Inverse Problem Theory

Methods for Data Fitting and Model Parameter Estimation

Albert Tarantola

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Methods for Data Fitting and Model Parameter Estimation

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PREFACE

Humans were naked worms; yet they had an *internal model* of the world. In the course of time up to the present, this model has been updated many times, following the development of new experimental possibilities (i.e., the developments of their senses) or the development of their intellect. Sometimes the updating has been only quantitative, sometimes it has been qualitative. Inverse problem theory tries to describe the rules human beings should use for quantitative updatings.

Let $\boldsymbol{S}$ represent a physical system (for instance the whole Universe, or a planet, or a quantum particle). Assume that we are able to define a set of *model parameters* which completely describes $\boldsymbol{S}$. These parameters may not all be directly measurable (for instance, the radius of the Earth's metallic core is not directly measurable). We can operationally define some *observable parameters* whose actual values hopefully depend on the values of the model parameters. To solve the *forward problem* is to predict the values of the observable parameters, given arbitrary values of the model parameters. To solve the *inverse problem* is to infer the values of the model parameters from given observed values of the observable parameters.

The set of observed values usually overdetermines some model parameters while leaving others underdetermined. Schematically, there are two reasons for underdetermination: intrinsic lack of data, and experimental uncertainties. To illustrate the first, consider for instance the problem of estimating the density distribution of matter inside a planet from knowledge of the gravitational field at its surface. It is well known that infinitely many different distributions of matter density give rise to identical exterior gravitational fields (Gauss' theorem), so there is no hope of obtaining a unique solution to the inverse problem using only gravitational data. Additional information has then to be used, such as, for instance, some a priori assumptions on density distribution, or an additional data set, such as seismic observations.

The second reason for underdetermination is uncertainty of knowledge: observed values always have experimental uncertainties, and physical theories allowing the resolution of the forward problem are always approximations of a more complex reality.

Data redundancy can, in general, easily be handled, and present-day methods do not differ essentially from those used, for instance, by Laplace in 1799, who introduced the "least-absolute-values" and the "minimax" criterion for obtaining the "best" solution, or by Legendre in 1801 and Gauss in 1809, who introduced the "least-squares" criterion.

Underdetermination is handled differently by differently thinking schools. Pure mathematicians like to refer to Hadamard's (1902, 1932) definition of "ill-posed problems": a problem is ill-posed if the solution is not unique or

if it is not a continuous function of the data (i.e., if to a "small" perturbation of data there corresponds an arbitrarily "large" perturbation of the solution). Examples of ill-posed problems are, for instance: i) the "analytic prolongement" of stationary fields (if a magnetic field of internal origin is given at a height h_1 over the surface of a planet, the problem of calculating the field at h_2 is well-posed if $h_2 \leq h_1$, and is ill-posed if $h_2 > h_1$; ii) the resolution of a diffusion equation (like the heat-transport equation) when the final conditions are given, instead of the initial conditions; iii) the inversion of integral operators (for instance, the typical problem of instrument deconvolution); iv) the resolution of discrete linear systems with a square matrix, if the latter is not regular.

In Hadamard's opinion, ill-posed problems do not have physical sense. General agreement exists today that ill-posed problems have "well-posed extensions" which are very meaningful. These well-posed extensions introduce a priori assumptions as to the unknowns. For example, Tikhonov (1963) assumes some "regularity" properties of the solution, while Franklin (1970) assumes given a priori statistics on the model space.

Some methods of inversion are known as "exact". They concern problems where the data set and the unknown set can be related by an inversible (generally nonlinear) application. Given the application solving the forward problem, the inverse problem consists in discovering the inverse application (in the usual mathematical sense of the word inverse). The whole field of "exact inversion" is neglected in this book, because these methods cannot deal with data uncertainty and data redundancy in a natural manner. They are interesting for solving mathematical inverse problems, not for data interpretation.

Inverse problem theory in the wide sense has been developed by people working with geophysical data. The reason is that geophysicists try to understand the Earth's interior but are doomed to use only data collected at the Earth's surface. Geophysical problems are always underdetermined in some sense, but as geophysical data contain a lot of information, it is worth-while to try to develop methods for extracting it. Since long, such methods have been only empirical. Backus (1970a, 1970b, 1970c) made the first systematic exploration of the mathematical structure of inverse problems. Backus and Gilbert (1967, 1968, 1970) introduced interesting concepts, such as, for instance, that of "model resolution". Their work was at the origin of a very fruitful development of quantitative methods of data interpretation in geophysics.

This book resolutely takes the viewpoint that the most general formulation of Inverse Problems is obtained when using the language of probability calculus, and when using a Bayesian interpretation of probability (Bayes, 1763). Inverse Problem Theory has to be developed from the consideration of uncertainties (either experimental, or in physical laws), and the right (well-posed) question to set is: given a certain amount of (a priori) information on

some model parameters, and given an uncertain physical law relating some observable parameters to the model parameters, in which sense should I modify the a priori information, given the uncertain results of some experiments? In my opinion, this in the only approach allowing us to analyze "error and resolution" in the "solution" with a convenient degree of generality, even for nonlinear forward problems.

The techniques used today for solving inverse problems are as multivariate as the problems themselves. One of the purposes of this book is to show that many of the methods used (linear programming, least-squares, maximum likelihood,...) can coherently be described from a few principles, i.e., that it is possible to build a *theory* for inverse problems.

The first part of this book deals exclusively with *discrete* inverse problems with a *finite* number of parameters. Some real problems are naturally discrete, others contain functions of a continuous variable, and can be discretized if the functions under consideration are smooth enough compared to the sampling length, or if the functions can conveniently be described by their development on a truncated basis.

The advantage of a discretized point of view for problems involving functions is that the mathematics are easier. The disadvantage is that some simplifications arising in a general approach can be hidden when using a discrete formulation (discretizing the forward problem and setting a discrete inverse problem is not always equivalent to setting a general inverse problem and discretizing for the practical computations).

