mathbf{m} + \mathbf{D}^T \mathbf{B} \mathbf{D} \mathbf{m} = \mathbf{A}^T \mathbf{E} \mathbf{y} + \mathbf{D}^T \mathbf{B} \mathbf{h} - \mathbf{D}^T \mathbf{B} \mathbf{D} \mathbf{m}^0 + \{\mathbf{A}^T \mathbf{E} \mathbf{A} \mathbf{m}^0 + \mathbf{D}^T \mathbf{B} \mathbf{D} \mathbf{m}^0\}$$

so that

$$\mathbf{m} = (\mathbf{A}^T \mathbf{E} \mathbf{A} + \mathbf{D}^T \mathbf{B} \mathbf{D})^{-1} [(\mathbf{W}\mathbf{A})^T \{\hat{\mathbf{d}}\} + \mathbf{D}^T \mathbf{B} \mathbf{h}] \quad (8.19)$$

where \mathbf{E} and the new data $\hat{\mathbf{d}}$ are as previously defined. The above estimator can easily

be shown to be consistent with the linear estimator given by eq. (6.2).

For the minimum-bias solution given by eq. (8.11), we have that

$$A^T E A m + \beta^2 I m = A^T E y - \beta^2 I m^0 + \{A^T E A m^0 + \beta^2 I m^0\}$$

giving the explicit solution for the model parameters

$$m = (A^T E A + \beta^2 I)^{-1} (W A)^T \{\hat{d}\} \quad (8.20)$$

which is also consistent with the linear analogue (eq. 6.1b).

For the solution for smooth models given by eq. (8.16), we have that

$$A^T E A m + \beta^2 H m = A^T E y - \beta^2 H m^0 + \{A^T E A m^0 + \beta^2 H m^0\}$$

giving the explicit relation

$$m = (A^T E A + \beta^2 H)^{-1} A^T \{\hat{d}\} \quad (8.21)$$

which is consistent with the linear solution for inversion with smoothness measures (equations 5.7 & 6.1a).

8.3 Relationships with standard methods

A comparison between the algorithms derived above and a few popular inversion schemes would perhaps throw more light on the principle and techniques of biased estimation. As in the linear methods, if $\beta \rightarrow 0$, then all the above iterative estimation formulae reduce to the weighted classical least squares update formula

$$m^{k+1} = m^k + [(W A)^T W A]^{-1} (W A)^T W y \quad (8.22)$$

where A and y are evaluated at m^k , highlighting the importance of β in biased estimation. Thus the stability characteristics and the effectiveness of the biased estimation methods depend largely on β and D .

Notice that eq. (8.11) differs from the usual damped least squares or ridge regression update formula (see e.g., Meju, 1992)

$$\mathbf{x} = [(\mathbf{W}\mathbf{A})^T \mathbf{W}\mathbf{A} + \beta I]^{-1} (\mathbf{W}\mathbf{A})^T \mathbf{W}\mathbf{y} \quad (8.23)$$

by the $-\beta^2 \mathbf{m}^0$ term. Equation (8.23) is the weighted variant of the ridge regression formula given by Marquardt (1963, 1970) and Hoerl & Kennard (1970). It is obvious that the above formula could only be derived from eq. (8.10b) by replacing the last term in braces on the right-hand side with $\beta \mathbf{x}^T \mathbf{D}^T \mathbf{D} \mathbf{x}$; but then we would not be dealing with the full linearized set of equations and this has implications for the intuitive arguments employed in the usual ridge regression formulations where the singular goal is to place a bound on the energy of the parameter increments. It is perhaps *apropos* to re-examine the popular ridge regression method within the framework of biased estimation.

Let us define the constrained inversion problem as *minimize* the Lagrangean function

$$\mathcal{L} = (\mathbf{W}\mathbf{d} - \mathbf{W}\mathbf{f}(\mathbf{m}))^T (\mathbf{W}\mathbf{d} - \mathbf{W}\mathbf{f}(\mathbf{m})) + \beta(\mathbf{m} - \mathbf{m}^0)^T(\mathbf{m} - \mathbf{m}^0) \quad (8.24)$$

where we are mainly searching for that bounded perturbation to our initial model that is optimal for fitting our data (cf. Marquardt, 1963). Note that we have neglected our usual operator \mathbf{D} since it is an identity matrix and all parameters have equal importance. Linearizing eq. (8.24) as usual gives the following approximation to the objective function:

$$\mathcal{L} = (\mathbf{W}\mathbf{y} - \mathbf{W}\mathbf{A}\mathbf{x})^T (\mathbf{W}\mathbf{y} - \mathbf{W}\mathbf{A}\mathbf{x}) + \beta \mathbf{x}^T \mathbf{x}$$

whose solution for \mathbf{x} is given by eq. (8.23). To fully understand this solution, let us analyse its consistency with the linear analogue represented by $\mathbf{m} = [\mathbf{G}^T \mathbf{G} + \beta I]^{-1} \mathbf{G}^T \mathbf{d}$ (i.e., eq. 5.10). From the normal equations, we have that

$$(\mathbf{A}^T \mathbf{E} \mathbf{A} + \beta I)[\mathbf{m} - \mathbf{m}^0] = \mathbf{A}^T \mathbf{E} \mathbf{y}$$

or

$$(\mathbf{A}^T \mathbf{E} \mathbf{A} + \beta I)\mathbf{m} = (\mathbf{W}\mathbf{A})^T[\mathbf{W}\mathbf{y} + \mathbf{W}\mathbf{A}\mathbf{m}^0] + \beta I\mathbf{m}^0$$

so that

$$\mathbf{m} = (\mathbf{A}^T \mathbf{E} \mathbf{A} + \beta I)^{-1} \{ (\mathbf{W}\mathbf{A})^T \hat{\mathbf{d}} + \beta \mathbf{m}^0 \} \quad (8.25)$$

where the quantity $\hat{d} = (\mathbf{W}\mathbf{y} + \mathbf{W}\mathbf{A}\mathbf{m}^0)$ is a form of data. It is obvious that the above relation will not yield the traditional damped least squares formula for a linear system (eq. 5.10). For a linear problem, eq. (8.25) will reduce to something in the form of the biased estimation formula given by eq. (5.2) if the term $\beta\mathbf{m}^0$ is equated to $\beta\mathbf{h}$, i.e., some 'assumed' *a priori* model. Operationally, the main difference between our biased scheme and the Marquardt algorithm is that a new *a priori* model (i.e., the previous iterate) is used at each iteration in the latter and this strategy is not in accord with the present philosophy of biased estimation. Paraphrased in a different way, treating the previous iterate as the *a priori* model is not consistent with our assumption that \mathbf{h} is independent of the observational data under consideration, and may lead to undesirable results. It is not the favoured approach to addressing the problem of non-uniqueness in non-linear inversion, albeit the most powerful minimization scheme (see Meju, 1992).

Using the quantity \mathbf{E} in place of $\mathbf{W}^T\mathbf{W}$ in eq. (8.9), we have that

$$\mathbf{m}^{k+1} = \mathbf{m}^k + \{[\mathbf{A}^T \mathbf{E} \mathbf{A} + \mathbf{B}]^{-1} [\mathbf{A}^T \mathbf{E} \mathbf{y} + \mathbf{B}(\mathbf{h} - \mathbf{m}^k)]\} \quad (8.26)$$

which is equivalent to the Bayesian estimation scheme of Jackson & Matsu'ura (1985, eq. 65-67) and comparable to Tarantola & Valette's (1982, eq. 49) nonlinear algorithm (see also Pous et al., 1987, eq. 3) if \mathbf{B} is interpreted statistically as the inverse *a priori* parameter covariance matrix (Meju, 1994d). Thus, using a simple algebra, we have in effect developed a scheme that is similar to the more mathematically rigorous schemes based on a probabilistic treatment of nonlinear inversion with prior data. However, note that the inversion philosophy and the usage of *a priori* information in Tarantola & Valette's landmark method differ somewhat from ours. We are primarily interested in forcing the final solution into close conformity with those parameter estimates known *a priori* and thus the last term on the right-hand side of eq. (8.26) is non-zero since only a few parameters estimates may be known *a priori* in typical practical situations. In Tarantola & Valette's algorithm, \mathbf{h} is simply the actual initial model \mathbf{m}^0 . In this case, as in Pous et al., (1987, eq. 6), the last term in eq.(8.26) would be equal to zero in the first iteration. We treated \mathbf{h} as being separate from \mathbf{m}^0 , more or less as in Jackson & Matsu'ura (1985). Note that in the algorithm of Jackson & Matsu'ura the quantity in braces in eq. (8.26) is multiplied by a suitably chosen factor b ($0 < b < 1$). It may thus be contended that our simple approach is somewhat general.

8.4 Implementation of constraints in iterative applications

The iterative constrained solution process can be effected as before with the augmented equations

$$\mathbf{y}_* = \begin{bmatrix} W\mathbf{y} \\ \gamma\Delta^k \end{bmatrix} \quad \text{and} \quad \mathbf{A}_* = \begin{bmatrix} W\mathbf{A} \\ \gamma\mathbf{D} \end{bmatrix} \quad (8.27)$$

where $\Delta^k = (\mathbf{h} - \mathbf{D}\mathbf{m}^k)$, \mathbf{m}^k are the parameter estimates at the previous (i.e., k^{th}) iteration, γ is the applicable Lagrange multipliers (β or β') and \mathbf{D} is the applicable problem regularization matrix. Note that \mathbf{m}^k is simply \mathbf{m}^0 in the first iteration and that Δ^k may not be a null-vector even though \mathbf{m}^0 may include the members of \mathbf{h} . An optimum value for β is found by trial and error. However, a recommended procedure is to select that value that gives an acceptable residual $|\mathbf{d} - \mathbf{f}(\mathbf{m}^k)|^2$ and yields a result that satisfies the imposed constraints.

It is pertinent to mention here that in inversion with smoothness measures (eq. 8.1b), if we wish to retain known estimates of the sought parameters while smoothing the variations between the unknowns, then an alternative technique that has been found to be effective in practice is to partition the augmenting data for \mathbf{A} and \mathbf{y} in the form

$$\mathbf{D} = \begin{bmatrix} \hat{\mathbf{D}} \\ \hat{\mathbf{F}} \end{bmatrix} = \begin{bmatrix} 1 & & & & \\ & \ddots & & & \\ & & 1 & & \\ & & & \dots & \dots \\ & & & 1 & -1 \\ & & & & \ddots \\ & & & & & 1 & -1 \end{bmatrix}; \quad \mathbf{h} = \begin{bmatrix} h_1 \\ \vdots \\ h_l \\ \vdots \\ 0 \\ \vdots \\ 0 \end{bmatrix} \quad (8.28)$$

and the applicable constraining equation is simply $\mathbf{D}\mathbf{m} = \mathbf{h}$ where $\hat{\mathbf{D}}$ is of dimension $l \times p$, $\hat{\mathbf{F}}$ is of dimension $(p-l-1) \times p$ and there are l known reliable estimates of \mathbf{m} .

A commonly used technique in geophysics is the inversion of combined data sets (Vozoff and Jupp, 1975; Gol'tsman, 1976) and is an effective means of deriving reliable estimates of the sought parameters. Experience has shown that this technique may not always yield unique parameter estimates especially if the constituent data components are inherently plagued by non-uniqueness. It may thus be more effective to incorporate prior estimates of the sought parameters if available. The algorithms described here are flexible and can be used in a joint inversion scheme with the data and constraining equations arranged in the form

$$A_* = \begin{bmatrix} A^1 \\ \vdots \\ A^j \\ \gamma D \end{bmatrix} \quad \text{and} \quad y_* = \begin{bmatrix} y^1 \\ \vdots \\ y^j \\ \gamma \Delta^k \end{bmatrix} \quad (8.29)$$

where the indices 1 to j refer to the weighted contributions from the j different data sets and the other symbols are as previously defined.

It is remarked here that we can also develop a hybrid practical technique that combines ridge regression-type solution stabilization measures (e.g., Meju, 1992) and biased estimation techniques by adding an additional term λI to $[A^T A_*]$ with $\gamma=1$ in eq.(8.27) where λ is a Marquardt damping factor. The algorithms and practical techniques described above are summarized in the following general algorithm.

8.5 Problem Session: Construction of Effective Biased Estimation Scheme

Let us attempt to use all that we have learnt so far to develop an effective practical algorithm for nonlinear biased estimation. A typical inverse problem is defined below.

Problem :

Given data d_i ($i=1, n$), determine optimal parameters, m^j ($j=1, p$) satisfying *a priori* information h_j .

Solution Procedure:

Step 1. Select an initial model m^0 containing *a priori* information.

Determine type of *a priori* constraints and form γD ; (where $\gamma=\beta$, a single undetermined multiplier or a diagonal matrix β consisting of zeros except at the positions corresponding to the reliable *a priori* information in m^0 where it is set to a small positive value)

Step 2. Calculate the augmenting data for y .

Loop ($i = n+1, n+p; k=1, p$)

$$y_i = \gamma(h_k - m_k^0)$$

End Loop

Step 3. Calculate $y_i = [Wd - Wf_i(m^0)]$; $i=1, n$.

$$\text{Calculate } SSE = \sum_{i=1}^{n+p} y_i^2$$

(SSE is used as a stopping criterion)

Step 4. Calculate $A_{ij} = \frac{\partial f_i(\mathbf{m}^0)}{\partial m^j}$

Form augmented Jacobian matrix

$$\mathbf{A}_* = \begin{bmatrix} \mathbf{W} \mathbf{A} \\ \gamma \mathbf{D} \end{bmatrix}$$

Step 5. Calculate $\mathbf{x} = [\mathbf{A}_*^T \mathbf{A}_*]^{-1} (\mathbf{A}_*^T \mathbf{y}_*)$

(where $\mathbf{y}_* = [y_1, y_2, \dots, y_{n+p}]^T$)

Step 6. Update parameter estimates

$$\mathbf{m}_{iter} = \mathbf{m}^0 + \mathbf{x}$$

$$\text{Calculate } SSE' = \sum \| \mathbf{d} - \mathbf{f}(\mathbf{m}_{iter}) \|^2 + \sum \| \gamma(\mathbf{h} - \mathbf{m}_{iter}) \|^2$$

If($SSE' \geq SSE$) STOP.

else

Set \mathbf{m}_{iter} to \mathbf{m}^0

Goto Step 2 (or Step 3, if $\mathbf{h} = [0, 0, \dots, 0]^T$)

Note that the solution (of the normal equations) for \mathbf{x} at Step 5 can be obtained using the singular value decomposition method (Eckart and Young, 1939; Lanczos, 1961).

8.6. Biased Estimation in Practice: Illustrative Examples

We will illustrate various aspects of iterative biased estimation using magnetotelluric (MT) data. The algorithm described by eq. (8.11) is applied to a synthetic data set in Figs. 8.1a and 8.1b to test its effectiveness. Notice in these figures that all the parameters of the actual model (A) were satisfactorily recovered (final models labelled F) using different poor starting models (S) and the problem regularization (or damping) factor $\beta=0.01$. The minimum-bias algorithm required about 7 iterations to achieve these results. Comparable results were also obtained with $\beta\mathbf{m}^0$ set to zero in eq. (8.11) to imitate the usual approach to nonlinear estimation but required about the same number of iterations. This suggests that both approaches could furnish reliable information from a data set of high quality.

1-D MODELS FOR SITE SYNTH-UL

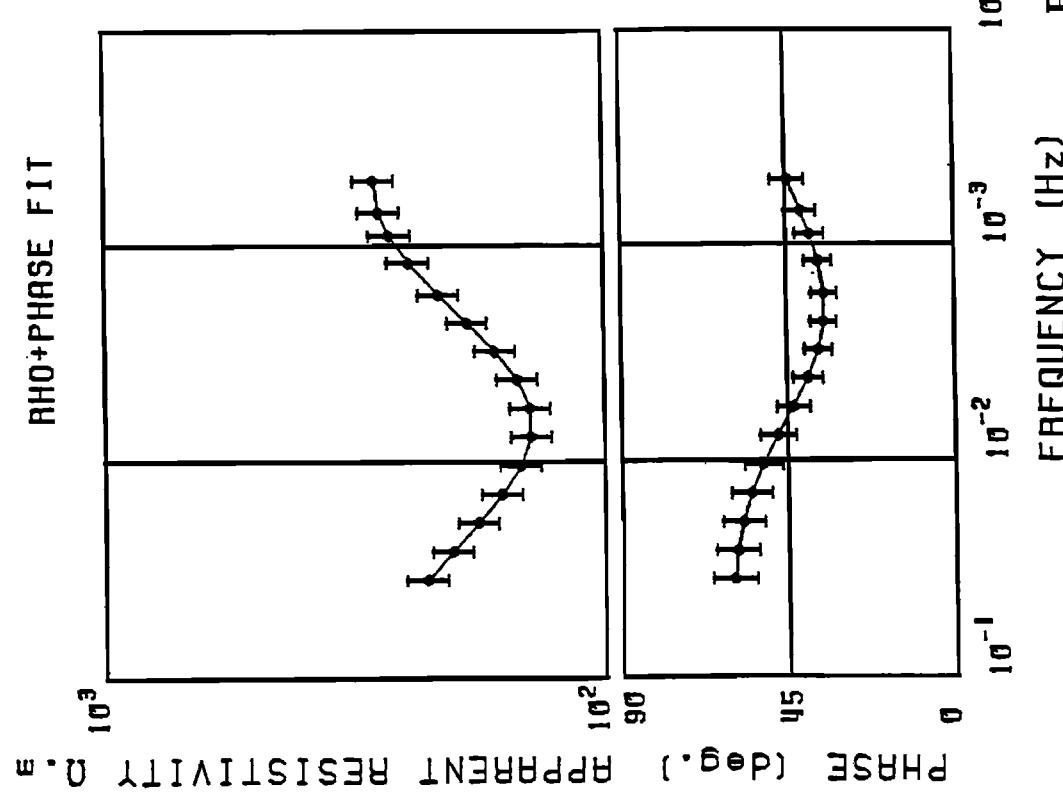


Fig. 8.1a Optimal model (F) derived from smooth starting model (S).
The true model (A) is also shown for comparison.

1-D MODELS FOR SITE SYNTH-UL

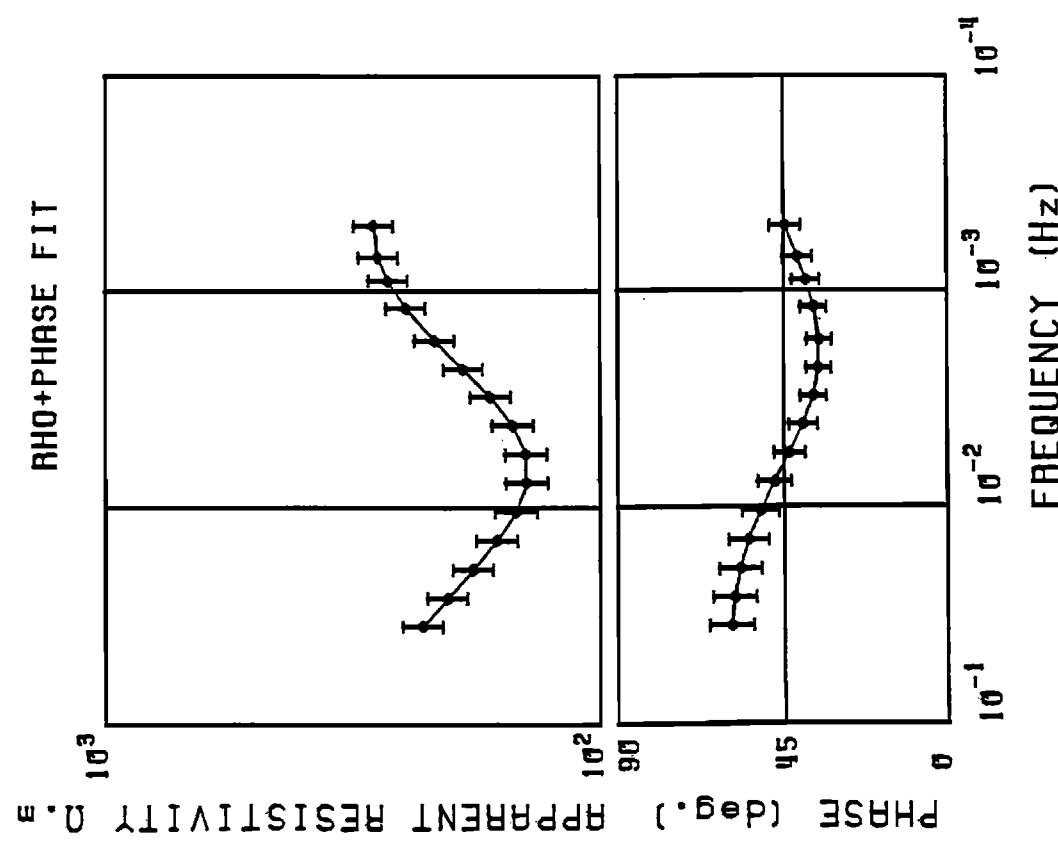


Fig. 8.1b Optimal inversion result (F) using a smooth starting model (S)

In Figs 8.2a and 8.2b the minimum-bias technique is applied to the well-known practical data - COPROD (Jones & Hutton, 1979) - using different values of β but the same poor starting model (labelled S). The result from a conventional ridge-regression inversion scheme (Meju, 1992) is also shown (as model 1) for comparison in these figures. All the optimal models have r.m.s. error of 1.0 ($\chi^2 \approx 30$) and are thus equivalent. It can be seen that the minimum-bias results vary with β and also differ from the ridge regression result in the top and bottom sections of the geoelectric profile. We are thus faced with the problem of non-uniqueness since all the models equally satisfy the given data. One way of addressing this problem would be to use *a priori* data, if available, in the inversion process. For convenience and to demonstrate the effectiveness of the maximum-bias algorithm in handling *a priori* data, let us assume that a previous study in the area furnished a resistivity of 500 $\Omega\text{-m}$ for the top 8 km of the Earth's crust. We wish to retain this value in the final solution (F) to the COPROD problem. For plotting convenience the assumed parameter estimate is included in the starting model (S) in this figure although this is not mandatory in the algorithm. The result of this illustrative exercise is shown in Fig. 8.3. Notice that the algorithm retained the desired prior estimate for the top layer's resistivity. Similar tests involving the other parameters of the model also proved successful suggesting that it is a potent technique for inversion with prior data. Note that all the above examples incorporated the constraints given by equation (8.1a).

To demonstrate the versatility of biased estimation, the smoothness constraints given by eq. (8.1b) have been employed with two different values of β in the estimation procedure yielding the smooth resistivity models shown in Fig. 8.4. Here, the Earth is parameterized into a succession of forty layers of different resistivities and predetermined fixed thickness (in log space). In both cases it is assumed that there are no known prior estimates of the layer resistivities and a half-space starting model of resistivity 100 $\Omega\text{-m}$ was adopted and the inversion process used eq. (8.16). Notice the good fit of the optimal models' responses to the COPROD data and that all the main subsurface features seen in the sparsely-parameterized models of Fig. 8.2 can also be identified in these smooth models. However, these smooth models also show a dependence on β (the symbols O and T in Fig. 8.4 represent results for different β values); the significance of this behaviour will be explored further in Chapter 10. In any case, we are again faced with the problem of non-uniqueness in this largely underdetermined (i.e., densely-parameterized) problem. We can address such problems using the biased

1-D MODELS FOR SITE COPROD

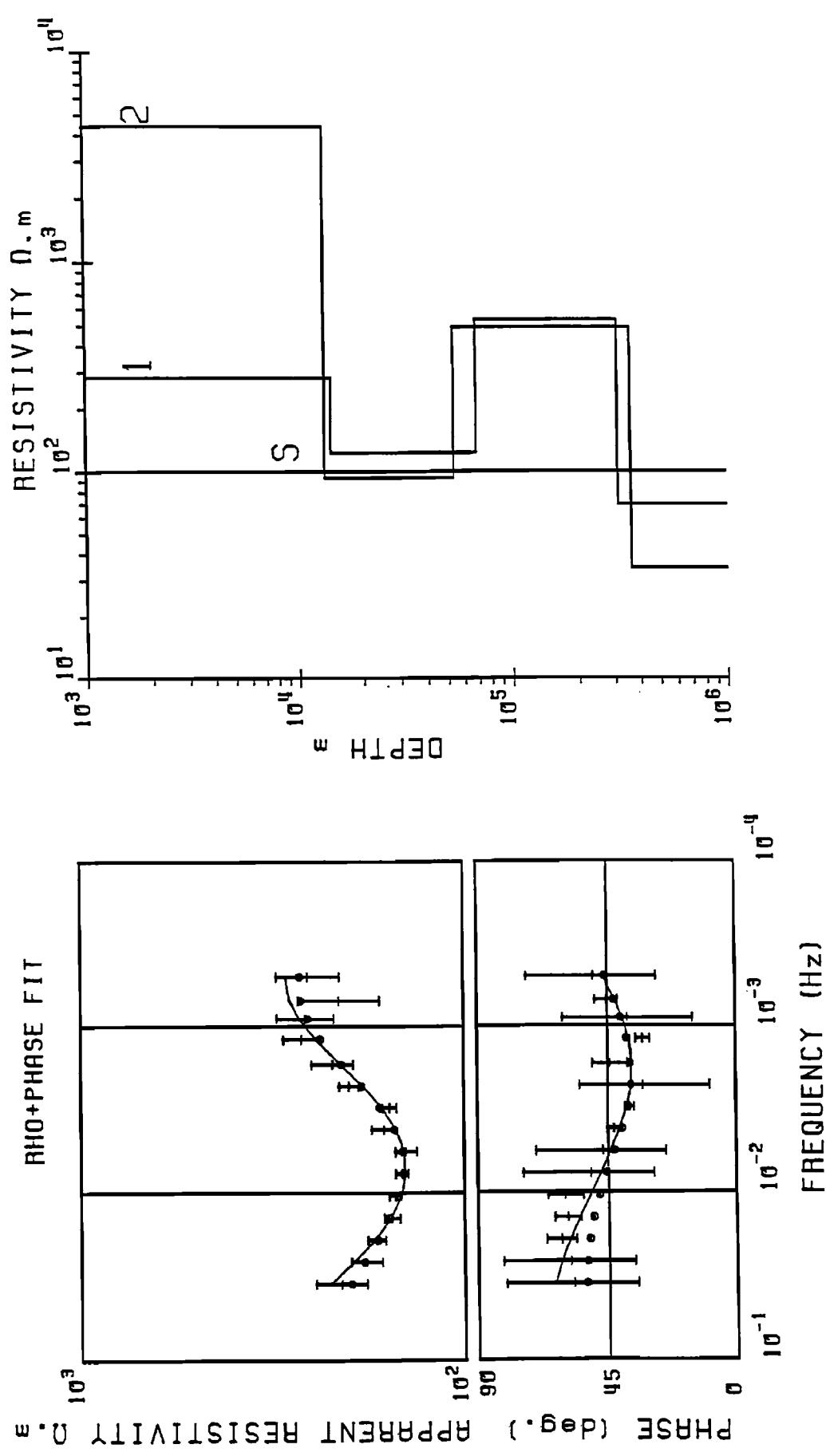


Fig. 8.2a Comparison of ridge regression (1) and biased estimation (2) results

1-D MODELS FOR SITE COPROD

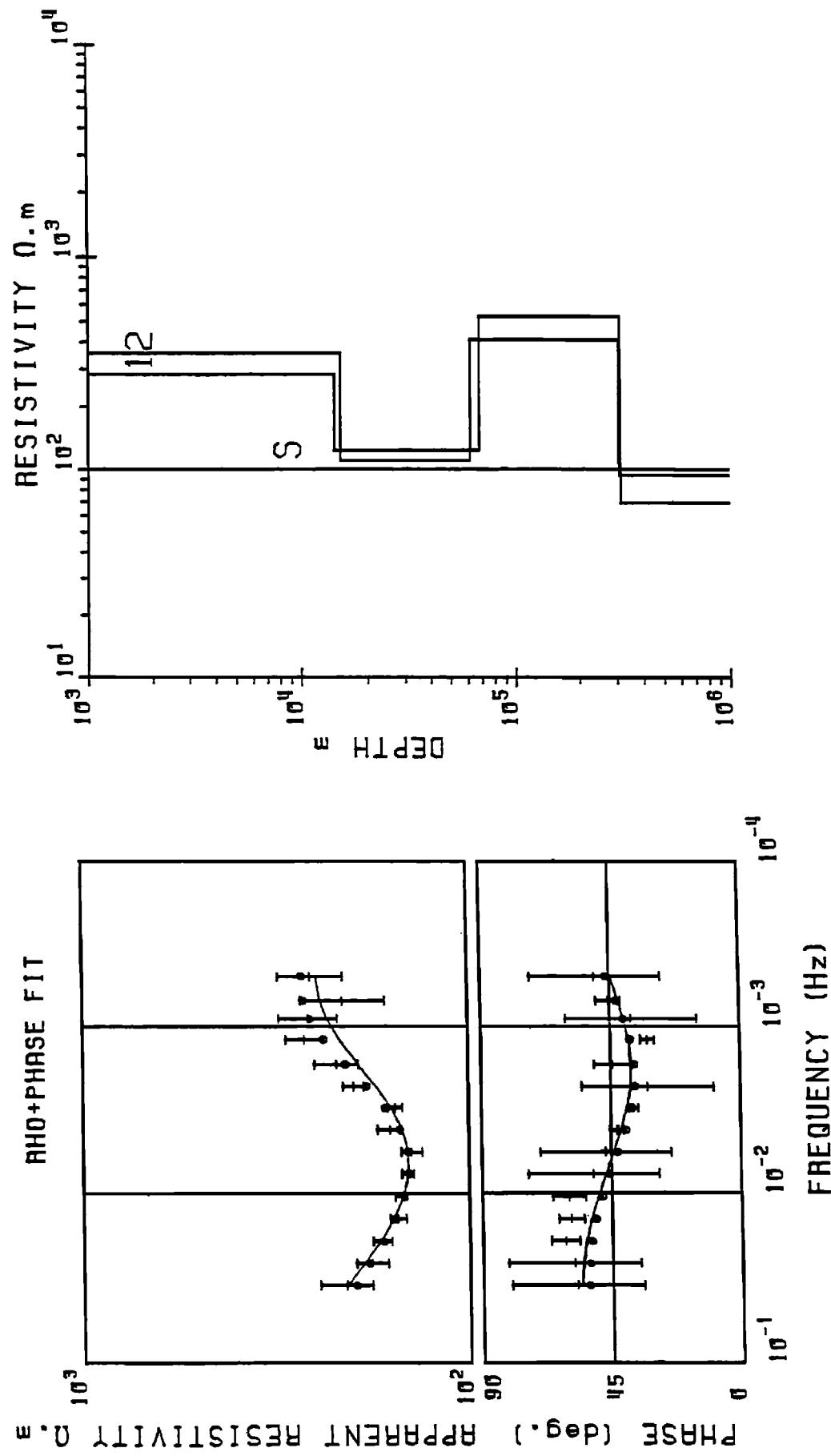


Fig. 8.2b Biased estimation model suggesting dependence on regularization factor

1-D MODELS FOR SITE COPROD

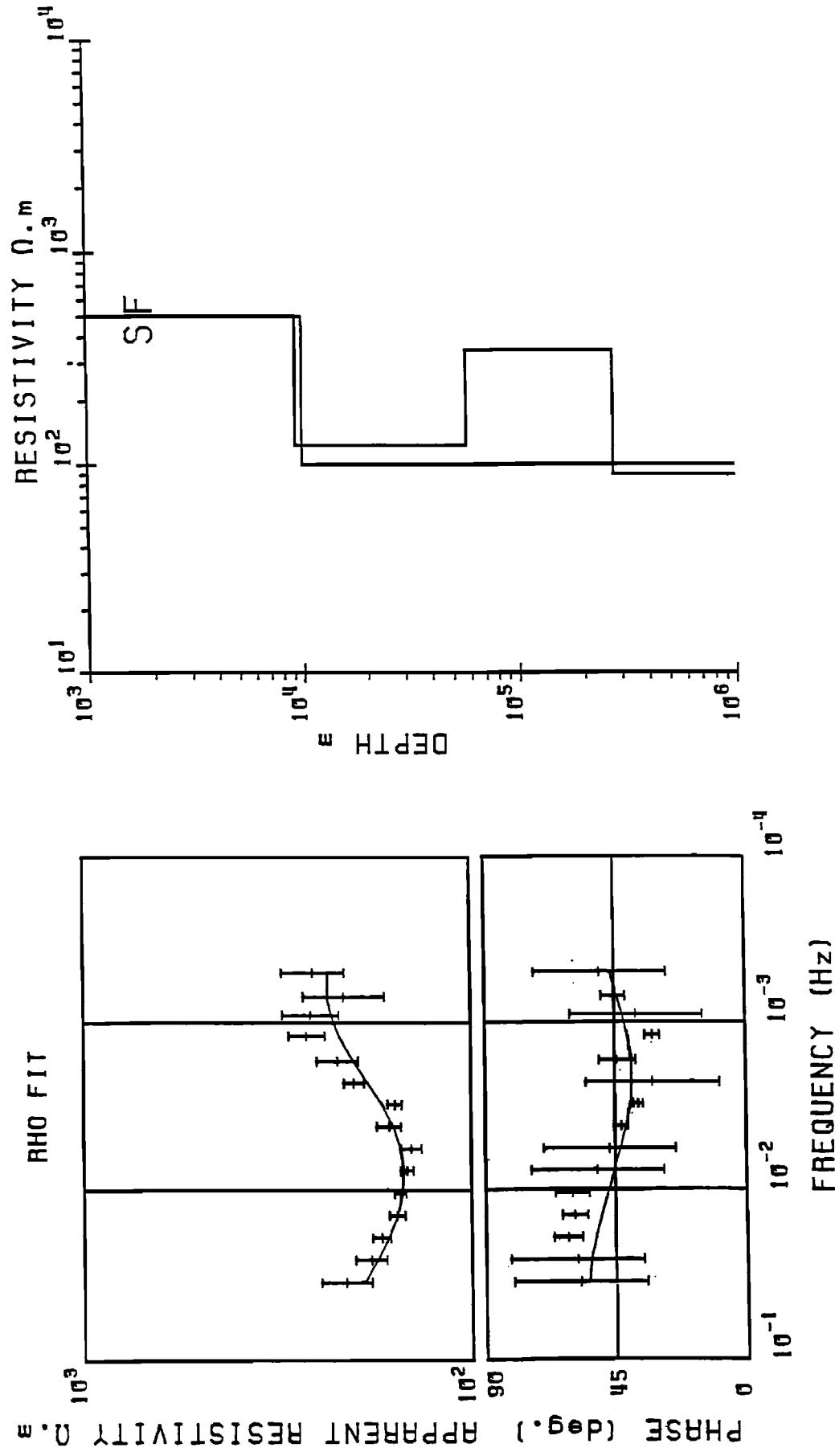


Fig. 8.3 Retention of specified parameter values in biased estimation

1-D MODELS FOR SITE COPROD

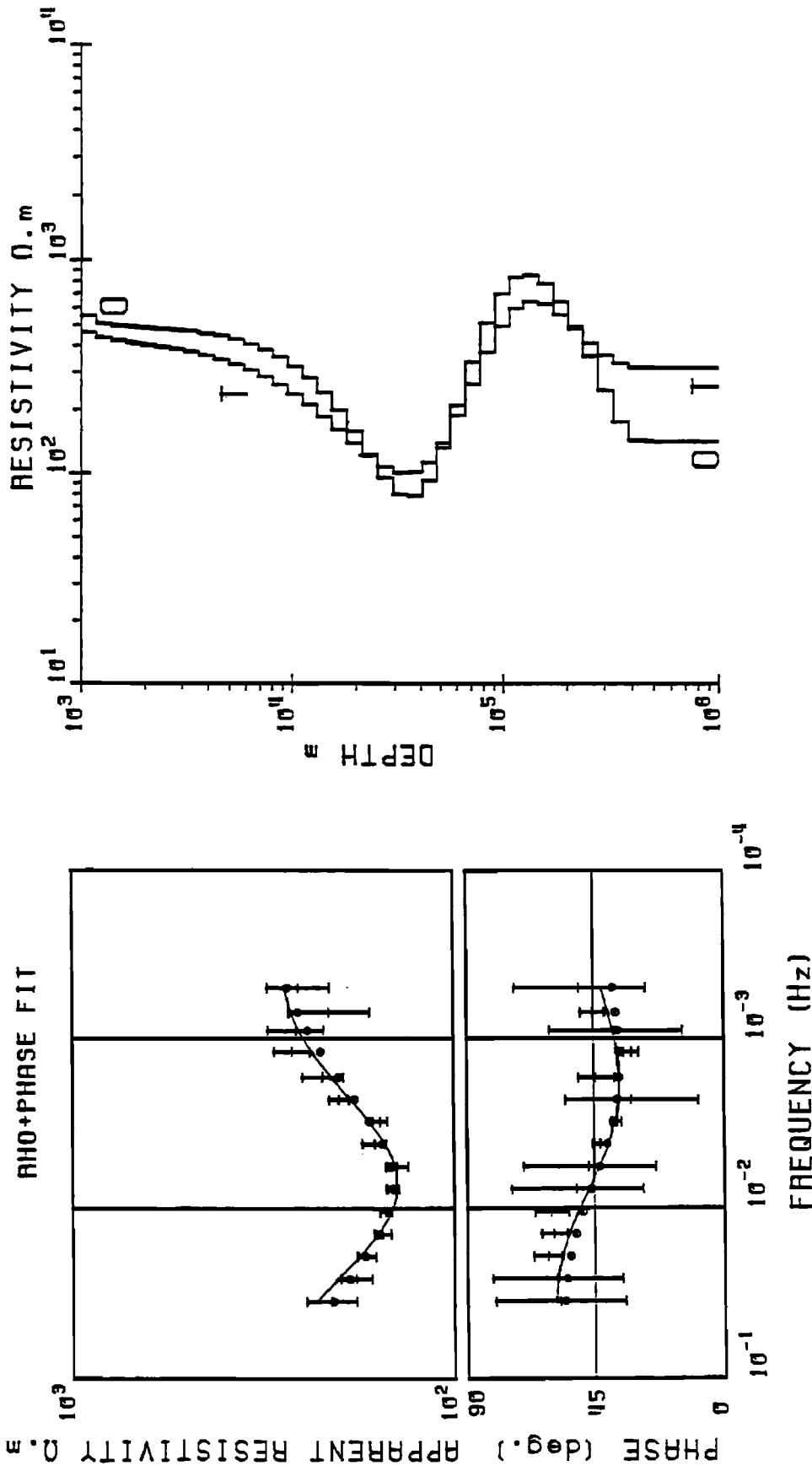


Fig. 8.4 Smooth models showing dependence on regularization factors

1-D MODELS FOR SITE COPROD

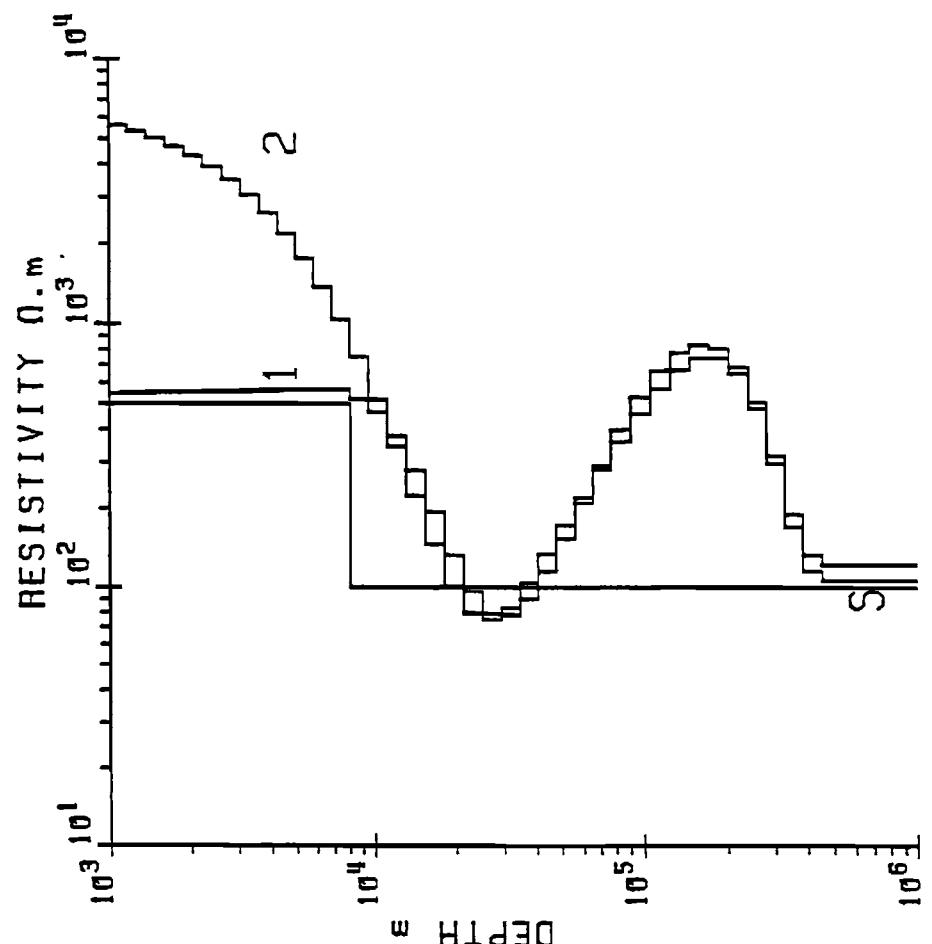
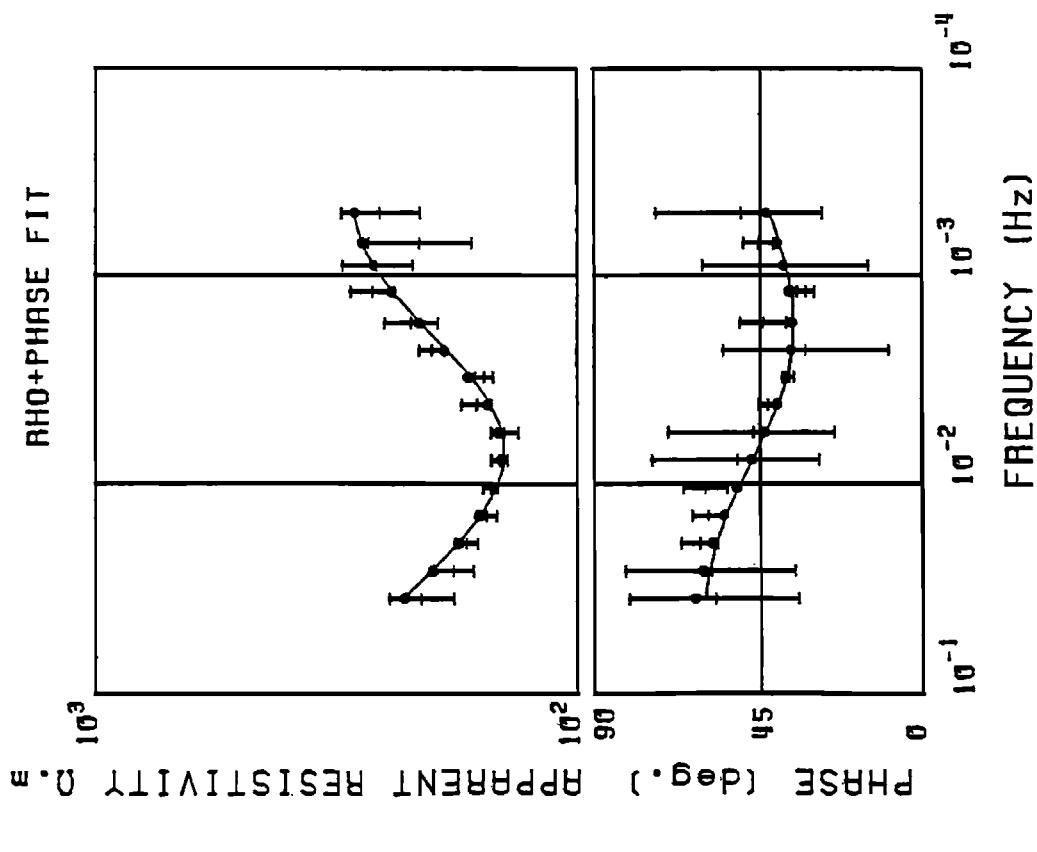


Fig. 8.5 Comparison of minimum-bias model (2) and hybrid model retaining specified parameters (1)

estimation techniques.

For illustration, let us assume that the top crust is not constrained by the COPROD data but that some prior estimates of the resistivity of this section of the geoelectric profile is available. We wish to demonstrate the effectiveness of the practical technique described by eq.(8.28). The result obtained using the *a priori* information that the top 8km of the Earth's crust has a resistivity of 500 Ωm (Model 1) is shown together with that obtained using a half-space starting model of 100 Ωm resistivity (Model 2) in Figure 8.5 for $\beta=0.6$. Notice that we are able to force the final solution to conform with the hypothetical *a priori* information in the top 8km (upper 14 layers) of the geoelectric crust while the rest of the profile was smoothed. Model 2 is again different from the two models shown in Fig. 8.4 for different values of β . It follows, therefore, that the use of hybrid constraints (eq. 8.28) may be the practical approach to reducing the inherent uncertainties in the interpretation of such densely-parameterized models.

9. SOLUTION APPRAISAL IN NONLINEAR INVERSION

An inversion process is incomplete without an analysis of the errors in the constructed solutions. When dealing with inexact experimental data, a fundamental task is the determination of how close to the truth (if there is one !) or how representative of the real world our inverse solution is. To shed some light on this issue, we will examine how the experimental errors translate into errors in the model estimates and use the well developed tools of linear appraisal (Section 6) to estimate approximate reliability of the non-linear solutions.

9.1 Assessing the Quality of the Solution

9.1.1 Goodness-of-fit

As for linear problems, and assuming that our data d_i are normally distributed about their expected values and with known uncertainties (or experimental errors), σ_i , the goodness-of-fit is defined by the statistical parameter q , calculated as

$$q = \sum_{i=1}^n \frac{(d_i - f_i(m))^2}{\sigma_i^2} \quad (9.1)$$

For n independent observations and p independent parameters, q is distributed as χ^2 with $(n-p)$ degrees of freedom. The expected value of q is n but in practice a model with $|n-p| < Q \lesssim n + \sqrt{2n}$ is acceptable. The Root Mean Square (rms) error given by

$$\text{rms} = \frac{1}{n} \sum_{i=1}^n \frac{(d_i^{\text{obs}} - f_i(m))^2}{\sigma_i^2}$$

or simply

$$\text{rms} = \frac{1}{n} \sum_{i=1}^n \|Wd_i^{\text{obs}} - Wf_i(m)\|^2 \quad \text{for a weighted solution.} \quad (9.2)$$

9.1.2 Parameter Resolution Matrix

The parameter resolution matrix of a linear system can be easily calculated and that was one motivation for re-casting our non-linear estimators in equivalent linear forms for the consistency analyses presented in Section 8.2.3. We will apply the straight-forward rule ($R = HA$, where H is the generalized inverse used) to three different cases. We will assume that the data equations have been standardized.

Case 1: Unconstrained solution

Using the relation $m = (A^T E A)^{-1} (W A)^T \{\hat{d}\}$, i.e., eq. 8.17, we find that

$$R = (A^T E A)^{-1} (W A)^T \cdot W A = I \quad (9.3)$$

If the inverse matrix exists, $R = I$, meaning that the model parameters may be fully or perfectly resolved by the data.

Case 2: Ridge regression solution

Using the re-interpreted Marquardt solution ($m = [A^T E A + \beta I]^{-1} [(W A)^T \hat{d} + \beta m^0]$, i.e., eq. (8.25), which uses the previous iterate as the *a priori* information, we have that

$$\begin{aligned} R &= ([A^T E A + \beta I]^{-1} (W A)^T \cdot W A) + ([A^T E A + \beta I]^{-1} \beta D^T \cdot \beta D) \\ &= (A^T E A + \beta I)^{-1} (A^T E A + \beta^2 I) \neq I. \end{aligned} \quad (9.4)$$

Thus the Marquardt solution does not have a perfect resolution matrix.

Case 3: Maximum-bias solution

Re-writing equation 8.19 as

$$m = (A^T E A + C^T C)^{-1} ((W A)^T \hat{d} + C^T h_*) \quad (9.5)$$

where $C = \beta D$, $h_* = \beta h$, and \hat{d} is as previously defined, we find that

$$\begin{aligned} R &= \{(A^T E A + C^T C)^{-1} (W A)^T \cdot W A\} + \{(A^T E A + C^T C)^{-1} C^T \cdot C\} \\ &= (A^T E A + C^T C)^{-1} (A^T E A + C^T C) = I \end{aligned} \quad (9.6)$$

showing that we have perfect resolution by incorporating *a priori* data in our solution process. The minimum-bias algorithm uses a set of independent *a priori* information (in the form of a null vector) and eq. (9.6) is thus applicable in this situation. Note here that the *a priori* estimates are assumed to be independent of the data unlike in the Marquardt case where the *a priori* data at successive iterations depend on the experimental data. In general, R is evaluated at an acceptable model. R may be interpreted as a gauge of the balance between the information provided by the data and those assumed *a priori*. If $R = I$, then each model parameter may be well determined. As in the linear case, the deviation of the rows of R from those of the identity matrix,

I, measures the lack of resolution for the corresponding model parameters.