The second part of the book deals with general inverse problems, which may contain such functions as data or unknowns. As this general approach contains the discrete case in particular, the separation into two parts corresponds only to a didactical purpose.

Although this book contains a lot of mathematics, it is not a mathematical book. It tries to explain how a method of acquisition of information can be applied to the actual world. Many intuitive arguments are discussed extensively, but not all have yet been justified mathematically. I hope that researchers in the physical sciences will find the compromise acceptable, and that researchers in applied mathematics will find some of the unsolved problems interesting.

Considerable effort has been made so that this book can serve either as a reference manual for researchers neeeding to refresh their memories on a given algorithm, or as a textbook for a course in Inverse Problem Theory.

Albert Tarantola
Paris, October 1986

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CHAPTER 1

THE GENERAL DISCRETE INVERSE PROBLEM

Far better an approximate answer to the *right* question,
which is often vague,
than an exact answer to the *wrong* question,
which can always be made precise.

John W. Tukey, 1962.

Central in this chapter is the concept of "state of information" over a parameter set. It is postulated that the most general way of describing a state of information over a parameter set is by defining a probability density over the corresponding parameter space. It follows that the results of the measurements of the observable parameters (data), the a priori information on model parameters, and the information on the physical correlations between observable parameters and model parameters can, all of them, be described using probability densities. The general Inverse Problem can then be set as a problem of "combination" of all this information. Using the point of view developed here, the solution of inverse problems, and the analysis of error and resolution, can be performed in a fully nonlinear way (but perhaps with a prohibitively large amount of computing time). In all usual cases, the results obtained with this method reduce to those obtained from more conventional approaches. All the results of the subsequent chapters are justified by the arguments developed here.

1.1: Model space and Data space

Let $\mathcal{S}$ be the *physical system* under study. For instance, $\mathcal{S}$ can be a galaxy for an astrophysicist, the Earth for a geophysicist, or a quantum particle for a quantum physicist.

The scientific procedure for the study of a physical system can be (rather arbitrarily) divided into the following three steps.

i) *Parametrization of the system* : discovery of a minimal set of *model parameters* whose values completely characterize the system (from a given point of view).

ii) *Forward modeling* : discovery of the *physical laws* allowing, for given values of the model parameters, of making predictions as to the results of measurements on some *observable parameters*.

iii) *Inverse modeling* : use of the actual results of some measurements of the observable parameters to infer the actual values of the model parameters.

Strong feed-backs exist between these steps, and a dramatic advance in one of them is usually followed by advances in the other two.

While the first two steps are mainly inductive, the third step is mainly deductive. This means that the postulates and rules of thinking that we follow in the two first steps are difficult to make explicit. On the contrary, the mathematical theory of logic (completed with the probability theory) seems to apply quite well to the third step, to which this book is devoted.

1.1.1: The model space

The choice of the model parameters to be used to describe a system is generally not unique.

Example 1: To describe the elastic properties of a solid, it is possible to use the tensor $c^{ijkl}(\mathbf{x})$ of elastic *stiffnesses* relating stress, $\sigma^{ij}(\mathbf{x})$, to strain, $\epsilon^{ij}(\mathbf{x})$, at each point $\mathbf{x}$ of the solid:

$$\sigma^{ij}(\mathbf{x}) = c^{ijkl}(\mathbf{x}) \; \epsilon^{kl}(\mathbf{x}) \; .$$

Alternatively, it is possible to use the tensor $s^{ijkl}(\mathbf{x})$ of elastic *compliances* relating strain to stress:

$\epsilon^{ij}(\mathbf{x}) = s^{ijkl}(\mathbf{x})\ \sigma^{kl}(\mathbf{x})$,

where the tensor $\mathbf{s}$ is the inverse of $\mathbf{c}$:

$c^{ijkl}\ s^{klmn} = \delta^{im}\ \delta^{jn}$.

The use of stiffnesses or of compliances is completely equivalent, and there is no "natural" choice. ■

A particular choice of model parameters is a *parametrization* of the system. Two different parametrizations are *equivalent* if they are related by a bijection.

Independently of any particular parametrization, it is possible to introduce an abstract space (set) of points, each representing a conceivable "model" of the system. This space is named the *model space* and is denoted by $\aleph$.

For quantitative discussions on the system, a particular parametrization has to be chosen. To define a parametrization means to define a set of experimental procedures allowing, at least in principle, to measure different characteristic of the system. Once a particular parametrization has been chosen, to each point of the model space a set of numerical values is associated, which can be represented by a point in space $\boldsymbol{M}$, isomorphic to a part of $\boldsymbol{R}^n$ ($\boldsymbol{R}$ denotes the real line, and n the number of parameters). The model space $\aleph$ is defined intrinsically, the space $\boldsymbol{M}$ depends on the particular parametrization chosen.

From a mathematical point of view, $\aleph$ is a (nonlinear) *manifold*, and $\boldsymbol{M}$ is a *chart* of $\aleph$.

Example 2: When a nuclear explosion takes place at the Earth's surface, it produces a seismic wave which propagates through the Earth. It is then possible to use the arrival times of the wave at some seismological observatories to estimate the location of the explosion. A "model" is then a particular location for the explosion, i.e., a geometrical point on the surface of the Earth. The model space $\aleph$ can be represented as the surface of a unit sphere (left of Figure 1.1). The model space is defined *intrinsically*, i.e., without reference to any particular system of coordinates. Nevertheless, for numerical computations, it is necessary to represent each point of the model space by its coordinates in a given coordinate system. To define a coordinate system over the model space is to give a *chart* $\boldsymbol{M}$ of the model space. Each model then corresponds to a point (in a part) of $\boldsymbol{R}^2$ (right of Figure 1.1). In this example, the word "chart" can be taken in its etymological sense. By extension, mathematicians call a "chart" any "mapping" between a n-dimensioned nonlinear manifold and a part of $\boldsymbol{R}^n$. It is an abuse of language that a map of the model space is often also named a "model space". The only in-

convenience of such abuse of language is that it can lead to the impression that a model space is necessarily a linear space, which is not true in general. For this particular problem, the model space may be furnished with a concept of *distance* between two arbitrary points (which can either be the euclidean length of the straight segment joining the two points through the sphere, or the length of the arc of great circle joining the points on the surface of the sphere). This is an exception rather than the rule, and usual model spaces cannot be furnished with a distance in such a natural way. ■

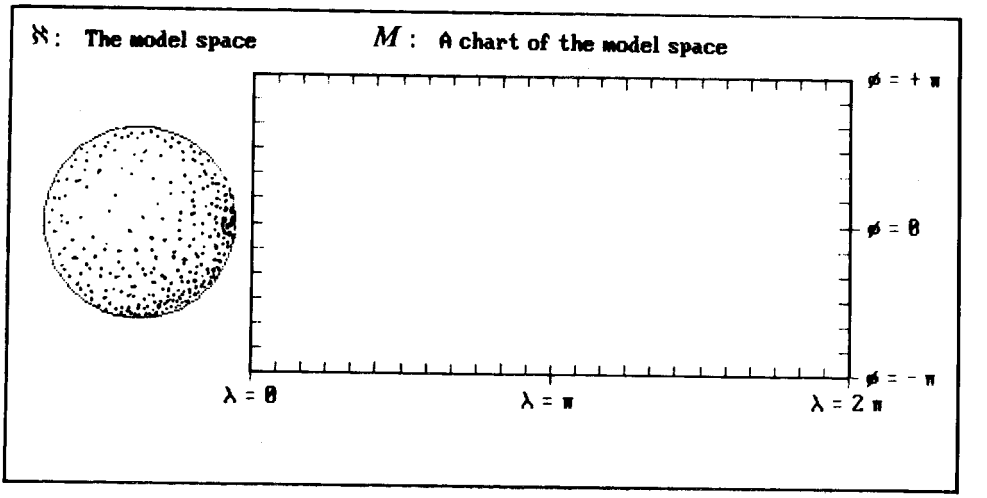


Figure 1.1: The model space $\mathfrak{M}$ is generally a nonlinear manifold (left of the figure). For numerical computations we introduce a chart of the manifold (right of the figure) which, by language abuse, is also named "model space" (see text for discussion).

The reader interested in the Theory of Differentiable Manifolds may refer, for instance, to Lang (1962), Narasimhan (1968), or Boothby (1975).

We have seen that a chart $\boldsymbol{M}$ of the model space $\mathfrak{M}$ is "isomorphic" to $\boldsymbol{R}^n$. The difference between a chart (of dimension n) and $\boldsymbol{R}^n$ is that each point of $\boldsymbol{R}^n$ is a set of pure real numbers, i.e., of *dimensionless* quantities. On the contrary, each point of a chart $\boldsymbol{M}$ is a set of n values with given *physical dimensions* (pressure, temperature, electric charge, ...).

Each point of $\mathfrak{M}$, or the corresponding point of $\boldsymbol{M}$, is named a *model*, and is represented by m .

Given a model space $\aleph$, when no confusion is possible, and by languistic abuse, the particular "chart" under consideration will also be named "model space". This corresponds to traditional terminology in inverse problem literature.

The number of model parameters needed for completely describing a system may be either finite or infinite.

Example 3: If the elastic properties of the solid in example 1 effectively vary from point to point, we need an infinite number of values to describe the system completely. If the solid is assumed homogeneous (i.e., if the values of the elastic parameters are independent of $\mathbf{x}$), then 21 parameters suffice for its complete description. ■

Let m^α represent a particular parameter (from a set which can either be finite or infinite). The parameter m^α may take its values in a discrete or in a continuous set. For instance, if m^α represents the mass of the Sun, we can assume a priori that it can take any value from zero to infinity; if m^α represents the spin of a quantum particle, we can assume a priori that it can only take discrete values. We will see later that the use of "delta functions" allows us to consider parameters taking discrete values as a special case of parameters taking continuous values. To simplify the discussions, the terminology used in this book will correspond to the assumption that all the parameters under consideration take their values in a continuous set. If this is not the case in a particular problem, the reader will easily make the corresponding corrections (see in particular problems 1.3 and 1.4).

The theory of infinite dimensional spaces needs a greater technical vocabulary than the theory of finite dimensional spaces. In what follows, and in all the first part of this book, I assume that the model space is *finite-dimensional*. The limitation to systems with finite number of parameters is severe from a mathematical point of view, because the kingdom of functions (even continuous) is infinitely much richer than the kingdom of finite-dimensioned spaces. But, as far as we can accept in some problems that the functions under consideration are *bandlimited*, it is always possible to consider a sampled version of these functions, and in this case there is no difference between the numerical results given by functional and by discrete approaches to Inverse Problem Theory (although the numerical algorithms may differ considerably, as it can be seen by comparing problem 1.2 with problem 7.1).

When a particular parametrization of the system has been chosen, each model can be represented by a particular set of values for the model parameters:

$$\mathbf{m} = \{ m^\alpha \} \qquad (\alpha \in \mathbf{I}_M) \tag{1.1}$$

where I_M represents a discrete finite *index set*. In as far as a particular parametrization of S is interpreted as a choice of coordinate lines over $\aleph$, the variables m^α can be named the *coordinate values* of $\mathbf{m}$ (with respect to the given coordinate lines).

By definition of our terminology, the following are synonymous:

i) to parametrize the physical system S,

ii) to define a coordinate system over the model space $\aleph$,

iii) to define a chart, M, of $\aleph$.