9.1.3 Trend Analysis of Residuals

The distribution of the misfit between the observed data and those computed for the optimal solution may reveal the presence of a trend (from positive to negative residuals, say) or the lack of it. Recall that we introduced this concept during the analysis of linear inversion with smoothness constraints. The following analysis leans heavily on that provided by Constantides (1987, Chap. 7). To examine any distribution patterns, it is instructive to plot the residuals against the independent experimental variable (e.g., geophone or electrode spacings, recording frequencies) and sometimes also the residuals versus observational data. The former will be mostly used here. A correct model will show some randomness in the distribution of residuals and the lack of randomness may suggest that some part of the model may have been better fitted than the others and therefore the optimal model is not the correct one. The four examples shown in Figures 9.1a-9.1d have been selected to illustrate some aspects of the problem and possible remedies are suggested. In Fig. 9.1a it would appear at a glance that the predicted data explain the field data adequately. However, analysis of the residuals show trends of increasing residuals in proportion to d . In this situation, it may be wise to normalise the residuals by dividing them by the associated data (Constantides, 1987), i.e.,

$$\hat{y} = \frac{d^{0bs} - d^{calc}}{d^{0bs}}$$

and the matrix A is scaled accordingly so that we are in effect solving a weighted system of equations for the parameter corrections. A different situation is seen in Fig. 9.1b where the residuals show a random distribution around zero. The model is deemed satisfactory in this case. In Fig. 9.1c is shown another interesting situation that might appear as a good fit at first sight. A careful examination will reveal the presence of an oscillatory pattern in the distribution of these residuals around zero. This might suggest inadequate prediction and the addition of a term that will introduce an oscillatory behaviour in the forward model may improve the fit to the data. In some cases, we may find that the residuals show a trend from positive to negative as in Fig. 9.1d. The situation illustrated in this figure imply low prediction of d at small values of the independent experimental variable and high prediction of d at high values of the measurement positions, say. A correction to the model to remedy this situation seems to be warranted but we must bear in mind that model resolution decreases with depth,

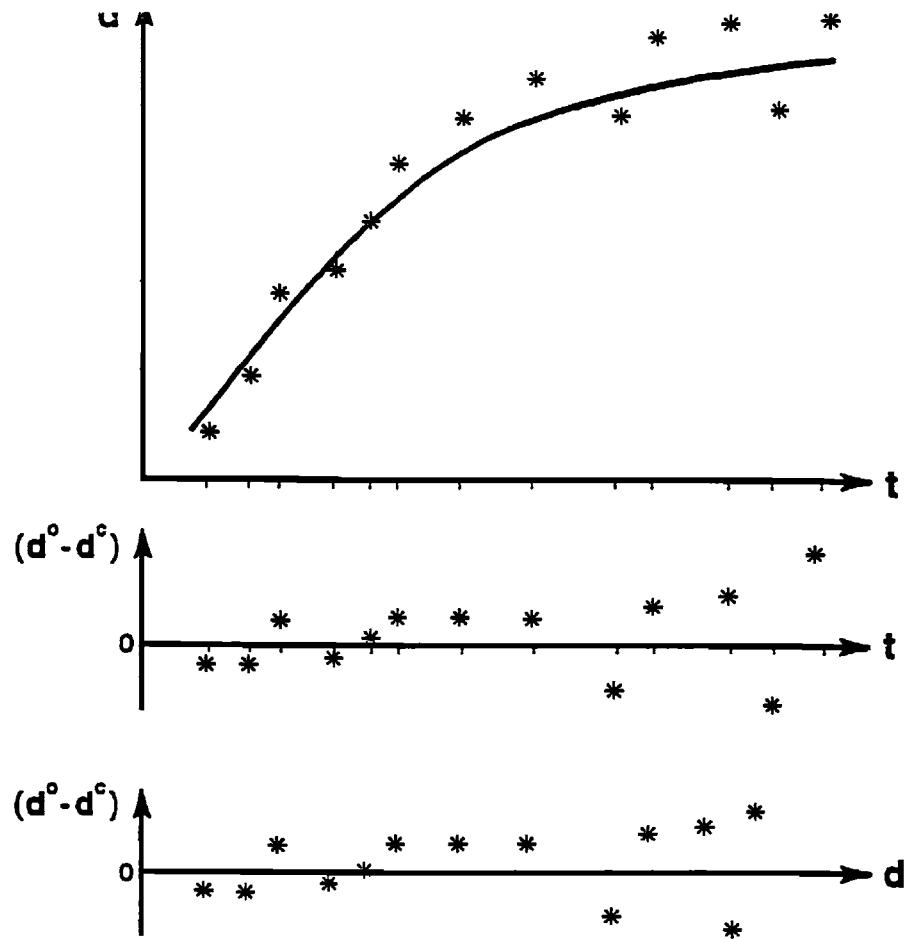


Figure 9.1a
Analysis of residuals showing trend of increasing
residuals in proportion to d

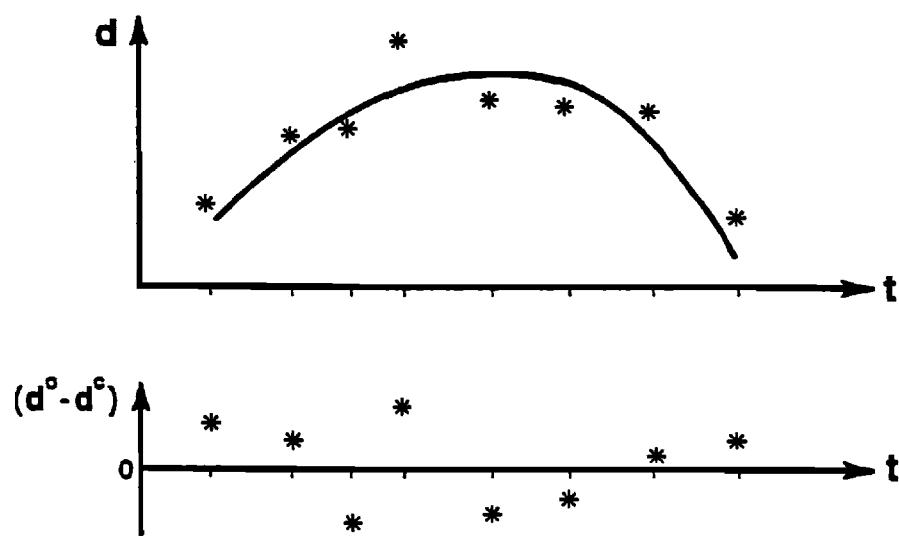


Figure 9.1b
Analysis of residuals showing a random trend

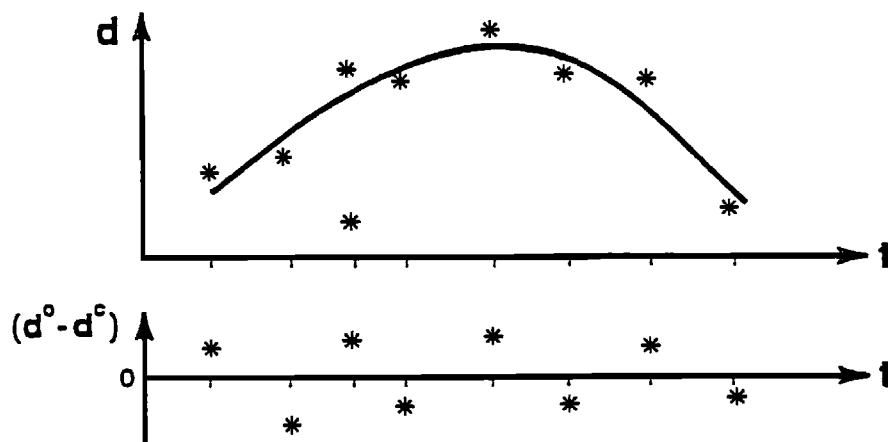


Figure 9.1c
Analysis of residuals showing oscillatory trend

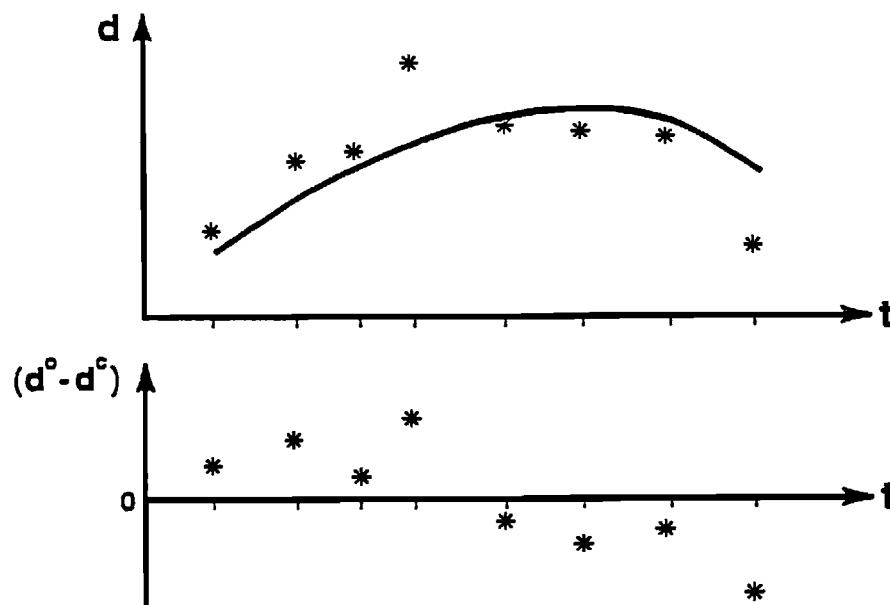


Figure 9.1d
Analysis of residuals showing trend from
positive to negative

(Fig. 9.1 after Constantinides, 1987)

Gaussian, uncorrelated and of equal variance σ^2 . The basic rule is that if $m^{est} = Ld$, then by law of propagation of errors, $Cov(m^{est}) = L[Cov(d)]L^T$ (see Meyer, 1976).

For the unconstrained (unbiased) solution given by equation 8.17, we have that

$$Cov(m^{est}) = \{(A^T EA)^{-1}(WA^T)\}[E \cdot Cov(\hat{d})] \{(A^T EA)^{-1}(WA)^T\}^T = (A^T EA)^{-1} \quad (9.7)$$

in the standardized framework. If the data equations were not normalized by the observational errors at the outset, the the right-hand side of eq. (9.7) must be preceded by σ^2 (the covariance of d) and the E term would not be present. It may be noted that for the unbiased statistically normalized solution, there is a simple relationship between the covariance and resolution matrices, i.e.,

$$R = Cov(m^{est})A^T EA. \quad (9.8)$$

For the minimum-bias solution given by eq. (8.20), we find that

$$\begin{aligned} Cov(m^{est}) &= \{(A^T EA + \beta^2 I)^{-1}(WA^T)\} [E \cdot Cov(\hat{d})] \{(A^T EA + \beta^2 I)^{-1}(WA)^T\}^T \\ &= (A^T EA + \beta^2 I)^{-1} A^T EA (A^T EA + \beta^2 I)^{-1} \end{aligned} \quad (9.9)$$

where the usual pre-multiplier σ^2 (from $Cov(d)=\sigma^2 I$) has disappeared as a consequence of the weighting procedure adopted in the biased estimation approach.

For inversion with reliable *a priori* estimates, the covariance for the maximum-bias solution (eq. 8.19) is

$$\begin{aligned} Cov(m^{est}) &= \{(A^T EA + D^T BD)^{-1}(WA)^T\}[E \cdot Cov(\hat{d})] \{(A^T EA + D^T BD)^{-1}(WA)^T\}^T \\ &\quad + \{(A^T EA + D^T BD)^{-1}(\beta D)^T\}[B \cdot Cov(h)] \{(A^T EA + D^T BD)^{-1}(\beta D)^T\}^T. \end{aligned} \quad (9.10)$$

Two interesting situations may develop that would affect the final form of the above expression. If there are no variations in the *a priori* parameters (which are assumed to be independent of the fitted data), then eq. (9.10) reduces to

$$Cov(m_d^{est}) = (A^T EA + D^T BD)^{-1} A^T EA (A^T EA + D^T BD)^{-1}. \quad (9.11a)$$

say in most geophysical exploration problems. If one is irrevocably committed to statistics, there is a simple test for randomness of residuals called the Runs Test.

9.1.3.1 The Runs test

This is used to test the randomness of a distribution of residuals. Let n_1 denote the total number of positive residuals, n_2 the total number of negative residuals, and r the number of times the sequence of residuals changes sign. The quantity, r is known as the number of runs. The distribution of r is approximated by the normal distribution and its mean and standard deviation are given by

$$\bar{r} = \frac{2n_1 n_2}{n_1 + n_2} + 1$$

$$\sigma = \left(\frac{2n_1 n_2 (2n_1 n_2 - n_1 - n_2)}{(n_1 + n_2)^2 (n_1 + n_2 - 1)} \right)^{\frac{1}{2}}$$

The standardized form of the variable is

$$Z = \frac{r - \bar{r}}{\sigma}$$

which is distributed with zero mean and unit variance. To test the hypothesis that Z is random, we need to compare Z with the normal standard distribution. If the value of Z falls in the region of acceptance of this test, then the hypothesis that the model is the correct one and that the residuals are randomly distributed can be accepted. If, on one hand, Z is too low, the model is inadequate; and a two-sided test must be performed. On the other hand, if Z is too high, then the data contain oscillations which must be accounted for by the model.

9.2 Model Bounds

The determination of bounding values on the optimal model parameters for a given set experimental data and associated errors is an important part of the inversion process. In fact, it should be looked upon as a logical completion of geophysical inversion.

9.2.1 Parameter Covariance matrix

The covariance matrices corresponding to the three cases mentioned above will be derived here using the standard procedure. The assumptions made are that the data are

However, in practice the matrix β is largely undetermined ($B = \beta^T \beta$) and the optimal set of values required to force the solution to satisfy the *a priori* data exactly can only be determined by trial-and-error. It follows that for each set of values used as the components of β , the resulting point estimates may be different. Put simply, the degree to which the optimal solution retains the specified h varies with β . It is possible to describe these variations statistically and determine the corresponding covariance matrix, but we shall choose to deduce an equivalent measure using a simple intuitive concept. Recall that in the original biased estimation formulations the data equations were weighted by the observational errors by way of the matrix W . In the same formulations, the extraneous data equations corresponding to our *a priori* information were pre-multiplied by the matrix β . It is easy to see that this operation is a weighting procedure and that both the W and β matrices serve the same function for the two kinds of data considered in the problem formulation. Now, by definition, $E = W^T W$, and therefore $Cov(d)$ is simply given by E^{-1} . The covariance of the variations in h is identically $B^{-1} = [\beta^T \beta]^{-1}$. The effect of these variations on $Cov(m^{est})$ in the standardized framework may thus be approximated by

$$Cov(m_h^{est}) = (A^T EA + D^T BD)^{-1} D^T BD (A^T EA + D^T BD)^{-1}. \quad (9.11b)$$

We may then determine the full covariance relation given by eq. (9.10) from the sum of the two sets of covariances defined in eq. 9.11a and 9.11b. This is simply

$$\begin{aligned} Cov(m^{est}) &= (A^T EA + D^T BD)^{-1} [A^T EA + D^T BD] (A^T EA + D^T BD)^{-1} \\ &= (A^T EA + D^T BD)^{-1}. \end{aligned} \quad (9.12)$$

It follows that for the maximum-bias solution, R and $Cov(m^{est})$ are related in the form

$$R = Cov(m^{est})(A^T EA + D^T BD). \quad (9.13)$$

The square roots of the diagonal elements of $Cov(m^{est})$ may be taken as the standard deviations of the least squares parameter estimates and may be used to estimate the bounds of the model parameters. In terms of confidence limits, the Covariance matrix allows us to define a confidence hyperellipsoid ($m^T Cov(m^{est}) m > 0$ for any m), in which we are $(100-\alpha)\%$ certain that the solution lies. We usually define the 95% confidence interval by choosing $\alpha \leq 5$.

9.3 Extreme Parameter sets : Most squares Inversion.

The iterative most squares method of extremal inversion (Meju and Hutton, 1992; Meju, 1994d) will be adopted as the mainstay of our model appraisal. We will determine the solution for a variety of practical situations. The problem definitions are the same as for the linear cases already considered and the details will not be recounted here for brevity. Essentially, having obtained an optimal least squares solution to an inverse problem, m we extremize the objective function $m^T b$ subject to the constraint that the residuals q (some combination of the data prediction error and solution length) are not greater than some threshold value q_T , where b is the parameter projection vector. The expected value of q_T is n (the number of data) or $n-l$ when the solution is effectively constrained to satisfy l known parameter estimates. We will drop the weighting term W here for notational simplicity but bear in mind that the data equations have been standardized.

Case 1: Unconstrained problem

To calculate the most-squares models for the Gauss-Newton solution, we need to extremize

$$m^T b + \frac{1}{2\mu} [(d - f(m))^T(d - f(m)) - q_T] . \quad (9.14)$$

This may be done in successive steps as for nonlinear least squares minimization.

Linearization of eq. (9.14) about an initial model will yield the function

$$(m^0 + x)^T b + \frac{1}{2\mu} [(y - Ax)^T(y - Ax) - q_T] \quad (9.15)$$

which is to be minimized or maximized to yield the parameter corrections x to be applied to m^0 until the condition $q = q_T$ is satisfied where $q = |d-f(m)|^2$. The most-squares solution for the parameter increments is simply (Meju & Hutton, 1992)

$$\hat{x} = (A^T A)^{-1}(A^T y - \mu b) \quad (9.16)$$

where

$$\mu = \pm \left(\frac{q_T - q_{LS}}{b^T [A^T A]^{-1} b} \right)^{\frac{1}{2}} \quad (9.17)$$

and is determined by the constraint $q = q_T$, and $q_{LS} = y^T y - y^T A (A^T A)^{-1} A^T y$.

Using the optimal least squares model as our initial model, the relevant iterative inversion formula is

$$\mathbf{m}^{k+1} = \mathbf{m}^k + (\mathbf{A}^T \mathbf{A})^{-1} (\mathbf{A}^T \mathbf{y} - \mu \mathbf{b}) \quad (9.18)$$

where \mathbf{m}^k is the refined model at iteration k , and \mathbf{A} and \mathbf{y} are evaluated at \mathbf{m}^k . The expected value of q_T is n , the number of the data. Note that if we preferred to solve explicitly for the parameter estimates rather than the perturbations, then we have that

$$\mathbf{m}^{est} = (\mathbf{A}^T \mathbf{A})^{-1} (\mathbf{A}^T \hat{\mathbf{d}} - \mu \mathbf{b}) \quad (9.19)$$

where $\hat{\mathbf{d}} = (\mathbf{y} + \mathbf{A}\mathbf{m}^0)$ and may be used in an iterative fashion. However, the above inversion formulae (9.18 and 9.19) are unstable algorithms especially if $\mathbf{A}^T \mathbf{A}$ is ill-conditioned. For this reason, Meju and Hutton (1992) suggested damping the absolute values of the parameter perturbations. This and other prescriptions for dealing with instability in iterative applications are discussed next.

Case 2: Damped solution

We already know that the process of damping involves adding fictitious (or extraneous) data to the actual observed data and that damping can be achieved in two ways. Thus, we can either define the statistical measure q as

$$q = (\mathbf{d} - \mathbf{f}(\mathbf{m}))^T (\mathbf{d} - \mathbf{f}(\mathbf{m})) + \beta(\mathbf{m} - \mathbf{m}^0)^T (\mathbf{m} - \mathbf{m}^0) \quad (9.20)$$

in line with the Marquardt-type approach, or as

$$q = (\mathbf{d} - \mathbf{f}(\mathbf{m}))^T (\mathbf{d} - \mathbf{f}(\mathbf{m})) + \beta^2 \mathbf{m}^T \mathbf{D}^T \mathbf{D} \mathbf{m} \quad (9.21)$$

in accord with the biased estimation philosophy; and in both cases we have placed some bound on the size of the parameter perturbations.

Considering the former definition of q (eq. 9.20), the linearized quantity to be minimized is (cf. Meju & Hutton, 1992)

$$(\mathbf{m}^0 + \mathbf{x})^T \mathbf{b} + \frac{1}{2\mu} \{ (\mathbf{y} - \mathbf{A}\mathbf{x})^T (\mathbf{y} - \mathbf{A}\mathbf{x}) + \beta \mathbf{x}^T \mathbf{x} - q_T \}. \quad (9.22)$$

Effecting the minimization in the usual manner, we have that

$$\frac{\partial}{\partial x} [(m^0 + x)^T b + \frac{1}{2\mu} \{x^T A^T A x - x^T A^T y - y^T A x + y^T y + \beta x^T x - q_T\}] = 0$$

or

$$[A^T A + \beta I]x = (A^T y - \mu b) \quad (9.23)$$

from which we obtain the damped most-squares parameter increments

$$x = [A^T A + \beta I]^{-1}(A^T y - \mu b) . \quad (9.24)$$

When the quadratic constraint ($q = q_T$) is satisfied, we find that

$$q_T = y^T y + x^T [A^T A + \beta I]x - 2x^T A^T y$$

or

$$q_T = y^T y + \mu^2 b^T (A^T A + \beta I)^{-1} b - y^T A (A^T A + \beta I)^{-1} A^T y \quad (9.25)$$

from which we obtain

$$\begin{aligned} \mu &= \left(\frac{q_T - y^T y + y^T A (A^T A + \beta I)^{-1} A^T y}{b^T [A^T A + \beta I]^{-1} b} \right)^{\frac{1}{2}} \\ &= \pm \left(\frac{q_T - q_{LS}}{b^T [A^T A + \beta I]^{-1} b} \right)^{\frac{1}{2}} . \end{aligned} \quad (9.26)$$

Nonlinearity is dealt with using the iterative formula

$$m^{k+1} = m^k + (A^T A + \beta I)^{-1}(A^T y - \mu b) \quad (9.27)$$

where A and y are evaluated at m^k .

If we elect to solve directly for parameter estimates rather than x , we have in this case,

$$m = [A^T A + \beta I]^{-1}(A^T \hat{d} + \beta m^0 - \mu b) \quad (9.28)$$

Adopting the alternative biased estimation strategy, the linearized function to be minimized is simply

$$\mathcal{L} = (\mathbf{m}^0 + \mathbf{x})^\top \mathbf{b} + \frac{1}{2\mu} \{(\mathbf{y} - \mathbf{Ax})^\top (\mathbf{y} - \mathbf{Ax}) + \beta^2 (\mathbf{m}^0 + \mathbf{x})^\top \mathbf{D}^\top \mathbf{D} (\mathbf{m}^0 + \mathbf{x}) - q_T\}. \quad (9.29)$$

Differentiating \mathcal{L} with respect to \mathbf{x} and setting equal to zero yields the normal equations,

$$[\mathbf{A}^\top \mathbf{A} + \beta^2 \mathbf{H}] \mathbf{x} = (\mathbf{A}^\top \mathbf{y} - \beta^2 \mathbf{H} \mathbf{m}^0 - \mu \mathbf{b})$$

from which we can obtain the solution for the relevant parameter perturbations

$$\mathbf{x} = [\mathbf{A}^\top \mathbf{A} + \beta^2 \mathbf{H}]^{-1} (\mathbf{A}^\top \mathbf{y} - \beta^2 \mathbf{H} \mathbf{m}^0 - \mu \mathbf{b}) \quad (9.30)$$

where $\mathbf{H} = \mathbf{D}^\top \mathbf{D}$. If we choose to solve explicitly for the parameter estimates, we find that

$$\mathbf{m} = [\mathbf{A}^\top \mathbf{A} + \beta^2 \mathbf{H}]^{-1} (\mathbf{A}^\top \hat{\mathbf{d}} - \mu \mathbf{b}) \quad (9.31)$$

where $\hat{\mathbf{d}}$ is as previously defined. Since eq. (9.30) must satisfy eq. (9.21), we have that

$$\mu = \pm \left(\frac{q_T - q_{LS}}{\mathbf{b}^\top [\mathbf{A}^\top \mathbf{A} + \beta^2 \mathbf{H}]^{-1} \mathbf{b}} \right)^{\frac{1}{2}} \quad (9.32)$$

where $q_{LS} = \mathbf{d}^\top \mathbf{d} + \beta^2 \mathbf{m}^{0\top} \mathbf{H} \mathbf{m}^0 - (\mathbf{y}^\top \mathbf{A} - \beta^2 \mathbf{m}^\top \mathbf{H}^\top) (\mathbf{A}^\top \mathbf{A} + \beta^2 \mathbf{H})^{-1} (\mathbf{A}^\top \mathbf{y} - \beta^2 \mathbf{H} \mathbf{m}^0)$.

Nonlinearity is dealt with using an iterative scheme as in the previous case.

Finally, if it is desired to retain any available reliable prior estimates in the extremal inversion, then we have to minimize the function

$$\mathbf{m}^\top \mathbf{b} + \frac{1}{2\mu} \{(\mathbf{d} - \mathbf{f}(\mathbf{m}))^\top (\mathbf{d} - \mathbf{f}(\mathbf{m})) + \beta [\mathbf{D}\mathbf{m} - \mathbf{h}]^\top \beta^\top [\mathbf{D}\mathbf{m} - \mathbf{h}] - q_T\} \quad (9.33)$$

The solution is therefore

$$\mathbf{x} = [\mathbf{A}^\top \mathbf{A} + \mathbf{B}\mathbf{H}]^{-1} \{ \mathbf{A}^\top \mathbf{y} + \mathbf{B}\mathbf{D}^\top (\mathbf{h} - \mathbf{D}\mathbf{m}^0) - \mu \mathbf{b} \}$$

or equivalently

$$\mathbf{m} = [\mathbf{A}^\top \mathbf{A} + \mathbf{B}\mathbf{H}]^{-1} \{ \mathbf{A}^\top \hat{\mathbf{d}} + \mathbf{B}\mathbf{D}^\top \mathbf{h} - \mu \mathbf{b} \} \quad (9.34)$$

where $\mathbf{B} = \beta^\top \beta$,

Most squares flow diagram

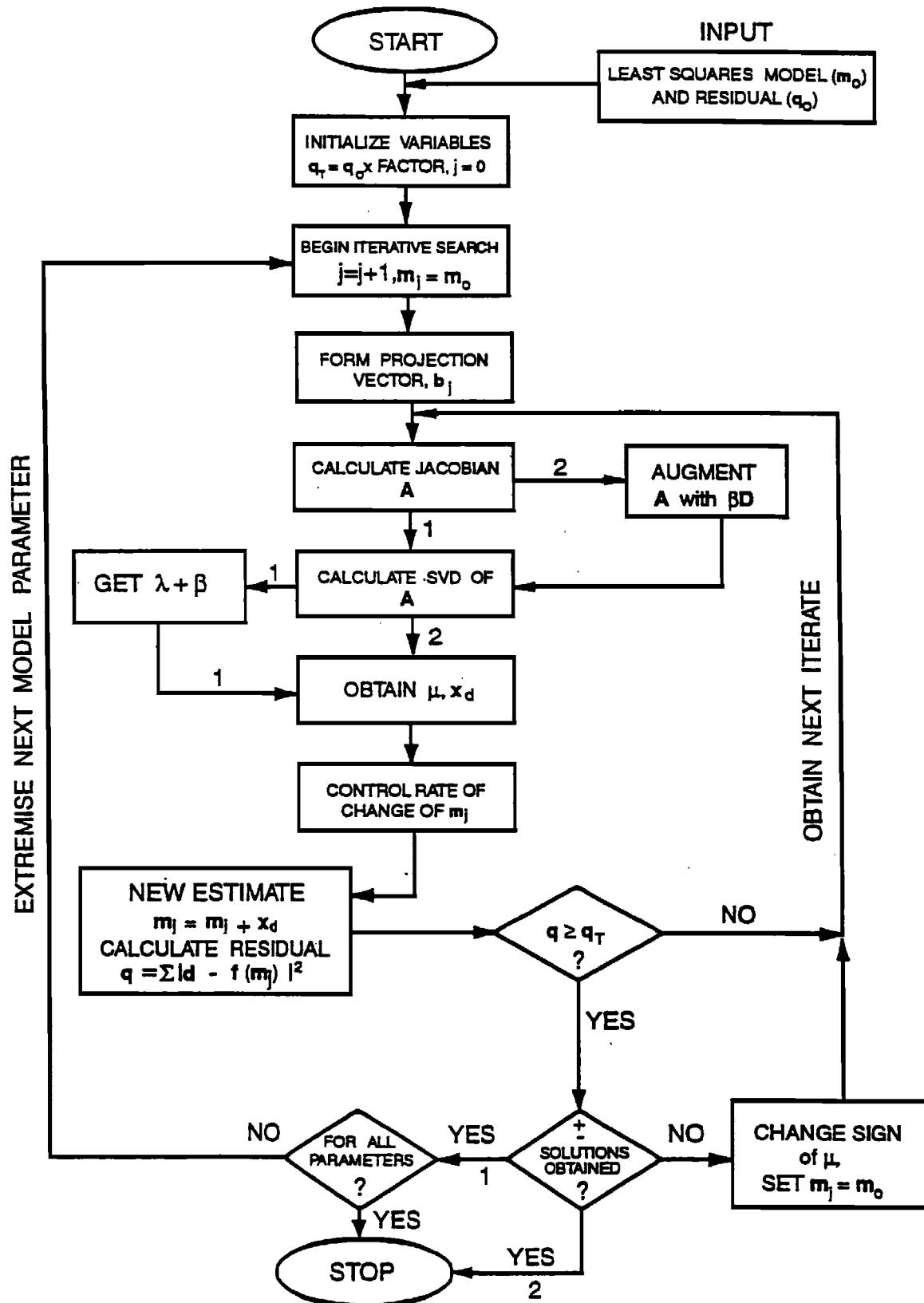


Figure 9.2

$$\mu = \pm \left(\frac{q_T - q_{LS}}{b^T [A^T A + BH]^{-1} b} \right)^{\frac{1}{2}} \quad (9.35)$$

and

$$q_{LS} = d^T d + B(h^T(h - Dm^0) + m^{0T} D^T(Dm^0 - h)) \\ - (y^T A - Bm^T H^T)(A^T A + BH)^{-1}(A^T y - BHm^0).$$

The most squares algorithm can be readily implemented and a flow diagram of an iterative scheme using the two methods of damping discussed above is shown in Fig. 9.2. Notice that the right-hand sides of equations 9.24 and 9.30 contain the damped least squares solution for all the parameters and an additional term that is specific to the parameter being extremized. The method uses a compensating relationship between the parameters and may be interpreted as providing the confidence limits of the optimal least squares model (Meju & Hutton, 1992). Provided that $q_T > q_{LS}$, there exists two solutions for μ for each parameter; and since none of the model parameters is kept fixed during each step of the iterative process, the method in effect generates $2p$ different models for the p model parameters that are consistent with the given data. Thus, the method may be useful for mapping out the parameter space for overdetermined nonlinear problems. An application of this method of analysis to the COPROD (Jones & Hutton, 1979) magnetotelluric data is shown in Fig. 9.3 for illustration. The maximum permissible residual, q_T was set to the number of data and the results show that the models are not constrained by the data in the top 10 km of the Earth's crust and at depth below about 300 km which agrees with Parker's (1982) maximum depth to which any model can be constrained by the COPROD data. It is obvious that the most-squares models throw some light on the variability of model space and show what features of the models are important or consistent with the field observations. It may be noted also that instead of extremizing each separate parameter, one can obtain a solution envelope by setting the projection vector as $b = [1, 1, \dots, 1]^T$ (Jackson, 1976). This would yield the upper and lower bounding models for the least squares model as demonstrated in Fig. 9.4a using magnetotelluric data. This procedure may be useful when dealing with smooth, densely parameterised models (eg. Constable et al., 1987; Meju & Hutton, 1992) as illustrated in Fig. 9.4b. Note that in generating the smooth models shown in this figure, the Earth was parameterized into a succession of layers of equal thickness (in log space) and that the smoothness measures were only applied to the layer resistivities.

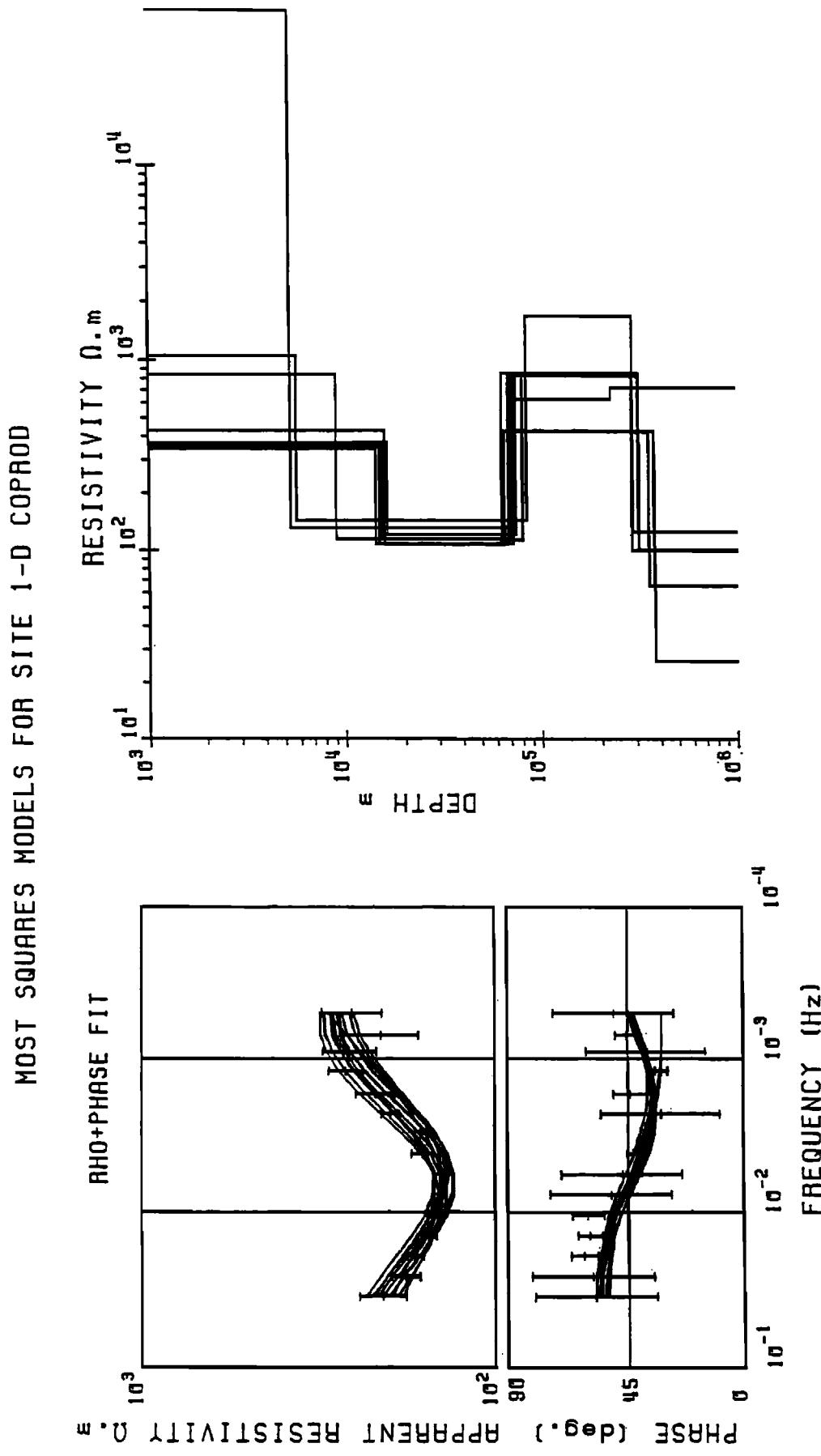


Fig. 9.3 Most-squares class of extreme models for MT data

MOST SQUARES MODELS FOR SITE SYNTH-4L

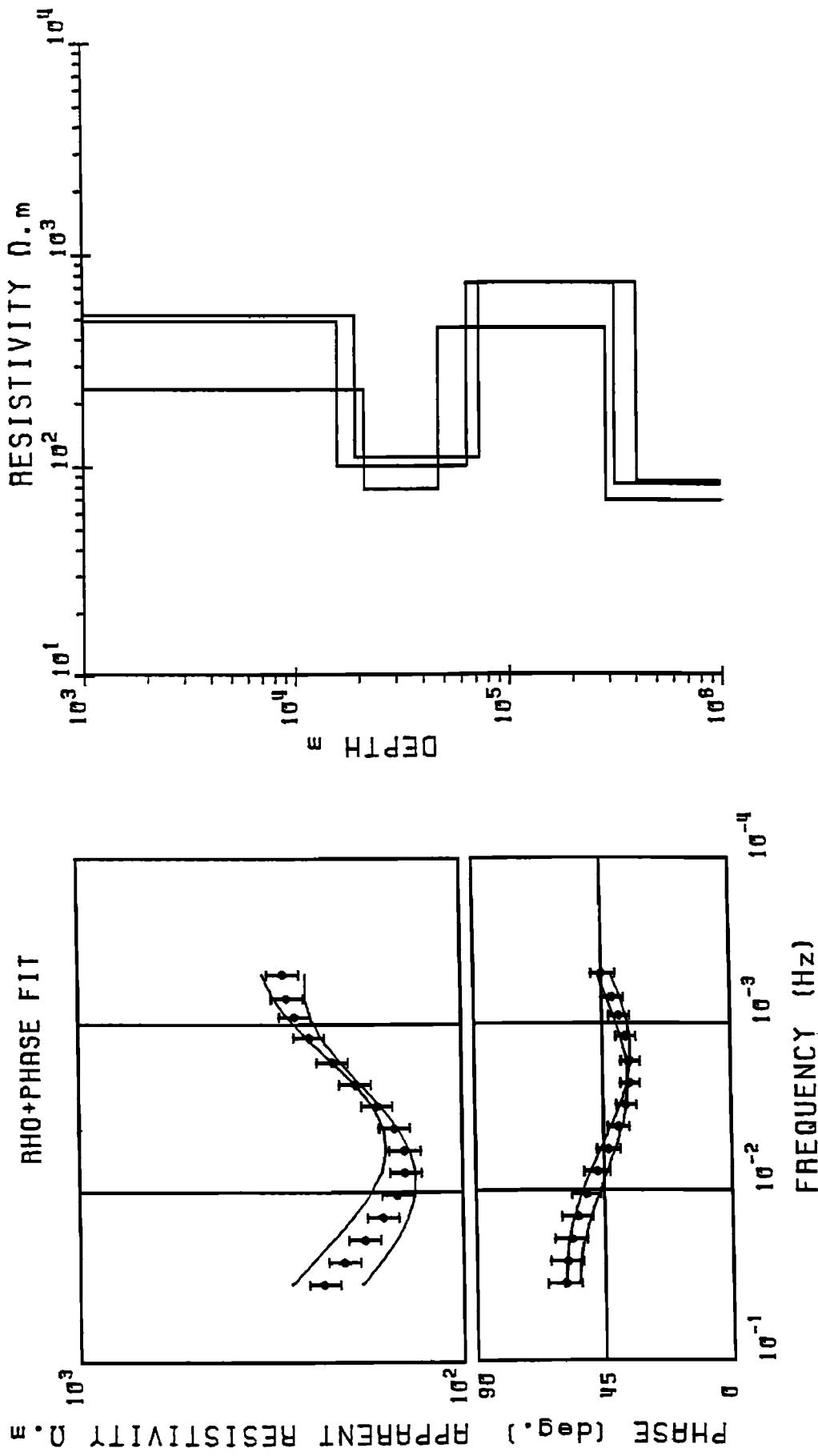


Fig. 9.4a. Most-squares solution envelopes for MT data (after Meju and Hutton, 1992)

MOST SQUARES MODELS FOR SITE SYNTH-4L

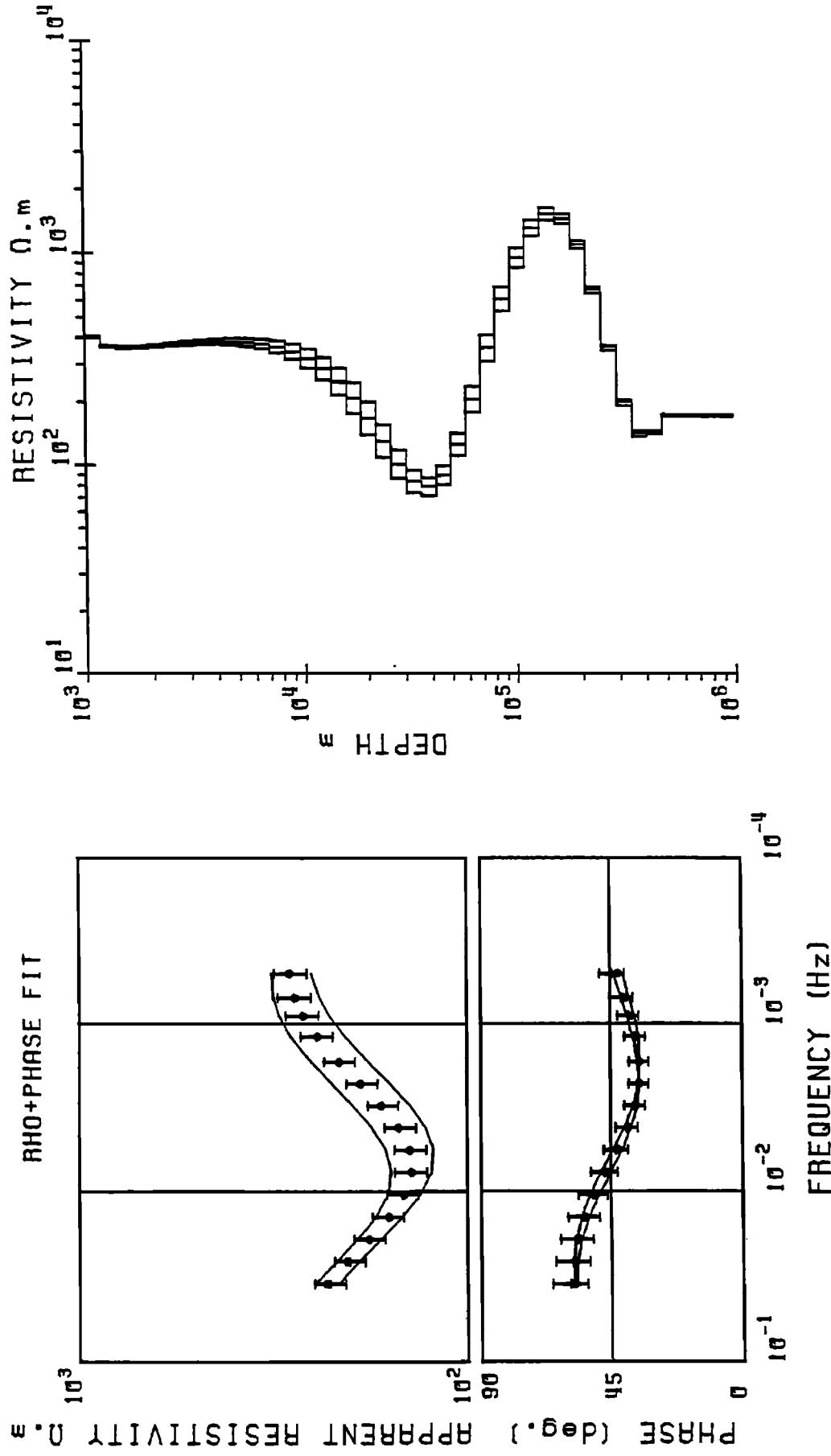


Fig. 9.4b Smooth solution envelopes for MT data (after MeJu and Hutton, 1992)

10. SAMPLE SPECIALIZED APPLICATIONS OF INVERSE THEORY

10.1 Processing of Time- or Space-Series Data

The Earth has sounds for those who listen but the music is always distorted by some unwanted tunes and inverse problem theory provides us with the filters for enhancing and understanding these sounds; geophysicists have mastered some of these sounds and are therefore in tune with the Earth. This is the author's favourite description of geophysical signal processing to the uninitiated and the full import of this simplifying assertion will become obvious in the following discussions.

10.1.1 Adaptive Signal Processing

Geophysical time- or space-series data are typically bedeviled by noise from various natural and artificial sources. These undesirable phenomena manifest as interference noise, random noise or nonlinear drift in the time-series data and we wish to remove them or minimize their effects using the tools provided by inverse problem theory. If the noise characteristics (or some reference desirable signals) are known, we could eliminate the noise in the data by simple filtering or by adaptive noise cancellation operations (e.g., Widrow and Hoff, 1960; Widrow et al., 1967; Wang and Treitel, 1971). Unfortunately, in typical geoexploration situations we do not know what the true signal is or what constitutes noise and processing the resulting time-series data becomes a difficult task and the main goal is to suppress the noise as best as we can. We will explain the undergirding principles of adaptive signal processing following some useful definitions. If the statistical properties (i.e., mean, variance, correlation functions, etc) characterising the data do not vary with recording time, then we may describe such a system as being stationary. If however, these statistical characteristics vary with measurement time, the system is said to be non-stationary.

Mathematical Model for a Stationary Linear System

Consider a linear time-invariant but otherwise unknown system whose sampled values of the output $y = (y_0, y_1, y_2, \dots, y_n)^T$ are related to the discrete system input $x = (x_0, x_1, x_2, \dots, x_n)^T = X^T$ and the impulse response function $w = (w_0, w_1, w_2, \dots, w_n)^T$ by the convolution

$$y_j = \sum_{i=0}^n w_i x_{j-i} = w^T X, \quad j=0,1,2,\dots . \quad (10.1.1)$$

A seismic trace, for example, can be approximated by the above finite discrete convolution and may be interpreted as representing the convolution of a reflection coefficient series with a reverberating pulse train. In any case, it should be noted that in addition to the usual input signal x_i , we need to supply an extraneous input signal (i.e., an estimate of the desired response) d_i containing the adaptive filter during the adaptation process, a kind of *a priori* information.

Inverse problem formulation

The inverse problem is simply stated as: Given the signals x_i and an estimate of the desired response d_i , find the impulse response w that is optimal in the least squares sense (i.e., the set of weights w ; yielding the best output).

Let us define the error between our desired response d_i (represented by the additional input signal) and the system output y_i (for the weight estimates, w_i) as

$$e_i = d_i - y_i;$$

or simply

$$e = d - w^T X = d - X^T w. \quad (10.1.2)$$

We wish to minimize the sum of squares of this error series, i.e.,

$$e^T e = (d - X^T w)^T (d - X^T w) = d^T d - 2d^T X^T w + w^T X X^T w.$$

The expected value of e^2 , given w is

$$\epsilon^2 = E(e^T e) = E(d^T d) - 2w^T E(d^T X) + w^T E(X X^T) w$$

where E is the expectation operator. Let the correlation vector $d^T X$ be denoted by ψ_{dx} or simply P and the autocorrelation matrix $X X^T$ be denoted by ψ_{xx} or R . Assuming that ψ_{dx} and ψ_{xx} approximate their expected values for this stationary process, we have that

$$\epsilon^2 = E(d^T d) - 2w^T \psi_{dx} + w^T \psi_{xx} w.$$

Minimization is effected by setting to zero the gradient of this quadratic function with respect to w .

Estimating gradients and optimal solution

The error gradient is simply

$$\nabla(\epsilon^2) = -2\psi_{dx} + 2\psi_{xx}w = -2(\psi_{dx} - \psi_{xx}w) \quad (10.1.3)$$

and equating it to zero for a minimum leads to the solution for the optimal weight vector

$$w^* = \psi_{xx}^{-1} \psi_{dx} = R^{-1}P \equiv [XX^T]^{-1}X^Td \quad (10.1.4)$$

which is the well-known Wiener-Hopf least mean square (LMS) error filter and can be used to find the minimum of the error surface through successive adjustment of the weights w . Note that this algorithm can be implemented in different ways using matrix inversion or gradient-type schemes. An iterative implementation using the method of steepest descent gives the adaptive process as (e.g., Widrow et al., 1975, 1976)

$$w^{j+1} = w^j + \beta(-\nabla_j) \quad (10.1.5)$$

where the estimated change in w^j is proportional to the negative of the error gradient and β is a scalar constant that controls the convergence and stability of the algorithm. Substituting the expression for the gradient vector (10.1.3) into this iterative algorithm, yields

$$w^{j+1} = w^j + \beta(2\{d - X^Tw^j\}X) = w^j + 2\beta eX \quad (10.1.6)$$

which is the popular Widrow-Hoff LMS algorithm and does not require the calculation of ψ_{dx} or ψ_{xx} . The useful output of this iterative filtering process (i.e., the clean signal) is the error series e . It can be shown that the Widrow-Hoff algorithm converges if β is assigned a value between 0 and $\frac{1}{\lambda}$, where λ is the largest eigenvalue of the input autocorrelation matrix XX^T . The algorithm also converges if β is replaced by $1/\text{trace}(\psi_{xx})$, where $\text{trace}(A)$ is the sum of the elements in the main diagonal of A (Wang, 1977).

A variant of the above adaptive algorithm is obtained by premultiplying the estimated error gradient at each iteration by an estimate of the inverse of the autocorrelation matrix yielding (see also, Widrow et al., 1975, 1976)

$$\begin{aligned}
\mathbf{w}^{j+1} &= \mathbf{w}^j - \beta R^{-1} \nabla_j \\
&= \mathbf{w}^j + 2\beta R^{-1} e^j X^j \equiv \mathbf{w}^j + 2\beta [XX^T]^{-1} X^T (\mathbf{d} - \mathbf{y})
\end{aligned} \tag{10.1.7}$$

which is an iterative inversion formula incorporating some kind of *a priori* data.

Time-varying Linear Systems with Non-Stationary Inputs

The task of suppressing or removing unwanted signals from geophysical time-series is a difficult one since the data often display non-stationary characteristics (such that their expected values are not constant). Several approaches have been developed to address such problems (e.g., Wang, 1977) but we will discuss a simple and effective adaptation of the Widrow-Hoff LMS algorithm – the correlated adaptive noise cancellation (CANC) algorithm of Hattingh(1988). Here, the required data sets are the primary signal containing the noise that is to be minimized d_i , and a reference signal x_i . Note the notational change from the previous treatment of adaptive noise cancellation. In the CANC algorithm, the reference signal input to the data adaptive filter, X is actually a tapped delay time version of the original reference signal with the time delay being equal to the filter length L , i.e.,

$$X = (x_i, x_{i-1}, \dots, x_{i-L+1})^T \tag{10.1.8}$$

where $L \leq i \leq n$. As before, the reference signal is merely used as a learning signal to adapt the filter coefficients. The filter output at the i^{th} instant for the given \mathbf{w} is thus

$$\mathbf{y} = \mathbf{w}^T X$$

and the error function to be minimized is simply

$$e_i = d_{(i-L/2)} - y_i. \tag{10.1.9}$$

In applying the Widrow adaptive algorithm $\mathbf{w}^{j+1} = \mathbf{w}^j + 2\beta e X$, we note here that $1 \leq j \leq L$. The recovered signal from this operation comes from the filter output y_i , and the extracted noise is contained in the error series e_i . A Fortran translation of the single-channel CANC algorithm given Hattingh(1988) is given in Fig. 10.1.1 and can be easily extended to handle multi-channel input.

```
      subroutine CANC(d,xx,y,nd,ns,L,beta,itern,iscale)
c correlated adaptive noise cancellation routine
c adapted from an original HP-Basic program by Hattingh,
c Computers & Geosciences, 14, 467-480, 1988.
c   d = primary signal ; xx = reference signal ; y = output signal
c   X = delayed reference signal ; w = filter coefficients (weights)
c   e = error signal
c   ns = actual number of samples in the time series d
c   nd = physical dimension of the vectors d & xx in control routine
c   L = filter length (typically about 2 times signal bandwidth)
c   beta = convergence factor (typically 0<beta<<1)
c   iter = number of iterations to be performed
c   iscale = 0 (no scaling) or 1 (each signal normalised by largest coefficient)
c-
      real d(nd), xx(nd), y(nd), X(nd),w(nd),e(nd)
c initializations
      iter=0
      L2=L/2
      do i=1,ns
        X(i)=0.0
        w(i)=0.0
        y(i)=0.0
        e(i)=0.0
      end do
      calculate and remove mean from prim. and ref. signals
      dsum=0.0
      xsum=0.0
      do i=1,ns
        dsum = dsum+d(i)
        xsum = xsum+xx(i)
      end do
      dmean=dsum/ns
      xmean=xsum/ns
      do i=1,ns
        d(i)=d(i)-dmean
      end do
```

```
    xx(i)=xx(i)-xmean
    end do
c note, at this stage, that for additional stability, we may employ a
c scaling operation of the signals using the largest coefficient of each
c time-series. final output may be de-scaled as required (not implemented).
    if(iscale.eq.1)then
c find largest sample value of each signal
    bigd=d(1)
    bigx=xx(1)
    do i=2,ns
        if(d(i).gt.bigd)then
            bigd=d(i)
        end if
        if(xx(i).gt.bigx)then
            bigx=xx(i)
        end if
    end do
c normalise the signals
    do i=1,ns
        d(i)=d(i)/bigd
        xx(i)=xx(i)/bigx
    end do
    endif
c ** end of scaling operations **
c apply CANC algorithm
10 continue
    do i=1+L, ns
c form delayed reference signal
        do k=1,L
            X(k)=xx(i-k)
        end do
c filter delayed reference signal
        do j=1,L
            y(i)=y(i)+w(j)*X(j)
        end do
c delay primary signal with lag L/2 and calculate error
```

```
e(i)=d(i-L2)-y(i)
calculate new filter coefficient using the Widrow-Hoff LMS algorithm
do j=1,L
    w(j)=w(j)+2.*beta*e(i)*X(j)
end do
end do
c      update count for next iteration
iter=iter+1
if(iter.LT.itern)then
c      zero filter output for next iteration
do i=1,ns
    y(i)=0.0
end do
c      repeat operations as specified by itern
goto 10
else
compensate for phase shift
do i=1,ns
    if(i.LE.L2)then
        y(i)=0.0
        e(i)=0
        else if(i.GE.(ns-L2))then
            y(i)=0.0
            e(i)=0.0
        else
            y(i)=y(i+L2)
            e(i)=e(i+L2)
        end if
    end do
end if
return
end
```

Fig. 10.1.1 A Fortran CANC routine.

10.1.2 Iterative Deconvolution of Seismograms from Ripple Fired Shots

The ever increasing environmental restrictions on the generation of high amplitude surface vibrations now make it difficult for large shots to be fired in long range crustal exploration seismology. The energy density of a shot may be reduced by firing a number of smaller shots spread out in time that together would generate effects that are comparable to a large shot. This is known as ripple firing of explosives and is now a standard practice in many rock quarries. Ripple fired shots generate seismograms containing overlapping pulse-shaped events (interfering arrivals of various phases from different shots) but the process can be modelled mathematically. From such confused signals, one hopes to deconvolve less noisy signals representing the seismogram that would have been recorded from a single large shot. This is a nonlinear inverse problem and it is possible using wave-shaping deconvolution and inversion techniques to recover a stacked, average source signal combining each individual shot. The main usefulness of inversion here is in optimizing the input spike time series for the wave-shaping deconvolution. The spike time series is then deconvolved from the whole field record to give a filtered source signal with a much reduced signal-to-noise ratio. Note that a field seismogram can be regarded as a nonlinear function of the positions and amplitudes of the spike input. Our model is the one-dimensional convolution of a source wavelet with a spike time series of a finite length plus additive noise, i.e.,

$$y = w * x + e . \quad (10.1.10)$$

The number of spikes in the input signal corresponds to the number of shots fired while the time separations of the spikes corresponds to the time delays between first arrivals from different shots at a receiver. The time delays consist of the actual firing delay of about 25ms and the delay owing to the different positions of the shots.