A chart of $\aleph$ is, by definition, isomorphic to R^n. In particular, a chart is a linear (vector) space. Given a particular chart M, it is then possible to define the *sum of two models*, $\mathbf{m}_1$ and $\mathbf{m}_2$, by the sum of its "components":

$$(m_1 + m_2)^\alpha = m_1^\alpha + m_2^\alpha \qquad (\alpha \in I_M) \tag{1.2}$$

and the *multiplication of a model by a real number* by the multiplication of all its "components":

$$(r\,m)^\alpha = r\,m^\alpha \qquad (\alpha \in I_M)\ (r \in R). \tag{1.3}$$

This justifies the name of "components" given to the coordinates m^α. Nevertheless, it should be emphasized that the previous definitions are *not intrinsic*, in the sense that the sum or the multiplication thus defined *depends* on the particular parametrization chosen for S. It is generally not possible to give an intrinsic definition of $\mathbf{m}_1 + \mathbf{m}_2$ or of $r\,\mathbf{m}$: the model space $\aleph$ is *not* a linear space in general.

Example 4: The homogeneous solid in example 1 can be described by the 21 elastic stiffnesses c^{ijkl} or, alternatively, by the 21 elastic compliances s^{ijkl}. Let $\mathbf{m}_1$ and $\mathbf{m}_2$ represent two different elastic solids. They can be represented either by c_1^{ijkl} and c_2^{ijkl}, or by s_1^{ijkl} and s_2^{ijkl}. The elastic solid defined by $c_1^{ijkl} + c_2^{ijkl}$ is different from the elastic solid defined by $s_1^{ijkl} + s_2^{ijkl}$: the sum of two models can not be defined intrinsically. ■

In fact, the theory of inversion can be developed completely without reference to any particular parametrization. We will see below that the only mathematical objects to be defined in order to deal with the most general formulation of inverse problems are *measures* over the model space (in the sense of the mathematical theory of integration). A measure over $\aleph$ is a mapping that, to any subset A of $\aleph$, associates a positive real number:

$$A \rightarrow P(A) \in R^+$$

named the *measure of* A . In general, $P(\aleph) = 1$, and the measure is named a *probability* over $\aleph$. Such measures can, in principle, be defined irrespectively of any particular parametrization of $\aleph$, i.e., independently of any particular chart. But once a particular chart M has been chosen, then it is very easy to describe a probability using a probability density.

In practical applications, we are always faced with a particular parametrization, and so long as it has been astutely chosen, we can forget all the subtleties distinguishing the abstract model space from the corresponding chart, name the last the model space, forget that the linear vector structure is not intrinsic, and go through the computations.

In defining the parametrization of a physical system, it has been said that the parameters have to be defined so as to be measurable "at least in principle". The following example illustrates this notion.

Example 5: The radius of the Earth's metallic core can be defined "experimentally" as the radius of the spherical region of the Earth where the mineral composition is predominantly metallic. Given a sample, we know how to determine its mineralogical composition. To measure the radius of the Earth's core, it "suffices" to make a (quite) deep hole, and analyze the obtained samples. The parameter "radius of the Earth's core" is perfectly defined, although only measurable "in principle". The use of physical laws allows us to predict the behaviour of seismic waves arriving at the surface of the Earth's core. The diffracted-reflected waves are directly observable at the Earth's surface. Thus, inverse problem theory allows us to obtain information on the radius of the core. ■

1.1.2: The data space

To obtain information on model parameters, we have to perform some observations during a physical experiment, i.e., we have to perform a measurement of some observable parameters.

Example 6: As discussed in example 5, for a geophysicist interested in understanding the Earth's deep structure, observations may consist, for instance, in recording a set of seismograms at the Earth's surface. ■

Example 7: For a particle physicist, observations may consist in a mesurement of the flux of particles diffused by a given target at different angles for a given incident particle flux. ■

The task of the experimenter is difficult, not only because he has to perform measurements as accurately as possible, but more essentially because he has to *imagine* new experimental procedures allowing him to measure observable parameters carrying a maximum of information on model parameters. For instance, it may be easy to determine the captain's age (for instance by stealing his passport), but there is little chance that this measurement will carry much information on the number of masts on the ship.

As was the case with model parameters, given experimental equipment, a certain freedom exists in choosing the observable parameters.

Example 8: Given a seismometer, we can choose as "output" a voltage proportional to the displacement of the mass, or to its velocity, or to its acceleration. ■

We thus arrive at the abstract idea of a *data space*, which can be defined as the space of all conceivable instrumental responses. Each particular realization is denoted by $\mathbf{d}$. When a particular choice has been made of the "observable parameters" (in the sense of example 8), a *chart* of the data space has been defined, which will be denoted $\boldsymbol{D}$, and which, by languistic abuse, will also be named "data space". Any conceivable result of the measurements can be written by the "components"

$$\mathbf{d} = \{ d^i \} \qquad (i \in I_D), \tag{1.4}$$

where I_D represents a discrete (and finite) index set. $\boldsymbol{D}$ is a linear space with the definitions

$$(\mathbf{d}_1 + \mathbf{d}_2)^i = d_1^i + d_2^i \qquad (i \in I_D) \tag{1.5}$$

$$(r\,\mathbf{d})^i = r\,d^i \qquad (i \in I_D)\ (r \in R). \tag{1.6}$$

Each vector $\mathbf{d}$ is then named a *data vector*, or *data set*.

1.1.3: The joint space $D \times M$

It is sometimes useful to introduce the product space $\boldsymbol{X} = \boldsymbol{D} \times \boldsymbol{M}$. Its elements are the couples $\mathbf{x} = (\mathbf{d}, \mathbf{m})$. As the elements of $\mathbf{d}$ are termed observable parameters and the elements of $\mathbf{m}$ are termed model parameters, the elements of $\mathbf{x}$ may be called *physical parameters*, or, for short, *parameters*. The space $\boldsymbol{X}$ is then named the *parameter space*.

$\boldsymbol{X}$ can be intuitively interpreted as representing a physical system $\boldsymbol{S}$ *extended* to contain also the measure instruments themselves. This space is much more fundamental than $\boldsymbol{D}$ and $\boldsymbol{M}$ and, in fact, for many problems

the separation of $\boldsymbol{X}$ into a data and a model space may be rather arbitrary.

The components of $\mathbf{x}$ can be viewed as coordinates in the parameter space $\boldsymbol{X}$. We can arbitrarily define another system of coordinates through a bijection

$$\mathbf{x}^* = \mathbf{x}^*(\mathbf{x}) \qquad \mathbf{x} = \mathbf{x}(\mathbf{x}^*) . \tag{1.7}$$

Such systems of coordinates are named *equivalent*. In section 1.2.3 I introduce the hypothesis that the system of coordinates is *minimal*.

The components of $\mathbf{m}$ are represented by the Greek indexes $\alpha,\beta,\ldots$; the components of $\mathbf{d}$ by the lower-case Latin indexes i,j,... . When necessary, the components of $\mathbf{x}$ are represented by upper-case Latin indexes:

$$\mathbf{x} = \{ x^A \} \qquad (A \in I_X) . \tag{1.8}$$

1.1.4: Notations

Authors dealing with discrete inverse problems usually consider a *column-matrix* notation for representing the elements of the model or the data spaces:

$$\mathbf{m} = \begin{bmatrix} m^1 \\ m^2 \\ \cdots \end{bmatrix}$$

$$\mathbf{d} = \begin{bmatrix} d^1 \\ d^2 \\ \cdots \end{bmatrix} .$$

In this book, the word "vector" always means "element of a linear vector space", and it will never be assumed that the natural representation of a vector is by using a column matrix.

Example 9: If the discrete model corresponds to a discretization of a function of *two* variables, say $f(x,y)$, the elements of the model space are naturally represented by

$$\mathbf{m} = \begin{bmatrix} m^{11} & m^{12} & \cdots \\ m^{21} & m^{22} & \cdots \\ \cdots & \cdots & \cdots \end{bmatrix} = \begin{bmatrix} f(x^1,y^1) & f(x^1,y^2) & \cdots \\ f(x^2,y^1) & f(x^2,y^2) & \cdots \\ \cdots & \cdots & \cdots \end{bmatrix}$$

so that the index set $\mathbf{I}_M$ is $N \times N$ (i.e., a set of couples of integers). In that case, a bidimensional array (i.e., a *matrix*) conveniently represents a model, and ranging the components of $\mathbf{m}$ into a column matrix is of no intuitive help (and is never needed in numerical computations). ■

If the components of a vector have to be explicited, the following abstract notation will be used:

$$\mathbf{m} = \{ m^\alpha \} \qquad (\alpha \in \mathbf{I}_M)$$

$$\mathbf{d} = \{ d^i \} \qquad (i \in \mathbf{I}_D) ,$$

which do not assume any particular arrangement.

Let, for instance, $\mathbf{G}$ represent a linear operator from M into D. We write

$$\mathbf{d} = \mathbf{G}\,\mathbf{m} . \tag{1.9a}$$

As $\mathbf{G}$ relates two discrete spaces, it can be shown that there exist constants $G^{i\alpha}$ $(i \in \mathbf{I}_D)$ $(\alpha \in \mathbf{I}_M)$ such that the linear equation (1.9a) can be written

$$d^i = \sum_{\alpha \in \mathbf{I}_M} G^{i\alpha}\, m^\alpha \qquad (i \in \mathbf{I}_D) . \tag{1.9b}$$

In general, the components of a linear operator like $\mathbf{G}$ may be represented as a multidimensional array (not necessarily a "matrix").

Example 10: For the model space of the previous example,

$$d^i = G^{i\,11}\, m^{11} + G^{i\,12}\, m^{12} + \ldots ,$$

where, in its turn, the index i may be multidimensional. ■

Of course, in as far as the number of components of $\mathbf{m}$ and $\mathbf{d}$ is finite, we can reclass them into column matrices, and linear operators like $\mathbf{G}$ can be represented by ordinary two-dimensional matrices. But the only effect of this is generally to destroy all the symmetries of the problem, and to suggest the use of matricial operations in problems where a slightly more abstract algebra may simplify notations and computations (see, for instance, problem 1.2). For a proper terminology, the array of numerical constants representing a linear operator should be named the *kernel* of the operator, and should not be identified with the operator itself, which is a more fundamental concept (for a given linear operator there are as many different ker-

nels as bases that we may choose in the corresponding linear spaces).

Let ϕ^α (resp. ψ^i) be constants such that $\Sigma\, m^\alpha\, \phi^\alpha$ (resp. $\Sigma\, d^i\, \psi^i$) makes sense (in particular in regard to the homogeneity of physical dimensions), and gives an (adimensional) real number. I define

$$\mathbf{m}^t\, \boldsymbol{\phi} \;=\; \sum_{\alpha \in I_M} m^\alpha\; \phi^\alpha \tag{1.10a}$$

$$\mathbf{d}^t\, \boldsymbol{\psi} \;=\; \sum_{i \in I_D} d^i\; \psi^i \;. \tag{1.10b}$$

In chapters 4 and 5, $\boldsymbol{\phi}$ (resp. $\boldsymbol{\psi}$) are identified as elements of the *dual* of $\boldsymbol{M}$ (resp. $\boldsymbol{D}$).