Field records of seismograms were obtained in an explosion seismology experiment using quarry blasts at Charnwood Lodge in Leicestershire, England (P.Maguire, 1991 unpub.). It was intended to fit the data for these ripple fired shots. The positions and amplitudes of the spikes in the input model were chosen as the model parameters. The model response is the synthetic seismogram produced by convolution. This inverse problem was solved using the ridge regression procedure outlined in section 7.4. One of the field records and the starting model for the iterative deconvolution are shown in Fig 10.1.2. The initial spike time series consists of equispaced spikes of equal amplitude and is

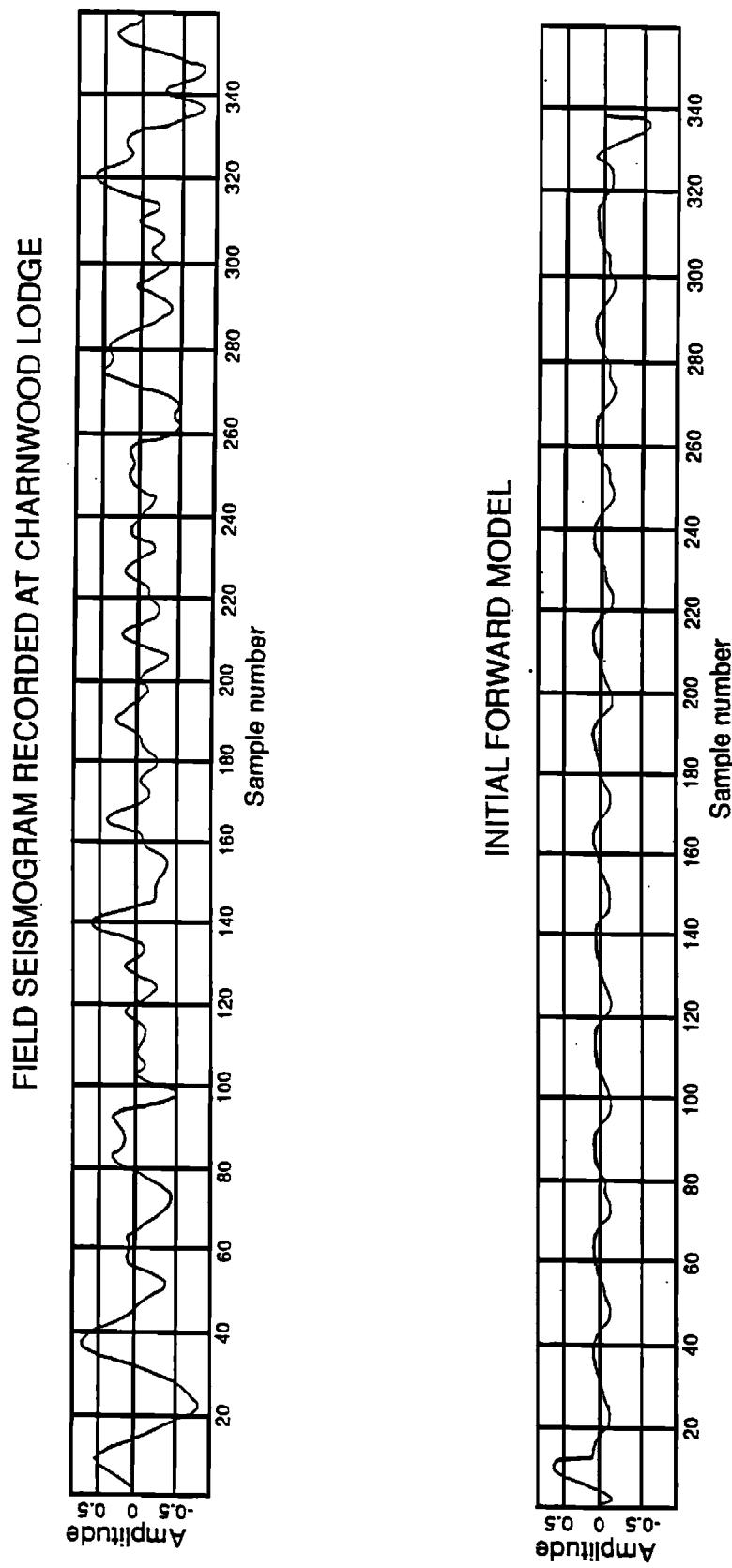


Fig. 10.1.2

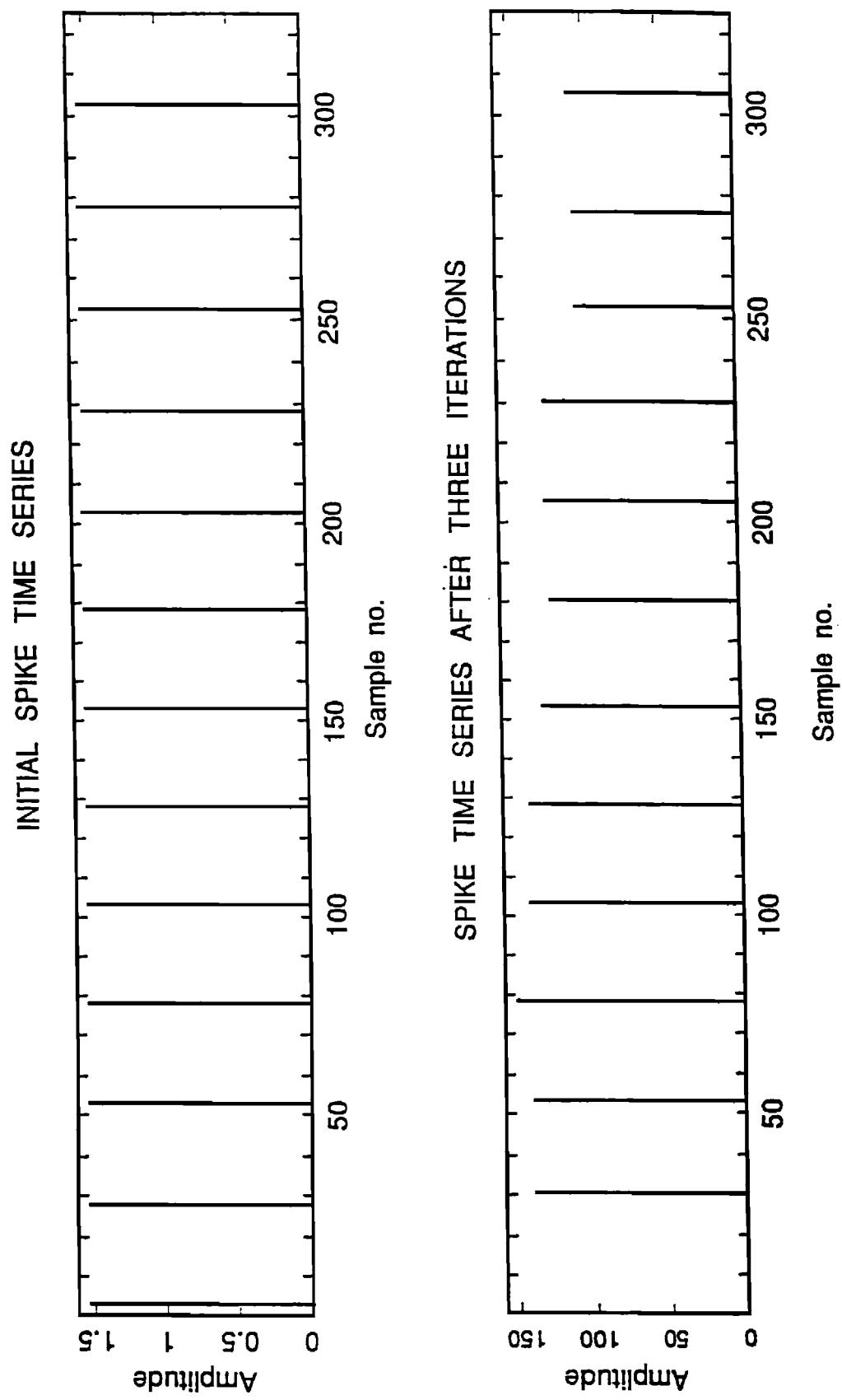


Fig. 10.1.3

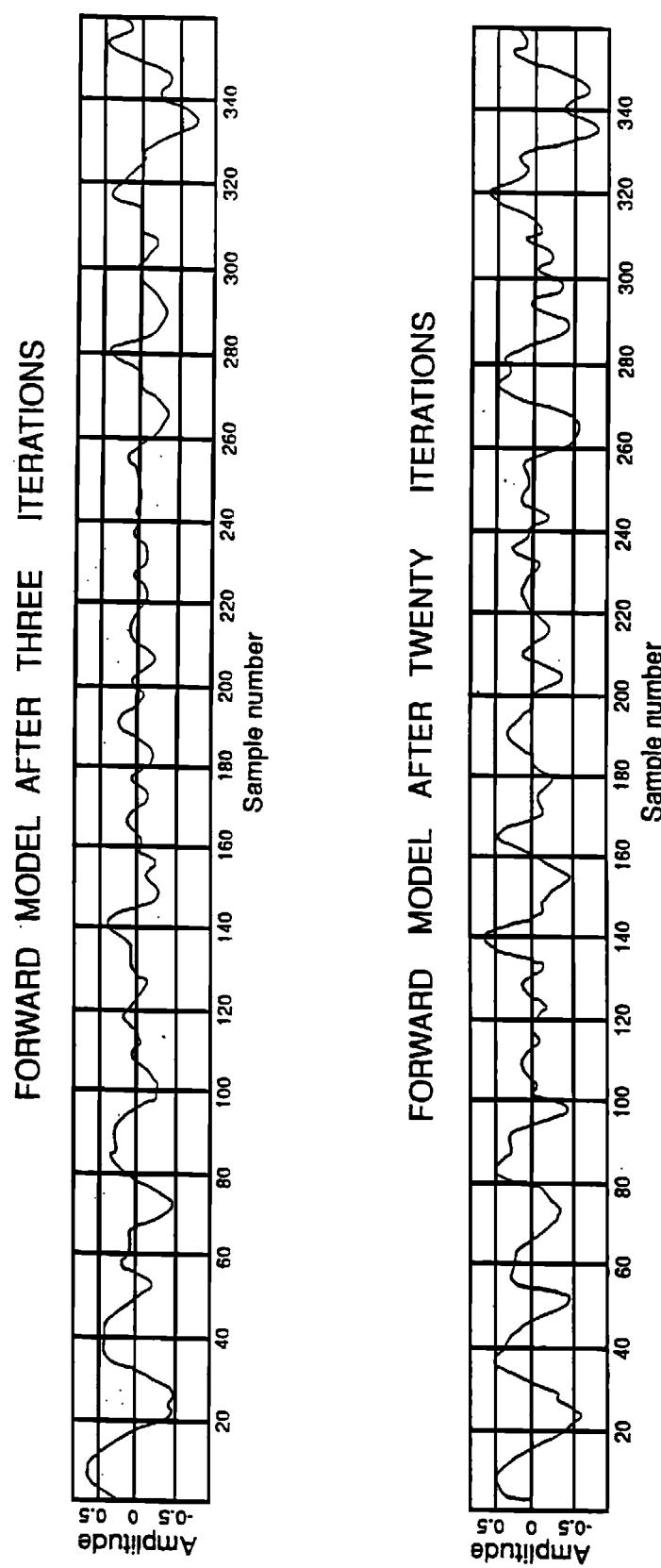


Fig. 10.1.4

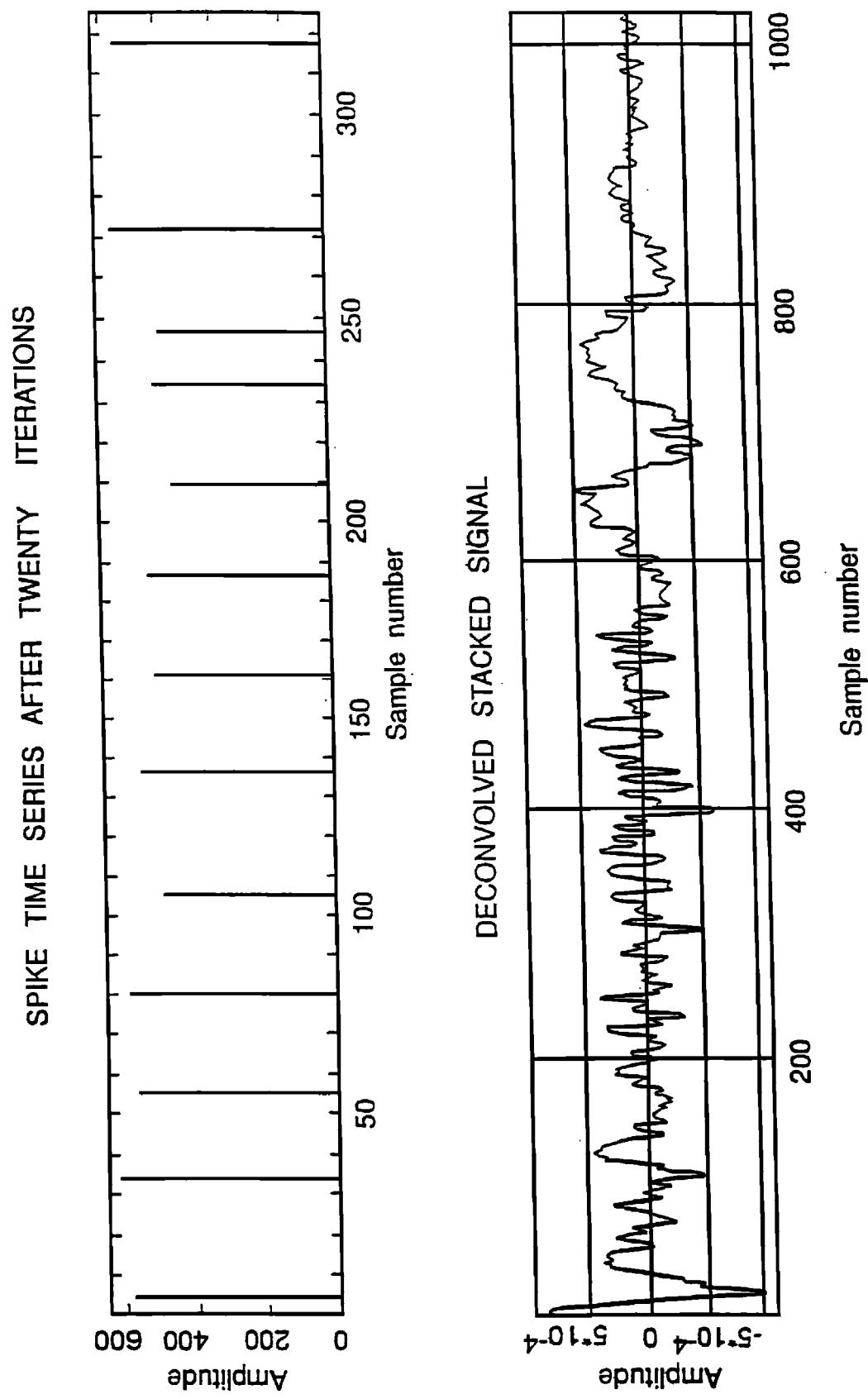


Fig. 10.1.5

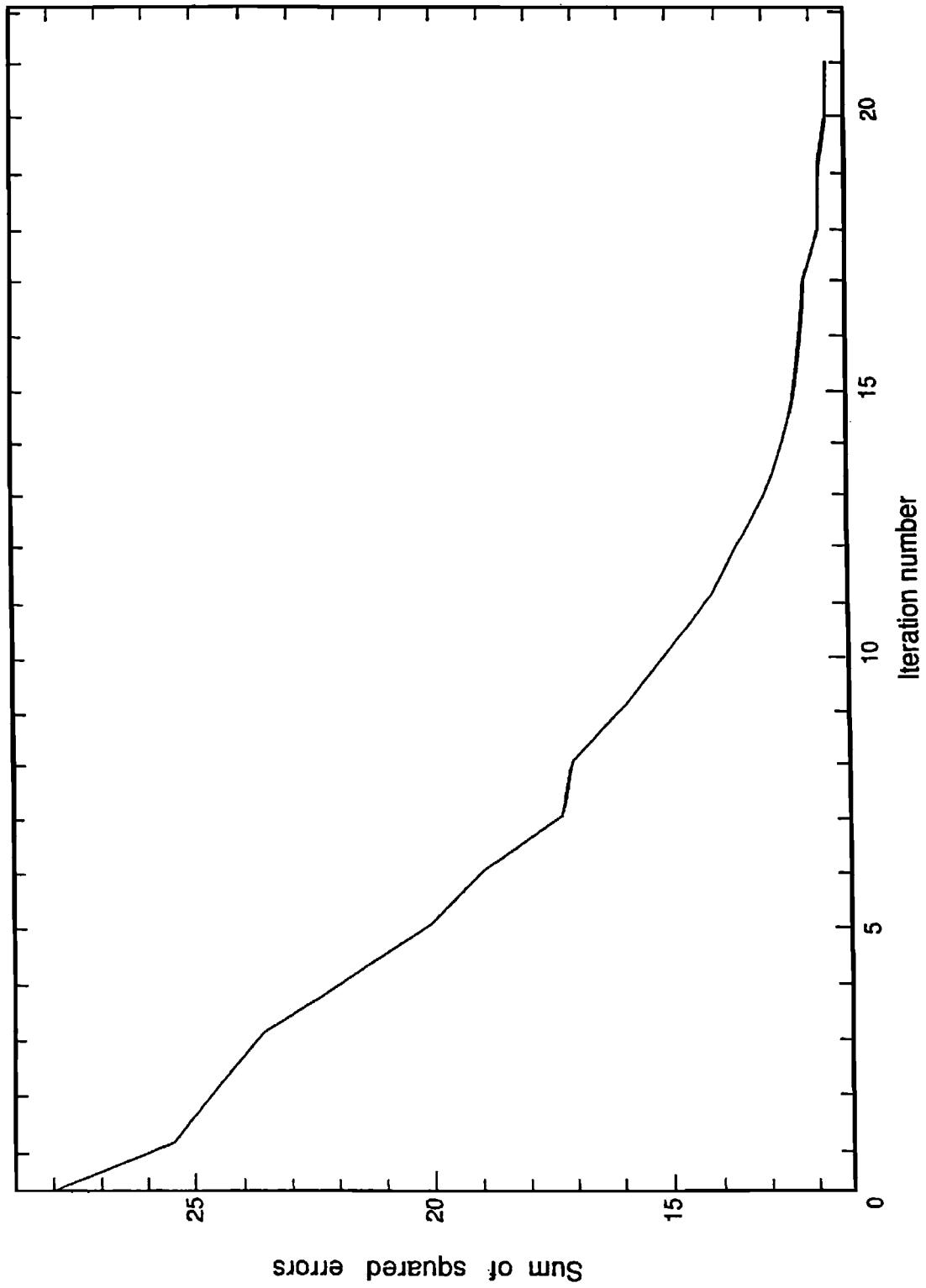


Fig. 10.1.6 Convergence characteristics of the algorithm

shown together with the spike time series after three iterations in Fig.10.1.3. The model estimates after three iterations and after 20 iterations are shown in Fig. 10.1.4. Notice the semblance of these estimates to the actual field seismogram shown in Fig. 10.1.2. The final spike time series and the deconvolved stacked signal are shown in Fig 10.1.5. The convergence characteristic of the algorithm is shown in Figure 10.1.6 in order that we can appreciate the effectiveness of the procedure. Notice that the sum of squares of residuals had decreased by more than two-fold to an acceptable level in 12 iterations and that the improvements after iteration 12 are negligible.

10.1.3 Residual Statics Estimation

When processing seismic reflection data it is important to account for the velocity variations in the weathering layer or we may end up with a distorted picture of the subsurface. Static time anomalies due to the weathering layer manifest in the form of signal misalignment on the seismic traces and lead to degraded wavelet character in common-datum-point (CDP) stacks. For reliable structural interpretations, we need to estimate the optimal distribution of time shifts required to correct for such static anomalies. Operationally, bulk time shifts are applied to individual seismic traces to compensate for these near-surface velocity variations. However, after the bulk time shifts, residual time differences between the traces may persist such that the desired reflection hyperbola may show random patterns leading to scattering of events after normal move-out (NMO) corrections. If the time shift is small in comparison with the spread length, the appropriate events may be lined up in an optimal way by estimating relative shifts after NMO corrections using Trace 1, say and the windows of strong reflections. This crude approach to residual statics analysis known as coherency stacking is not governed by any physical law. Note, however, that reasonable results may be obtained if the time shifts are small with respect to the spread length. Information about the near-surface weathering zone may also be furnished by uphole tests in a borehole through the weathered layer, refraction seismics or refraction first breaks on the reflection records (this may be a problem since the recording arrays in reflection surveys are typically designed to eliminate refractions). It is possible to set up a system of equations for estimating static time corrections for CDP seismic reflection data (Tanner et al., 1974). Wiggins et al.(1976) cast the problem as a linear inverse problem and the following analysis derives from their landmark paper.

The residual statics problem

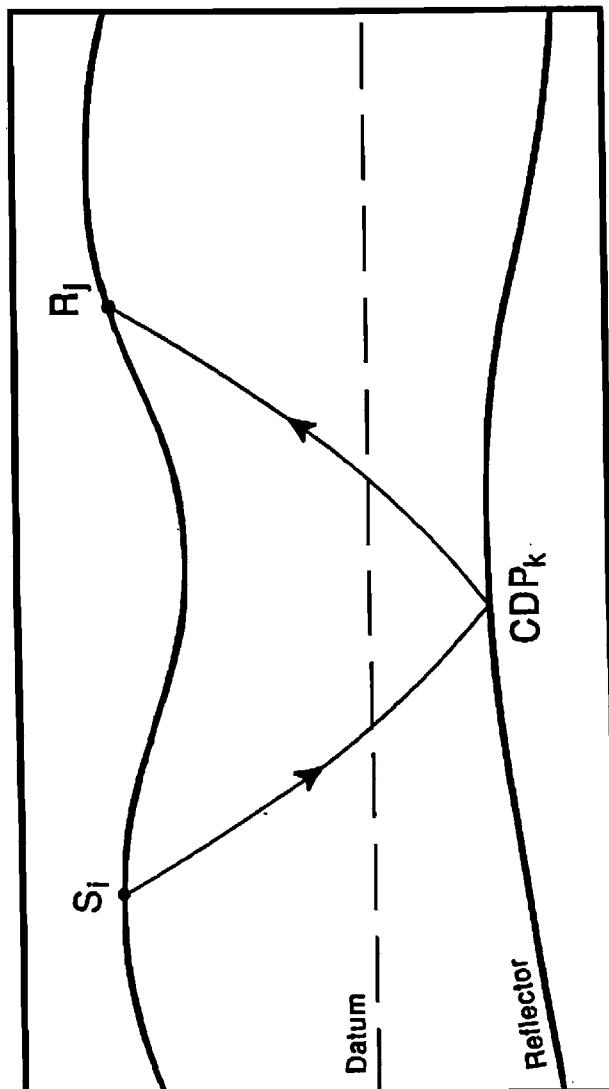


Figure 10.1.7

10.1.3.1 Problem formulation for linear survey lines

Consider the ray path from source position S_i to a subsurface reflector and thence to a surface receiver R_j , as illustrated in Fig. 10.1.7. Assuming surface consistency (i.e., that the static shift associated with surface point S is independent of the ray path and of whether S is a shot or receiver – provided that datum corrections have been applied) and subsurface consistency (i.e., residual NMO is assumed to be independent of offset), the total travel time from shot location S_i to the buried reflector at the k^{th} CDP to the receiver location R_j (i.e., a given reflection event on the ij trace) is given by

$$T_{ij} = S_i + R_j + N_k + M_k x_{ij}^2 \quad (10.1.11)$$

where T_{ij} is the travel time for the chosen horizon on trace ij , S_i is the travel time from the source to the datum plane for the i^{th} shot, R_j is the travel time from the receiver position R_j to datum plane, N_k is the normal incidence two-way travel time from datum to the reflector at the k^{th} CDP position, M_k is the time averaged residual NMO and x_{ij} is the distance from the i^{th} shot to the j^{th} receiver.

The above relation holds for every source-receiver combination along a survey line. It follows therefore that for ns shots and nt receivers, there are $n = ns \times nt$ such equations. The desired time terms for static corrections are S_i, R_j, N_k and M_k and we can pose the problem in the form $\mathbf{d} = \mathbf{Gm}$ where \mathbf{d} is the vector of observed travel times T_{ij} , \mathbf{m} is the vector of the sought time terms and \mathbf{G} is the coupling or coefficient matrix for the n equations. For illustration, consider the simple source-receiver configuration shown in Fig. 10.1.8 for a seismic line shot off-end. The system consists of four shot points (i.e., $ns = 4$) and four receivers (i.e., the number of traces per shot, $nt = 4$) and the

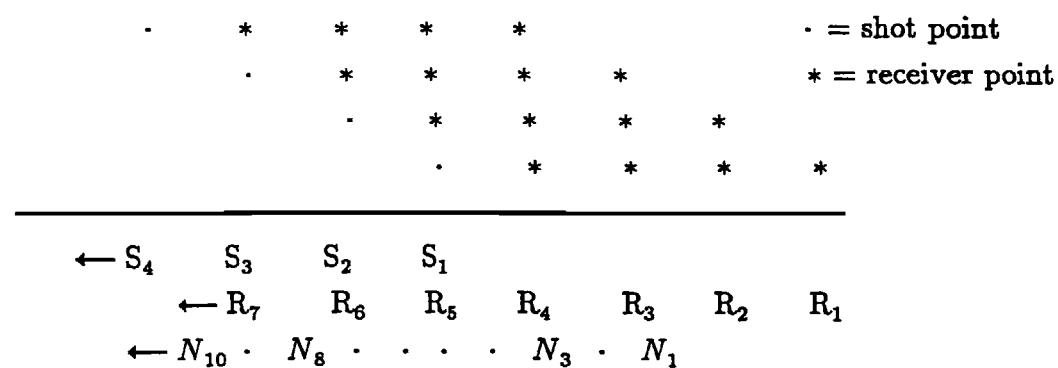


Fig. 10.1.8 Illustration of the CDP geometrical relationships
(after Wiggins et al., 1976)

shot spacing is equal to the constant receiver spacing. We thus have sixteen observed data values ($n=16$). It is obvious from Fig. 10.1.8 that there are seven unique receiver positions (i.e., $nr = ns+nt-1$) and ten unique CDP positions ($ng=nm=nt+2[ns-1]$) so that there are thirty-one ($p = ns+nr+ng+nm$) model parameters for this simple problem.

The above problem can be posed in matrix form with

$$\mathbf{m} = [S_1, \dots, S_4, R_1, \dots, R_7, N_1, \dots, N_{10}, M_1, \dots, M_{10}]^T$$

$$\mathbf{d} = [T_{11}, T_{12}, T_{13}, T_{14}, T_{22}, T_{23}, T_{24}, T_{25}, T_{33}, T_{34}, T_{35}, T_{36}, T_{44}, T_{45}, T_{46}, T_{47}]$$

and the coefficient matrix G as given in Fig. 10.1.9.

$$\left| \begin{array}{ccccccccc|ccccccccc} 1 & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & 16 & \cdot & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & 9 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & 4 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & 16 & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & 9 & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 4 & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & 16 & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & 9 & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 4 & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & & 16 & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & & 9 & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & & 4 & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & 1 & \cdot & 1 & \cdot & \cdot & \cdot & & & 1 & \cdot & \cdot & \cdot \end{array} \right|$$

$\uparrow \quad \uparrow \quad \uparrow \quad \uparrow \quad \uparrow \quad \uparrow \quad \dots \quad \uparrow \quad \uparrow \quad \uparrow \quad \uparrow \quad \uparrow \quad \dots \quad \uparrow \quad \uparrow \quad \uparrow$
 $S_1 \dots S_4 \quad R_1 \quad \dots \quad R_4 \quad N_1 \quad \dots \quad N_{10} \quad M_1 \quad \dots \quad M_{10}$

Fig. 10.1.9 The G matrix for the problem involving the CDP geometry shown in Fig. 10.1.8. The dots correspond to zeros and the columns of G are identified with the corresponding parameters of the problem using the usual symbols at the bottom (after Wiggins, et al. 1976).

The problem is undetermined since $n < p$. For such a short spread, increasing the shot points would increase the indeterminacy. For instance, if ns is increased to eight, we

have that $p=55$ and $n=32$. The problem is said to be ill-posed and needs to be regularized. Note, however, that if we employ a 24-trace receiver group system, the problem becomes overdetermined for greater than three shots as shown in Table 10.1.1. It is stressed that even in this overdetermined situation, there is still some indeterminacy in the set up as there are not enough independent equations to constrain the individual parameters.

<i>nt</i>	<i>ns</i>	<i>nr</i>	<i>ng</i>	<i>p</i>	<i>n</i>
24	3	26	28	85	72
24	4	27	30	91	93
24	12	35	46	139	288
24	24	47	70	211	576

Table 10.1.1 Survey design parameters

Problem solution and useful computational strategies

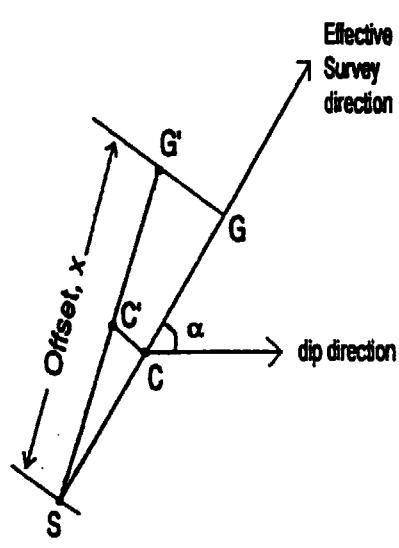
For such underconstrained problems, we need to use a constrained inversion method. We may obtain the least squares solution

$$\mathbf{m} = [\mathbf{G}^T \mathbf{G} + \beta^2 \mathbf{I}]^{-1} \mathbf{G}^T \mathbf{d}$$

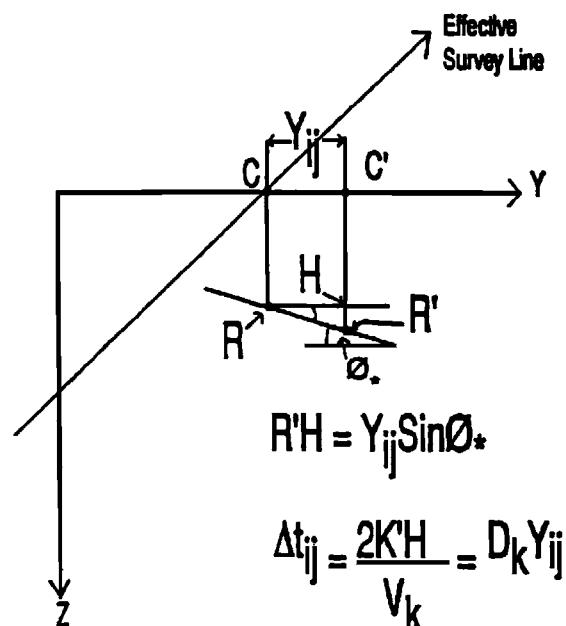
using either the biased estimation approach as in the comparable delay-time problem treated in Chapter 5 or by direct augmentation of the singular values of the problem for problems of moderate sizes. Because of the large size of equations involved for typical field surveys, the Gauss-Seidel iterative method of solution is often employed in the solution of the above system of matrix equations. While it may be practicable to augment the matrix \mathbf{G} with $\mathbf{D} = \mathbf{I}$, there may be other strategies that will cut down the size of the problem. For example, M_k is unlikely to vary greatly from one CDP position to another and it may thus be useful to average the coefficients over some “distance window” along a survey line (Hatton, et al., 1986). Thus, coefficients M_i to M_{i+l} may be averaged (i.e., reduced to one column) to give M_j simply by adding together columns i to $i+l$ of the matrix \mathbf{G} .

10.1.3.2 Estimation of Three-dimensional Residual Statics.

When computing residual statics for non-linear recording lines of 3-D surveys, the effect



(a)



(b)

Fig 10.1.10 (a) A deviated survey line \$S-G'\$ and its projection along the effective survey line \$S-G\$. The distance \$x\$ is the source-receiver offset and its midpoint is \$C'\$. The midpoint of the CDP gather is denoted by \$C\$. The angle between the source-receiver direction and the true dip direction is denoted by \$\alpha\$.
 (b) A cross-section taken perpendicular to the nonlinear survey line at the \$K^{th}\$ CDP. For the single cross-dipping planar reflector, \$\Delta t_{ij}\$ is the time difference in reflection time between a trace with its midpoint on the effective survey line (normal to the plane of the figure and denoted by \$C\$) and one displaced a distance \$y_{ij}\$ from it (denoted by \$C'\$). \$\theta_*\$ is the apparent reflector dip.

of dip on the residual NMO term M_k and the effect of deviation of source-receiver midpoint from the k^{th} CDP on the dip moveout term should be taken into account. As in the 2-D case, we assume that static corrections are surface and subsurface consistent. The observed traveltime for any given reflection event on the trace being considered is then given by the sum of six terms (Zai-tian, 1988)

$$T_{ijk} = S_i + R_j + N_k + M_k x_s^2 + M'_k x_c^2 + D_k y_s \quad (10.1.12)$$

where M_k is the time-averaged residual NMO coefficient along the strike direction at the k^{th} CDP position, M'_k is the time-averaged residual NMO coefficient along the dip direction at CDP k , $x_s = x \sin\alpha$, $x_c = x \cos\alpha$, $D_k = \frac{2\sin\phi}{v_{rms}}$ is the apparent-dip (or cross-dip) correction coefficient, $y_s = y \sin\alpha$, and M_k and M'_k are constant for the CDP gather. Here, x is the source-receiver offset, y is the distance between the source-receiver midpoint and the CDP point, v_{rms} is the RMS velocity along strike, ϕ is the true dip angle of the reflector and α is the angle between the true dip direction and the source-receiver direction (see Fig. 10.1.10).

The meaning of the cross-dip term $D_k y_s$ can be understood from Fig. 10.1.10a and 10.1.10b where it can be deduced that the time difference due to the deviation of the source-receiver from the effective (or projected) survey line is given by

$$\begin{aligned} \Delta t_i &= \frac{2R' H}{v} \\ \text{or} \quad \Delta t_i &= \frac{2y \sin\phi_*}{v_\alpha} = \frac{2y \sin\phi \cos(\alpha + \frac{\pi}{2})}{v_\alpha} \\ &= \frac{2y \sin\phi \cdot (-\sin\alpha)}{v_\alpha} = D_k y_s \end{aligned} \quad (10.1.13)$$

where $\phi_* = \phi \cos(\alpha + \frac{\pi}{2})$.

To understand the meaning of the terms M_k and M'_k , we simply note that the time-distance relation for a 3-D point source can be written as (Zai-tian, 1988)

$$t^2 = t_0^2 + \frac{x^2}{v_{rms}^2} \left\{ 1 - \sin^2\phi \cos^2(\alpha - \alpha_0) \right\} \quad (10.1.14)$$

where α is the azimuth of an offset position, α_0 is the azimuth of the true dip direction and the other symbols have been previously defined. Now, if $\alpha_0 = 0$ in the above time-distance relation (10.1.14), we have that

$$t^2 = t_0^2 + \frac{x^2}{v_{rms}^2} \{1 - \sin^2\phi \cos^2\alpha\}. \quad (10.1.15)$$

Now again, since $\{1 - \sin^2\phi \cos^2\alpha\} = \{1 - \cos^2\alpha + \cos^2\phi \cos^2\alpha\} = \{\sin^2\alpha + \cos^2\phi \cos^2\alpha\}$, it follows that.

$$t^2 = t_0^2 + \frac{x^2 \sin^2\alpha}{v_{rms}^2} + \frac{x^2 \cos^2\alpha}{v_\phi^2} \quad (10.1.16)$$

where $v_\phi = \frac{v_{rms}}{\cos\phi}$ is the NMO velocity along the true dip direction. Thus, the residual NMO is given by (Zai-tian, 1988)

$$\begin{aligned} \delta\Delta t &= \frac{1}{2t_0} \left(\frac{1}{v_{rms}^2} - \frac{1}{v_\phi^2} \right) x^2 \sin^2\alpha + \frac{1}{2t_0} \left(\frac{1}{v_\phi^2} - \frac{1}{v_{rms}^2} \right) x^2 \cos^2\alpha \\ &= M_k x^2 \sin^2\alpha + M'_k x^2 \cos^2\alpha = M_k x_s^2 + M'_k x_c^2 \end{aligned} \quad (10.1.17)$$

where v_{rms} and v_ϕ are the uncorrected velocities applied to NMO correction. It should be noted that $v_\phi = v_{rms}$ when $\phi = 0$ and if in addition $\alpha = 0$, we have that

$$\delta\Delta t = \frac{1}{2t_0} \left(\frac{1}{v_{rms}^2} - \frac{1}{v_{rms}^2} \right) x^2 = \hat{M}_k \quad (10.1.18)$$

so that eq. (10.1.12) simplifies to

$$T_{ijk} = S_i + R_j + N_k + \hat{M}_k x_{ij}^2 \quad (10.1.19)$$

which is equivalent to the expression for the linear survey problem.

In the general 3-D situation, S_i , R_j , N_k , M_k , M'_k and D_k are the sought parameters m , and eq.(10.1.12) is posed in the usual form

$$d = \bar{G}m$$

where the vector d contains the observed reflection times and \bar{G} is similar in form to that of the linear survey line (the elements are modified to account for the new structural effects). The problem can be solved as in the 2-D case using the LU or singular-value decomposition techniques. It should be noted, however, that the problem is undersconstrained and will require some problem regularization measures to stabilize the solution process. It is remarked that the typically large system of linear equations can be economically solved in an approximate manner using simple projection schemes.

10.1.4 Reduction of Line Intersection Errors in Network-type Surveys

Land, marine and airborne geophysical survey data may be in error due to a number of causes. In typical network-type surveys, navigational inaccuracies (including altitude differences between intersecting lines), instrumental bias and drift, and temporal effects arising from oceanographic, atmospheric and ionospheric phenomena may impart systematic and/or non-systematic bias on the field records. Consequently, the data recorded at coincident locations at different times in intersecting survey lines may show corresponding discrepancies dubbed crossover or intersection errors (or simply mis-ties). The magnitude of these mis-ties may vary greatly depending on the causative factors (e.g., navigational errors are often dependent on the quality of the navigation system used in the survey) and the desired level of accuracy in a survey may dictate what we consider to be a significant source of error. For example, diurnal drift may be considered the main source of error for a ± 1 gamma aeromagnetic survey, with good positional control using Doppler navigation (or section roads) and tracking camera for accurate path recovery while in high sensitivity ± 0.1 gamma survey, positional and diurnal drift errors become equally important (Yarger et al., 1978). For a reliable interpretation, we need to adjust the raw data sets by some unknown amount which may be determined using some *a priori* information such as base station measurements.

We are interested in crossover adjustment procedures without complimentary base station data. Traditionally, manual loop closure methods are applied in seismic, gravimetric, magnetic and geodetic surveying but this practice has now been widely replaced by automated error estimation schemes. We will look at the building blocks of this mathematical approach and for a better overall understanding of the undergirding principles, we will try and blend the problems of network adjustment in magnetic, gravimetric and geodetic surveying using a specific case. It is easy to extend the developments once the procedure is understood and it is therefore instructive to start with a simple problem.

Consider a small survey network consisting of four approximately north-south (N) traverses and three approximately east-west (E) tie-lines (Fig. 10.1.11). In effect, we have seven lines ($p=7$) and twelve intersections (i.e., $n=12$). At the i^{th} intersection, there are two observations, r_{N_i} and r_{E_i} ; but the actual value of the sought physical quantity at that point may be different from both observations. Note that these

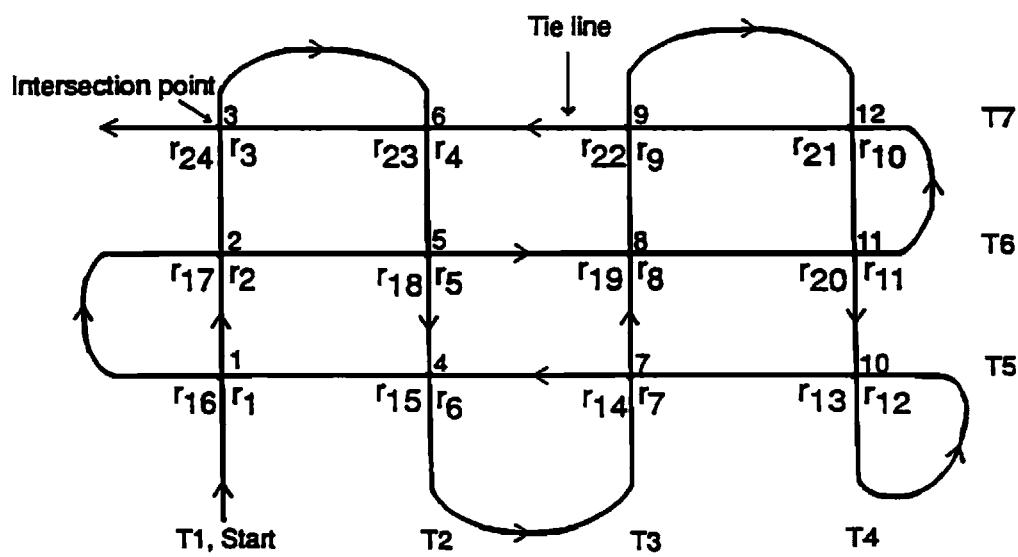


Fig. 10.1.11 Sample survey plan. T1 to T7 are the tracklines and r_1 to r_{24} represent the readings at different times at the twelve (1 to 12) points of intersection

readings could be gravity or magnetic field data or in the case of satellite altimetry, the distance from the satellite to the earth's surface directly below.

If we are dealing with altimeter data, the problem is straightforward. The measured values of the satellite-to-earth distance r are known; the height h , of the satellite (above a reference datum) is generally constant along an orbit but its exact value is unknown. The ground's elevation at any location is given by $(h - r)$ and may assume different values for different tracks. The discrepancy in elevation estimates at a line intersection is given by (see Menke, 1984)

$$e_i = (h_N - r_N)_i - (h_E - r_E)_i$$

which, with the order of the terms changed, leads to

$$e_i = (h_N - h_E)_i - (r_N - r_E)_i \quad (10.1.20)$$

Now, since the quantity h_i is our desired parameter at a particular point, and the crossover observation is given by $d_i = (r_N - r_E)_i$, we may rewrite eq.(10.1.20) as

$$e_i = \delta_{ij}h_j - d_i \quad (10.1.21)$$

which is in the familiar form $e = Gm - d$.

For conventional airborne potential field measurements, the problem is somewhat similar but can be formulated differently depending on the task at hand. In general, an important objective of magnetic, gravimetric and indeed other geophysical surveys is the determination of accurate field values at the observational stations. The height of the aircraft is usually fairly constant as in satellite altimetry but usually known while the exact value of the desired physical field F is unknown. The mis-tie between track k when it intersects track l , say, is simply $d = (r_N - r_E)$ and the sought line adjustment coefficients are obtained from the least squares problem $Gm = d$ where, as for the satellite altimetry problem, and for the sample 7-line survey network (Fig. 10.1.11), the coefficient matrix and the discrepancy vector are given by

$$G = \begin{bmatrix} 1 & & -1 & & & & \\ 1 & & & -1 & & & \\ 1 & & & & -1 & & \\ & 1 & & -1 & & & \\ & 1 & & & -1 & & \\ & & 1 & & -1 & & \\ & & 1 & & & -1 & \\ & & & 1 & & -1 & \\ & & & & 1 & & -1 \\ & & & & & 1 & \\ & & & & & & -1 \end{bmatrix} \quad \text{and } d = \begin{bmatrix} r_1 - r_{16} \\ r_2 - r_{17} \\ r_3 - r_{24} \\ r_6 - r_{15} \\ r_5 - r_{18} \\ r_4 - r_{23} \\ r_7 - r_{14} \\ r_8 - r_{19} \\ r_9 - r_{22} \\ r_{12} - r_{13} \\ r_{11} - r_{20} \\ r_{10} - r_{21} \end{bmatrix} \quad (10.1.22)$$

where only the non-zero entries of the 12×7 coefficient matrix are shown.

For small-size surveys such as the example adopted here, we may solve the problem using any of the regularized matrix inversion solution techniques discussed in the previous chapters. The required quantities for calculating the solution are $G^T G$ and $G^T d$. For the case treated here, $G^T G$ is simply

$$G^T G = \begin{bmatrix} 3 & 0 & 0 & 0 & -1 & -1 & -1 \\ 0 & 3 & 0 & 0 & -1 & -1 & -1 \\ 0 & 0 & 3 & 0 & -1 & -1 & -1 \\ 0 & 0 & 0 & 3 & -1 & -1 & -1 \\ -1 & -1 & -1 & -1 & 4 & 0 & 0 \\ -1 & -1 & -1 & -1 & 0 & 4 & 0 \\ -1 & -1 & -1 & -1 & 0 & 0 & 4 \end{bmatrix}. \quad (10.1.23)$$

A few structural pointers can be gleaned from the above formulations. Notice that if the matrix G is augmented by a scaled version of itself (i.e., $\beta G \equiv \beta D$) and the discrepancy vector d is correspondingly augmented with zeros, we in effect end up with a smooth inversion formula.

$$m = [(WG)^T WG + \beta^2 H]^{-1} (WG)^T Wd \quad (10.1.24)$$

and, as in the refraction seismology experiment in Chapter 5, we could examine the trajectory of the solutions in β -space. The data weighting term W is introduced here for statistical considerations and is a flexible strategy for controlling the influence of a given observation on the final solution. Note that there are several forms of weighting. In magnetic surveys, for example, the data equations may be inversely weighted according to an estimate of the local field gradient using, say (see Ray, 1985)

$$W_{ij} = \left\{ \left(\frac{r_N}{t_N} \right)^2 + \left(\frac{r_E}{t_E} \right)^2 + 1 \right\}^{-\frac{1}{2}} \quad (10.1.25)$$

where the corresponding r and t represent the field readings and times at a given point of intersection.

It is obvious that the structure of the matrix G also allows the incorporation of *a priori* constraints in the solution process. For instance, a high quality line (or line segment) could be held fixed simply by adding the appropriate extra row of constraints onto G and appending the well estimated *a priori* data onto d as described in Chapter 5.

So far, we have concerned ourselves with the solution of small-size matrix equations. In typical large, finely gridded surveys, the dimensions of the matrix G may be of the order of 1000×1000 (or even greater) so that the application of simple matrix decomposition techniques in routine processing becomes an extremely difficult task using present-day computers. The usual approach uses iterative gradient-type solutions and the interested reader is referred to the easily digestible schemes described in Cloutier (1983) and Menke (1984) among others. However, it may be pointed out that matrix decomposition and inversion of large-size surveys is not an impossible task. An ingenuous manipulation of the matrix G may render the problem solvable in an efficient manner. It can be seen from eq. (10.1.22) that as more survey lines are added, the matrix G increases in size but maintains a consistent block-structure for its non-zero components (Ray, 1985), viz :

The small diagonal blocks are dense while the large block on the righthand-side is typically sparse. This structure can be exploited in the solution scheme. For example, the problem may be solved by direct application of block orthogonal decomposition using ridge regression (Ray, 1985).

While the above simplistic treatment will serve to cement the basic tools of track adjustment, it is remarked that in routine magnetic processing for example, the problem is set up to remove a bias from all the lines as above but with an additional goal of removing tilt from one of the traverses and one of the tie-lines. In this situation, there would be an additional column in G for each of the lines used for the tilt correction .

10.2 Layered-Earth Inversion of Reflection Seismograms

In this introduction to seismogram inversion, we shall restrict our discussion to cases in which the earth can be considered to consist of horizontal layers characterised by constant material properties (density ρ_j , velocity v_j and thickness h_j) as depicted in Figure 10.2.1. The ground is excited by some energy input derived from an explosive

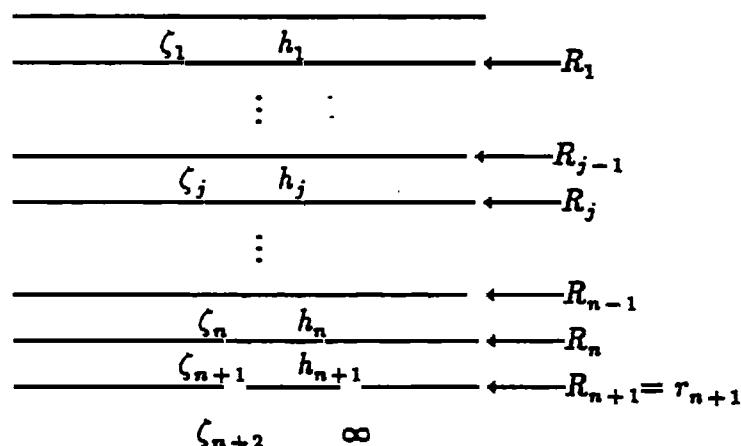


Fig. 10.2.1 An $(n+2)$ -layered Earth model. $\zeta_j = \rho_j v_j$ is the acoustic impedance of the j^{th} layer of velocity v_j , density ρ_j and thickness h_j .

source, say and part of this energy is reflected back towards the surface at each of the interfaces in the model. The signals can be observed at the surface or in boreholes as functions of time and spatial position. The reflection traveltime data recorded at an observation point constitutes a seismic trace. A typical seismogram consists of several seismic traces. We will look at two measurement geometries:

- (1) Horizontal source-receiver surface array configurations and
- (2) Surface-and-borehole source and receiver arrays.

10.2.1 Iterative Inversion of Normal Incidence Surface Seismic Traces

Consider the problem of recovering the acoustic impedance structure of the subsurface from normal incidence (or zero-offset) reflection seismograms recorded on the surface using horizontal source-receiver array configurations (e.g., Cooke and Schneider, 1983; Oldenburg et al., 1983). The subsurface is parameterized into discrete intervals of constant impedance. A common type of parameterization uses equispaced samples of the same dimension as the observed data. If we can simulate seismograms corresponding to any given distribution of acoustic impedances, then the above problem can be solved using inverse theory. There are many methods of solving such problems and the common tasks include the calculation of the forward solution and the matrix of partial derivatives (or gradients of the objective function) for linearized solution processes.

The forward problem

We shall adopt the familiar convolutional model for the forward process. Essentially, a layered-earth response function is convolved with a seismic source wavelet to simulate the filter and phase shift effects of the earth and recording system yielding

$$S(t) = R(t) * W(t) \quad (10.2.1)$$

where the $R(t)$ is the earth reflectivity function, $*$ is the convolutional operator and $W(t)$ is the source wavelet. Using the z-transform method, a recursive relation for the reflectivity function is given by (Cooke and Schneider, 1983)

$$R_j(Z) = \frac{(r_j + R_{j+1}Z)}{(1 + r_j R_{j+1}Z)}, \quad j = n, n-1, \dots, 2, 1 \quad (10.2.2)$$

where r_j is the pressure amplitude reflection coefficient at the boundary between layers j and $j+1$ (see Fig. 10.2.1) and is defined as

$$r_j = \frac{(\zeta_{j+1} - \zeta_j)}{(\zeta_{j+1} + \zeta_j)} \quad (10.2.3)$$

and the acoustic impedance ζ_j is the product of the density and velocity of the j^{th} layer. If we define $R_{n+1} = r_{n+1}$ and then apply the above recursive relations, we would obtain the reflectivity function $R(t)$ required in our convolutional model.

Formulating the inverse problem

We are interested in finding the acoustic impedance structure that will generate the

synthetic seismogram $S(t)$ that fits our field seismogram $\hat{S}(t)$ best in the least squares sense. That is, we want to minimize the residual

$$e = (\hat{S} - S)^T (\hat{S} - S) \quad (10.2.4)$$

subject to physical or geological constraints. This is a nonlinear problem in ζ and we therefore opt for an iterative linearized solution process.

To start with and for notational consistency, we note that eq.(10.2.1) may be written as

$$S = W * R = f(m)$$

so that the field records may be expressed simply as

$$\hat{S} = f(m) + e. \quad (10.2.5)$$

Expanding $f(m)$ about an initial models m^0 in Taylor series and neglecting high order terms as usual gives

$$f(m) = f(m^0) + \frac{\partial f(m^0)}{\partial m^0} (m - m^0)$$

or equivalently

$$\{f(m) - f(m^0)\} = \left\{ \frac{\partial f(m^0)}{\partial m^0} \right\} \{m - m^0\}$$

so that eq. (10.2.5) may be written in our familiar matrix notation as

$$y = Ax + e$$

where

$$A = W * \frac{\partial R^0}{\partial m^0}$$

and is obtained by differentiating equation (10.2.1) with respect to the chosen model parameterization (i.e., the acoustic impedance profile or the reflection coefficient series), and R^0 is the reflectivity function corresponding to the initial model parameters m^0 . Notice that the source wavelet W is independent of the layer sequence and is here convolved with another time series $\partial R^0 / \partial m^0$ in the same way as for the generation of

a synthetic seismogram. We may therefore develop a recurrence relation for calculating the partial derivatives A .

Computation of partial derivatives

If one is inverting a seismogram for ζ , we note from eqs. (10.2.1 to 10.2.3) that the reflectivity function R is a function of r which is in turn a function of ζ . Thus,

$$\frac{\partial R}{\partial \zeta} = \frac{\partial R}{\partial r} \cdot \frac{\partial r}{\partial \zeta} \quad (10.2.6)$$

where $\frac{\partial R}{\partial r} = \frac{(1 - (R_{j+1}Z)^2)}{(1 + r_j R_{j+1}Z)^2}$ and $\frac{\partial r}{\partial \zeta} = \frac{-2\zeta_{j+1}}{(\zeta_{j+1} + \zeta_j)^2}$.

Solving the inverse problem

In typical practical situations, we are required to solve matrix equations of large sizes. In the present formulation, it is the least squares normal equations

$$A^T A x = A^T y$$

that have to be solved for the parameter corrections x . Depending on the auxiliary constraints imposed on the solution process, we may use the constrained matrix-inversion techniques developed in the previous chapters or gradient-type algorithms.

Conjugate-gradient approach

Gradient-type schemes are attractive in that they do not require matrix decomposition or inversion. A standard conjugate-gradient least squares inversion algorithm is given below for illustration:

Step 1: Initialize parameter vector x and error vector e

set $x^0 = 0$

$$e_0 = (A^T A x^0 - A^T y)$$

$$d_0 = -e_0$$

define a fixed percentage (ϵ) of e_0 for use as a stopping criterion

$$\text{set } tol = \epsilon |e^0|$$

or Otherwise

Step 2: Iterate for best fit model, computing new A and y at each iteration

LOOP (for $i=1,n$)

get:

$$b_i = A^T A d_{i-1}$$

$$\Delta_i = \frac{|e_{i-1}|^2}{d_{i-1} b_i}$$

improve previous estimate in Δ -step and get new error

get:

$$x^i = x^{i-1} + \Delta_i d_{i-1}$$

$$e_i = e_{i-1} + \Delta_i b_i$$

convergence test

If $|e_i| < tol$, STOP

Else

$$\text{set } \mu_i = \frac{|e_i|^2}{|e_{i-1}|^2}$$

select new conjugate direction

$$\text{get } d_i = -e_i + \mu_i d_{i-1}$$

END LOOP

Note that a new Jacobian matrix A and discrepancy (or data misfit) vector y are required at each iteration in Step 2 of the above algorithm. In principle, the algorithm never diverges and the stopping criterion is therefore designed such that the iteration stops once the residuals have gone down to a predetermined tolerable value, tol .