Given the linear operator $\mathbf{G}$ of equations (1.9), mapping the model space into the data space, the *transpose* of $\mathbf{G}$ is denoted $\mathbf{G}^t$, and is a linear operator defined by the identity

$$\mathbf{m}^t\; (\,\mathbf{G}^t\, \boldsymbol{\psi}\,) \;=\; (\,\mathbf{G}\,\mathbf{m}\,)^t\; \boldsymbol{\psi}\;, \tag{1.11a}$$

valid for any $\mathbf{m}$ and $\boldsymbol{\psi}$. In chapters 4 and 5, $\mathbf{G}^t$ is identified as an operator mapping the dual of the data space into the dual of the model space. As $\mathbf{G}^t$ maps two discrete spaces, there exist constants $(G^t)^{\alpha i}$ such that

$$(\mathbf{G}^t\, \boldsymbol{\psi})^\alpha \;=\; \sum_{i \in I_D} (G^t)^{\alpha i}\; \psi^i \;,$$

and it can then easily be shown from the general definition (1.11a) that

$$(G^t)^{\alpha i} \;=\; (G)^{i \alpha} \;. \tag{1.11b}$$

In the particular case of matricial kernels, this last formula corresponds to the usual definition of matrix transposition.

The *inverse* of a linear operator, if it exists, is introduced by the usual definition. For instance, the operator $\mathbf{S}$ with components $S^{\alpha\beta}$ $(\alpha \in I_M)$ $(\beta \in I_M)$ is the inverse of $\mathbf{Q}$, with components $Q^{\alpha\beta}$ if

$$\sum_{\beta \in I_M} S^{\alpha\beta}\; Q^{\beta\gamma} \;=\; \sum_{\beta \in I_M} Q^{\alpha\beta}\; S^{\beta\gamma} \;=\; \delta^{\alpha\gamma} \;, \tag{1.12a}$$

where $\delta^{\alpha\gamma}$ represents the Kronecker's symbol (1 if $\alpha = \gamma$, 0 otherwise). We then write

$$S = Q^{-1} \qquad Q = S^{-1} . \tag{1.12b}$$

With the notations introduced by equations (1.10), (1.11), and (1.12), general linear equations look like ordinary matricial equations, but keep a much more general sense.

1.2: States of Information

1.2.1: The mathematical concept of probability

Let X represent an arbitrary set. By definition, a measure over X is a rule that to any subset A of X a real positive number $P(A)$ is associated, named the *measure of* A and satisfying the two properties

i) If $\varnothing$ represents the empty set, then

$$P(\varnothing) = 0 . \tag{1.13}$$

ii) If $A_1, A_2, \ldots$ represents a disjoint sequence of sets of X, then

$$P\left[\sum_i A_i\right] = \sum_i P(A_i) . \tag{1.14}$$

$P(X)$ is not necessarily finite. If it is, then P is termed a *probability* (or *probability measure*) over X. In that case, P is usually normalized to unity: $P(X) = 1$.

Example 11: Let X be the set {HEAD, TAIL}. Setting

$$P(\varnothing) = P(\text{neither HEAD nor TAIL}) = 0 ,$$

$$P(\text{HEAD}) = r ,$$

$$P(\text{TAIL}) = 1 - r ,$$

and

$$P(\text{HEAD} \cup \text{TAIL}) = P(\text{HEAD or TAIL}) = 1 ,$$

where r is a real number $0 \leq r \leq 1$, defines a probability over X. ■

Example 12: Let X be the surface of a sphere, π_0 a particular point on the surface, and H_0 the hemisphere centered at π_0. To any subset A of points on the surface of the sphere, a number $P(A)$ proportional to the surface of the set of points lying on H_0 is associated. This defines a probability over X. This probability has been defined *independently* of any choice of coordinates over the surface. ■

Let P be a measure over a nonlinear manifold X. Assume that a particular coordinate system has been chosen over X. Let $\mathbf{x} = \{x^1, x^2, \ldots\}$ denote the coordinates of a point. If a function $f(\mathbf{x})$ exists such that for any $A \subset X$,

$$P(A) = \int_A d\mathbf{x}\, f(\mathbf{x}) , \tag{1.15}$$

where, for short, the following notation has been used

$$\int_A d\mathbf{x} \equiv \int dx^1 \int dx^2 \ldots \qquad \text{(over } A\text{)} ,$$

then $f(\mathbf{x})$ is termed the *measure density function* representing P (with respect to the given coordinate system). If P is a probability (i.e., if $P(X)$ is finite), then $f(\mathbf{x})$ is termed a *probability density function.*

Example 13: Let X, π_0, and H_0 be as defined in the previous example. Let us consider a particular choice of coordinates over the surface of the sphere, such as for instance spherical coordinates (θ,ϕ). Letting $f(\theta,\phi)$ be a function defined by

$$\begin{aligned} f(\theta,\phi) &= \sin\theta && \text{on } H_0 \\ f(\theta,\phi) &= 0 && \text{outside } H_0 , \end{aligned}$$

and as the surface element over the surface on a sphere is $dS = \sin\theta\, d\theta\, d\phi$, the probability defined in the previous example can be written

$$P(A) = \int d\theta \int d\phi\, \frac{f(\theta,\phi)}{4\pi} \qquad \text{(over } A\text{)} .$$

The function $f(\theta,\phi)/4\pi$ defines a *probability density* over the surface of the sphere. Let (u,v) be a new choice of coordinates over the sphere. To the *same* probability P there corresponds a new probability density $g(u,v)$ which is, in general, *different* from the old one. ■

Example 14: Let X be the positive part of the real line, $X = R^+ = (0,+\infty)$, and let $f(x)$ be the function $1/x$. The integral (1.15) then defines a measure over X, but not a probability (because $P(R^+) = \infty$). The function $f(x)$ is then a *measure density* but not a probability density. ■

To develop our theory, we will effectively need to consider non-normalizable measures (i.e., measures which are not a probability). These measures cannot describe the probability of a given subset A of the parameter space under consideration: they can only describe the *relative probability* of two subsets A_1 and A_2. We will see that this is sufficient for our needs. To simplify the discussion, I will use the languistic abuse of naming "probability" an arbitrary measure.