10.2.2 Inversion of Vertical Seismic Profile (VSP) Data

The seismic wave field generated by a source fired at the surface (or a set of shots set off at varying offsets and azimuth to a well-head) can be recorded at different depths in a borehole (Fig. 10.2.2). It is also common to have surface receivers and borehole sources. We will adopt the surface-shot borehole-receiver arrangement in this discussion but bear in mind that the various arrays are generally termed Vertical Seismic Profiles. A major difference between VSP data and horizontal surface array data is that the wave field approaches the VSP receivers from above and below. It is customary to separate the upward and downward propagating wave fields (e.g., Seeman and Horowicz, 1983) and the inverse problem can therefore be easily tackled using any of the methods that hold good for the comparable surface array data. Recall that the inversion of horizontal surface array data suffers from nonuniqueness owing to an array of factors of which the

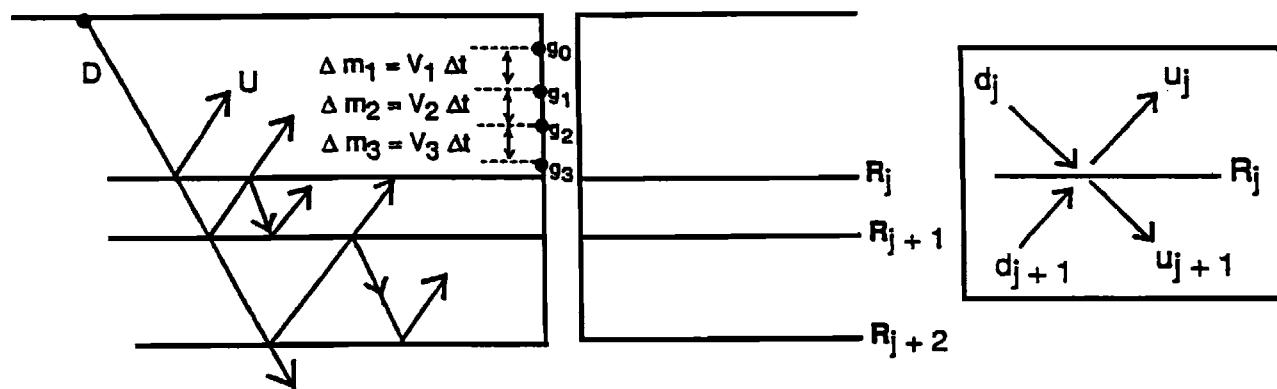


Fig. 10.2.2 A surface-source borehole-receiver array system

bandlimited nature of the data is most problematical. This problem is somewhat less in the VSP problem where we are provided with some useful constraints in the form of a good description of the downgoing wavelet and its amplitude relative to the upward propagating wavefield (Grivelet, 1985). Let us now examine some common applications of inverse theory in VSP data processing.

Posing the separation of upgoing and downgoing wave fields as an inverse problem

Consider the hypothetical situation illustrated in Fig. 10.2.2 where there are four receivers (g_0 to g_3) clamped against the wall of a borehole above a horizontal reflector (characterised by reflectivity R_1) and a shot is set off on the surface. For simplicity, let us assume that any changes in the shape of the source wavelet during propagation is negligible between the receiver positions and that the time delays Δt between any two contiguous receiver positions are the same. We can therefore express the recorded data at positions g_0 to g_3 as (see Hatton et al., 1986, p.153)

$$\begin{aligned} s_0(t) &= u_0(t) + d_0(t) \\ s_1(t) &= u_0(t-\Delta t) + d_0(t+\Delta t) \\ s_2(t) &= u_0(t-2\Delta t) + d_0(t+2\Delta t) \\ s_3(t) &= u_0(t-3\Delta t) + d_0(t+3\Delta t) \end{aligned} \tag{10.2.7}$$

where u_0 and d_0 are, respectively, the upward and downward propagating wave fields at the chosen reference level g_0 . It may be noted that in practical situations, we would have an extra term for additive noise in the righthand side of eq. (10.2.7).

It is instructive to obtain the relations for the various frequency components of the recorded signals. To do this, we simply express eq.(10.2.7) in the frequency domain. Thus, at any frequency, we have that

$$\begin{aligned} S_0(f) &= U_0(f) + D_0(f) \\ S_1(f) &= \exp(-i\omega\Delta t)U_0(f) + \exp(i\omega\Delta t)D_0(f) \\ S_2(f) &= \exp(-i\omega2\Delta t)U_0(f) + \exp(i\omega2\Delta t)D_0(f) \end{aligned}$$

$$S_3(f) = \exp(-i\omega 3\Delta t)U_0(f) + \exp(i\omega 3\Delta t)D_0(f) \quad (10.2.8)$$

which, in our familiar matrix form, is simply

$$\begin{bmatrix} S_0 \\ S_1 \\ S_2 \\ S_3 \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ e^{-i\omega\Delta t} & e^{i\omega\Delta t} \\ e^{-i\omega 2\Delta t} & e^{i\omega 2\Delta t} \\ e^{-i\omega 3\Delta t} & e^{i\omega 3\Delta t} \end{bmatrix} \begin{bmatrix} U_0 \\ D_0 \end{bmatrix}. \quad (10.2.9)$$

In general, eq.(10.2.9) is in the form $d = Gm$ where d contains the Fourier transforms of the data recorded at each receiver position and m is the solution for U_0 and D_0 for all frequency components. The solution to the above problem can be obtained using any of the standard inversion algorithms employing regularized G -matrix or solution simplicity measures. For example, using the ridge regression algorithm, we have that

$$m = [G_*^T G + \beta^2 I]^{-1} G_*^T d \quad (10.2.10)$$

where G_* is the complex conjugate of G . The desired time domain estimates of the upward and downward propagating wave fields (u_0 and d_0) are given by the inverse Fourier transform of m , i.e.,

$$\begin{bmatrix} u_0 \\ d_0 \end{bmatrix} = F^{-1} \begin{bmatrix} U_0 \\ D_0 \end{bmatrix} \quad (10.2.11)$$

where F^{-1} denotes the inverse Fourier transform.

Having separated the VSP wave field components, and assuming that the data have been subsequently corrected for spherical spreading, let us now proceed to show how useful structural information about the subsurface may be reconstructed from the upgoing waves.

Recovery of the acoustic impedance profile

Our model here consists of a stack of horizontal layers of equal two-way travel-time excited by compressional plane waves travelling at normal incidence, and the structure can be characterised as a time-series of reflection coefficients of acoustic impedances as for the comparable surface reflection problem. We want to find the model parameters

(impedances of reflection coefficients) that will generate a synthetic seismogram that matches our field records best in the least squares sense. As before, we would require to compute synthetic seismograms and their partial derivatives (or gradients). For the forward problem, we compute the upgoing and downgoing waves for an elementary surface (Fig. 10.2.2 top right inset) as (Grivelet, 1985)

$$u_j = -r_j d_j + (1 + r_j) u_{j+1}$$

and

$$d_{j+1} = (1 - r_j) d_j + r_j u_{j+1}. \quad (10.2.12)$$

Next, we obtain the impulse response sequence I as $I_j = u_j$ ($j=1,2,\dots,N$). The impulse response is then convolved with a wavelet W to yield the synthetic seismogram $S(t)$. Note that the actual observed downgoing wave field contains the direct pulse and the associated multiples generated above the recording level and can be transformed into a zero-phase wavelet by application of a wave-shaping filter (Grivelet, 1985). This wave-shaped downgoing wave may be used to approximate W yielding

$$S(t) = W(t) * I(t). \quad (10.2.13)$$

The inverse problem is then stated as: minimize $\sum |\hat{S} - S|^2$ subject to any given constraints where \hat{S} is the observed seismogram for the wave-shaped upgoing waves. The problem is nonlinear and can be solved using any of the standard generalized matrix inversion methods or gradient-type algorithms. The initial model for the iterative inversion may be obtained using, say, a recursive event detection algorithm (e.g., Grivelet 1985). Linearization will yield the expression

$$\mathbf{y} = \mathbf{Ax} + \mathbf{e}$$

where

$$\mathbf{A} = W(t) * \frac{\partial I^0}{\partial m_j} \quad (10.2.14)$$

and is obtained from eq.(10.2.12) for the chosen model parameterization (i.e., reflection coefficients r_j or acoustic impedances ζ_j), for example, we may write

$$\frac{\partial I}{\partial \zeta} = \frac{\partial I}{\partial r} \cdot \frac{\partial r}{\partial \zeta} \quad (10.2.15)$$

where $\frac{\partial I}{\partial r} = -d_j + u_{j+1}$ and $\frac{\partial r}{\partial \zeta} = \frac{-2\zeta_{j+1}}{(\zeta_{j+1} + \zeta_j)^2}$.

10.2.3 Limitations of Normal Incidence (Zero-Offset) Inversion

Note from eq.(10.2.3) that if one of the impedances is known, ζ_1 say, then one may construct an impedance profile by recursive inversion using the relation (see e.g., Lavergne and Willm, 1976)

$$\zeta_{j+1} = \zeta_j \frac{(1 + r_j)}{(1 - r_j)} \quad (10.2.16)$$

where it is assumed that the seismic trace is noise free and has been rid of the source wavelet, multiples and effects of spherical spreading, transmission losses and scaling. It is obvious that all these conditions are seldom met in routine data processing. The iterative inversion approach described above are thus more popular, but they have their drawbacks too. For example, the data are band-limited and the results are nonunique without the use of *a priori* information. The data suffer from the lack of low- and high-frequency information about the impedance structure. This can be seen simply by restating eq.(10.2.1) as (Oldenburg et al., 1983)

$$S(t) = F^{-1}[R(f), W(f)] \quad (10.2.17)$$

where F^{-1} is the inverse Fourier transform operator and $R(f)$ and $W(f)$ are the Fourier transforms of $R(t)$ and $W(t)$ respectively. It is obvious that the seismogram contains energy only at those frequencies where $R(f)$ and $W(f)$ are non-zero. Note that real data are band-limited in frequency only because of the measurement system; the function $S(t)$ is broadband but $W(t)$ is always band-limited so that $S(t)$ does not contain much information outside this bandwidth. It should be pointed out here that Oldenburg et al., (1983) developed methods for predicting the missing low- and high-frequency information from band-limited normal incidence reflection seismograms; in any case, this method does not hold good for very low frequencies since such frequencies (down to zero) are only present in moveout data (see McAulay, 1985).

It is a well known fact that the most desired parameter in seismic data processing is velocity. In normal incidence or post-stack inversion, unambiguous determination of separate layer velocities and densities is not possible because velocity and density arise only as a product in the reflection coefficient. Moreover, it is difficult to model the exact manner in which some of the observed undesirable features such as interbed multiples are stacked. The inversion of pre-stack data helps overcome such problems and will be introduced next.

10.2.4 Plane-Layer Inversion of Pre-stack Seismograms for Velocity and Density Profiles

In prestack or nonnormal incidence considerations, the traveltimes across a given layer depend upon the angles of the plane-wave components which are functions of the compressional and shear velocities in the layers but not of density. This means that velocities and densities may be determined separately for such problems. The landmark plane-layer point-source model of McAulay (1985) will be adopted in our discussion of seismogram inversion for velocity and/or density profiles. Essentially, a point-source is accounted for using a spherical expansion into plane waves; and an extension of the plane wave reflection response to the non-normal incidence situation and the incorporation of surface effects completes the formalism.

A radiating spherical wave from a point source can be expanded into a set of plane waves each reflected from the succession of horizontal layers (see Fig. 10.2.3),

$$U(r, \omega) = ik_0 \int_{\phi=0}^{\pi/2 - i\infty} R(\phi, \omega) J_0(k_0 r \sin\phi) \exp[i(h_s + h_r)k_0 \cos\phi] \sin\phi d\phi \quad (10.2.18)$$

where $R(\phi, \omega)$ is the reflection coefficient for a plane wave at frequency ω and striking the stack of layers at an angle ϕ from the vertical, $i = \sqrt{-1}$, $k_0 = \omega/v_0$ is the wave-number for the medium at the surface having a velocity v_0 , h_s and h_r are respectively the heights of the source and receiver above the topmost interface, and J_0 is the zero order Bessel function. For a known source of strength P , the response at a receiver located at a specific point in space is determined by summing the effects over all angles in the above equation and transforming from frequency to time domain. The layered-earth response function R is determined separately for each plane wave and each frequency component of the source field.

McAulay's algorithm for calculating R

The non-normal incidence reflection response R for the compressional wave case is considered here. For the j^{th} layer of density ρ_j and velocity v_j , the upward and downward components of the wave pressure are written in terms of that at the same position in an adjacent layer ($j+1$). From Fig. 10.2.4, we have that

$$D'_{j+1} = t_j D_j + \bar{c}_j U'_{j+1} \quad (10.2.19)$$

and

$$U_j = c_j D_j + \bar{t}_j U'_{j+1}. \quad (10.2.20)$$

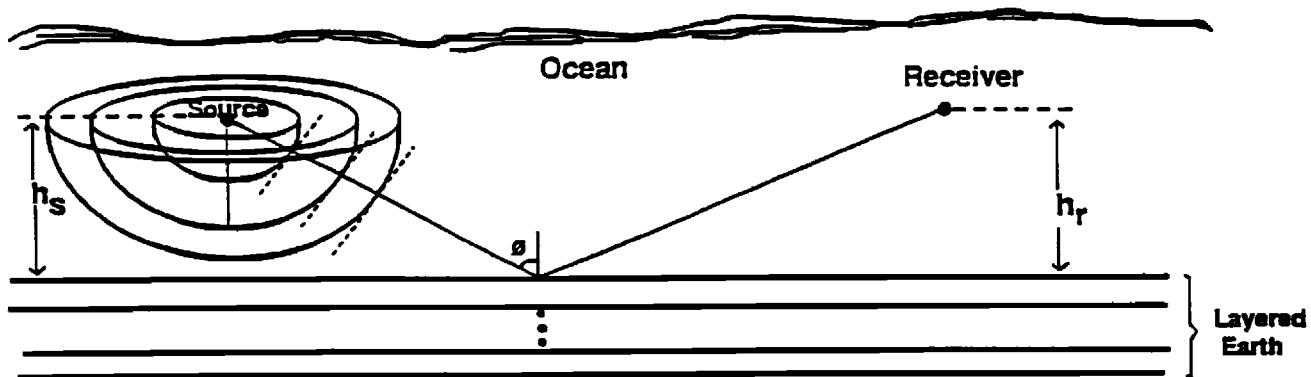


Fig. 10.2.3 Point source model for a horizontal structure with an ocean surface (after McAulay, 1985)

Now, from eq.(10.2.19),

$$D_j = \frac{1}{t_j}(D'_{j+1} - \bar{c}_j U'_{j+1}) = \frac{1}{t_j}(D'_{j+1} + c_j U'_{j+1})$$

which may be substituted into eq. (10.2.20) to yield

$$U_j = \frac{1}{t_j} \{c_j D'_{j+1} + U_{j+1}(t_j \bar{t}_j - c_j \bar{c}_j)\} = \frac{1}{t_j} \{c_j D'_{j+1} + U'_{j+1}\}$$

so that

$$\begin{bmatrix} U_j \\ D_j \end{bmatrix} = \frac{1}{t_j} \begin{bmatrix} 1 & c_j \\ c_j & 1 \end{bmatrix} \begin{bmatrix} U'_{j+1} \\ D'_{j+1} \end{bmatrix} \quad (10.2.21)$$

where $\bar{c}_j = -c_j$ and $t_j \bar{t}_j - c_j \bar{c}_j = 1$. The reflection coefficient c_j for a wave at non-normal incidence having approached the interface from the medium having impedance ζ_j is given by

$$c_j = \frac{\zeta_{j+1} - \zeta_j}{\zeta_{j+1} + \zeta_j} \quad (10.2.22)$$

where for the plane-wave whose direction is at an angle θ_j with respect to the vertical, the acoustic impedance is defined as

$$\zeta_j = \frac{\rho_j v_j}{\cos \theta_j} = \frac{\rho_j \omega}{p_j} \quad (10.2.23)$$

and the horizontal component of the wavefield in layer j is $k_j \cos \theta_j = \frac{\omega}{v_j} \cos \theta_j = p_j$. For computational ease, we may write the angle of the plane wave in each layer in terms of the vertical component of the wavenumber at the surface medium as

$$p_j = (k_j^2 - p_0^2)^{\frac{1}{2}}$$

whence

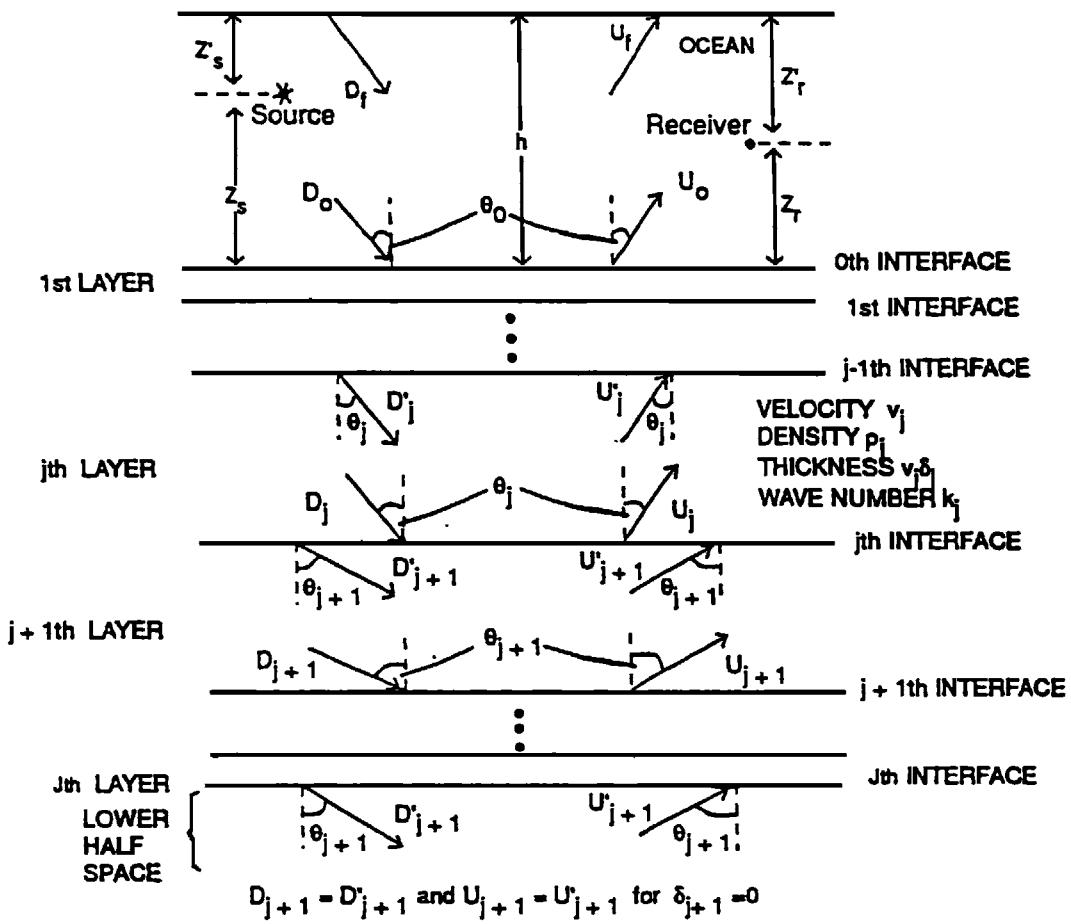
$$\zeta_j = \rho_j \left\{ \frac{1}{v_j^2} - \frac{p_0^2}{\omega^2} \right\}^{\frac{1}{2}}. \quad (10.2.24)$$

From the set-up in Fig. 10.2.4, the propagation from one layer onto another (across the j^{th} layer, say) assuming time dependence of the form $e^{i\omega t}$ is described by

$$D_j = D'_j \exp(i v_j \delta_j p_j)$$

and

$$U_j = U'_j \exp(-i v_j \delta_j p_j)$$



**Fig. 10.2.4 Set up for non-normal incidence reflection coefficient computations
(after McAulay, 1985)**

where δ_j is the normal incidence traveltime across the j^{th} layer. If we denote the phase delay across this layer by the exponential factor

$$E_j = \exp(2iv_j\delta_j p_j) = \exp(2i\delta_j[\omega^2 - p_0^2 v_j^2]^{\frac{1}{2}})$$

then we have that

$$\begin{bmatrix} U'_{j+1} \\ D'_{j+1} \end{bmatrix} = \begin{bmatrix} E_{j+1}^{\frac{1}{2}} & 0 \\ 0 & E_{j+1}^{-\frac{1}{2}} \end{bmatrix} \begin{bmatrix} U_{j+1} \\ D_{j+1} \end{bmatrix} \quad (10.2.25)$$

thus allowing us to rewrite eq. (10.2.21) as

$$\begin{bmatrix} U_j \\ D_j \end{bmatrix} = \frac{1}{t_j E_{j+1}^{1/2}} \begin{bmatrix} E_{j+1} & c_j \\ c_j E_{j+1} & 1 \end{bmatrix} \begin{bmatrix} U_{j+1} \\ D_{j+1} \end{bmatrix}. \quad (10.2.26)$$

Recursive application of equation (10.2.26) yields the relation between the upward and downward wave pressures just above the top interface U_0 and D_0 and those one layer thickness below the bottom interface, U_{J+1} and D_{J+1}

$$\begin{bmatrix} U_0 \\ D_0 \end{bmatrix} = \left\{ \prod_{j=0}^J q_j P_j \right\} \begin{bmatrix} U_{J+1} \\ D_{J+1} \end{bmatrix} = qW \begin{bmatrix} U_{J+1} \\ D_{J+1} \end{bmatrix} \quad (10.2.27)$$

where

$$q_j = \frac{1}{t_j E_{j+1}^{1/2}}, \quad P_j = \begin{bmatrix} E_{j+1} & c_j \\ c_j E_{j+1} & 1 \end{bmatrix} \quad \text{and} \quad W = \begin{bmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{bmatrix} = \prod_{j=0}^J P_j = P_0 P_1 \dots P_J.$$

It is obvious that P is a propagator matrix that facilitates the computation of upgoing and downgoing wave components just above the j^{th} layer (i.e., U_j and D_j) from those just above the $(j+1)$ -layer.

To obtain the reflection response R , we assume that no field enters into the stack of layers from the bottom half-space, i.e., $U_{J+1}=0$. Using this radiation condition, R is derived from eq.(10.2.27) simply as

$$R = \frac{U_0}{D_0} = \frac{w_{12}}{w_{22}}. \quad (10.2.28)$$

Where a body of water is present above the stack of layers (Fig. 10.2.3), the free surface is taken into account simply by adjusting the reflection coefficient R to this surface, thus

$$R_f = \frac{U_f}{D_f} = \frac{e^{ip_0 h} U_0}{e^{-ip_0 h} D_0} = e^{2ip_0 h} \cdot R \quad (10.2.29)$$

where $p_0 = k_0 \cos \theta_0$ and h is the thickness of the water column. For a shot fired in water at a depth h_s from this surface, the field received at a receiver position in the same medium at a depth h_r from the free surface is given by

$$R_r = \frac{R_f}{(1 + r_0 R_f)} \gamma \quad (10.2.30)$$

where

$$\gamma = e^{-2p_0 h_r} \left([1 - r_0 e^{2ip_0 h_r}] \cdot e^{ip_0 (h_r - h_s)} \{1 - r_0 e^{2ip_0 h_s}\} \right)$$

and we have neglected the direct wave and its surface reflection; the measure $[R_f/(1+r_0 R_f)]e^{-2p_0 h_r}$ is the response modified for the surface reverberation adjusted to the receiver and for a surface reflection coefficient of $-r_0$, $[1-r_0 e^{2ip_0 h_r}]$ is the receiver ghost and $e^{ip_0 (h_r - h_s)}\{1-r_0 e^{2ip_0 h_s}\}$ is the source ghost adjusted to the receiver depth. It may be noted that incorporating surface effects in the problem formulation allows us to accurately simulate some observed phenomena. For example, in practical situations the reflection energy arriving at the surface is reflected into the body of water because of the high reflectivity at the water-air interface; this energy may bounce back and forth between the surface and the solid substratum on which the water rests generating severe multiples. The algorithm described above effectively simulates primaries, interbed multiples, surface multiples, ghosts, lateral waves (refractions) and combinations of the waves.

Computation of partial derivatives of R

The partial derivatives of R with respect to the model parameters, m (i.e., velocities, v_j and densities, ρ_j), can be derived from eqs. (10.2.28 - 10.2.30) for the appropriate experimental set-up. Using eq. (10.2.28), we have (see McAulay, 1985)

$$\frac{\partial R}{\partial m_j} = \frac{w_{22}(\partial w_{12}/\partial m_j) - w_{12}(\partial w_{22}/\partial m_j)}{w_{22}}. \quad (10.2.31)$$

If the surface effects are taken into account, then we need the partial derivatives

$$\frac{\partial R_r}{\partial m_j} = \frac{\gamma \{(1 + r_0 R_f)(\partial R_f / \partial m_j) - r_0 R_f (\partial R_f / \partial m_j)\}}{(1 + r_0 R_f)^2} = \frac{\gamma}{(1+r_0 R_f)^2} \cdot \frac{\partial R_f}{\partial m_j} \quad (10.2.32)$$

where

$$\frac{\partial R_f}{\partial m_j} = \exp(2ip_0h) \frac{\partial R}{\partial m_j}$$

and $p_0 = k_0 = \frac{\omega}{v_0}$.

To complete the computation of partial derivatives, we need the function $\frac{\partial R}{\partial m_j}$ and this requires the evaluation of $\frac{\partial W}{\partial m_j}$ or simply $\frac{\partial W}{\partial v_j}$ and $\frac{\partial W}{\partial \rho_j}$.

Recall that we defined the propagator matrix P_j as a function of E_{j+1} and c_j so that P_{j-1} is a function of E_j and c_{j-1} . Therefore, depending on the model parameter being considered, P_j and P_{j-1} are both functions of m . In general, we write

$$\frac{\partial W}{\partial m_j} = \prod_{k=0}^{j-1} P_k \left(\frac{\partial P_j}{\partial m_j} \right) \prod_{k=j+1}^J P_k + \prod_{k=0}^{j-2} P_k \frac{\partial P_{j-1}}{\partial m_j} \prod_{k=j}^J P_k. \quad (10.2.33)$$

Now

$$\frac{\partial P_j}{\partial m_j} = \left\{ \frac{\partial P_j}{\partial E_{j+1}} \cdot \frac{\partial E_{j+1}}{\partial m_j} \right\} + \frac{\partial P_j}{\partial c_j} \cdot \frac{\partial c_j}{\partial m_j} \quad (10.2.34)$$

and

$$\frac{\partial P_{j-1}}{\partial m_j} = \left\{ \frac{\partial P_{j-1}}{\partial E_j} \cdot \frac{\partial E_j}{\partial m_j} \right\} + \frac{\partial P_{j-1}}{\partial c_{j-1}} \cdot \frac{\partial c_{j-1}}{\partial m_j} \quad (10.2.35)$$

where

$$\frac{\partial P_j}{\partial c_j} = \begin{bmatrix} 0 & 1 \\ E_{j+1} & 0 \end{bmatrix}, \quad \frac{\partial P_{j-1}}{\partial E_j} = \begin{bmatrix} 1 & 0 \\ c_{j-1} & 0 \end{bmatrix} \text{ and } \frac{\partial P_{j-1}}{\partial c_{j-1}} = \begin{bmatrix} 0 & 1 \\ E_j & 0 \end{bmatrix}.$$

For the velocity parameter, we have from eq. (10.2.34) that

$$\frac{\partial P_j}{\partial v_j} = \frac{\partial P_j}{\partial c_j} \cdot \frac{\partial c_j}{\partial v_j}$$

$$\text{since } \frac{\partial E_{j+1}}{\partial v_j} = 0 \text{ and } \frac{\partial c_j}{\partial v_j} = \frac{-2\zeta_{j+1}\zeta_j}{(\zeta_{j+1} + \zeta_j)^2} \cdot \frac{\omega^2}{p_j^2 v_j^3};$$

and for eq. (10.2.35), we have

$$\frac{\partial E_j}{\partial v_j} = \frac{-2i\delta E_j p_j^2}{p_j} \text{ and } \frac{\partial c_{j-1}}{\partial v_j} = \frac{2\zeta_{j-1}\zeta_j}{(\zeta_{j-1} + \zeta_j)^2} \cdot \frac{\omega^2}{p_j^2 v_j^3}$$

so that

$$\begin{aligned} \frac{\partial W}{\partial v_j} = & \prod_{k=0}^{j-1} P_k \left\{ \begin{bmatrix} 0 & 1 \\ E_{j+1} & 0 \end{bmatrix} \frac{-2\zeta_{j+1}\zeta_j}{(\zeta_{j+1} + \zeta_j)^2} \cdot \frac{\omega^2}{p_j^2 v_j^3} \right\} \prod_{k=j+1}^J P_k \\ & + \prod_{k=0}^{j-2} P_k \left\{ \begin{bmatrix} 1 & 0 \\ c_{j-1} & 0 \end{bmatrix} \left(\frac{-2i\delta E_j p_j^2}{p_j} \right) + \begin{bmatrix} 0 & 1 \\ E_j & 0 \end{bmatrix} \left(\frac{2\zeta_{j-1}\zeta_j}{(\zeta_{j-1} + \zeta_j)^2} \cdot \frac{\omega^2}{p_j^2 v_j^3} \right) \right\} \prod_{k=j}^J P_k. \end{aligned}$$

Similarly, for the density parameter, we have that

$$\frac{\partial P_j}{\partial \rho_j} = \frac{\partial P_j}{\partial c_j} \cdot \frac{\partial c_j}{\partial \rho_j}$$

where

$$\frac{\partial c_j}{\partial \rho_j} = \frac{-2\zeta_{j+1}\omega}{(\zeta_{j+1} + \zeta_j)^2 p_j}$$

and

$$\frac{\partial P_{j-1}}{\partial \rho_j} = \frac{\partial P_{j-1}}{\partial c_{j-1}} \cdot \frac{\partial c_{j-1}}{\partial \rho_j}$$

where

$$\frac{\partial c_{j-1}}{\partial \rho_j} = \frac{2\zeta_{j-1}\omega}{(\zeta_{j-1} + \zeta_j)^2 p_j}$$

giving

$$\begin{aligned} \frac{\partial W}{\partial \rho_j} = & \prod_{k=0}^{j-1} P_k \left\{ \begin{bmatrix} 0 & 1 \\ E_{j+1} & 0 \end{bmatrix} \frac{-2\zeta_{j+1}\zeta_j\omega}{(\zeta_{j+1} + \zeta_j)^2 p_j} \right\} \prod_{k=j+1}^J P_k \\ & + \prod_{k=0}^{j-2} P_k \left\{ \begin{bmatrix} 0 & 1 \\ E_j & 0 \end{bmatrix} \frac{2\zeta_{j-1}\omega}{(\zeta_{j-1} + \zeta_j)^2 p_j} \right\} \prod_{k=j}^J P_k. \end{aligned}$$

It may be noted that the matrix of partial derivatives is of dimension $n \times np$, i.e., number of observations by number of model parameters where in the frequency-wavenumber domain case the number of observations is equal to the number of frequencies times the number of horizontal wavenumbers or angles. The partial derivatives are computed during the forward evaluations resulting in considerable savings in computing costs. The inverse problem can be solved using any of the standard methods of iterative inversion but the conjugate-gradient method is commonly used (see Section 10.2.1).

10.3 Layered-Earth Inversion of Electromagnetic and Electrical Resistivity Soundings

Electromagnetic (EM) and electrical resistivity methods of geophysical exploration are widely used in mining, geothermal, petroleum, hydrogeological and geotechnical investigations as well as in geological mapping. The transient or time-domain electromagnetic (TEM or TDEM) and magnetotelluric (MT) methods are the most popular deep-probing EM methods. The observational data are typically presented in the form of apparent resistivity and/or TEM voltage decay or MT phase sounding curves. The Schlumberger and Wenner dc resistivity techniques are hugely popular electrical methods and the field recordings are in the form of apparent resistivity (or simply resistance) sounding curves. Data interpretation was traditionally carried out by curve matching, a practice now replaced by forward modelling on computers and automated inversion techniques. Let us now examine how such depth-sounding data may be inverted for subsurface resistivity structure.

10.3.1 The Inverse Problem

The inverse problem of EM or electrical depth sounding involves finding a model that fits the observed data best or within some preset conditions. The problem can therefore be formulated in a number of ways depending on the ultimate goal or type of constraining conditions imposed on the problem. In general, model construction involves minimizing the differences between our n values of observational data, d and those predicted via the nonlinear forward functional, $f(m)$ whilst satisfying any constraints imposed on the problem. The form of constraints depends on our informed expectations of the subsurface resistivity structure or the actual values of the sought model parameters derived from some other experiments at the same location, say. Thus, for example, if we expect that there are no sharp discontinuities in resistivity in the subsurface, then it may be wise to seek smooth models. If, on the other hand, we expect some distinct geoelectrical units in accord with geological wisdom, then it may be desirable to construct conventional layered (i.e., sparsely-parameterized) models. Also, a better picture of the subsurface may be obtained under certain circumstances by modelling a combination of different geophysical data sets. Along these lines, we may also elect to retain some prior estimates of the sought parameters in the final solution to our inverse problem. A practical construction algorithm should be flexible enough to accommodate most of the interpretational features highlighted above. It is also expected that the inverse solution process be numerically stable.

10.3.2 Linearizing Parameterizations

The goal of layered-earth inversion is to find an earth-type resistivity structure that will reproduce our field observations. The earth is parameterized into a succession of layers of resistivities, ρ_i and thicknesses, h_i . The quantities, ρ and h are the parameters of our Earth-model and may assume a wide range of values. It is well known that the apparent resistivities display a log-normal distribution and because a wide range of values are considered in typical inverse problems, their logarithms are used instead of the original data themselves. We also use the logarithms of ρ and h as the sought parameters. For the apparent resistivity data, we may also re-define the observational errors (e.g., Pedersen and Hermance, 1986; Meju, 1992) as

$$\epsilon_i = \log(d_i + \epsilon_i^0) - \log(d_i)$$

where ϵ_i^0 is the i^{th} observed standard deviations. It is also desirable to use logarithmic differences when calculating partial derivatives with a finite-difference scheme.

10.3.3 Forward Problems and Computational Considerations

To conduct a search for models that explain our field data, we need to be able to simulate the observable responses of hypothetical earth-models to inductive energizations or current excitations for a given measurement configuration. This is perhaps the most important task in data inversion and constitutes the forward problem. Thus, before implementing an inversion scheme, it is instructive to ascertain that there exists an efficient, stable numerical scheme for solving the EM layered-earth forward problem. For illustration, the inverse Laplace-transform method of Knight and Raiche (1982) and Raiche (1984) will be adopted for the TEM method and the algorithm given in Word, Smith and Bostick (1970) would be used for the MT forward problem. For the electrical resistivity simulations, we will use the linear filter method (Koefoed, 1970; Ghosh, 1971; Johansen, 1975). The relevant theories are summarized below.

10.3.3.1 The TEM Forward Problem

In the TEM forward problem, we attempt to simulate the ground's responses to inductive energization. One way of doing this is to calculate the mutual impedance, Z between the transmitter (Tx) and Receiver (Rx) loops, located on the ground's surface, as a function of measurement (or delay) times t . The Rx may be a small multi-turn coil

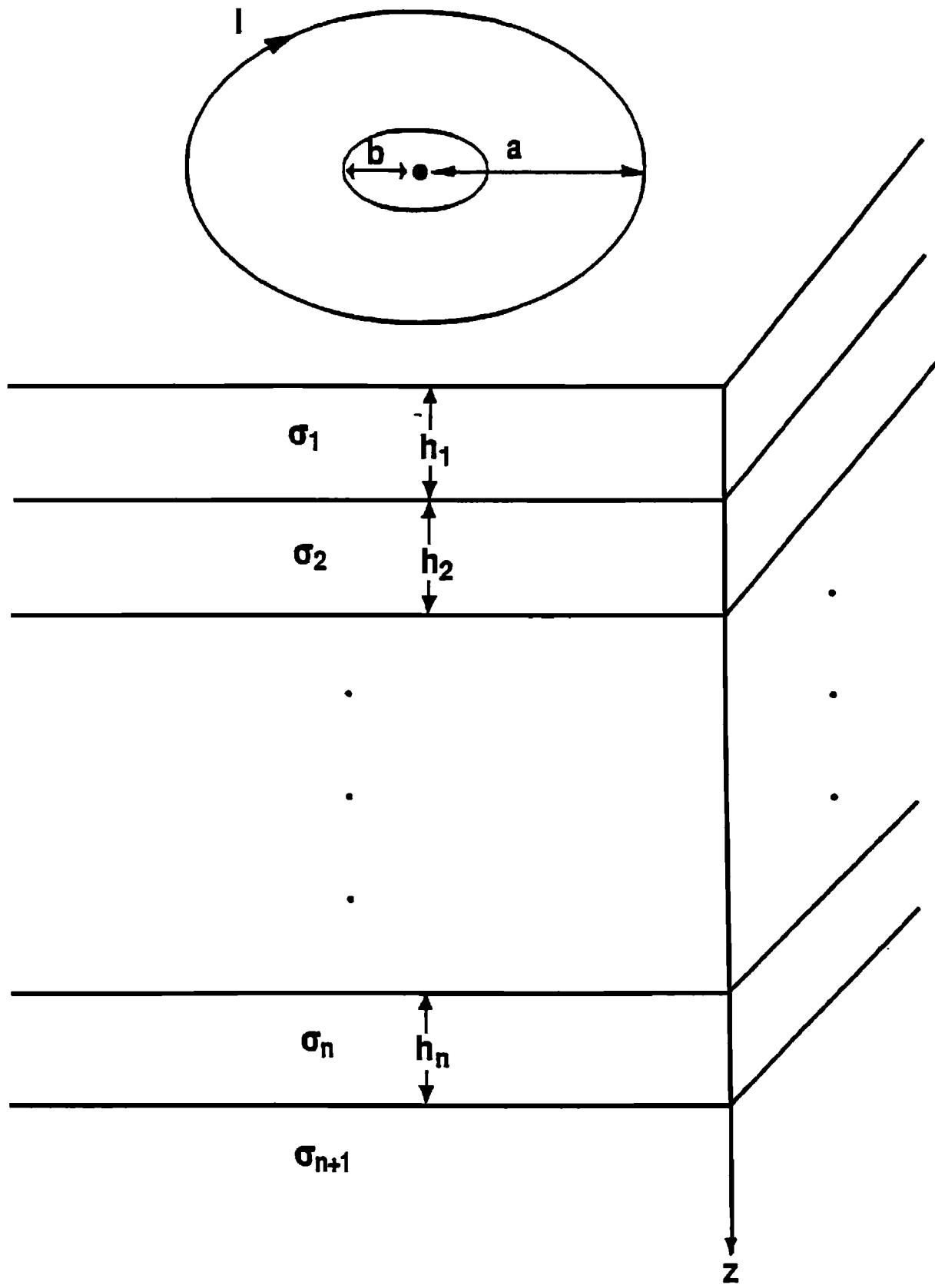


Fig. 10.3.1 TEM loops on layered-ground

placed at the centre of the Tx loop (an arrangement referred to as the central-loop or in-loop configuration) or the Tx can serve as the Rx during the transmitter-off time (the coincident-loop measurement configuration). In a layered-earth situation, for a Tx loop of radius a and Rx loop of radius b , (see Fig. 10.3.1) we have that (Knight and Raiche, 1982)

$$Z(t) = -\pi\mu ab \int_0^\infty L_p^{-1}\{I(p)pA_0(m, p, \lambda)\}J_1(\lambda a)J_1(\lambda b)d\lambda \quad (10.3.1)$$

where $A_0(m, p, \lambda)$ is the layered-earth impedance function, m represents the parameters of the Earth-model (i.e., resistivities ρ_j - or their reciprocals, conductivities σ_j - and thicknesses, h_j of the layers), p is the Laplace transform variable corresponding to $-i\omega$ where ω is the angular frequency, λ is the integration variable for the inverse Hankel transform, $I(p)$ represents the Laplace transform of the normalized current waveform and is equal to $-p^{-1}$ for step function turn-off, J_1 is the Bessel function of order 1, and L_p^{-1} is the inverse Laplace transform operator with respect to p ; $\mu = 4\pi \cdot 10^{-7}$ henries/m is the magnetic permeability of free-space and i is the imaginary unit.

Evaluation of eq.(10.3.1) can be facilitated using the Gaver-Stehfest method given in Raiche and Knight and the linear filter method. Note that the manner in which the current is switched off influences the TEM records and must be accounted for during data analysis. If we incorporate the effect of Tx turn-off time, t_0 in our calculations, then eq. (10.3.1) simplifies to (Raiche, 1984)

$$Z^{cn}(t) = \frac{\pi\mu a}{2t_0} \cdot \frac{A_R}{A_T} \int_0^\infty G(\xi^2\tau, m)J_1(\xi)\xi d\xi \quad (10.3.2)$$

for the central-loop configuration, and

$$Z^{cd}(t) = \frac{\pi\mu a}{t_0} \int_0^\infty G(\xi^2\tau, m)J_1^2(\xi)d\xi \quad (10.3.3)$$

for the coincident-loop configuration. In equations (10.3.2) and (10.3.3), we have that

$$G(\xi^2\tau, m) = F(\xi^2\tau') - F(\xi^2\tau)$$

where $F(\xi^2\tau) = -L_p^{-1} \left| \frac{A_0(p)}{p} \right|$, t_0 is the ramp (turn-off time), A_R is the effective area of the Rx loop, A_T is the area of the Tx loop, and the normalized times τ and τ' are given by

$\tau' = \frac{(t-t_0)}{\sigma\mu a^2}$, $\tau = \frac{t}{\sigma\mu a^2}$ for the SIROTEM-type systems and

$\tau' = \frac{t}{\sigma\mu a^2}$, $\tau = \frac{(t+t_0)}{\sigma\mu a^2}$ for the Geonics EM37-type systems.

and $\sigma=\sigma_1$ in the layered-earth case. Digital filters (e.g., Anderson, 1979) may be used to perform the inverse Hankel transforms. Note that equation (10.3.3) may be re-written with a different kernel as

$$Z^{cd}(t) = \frac{\pi\mu a}{t_0} \int_0^\infty \{G(\xi^2\tau, m)J_1(\xi)\}J_1(\xi)d\xi \quad (10.3.4)$$

to effect the numerical integration with Anderson's (1979) digital filters. The kernel (in curly brackets) will thus require the evaluation of the J_1 Bessel function.

Algorithm for calculating A_0

The layered-earth impedance function, A_0 is found by a back-substitution process (see Knight and Raiche, 1982; Raiche, 1984). For a structure with n layers above a uniform half-space of conductivity σ_{n+1} (Fig. 10.3.1), the reflection coefficient at the interface between layer j of conductivity σ_j and layer $j+1$ of conductivity σ_{j+1} is

$$R_j = \frac{s_j - s_{j+1}}{s_j + s_{j+1}} \quad (10.3.5)$$

where $s_j = (\lambda^2 - i\omega\mu\sigma_j)^{1/2}$. Defining the exponential factor $E_j = \exp(-2s_j h_j)$ and working up from the bottom of the sequence of layers, we calculate

$$F_{n+1} = 0 \quad (10.3.6)$$

for the basal half-space,

$$F_n = R_n E_n \quad (10.3.7)$$

for the overlying layer n , and

$$F_j = E_j \frac{(R_j + F_{j+1})}{(1 + R_j F_{j+1})} \quad (10.3.8)$$

for any layer j ($0 < j < n$) on top of layer n .

Using this recursive relation, the function A_0 is simply

$$A_0 = \frac{(R_0 + F_1)}{(1 + R_0 F_1)}. \quad (10.3.9)$$

Ramp function apparent resistivity approximations

For modelling purposes it is customary to define an apparent resistivity (reciprocal of apparent conductivity) for which no simple expression exists and may change with measurement time. The asymptotic expressions for the step function apparent resistivity as $t \rightarrow 0$ (the so-called early time) and as $t \rightarrow \infty$ (late time) are respectively (Spies and Eggers, 1986)

$$\rho_a^{\text{early}} = \frac{a^3 v}{3 \mathcal{A}_R I} \quad \text{and} \quad \rho_a^{\text{late}} = \frac{I^{2/3} a^{4/3} \mathcal{A}_R^{2/3} \mu^{5/3}}{20^{2/3} \pi^{1/3} t^{5/2} v^{2/3}}$$

where v is the voltage at the Rx coil, I is the Tx current and the other symbols have their usual meanings.

Following Raiche (1984), the ramp-adjusted apparent resistivity can be approximated from the modified expression for Z which, for the coincident-loop geometry, is

$$Z_a^{cd}(t) = \frac{2\pi a \pi^{1/2} X^{3/2}}{t} \sum_{k=0}^{\infty} \frac{(-)^k (2k+2)! X^k}{k! (k+1)! (k+2)! (2k+5)} T_z(k) \quad (10.3.10)$$

where

$$T_z(k) = \frac{1}{t_0/t(k+3/2)} \left\{ \frac{1}{(1 - t_0/t)^{k+3/2}} - 1 \right\} \quad \text{and} \quad X = \frac{\sigma \mu a^2}{4t_0} .$$

For the central-loop geometry, we have that (e.g., Sandberg, 1988)

$$Z_a^{cn}(t) = \frac{(\pi \mu a)^{1/2}}{2t_0} \cdot \frac{\mathcal{A}_R}{\mathcal{A}_T} \sum_{k=0}^{\infty} \frac{(-)^k}{4^k k! (2k+3) (2k+5)} \left\{ \frac{1}{\tau'^{k+3/2}} - \frac{1}{\tau^{k+3/2}} \right\} . \quad (10.3.11)$$

Iterative procedures (e.g., Spies and Raiche, 1980; Sandberg 1988) are used to correct the approximations until the final value of the apparent resistivity is found. We will now show how to develop analytical expressions for the partial derivatives required in TEM data inversion.

Computation of partial derivatives of A_0

The partial derivatives required in the inversion processes can be calculated from equation (10.3.1). Examining this equation, it is obvious that the derivatives with respect to the model parameters, m will only involve the layered-earth function A_0 . Thus we require the derivatives, $\partial A_0 / \partial m_j$, which may be obtained by differentiating equation (10.3.9). As in the preceding section, a recursive relationship for these partial derivatives can be developed. Noting that m_j may be either σ_j or h_j , then for the j

layers on top of layer n resting on the basal half-space (Fig. 10.3.1), we may write

$$\frac{\partial A_0}{\partial m_j} = \frac{\partial A_0}{\partial F_1} \cdot \frac{\partial F_1}{\partial F_2} \cdot \frac{\partial F_2}{\partial F_3} \cdot \frac{\partial F_3}{\partial F_4} \cdots \frac{\partial F_{j-1}}{\partial F_j} \cdot \frac{\partial F_j}{\partial m_j}. \quad (10.3.12)$$

The first term on the right-hand side of equation (10.3.12) is obtained from the straightforward differentiation of eq. (10.3.9) as

$$\frac{\partial A_0}{\partial F_1} = \frac{(1 + R_0 F_1) - R_0(R_0 + F_1)}{(1 + R_0 F_1)^2} = \frac{(1 - R_0^2)}{(1 + R_0 F_1)^2}. \quad (10.3.13)$$

To obtain expressions for $\partial F_j/\partial m_j$ and $\partial F_j/\partial F_{j+1}$, we simply differentiate equation (10.3.8). First, let us find $\partial F_j/\partial \sigma_j$. Here F_j is of the functional form $F = W \frac{U}{D}$ where W, U, D and also F are functions of σ . We therefore use logarithmic differentiation. By this technique,

$$\frac{\partial F}{\partial \sigma} = F \left\{ \frac{1}{W} \frac{\partial W}{\partial \sigma_j} + \frac{1}{U} \frac{\partial U}{\partial \sigma_j} - \frac{1}{D} \frac{\partial D}{\partial \sigma_j} \right\}$$

so that

$$\begin{aligned} \frac{\partial F_j}{\partial \sigma_j} &= \frac{i\mu\omega}{s_j} F_j \left\{ h_j + \frac{[(s_j - s_{j+1}) - (s_j + s_{j+1})]}{2(R_j + F_{j+1})(s_j + s_{j+1})^2} - F_{j+1} \frac{[(s_j - s_{j+1}) - (s_j + s_{j+1})]}{2(1 + R_j F_{j+1})(s_j + s_{j+1})^2} \right\} \\ &= \frac{i\mu\omega}{s_j} F_j \left\{ h_j - \frac{s_{j+1}}{(R_j + F_{j+1})(s_j + s_{j+1})^2} + \frac{s_{j+1} F_{j+1}}{(1 + R_j F_{j+1})(s_j + s_{j+1})^2} \right\}. \end{aligned} \quad (10.3.14)$$

For $\partial F_j/\partial h_j$, we simply obtain

$$\frac{\partial F_j}{\partial h_j} = -2s_j F_j \quad (10.3.15)$$

and using the quotient rule in differentiation, we find that

$$\frac{\partial F_j}{\partial F_{j+1}} = \frac{(1 + R_j F_{j+1}) E_j - (R_j + F_{j+1}) E_j R_j}{(1 + R_j F_{j+1})^2} = \frac{(1 - R_j^2) E_j}{(1 + R_j F_{j+1})^2}. \quad (10.3.16)$$

Along similar lines, for layer n and the basal half-space, we have that

$$\frac{\partial A_0}{\partial m_k} = \frac{\partial A_0}{\partial F_1} \cdot \frac{\partial F_1}{\partial F_2} \cdot \frac{\partial F_2}{\partial F_3} \cdots \frac{\partial F_{n-1}}{\partial F_n} \cdot \frac{\partial F_n}{\partial m_k} \quad (10.3.17)$$

where m_k could be h_n , σ_n , or σ_{n+1} . Note that equation (10.3.17) uses the intermediate results obtained for $\partial A_0/\partial m_j$ above and we therefore require only $\partial F_n/\partial \sigma_n$,

$\partial F_n / \partial h_n$ and $\partial F_n / \partial \sigma_{n+1}$. These are respectively given by

$$\begin{aligned}\frac{\partial F_n}{\partial \sigma_n} &= \frac{i\omega\mu}{s_n} F_n \left\{ h_n - \frac{1}{2(s_n - s_{n+1})} + \frac{1}{2(s_n + s_{n+1})} \right\} \\ &= \frac{i\omega\mu}{s_n} F_n \left\{ h_n - \frac{s_{n+1}}{2(s_n^2 - s_{n+1}^2)} \right\} \quad (10.3.18)\end{aligned}$$

$$\frac{\partial F_n}{\partial h_n} = -2s_n F_n \quad (10.3.19)$$

and

$$\begin{aligned}\frac{\partial F_n}{\partial \sigma_{n+1}} &= E_n \left\{ \frac{(s_n + s_{n+1}) \cdot \frac{i\omega\mu}{2s_{n+1}} - (s_n - s_{n+1}) \cdot \frac{-i\omega\mu}{2s_{n+1}}}{(s_n + s_{n+1})^2} \right\} \\ &= \frac{2i\omega\mu E_n s_n}{(s_n^2 + s_{n+1}^2)^2} . \quad (10.3.20)\end{aligned}$$

The partial derivatives of the TEM response is simply determined by replacing A_0 in equation (10.3.1) with $\partial A_0 / \partial m$ given above. Note that since Anderson's filter weights (Anderson, 1979, eq.[5]) are independent of the layer-sequence, they can be used to evaluate these partial derivatives.

10.3.3.2 The MT Forward Problem

In the magnetotelluric situation, a well-known expression for computing the EM impedance measurable on the surface of an n -layered (homogeneous and isotropic) earth is (Word, Smith and Bostick, 1970).

$$Z_j = \frac{\gamma_j \cdot \frac{\gamma_j(1 - E_j) + Z_{j+1}(1 + E_j)}{\gamma_j(1 + E_j) + Z_{j+1}(1 - E_j)}}{\gamma_j} \quad (10.3.21)$$

where the induction parameter $\gamma_j = (i\omega\mu\sigma_j)^{\frac{1}{2}}$, the exponential factor $E_j = \exp(-2\gamma_j h_j)$ and for the terminating half-space $Z_n = (i\omega\mu\rho_n)^{\frac{1}{2}}$. For ease of discussion let us simplify this further. For the j^{th} layer of resistivity ρ_j and thickness h_j , define an intrinsic impedance $w_j = \frac{\gamma_j}{\sigma_j} = (i\omega\mu\rho_j)^{\frac{1}{2}}$ and the impedance at the top of this layer looking down as

$$Z_j = w_j \cdot \frac{1 - R_j E_j}{1 + R_j E_j} , \quad j=n-1, \dots, 1 \quad (10.3.22)$$

where the reflection coefficient R_j is given by

$$R_j = \frac{w_j - Z_{j+1}}{w_j + Z_{j+1}} \quad (10.3.23)$$

and $Z_n = w_n$. Recursive application of eq.(10.3.22) starting from the bottom ($j=n-1$) yields the impedance at the surface Z_1 for the desired range of measurement frequencies and these are complex values.

For modelling purposes, it is customary to define the Cagniard apparent resistivity

$$\rho_a = \frac{1}{\omega \mu} |Z_1|^2 \quad (10.3.24)$$

and phase of the impedance

$$\phi = \tan^{-1} \left\{ \frac{\text{Im}(Z_1)}{\text{Re}(Z_1)} \right\}. \quad (10.3.25)$$

Derivation of MT partial derivatives

Since the evaluation of the MT forward problem is almost a trivial problem on modern computers, for the uninitiated the partial derivatives required for inversion may be easily computed using a finite difference scheme (e.g., Meju, 1992). However, we will show how to derive the necessary analytical expressions for the partial derivatives.