If a measure is normalizable (i.e., if it is a probability), it is immaterial whether it has effectively been normalized or not. In this book, two probabilities P_1 and P_2 which are proportional,

$$P_1(A) \equiv r\, P_2(A) \quad \text{(for any } A\text{)} \quad \text{(r given a positive real number)}, \qquad (1.16)$$

are identified. This gives much lighter notations, because the probability densities under consideration do not need to be systematically normalized. Note that the constant r in (1.16) has to be adimensional.

To allow more generality to the notations, I assume that the "functions" representing probability densitites are, in fact, distributions, i.e., generalized functions containing in particular Dirac's "delta function".

It should be noticed that, as a probability is a real number, and as the components $x^1,x^2,...$ in general have physical dimensions, the physical dimension of a probability density is a *density* of the considered space, i.e., it has as physical dimensions the inverse of the physical dimensions of the volume element of the considered space.

Example 15: Let v be a velocity and m a mass. The respective physical dimensions are $L\,T^{-1}$ and M. Let $f(v,m)$ be a probability density on (v,m). For the probability

$$P(\, v_1 \le v \le v_2 \text{ and } m_1 \le m \le m_2\,) = \int_{v_1}^{v_2} dv \int_{m_1}^{m_2} dm\; f(v,m)$$

to be a real number, the physical dimensions of f have to be $M^{-1}\,L^{-1}\,T$. ■

Let P be a probability over X, and $f(x)$ be the probability density representing P in a given coordinate system. Let

$$\mathbf{x}^* = \mathbf{x}^*(\mathbf{x}) \tag{1.17}$$

represent a *change of coordinates* over X, and let $f^*(\mathbf{x}^*)$ be the probability density representing P in the new coordinates:

$$P(A) = \int_A d\mathbf{x}^* \, f^*(\mathbf{x}^*) \, .$$

By definition of $f(\mathbf{x})$ and $f^*(\mathbf{x}^*)$, for any $A \subset X$

$$\int_A d\mathbf{x} \, f(\mathbf{x}) = \int_A d\mathbf{x}^* \, f^*(\mathbf{x}^*) \, ,$$

using the elementary properties of the integral, the following important property can be deduced

$$f^*(\mathbf{x}^*) = f(\mathbf{x}) \left| \frac{\partial \mathbf{x}}{\partial \mathbf{x}^*} \right| , \tag{1.18}$$

where $|\partial \mathbf{x}/\partial \mathbf{x}^*|$ represents the absolute value of the Jacobian of the transformation.

Let $\mathbf{x}$ and $\mathbf{y}$ be two vector parameter sets, and let $f(\mathbf{x},\mathbf{y}$ be a normalized probability density. Two definitions are important: the *marginal probability density* for $\mathbf{y}$,

$$f_Y(\mathbf{y}) = \int_X d\mathbf{x} \, f(\mathbf{x},\mathbf{y}) \, , \tag{1.19a}$$

and the *conditional probability density* for $\mathbf{x}$ given $\mathbf{y} = \mathbf{y}_0$,

$$f_{X|Y}(\mathbf{x}|\mathbf{y}_0) = \frac{f(\mathbf{x},\mathbf{y}_0)}{\displaystyle\int_X d\mathbf{x} \, f(\mathbf{x},\mathbf{y}_0)} \, . \tag{1.19b}$$

From these definitions it follows that the joint probability density equals the conditional probability density times the marginal probability density:

$$f(\mathbf{x},\mathbf{y}) = f_{X|Y}(\mathbf{x}|\mathbf{y}) \, f_Y(\mathbf{y}) \, , \tag{1.20a}$$

and the *Bayes theorem*:

$$f_{Y|X}(y|x) = \frac{f_{X|Y}(x|y)\, f_Y(y)}{\int_Y dy\, f_{X|Y}(x|y)\, f_Y(y)} . \qquad (1.20b)$$

The Bayes theorem is a mathematical tautology, which cannot be applied to solve real world problems, unless physical postulates attach a particular interpretation to the probability densities and associated marginal and conditional probabilities.

1.2.2: The interpretation of a probability

It is possible to associate more than one intuitive meaning to any mathematical theory. For instance, the axioms and theorems of a three-dimensional vector space can be interpreted as describing the physical properties of the sum of forces acting on a point material particle, as well as describing the physiological sensations produced in our brain when our retina is excited by a light composed by a mixing of the three fundamental colors (e.g., Feynmann, 1963). Hofstadter (1979) gives a lot of examples of different valid intuitive meanings that can be associated with a given formal system.

There are two different usual intuitive interpretations of the axioms of probability as introduced in the previous section.

The first interpretation is purely statistical: when some physical "random" process takes place it leads to a given "realization". If a great number of realizations have been observed, these can be described in terms of "probabilities", which follow the axioms of the previous section. The physical parameter allowing of describing the different realizations is termed a *random variable*. The mathematical theory of statistics is the natural tool for analyzing the outputs of a random process.

Example 16: After one million throws of a biased coin, I have observed $6.2\ 10^5$ HEADS and $3.8\ 10^5$ TAILS. This gives the probability

$$P(\varnothing) = P(\text{neither HEAD nor TAIL}) = 0 ,$$

$$P(\text{HEAD}) = 0.62 ,$$

$$P(\text{TAIL}) = 0.38 ,$$

and

$$P(\text{HEAD} \cup \text{TAIL}) = P(\text{HEAD or TAIL}) = 1 . \blacksquare$$

The second interpretation is in terms of *subjective degree of knowledge* of the "true" value of a given physical parameter. By "subjective" is meant that it represents the knowledge of a given individual, obtained using rigorous scientific (objective) methods, but that this knowledge may vary from individual to individual because each may possess different data sets.