First, it may be noted that one can invert the apparent resistivity or phase information either separately or jointly. We therefore require $\frac{\partial \rho_a}{\partial m_j}$ and $\frac{\partial \phi}{\partial m_j}$ where the model parameters m_j are the layer resistivities and thicknesses. Now, recall that ρ_a and ϕ are derived from complex values Z_1 ; we determine their partial derivatives as

$$\frac{\partial \rho_a}{\partial m_j} = \frac{\partial \rho_a}{\partial Z_1} \cdot \frac{\partial Z_1}{\partial m_j} = \frac{2}{\omega \mu} \left\{ \text{Re}[Z_1] \cdot \text{Re}\left[\frac{\partial Z_1}{\partial m_j}\right] + \text{Im}[Z_1] \cdot \text{Im}\left[\frac{\partial Z_1}{\partial m_j}\right] \right\} \quad (10.3.26)$$

and

$$\frac{\partial \phi}{\partial m_j} = \frac{\partial \phi}{\partial Z_1} \cdot \frac{\partial Z_1}{\partial m_j} = \frac{1}{|Z_1|^2} \left\{ \text{Re}[Z_1] \cdot \text{Im}\left[\frac{\partial Z_1}{\partial m_j}\right] - \text{Im}[Z_1] \cdot \text{Re}\left[\frac{\partial Z_1}{\partial m_j}\right] \right\} \quad (10.3.27)$$

or

$$\frac{\partial \phi}{\partial m_j} = \frac{Re(Z_1) \cdot Im(\frac{\partial Z_1}{\partial m_j}) - Im(Z_1) \cdot Re(\frac{\partial Z_1}{\partial m_j})}{(Re(Z_1))^2 + (Im(Z_1))^2}. \quad (10.3.28)$$

To evaluate the above expressions, we require the quantity $\left\{ \frac{\partial Z_1}{\partial m_j} \right\}$. As in the TEM problem, for $j = 1, \dots, n-1$, we may write

$$\frac{\partial Z_1}{\partial m_j} = \left\{ \frac{\partial Z_1}{\partial Z_2} \frac{\partial Z_2}{\partial Z_3} \dots \frac{\partial Z_{j-1}}{\partial Z_j} \right\} \frac{\partial Z_j}{\partial m_j}. \quad (10.3.29)$$

We can compute the quantities in curly brackets from eq.(10.3.22) as

$$\begin{aligned} \frac{\partial Z_j}{\partial Z_{j+1}} &= w_j \left\{ \frac{(1+R_j E_j)[E_j \cdot \frac{2w_j}{(w_j + Z_{j+1})^2}] - (1-R_j E_j)[E_j \cdot \frac{-2w_j}{(w_j + Z_{j+1})^2}]}{(1+R_j E_j)^2} \right\} \\ &= \frac{4w_j^2 E_j}{(w_j + Z_{j+1})^2 (1+R_j E_j)^2}. \end{aligned} \quad (10.3.30)$$

Now

$$\frac{\partial Z_1}{\partial h_j} = w_j \frac{\partial \left(\frac{1-R_j E_j}{1+R_j E_j} \right)}{\partial h_j} = w_j \left\{ \frac{(1+R_j E_j) \cdot \partial U / \partial h_j - (1-R_j E_j) \cdot \partial D / \partial h_j}{(1+R_j E_j)^2} \right\}$$

and

$$\frac{\partial U}{\partial h_j} = 2R_j \gamma_j E_j \text{ and } \frac{\partial D}{\partial h_j} = -2R_j \gamma_j E_j.$$

Therefore,

$$\frac{\partial Z_1}{\partial h_j} = \frac{4\gamma_j w_j E_j R_j}{(1+R_j E_j)^2}$$

or if we want the same denominator as in eq. (10.3.30) for computational ease

$$\frac{\partial Z_1}{\partial h_j} = \frac{4i\omega\mu E_j [w_j - Z_{j+1}] \{w_j + Z_{j+1}\}}{(1+R_j E_j)^2 [w_j + Z_{j+1}] \{w_j + Z_{j+1}\}} = \frac{4i\omega\mu E_j (w^2 - Z_{j+1}^2)}{(1+R_j E_j)^2 (w_j + Z_{j+1})^2}. \quad (10.3.31)$$

Next, find $\partial Z_1 / \partial \rho_j$ using eq. (10.3.22). Here Z_j is of the functional form $Z = W \frac{U}{D}$ where W, U, D and also Z are functions of ρ . We therefore use logarithmic differentiation.

By this technique,

$$\frac{\partial Z}{\partial \rho} = Z \left\{ \frac{1}{W} \frac{\partial W}{\partial \rho_j} + \frac{1}{U} \frac{\partial U}{\partial \rho_j} - \frac{1}{D} \frac{\partial D}{\partial \rho_j} \right\} \quad (10.3.32)$$

so that

$$\begin{aligned} \frac{\partial Z_j}{\partial \rho_j} &= Z_j \left\{ \frac{1}{w_j} \cdot \frac{\partial w_j}{\partial \rho_j} + \frac{1}{(1-R_j E_j)} \cdot \frac{\partial(1-R_j E_j)}{\partial \rho_j} - \frac{1}{(1+R_j E_j)} \cdot \frac{\partial(1+R_j E_j)}{\partial \rho_j} \right\} \\ &= i\omega\mu Z_j \left\{ \frac{1}{2w_j^2} - \left\{ \frac{h_j}{\gamma_j \rho_j^2} + \frac{2Z_{j+1}}{2w_j(w_j^2 - Z_{j+1}^2)} \right\} \left\{ \frac{2R_j E_j}{(1-R_j^2 E_j^2)} \right\} \right\} \end{aligned} \quad (10.3.33)$$

which simplifies further to

$$\begin{aligned} \frac{\partial Z_j}{\partial \rho_j} &= \frac{Z_j}{2\rho_j} - \frac{2i\omega\mu R_j E_j Z_j}{(1 - R_j^2 E_j^2) w_j} \left\{ \frac{h_j}{\rho_j} + \frac{Z_{j+1}}{(w_j^2 - Z_{j+1}^2)} \right\} \\ &= \frac{Z_j}{2\rho_j} - \frac{2i\omega\mu}{(1 + R_j E_j)^2 (w_j + Z_{j+1})^2} \left\{ \frac{h_j (w_j^2 - Z_{j+1}^2)}{\rho_j} + Z_{j+1} \right\}. \end{aligned} \quad (10.3.34)$$

For the terminating substratum, we have that

$$\frac{\partial \rho_a}{\partial \rho_n} = \left\{ \frac{\partial \rho_a}{\partial Z_1} \right\} \frac{\partial Z_1}{\partial \rho_n} \quad (10.3.35)$$

and

$$\frac{\partial \phi}{\partial \rho_n} = \left\{ \frac{\partial \phi}{\partial Z_1} \right\} \frac{\partial Z_1}{\partial \rho_n} \quad (10.3.36)$$

which are respectively similar to eqs. (10.3.26) and (10.3.27) with

$$\frac{\partial Z_1}{\partial \rho_n} = \left(\frac{\partial Z_1}{\partial Z_2} \frac{\partial Z_2}{\partial Z_3} \dots \frac{\partial Z_{n-2}}{\partial Z_{n-1}} \frac{\partial Z_{n-1}}{\partial Z_n} \right) \frac{\partial Z_n}{\partial \rho_n} \quad (10.3.37)$$

where the quantities in bracket are furnished by eq. (10.3.30) and

$$\frac{\partial Z_n}{\partial \rho_n} = \frac{i\omega\mu}{2w_n^{1/2}} = \frac{(i\omega\mu/\rho_n)^{1/2}}{2} = \frac{\gamma_n}{2}. \quad (10.3.38)$$

10.3.3.3 The Schlumberger Forward Problem

For the Schlumberger dc resistivity method, the layered-earth forward response is given by (Koefoed, 1970)

$$\rho_a(L) = L^2 \int_0^\infty T(\lambda) J_1(\lambda L) \lambda d\lambda \quad (10.3.39)$$

where L is half the current electrode spacing and the resistivity transform $T(\lambda)$ is calculated recursively. For an n -layered earth (Fig. 10.3.2), we start



Fig. 10.3.2 A layered-earth model for the dc Schlumberger problem.

from the bottom and obtain the resistivity transform at the top of the infinite substratum as $T_n = \rho_n$. For notational simplicity, let us define the exponential factor

$$E_i = \exp(-2h_i \lambda)$$

and the reflection coefficient

$$R_i = \frac{(\rho_i - \rho_{i+1})}{(\rho_i + \rho_{i+1})}.$$

For layer $n-1$ resting on this substratum, the transform is (Koefoed, 1970)

$$T_{n-1}(\lambda) = \rho_{n-1} \left(\frac{1 - R_{n-1} E_{n-1}}{1 + R_{n-1} E_{n-1}} \right). \quad (10.3.40)$$

For any other overlying layer j (i.e., $j = n-2, n-3, \dots, 2, 1$),

$$T_j(\lambda) = \frac{W_j + T_{j+1}(\lambda)}{1 + W_j T_{j+1}(\lambda)/\rho_j^2} \quad (10.3.41)$$

where

$$W_j = \rho_j \left(\frac{1 - E_j}{1 + E_j} \right).$$

The above recursive relation is used to calculate $T(\lambda) = T_1(\lambda)$ required in eq. (10.3.39). Eq. (10.3.39) is easily evaluated by convolution using digital filters (e.g., Ghosh, 1971; Johansen, 1975) on a computer. The problem is recast in the form

$$\rho_a = \sum_{k=k_{min}}^{k_{max}} T(\lambda) f_k \quad (10.3.42)$$

where the coefficients of a moving average filter are represented by f_k .

Partial derivatives for the Schlumberger problem

Using linear filters for evaluating eq. (10.3.39), the derivatives required for the inverse calculations may be obtained simultaneously as

$$\frac{\partial \rho_a}{\partial m_j} = \sum \frac{\partial T(\lambda_k)}{\partial m_j} f_k. \quad (10.3.43)$$

Now, for layers $j = n-2, n-3, \dots, 1$ we have that

$$\frac{\partial T}{\partial m_j} = \left\{ \frac{\partial T_1}{\partial T_2} \frac{\partial T_2}{\partial T_3} \dots \frac{\partial T_{j-1}}{\partial T_j} \right\} \frac{\partial T_j}{\partial m_j}. \quad (10.3.44)$$

From eq. (10.3.41) and using the quotient rule, we have that

$$\frac{\partial T_j}{\partial h_j} = \frac{((1 + W_j T_{j+1}/\rho_j^2) \cdot (\partial U / \partial h) - (W_j + T_{j+1}) \cdot (\partial V / \partial h))}{(1 + W_j T_{j+1}/\rho_j^2)^2} \quad (10.3.45)$$

where $\frac{\partial U}{\partial h} \equiv \frac{\partial W}{\partial h} = \frac{\partial W_j}{\partial E_j} \cdot \frac{\partial E_j}{\partial h_j}$, $\frac{\partial W_j}{\partial E_j} = \frac{-2}{(1 + E_j)^2}$ and $\frac{\partial E}{\partial h} = -2\lambda E_j$,

so that

$$\frac{\partial U}{\partial h} = \frac{4\lambda E_j \rho_j}{(1+E_j)^2}.$$

Following the same line of reasoning, we have that

$$\frac{\partial V}{\partial h} = \frac{T_{j+1}}{\rho_j^2} \cdot \frac{\partial U}{\partial h}$$

giving

$$\frac{\partial T_j}{\partial h_j} = \left\{ \frac{(1 - T_{j+1}^2/\rho_j^2)}{(1 + W_j T_{j+1}/\rho_j^2)^2} \right\} \cdot \frac{4\lambda\rho_j E_j}{(1+E_j)^2}. \quad (10.3.46)$$

Proceeding in a similar fashion, we have that

$$\frac{\partial T_j}{\partial T_{j+1}} = \frac{(1 - W_j^2/\rho_j^2)}{(1 + W_j T_{j+1}/\rho_j^2)^2}. \quad (10.3.47)$$

For $\partial T/\partial \rho$, we apply the method of logarithmic differentiation and obtain

$$\frac{\partial T_j}{\partial \rho_j} = \left\{ \frac{(1 - T_{j+1}^2/\rho_j^2)}{(1 + W_j T_{j+1}/\rho_j^2)^2} \right\} \cdot \frac{W_j}{\rho_j} + \frac{2(W_j + T_{j+1})W_j T_{j+1}}{(1 + W_j T_{j+1}/\rho_j^2)^2 \rho_j^3}. \quad (10.3.48)$$

As before, we may write for the terminating half-space

$$\frac{\partial T_1}{\partial \rho_n} = \left(\frac{\partial T_1}{\partial T_2} \frac{\partial T_2}{\partial T_3} \dots \frac{\partial T_{n-2}}{\partial T_{n-1}} \right) \cdot \left\{ \frac{\partial T_{n-1}}{\partial T_n} \right\} \frac{\partial T_n}{\partial \rho_n}$$

noting that $\frac{\partial T_n}{\partial \rho_n} = 1$ and $\frac{\partial T_{n-1}}{\partial T_n} = \frac{\partial T_{n-1}}{\partial \rho_n}$.

Thus, for the infinite substratum and the overlying layer, we obtain from eq. (10.3.40)

$$\frac{\partial T_{n-1}}{\partial \rho_{n-1}} = \frac{T_{n-1}}{\rho_{n-1}} - \frac{4R_{n-1}E_{n-1}\rho_{n-1}\rho_n}{(1 + R_{n-1}E_{n-1})^2(\rho_{n-1} + \rho_n)^2} \quad (10.3.49)$$

$$\frac{\partial T_{n-1}}{\partial h_{n-1}} = \frac{4\lambda R_{n-1}^2 E_{n-1} \rho_{n-1}^2}{(1 + R_{n-1}E_{n-1})^2} \quad (10.3.50)$$

and

$$\frac{\partial T_{n-1}}{\partial \rho_n} = \frac{4R_{n-1}E_{n-1}\rho_{n-1}^2}{(1 + R_{n-1}E_{n-1})^2(\rho_{n-1} + \rho_n)^2}. \quad (10.3.51)$$

10.3.3.4 The Wenner Problem

The Wenner arrangement is modelled by a similar set of equations to those given above for the Schlumberger configuration. The simple demonstration program for Wenner inversion WENINV given in the appendix contains the forward routine FWRD which uses the filter coefficients of Biwen and Barker (1994).

10.3.3.5 Approximate Partial Derivatives

In all the above forward problem descriptions, the expressions for computing the required first partial derivatives with respect to the model parameters were obtained analytically. In all cases, finite difference approximations may also be used. Note that if a finite difference approximation is used with the said linearizing parameterizations then the computational formula for the partial derivatives may be of the form

$$A_{ij} = \frac{\log(F_i(m_j + \delta)) - \log(F_i(m_j))}{\delta} \quad (10.3.52)$$

for the forward difference technique (e.g., Meju, 1992) or

$$A_{ij} = \frac{\log(F_i(m_j + \delta)) - \log(F_i(m_j - \delta))}{2\delta} \quad (10.3.53)$$

for the central difference technique. The former technique has been successfully applied to EM and DC resistivity inversion by ridge regression (see Meju, 1992) and is implemented in the simple demonstration program WENINV listed in Appendix B. The perturbation factor δ is determined empirically. In WENINV (and the MT program MTINV given in Meju, 1992), for example, a value of 0.03 is used and the perturbed model parameter is simply:

$$(m_j \pm \delta) = \text{antilog} (\log(m_j) \pm 0.03). \quad (10.3.54)$$

It may be pointed out here that the linearizing parameterizations described earlier demands that we use as derivatives for the apparent resistivities

$$A_{ij} = \frac{\partial \ln \rho_a}{\partial m_j} = \frac{1}{\rho_a} \frac{\partial \rho_a}{\partial m_j}. \quad (10.3.55)$$

10.3.4 Resistivity Model Construction Methods

For the resistivity inverse problem, we state the model construction problem as:

" Given a finite collection of inexact observational data, find a statistically acceptable model that explains the observational data and their associated uncertainties and satisfies any constraints imposed on the problem by physical considerations".

Since the forward functional is nonlinear with respect to the model parameters m , an iterative procedure must be used to solve the problem. For instance, in inversion with null priors or smoothness measures, the formal iterative formula is given as

$$m^{k+1} = m^k + [(WA)^T WA + \beta^2 H]^{-1} [(WA)^T Wy - \beta^2 m^k]$$

or

$$m^{k+1} = [(WA)^T WA + \beta^2 H]^{-1} (WA)^T \hat{d}_k \quad (10.3.56)$$

where $\hat{d}_k = (Wy + WAm^k)$. The partial derivatives $A_{ij} = \partial f(m^k)/\partial m_j$ are evaluated at m^k and the iteration is begun at $k=0$. The partial derivatives may be calculated analytically using the expressions derived above or by simple numerical finite differencing and the quantities on the right-hand side of eq. (10.3.56) are easily determined using the singular value decomposition method. The computational advantages accruing from such an approach are widely known. The above inversion method is flexible. For example, if we wish to interpret a combination of EM and electrical or some other complimentary data set (e.g., Vozoff and Jupp, 1975; Raiche et al., 1985), then we simply replace the matrix A and the vector y with the augmented analogues A_* and y_* which are of the form

$$A_* = \begin{bmatrix} A_1 \\ A_2 \end{bmatrix}; \quad y_* = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

where the subscripts 1 and 2 indicate the contributions from the separate but complimentary data sets to be jointly inverted. Note that more than two data sets can be combined and inverted simultaneously.

In generating smooth models, if we wish to retain known estimates of the sought parameters while smoothing the variations between the unknowns, then an alternative technique that has been found to be effective in practice is to partition the augmenting data for A and y in the form

$$\beta D = \beta \begin{bmatrix} \hat{I} \\ \hat{D} \end{bmatrix} = \beta \begin{bmatrix} 1 & 0 & \dots \\ \vdots & \ddots & \\ \dots & 0 & 1 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \dots & 0 & 1 & -1 & \\ & & & \ddots & \\ & & & & 0 & 1 & -1 \end{bmatrix}; \quad \beta h = \beta \begin{bmatrix} h_1 \\ h_l \\ \vdots \\ b_1 \\ \vdots \\ b_k \end{bmatrix}$$

and the applicable constraining equation is simply $Dm = h$ where \hat{I} is of dimension $l \times p$, \hat{D} is of dimension $(p-l-1) \times p$, $b_j = -\{\hat{D}m\}_j$; and $k = (p-l-1)$ and there are l known reliable estimates of m .

A common and very effective derivative regularization measure is to add a small biasing constant to the main diagonal of $(WA)^T WA$ giving the iterative formula (e.g., Meju, 1992) $m^{k+1} = m^k + [(WA)^T WA + \beta^2 I]^{-1} [(WA)^T Wy]$ which is the standardized version of the very popular ridge regression formula.

Useful additional stabilizing operations in the solution process

During parameter updating, some auxiliary physical constraints may come into play for added stability. It is recommended to employ the smoothness criterion of Jackson (1973) which ensures that the rms size of the parameter perturbations is not greater than unity. The smoothness criterion, sc is defined as

$$sc = [\frac{1}{p} \sum_{j=1}^p (x_j)^2]^{\frac{1}{2}} \leq 1 \quad (10.3.57)$$

where x_j are the calculated parameter corrections. For example, at each iteration any perturbation x_j greater than 1 is regarded as unsuccessful or physically unrealizable and may be multiplied by a factor (<1) that decreases the length without changing its direction. Thus, the formal estimation formula given by eq. (10.3.56) is replaced by the practical formula

$$m^{k+1} = m^k + sc \{ [(WA)^T WA + \beta^2 H]^{-1} [(WA)^T Wy - \beta^2 m^k] \} \quad (10.3.58)$$

where $0 < sc \leq 1$ is the *ad hoc* multiplication factor. Note that while this operation prevents the solution from wildly "over-shooting" the linear range, it does slow the convergence. Also for physical reasons, a commonly used constraint is that the model parameters, m are non-negative scalar functions.

It may also be desirable to scale each column of the matrix A by the root mean sum of

squares value of the coefficients as it can speed up the convergence of the iterative process (Marquardt, 1963). However, this should be done only when the elements of one row are markedly different from those in another row because of the round-off errors incurred during scaling (Meju, 1992). A simple routine for effecting this technique is listed in Fig. 10.3.3 and can be called at each iteration in an inversion program.

```

      subroutine SCALEJ(ncol,nrow,A,s)
c      scales the elements of each column of the matrix A by the
c      root mean sum of squares value of the coefficients, sj.
      real A(nrow,ncol), s(ncol)
c      effect the scaling procedure for every column of A
      do j=1,ncol
        sum=0.0
c      obtain the scaling factors, sj
        do i=1,nrow
          sum=sum + A(i,j)**2
        end do
        s(j)=sqrt(sum/float(nrow))
c      scale each element of the jth column by sj
        do i=1,nrow
          A(i,j)=A(i,j)/s(j)
        end do
      end do
      return
    end
  
```

Fig. 10.3.3 A simple routine for scaling the Jacobian matrix.

Note that the original matrix A is effectively transformed to a scaled version A^* . This scaled matrix is

$$A_{ij}^* = \frac{A_{ij}}{s_j} = C^{-1}A_{ij}$$

$$\text{where } s_j^2 = \frac{1}{n} \sum_{i=1}^n (A_{ij})^2$$

and the diagonal scaling matrix is of the form

$$C = \begin{bmatrix} s_1 & 0 & \dots & 0 \\ 0 & s_2 & 0 & \dots & 0 \\ \vdots & 0 & \ddots & \ddots & \vdots \\ 0 & \vdots & 0 & \ddots & 0 \\ 0 & 0 & \dots & 0 & s_p \end{bmatrix}.$$

Note that if a scaling operation is effected, then the resulting least squares solution must be de-scaled to obtain the actual parameter perturbations or direct estimates. Let $Z=WA$, where W is the weighting matrix of the observational errors defined previously. The damped least squares estimate of the scaled parameter change vector x_s (see eq. 10.3.56) is

$$\begin{aligned} x_s &= [(C^{-1}Z)^T(C^{-1}Z) + \beta^2 H]^{-1}(C^{-1}Z)^T(Wy) \\ &= C[Z^T Z + \beta^2 H]^{-1}Z^T(Wy) \\ &= Cx. \end{aligned}$$

Therefore, to obtain the actual parameter perturbations we have to rescale the resultant solution in the form $x = C^{-1}x_s$.

10.3.5 Model Appraisal

During model search, an acceptance criterion may be that the sum of squares of the error weighted residuals is less than $n + \sqrt{2n}$, (i.e., within one standard deviation of the mean of the associated random variable) (see Parker, 1982). The covariance information is calculated using the relevant expression derived previously. However, it may be necessary to control the rate of change (or the size) of the most squares solutions (e.g., Meju and Hutton, 1992; Meju, 1994d). For example, in extremization with null priors we could apply Jackson's smoothness criterion yielding the practical most squares formula

$$m_{ms}^{k+1} = m_{ms}^k + sc\{(WA)^T WA + \beta^2 I\}^{-1}\{(WA)^T Wy - \beta^2 m^k - \mu b\} \quad (10.3.59)$$

where the symbols are as previously defined.

10.3.6 Sample Applications in EM Data Interpretation

In the absence of *a priori* information, a useful strategy in the inversion of practical

1-D MODELS FOR SITE : IRS29

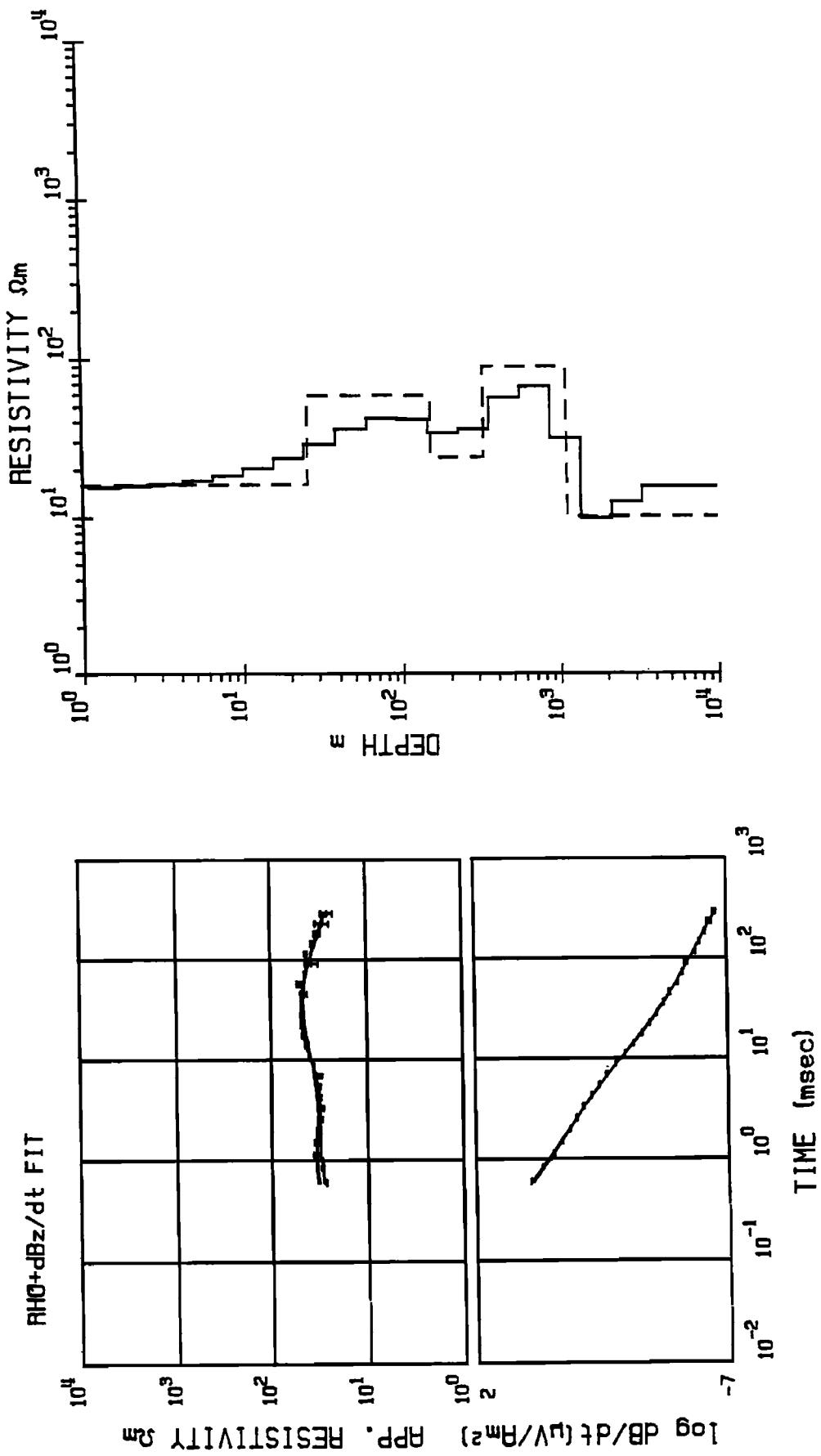


Fig. 10.3.4 Optimal smooth and rough models for TEM data

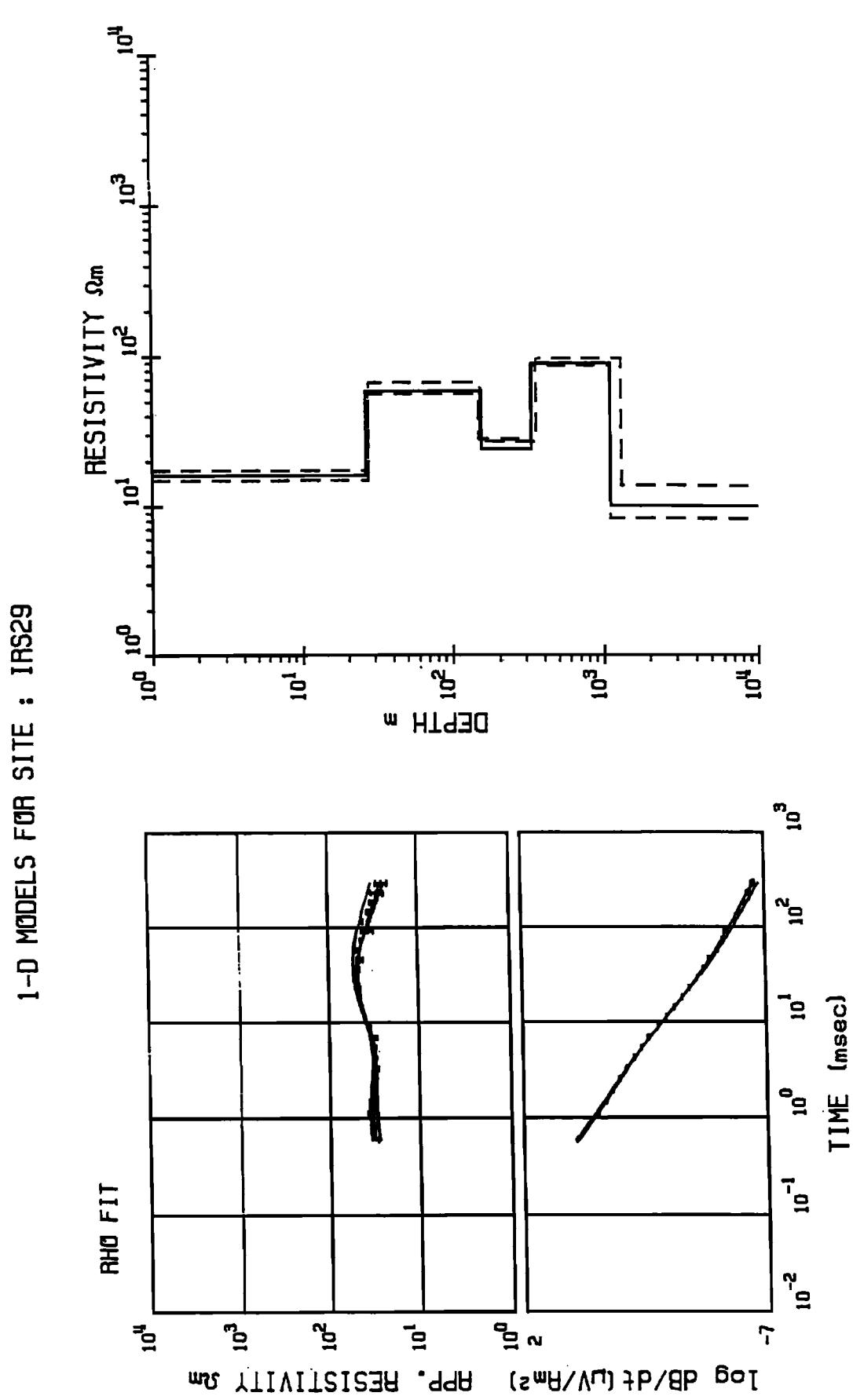


Fig. 10.3.5a Most-squares solution envelopes for TEM data

1-D MODELS FOR SITE : IRS29

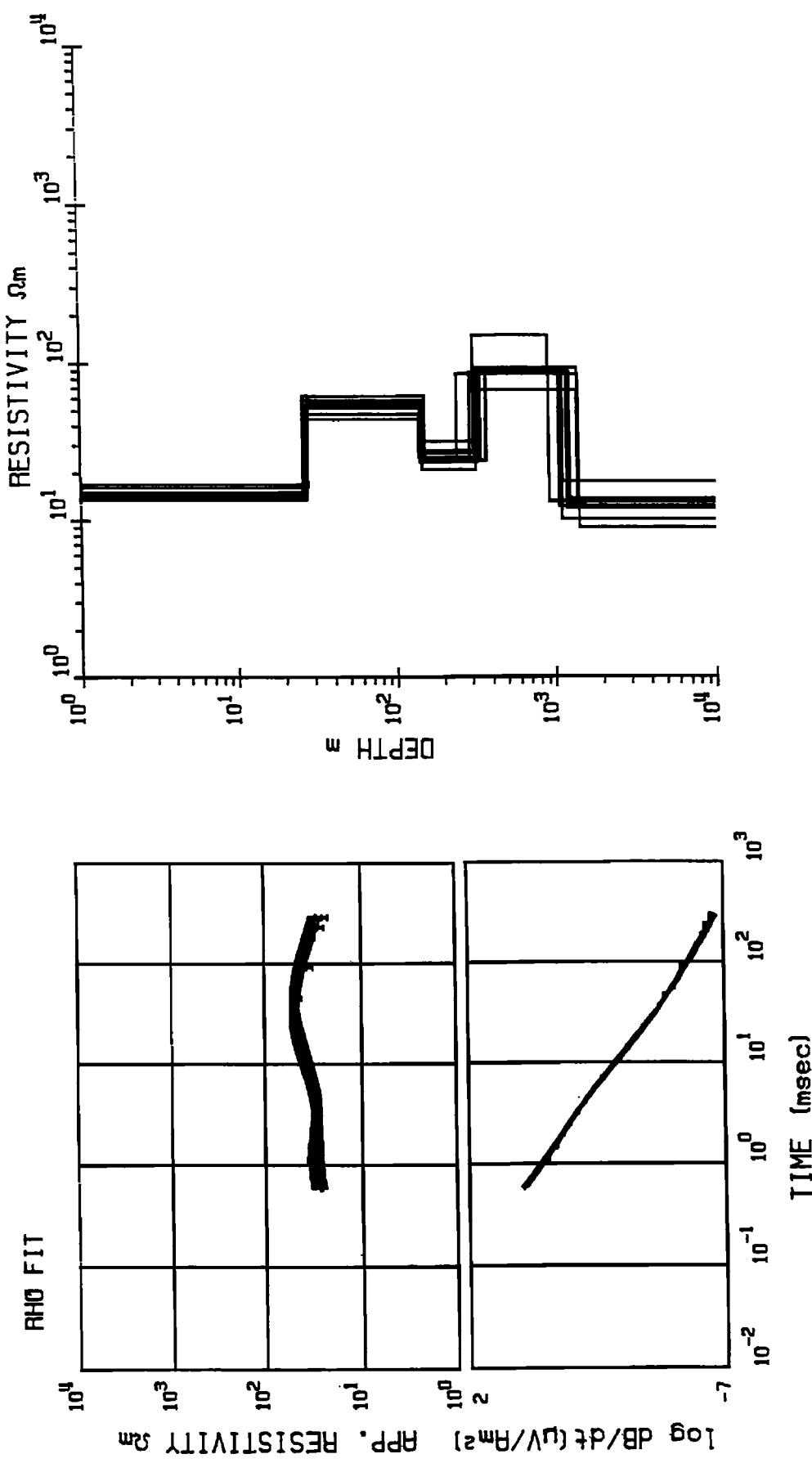


Fig. 10.3.5b Most-squares class of extreme models for TEM data

data may involve the construction of optimal smooth models using a featureless initial model (i.e., a half-space) which are then used to guide the search for acceptable simpler models. The underlying philosophy in this method of interpretation is that any significant features retained in the smooth model may be present in the subsurface and thus warrants further exploration using simpler parametric inversion procedures. The results of such an application of inverse theory are shown in Fig. 10.3.4 for TEM data. Notice the concordant features present in both kinds of subsurface models. Applications of the most squares appraisal scheme in the determination of the solution envelopes and the extreme class of models for the optimal least squares 5-layer model for the TEM data are shown respectively in Figs. 10.3.5a (broken lines) and 10.3.5b. It is obvious that the most-squares models adequately describe the field observations and their associated uncertainties as well as highlight the variability of model space.

10.3.6.1 Joint inversion of TEM and MT soundings

To demonstrate another aspect of EM inversion, we undertake a joint inversion of TEM and MT data recorded at the same station. The MT data are very similar in the two orthogonal measurement directions and of good quality (Meju et al., 1993) and one set of apparent resistivity and phase curves has been chosen for this exercise. The MT data are in accord with the TEM data – plotted at their equivalent frequencies (Meju, 1994f) – as shown in the lefthand panels of Fig. 10.3.6. Note that for each method, there are two interpretable data sets and any combination of data between the methods would suffice in a joint interpretation scheme. However, the optimal model shown in this figure was obtained by simultaneous inversion of all the available data (i.e., apparent resistivity, TEM voltage decay and MT phase curves). It is easy to show that inverting each individual EM data set would not yield a more detailed subsurface picture. In other words, we identify a better model by combining various geophysical observations (Gol'stman, 1976). The above combined data interpretation strategy holds good if there are no lateral changes in the earth's resistivity structure in the neighbourhood of the observational station. It is quite common to find the TEM and MT apparent resistivities in disagreement and this often suggests that there are lateral changes in the subsurface geology in the vicinity of the particular station and presents a different interpretation problem. So how can such discrepancies arising mainly from static distortion of MT data (analogous to static time shifts in reflection seismics) be resolved using inverse problem theory? We will look at a simple inversion strategy for dealing with problems of this kind next.

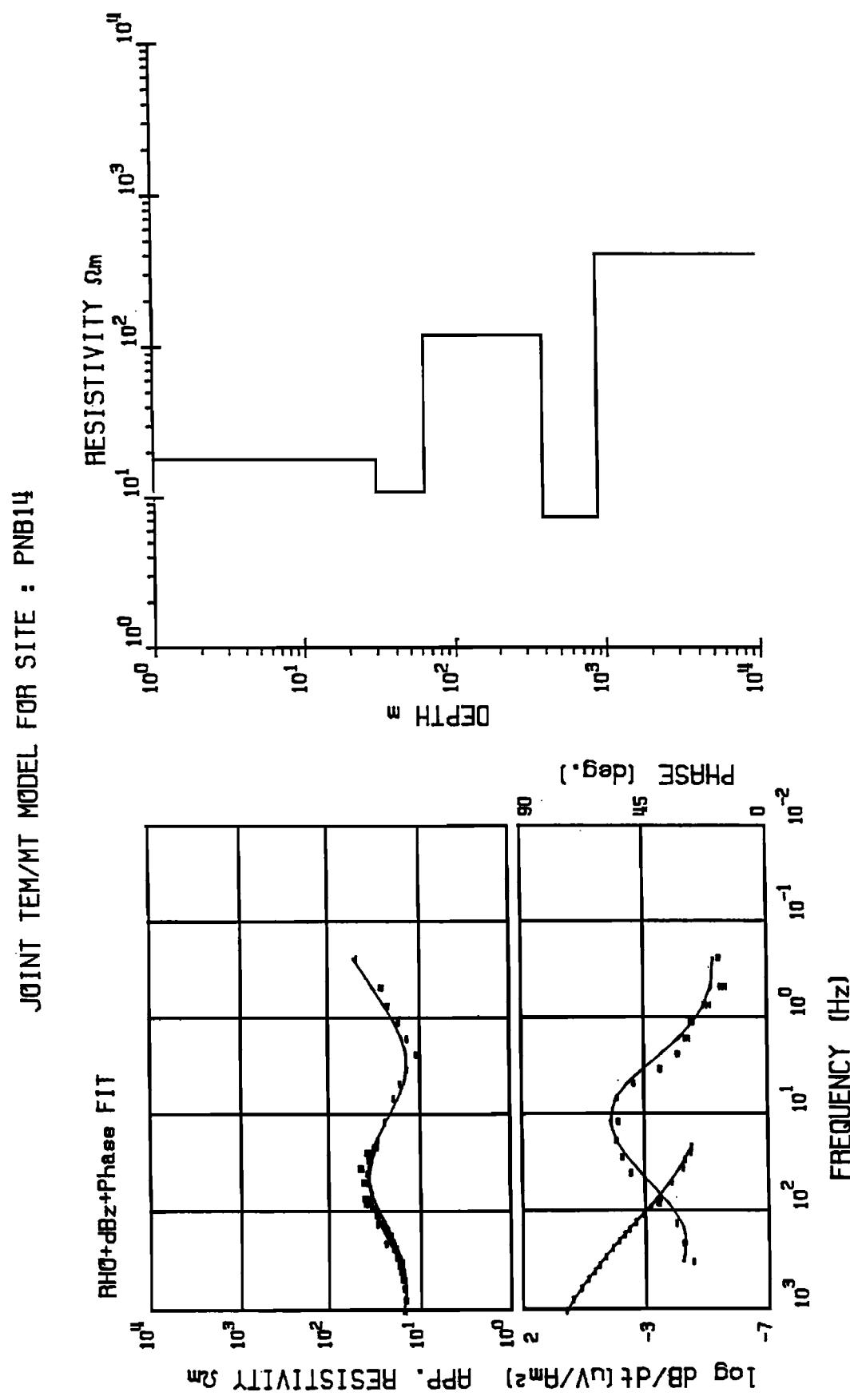


Fig. 10.3.6 Joint inversion of all available TEM and MT data

10.3.6.2 Dealing with the static shift problem in MT interpretation

Field and theoretical studies have shown that in the presence of small-scale surface or near-surface inhomogeneities, magnetotelluric MT apparent resistivity sounding curves are typically shifted by a multiplicative factor that is constant at all frequencies with the impedance phase data being unaffected. MT static shift is essentially a galvanic response associated with three-dimensional (3-D) bodies (e.g., Berdichevsky and Dmitriev, 1976) and the direction and possibly the amount of shift depends on the resistivity characteristics of the 3-D bodies. Two-dimensional (2-D) numerical modelling studies suggest that conductive inhomogeneities cause a downward shift while the reverse is the case for resistive bodies which also have a slightly larger multiplicative static shift (Jones, 1986). When interpreting MT soundings, conventional wisdom is to first identify any possible shifts and then seek some efficient corrective measures for the biased apparent resistivity curves. An approach to solving the static shift problem in the absence of any complimentary information is to shift the suspected sounding curve to some reference level determined with the aid of some statistical identification or characterisation criteria (e.g., Jones, 1988). A more unique extension of this practice uses complimentary surface measurements (e.g., Sternberg et al., 1988) or *a priori* data from boreholes (although access to borehole information is often limited in many routine surveys).

The favoured approach involves the use complimentary surface TEM data but unlike the conventional two-stage techniques involving firstly, the determination of the correct apparent resistivity level using TEM data and shifting of the entire MT apparent resistivity curve by a constant amount before interpretation (e.g., Sternberg, 1988; Pellerin and Hohmann, 1990), we will adopt a one-stage technique involving only the undistorted and equivalent MT phase information (Meju, 1994e). The underlying philosophy here is that if the right level of apparent resistivity is furnished by some other surface method, then one only needs to jointly invert the MT phase and this complimentary data set to recover the correct subsurface resistivity distribution thus eliminating the need for apparent resistivity data correction and leading to a simpler and more efficient interpretation scheme. There are some effective practical considerations to be borne in mind when adopting this approach. For the joint inversion problem, our popular inversion formula for single data sets expands to (Meju, 1994e)

$$x = [A^T A + \beta^2 I]^{-1} (A^T y - \beta^2 m^0)$$

where

$$\mathbf{y}_* = \begin{bmatrix} \mathbf{y}_t \\ \mathbf{y}_\phi \end{bmatrix} = \begin{bmatrix} \mathbf{d}_t - f_t(\mathbf{m}^0) \\ \mathbf{d}_\phi - f_\phi(\mathbf{m}^0) \end{bmatrix} \quad (\text{dimension: } [nt + n\phi] \times 1)$$

and

$$\mathbf{A}_* = \begin{bmatrix} \mathbf{A}_t \\ \mathbf{A}_\phi \end{bmatrix} = \begin{bmatrix} \partial f_t(\mathbf{m}^0)/\partial \mathbf{m}^0 \\ \partial f_\phi(\mathbf{m}^0)/\partial \mathbf{m}^0 \end{bmatrix} \quad (\text{dimensions: } [nt + n\phi] \times np)$$

for the nt (≥ 1) TEM apparent resistivity data, $n\phi$ phase measurements, and np model parameters. The subscripts t and ϕ denote the respective contributions to the system of equations from TEM and MT phase data. It should be noted that one may also elect to invert the phase information for the two orthogonal measurement directions with the TEM data for an effective interpretive model for the station of interest using the above formulations.

It is good practice in inversion to scale each observation by its associated uncertainty so that poorly estimated data have relatively less influence on the solution. In this situation, the weighted solution is simply (Meju, 1994e)

$$\mathbf{x} = [(W\mathbf{A})_*^T (W\mathbf{A})_* + \beta^2 I]^{-1} \{ (W\mathbf{A})_*^T (W\mathbf{y})_* - \beta^2 \mathbf{m}^0 \}$$

where the diagonal weighting matrix W contains the reciprocals of the observational errors. The above parameter corrections \mathbf{x} are applied to \mathbf{m}^0 in successive applications to recover the desired model parameters, \mathbf{m} .

However, it may be noted that these two sets of data to be inverted have different magnitudes. It is therefore instructive to normalise them to some common-scale before they are assembled in \mathbf{y}_* and \mathbf{A}_* . Now, as in conventional simultaneous inversion of MT apparent resistivity and phase data, the logarithms of the TEM data are considered in this scheme with the actual phase data, that is,

$$\mathbf{y}_t = \{\ln d_t - \ln f_t(\mathbf{m}^0)\}$$

and

$$\mathbf{A}_t = \partial \{\ln f_t(\mathbf{m}^0)\} / \partial \mathbf{m}^0.$$

The components of \mathbf{m} are also taken to be the logarithms of the resistivities and thicknesses of the sought subsurface model. However, since the phase data could vary from 0 to 90 say, for some given problem while the transformed apparent resistivities

JOINT TEM/MT MODEL FOR SITE : PNB22

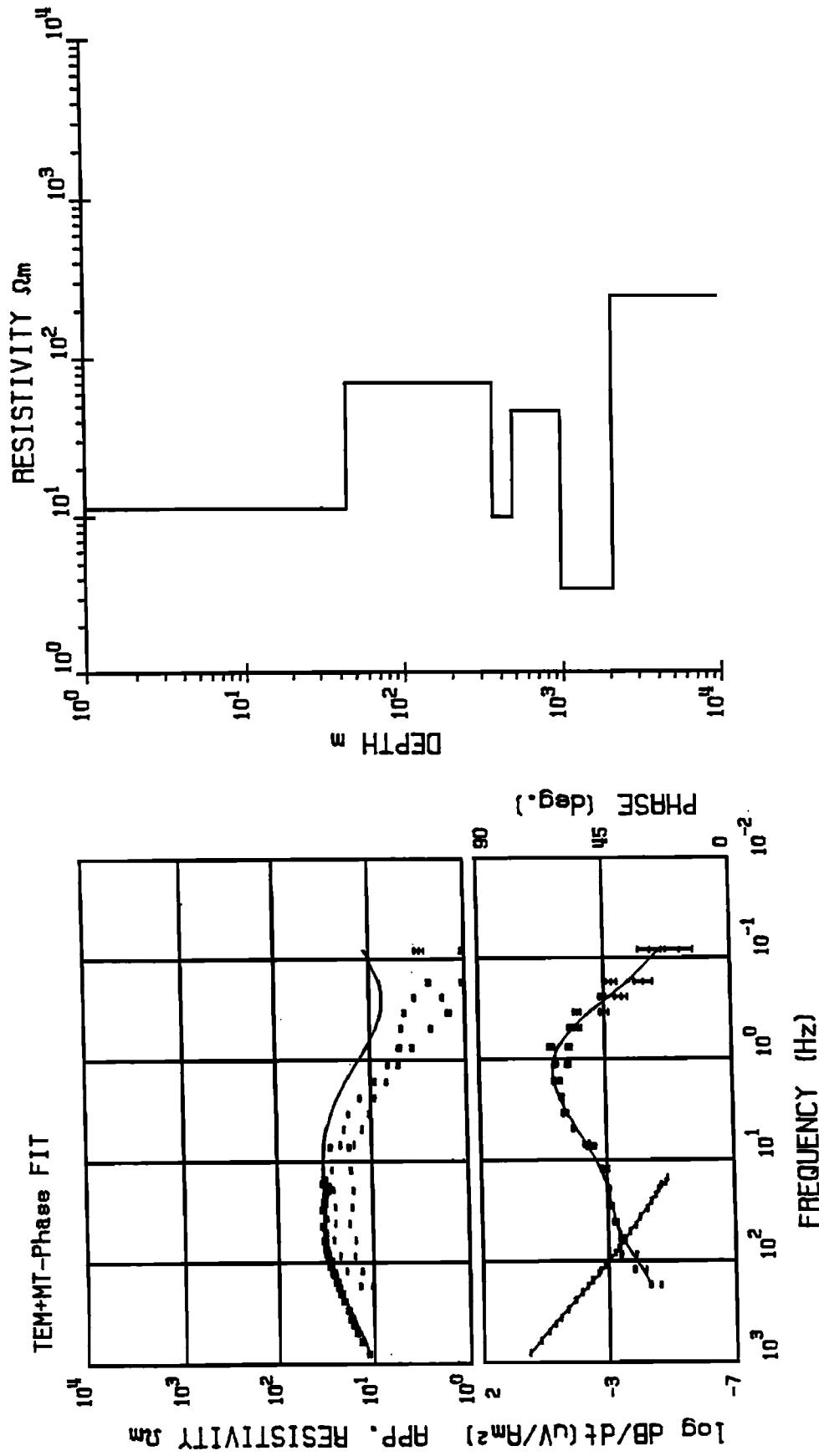


Fig. 10.3.7 Joint inversion of TEM and MT phase data (after Meju, 1994e)

would typically assume a range of values that is less than one-tenth of that of the phase data, a useful practical strategy might be to normalize the contributions from the phase data to the system of equations by some constant factor (~ 10).

An application of this inversion strategy to TEM and biased MT data from the same station in a sedimentary basin (Meju, 1994b) is shown in Fig. 10.3.7. Notice the good fit of the optimal joint model responses to the field MT-phase and TEM data. Since MT phase data should be the same in both directions in an ideal layered earth situation, it is a good practice to seek a representative model by inverting the combined phase data in areas where a horizontally stratified structure can be assumed as a working model. As shown in Meju (1994e), another advantage of this approach is that TEM data of limited bandwidth (i.e., with little or no overlap with MT phase curves) may suffice for recovering the true resistivity structure from the MT-phase data.

10.3.6.3 Joint inversion of central- and coincident-loop TEM soundings

As a way of addressing the problem of lateral variations within the Tx loop area in TEM inversions, it may be useful to define an effective resistivity distribution underneath a particular site by jointly inverting the central- and coincident-loop depth-sounding data as illustrated in Fig. 10.3.8a. It is clear from this figure that the central and coincident loop data are in excellent agreement suggesting negligible lateral variations within the area covered by the Tx loop for the sampled depth zones. A local areal average may also be defined by the joint inversion of multiple-station (i.e. combined) data as illustrated in Fig. 10.3.8b. Such areal representative models may find use in regional surveys where the gross features of the subsurface resistivity variations are desired.

10.3.7 Inversion of dc Resistivity Data

All the inversion applications demonstrated above using EM data hold good for dc apparent resistivity data and it would serve no further purpose to recount them here. However, it may be noted that it is common practice to simultaneously invert dc and EM data for better model verification (e.g., Vozoff & Jupp, 1975). It may also be necessary to scale the elements of the Jacobian matrix if they differ markedly in size for the different types of data involved in the joint inversion process. The computer program WENINV listed in the appendix performs only single-station data inversion but can be easily modified to handle multiple data sets.

1-D MODEL FOR SITE : CYP7 (CC+CN)

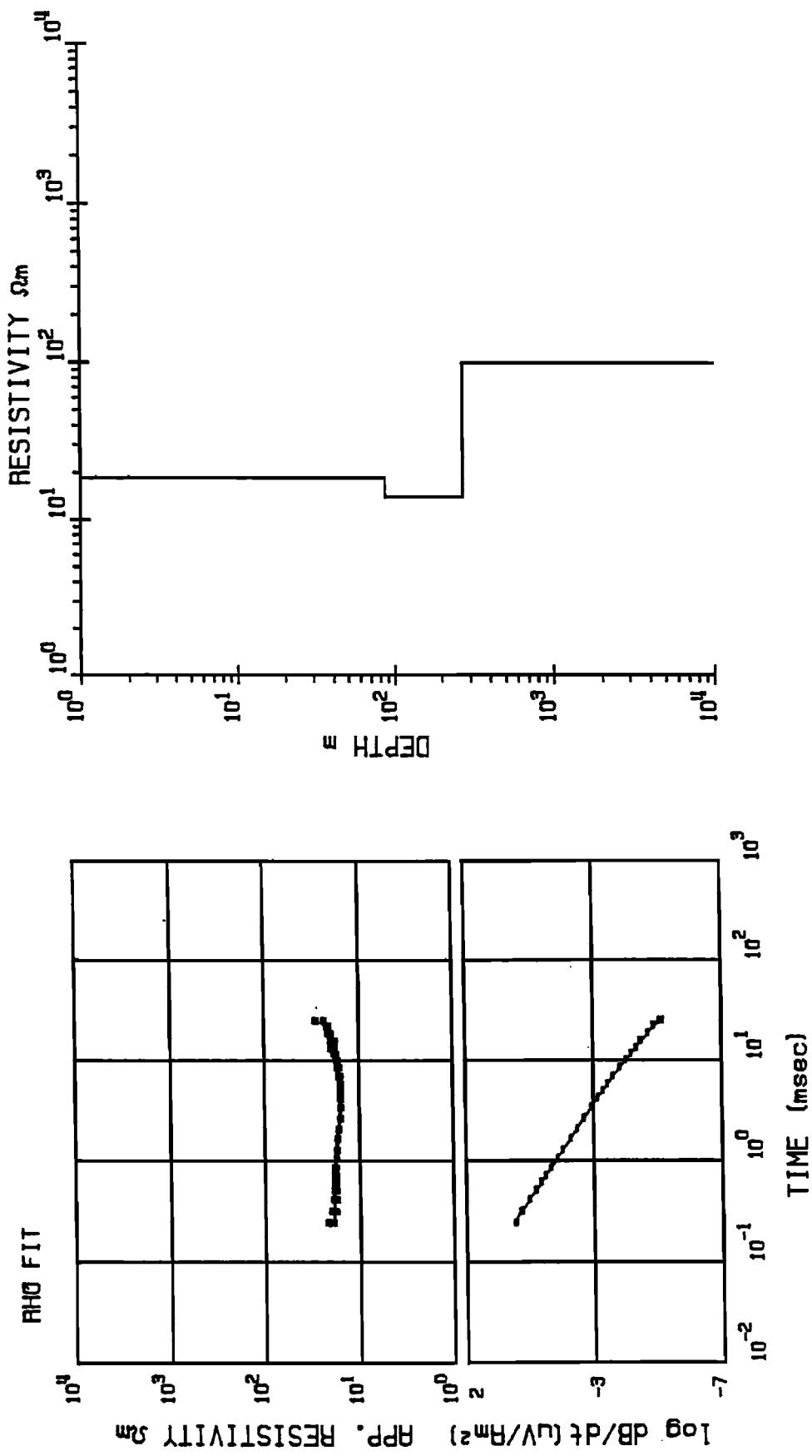


Fig. 10.3.8a Effective site resistivity from coincident- and central-loop TEM data

1-D MODEL FOR SITE : CYP7+CYP8 (CC)

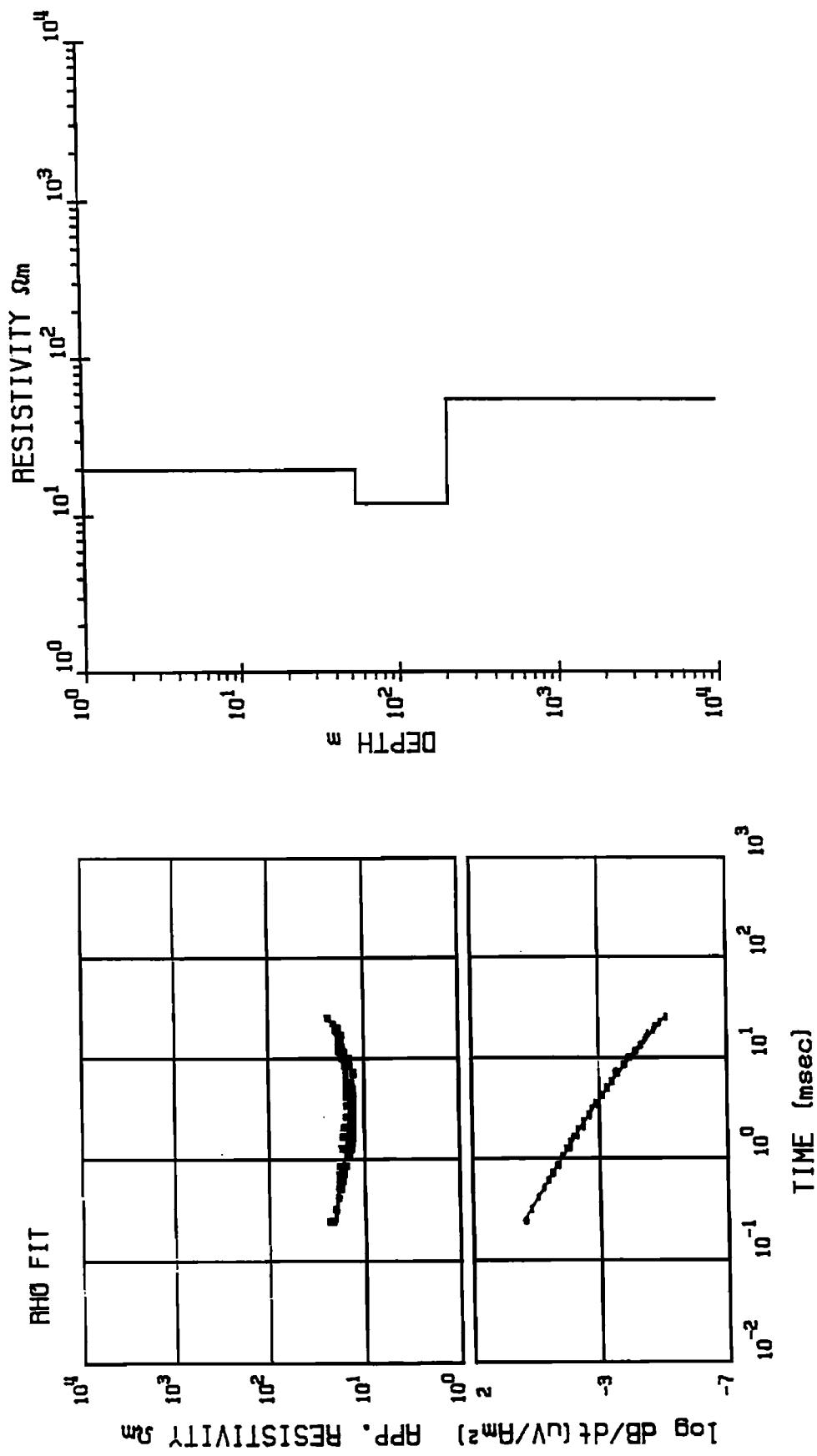


Fig. 10.3.8 Mean resistivity distribution from multi-station TEM data

10.4 Estimation of Effective Depth of Inference Using Smooth Models

10.4.1 Aspects of smooth model construction

Recall from Chapter 6 that smooth models may be constructed by minimizing the cost function

$$\phi = (\mathbf{W}\mathbf{d} - \mathbf{W}\mathbf{f}(\mathbf{m}))^\top(\mathbf{W}\mathbf{d} - \mathbf{W}\mathbf{f}(\mathbf{m})) + \beta^2(\mathbf{m}^\top \mathbf{H}\mathbf{m}) \quad (10.4.1)$$

or the mathematically equivalent function (since β is undetermined)

$$\phi = \beta^{-2}\{(\mathbf{W}\mathbf{d} - \mathbf{W}\mathbf{f}(\mathbf{m}))^\top(\mathbf{W}\mathbf{d} - \mathbf{W}\mathbf{f}(\mathbf{m}))\} + (\mathbf{m}^\top \mathbf{H}\mathbf{m}). \quad (10.4.2)$$

The constrained linearized solution is simply

$$\mathbf{x}_s = [(\mathbf{W}\mathbf{A})^\top(\mathbf{W}\mathbf{A}) + \beta^2 \mathbf{H}]^{-1}[(\mathbf{W}\mathbf{A})^\top(\mathbf{W}\mathbf{y}) - \beta^2 \mathbf{H}\mathbf{m}_0]. \quad (10.4.3)$$

or

$$\mathbf{m}_s = [(\mathbf{W}\mathbf{A})^\top(\mathbf{W}\mathbf{A}) + \beta^2 \mathbf{H}]^{-1}(\mathbf{W}\mathbf{A})^\top \hat{\mathbf{d}}_1 \quad (10.4.4)$$

where $\hat{\mathbf{d}}_1 = \{(\mathbf{W}\mathbf{y}) + (\mathbf{W}\mathbf{A})\mathbf{m}_0\}$ and the other symbols have their usual meanings.

Implementation of the smooth model algorithm

The smooth model algorithm is simple and can be readily implemented as a biased estimation procedure. Basically, the first difference operator \mathbf{D} is premultiplied by β (chosen as a value less than or equal to unity) and appended onto the actual weighted matrix of partial derivatives ($\mathbf{W}\mathbf{A}$). The weighted discrepancy vector $\mathbf{W}\mathbf{y}$ is also augmented with the extraneous data ($-\beta\mathbf{D}\mathbf{m}_k$ or simply zeros) forming \mathbf{y}_* . The main task here is the determination of the inverse matrix $[(\mathbf{W}\mathbf{A})^\top \mathbf{W}\mathbf{A} + \beta^2 \mathbf{H}]^{-1} = (\mathbf{A}_*^\top \mathbf{A}_*)^{-1}$. Using the SVD technique, the $(n+l) \times p$ augmented matrix, \mathbf{A}_* is decomposed into a product of three other matrices, i.e., $\mathbf{A}_* = \mathbf{U}\Lambda\mathbf{V}^\top$, where \mathbf{U} and \mathbf{V} are the data space and parameter space eigenvectors respectively and Λ is a diagonal matrix of the singular values of \mathbf{A}_* . In terms of SVD, the constrained least squares solution given by equation (10.4.3) is simply

$$\mathbf{x}_s = \mathbf{V}\Lambda^{-1}\mathbf{U}^\top(\mathbf{y}_*).$$

Note that since we have regularized \mathbf{A} by augmenting it with \mathbf{D} , it is non-singular. However, depending on the value of the regularization parameter β used, some of the

singular values of the regularized derivatives may still be quite small producing undesirable effects on inverting the matrix $A^T A$. A simple and effective routine for implementing this procedure PREP, is given in Fig. 10.4.1. It can be used in any conventional layered-earth inversion scheme to generate the initial model and the augmenting equations for smooth models. It is called once before the iteration process; note that while the actual data segments of A and y are modified when new partial derivatives and data misfit vector are evaluated, their augmenting data are not changed in the above solution process. However, a routine for appending the appropriate extraneous data onto A and y , FSTDIF is included in PREP and may be called at each iteration. The depth estimates returned by PREP should be held constant in the inversion process while the model resistivities are optimized.

```

subroutine PREP(nrow,beta,A,Y,rm,dm,nL,ncol,ndat)
constructs an approximate initial model for smooth MT inversion
c Input: jacobian matrix A, discrepancy vector Y, actual nrow in A
c          and damping factor beta.
c Output: rm,dm=initial model parameters (rm=resistivity ; dm=depths in metres);
c          augmented A,Y, ncol and nrow of new A,y : uses the routine FSTDIF.
c          Returned model has nL layers and nD interfaces.
c Routine set for 50 data points and 20 layers. Thus A((50+50+20),(20+20))
c and Y(50+50+20) to allow for joint data sets. change as required but keep
c physical dimensions of arrays same as in calling routine.
c Nrow=nfreq when fitting only app.rho or phase; nrow=2*nfreq when
c fitting app rho and phase simultaneously. Field data stored in common block
c FDATA. AR1=app.rho; Ar2=apprho errors; ph1=phase in degrees.
c ph2=phase errors, freq=frequencies in Hz.

common /FDATA/ freq,ar1,ar2,ph1,ph2,nfreq
real freq(50),ar1(50),ar2(50),ph1(50),ph2(50),a(120,40)
real y(120),rm(20),dm(20),db(50)
character*1 ans
ndat=nrow
nL=20
nL2=nL-2
nD=nL-1
ncol=nL
nrow=ndat+nD

```

```
write(*,'(/A)')' please note : initial model is a half-space '
write(*,'(/A,$)')' want to specify half-space resistivity ? y:n'
read(*,'(A1)') ans
if(ans.eq.'Y'.OR.ans.eq.'y')then
    write(*,(" please enter half-space resistivity "))
    read(*,*)rhoHS
    else
c      calculate average resistivity from given data ar1
        rhoHS=0.0
        do 1 i=1,nfreq
            rhoHS=rhoHS+ar1(i)
1      continue
        rhoHS=rhoHS/nfreq
    endif
    write(*,'(A,$)')' want to specify min/max depths ? y:n '
    read(*,'(A1)')ans
    IF(ans.eq.'Y'.OR.ans.eq.'y')then
        write(*,*)' enter approx. top and bottom depths in metres '
11   read(*,*) sma,big
        if(big.LE.sma)then
            write(*,*)' warning: your max. depth is less than min depth'
            write(*,*)' enter new depths to top and bottom of half-space'
            GOTO 11
        endif
        top=alog10(sma)
        bot=alog10(big)
        ELSE
c      find minimum and maximum penetration depths
c      using Bostick's algorithm
        pi=acos(-1.)
        amu0=4.*pi*1.E-7
        do 2 i=1,nfreq
            f=1./sqrt(2.*pi*amu0*freq(i))
            db(i)=sqrt(ar1(i))*f
2      continue
        big=db(1)
```

```

sma=db(1)
do 10 i=1,nfreq
  st=db(i)
  if(st.GT.big)then
    big=st
  elseif(st.LT.sma)then
    sma=st
  endif
10  continue
  sma=sma/nL
c change above line to SMA=10.**LD0+0.1 if LD0 is log of
c minimum plotting depth in your plotting routine
  top=alog10(sma)
  big=big*1.8
  bot=alog10(big)
  ENDIF
c construct smooth model. first put rm=rho-halfspace
  do 20 l=1,nL
    rm(i)=rhoHS
20  continue
c next compute depth range and subdivide to get
c ND equi-spaced layer boundaries
  rng=top-bot
  dd=rng/nL2
  do 40 i=1,nL2
    k=i+1
    dt=dd*FLOAT(i)
    dm(k)=10**((top+dt)
40  continue
  dm(1)=sma
  dm(nd)=big
c set up augmenting equations in jacobian matrix A and
c discrepancy vector y
  call FSTDIF(nn,m2,beta,ncol,ndat,nrow,A,Y)
  return
  end

```

C-----

```

subroutine FSTDIF(nn,m2,beta,ncol,ndat,nrow,A,Y)
c first difference operator for smooth models. augment A and y.
real A(nn,m2),Y(nn)
nfl=ndat+1
do 10 i=nfl,nrow
Y(I)=0.0
IR=i-ndat
IR2=IR+1
do 20 j=1,ncol
20 A(i,j)=0.0
A(i,IR)=1.0*beta
A(i,IR2)=-1.0*beta
10 continue
return
end

```

Fig. 10.4.1 A simple data preparation routine for MT inversion for smooth models.

Determination of suitable starting models

The main attractions of inversion for smooth models are reflected in the commonly held views that the optimal models are independent of the initial half-space model and that any significant features resulting therefrom may be justified by the data. It is not difficult to conceive that inversion for smooth models is most effective if the search is initiated with a half-space model or a smooth model derived for instance from a simple resistivity-versus-depth data transformation (Meju, 1988); the minimization path is well defined and the smoothness constraints, though contradictory in a sense to the requirement to satisfy the data, lead to a stable inversion process. Importantly, since the solution is biased towards the initial *a priori* information, the reconstructed smooth model will retain some of the desirable features of our initial smooth model; and because the data (providing they are of reasonable quality) tend to predominate somewhat over contrasting *a priori* information, we in effect retrieve a smooth model that is consistent with our observations. It is easy to show the reliance of such models on the initial conditions which is contrary to the popular belief.

In Figs. 10.4.2 and 10.4.3 are shown the results of inversion of synthetic magneto-telluric (MT) data using different initial models with the earth-model parameterised

1-D MODELS FOR SITE MT3L

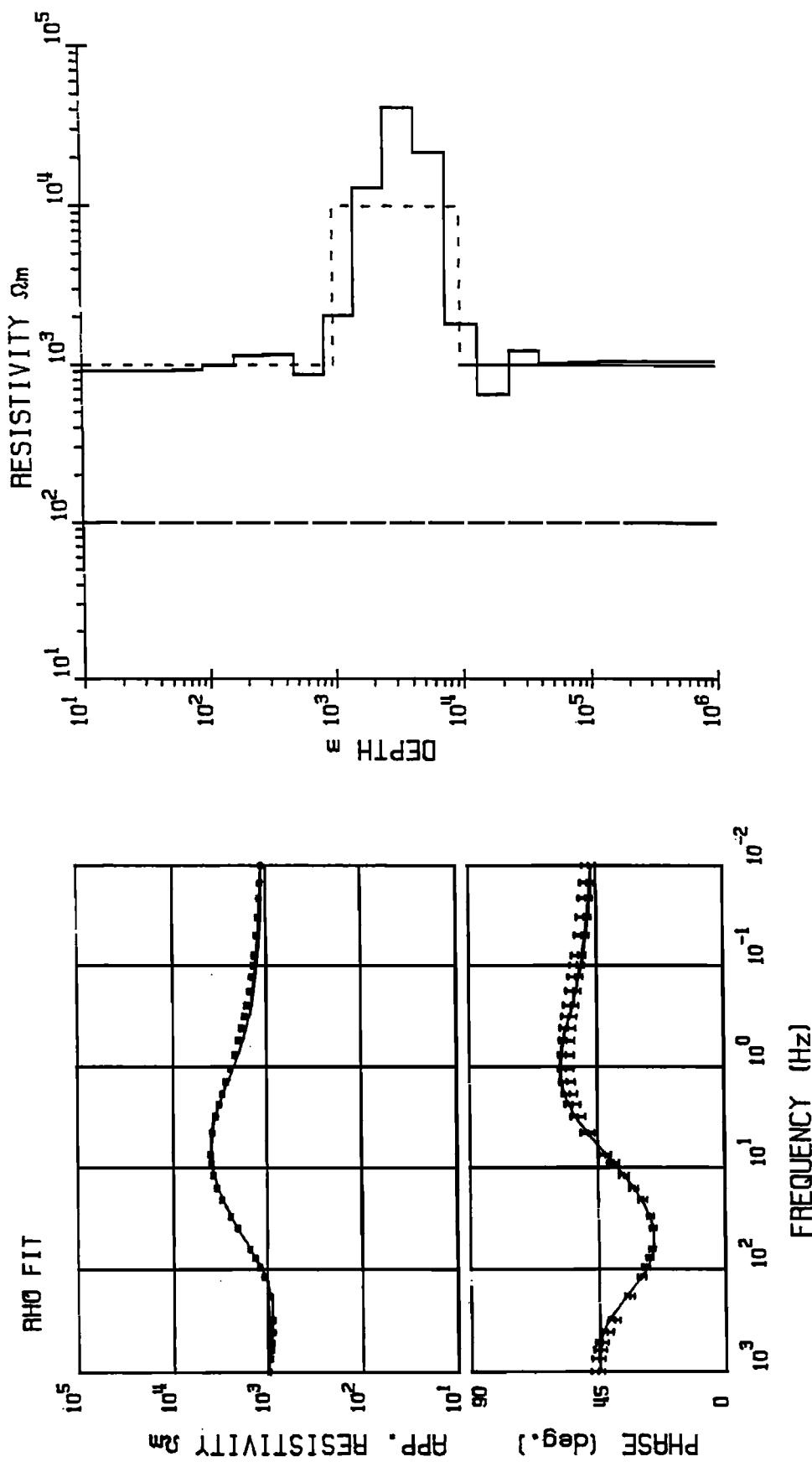


Fig. 10.4.2a. Inversion with the smoothest initial model

1-D MODELS FOR SITE MT3L

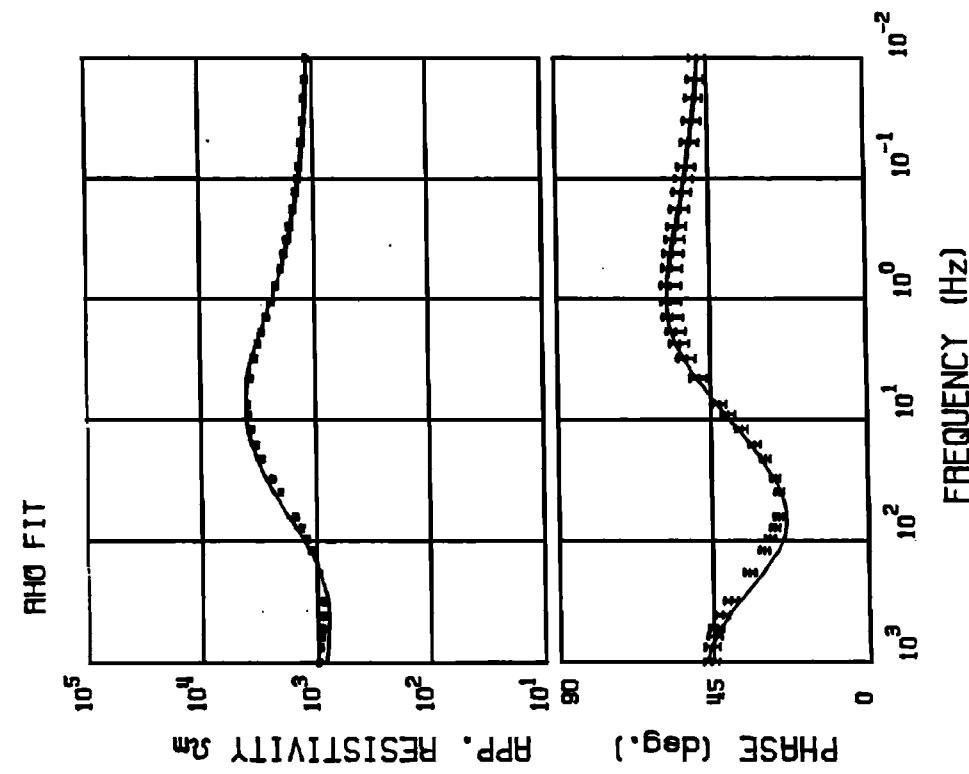


Fig. 10.4.2b Inversion with approximately smooth initial model

1-D MODELS FOR SITE MT3L

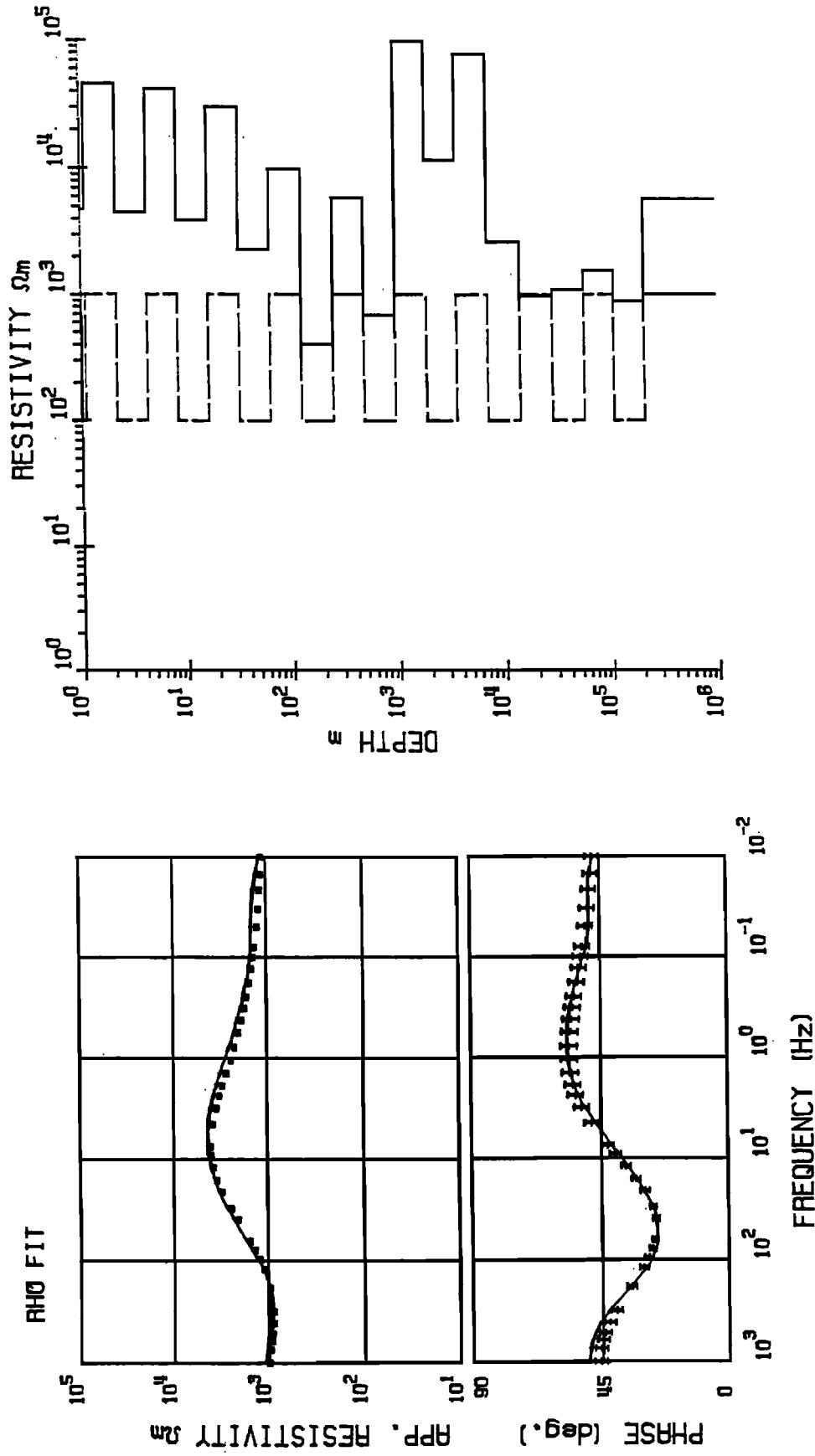


Fig. 10.4.3 Inversion with non-smooth initial model

1-D MODELS FOR SITE COPROD

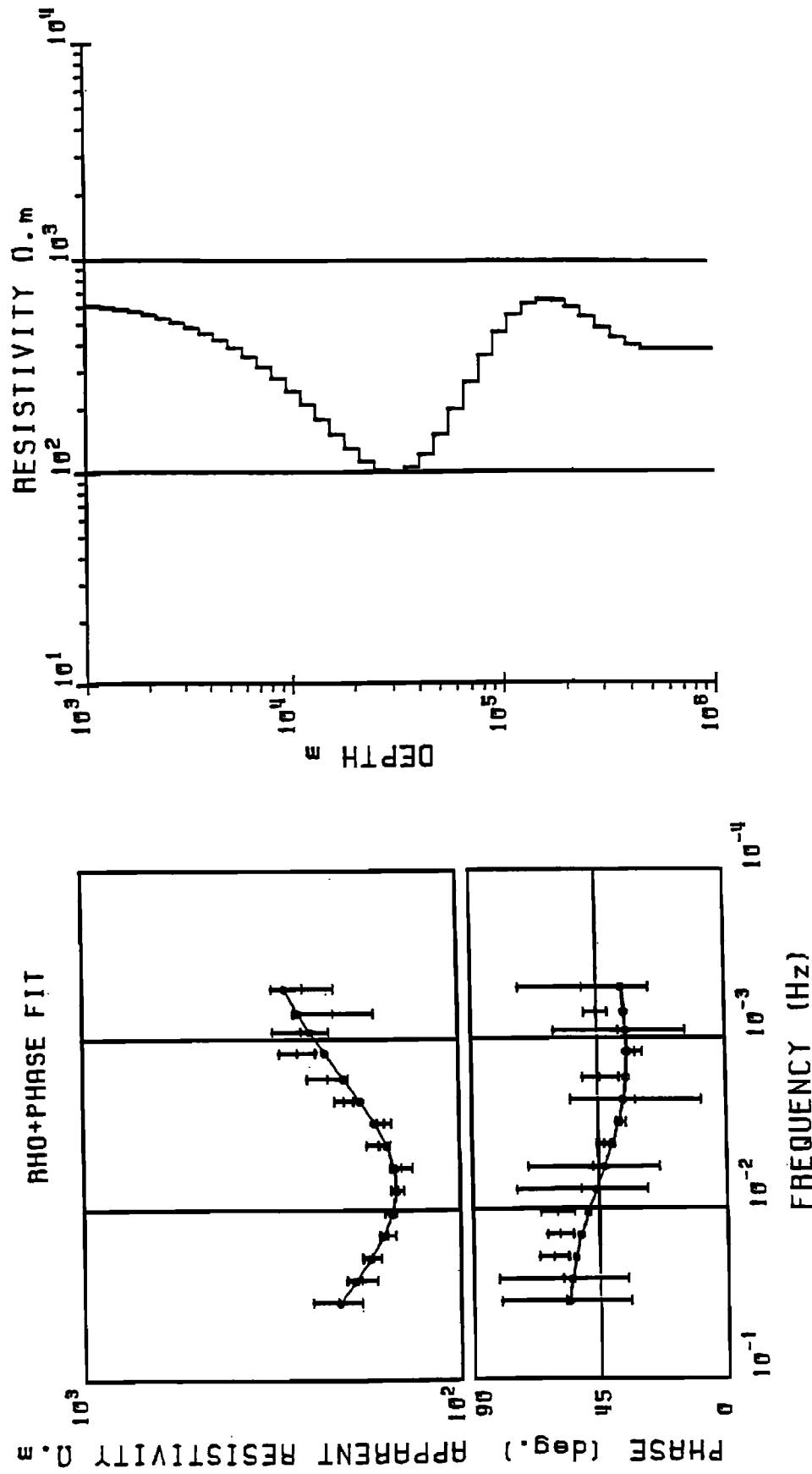


Fig. 10.4.4 Optimal models from initial half-space models of different resistivities

into a succession of twenty layers of constant thickness (in log space) and with β assigned a fixed value of 0.1. In all the figures, the initial model is represented by long dashed lines and the optimal models by solid lines. The true model used to compute the test data is also shown in Fig. 10.4.2a (short dashed lines). It is obvious that only the models reconstructed from the smooth initial models (Figs. 10.4.2a and 10.4.2b) retained the desired smooth features and resemble the true model adopted for the exercise (shown on righthand plot of Figure 10.4.2a). As shown in Fig. 10.4.3, the test employing a non-smooth initial model was unsuccessful.

Convergence characteristics

The biased estimation approach described above offers a computational advantage in the sense that a fixed value of the quadratic factor β is used throughout an inversion application. Note, however, that in the above examples it was deemed necessary, as a practical constraint, to place a bound on the size of the parameter perturbations using Jackson's (1973) smoothness criterion. Thus the lengths of the perturbations were decreased to about 30% of the actual value if they exceeded some fixed value. This operation decreased the speed of convergence but provided additional stability to the solution process. The smooth model shown in Fig. 10.4.2a was generated after only 6 iterations.

Having accepted that half-space models are convenient starting points for generating smooth models, it is instructive to see whether the algorithm will converge to the same or similar optimal model for different half-space resistivities for a given data set. The method was applied to the MT COPROD (Jones and Hutton, 1979) apparent resistivity and phase data using the $100\Omega m$ and $1000\Omega m$ initial models and the results are shown in Fig. 10.4.4. Notice that the optimal models from the two different starting models are exactly the same ($\chi^2=29.3$ for both). A value of 0.6 was employed for β and the earth model was parameterized into a succession of forty layers in these examples.

10.4.2 Geometric interpretation of smooth inversion: intuitive concepts and implications
The quadratic factor β and the measures q_2 and q_1 are the essential ingredients in the generation of smooth models as illustrated in the following interpretative analysis aimed at providing a clearer understanding of the smooth model construction process, and especially those aspects that may have practical implications. Let us consider first the hypothetical situation where the desired solution can be found in one step as the interpretative analysis would then lean on that provided for constrained linear inversion.

Notice that equations (10.4.1) and (10.4.2) may be written in shorthand form as

$$\phi = q_1 + \beta q_2 \quad (10.4.5)$$

and

$$\phi = \beta^{-1} q_1 + q_2 \quad (10.4.6)$$

The measure q_2 is zero when $m_1=m_2=\dots=m_p$, that is, $Dm=h=0$ as for an initial half-space model (a situation that fulfils one of the conditions in our problem definition). For ease of discussion, it will be assumed that there is a point in model-space where q_2 is effectively minimized and denoted by B in Fig. 10.4.5. Similarly, q_1 attains a minimum at some other point in function space denoted by A in this figure. The reader is reminded that in reality the contours (i.e., l -dimensional hypersurfaces of constant q_1 and q_2) in Fig. 10.4.5 can be highly distorted in shape. Geometrically, the situation may be better imagined as a scenery with chains of mountains and valleys of various forms and sizes with the locations of the minima of q_1 (and sometimes q_2) completely unknown. Again, for ease of discussion these minima are likened to two main valleys in the conceptual chain, one of which is a large-scale depression or regional feature with the deepest point corresponding to the minimum in q_1 (represented by point A in Fig. 10.4.5). The deepest point in the other major valley would correspond to point B. If equation (10.4.5) or (10.4.6) is minimized using the inversion formula (10.4.4), it is conceivable that for smooth initial models, the solution will in general travel from B to A as β is varied from an infinitely large value to zero, say in a line-search scheme. Since the quantities q_1 and q_2 can be computed for the solution obtained for any particular value of β , the travel path of the smooth solutions can be monitored as β is varied. Such a solution trajectory is also illustrated in Fig. 10.4.5 for the hypothetical situation.

A characteristic feature of nonlinear problems is that the travel path of the solution may be dotted with minor depressions and ridges (i.e., a rugged topography) preventing the journey sometimes from reaching a successful completion. Another undesirable feature is that a false trail may be followed in the search for a minimum resulting in an unwanted solution, i.e., the searched valleys are different from our target valley whose bottom-point is A. However, the use of *a priori* information (Jackson, 1979) in the search process may alleviate some of these problems as such prior data often help define a fruitful search direction as well as ease the travel process. In the absence of *a priori* information, any minima-seeking algorithm can at best hope to avoid some of the minor valleys in the travel path of the solution but there is usually no guarantee that the deepest valley will be searched or its deepest point found. In the smooth model

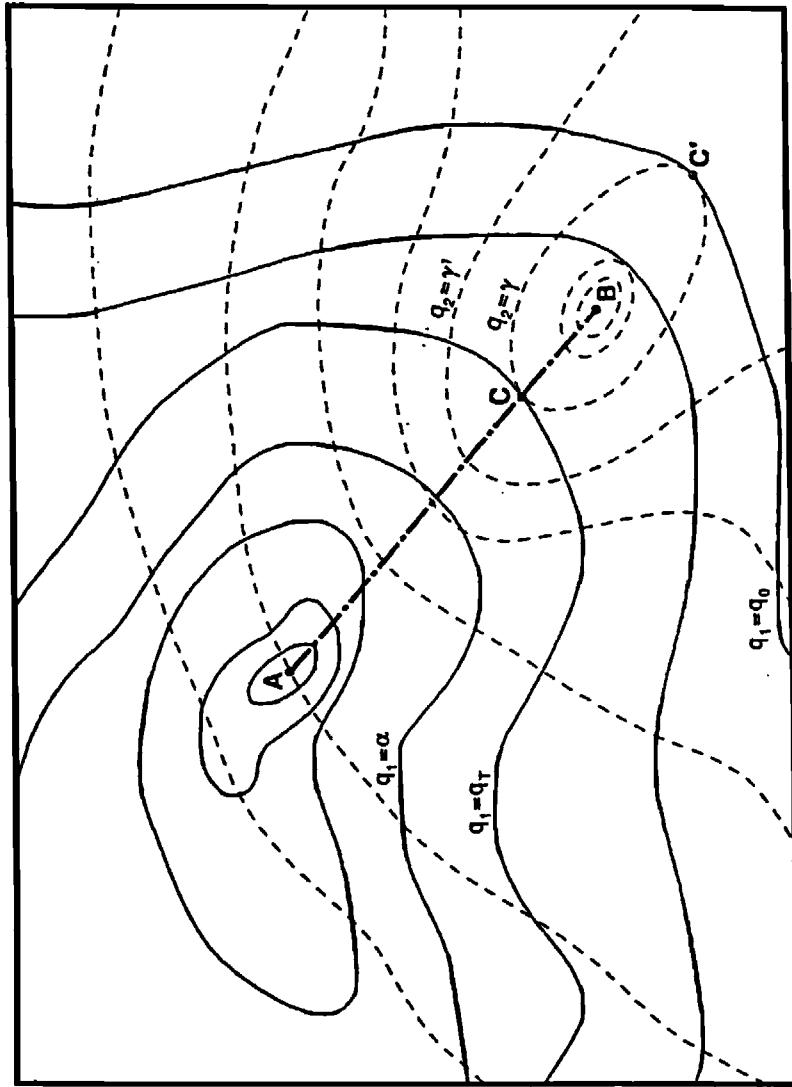


Fig. 10.4.5 A 2-D simplification of solution trajectory in function space

problem, we have incorporated prior constraints on the desired form of the solution. Apropos therefore, is the selection of suitable initial models in inversion with smoothness constraints. Metaphorically speaking, the smoothness measure $\beta(m^T H m)$ is a good pathfinder but mostly for a restricted class of prospectors - smooth initial models. However, it may be pointed out that not all smooth models constitute good initial models. Owing to the linearizing parameterizations employed in the solution process, the suitability of the initial model depends on the length of the potential travel path in function space, i.e., between our hypothetical minima A and B (a distance dubbed AB here). For smooth initial models, the size of AB spells the difference between rapid and slow convergence or between success and failure in inversion for there is a threshold distance beyond which a given initial model becomes unsuitable and the algorithm may fail to converge to a desirable solution. If the initial model is not smooth, then q_2 may attain a minimum at several locations in the p -dimensional space and the solution faces a more difficult journey over the rugged terrain. The end result may be undesirable and the solution procedure would require special path-finding measures such as hybrid inversion schemes.

Extending this over-simplified analysis to the more general situation where the solution satisfying the constraints $q_1 = q_T$ and $q_2 = \gamma$ say is sought in Fig. 10.4.5, it can be deduced that the desired point in our q_1 valley is posit not at A but at some other point C, say on the valley side nearer B. To get to this point from B requires a suitable choice of the quadratic factor β ; one can easily overshoot the point C (thus missing the desired solution) by using coarse steps in (or unrealistic values of) β . The dense β -sampling procedure adopted by Constable et al., (1987) may be the favoured strategy in this situation. However, since the solution must lie somewhere between A and B in our hypothetical analysis, we may restrain the range of values of β required in a line-search process. Now, depending on the initial model (with $q_1 = q_0$, say), we may obtain the undesirable solution C' which also satisfies the smoothness constraint. This may be the case for non-smooth initial models (where the point B may be enclosed by the $q_1 = q_0$ contour in Fig. 10.4.5) and *a fortiori* for using half-space initial models.

In the foregoing analyses, it has been emphasised that a suitable choice of β and an appropriate initial model are a *sine qua non* for the inversion for smooth models. It is stressed, however, that while this contention is correct for the biased estimation approach, it does not imply that non-smooth initial models will always lead to failure or non-convergence in smooth model construction schemes since it is possible to adapt some other effective practical strategies to such problems (as discussed later).

Subsurface characterisation at the datum-scale

On the interpretational front, the behaviour of the optimal solutions reconstructed from half-space models for various values of β can also be visualised within a geometrical framework. Here, they are analysed for consistency and/or dependence on β with a view to deriving some model interpretational guides. Note that in every sense generating the smoothest model entails forcing the solution towards conformity with $h=0$.

Thus initiating the search with a half-space model, as is common practice, is consistent with the adopted *a priori* constraints in equations (10.4.1) and (10.4.2). Since the form of the solution is well defined *ab initio*, the stabilized successive approximations simply serve to improve the fit to the given data; the solution is usually safely guided towards some sort of minimum in q_1 . Obviously, the degree to which this initial constraint is satisfied depends on the value assigned to β . Interestingly, as the influence exerted by β on the travel path of a particular solution is counteracted by the requirement to also satisfy the data to be inverted, a useful attendant feature is that for some values of β the form of the resultant model would differ significantly at those subsurface positions where the solution paths are not constrained by the observational data (i.e., the under-determined parts) but may be similar elsewhere. If this contention is correct, then the subsurface may be adequately characterised at the datum-scale using the information pooled from the smoothest models constructed for a range of β . It may thus be possible to estimate an approximate depth of investigation for a given data set without recourse to rigorous mathematical analysis (Meju, 1993) as demonstrated next.

10.4.3 Pooled model interpretation: the effective depth of investigation

Let us examine the morphology of the solutions in β -space. The relationships between the models derived for a range of β values were shown in Fig. 10.4.6 for the COPROD data sets respectively. Notice that the models show concordant features in the depth range $\sim 14\text{km}$ to $\sim 300\text{km}$ but differ significantly outside this zone. Meju(1993) interpreted the discordance in structure outside this depth range as being due to the fact that the models are not constrained by the data at those positions. This interpretation is in accord with the maximum depth determined by Parker (1982) to which any model can be constrained by the COPROD data and is also consistent with the most-squares analysis of the data (Meju and Hutton, 1992). Note that such consistent patterns have been obtained for a variety of resistivity depth sounding data. In the MT situation, the pattern may be diffuse at depth for those data sets in which the models

1-D MODELS FOR SITE COPROD

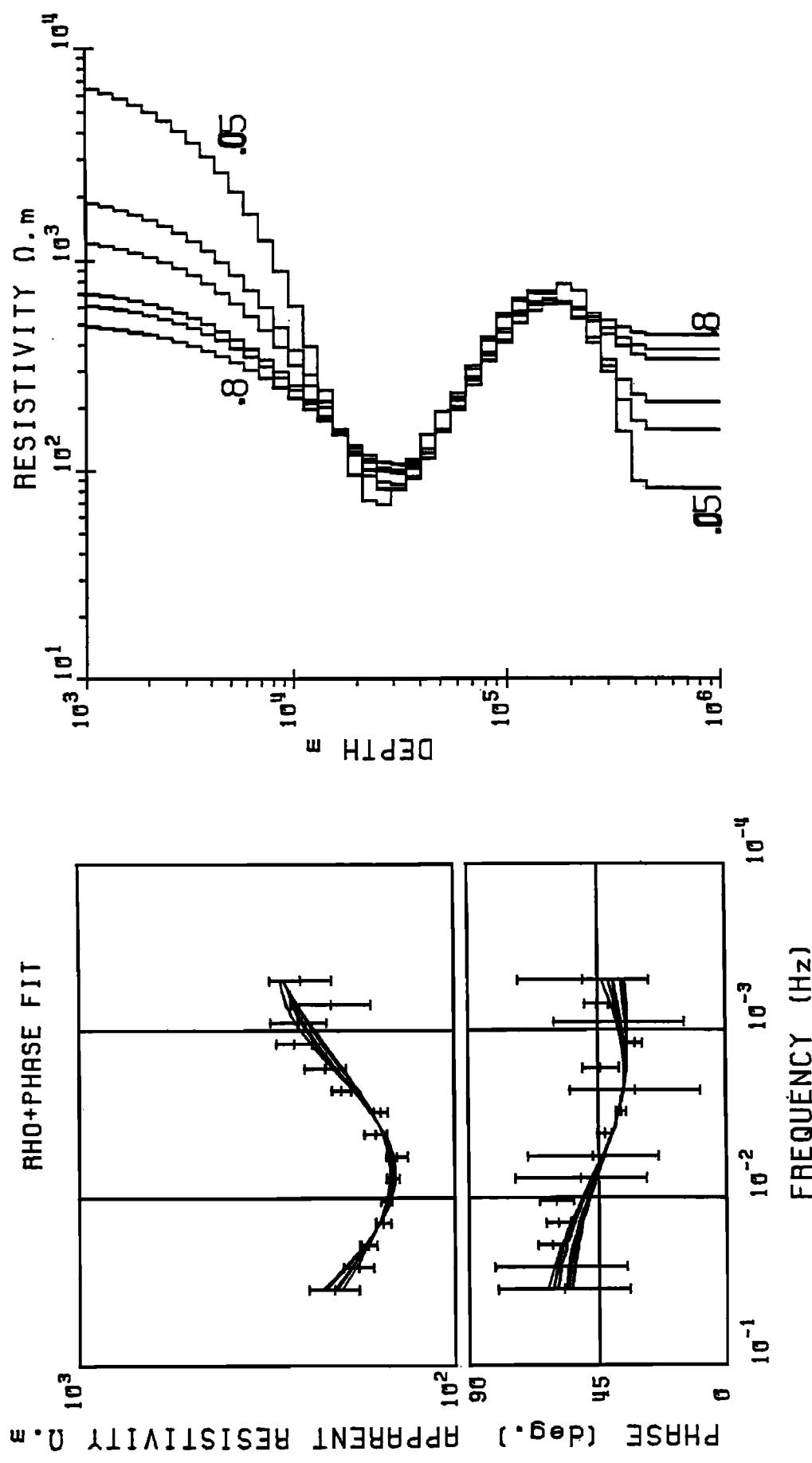


Fig. 10.4.6 Effective depth of inference (zone of structural concordance pooled models) for COPROD data

1-D MODELS FOR SITE : EM42-IR29

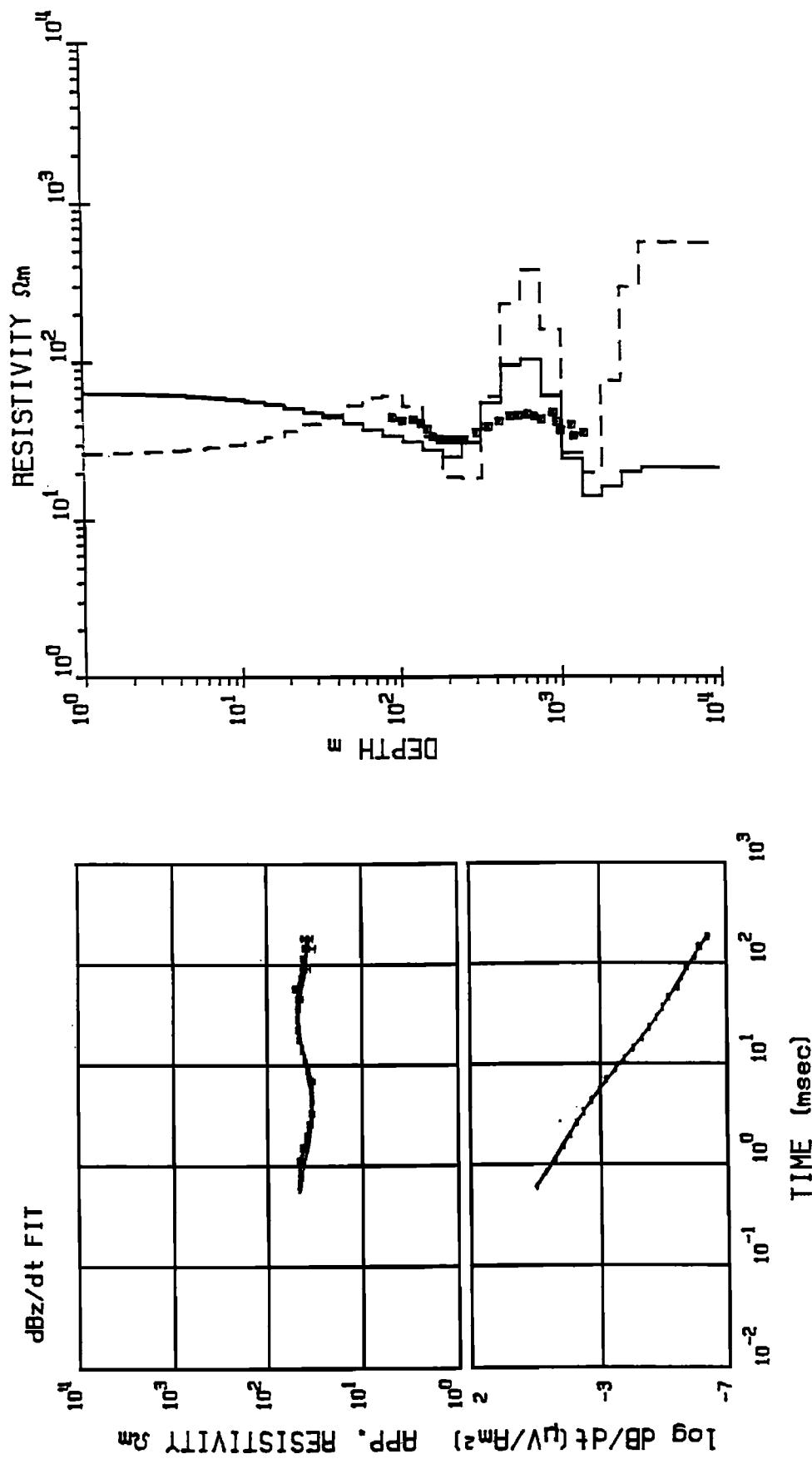


Fig. 10.4.7 Comparison of effective depths from smooth models and direct depth imaging for TEM data

show a monotonically decreasing resistivity with depth; but even in such cases, some discernible trend is present especially in the upper section of the geoelectric profiles. Such a method may thus have applications in simple determinations of the approximate depth of inference for a given set of practical data. An obvious method of efficiently deriving this useful information will be to generate optimal smooth models for two values of β that are about an order of magnitude apart as illustrated for TEM data in Fig. 10.4.7. The agreement between this TEM interpretation and the resistivity-versus-depth information derived using a recently developed direct-depth TEM data transformation technique (see Meju, 1999a, 1994f) is obvious in this figure.

10.5 Simultaneous Inversion of Multi-Station data with Spatial Constraints

Consider the process of interpreting geophysical soundings from a profile across a sedimentary basin. In the absence of any deformational activities, and assuming that the subsurface consists of a succession of horizontal or near-horizontal beds of sedimentary rocks - an ideal situation - we expect the physical property of a given rock bed to be fairly uniform laterally, only differing significantly from that of the underlying or overlying bed. The interpretation of field measurements along a profile in this case is a straightforward task. Unfortunately, in most basin exploration situations we find that there are lateral changes in the Earth's structure and this introduces some bias in the field data. For example, in resistivity surveying, the recorded apparent resistivity sounding curves at some locations along the said profile may be shifted along the vertical axes or show a large scatter in their distribution. In the magnetotelluric (MT) situation this may manifest as a static (frequency independent) shift of the apparent resistivity curves but not the EM impedance phase data but the direction and magnitude of the shift are not known except where there are some other complementary information available at the given observational site. The inversion of such a biased and/or noise degraded data set will not yield a reliable picture of the subsurface at the affected site. In the MT case, it is known that a plethora of models can reproduce a given phase curve and some information not contained in the data from the affected observational site must be used to determine the correct levels of the apparent resistivity curves or the appropriate model parameters.

The recovery of the correct parameters for a biased data set selected from a pool of other related data sets, some of which are unbiased, can be posed as an inverse problem (Meju, 1988). We simply use the reliable data as *a priori* information and impose some

penalties on the solution for the biased site. An effective penalty for such a site is that the solution be as close as possible to those of the neighbouring observational locations. We therefore state the optimization problem as:

Given sets of conflicting observations from different positions along a survey line, some of which satisfy some normality conditions, find the smoothest lateral distribution of physical properties that explains the observations.

Here, we are interested in obtaining a laterally smooth interpretive cross-section. We start off with a smooth profile (i.e., the same model is used for all sites) and invert all the various data sets simultaneously with the constraint that differences in the layer parameters between physically adjacent stations be minimal and that the solutions be statistically stable. This, in effect, may be termed a $1\frac{1}{2}$ -dimensional problem and the inversion technique will be demonstrated using a two-station example (extension to higher dimensions is straightforward) which in the MT case may be effected by the simultaneous inversion of the phase data from a problematical site and the unbiased apparent resistivity and phase data from the neighbouring location. The data and constraining equations are partitioned in the form $A_* \mathbf{x}_* = \mathbf{y}_*$ and given by (Meju, 1988)

$$\begin{bmatrix} A_1 & \dots & 0 \\ \dots & \dots & \dots \\ 0 & \dots & A_1 \\ \dots & \dots & \dots \\ 1 & \dots & -1 \\ 1 & \dots & -1 \\ \dots & \dots & \dots \\ 1 & \dots & -1 \end{bmatrix} \begin{bmatrix} \mathbf{x}_{11} \\ \mathbf{x}_{21} \\ \vdots \\ \mathbf{x}_{p1} \\ \dots \\ \mathbf{x}_{12} \\ \mathbf{x}_{22} \\ \vdots \\ \mathbf{x}_{p2} \end{bmatrix} = \begin{bmatrix} \mathbf{y}_{11} \\ \mathbf{y}_{21} \\ \vdots \\ \mathbf{y}_{n1} \\ \dots \\ \mathbf{y}_{12} \\ \mathbf{y}_{22} \\ \vdots \\ \mathbf{y}_{n'2} \\ \dots \\ h_1 \\ h_2 \\ \vdots \\ h_p \end{bmatrix} \quad (10.5.1)$$

where A_* is an $(n+n'+p) \times (p+p)$ global matrix containing the partial derivatives A_1, A_2 plus the $p \times 2p$ smoothness matrix for the two stations, \mathbf{x}_* contains the solution vectors \mathbf{x}_1 and \mathbf{x}_2 each of dimension $p \times 1$, and the vector \mathbf{y}_* contains the discrepancy vectors $\mathbf{y}_{1(n \times 1)}$ and $\mathbf{y}_{2(n' \times 1)}$ plus the augmenting data h_1, \dots, h_p which are the desired differences in the values of the corresponding layer parameters. In this example h is the null vector.

The coupled optimization problem is stated as minimize the Lagrangean function

$$\mathcal{L}(\mathbf{m}_*) = (\mathbf{d}_* - f(\mathbf{m}_*))^T (\mathbf{d}_* - f(\mathbf{m}_*)) + \beta^2 (\mathbf{m}_*^T \mathbf{D}_*^T \mathbf{D}_* \mathbf{m}_*) \quad (10.5.2)$$

or its linearized equivalent

$$\mathcal{L}(\mathbf{m}_*^0 + \mathbf{x}_*) = (\mathbf{y}_* - \mathbf{A}_* \mathbf{x}_*)^T (\mathbf{y}_* - \mathbf{A}_* \mathbf{x}_*) + \beta^2 \{ (\mathbf{m}_*^0 + \mathbf{x}_*)^T \mathbf{D}^T \mathbf{D} (\mathbf{m}_*^0 + \mathbf{x}_*) \} \quad (10.5.3)$$

where β is an undetermined multiplier, \mathbf{m}_* is the sought joint set of model parameters and \mathbf{m}_*^0 is our common starting model. We have that

$$\frac{\partial \mathcal{L}}{\partial \mathbf{x}_*} = -2\mathbf{A}_*^T \mathbf{y}_* + 2\mathbf{A}_*^T \mathbf{A}_* \mathbf{x}_* + 2\beta^2 \mathbf{H} \mathbf{m}_*^0 + 2\beta^2 \mathbf{H} \mathbf{x}_* = 0$$

or

$$\mathbf{A}_*^T \mathbf{A}_* \mathbf{x}_* + \beta^2 \mathbf{H} \mathbf{x}_* = \mathbf{A}_*^T \mathbf{y}_* - \beta^2 \mathbf{H} \mathbf{m}_*^0$$

from which we obtain the solution

$$\mathbf{x}_* = [\mathbf{A}_*^T \mathbf{A}_* + \beta^2 \mathbf{H}]^{-1} [\mathbf{A}_*^T \mathbf{y}_* - \beta^2 \mathbf{H} \mathbf{m}_*^0]. \quad (10.5.4)$$

We can also view the problem from a naive (less formal) but more illuminating angle and state the linearized inverse problem as the search for the smoothest solution amongst all possible solutions with $|\mathbf{y}_* - \mathbf{A}_* \mathbf{x}_*|^2 \leq q_T$ (the maximum tolerable misfit), as judged by the the quadratic measure $|\mathbf{x}_1 - \mathbf{x}_2|^2$. We define the Lagrangean function in component form as (Meju, 1988)

$$\begin{aligned} \mathcal{L}(\mathbf{x}_1, \mathbf{x}_2) = & \sum_{j=1}^p (x_{1,j} - x_{2,j})^T (x_{1,j} - x_{2,j}) + \mu^{-1} \left\{ \sum_{i=1}^n [y_{1,i} - \sum_{j=1}^p A_{1,i,j} x_{1,j}]^2 \right. \\ & \left. + \sum_{k=1}^{n'} [y_{2,k} - \sum_{j=1}^p A_{2,k,j} x_{2,j}]^2 - q_T \right\} \end{aligned} \quad (10.5.5)$$

where μ is an undetermined multiplier and the subscripts 1 and 2 indicate the observational station contributing the data; these data have been standardized but the W term is neglected for clarity. Setting the derivatives of \mathcal{L} with respect to the model parameters to zero, we obtain for the first linear approximation (Meju, 1988),

$$\frac{\partial \mathcal{L}(\mathbf{x}_1, \mathbf{x}_2)}{\partial x_{1,j}} = \mathbf{x}_1 - \mathbf{x}_2 + \mu^{-1} (\mathbf{A}_1^T \mathbf{A}_1 - \mathbf{A}_1^T \mathbf{y}_1) = 0$$

giving

$$(A_1^T A_1 + \mu I) x_1 = A_1^T y_1 + \mu x_2$$

and

$$\frac{\partial \mathcal{L}(x_1, x_2)}{\partial x_{2j}} = x_2 - x_1 + \mu^{-1} (A_2^T A_2 - A_2^T y_2) = 0$$

giving

$$(A_2^T A_2 + \mu I) x_2 = A_2^T y_2 + \mu x_1$$

so that

$$x_1 = (A_1^T A_1 + \mu I)^{-1} (A_1^T y_1 + \mu x_2) \quad (10.5.6)$$

and

$$x_2 = (A_2^T A_2 + \mu I)^{-1} (A_2^T y_2 + \mu x_1). \quad (10.5.7)$$

The above equations (10.5.6 and 10.5.7) must be solved simultaneously for the solutions and may be applied successively to recover the desired model. It is clear that the above solutions are coupled via μ . If the constraining equations are weighted more heavily than the data equations then the differences between the values of the parameters are minimized at the expense of increasing the prediction error of the other equations. A very small value of μ would produce the usual rough models. The regularization factor μ is determined by trial and error and a value is accepted if the permissible misfit q_T is satisfied. This technique was suggested for the magnetotelluric static shift problem (Meju, 1988) and may be interpreted as moving a resolving kernel across the surface instead of down the geoelectric section as is customary in geophysical inversion of one-dimensional depth-soundings. With appropriate constraints for example, one might deduce a smoother and less distorted resistivity cross-section for a set of depth soundings than would be obtained using conventional interpretation strategies. We will now proceed to proper multi-dimensional inversion of geophysical data.

10.6 Inversion of Potential Field Data

We have shown how potential field data may be corrected for temporal and spatial variations during routine processing by application of inverse problem theory. We shall look at another aspect of data analysis in which geological targets of interest are delineated using field data. This process will be referred to as data interpretation.

10.6.1 Interpretation of Aeromagnetic Data

A rapid and cost-effective way of exploring vast land areas is by airborne magnetic surveys. Aeromagnetic surveys find application in mineral exploration in basement areas and in petroleum exploration of sedimentary basins among other uses. Consider the problem of interpreting aeromagnetic data from a sedimentary basin with the objective of determining the depth to the basement and any structural features that may be important in petroleum resource evaluation. The intrabasement anomalies often targeted for analysis may be due to several independent two-dimensional (2-D) or three-dimensional (3-D) bodies of arbitrary shapes some of which can be approximated by prisms having arbitrary orientations and magnetizations.

10.6.1.1 2-D Interpretation of Intrabasinal Anomalies

The observable response due to a simple 2-D body (e.g., a dyke-like feature) may be simulated as that of a vertical semi-infinite 2-D prism (see Fig. 10.6.1). Thus, shallow sources due to faults and vertical intrusions in a sedimentary basin could be modelled as thin prisms while the topography of the basement may be approximated by deep sources in the form of thick prisms. Considering the vertical prism model shown in Fig. 10.6.1, there are six parameters of interest to us, namely the depth to the top of the prism z_j , the horizontal positions of the two edges of the prism x_i and x_{j+1} , the intensity of magnetisation J_j , the inclination of magnetisation I_j , and the general datum term ΔT_0 . In typical exploration situations, there could be several 2-D bodies in the surveyed area such that our field observations may have contributions from more than one prisms in our model for the basin. For this idealized scenery, we note that the observable magnetic field intensity at a point x_i due to the j^{th} prism may be obtained as (Leite & Leao, 1985)

$$\Delta T_j(x_i) = 2J_j \left\{ A_{0j} \left\{ \tan^{-1}(C_{ij}/z_j) - \tan^{-1}(D_{ij}/z_j) \right\} + 0.5B_{0j} \ln(E_{ij}/F_{ij}) \right\} \quad (10.6.1)$$

and the total contribution due to k independent bodies for the i^{th} datum ($i = 1, 2, \dots, n$) is simply

$$\Delta T(x_i) = \sum_{j=1}^k \Delta T_j(x_i) + \Delta T_0 \quad (10.6.2)$$

where $A_{0j} = \alpha_0 \alpha_j - \gamma_0 \gamma_j$, $B_{0j} = \alpha_0 \gamma_j + \alpha_j \gamma_0$, $C_{ij} = x_j - x_i$, $D_{ij} = x_{j+1} - x_i$, $E_{ij} = D_{ij}^2 + z_j^2$ and $F_{ij} = C_{ij}^2 + z_j^2$.

The quantities α_j and γ_j are the direction cosines of the magnetization vector of the j^{th}

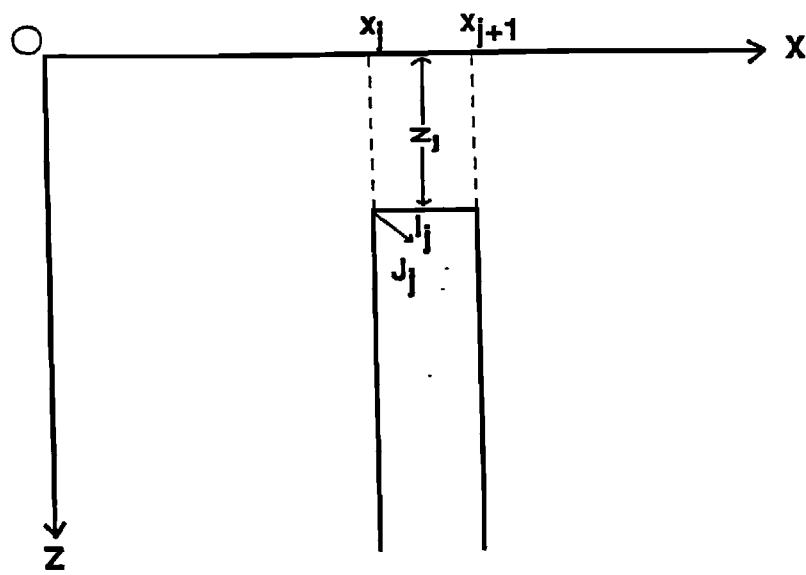


Fig. 10.6.1 Vertical prism model for the magnetic computations. The prism extends over a long distance in the strike direction, Y.

body while α_0 and γ_0 are those of the geomagnetic field vector of magnitude T and are given by

$$\alpha_j = \cos I_j \cos D_j \quad (10.6.3)$$

and

$$\gamma_j = \sin I_j, \quad (10.6.4)$$

for $j = 0, \dots, k$, where D is the declination.

Calculation of Partial Derivatives

The partial derivatives required for the inverse problem of determining the parameters of the 2-D bodies from practical data are obtained by differentiating eq. (10.6.2) with respect to each of the six model parameters. Thus, as in Leite and Leao, we have that

$$\frac{\partial \Delta T(x_i)}{\partial z_j} = 2J_j \left\{ A_{0j}(D_{ij}/E_{ij} - C_{ij}/F_{ij}) + B_{0j}(z_j/E_{ij} - z_j/F_{ij}) \right\} \quad (10.6.5)$$

$$\frac{\partial \Delta T(x_i)}{\partial x_j} = 2J_j \left\{ A_{0j}(z_j/F_{ij}) - B_{0j}(C_{ij}/F_{ij}) \right\} \quad (10.6.6)$$

$$\frac{\partial \Delta T(x_i)}{\partial x_{j+1}} = 2J_j \left\{ -A_{0j}(z_j/E_{ij}) + B_{0j}(D_{ij}/E_{ij}) \right\} \quad (10.6.7)$$

$$\frac{\partial \Delta T(x_i)}{\partial J_j} = \frac{\Delta T_j(x_i)}{J_j} \quad (10.6.8)$$

$$\frac{\partial \Delta T(x_i)}{\partial \Delta T_0} = 1 \quad (10.6.9)$$

and

$$\frac{\partial \Delta T(x_i)}{\partial I_j} = 2J_j \left\{ A'_{0j} \left\{ \tan^{-1}(C_{ij}/z_j) - \tan^{-1}(D_{ij}/z_j) \right\} + 0.5B'_{0j} \ln(E_{ij}/F_{ij}) \right\} \quad (10.6.10)$$

where $A'_{0j} = (-\alpha_0 \sin I_j \cos D_j) - \gamma_0 \cos I_j$ and $B'_{0j} = (\alpha_0 \cos I_j - \gamma_0 \sin I_j \cos D_j)$.

A typical inversion algorithm would require as input the geomagnetic field and a guess model assuming that the field data have already been subjected to the standard

processing techniques (e.g., smoothing and regional-residual separation). The solution to the inverse problem $\text{minimize } q(\mathbf{m}) = | \mathbf{d} - \mathbf{f}(\mathbf{m}) |^2$ may be obtained using any standard optimization method but the most popular schemes are the regularized matrix inversion methods and the conjugate-gradient techniques.

10.6.2 Interpretation of Gravity Data

The interpretation of gravity anomalies due to 2-D and 3-D structures of arbitrary shapes is an inverse problem that can be handled using the generalized matrix inversion techniques discussed previously. The key task here is the solution of the forward problem. If the forward solution is known for bodies of uniform densities and irregular shapes, then we can easily retrieve the subsurface density distribution (or the parameters of the 2-D/3-D bodies) that will explain a given set of observations. In the application of inverse theory, we need to compute the partial derivatives of the models and have to incorporate some form of constraints on the solution process to avoid instabilities. The gravity problem is generally non-unique, and it is thus desirable to incorporate any available (and reliable) *a priori* information in the problem formulation. Since the forward problem holds the key to a successful interpretation, it is appropriate that we start by considering 2-D forward models of the subsurface. The well-known Pedersen (1977) model and some applications of the hugely popular Talwani method (Talwani et al., 1959) will be discussed.

10.6.2.1 Interpretation of Intrabasinal Anomalies using Pedersen's 2-D Model

Consider the problem of sedimentary basin evaluation for hydrocarbon resources. An important interpretation problem here is the determination of a single 2-D interface between the sediments and the basement as this information can be used to delineate areas worthy of further detailed exploration. For such a task, we can adopt Pederson's mathematical model.

Let ρ_1 and ρ_2 be the densities of the sediments and basement respectively and consider the observed gravity field along a profile to be the sum of the signatures contributed by a stack of prisms or overlapping dyke-like bodies which extend infinitely in the strike direction and whose upper surface define the sediment-basement boundary (see Fig. 10.6.2). The density contrast between the basement and the sediments is $\Delta\rho = \rho_1 - \rho_2$. In many practical situations, the gravity data are processed to yield the

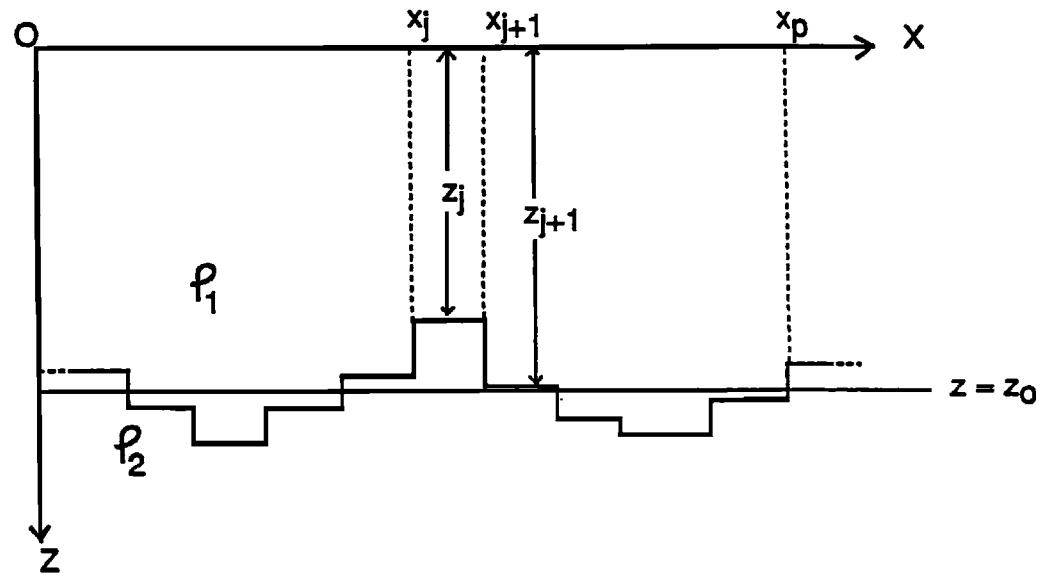


Fig. 10.6.2 Contiguous prisms representing basement of density ρ_2 with overlying sediments of density ρ_1 .

residual anomalies implying that the regional gravity effect associated with some reference depth z_0 has been removed. In this situation, for prismatic bodies with the j^{th} prism having edges x_j and x_{j+1} (Fig. 10.6.2), the observable gravity response at some profile position x_i is given by

$$\begin{aligned}\Delta g(x_i) = & -G\Delta\rho \sum_{j=2}^{m-1} \left\{ C_{ji} \ln \frac{C_{ji}^2 + z_j^2}{C_{ji}^2 + z_0^2} - D_{ji} \ln \frac{D_{ji}^2 + z_j^2}{D_{ji}^2 + z_0^2} + 2z_j \left(\tan^{-1} \frac{C_{ji}}{z_j} - \tan^{-1} \frac{D_{ji}}{z_j} \right) \right. \\ & \left. - 2z_0 \left(\tan^{-1} \frac{C_{ji}}{z_0} - \tan^{-1} \frac{D_{ji}}{z_0} \right) \right\} - G\Delta\rho \sum_{j=1,m} \left\{ \pi(z_j - z_0) + \delta_j D_{ji} \ln \frac{D_{ji}^2 + z_0^2}{D_{ji}^2 + z_j^2} \right. \\ & \left. + 2\delta_j z_0 \tan^{-1} \frac{D_{ji}}{z_0} - 2\delta_j z_j \tan^{-1} \frac{D_{ji}}{z_j} \right\} \end{aligned} \quad (10.6.11)$$

where $C_{ji} = (x_{j+1} - x_i)$ and $D_{ji} = (x_j - x_i)$, G is the universal gravitational constant, and δ_j is equal to -1 if $j=1$ and equal to 1 if $j=m$ (note that in the last summation j is either 1 or m).

If ρ_1 , ρ_2 and z_0 are specified and it is intended to find the 2-D topography, i.e., the set of values z_j that would explain the field observations, then the partial derivatives of the model data with respect to the parameters z_j are given by (Pedersen, 1977)

$$\frac{\partial \Delta g(x_i)}{\partial z_j} = \begin{cases} -2G\Delta\rho \left\{ \tan^{-1}(C_{ji}/z_j) - \tan^{-1}(D_{ji}/z_j) \right\} & , j = 1, 2, \dots, m-1 \\ -G\Delta\rho \left\{ \pi - 2\delta_j \tan^{-1}(D_{ji}/z_j) \right\} & , j = 1, m \end{cases} \quad (10.6.12)$$

where $i=1,2,\dots,n$ are the indices of the observational stations. For a more general 2-D interpretation, we shall examine the Talwani model next.

10.6.2.2 Modelling of 2-D bodies of arbitrary shapes using Talwani's method

A 2-D subsurface feature of irregular shape may be conceptually viewed as a polygon having a similar shape and physical property – a kind of scaled down model of the real body. The gravitational attraction of such an n -sided polygon can be calculated and constitutes the forward problem. Consider the 2-D body shown in Fig. 10.6.3. If we

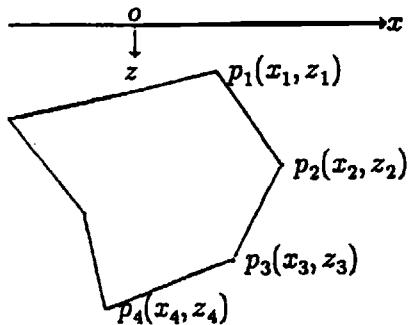


Fig. 10.6.3 Cross-section of a polygon representing a 2-D subsurface body.

assume that it extends to great distances in the strike direction (which is mutually perpendicular to the x- and z-directions), then the attraction at an observational position, O along the x-axis is given by (see also Grant & West, 1967)

$$\Delta g = 2G\Delta\rho \sum_{k=1}^{n_{sides}} \left\{ \frac{b_k}{(1+a_k^2)} \right\} \left\{ \frac{1}{2} \ln \left(\frac{x_{k+1}^2 + z_{k+1}^2}{x_k^2 + z_k^2} \right) \right\} + a_k \left\{ \tan^{-1} \left(\frac{x_{k+1}}{z_{k+1}} \right) - \tan^{-1} \left(\frac{x_k}{z_k} \right) \right\} \quad (10.9.1)$$

where $a_k = (x_{k+1}-x_k)/(z_{k+1}-z_k)$, $b_k = (x_k z_{k+1} - x_{k+1} z_k)/(z_{k+1}-z_k)$, G is the universal gravitational constant, and $\Delta\rho$ is the density contrast of the body with the surrounding medium.

The parameters of the model are the density contrast with the surrounding medium $\Delta\rho$ and the (horizontal and vertical) coordinates of the n -sided 2-D body. The computation of the partial derivatives of the model is straightforward and in the case of the density parameter we simply have that

$$\frac{\partial \Delta g}{\partial \Delta\rho} = 2G \sum_{k=1}^{n_{sides}} \left\{ \frac{b_k}{(1+a_k^2)} \right\} \left\{ \frac{1}{2} \ln \left(\frac{x_{k+1}^2 + z_{k+1}^2}{x_k^2 + z_k^2} \right) \right\} + a_k \left\{ \tan^{-1} \left(\frac{x_{k+1}}{z_{k+1}} \right) - \tan^{-1} \left(\frac{x_k}{z_k} \right) \right\}. \quad (10.9.2)$$

10.6.2.3 Implementing a Gravity Inversion Algorithm

The idea here is to point out that apart from the forward problem, the main difference between one-dimensional inversion and multi-dimensional inversion is in the dimensions of the vectors and matrices involved. An optimization or minimization routine used for resistivity inversion say, can easily be adapted to handle the gravity or magnetic problem. For illustration, the ridge regression routine used in the 1-D Wenner resistivity

inversion (Sec. 10.3.3.4) is adapted to a 2-D gravity inversion problem using a variant of the popular Talwani forward algorithm. The program (GRAVINV) is listed in Appendix C and is self-explanatory but we will explain one important practical aspect of gravity data analysis. A common, but by no means mandatory, pre-interpretation practice is to separate out regional effects from the observed data. The resulting data set is referred to as the residual gravity anomaly. It is therefore a good practice to build this aspect of data processing into an inversion program. There are several ways of estimating regional gradients but we will restrict ourselves to simple trend estimation using the method of least squares. A simple implementation of the classical least squares scheme is illustrated in the sub-program SIMPREG listed below.

```

      subroutine SIMPREG(n,x,y,y2,ey2)
c   a simple routine for estimating the regional trend for potential field data
c   using a linear regression technique. estimates regional gradient
c   and the associated errors based on data scatter, aerr and berr.
c   input: x=position; y=potential field data; n=number of data.
c   output: y2= regional trend ; ey2=estimation error in y2.
c-----
      dimension x(100),y(100),xx(100),xy(100),ey2(100),y2(100)
c   initializations
      sumx=0.0
      sumxx=0.0
      sumxy=0.0
      sumy=0.0
      calculate required quantities xx,xy and sums
      do 10 i=1,n
         xx(i)=x(i)*x(i)
         xy(i)=x(i)*y(i)
         sumx=sumx+x(i)
         sumxx=sumxx+xx(i)
         sumxy=sumxy+xy(i)
         sumy=sumy+y(i)
10   continue
      calculate the common denominator and the desired regression parameters.
      den=n*sumxx-(sumx*sumx)
      b=(n*sumxy-(sumx*sumy))/den

```

a=(sumy*sumxx-sumx*sumxy)/den
calculate root mean square errors in a,b.

```
sse=0.0
do 20 i=1,n
  e=y(i)-a-(b*x(i))
  sse=sse+(e*e)
20  continue
rmsq=sse/(n-2)
aerr=rmsq*sumxx/den
berr=n*rmsq/den
do 30 i=1,n
  y2(i)=a+b*x(i)
  fmin=(a-aerr)+(b-berr)*x(i)
  fmax=(a+aerr)+(b+berr)*x(i)
  ey2(i)=(abs(fmin)+abs(fmax))/2.
30  continue
return
end
```

This subroutine is used in the gravity inversion program listed in the appendix where the residual anomaly is simply taken as the difference between the observed gravity anomaly and the calculated regional trend. The computer program allows for the interpretation of either the original field data or the residual anomaly.

10.6.2.4 Aspects of Gravity Inverse Problem

The general inverse problem is nonlinear but we can reduce the non-linearity by choosing an appropriate parameterization. Consider the inverse problem in which the dimensions of a body are specified and we are required to determine its density from some given gravity observations. As demonstrated by the test summarised in Figure 10.6.4a, as the bulk density of a body of fixed geometrical dimensions is varied, the gravity response at an observational point, O situated at a distance d from the body shows a linear relationship. The slope of this linear change in gravity response depends on the separation, d . On the other hand, if the density of a body is specified (e.g., from intersecting borehole measurements) and we are required to determine its shape from the observed gravity data, then we are dealing with a different kind of inverse problem.

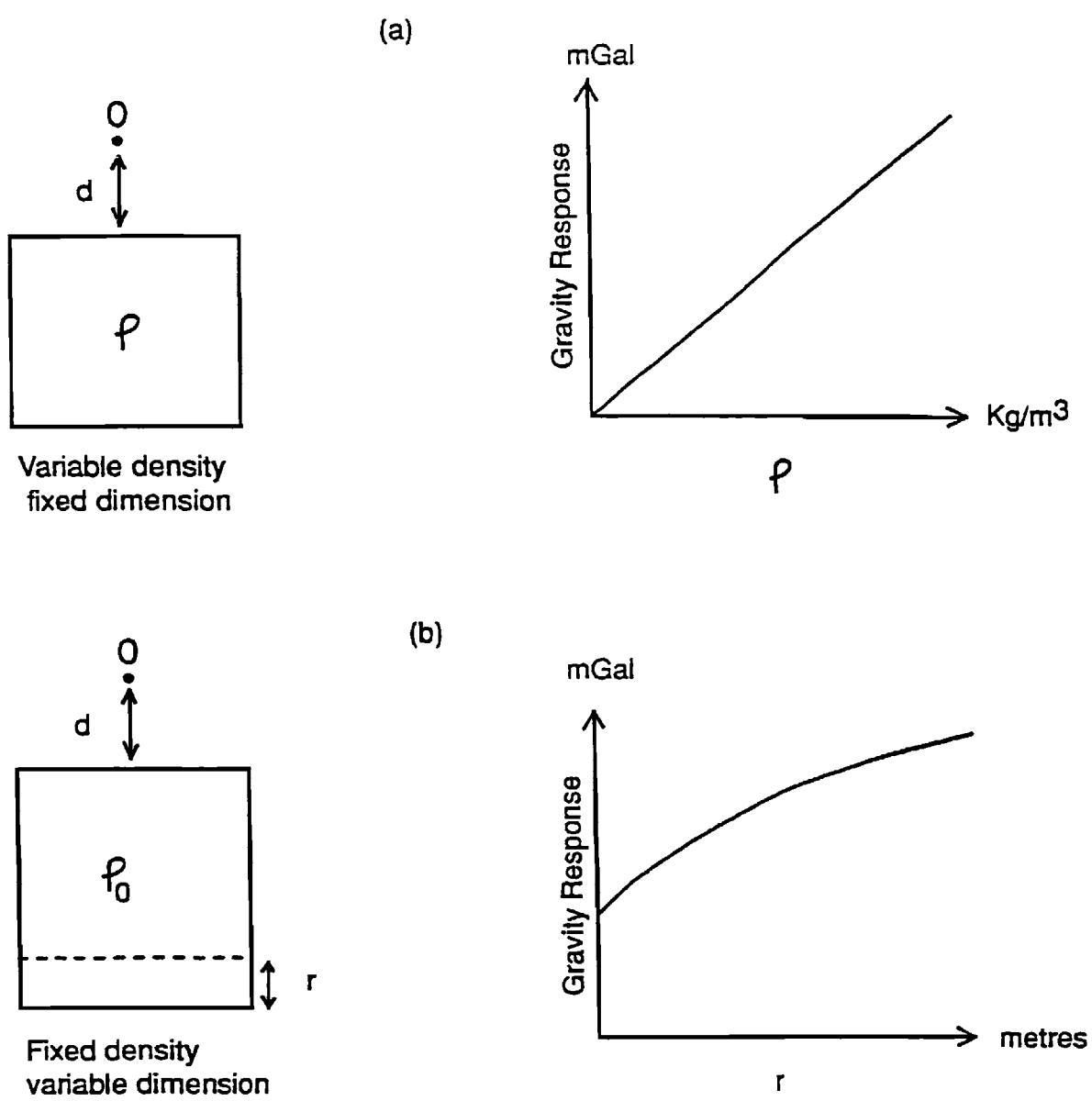


Fig. 10.6.4 Gravity response at a point O as (a) ρ is varied with block size held constant and (b) ρ is fixed as block size is varied

As illustrated for a simple body of fixed density in Fig. 10.6.4b, the response at point O as the physical dimensions of the test body is varied by extending or shortening its base shows a non-linear relationship. The gravity effect of varying both the shape and density to fit a given set of experimental data will obviously show a non-linear behaviour and is left to the imagination of the reader. In any case, it can be gleaned from these simple tests that we could in principle reduce the inherent non-linearity in the interpretation of practical data by using *a priori* information derived from say, geological data or other geophysical results from the area. Let us now demonstrate the above concepts using typical crustal exploration data.

In Fig. 10.6.5 is shown a 2-D model for magnetotelluric (MT) and gravity data across the Caledonides of Scotland (Meju, 1988). The geometrical shapes in the model were determined by separate 2-D modelling studies of MT data across the region. The resulting model was used initially to fix the geometry of the gravity interpretation problem which reduced it to the search for the optimal density distribution that will explain the gravity anomalies. At some locations not constrained by the MT data, the shapes of the bodies were inferred from geological considerations. This is the simplest approach to gravity inversion. Notice the good fit of the integrated model response to the data. The same gravity data were inverted for the subsurface density distribution, this time allowing both the shapes and density contrasts of the bodies to be varied. The results are shown in Fig. 10.6.6. This operation required a powerful two-stage minimization by ridge regression as described in Chapter 7 (see also Meju, 1992). Note the good fit between the model response and the field data and the structural concordance with the model shown in Fig. 10.6.5. The agreement between the model shown in Fig. 10.6.5 and high resolution seismic reflection images of the deep crust and upper mantle in the region was demonstrated in Meju (1988) and underlines the need for an integrated approach to geophysical data analysis.

10.6.3 Joint Inversion of Magnetic and Gravity Data

Magnetic and gravity anomalies may have the same source (or at least the signatures may be due to structures which have some common geometric elements) and useful information can be obtained when both data sets are simultaneously inverted for the shape and position of the causative bodies characterised by constant unknown density and susceptibility contrasts. This is a nonlinear inverse problem and may be formulated as in our previous treatment of joint inversion of resistivity data.

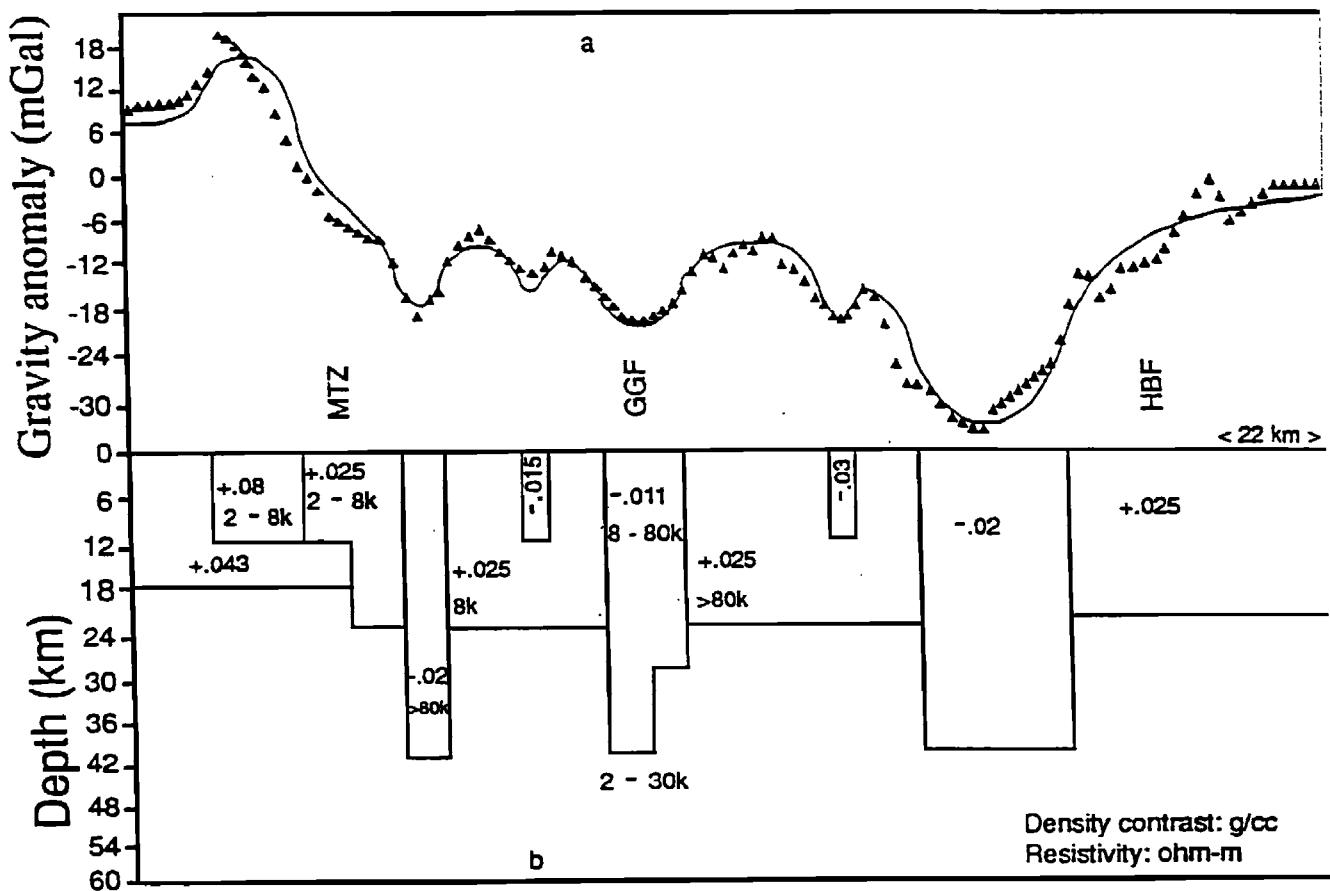


Fig. 10.6.5 An integrated geophysical model for the Caledonides of northern Scotland (Meju, 1988). (a) Bouguer gravity anomaly; (b) MT/gravity model.

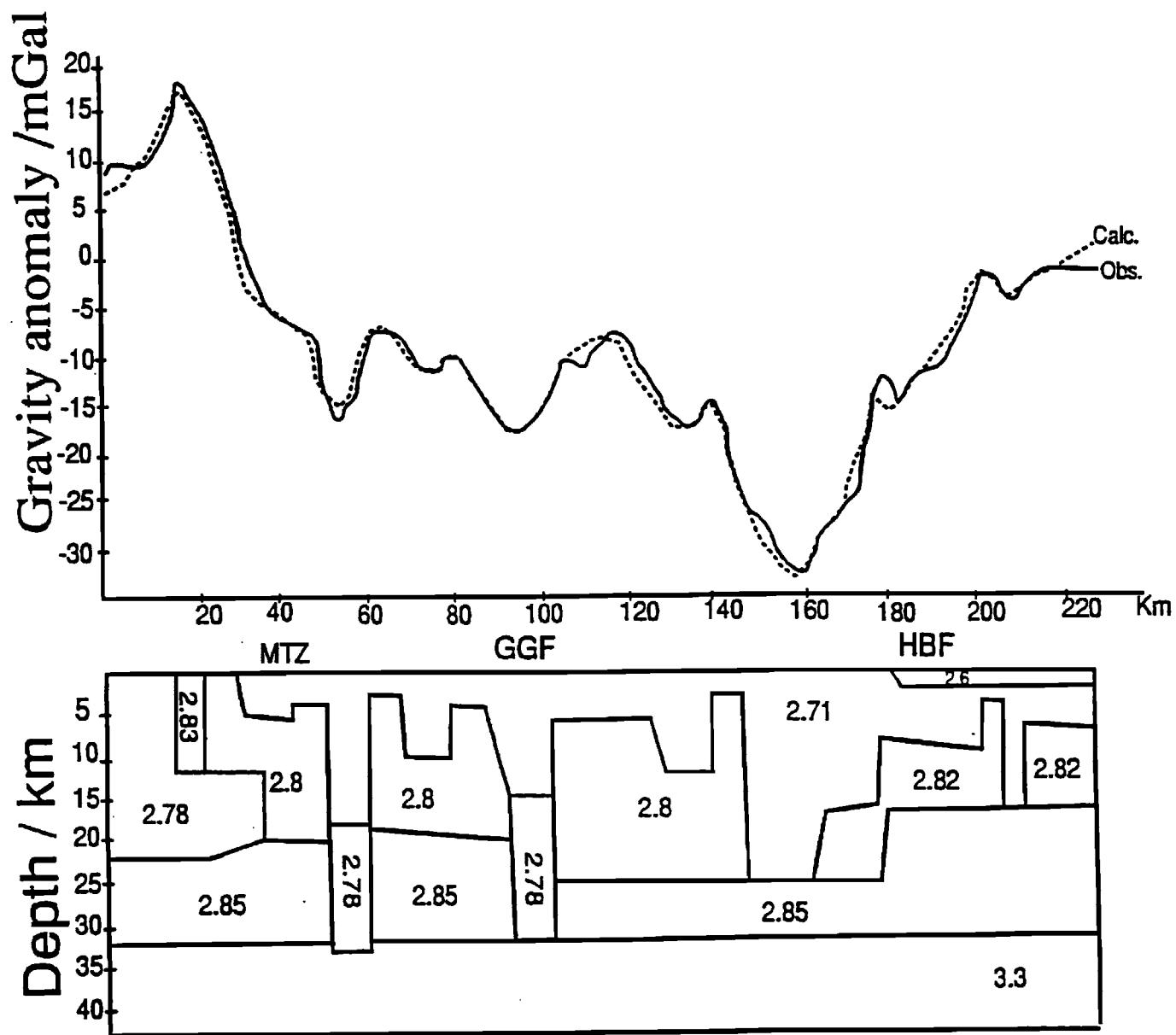


Fig. 10.6.6 A 2D regional gravity model for the Caledonides of Northern Scotland

If the observed magnetic and gravity data are d_m and d_g respectively, they are related to the np model parameters \mathbf{m} characterising the anomalous subsurface bodies by

$$d_m = f_m(\mathbf{m}) + e_m$$

and

$$d_g = f_g(\mathbf{m}) + e_g$$

where the nonlinear forward functionals f_m and f_g have been described in the preceding sections and e_m and e_g are the vectors of additive noise in the measurements. The joint data set is simply

$$\mathbf{d} = \begin{bmatrix} d_m \\ \dots \\ d_g \end{bmatrix}$$

and is of dimension $(nm + ng) \times 1$ where there are nm magnetic observations and ng gravity data. Similarly, the joint prediction model may be expressed as

$$f(\mathbf{m}) = \begin{bmatrix} f_m(\mathbf{m}) \\ \dots \\ f_g(\mathbf{m}) \end{bmatrix}$$

leading to the relation

$$\mathbf{d} = f(\mathbf{m}) + \mathbf{e}.$$

Linearizing about an initial model \mathbf{m}^0 leads to the familiar problem

$$\mathbf{y} = \mathbf{Ax} + \mathbf{e}$$

where \mathbf{x} is the sought parameter correction vector,

$$\mathbf{y} = \begin{bmatrix} \mathbf{y}_m \\ \dots \\ \mathbf{y}_g \end{bmatrix} \text{ and } \mathbf{A} = \begin{bmatrix} \mathbf{A}_m \\ \dots \\ \mathbf{A}_g \end{bmatrix}.$$

Here, $\mathbf{y}_m = d_m - f_m(\mathbf{m}^0)$, $\mathbf{y}_g = d_g - f_g(\mathbf{m}^0)$, $\mathbf{A}_m = \partial f_m(\mathbf{m}^0) / \partial \mathbf{m}^0$ and $\mathbf{A}_g = \partial f_g(\mathbf{m}^0) / \partial \mathbf{m}^0$. Note that the matrix of partial derivatives, \mathbf{A} is of dimension $(nm + ng) \times np$ and the column vector \mathbf{y} is of dimension $(nm + ng) \times 1$. The system of equations may be solved using any of the standard procedures. It should be pointed out that since the gravity and magnetic data are in different units, a useful stabilizing strategy in joint inversion is

to employ some form of scaling for y_m , y_g , A_m and A_g before they are assembled in the joint matrix A and joint vector y . After solving the least squares normal equations, the resulting solution must be appropriately re-scaled to yield the correction vector π . A constrained inversion formula is recommended for solving the inverse problem and any available *a priori* information may be scaled and appended onto the system of equations for better model identification.

Acknowledgements: Some of the data used in the exercises in this course note were taken from published and unpublished accounts and the author is eternally grateful to the various sources.

REFERENCES

- Anderson, W.L., 1979. Numerical integration of related Hankel transforms of orders 0 and 1 by adaptive digital filtering. *Geophysics*, 44, 1287-1305.
- Backus, G.E. & Gilbert, J.F., 1967. Numerical application of a formalism for geophysical inverse problems. *Geophys. J.R. Astr. Soc.*, 13, 247-276.
- Backus, G.E. & Gilbert, J.F., 1968. The resolving power of gross earth data. *Geophys. J. R. Astr. Soc.*, 16, 169-205.
- Backus, G.E. & Gilbert, J.F., 1970. Uniqueness in the inversion of inaccurate gross earth data. *Phil. Trans. R. Soc. A*, 266, 123-192.
- Biwen, X., and Barker R., 1993. Filter coefficients for offset Wenner and Wenner resistivity sounding interpretation. *Computers & Geosciences* (in press).
- Cloutier, J.R., 1983. A technique for reducing low-frequency, time-dependent errors present in network-type surveys. *J. Geophys. Res.*, 88, 659-663.
- Constable, S.C., Parker, R.L., & Constable, C.G., 1987. Occam's inversion: A practical algorithm for generating smooth models from electromagnetic sounding data, *Geophysics*, 52, 289-300.
- Constantinides, A., 1987. *Applied Numerical Methods with personal computers*. McGraw-Hill Book Co.
- Cooke, D.A., and Schneider, W.A., 1983. Generalized linear inversion of reflection seismic data. *Geophysics*, 48, 665-676.
- Duijndam, A.J.W., 1988. Bayesian estimation in seismic inversion. Part I : Principles, *Geophysical Prospecting*, 36, 878-898.
- Duijndam, A.J.W., 1988. Bayesian estimation in seismic inversion. Part II: Uncertainty Analysis, *Geophysical Prospecting*, 36, 899-918.
- Eckart, C. & Young, G., 1939. A principal axis transformation for non-Hermitian matrices, *Amer. Math. Soc. Bull.*, 45, 118-121.
- Gaver, D.P., 1966. Observing stochastic processes and approximate transform inversion. *Oper. Res.*, 14, 444-459.
- Ghosh, D.P., 1971. The application of linear filter theory to the direct interpretation of geoelectrical resistivity sounding measurements. *Geophys. Prosp.*, 19, 192-217.
- Gol'tsman, F.M., 1976. The combination of observations in the identification of geophysical objects, *Izv., Earth Physics*, no. 7, 40-54.
- Gol'tsman, F.M., 1975. Statistical theory for the interpretation of geophysical fields, *Izv., Earth Physics*, no.1, 29-53., translated by M.N.Pillai.
- Gol'tsman, F.M., 1971. Statistical models of interpretation. Science (Nauka) Press, Moscow.

- Grant, F.S., and West, G.F., 1967. Interpretation theory in applied geophysics. McGraw Hill. New York.
- Grivelet, P.A., 1985. Inversion of vertical seismic profiles by iterative modeling. *Geophysics*, 50, 924-930.
- Hattingh, M., 1988. A new data adaptive filtering program to remove noise from geophysical time- or space-series data. *Computers & Geosciences*, 14, 467-480.
- Hatton, L., Worthington, M.H. & Makin, J., 1986. *Seismic Data Processing: Theory and Practice*. Blackwell Scientific Publications, pp.139-163.
- Hoerl, A.E. & Kennard, R.W., 1970. Ridge regression: biased estimation for nonorthogonal problems, *Technometrics*, 12, 55-67.
- Jackson, D.D., 1979. The use of *a priori* data to resolve non-uniqueness in linear inversion, *Geophys. J. R. astr. Soc.*, 57, 137-157.
- Jackson, D. D, 1973. Marginal solutions to quasi-linear inverse problems in geophysics: the edgehog method. *Geophys. J. Roy. Astr. Soc.*, 35, 121-136.
- Jackson, D.D., 1972. Interpretation of inaccurate, insufficient, and inconsistent data, *Geophys. J. R. astr. Soc.*, 28, 97-109.
- Jackson, D.D. & Matsu'ura, M., 1985. A Bayesian approach to nonlinear inversion, *J. Geophys. Res.*, 90, 581-591.
- Johansen, H.K., 1975. An interactice computer/graphic-display-terminal system for interpretation of resistitivity soundings. *Geophys. Prosp.*, 23, 449-458.
- Jones, A.G. & Hutton, R., 1979. A multi-station magnetotelluric study in southern Scotland II. Monte-Carlo inversion of the data and its geophysical and tectonic implication, *Geophys. J. R. astr. Soc.*, 56, 351-358.
- Knight, J. H. and Raiche, A. P., 1982. Transient electromagnetic calculations using the Gaver-Stehfest inverse Laplace transform method. *Geophysics*, 47, 47-50.
- Koefoed, O., 1970. A fast method for determining the layer distribution from the raised kernel function. *Geophys. Prosp.*, 18, 564-570.
- Lambeck, K., 1980. *The Earth's variable rotation: geophysical causes and consequences*. Cambridge University Press, 449p.
- Lanczos, C., 1961. *Linear Differential Operators*, Chap. 3, Van Nostrand, London.
- Lavergne, M., and Willm, C., 1976. Inversion of seismograms and pseudo velocity logs. *Geophys. Prosp.*, 25, 231-250.
- Leite, L.W.B., and Leao, J.W.D., 1985. Ridge regression applied to the inversion of two-dimensional aeromagnetic anomalies. *Geophysics*, 50, 1294-1306.
- Levenberg, K., 1944. A method for the solution of certain nonlinear problems in least squares. *Quart. Appl. Math.*, 2, 164-168.

- Marquardt, D.W.,1970. Generalized inverses, ridge regression, biased linear estimation and nonlinear estimation, *Technometrics*, 12, 591-612.
- Matsu'ura, M. & Hirata, N., 1982. Generalized least-squares solutions to quasi-linear inverse problem with a priori information, *J. Phys. Earth*, 30, 451-468.
- McAulay, A.D.,1985. Prestack inversion with plane-layer point-source modelling. *Geophysics*, 50, 77-89.
- Meju, M.A., 1994f. Simple effective resistivity-depth transformations for in-field or real-time data processing. *First Break* (in review).
- Meju, M.A.,1994e. Joint inversion of TEM and MT-phase data: A simple effective remedy for static shift in MT soundings. *Geophysics* (in review).
- Meju, M.A.,1994d. Biased estimation: a simple framework for inversion and uncertainty analysis with prior information. *Geophys. J. Int.*, (in press).
- Meju, M.A., 1994c. A general program for linear parameter estimation and uncertainty analysis. *Computers & Geosciences*, 20, 197-220.
- Meju, M.A., 1994b. Joint TEM and AMT surveys: cost-effective exploration in frontier basin regions. *Proceedings of 10th Petroleum Congress and Exhibition of Turkey*, Ankara; *Geophysics volume*, 157-176.
- Meju, M.A.,1994a. Assessing the role of infiel resistivity image processing in shallow subsurface investigations. *Proceedings of the Symposium on the Application of Geophysics to Engineering and Environmental Problems*, Boston; 19-40.
- Meju, M.A.,1992. An effective ridge regression procedure for resistivity data inversion, *Computers & Geoscience*, 18, 99-118.
- Meju, M.A.,1988. The deep electrical structure of the Great Glen Fault, Scotland. PhD thesis, University of Edinburgh (Jan. 1988)
- Meju, M.A., Fontes, S.L. and Oliveira, M.F.B., 1993. Joint TEM/AMT feasibility studies in Parnaiba Basin, Brazil: geoelectrostratigraphy and groundwater resource evaluation in Piaui State. *3rd International Congress of the Brazilian Geophysical Society*, Rio de Janeiro. Expanded Abstracts, 1373-1378.
- Meju, M.A. and Hutton, V.R.S.,1992. Iterative most-squares inversion : application to magnetotelluric data, *Geophys. J. Int.* 108,758-766.
- Menke,1984. *Introduction to Geophysical Data Analysis: Discrete inverse theory*, Academic Press Inc., Orlando, Florida.
- Meyer,S.L., 1976. *Data Analysis for Scientists and Engineers*. John Wiley, New York.
- Oldenburg, D.W., Scheuer, T., and Levy, S., 1983. Recovery of the acoustic impedance from reflection seismograms. *Geophysics*, 48, 1318-1337.
- Parker, R.L.,1982. The existence of a region inaccessible to magnetotelluric sounding,

- Geophys. J. R. Astr. Soc., 68, 165-170.
- Parasnis, D.S., 1986. Principles of applied geophysics. Chapman and Hall.
- Pedersen, L.B., 1977. Interpretation of potential field data, a generalized inverse approach. Geophys. Prosp., 25, 199-230.
- Pedersen, J. and Hermance, J. F., 1986. Least-squares inversion of one-dimensional magnetotelluric data: an assessment of procedures employed by Brown University. Surveys in Geophysics, 8(2), 187-231.
- Pous, J., Marcuello, A. & Queralt, P., 1987. Resistivity inversion with a priori information, Geophys. Prosp., 35, 590-603.
- Press, W.H., Flannery, B.P., Teukolsky, S.A., and Vetterling, W.T., 1986. Numerical recipes: the art of scientific computing. Cambridge University Press, Cambridge. 818p.
- Raiche, A. P., 1984. The effect of ramp function turn-off on the TEM response of layered earth. Expl. Geophys., 15, 37-41.
- Raiche, A. P., Jupp, D.L.B., Rutter, H. and Vozoff, K., 1985. The joint use of coincident loop transient electromagnetic and Schlumberger sounding to resolve layered structures. Geophysics, 50, 1618-1627.
- Ray, R.D., 1985. Correction of systematic error in magnetic surveys: An application of ridge regression and sparse matrix theory. Geophysics, 50, 1721-1731.
- Seeman, B., and Horowicz, L., 1983. Vertical seismic profiling: separation of upgoing and downgoing acoustic waves in a stratified medium. Geophysics, 48, 555-568.
- Spies, B. R. and Eggers, D.E., 1986. The use and misuse of apparent resistivity in electromagnetic methods. Geophysics, 51, 1462-1471.
- Stehfest, H., 1970b. Remark on Algorithm 368, Numerical inversion of Laplace transforms. Comm. Assn. Comp. Mach., 13, 624.
- Stehfest, H., 1970a. Algorithm 368, Numerical inversion of Laplace transforms. Comm. Assn. Comp. Mach., 13, 47-49.
- Stroud, K.A., 1986. Further Engineering Mathematics: Programmes and Problems. Macmillan Education Ltd. (reprinted 1987).
- Talwani, M., Worzel, J.L., and Landisman, M., 1959. Rapid gravity computations for two-dimensional bodies with application to the Mendocino submarine fracture zone. J. Geophys. Res., 64, 49-59.
- Tanner, M.T., Koehler, F., and Alhilali, K.A., 1974. Estimation and correction of near-surface time anomalies, Geophysics, 39, 441-463.
- Tarantola, A. & Valette, B., 1982. Generalized nonlinear inverse problems solved using the least squares criterion, Review of Geophysics and Space Physics, 20, 219-232.

- Tikhonov, A.N., 1963. Regularization of ill-posed problems, *Doklady Akad. Nauk SSSR*, 153, 1-6.
- Tikhonov, A.N. & Arsenin, V.Y., 1977. *Solution of ill-posed problems*, John Wiley and Sons, Inc.
- Tikhonov, A.N. & Glasko, V.B., 1965. Application of a regularization method to nonlinear problems, *J. Comp. Math. and Math. Physics*, 5, no. 3, 1965.
- Tikhonov, A.N. & Glasko, V.B., 1975. Application of the regularization method to geophysical interpretation problems, *Izv., Earth Physics*, no.1, 38-48, translated by M.N. Pillai.
- Twomey, 1977. *An Introduction to the Mathematics of Inversion in Remote Sensing and Indirect Measurements*, Elsevier Scientific Publ. Co., Amsterdam.
- Vozoff, K., & Jupp, D.L.B., 1975. Joint inversion of geophysical data, *Geophys. J. R. astr. Soc.*, 42, 977-991.
- Wang, R.J., 1977. Adaptive predictive deconvolution of seismic data. *Geophys. Prosp.*, 25, 342-381.
- Wang, R.J., and Trietel, S., 1971. Adaptive signal processing through stochastic approximation. *Geophys. Prosp.*, 19, 718-728
- Widrow, B., and Hoff, M., Jr., 1960. Adaptive switching circuits. *IRE WESCON Conv. Rec.*, pt. 4, 96-104.
- Widrow, B., Glover, J.R. Jr., McCool, J.M., Kaunitz, J., Williams, C.S., Hearn, R.H., Zeidler, J.R., Dong, E. Jr., and Goodlin R., 1975. Adaptive noise cancelling: principles and applications. *Proc. IEEE*, 63, 1692-1716.
- Widrow, B., Mantey, P., Griffiths, L., and Goode, B., 1967. Adaptive antenna systems. *Proc. IEEE*, 55, 2143-2159.
- Widrow, B., McCool, J.M., Larimore, M.G., and Johnson, C.R., Jr., 1976. Stationary and nonstationary characteristics of the LMS adaptive filter. *Proc. IEEE*, 64, 1151-1162.
- Wiggins, R., Larner, K., and Wisecup, R.D., 1976. Residual statics analysis as a general linear inverse problem. *Geophysics*, 41, 922-938.
- Word, D.H., Smith, H.W., and Bostick, F. X., Jr., 1970. An investigation of the magnetotelluric tensor impedance method. Tech. Rep. No. 82, Electr. Geophys. Res. Lab., University of Texas, Austin. 264p.
- Yarger, H.L., Robertson, R.R., and Wentland, R.L., 1978. Diurnal drift removal from aeromagnetic data using least squares. *Geophysics*, 46, 1148-1156.
- Zai-tian, Ma, 1988. Problems of three-dimensional seismic data processing. *Chinese J. Geophys.*, 31, 147-156.

APPENDIX A

SVDINV: A computer program for linear inversion and detailed error analysis program SVDINV

c a detailed illustration of generalised matrix inversion
c using the singular value decomposition (svd) method.
c solves the linear inverse problem of the form d=gm
c and performs uncertainty analyses (model resolution,
c parameter covariances and least squares standard
c deviations, most-squares solution envelopes and extreme
c parameter sets, i.e., model bounds).
c adapted from M.A.Meju, 1994a, Comp. & Geosc.,20,197-220

c-----

```
real g(100,40),u(100,40),ut(40,100),v(40,40),q(40),d(100)
+ ,vqi(40,40),utd(40),gm(100),vt(40,40),r(40,40),cov(40,40)
+ ,stdev(40),qi(40),x(100),m(40)
character*16 infil,outfil,ans*1
```

c describe program capabilities

```
write(*,*)
write(*,*)' This program can tackle the following linear problems'
write(*,*)' (1) simple straight-line fitting for intercept and '
write(*,*)' slope (i.e.,two-parameter problems); [x,y] data'
write(*,*)' pairs required as input in this situation'
write(*,*)' (2) multiple-parameter linear inverse problems; data'
write(*,*)' vector d and design matrix G required as input'
```

c determine form of data and select appropriate input style

```
write(*,'(/a,$)')' is this a simple straight-line problem? [Y:N]'
read(*,'(a1)')ans
if(ans.eq.'Y'.or.ans.eq.'y')then
```

c read [x,y] data pairs and form G-matrix

```
call getdat(ndat,x,d)
ncol=2
do i=1,ndat
g(i,1)=1.
g(i,2)=x(i)
end do
else
```

```

c read data and components of G-matrix from a diskfile
  write(*,'(a,$)')' enter ndat,nparm:>
  read(*,*)ndat,ncol
  write(*,'(a,$)')' enter input filename for d & G :>
  read(*,'(a)')infil
  open(unit=1,file=infil,status='old')
  write(*,'(/a)')' reading data vector d '
    do i=1,ndat
      read(1,*) d(i)
    end do
  write(*,'(/a)')' reading G matrix, row by row '
    do i=1,ndat
      read(1,*)( g(i,j),j=1,ncol)
    end do
  close(1)
  endif
c open result file
  write(*,'(//a,$)')' enter output filename for results:>
  read(*,'(a)')outfil
  open(unit=3,file=outfil,status='new')
c select mode of operation
  write(*,'(/a,$)')' use damping technique ? [y:n] '
  read(*,'(a1)')ans
  if(ans.eq.'Y'.or.ans.eq.'y')then
    write(*,'(/a/)')' select damping type for problem regularisation'
    write(*,*)' for smoothest measures(flat solution), enter [1]'
    write(*,*)' for bias estimation proper (D=I), enter [2]'
    write(*,*)' for Marquardt-Levenberg damping, enter [3]'
    write(*,'(/a,$)')' enter 1, 2 or 3 :>
    read(*,'(I1)')iopt
    write(*,'(a,$)')' enter damping factor (beta) :>
    read(*,*)beta
  constraining equations for the design matrix G. Note: if last parameter is
  c well determined, it may be allowed to float with the others constrained.
  if(iopt.eq.1.or.iopt.eq.2)then
    write(*,'(a,$)')' constrain: ALL [1], all but last [2] ? [1:2]>

```

```
read(*,'(I1)')minus
if(iopt.eq.2)then
minus=minus-1
endif
nrow=ndat+ncol-minus
k=0
do i=ndat+1,nrow
k=k+1
d(i)=0.0
  do j=1,ncol
    g(i,j)=0
  end do
  if(iopt.eq.2)then
    g(i,k)=beta*1.0
  elseif(iopt.eq.1)then
    g(i,k)=beta*1.0
    g(i,k+1)=-beta*1.0
  endif
end do
elseif(iopt.eq.3)then
nrow=ndat
endif
else
c solution damping not required
beta=1.
nrow=ndat
endif
call svd(nrow,ncol,g,u,v,q)
do i=1,ncol
calculate u-transpose
  do j=1,nrow
    ut(i,j)=u(j,i)
  end do
calculate v divided by lambda
  do k=1,ncol
    if(iopt.eq.3)then
```

```

c effect Marquardt-Levenberg-type damping of the singular values
  q(i)=q(i)/(q(i)+beta)**2.
  vqi(k,i)=v(k,i)*qi(i)
  else
    vqi(k,i)=v(k,i)/q(i)
  endif
end do
end do

calculate the inner product ut*d
call inprod(40,100,ncol,nrow,ut,d,utd)

calculate the regression estimates m
call inprod(40,40,ncol,ncol,vqi,utd,m)
write(3,'(/a)')' here are the least squares estimates '
write(3,*) (m(i),i=1,ncol)
write(3,'(/a)')

call inprod(100,40,nrow,ncol,g,m,gm)

calculate data misfit, sumd=|d-Gm|**2 & total misfit,sumt=sumd+|Dm-h|**2
sumt=0.0
do i=1,nrow
  sumt=(d(i)-gm(i))**2+sumt
  if(i.le.ndat)then
    sumd=sumt
  endif
end do
write(3,*)" data misfit d+constr. misfit damping factor"
write(3,*)sumd,sumt,beta

calculate model resolution matrix, r
c first, form v-transpose; then get matrix-product v.vt
  do i=1,ncol
    do j=1,ncol
      if(iopt.eq.3)then
        v(j,i)=v(j,i)*q(i)*qi(i)
      endif
      vt(i,j)=v(j,i)
    end do
  end do

```

```

call mxprod(40,40,ncol,ncol,v,vt,r)
write(3,'(/a)')' resolution information'
do i=1,ncol
  write(3,*)(r(i,j),j=1,ncol)
end do

calculate parameter covariance matrix, cov
  write(*,'(/a,$)')' do you know the variance of data errors? [Y:N]?
  read(*,'(a1)')ans
  if(ans.eq.'Y'.or.ans.eq.'y')then
    write(*,'(a,$)')' enter the variance :> '
    read(*,*)sigma2
  else
    if(ndat.gt.ncol)then
      sigma2=sumd/(ndat-ncol)
    else
      sigma2=sumd
    endif
  endif
  do i=1,ncol
    do j=1,ncol
      if(iopt.eq.3)then
        cov(j,i)=sigma2*r(j,i)/(q(i)+beta)/(q(i)+beta)
      else
        cov(j,i)=sigma2*r(j,i)/q(i)/q(i)
      endif
    end do
  end do

calculate standard deviations (sqrt of diagonal elements of cov-matrix)
  stdev(i)=sqrt(cov(i,i))
  end do
  write(3,'(/a)')' covariance information'
  do i=1,ncol
    write(3,*)(cov(i,j),j=1,ncol)
  end do
  write(3,'(/a)')' standard deviations of estimates'
  write(3,*) (stdev(i),i=1,ncol)

calculate extreme parameter sets or solution envelopes

```

```
call mostsq(iopt,nrow,ncol,g,d,m,sumt,v,vt,q,qi)
close(3)
stop
end

c-----
subroutine GETDAT(ndat,x,y)
dimension x(100),y(100)
character*20 infile,outfile
nerr=0
write(*,'(/a)')
write(*,*)' [x,y] data pairs for line-fitting to be read next!'
write(*,'(/a,$)')' are the data stored as a diskfile ? [Y:N] > '
read(*,'(a1)')ans
if(ans.eq.'y'.or.ans.eq.'Y')then
goto 96
97  write(*,95)infile
nerr=nerr+1
95  format(/' !!! error in opening diskfile: ',a20,' try again !!!')
if(nerr.gt.5)return
96  write(*,'(/a,$)')' enter name of data file (max.20 chars) > '
read(*,'(a20)')infile
open(unit=3,err=97,file=infile,status='old')
n=1
1   read(3,*,err=98)x(n),y(n)
n=n+1
goto 1
98  ndat=n-1
write(*,10)infile,ndat
10  format(/1x,a20,: number of data read = ',i3)
close(unit=3,status='keep')
else
write(*,*)'
write(*,*)' please enter your data line by line: x,y <return> '
write(*,*)' terminate data entry with any character, e.g., * '
n=1
2   read(*,*,err=99)x(n),y(n)
```

```
n=n+1
goto 2
99 ndat=n-1
write(*,11)ndat
11 format(/1x,' please note: number of data read = ',i3)
write(*,'(/a,$)')' save these data in a diskfile ? [Y:N] > '
read(*,'(a1)')ans
if(ans.eq.'y'.or.ans.eq.'Y')then
write(*,'(/a,$)') enter name for diskfile (max.20 chars.) > '
read(*,'(a20)')outfile
open(unit=3,file=outfile,status='new')
do i=1,ndat
  write(3,*) x(i),y(i)
end do
close(unit=3,status='keep')
endif
endif
return
end
```

```
c-----_
      subroutine INPROD(mm,nn,m,n,amx,v1,v2)
c multiplies the matrix amx by vector v1 and returns vector v2
      dimension v1(nn),v2(mm),amx(mm,nn)
      do i=1,m
        sum=0.0
        do j=1,n
          sum=v1(j)*amx(i,j)+sum
        end do
        v2(i)=sum
      end do
      return
    end
```

```
c-----_
      subroutine MXPROD(mm,nn,m,n,a,b,c)
c performs matrix multiplication
      dimension a(mm,nn),b(nn,mm),c(mm,mm)
```

```

do i=1,m
do j=1,m
sum=0.0
do k=1,n
sum=sum+a(i,k)*b(k,j)
end do
c(i,j)=sum
end do
end do
return
end

c-----
subroutine MOSTSQ(iopt,ndat,ncol,G,d,m,qls,v,vt,q,qi)
c linear extremal inversion using the most-squares method.
real g(100,40),d(100),v(40,40),vt(40,40),q(40),qi(40)
+,vqi2(40,40),b(40),vtb(40),vqb(40),ym(100),yp(100),xm(40),xp(40)
real mu,mul,m(40),msp(40,40),msm(40,40)
character*1 opt
logical lenv
write(*,'(/a)')' do you want solution envelopes (E) or extreme
+parameter sets (S) ? '
write(*,'(a,$)')' please enter E or S :> '
read(*,'(a1)')opt
if(opt.eq.'E'.or.opt.eq.'e')then
lenv=.true.
nkol=1
else
lenv=.false.
nkol=ncol
endif
c initialise solution arrays
do i=1,nkol
do j=1,ncol
msp(i,j)=m(j)
msm(i,j)=m(j)
end do

```

```
    end do
    iflag=0
calculate the limits of model parameters consistent with the data
c by a method akin to Jackson (1976)-JGR,v.81,no.5,p.1027-1030.
c-----main loop for nkol extremizations-----
    do ns=1,nkol
c first, form projection vector,b
    do i=1,ncol
        if(lenv)then
            b(i)=1.0
        else
            b(i)=0.0
        endif
    end do
    if(iflag.eq.0)then
c get the maximum permissible misfit (i.e., threshold residual)
        write(*,35)qls
35    format(/1x,' note that least squares residuals, qls =',f14.10)
        write(*,'(/a,$)')' enter desired threshold residual Qt (>Qls) :> '
        read(*,*)qt
c if Qt less than optimal least squares misfit (Qls), skip analysis.
        if(qt.lt.qls)then
            write(*,*)' Qt < Qls, search terminated'
            return
        endif
        endif
        iflag=1
calculate relevant quantities
        b(ns)=1.
        do j=1,ncol
            do i=1,ncol
                if(iopt.eq.3)then
                    vqi2(i,j)=v(i,j)*qi(j)**2.
                else
                    vqi2(i,j)=v(i,j)/q(i)/q(j)
                endif
            end do
        end do
    end do
end iflag
```

```
    end do
    end do
call inprod(40,40,ncol,ncol,vt,b,vtb)
call inprod(40,40,ncol,ncol,vqi2,vtb,vqb)
mul=0.0
do i=1,ncol
if(iopt.eq.3)then
  mul=(vtb(i)*qi(i))**2+mul
else
  mul=(vtb(i)/q(i))**2+mul
endif
end do
mu=sqrt((qt-qls)/mul)
do i=1,ncol
  xms=mu*vqb(i)
calculate and save most-squares estimates
  msm(ns,i)=m(i)-xms
  xm(i)=msm(ns,i)
  msp(ns,i)=m(i)+xms
  xp(i)=msp(ns,i)
end do
calculate residuals for estimates
call inprod(100,40,ndat,ncol,g,xm,ym)
call inprod(100,40,ndat,ncol,g,xp,yp)
sump=0.0
summ=0.0
do i=1,ndat
  sump=sump+(d(i)-yp(i))**2.
  summ=summ+(d(i)-ym(i))**2.
end do
write(*,*)' param.no. misfit-plus misfit-minus Qt'
write(*,*) ns,sump,summ,qt
end do
c -----end of main loop-----
if(lenv)then
  write(3,'(/a)')' most-squares upper and lower solution envelopes'
```

```

else
  write(3,'(/a)')'  most-squares extreme parameter sets '
endif
write(3,*)' plus solutions'
do ns=1,nkol
  write(3,*)(msp(ns,i),i=1,ncol)
end do
write(3,*)' minus solutions'
do ns=1,nkol
  write(3,*)(msm(ns,i),i=1,ncol)
end do
return
end

```

subroutine SVD(n,m,a,u,v,q)

c Singular Value Decomposition routine. Based on R.L.Parker's Fortran
 c translation of an original Algol program from: Wilkinson & Reinsch,1971,
 c Handbook for Automatic Computation Vol 2 - Linear Algebra, pp140-144.
 c Method: The matrix A(n,m) is decomposed. Singular values in Q,
 c Pre-matrix in U. Post-matrix in V. The array E is used as working space.

REAL a(100,40),u(100,40),v(40,40),q(40),e(400)

tol = 1.0e-77

eps = 1.0e-10

do i=1,n

do j=1,m

u(i,j) = a(i,j)

end do

end do

c Householder reduction to bi-diagonal form

g = 0.0

x = 0.0

do i=1,m

e(i) = g

s = 0.0

l = i+1

do j=i,n

```

      s = u(j,i)**2 + s
    end do
    if (s .ge. tol) then
      f      = u(i,i)
      g      = -sign(sqrt(s),f)
      h      = f*g-s
      u(i,i) = f-g
      if (l.le.m) then
        do j=l,m
          s = 0.0
          do k=i,n
            s = u(k,i)*u(k,j) + s
          end do
          f = s/h
          do k=i,n
            u(k,j) = u(k,j) + f*u(k,i)
          end do
        end do
      end if
    else
      g = 0.0
    end if
    q(i) = g
    s   = 0.0
    if (l.le.m) then
      do j=l,m
        s = u(i,j)**2 + s
      end do
    end if
    if (s.ge.tol) then
      f = u(i,i+1)
      g = -sign(sqrt(s),f)
      h = f*g-s
      u(i,i+1) = f-g
      if (l.le.m) then
        do j=l,m

```

```

e(j) = u(i,j)/h
end do
end if
if (l.gt.n) go to 40
do j=1,n
  s = 0.0
  if (l.le.m) then
    do k=l,m
      s = u(j,k)*u(i,k) + s
    end do
    do k=l,m
      u(j,k) = u(j,k) + s*e(k)
    end do
  end if
end do
else
  g = 0.0
end if
40  y = abs(q(i)) + abs(e(i))
  if (y .gt. x) x=y
end do
c  Accumulation of right-hand transforms (v)
  do iback=1,m
    i = m+1-iback
    if (g .ne. 0.0) then
      h = u(i,i+1)*g
      if (l.le.m) then
        do j=l,m
          v(j,i) = u(i,j)/h
        end do
        do j=l,m
          s = 0.0
          do k=l,m
            s = u(i,k)*v(k,j) + s
          end do
          do k=l,m

```

```

    v(k,j) = v(k,j) + s*v(k,i)
end do
end do
end if
end if
if (l.le.m) then
do j=l,m
    v(j,i) = 0.0
    v(i,j) = 0.0
end do
end if
v(i,i) = 1.0
g      = e(i)
l      = i
end do
c   Accumulation of left-hand transforms
do iback=1,m
    i = m+1-iback
    l = i+1
    g = q(i)
    if (l.le.m) then
        do j=l,m
            u(i,j) = 0.0
        end do
    end if
    if (g .ne. 0.0) then
        h = u(i,i)*g
        if (l.le.m) then
            do j=l,m
                s = 0.0
                do k=l,n
                    s = u(k,i)*u(k,j) + s
                end do
                f = s/h
                do k=i,n
                    u(k,j) = u(k,j) + f*u(k,i)
                end do
            end do
        end if
    end if
end do

```

```
    end do
    end do
end if
do j=i,n
  u(j,i) = u(j,i)/g
end do
else
  do j=i,n
    u(j,i) = 0.0
  end do
end if
u(i,i) = u(i,i) + 1.0
end do
c  Diagonalization of bi-diagonal form
eps = eps*x
do kback=1,m
  k = m+1-kback
c  Test F-splitting
10  do lback=1,k
    l = k+1-lback
    if (abs(e(l)).le. eps) goto 30
    if (abs(q(l-1)) .le. eps) goto 20
  end do
c  Cancellation of e(l), if (l.gt.1)
20  c = 0.0
    s = 1
    l1 = l-1
    do i=l,k
      f = s*e(i)
      e(i) = c*e(i)
      if (abs(f) .gt. eps) then
        g = q(i)
        q(i) = sqrt(f*f + g*g)
        h = q(i)
        c = g/h
        s = -f/h
```

```

do j=1,n
    y      = u(j,l1)
    z      = u(j,i)
    u(j,l1) = y*c + z*s
    u(j,i) = -y*s + z*c
end do
end if
end do
c   Test F-convergence
30  z = q(k)
if (l .ne. k) then
c       Shift from bottom 2 x 2 minor
    x = q(l)
    y = q(k-1)
    g = e(k-1)
    h = e(k)
    f = ((y-z)*(y+z) + (g-h)*(g+h))/(2.0*h*y)
    g = sqrt(f*f + 1.0)
    f = ((x-z)*(x+z) + h*(y/(f + sign(g,f))-h))/x
c       Next q-r transformation
    c = 1.0
    s = 1.0
    lplus = l + 1
    do i=lplus,k
        g = e(i)
        y = q(i)
        h = s*g
        g = c*g
        z = sqrt(f*f + h*h)
        e(i-1) = z
        c = f/z
        s = h/z
        f = x*c+g*s
        g = -x*s+g*c
        h = y*s
        y = y*c
    end do
end if
end do

```

```

do j=1,m
    x      = v(j,i-1)
    z      = v(j,i)
    v(j,i-1) = x*c+z*s
    v(j,i)  = -x*s+z*c
end do
z      = sqrt(f*f + h*h)
q(i-1) = z
c      = f/z
s      = h/z
f      = c*g+s*y
x      = -s*g+c*y
do j=1,n
    y=u(j,i-1)
    z=u(j,i)
    u(j,i-1)=y*c + z*s
    u(j,i)=-y*s + z*c
end do
end do
e(1) = 0.0
e(k) = f
q(k) = x
goto 10
end if
c   Convergence
if (z .lt. 0.0).then
c     q is made non-negative
    q(k) = -z
    do j=1,m
        v(j,k) = -v(j,k)
    end do
end if
end do
return
end

```

APPENDIX B

WENINV: A simple demonstration program for nonlinear inversion of Wenner soundings by ridge regression.

program WENINV

C A simple demonstration of nonlinear dc resistivity
C inversion by ridge regression using the SVD method.
C The Wenner/Offset Wenner configuration is assumed and
C inverts data at spacings of 0.5,1,2,4,8,16,.....
C Handles a maximum of 5 layers in the present form.
C Alteration to handle more layers is trivial.
C Author: Meju, M.A.

COMMON/SOLUTION/MOD,N2

REAL RM(5),DM(4),Y(22),MOD(9),DOBS(22),AB(22),DCALC(22)

REAL A(22,9),U(22,9),V(9,9),Q(9),DMB(4),RMB(5)

INTEGER EXITIT

CHARACTER*20 INFILE

C set up flags and perform initializations

SSQ=1.E+10

TOL=0.0003

EXITIT = 0

INTIT=0

N2=1

c read field data stored as [ab,d] pairs: ab=experimental geometry, d=data.

WRITE(*,'(/A,\$)') ' ENTER DATA FILENAME :> '

READ(*,'(A20)')INFILE

OPEN(UNIT=3,FILE=INFILE,STATUS='OLD')

N=1

10 READ(3,*END=99) AB(N),DOBS(N)

N=N+1

GOTO 10

99 CONTINUE

NDAT=N-1

CLOSE(UNIT=3,STATUS='KEEP')

WRITE(*,20)INFILE,NDAT

20 FORMAT(/2X,A20, ' NUMBER OF DATA READ = ',i3)

C read guess model; input parameters are NLAY layer resistivities, RM

```

C and NLAY-1 depths to layer boundaries from the surface, DM.
  WRITE(*,'(/A,$)') ' ENTER NUMBER OF LAYERS IN GUESS MODEL :> '
  READ(*,*) NLAY
  NCOL=NLAY*2-1
  WRITE(*,'(/A)') ' NOW ENTER LAYER RESISTIVITIES (ohm-m): '
  READ(*,*)(RM(I),I=1,NLAY)
  WRITE(*,'(/A)') ' Now enter DEPTHS (metres) to layer BOUNDARIES :'
  READ(*,*)(DM(I),I=1,NLAY-1)

C initiate iterative refinement of guess model
1  CONTINUE
c first solve the forward problem giving DCALC and form discrepancy
c vector Y = Dobs-Dcalc. Obtain Sum of Squares Error, SSE=Y**2.
  CALL MISFIT(NLAY,RM,DM,NDAT,DOBS,DCALC,Y,SSE)
  WRITE(*,30) EXITIT,SSE
30  FORMAT(/' Iteration number = ',I4,: Sum of squares error = ',F10.4)
C check for convergence. are stopping criteria satisfied ?
  IF(SSQ.LT.SSE) THEN
    WRITE(*,*)' DIVERGENCE : ITERATION STOPPED'
    GOTO 999
  END IF
  IF (ABS(SSQ-SSE).LE.TOL) THEN
    WRITE(*,*)' SLOW CONVERGENCE : ITERATION ABORTED'
    GOTO 999
  ENDIF
  SSQ=SSE
C save best solution in arrays RMB and DMB
  DO 40 I=1,NLAY-1
    RMB(I)=RM(I)
    DMB(I)=DM(I)
40  CONTINUE
  RMB(NLAY)=RM(NLAY)
C write out current model
  WRITE(*,'(/A)')' CURRENT MODEL IS AS FOLLOWS '
  WRITE(*,*)(RMB(I),I=1,NLAY)
  WRITE(*,*)(DMB(I),I=1,NLAY-1)
C calculate partial derivatives for the inverse problem

```

```

        CALL PARTIAL(NDAT,DCALC,NLAY,RM,DM,A)
C calculate SVD of A
        CALL SVD(NDAT,NCOL,A,U,V,Q)
c calculate model correction by ridge regression and return updated model
c MOD in common block /SOLUTION/
        CALL RIDGE(Y,NCOL,NDAT,U,V,Q,SSQ0,INTIT,NLAY,RM,DM,DOBS)
C check that control flag is in order and update parameters
        IF(N2.EQ.0)THEN
          GOTO 999
        ELSEIF(N2.EQ.1)THEN
          DO 50 I=1,NLAY-1
            J=I+NLAY
            RM(I)=MOD(I)
            DM(I)=MOD(J)
50      CONTINUE
            RM(NLAY)=MOD(NLAY)
        ENDIF
        EXITIT=EXITIT+1
C repeat iterative operation
        GOTO 1
999  CONTINUE
        WRITE(*,'(/A/)')' *****INVERSION COMPLETED***** '
        WRITE(*,*)' Here are the optimum parameters: RHOS AND DEPTHS'
        WRITE(*,*)(RMB(I),I=1,NLAY)
        WRITE(*,*)(DMB(I),I=1,NLAY-1)
        STOP
        END
C-----
C----- subroutine RIDGE(Y,NCOL,NROW,U,V,Q,SSQ0,INTIT,NR,RM,DM,DOBS)
C RIDGE REGRESSION ROUTINE. M.A.MEJU 1986
C Ref: Meju,M.A.,1992. Computers & Geoscience, vol. 18,99-118.
        COMMON /SOLUTION/P,N2
        REAL Q(9),V(9,9),U(22,9),X(9),QK(0:10)
        + , Y(22),YT(22),UT(9,22),VQ(9,9),UTY(9)
        + , DOBS(22),DCALC(22)
        + , RM(5),DM(4),RT(5),DT(4),H(4),RMD(9),P(9)

```

```
C INITIAL CONSTANTS AND FLAGS
ND=NR-1
FC=1./10.
N2=0
SSQT0=SSQ0
ND=NR-1
NPARM=NR+ND
C SET MARQUARDT DAMPING FACTORS FOR RIDGE REGRESSION
C FIND SMALLEST/LARGEST SINGULAR VALUES QS AND QL
QL=0.00000001
QS=10000000.
DO 10 I=1,NCOL
IF(Q(I).GT.QL)THEN
QL=Q(I)
ELSEIF(Q(I).LT.QS)THEN
QS=Q(I)
END IF
10 CONTINUE
QL=10*QL
QS=QS/10.
CALCULATE TEN SAMPLES OF THE FUNCTION QK = A + BK**2
DO 20 K=1,10
QK(K)=(100*QS-QL+(QL-QS)*FLOAT(K)**2)/99.
20 CONTINUE
QK(0)=0.0
DO 30 IK=1,11
INTIT=INTIT+1
CALCULATE DAMPING FACTOR
BETA=QK(11-IK)**2
C damp Q to avoid singularities, get Q-inverse, and U-transpose
DO 40 I=1,NCOL
QI=Q(I)/(Q(I)**2+BETA)
DO 50 J=1,NROW
UT(I,J)=U(J,I)
50 CONTINUE
CALCULATE V/LAMBDA
```

```
DO 60 K=1,NCOL
  VQ(K,I)=QI*V(K,I)
60  CONTINUE
40  CONTINUE
CALCULATE INNER PRODUCT UT*Y
  CALL INPROD(9,22,NCOL,NROW,UT,Y,UTY)
CALCULATE REGRESSION ESTIMATE X.
  CALL INPROD(9,9,NCOL,NCOL,VQ,UTY,X)
  NN=0
c place bounds on size of perturbations using the Smoothness Criterion of
c JACKSON(1973) GJRAS 35,121-136.
c If SQRT(SUMSQ(X)/NCOL).GT.1, solution not physically realizable.
c therefore, DECREASE SIZE OF X WITHOUT CHANGING ITS DIRECTION
72  SMC=0.0
    DO 80 M=1,NCOL
      SMC=X(M)**2+SMC
C IF X TOO LARGE,SET FLAG NN=1
  IF(ABS(X(M)).GT.3.0)NN=1
80  CONTINUE
  SMC=SQRT(SMC/FLOAT(NCOL))
  IF(SMC.GT.1.0)THEN
C* DECREASE MAGNITUDE OF PARAMETER INCREMENTS
  DO 73 K=1,NCOL
73  X(K)=X(K)*0.9
  GOTO 72
  END IF
C**END OF AMPLITUDE CHECK; PROCEED WITH LINE SEARCH IF NN=0
  IF(NN.EQ.0)THEN
    DD=0.0
    H(1)=DM(1)
    DO 75 I=2,ND
      H(I)=DM(I)-DM(I-1)
75  CONTINUE
C UPDATE PARAMETER VALUE AFTER RE-SCALING X
CONTROL RATE OF CHANGE OF PARAMETERS BY FACTOR, FC (30%)
  DO 90 I=1,NR
```

```

RMD(I)=10.**( ALOG10(RM(I))+X(I)*FC)
IF(I.LE.ND)THEN
J=I+NR
H(I)=10.**( ALOG10(H(I))+X(J)*FC)
DD=DD+H(I)
RMD(J)=DD
ENDIF
90 CONTINUE
CHECK FOR NEGATIVE MODEL PARAMETERS
DO 92 I=1,NCOL
IF(RMD(I).LT.0.)THEN
WRITE(*,'(A)')' NEGATIVE PARAMETER FOUND !'
RETURN
END IF
92 CONTINUE
C pass the elements of RMD back into resistivity and depth parameters
DO 95 I=1,ND
J=I+NR
RT(I)=RMD(I)
DT(I)=RMD(J)
95 CONTINUE
RT(NR)=RMD(NR)
CALL MISFIT(NR,RT,DT,NROW,DOBS,DCALC,YT,SSQT)
IF(INTIT.LE.11)THEN
IF(IK.EQ.1)THEN
WRITE(*,'(A)')' **STAGE 2 (INTERNAL) ITERATIONS :RIDGE** '
WRITE(*,'(" ESTIMATED MISFIT AND DAMPING FACTOR")')
END IF
WRITE(*,*)SSQT,BETA
ENDIF
C STOPPING CRITERION
IF(SSQT.GT.SSQT0)THEN
RETURN
ELSE
SSQT0=SSQT
END IF
CHECK THAT INTERFACE DEPTHS ARE IN ORDER

```

```
DO 100 J=2,ND
IF(DT(J-1).GE.DT(J))THEN
  WRITE(*,'(A)') ' ABNORMAL INTERFACE POSITION FOUND '
  RETURN
END IF
100 CONTINUE
C SAVE BEST-FIT SOLUTION
  DO 110 I=1,NPARM
    P(I)=RMD(I)
110 CONTINUE
N2=1
BETA0=BETA
END IF
END IF
30 CONTINUE
RETURN
END
c-----
      subroutine INPROD(mm,nn,m,n,matrix,vec,x)
c multiplies a matrix by vector vec and returns vector x
      real vec(nn),x(mm),matrix(mm,nn)
      do 10 i=1,m
        sum=0.0
        do 20 j=1,n
          sum=vec(j)*matrix(i,j)+sum
20      continue
        x(i)=sum
10      continue
      return
      end
c-----
      subroutine MISFIT(NLAY,RM,DM,NDAT,DOBS,DCALC,Y,SSE)
C call forward routine FWRD, obtains model responses FCALC
C and discrepancy vector Y as well as residual error SSE.
      REAL RM(5),DM(4),Y(22),DOBS(22),DCALC(22)
      CALL FWRD(NLAY,RM,DM,DCALC)
```

```
SSE=0.0
DO 10 I=1,NDAT
Y(I)=ALOG10(DOBS(I)/DCALC(I))
SSE=SSE+Y(I)**2
10    CONTINUE
CONTINUE
END
c-----
subroutine FWRD(nlay,rm,dm,Arho)
c   Computes layered earth response for the DC Wenner/Offset Wenner case.
c   Responses = apparent resistivities (Arho) at spacings a =0.5,1,2,4,...1024.
c   model parameters are rm and hm.  rm = layer resist.; h = layer thicknesses;
c   t = resistivity transforms; c = filter coefficients of Biwen and Barker (1994).
real t(21), c(11), rm(5), hm(4), Arho(22), dm(4)
data c/-0.000409, -0.009047, 0.065211, -0.174571, 0.38731,
&-0.0431, 2.093407, -1.622722, 0.338352, -0.039963, 0.004206/
c   get layer thicknesses
hm(1) = dm(1)
if(nlay.gt.2)then
do 100 i=2, nlay-1
hm(i)=dm(i)-dm(i-1)
100  continue
endif
c   calculate resistivity transforms
xr=0.5/64.
do 200 nk=1,21
xr=xr*2.
xx=alog(xr)+0.246844
x=exp(xx)
bb=rm(nlay)
if(nlay.gt.1)then
do 300 kk=1,nlay-1
rw=rm(nlay-kk)
zw=hm(nlay-kk)/x
th=tanh(zw)
bb=(bb+th*rw)/(1.+th*bb/rw)
```

```
300 continue
    endif
    t(nk)=bb
200 continue
c   **evaluate convolution**
    do 400 nk=1,11
        rrm=0.0
        do 500 nkk=1,11
            rrm=rrm+t(nkk+nk-1)*c(12-nkk)
500 continue
    jt=nk
    Arho(jt)=rrm
400 continue
    return
end
C-----
      subroutine PARTIAL(NDAT,DCALC,NLAY,RM,DM,A)
Compute partial derivative by numerical forward differencing
c perturb each model, find forward response, subtract calc (unperturbed
c response from subroutine MISFIT) from perturbed response and fill up
c corresponding columns of A-matrix. NOTE: for rapid convergence, forward
c differences not divided by perturbation factor DEL but solution scaled
c accordingly in RIDGE later.
      REAL A(22,9),DCALC(22),PDATA(22),RM(5),DM(4)
      DEL=0.03
      DO 10 J=1,NLAY
      SAFE=RM(J)
C perturb by del-m in log space
      RM(J) = 10.**( ALOG10(RM(J))+DEL)
      CALL FWRD(NLAY,RM,DM,PDATA)
C   FILLING COLUMNS OF MATRIX A
      DO 20 I=1,NDAT
      A(I,J) = ALOG10(PDATA(I)/DCALC(I))
20  CONTINUE
      RM(J) = SAFE
10  CONTINUE
```

C repeat for depth parameters

```
DO 30 J = 1,NLAY-1
SAFE = DM(J)
DM(J)=10.**( ALOG10(DM(J))+DEL)
CALL FWRD(NLAY,RM,DM,PDATA)
```

C FILLING COLUMNS OF MATRIX A

```
DO 40 I=1,NDAT
A(I,J+NLAY) = ALOG10(PDATA(I)/DCALC(I))
```

40 CONTINUE

```
DM(J) = SAFE
```

30 CONTINUE

```
RETURN
```

```
END
```

c-----

```
subroutine SVD(n,m,a,u,v,q)
```

C insert original routine from SVDINV here to use this program.

```
return
```

```
end
```

APPENDIX C

GRAVINV: A simple program for two-dimensional gravity inversion by ridge regression

```

program GRAINV
c forward and inverse modelling program for 2-dimensional interpretation
c of gravity data. The forward problem is solved using the Talwani
c method and the inverse problem uses ridge regression techniques.
c The matrix inversion employs the singular value decomposition method.
c Channel Assignments: chan. 1 (input)-field data and model parameters
c                      chan .3 (output)-modelling results
c language: FORTRAN77
c Author : M.A.Meju,1993
c Modification History
c Version 1.0: original development, 1993 July; 50 prisms each having
c a maximum of 50 vertices.
c-----
```

```

real fx(100),fz(100),x(50,50),z(50,50),rho(50),gcal(100)
+ ,rhoc(50),rhob(50),anom(100),y(100),ey(100),reg(100),
+ a(100,50),u(100,50),v(50,50),q(50)
integer exitit,nsides(50)
common /sol/ rhoc,nn2
common /model/ x,z,npol,nsides,rho
common /fdata/ anom,fx,fz,ndat
character*1 head(20),ans,opt,dset,ans1,dtype
logical linv
c
c set up plotting parameters
c call pltparm(user supplied)
isc=0
linv=.false.
c read field data (station locations and gravity anomalies)
19 continue
call getdata(fx,fz,anom,ey,ndat,head,nc)
c compute regional trend, residual anomaly and display all data sets
write(*,'(//a)') ' NB: 2 forms of the Field Data displayed next: '
write(*,*)' the actual Bouguer anomaly and the residuals '
```

```
17 continue
call plotting routine. NB: gravplot should call SIMPREG here to estimate
c the regional field REG (see Sect. 10.6.2.3).
call gravplot(npol,nsides,x,z,ndat,fx,anom,gcal,head,nc,0,
+ 0,reg,ey)
write(*,'(a,$)')' change plot scale ? [Y:N] > '
read(*,'(a1)')ans
if(ans.eq.'Y'.or.ans.eq.'y')then
c      call chpltsc (user supplied)
      isc=1
      endif
write(*,'(/a,$)')' another field data display ? [Y:N] > '
read(*,'(a1)')ans
if(ans.eq.'Y'.or.ans.eq.'y')then
  write(*,'(/a,$)')' Same [S] or Another [A] data-set ? [S:A] > '
  read(*,'(a1)')dset
  if(dset.eq.'S'.or.dset.eq.'s')then
    goto 17
  elseif(dset.eq.'A'.or.dset.eq.'a')then
    goto 19
  endif
  endif
c determine what form of data is to be interpreted
  write(*,'(/a)')' note: either of the 2 forms of the data may be '
  write(*,'*)' interpreted: i.e., Bouguer or Residual anomaly. '
  write(*,'(/a,$)')' model bouguer(B) or residual(R) data ? [B:R]> '
  read(*,'(a1)')dtype
  if(dtype.eq.'R'.or.dtype.eq.'r')then
    do i=1,ndat
      anom(i)=anom(i)-reg(i)
    end do
    endif
c set reg to zero as this constant bias is added onto forward response
  do i=1,ndat
    reg(i)=0.0
  end do
```

```
c determine relevant operation : inversion of forward modelling
write(*,'(/a)')' please select desired operation '
write(*,'(a,$)')' Enter I (Inversion) or F (Forward modelling):>
read(*,'(A1)') ans1
if(ans1.eq.'I'.or.ans1.eq.'i')then
    linv=.true.
    else
        linv=.false.
    endif
write(*,'(/A)') ' note: constructed model read next from a file '
53 call getmod(npol,nsides,x,z,rho)
nparin=npol
18 continue
if(.not.linv)then
25 continue
write(*,'(a)')' Your current model is as follows: '
call print(npol,rho)
call misfit(ey,y,anom,reg,ndat,ssq,npol,nsides,x,z,fx,fz,rho,gcal,
+ a)
call gravplot(npol,nsides,x,z,ndat,fx,anom,gcal,head,nc,1,0,
+ reg,ey)
if(isc.eq.0)then
    write(*,'(a,$)')' change plot scale ? [Y:N] >
    read(*,'(a1)')ans
    if(ans.eq.'Y'.or.ans.eq.'y')then
c        call chpltsc(user supplied)
        isc=1
        endif
        isc=1
        endif
c model changing part
write(*,'(a,$)')' stop interactive modelling now ? y:n >
read(*,'(a1)') ans
if(ans.eq.'Y'.OR.ans.eq.'y')then
    write(*,'(A,$)')' PROCEED TO AUTOMATIC INVERSION ? Y:N >
    read(*,'(A1)') opt
```

```
if(opt.eq.'Y'.OR.opt.eq.'y')then
  goto 35
else
  write(*,'(/a/)')' End of modelling session: Have a nice day !'
  do i=1,npol
    rhob(i)=rho(i)
  end do
  goto 5
endif
endif
call adjust(rho)
goto 25
endif

35 continue
c**END OF INTERACTIVE FORWARD MODELLING**
nrow=ndat
ncol=npol
c initialize variables
tol=0.001
stol=10000000.
NN2=1
SSQ0=10000000.
intit=0
exitit=0
c START THE ITERATIVE PROCESS
1  continue
  write(*,102) exitit
102 format(/' EXT. ITERATION NUMBER : ',I2)
c print current model
  if(exitit.LE.15) call print(npol,rho)
  exitit=exitit+1
c calculate relative difference between field data and initial model
c response and form discrepancy vector, Y. Vector scaled to reflect
c differing observational errors (where given). Calculate sum of
c squares of residuals, SSQ
  call misfit(ey,y,anom,reg,ndat,ssq,npol,nsides,x,z,fx,fz,rho,gcal
```

```
+ ,a)
      write(*,103)SSQ
103  format(/' SSQ = ',F11.5)
C STOPPING CRITERION 1: if SSQ larger than previous iterate's, STOP
      if(SSQ0.LT.SSQ)then
        goto 2000
      endif
c save best solution in array RHOB
      SSQ0=SSQ
      do 40 i=1,npol
        rhob(i)=rho(i)
40    continue
      chisq=SSQ0
      flag=stol-chisq
c STOPPING CRITERION 2:
      if(flag.GE.tol)then
        goto 80
      else
        goto 2000
      endif
80    continue
c calculate the SVD of A
      call svd(nrow,ncol,A,u,v,q)
c apply ridge regression for optimal solution
c...this is a two stage solution process...
      call ridge(y,ey,ncol,nrow,a,u,v,q,ssq0,intit,reg)
c STOPPING CRITERION 3: if damping fails first time, skip ridge
c regression
      if(NN2.EQ.0)then
        goto 2000
      elseif(NN2.EQ.1)then
        do k=1,npol
          rho(k)=rhoc(k)
        enddo
      endif
      stol=chisq
```

```

GOTO 1
2000 CONTINUE
c...INVERSION COMPLETE, PRINT RESULTS
write(*,'(/A)')' **END OF MODEL SEARCH** '
write(*,'(/)')
write(*,'(" EXT.ITERATIONS INT.IT  SUM-SQUARE MISFIT"))')
write(*,*)extit-1,intit,chisq
6 continue
call gravplot(npol,nsides,x,z,ndat,fx,anom,gcal,head,nc,
+ 1,1,reg,ey)
write(*,'(A,$)')' CHANGE PLOT SCALE ? [Y:N] > '
read(*,'(A1)')ans
if(ans.EQ.'Y'.OR.ans.EQ.'y')then
c   call chpltsc(user supplied)
isc=1
goto 6
endif
C...WRITE OUT RESULTS TO OUTPUT FILE.
5  write(*,'(A,$)')' WRITE RESULTS TO A FILE ? [Y:N] > '
read(*,'(A1)')ans
if(ans.EQ.'Y'.OR.ans.EQ.'y')then
  call output(head,chisq,npol,rhob)
endif
write(*,'(A,$)')' SAVE RESULTS AS A PLOTFILE ? [Y:N] > '
read(*,'(A1)')ans
if(ans.EQ.'Y'.OR.ans.EQ.'y')then
  call gravplot(npol,nsides,x,z,ndat,fx,anom,gcal,head,nc,
+ 1,1,reg,ey)
endif
write(*,'(A,$)')' TERMINATE MODELLING SESSION ? [Y:N] > '
read(*,'(A1)')ans
if(ans.EQ.'N'.OR.ans.EQ.'n')then
  write(*,'(A,$)')' model same(S) or another(A) data-set ? [S:A]> '
  read(*,'(A1)') dset
  if(dset.EQ.'A'.OR.dset.EQ.'a')then
    goto 19

```

```

elseif(dset.EQ.'S'.OR.dest.EQ.'s')then
  write(*,'(A)')' return to Forward modeling(F), Inversion(I) ?'
  read(*,'(A1)')ans1
  if(ans1.EQ.'F'.OR.ans1.EQ.'f')then
    linv=.false.
    goto 18
  elseif(ans1.EQ.'I'.OR.ans1.EQ.'i')then
    write(*,'(A)')' YOUR CURRENT MODEL IS AS FOLLOWS: '
    call print(npol,rho)
    call adjust(rho)
    goto 35
  endiff
  endiff
  endiff
52   write(*,'(/a/)')' End of modelling session: Have a nice day !'
  stop
end

c-----
c
c          **SUBROUTINES**
c
c-----
subroutine getdata(fz,fz anom,error,ndat,head,nc)
c  reads gravity measurement locations and field observations
c  and associated uncertainties
c  Input Structure: two data formats are accepted and declared via control CONS.
c  (1) position(m) and anomaly(mgals) for which CONS = 0      OR
c  (2) position(m), anomaly(mgals) and topo-height(m) for which CONS =1
  real fz(100),fx(100),anom(100),error(100)
  character*20 infile
  character*1 head(20)
c  read project header
  write(*,'(/a/)')' Enter Profile/project header or title (A20) '
  read(*,'(20a1)')head
  write(*,'(/A,$)')' enter filename for field data (a20): > '
  read(*,'(a20)')infile

```

```

      open(unit=1,file=infile,status='old')
c   read input data-type control
      read(1,* )cons
      do n=1,1000
         if(cons.eq.0)then
            read(1,* ,end=999) fx(n),anom(n)
            fz(n)=0.0
         else
            read(1,* ,end=999) fx(n),anom(n),fz(n)
         endif
      end do
999  ndat=n-1
      write(*,10) head,ndat
10   format(' ',20a1,' number of gravity stations read = ',i3/)
      close(1,status='keep')
      do i=1,20
         k=21-i
         if(head(k).ne.' ')goto 20
      end do
20   nc=k
calculate weighting factors to be used for data standardization
c set errors to unity **actual errors not read in this version**
      do i=1,ndat
         error(i)=1.0
      end do
      return
      end

c-----
      subroutine getmod(npoly,nsides,x,z,rho)
c reads input model geometry.
c INPUT FILE structure:
c Data 1: number of polygons, NPOL.
c (polygons assigned number 1 to NPOL for identification purposes,POLNUM)
c Data 2: for each polygon there are two lines of input.
c Line1: body id(POLNUM), no. of sides(NSIDES), den. contrast(g/cc)RHO
c Line2: nsides pairs of x- and z-coordinates of body read clockwise

```

```
c           and closing at starting point.  
c  
c     real x(50,50),z(50,50),rho(50)  
c     integer nsides(50)  
c     character*20 infile  
c   read input filename  
c     write(*,'(/A,$)') ' enter input-model filename (a20): > '  
c     read(*,'(a20)') infile  
c     open(unit=1,file=infile,status='old')  
c   read number of prisms and topo info  
c     read(1,*) npol  
c   read model parameters  
c     do k=1,npol  
c       read(1,*) polnum,nsides(k),rho(k)  
c       read(1,*)(x(i,k),z(i,k),i=1,nsides(k))  
c     end do  
c     close(1,status='keep')  
c   return  
c  
c-----  
c     subroutine adjust(rho)  
c     real rho(50)  
c     character*1 ans  
c     write(*,'(a,$)') ' change the density of a polygon ? Y:N > '  
28   read(*,'(a1)') ans  
c     if(ans.eq.'Y'.or.ans.eq.'y')then  
c       write(*,'(A,$)') ' type in polygon number > '  
c       read(*,*)nlay  
c       write(*,'(a,$)') ' enter new density contrast: > '  
c       read(*,*) rho(nlay)  
c       write(*,'(A,$)') ' change another polygon ? Y:N > '  
c       goto 28  
c     end if  
c   return  
c  
c-----
```

```
subroutine tal2dfwd(reg,ndat,npol,x,z,fx,fz,rho,nsides,gcal,a)
c a modified version of the original Talwani algorithm. adapted from
c R.Hipkin, University of Edinburgh
integer nsides(50)
real x(50,50),z(50,50),exx(50),zee(50),r(50),rho(50),delz(100)
+ ,fx(100),fz(100),spdelz(50),sselz(100),theta(100),gcal(100)
+ ,a(100,50),reg(100)
pi2=8*atan(1.0d0)
pi=4*atan(1.0d0)
pih=2*atan(1.0d0)
do k=1,ndat
    sselz(k)=reg(k)
c     sselz(k)=0.0
end do
c main loop
do 11 nl=1,npol
    nvert=nsides(nl)-1
    do 420 k=1,ndat
        sdelz=0
        exx(1)=x(1, nl)-fx(k)
        zee(1)=z(1, nl)-fz(k)
        r(1)=exx(1)**2+zee(1)**2
        if(exx(1).lt.0.0)then
            if(zee(1).lt.0.0)then
                theta(1)=atan(zee(1)/exx(1))-pi
                else
                    theta(1)=atan(zee(1)/exx(1))+pi
            endif
        elseif(exx(1).eq.0.0)then
            if(zee(1).lt.0.0)then
                theta(1)=-1.570796327
            elseif(zee(1).eq.0.0)then
                theta(1)=0.0
            elseif(zee(1).gt.0.0)then
                theta(1)=1.570796327
            endif
        endif
    end do 420
11 continue
end subroutine tal2dfwd
```

```

elseif(exx(1).gt.0.0)then
theta(1)=atan(zee(1)/exx(1))
endif
do 410 i=1,nvert
exx(i+1)=x(i+1,nl)-fx(k)
zee(i+1)=z(i+1,nl)-fz(k)
r(i+1)=exx(I+1)**2.+zee(I+1)**2.
if(exx(i+1).lt.0.0)then
if(zee(I+1).lt.0.0)then
theta(I+1)=atan(zee(I+1)/exx(I+1))-pi
else
theta(I+1)=atan(zee(I+1)/exx(I+1))+pi
endif
elseif(exx(i+1).eq.0.0)then
if(zee(i+1).lt.0.0)then
theta(i+1)=-pih
elseif(zee(i+1).eq.0.0)then
theta(i+1)=0.0
elseif(zee(i+1).gt.0.0)then
theta(i+1)=pih
endif
elseif(exx(i+1).gt.0.0)then
theta(i+1)=atan(zee(i+1)/exx(i+1))
endif
check=exx(i)*zee(i+1)-zee(i)*exx(i+1)
if(check.eq.0.0)then
delz(i)=0.0
else
omega=theta(i)-theta(i+1)
if((abs(omega)-pi).le.0.0)then
dtheta=omega
elseif((abs(omega)-pi).gt.0.0)then
if(omega.lt.0.0)then
dtheta=omega+pi2
else
dtheta=omega-pi2

```

```

        endif
    endif
    delz(i)=(check/((exx(i+1)-exx(i))**2+(zee(i+1)-zee(i))**2))*(((ex
    + x(i+1)-exx(i))*dtheta)+0.5*(zee(i+1)-zee(i))*alog(r(i+1)/r(i)))
    endif
    sdelz=sdelz+delz(i)
    exx(i)=exx(i+1)
    zee(i)=zee(i+1)
    r(i)=r(i+1)
    theta(i)=theta(i+1)

410 continue
    spdelz(k)=13.34*rho(nl)*sdelz
    sselz(k)=sselz(k)+spdelz(k)
    gcal(k)=sselz(k)
    a(k,nl)=gcal(k)/rho(nl)

420 continue
c main loop ends
11 continue
    return
    end

c-----
subroutine misfit(ey,y,anom,reg,ndat,ssq,npol,nsides,x,z,fx,fz,
+ rho,gcal,a)
integer nsides(50)
real anom(100),y(100),x(50,50),z(50,50),rho(50),fx(100)
+ ,fz(100),gcal(100),a(100,50),ey(100),reg(100)
compute model response
call tal2dfwd(reg,ndat,npol,x,z,fx,fz,rho,nsides,gcal,a)
sum=0.0
compute discrepancy vector y, and sum of squared error ssq
c **activate as necessary: data normalized by associated standard errors, ey
    do i=1,ndat
c**      y(i)=(anom(i)-gcal(i))/ey(i)
        y(i)=anom(i)-gcal(i)
        sum=sum+y(i)**2.
    end do

```

```

c**      do k=1,npol
c**      do i=1,ndat
c**          a(i,k)=a(i,k)/ey(i)
c**      end do
c**      end do
c**      ssq=sum
c**      return
c**      end
c-----
c      subroutine ridge(y,ey,ncol,nrow,a,u,v,q,ssq0,intit,reg)
c ridge regression routine. Max Meju, 1986. See also
c M.A.Meju, 1992, Computers & Geoscience, vol.18, no.2/3,pp99-118.
c common /sol/p,n2
c common /model/ xx,zz,npol,nsides,rho
c common /fdata/ anom,fx,fz,ndat
c real fx(100), fz(100), xx(50,50), zz(50,50), rho(50), p(50), rhom(50)
c + , anom(100), y(100), ey(100), a(100,50), u(100,50), v(50,50), q(50)
c + , x(50), qk(0:10), yt(100), ut(50,100), vq(50,50), uty(50), ax(100)
c + , gcal(100), reg(50)
c integer nsides(50)
c set initial constants and flags
c      fc=1./10.
c      n2=0
c      ssqt0=ssq0
c set Marquardt damping factors for ridge regression
c find smallest & largest singular values Qs & Ql
c      ql=0.00000001
c      qs=10000000.
c      do 10 I=1,ncol
c          if(q(i).gt ql)then
c              ql=q(i)
c          elseif(q(i).lt.qs)then
c              qs=q(i)
c          end if
c 10    continue
c      ql=10*ql

```

```
qs=qs/10.  
calculate 10 samples of the damping function Qk = a + bk**2  
    do 20 k=1,10  
        qk(k)=(100*qs-ql+(ql-qs)*float(k)**2)/99.  
20    continue  
    qk(0)=0.0  
c---main optimization loop---  
    do 30 ik=1,11  
        intit=intit+1  
calculate damping factor beta  
    beta=qk(11-ik)**2  
c damp q to avoid singularities, get inverse q and u-transpose  
    do 40 i=1,ncol  
        qi=q(i)/(q(i)**2+beta)  
        do 50 j=1,nrow  
            ut(i,j)=u(j,i)  
50    continue  
compute v/q  
    do 60 k=1,ncol  
        vq(k,i)=qi*v(k,i)  
60    continue  
40    continue  
compute inner product ut*y  
    call inprod(50,100,ncol,nrow,ut,y,uty)  
calculate regression estimate x  
    call inprod(50,50,ncol,ncol,vq,uty,x)  
    call inprod(100,50,nrow,ncol,a,x,ax)  
    nn=0  
c place bounds on the size of perturbations using the smoothness  
c criterion of Jackson (1973) GJRAS 35,121-136.  
c if sqrt(sumsq(x)/ncol).gt.1.), solution not physically realizable  
c therefore decrease size of x without changing its direction  
72    smc=0.0  
    do 80 m=1,ncol  
        smc=smc+x(m)**2  
c      if too large. set flag nn to 1
```

```
if(abs(x(m)).gt.3.0)nn=1
80    continue
      smc=sqrt(smc/float(ncol))
      if(smc.gt.1.0)then
        do 73 k=1,ncol
73    x(k)=x(k)*0.9
        goto 72
      end if
c end of amplitude check. proceed with 1-d line search if nn=0.
c update parameter value after re-scaling x.
c control rate of change of parameters by factor fc (30%).
      do 90 i=1,ncol
        rhom(I)=rho(i)+x(i)*fc
90    continue
      call misfit(ey,yt,anom,reg,ndat,ssqt,npol,nsides,xx,zz,fx,fz,rho,
+ gcal,a)
      if(intit.le.11)then
        if(ik.eq.1)then
          write(*,'(/a)')'*Stage 2 Minimization by Ridge regression**'
          write(*,'(" Estimated Misfit and Damping factor")')
        end if
        write(*,*)ssqt,beta
      endif
c stopping criterion
      if(ssqt.gt.ssqt0)then
        return
      else
        ssqt0=ssqt
      c save best solution in array p
        do 110 i=1,ncol
          p(i)=rhom(i)
110    continue
        n2=1
      endif
30    continue
      return
```

```
end  
c-----  
    subroutine inprod(mm,nn,m,n,vx,y,a)  
c matrix vx multiplied by vector y gives vector a  
    real y(nn),a(mm),vx(mm,nn)  
    do 10 i=1,m  
        sum=0.0  
        do 20 j=1,n  
            sum=sum+y(j)*vx(i,j)  
20    continue  
    a(i)=sum  
10    continue  
    return  
    end  
c-----  
    subroutine output(head,ssq,npol,rho)  
    real rho(50)  
    character*20 outfile  
    character*1 head(20)  
c    open output file  
    write(*,'(a,$)') ' type in output filename (a20) :> '  
    read(*,'(a)')outfile  
    open(unit=3,file=outfile,status='new')  
    write(3,10) head  
10    format(/1X,'2-D Gravity Model for Site : ',20a1)  
    write(3,'(/A)') ' Best Fit Model '  
    write(3,15)ssq  
15    format(1X,' chi-squared misfit = ',f9.3)  
    write(3,20)  
20    format(/1X,' polygon no. density constraint ')  
    do i=1,npol  
        write(3,*)i, rho(i)  
    end do  
    close(3)  
    return  
    end
```

```

c-----  

      subroutine print(npol,rho)  

c prints current parameter estimates  

      real rho(50)  

      write(*,10)  

10   format(/1X,'polygon no. density contrast ')  

      do 20 I=1,npol  

      write(*,*)I, rho(i)  

20   continue  

      return  

      end  

c-----  

c      subroutine svd(n,m,a,u,v,q)  

c      **insert the routine listed in SVDINV here***  

c      return  

c      end  

c-----  

c      ** plot routines supplied by user **  

c-----  

c      subroutine gravplot(npol,nsides,x,z,ndat,fx,anom,gcal,head,nc,0,  

c      + 0,reg,ey)  

c      ***User to supply plotting routine**  

c      return  

c      end

```