Example 17: What is the radius of the Earth's metallic core? Nobody knows exactly. But with the increasing accuracy of seismic measurements, the *information* we have on this parameter continuously improves. The opinion maintained in this book is that the more general (and scientifically rigorous) answer it is possible to give at any moment to that question is found by defining a rule giving the probability of the true value of the radius of the Earth's core being within r_1 and r_2 for any couple of values r_1 and r_2. That is to say, the most general answer consists in the definition of a *probability* over the physical parameter representing the radius of the core. ■

This subjective interpretation of the postulates of the probability theory is usually named *Bayesian*, in honor of Bayes (1763). It is not in contradiction with the statistical interpretation. It simply applies to different situations.

One of the difficulties of the approach is that, given a state of information on a set of physical parameters, it is not always easy to decide which probability "models" it best. I hope that the examples in this book will help to show that it is possible to use some common sense rules to give an adequate solution to this problem.

I set explicitly the following postulate:

> Let X be a discrete parameter space
> with a finite number of parameters.
> The most general way we have
> for describing any ***state of information*** on X
> is by defining a **probability** (in general, a measure) over X.

Let P denote the probability corresponding to a given state of information on X, and $f(\mathbf{x})$ the associaled probability density:

$$P(A) = \int_A d\mathbf{x}\ f(\mathbf{x}) \qquad \text{for any } A \subset X.$$

The probability $P(\cdot)$ or the probability density $f(\cdot)$ are said to *represent*

For practical applications of the probability theory, it is also necessary to give an intuitive content to the definition of marginal probability. Let $f(y,z)$ be the probability density representing a certain state of information on the parameters (y,z). From the definition in the preceding section and the previous discussion, we can see that all the information on the parameters y is contained in the marginal probability density $f_Y(y) = \int dz\, f(y,z)$. The probability density $f(y,z)$ does not contain more information on y; it contains only information about the "correlations" between the parameters y and z.

Box 1.1: Central estimators and estimators of dispersion

a) One-dimensional case. Given a normalized one-dimensional probability density function $f(x)$, consider the expression

$$s_p(m) = \left(\int_{-\infty}^{+\infty} dx \; |x - m|^p \; f(x) \right)^{1/p} . \qquad (1)$$

For given p, the value of m which makes s_p minimum is termed the *center of* $f(x)$ *in the* ℓ_p *norm sense*, and is denoted by m_p. The value m_1 is termed the *median*, m_2 the *mean* (or *mathematical expectation*), and m_∞ the *mid-range*. The following properties hold:

median (minimum ℓ_1 norm):

$$\int_{-\infty}^{+\infty} dx \; |x-m_1| \; f(x) \text{ minimum } \Leftrightarrow \int_{-\infty}^{m_1} dx \; f(x) = \int_{m_1}^{+\infty} dx \; f(x) = \frac{1}{2}$$

mean (minimum ℓ_2 norm):

$$\int_{-\infty}^{+\infty} dx \; (x-m_2)^2 \; f(x) \text{ minimum } \Leftrightarrow m_2 = \int_{-\infty}^{+\infty} dx \; x \; f(x)$$

mid-range (minimum ℓ_∞ norm):

$$\lim(p \to \infty) \int_{-\infty}^{+\infty} dx \; |x-m_\infty|^p \; f(x) \text{ minimum } \Leftrightarrow m_\infty = \frac{x_{sup} + x_{inf}}{2} ,$$

where x_{sup} (resp. x_{inf}) is the maximum (resp. minimum) value of x for which $f(x) \neq 0$.

(...)

The value of $s_p(m)$ at the minimum is termed the *dispersion of* $f(x)$ *in the* ℓ_p *norm sense*, and is denoted by σ_p :

$$\sigma_p = s_p(m_p) . \tag{2}$$

The value σ_1 is termed the *mean deviation* , σ_2 the *standard deviation*, and σ_∞ the *half-range* . The following properties hold:

mean deviation (minimum ℓ_1 norm):

$$\sigma_1 = \int_{-\infty}^{+\infty} dx \; |x-m_1| \; f(x) \quad \Leftrightarrow \quad \sigma_1 = \int_{m_1}^{+\infty} dx \; x \; f(x) - \int_{-\infty}^{m_1} dx \; x \; f(x)$$

standard deviation (minimum ℓ_2 norm):

$$\sigma_2^2 = \int_{-\infty}^{+\infty} dx \; (x-m_2)^2 \; f(x) \quad \Leftrightarrow \quad \sigma_2^2 = \int_{-\infty}^{+\infty} dx \; x^2 \; f(x) - m_2^2$$

half-range (minimum ℓ_∞ norm):

$$\sigma_\infty = \lim_{p \to +\infty} \left(\int dx \; |x-m_\infty|^p \; f(x) \right)^{1/p} \quad \Leftrightarrow \quad \sigma_\infty = \frac{x_{sup} - x_{inf}}{2}$$

b): Multidimensional case. Given a probability density function $f(\mathbf{x})$ defined for the vector variable $\mathbf{x} = (x^i \; ; \; i \in I_X)$, consider the operator $\mathbf{C}_2(\mathbf{m})$ defined by its components

$$C_2^{ij}(\mathbf{m}) = \int_{-\infty}^{+\infty} dx \; (x^i-m^i) \; (x^j-m^j) \; f(\mathbf{x}) . \tag{3}$$

The vector $\mathbf{m}_2$ which minimizes the diagonal elements of $\mathbf{C}_2(\mathbf{m})$ is termed the *mean* (or mathematical expectation) of $\mathbf{x}$ *in the* ℓ_2 *norm sense*. It is given by

$$\mathbf{m}_2 = \int_{-\infty}^{+\infty} dx \; \mathbf{x} \; f(\mathbf{x}) .$$

The value at $\mathbf{m} = \mathbf{m}_2$ of the operator (3) is termed the *covariance* of $\mathbf{x}$ *in the* ℓ_2 *norm sense*, and is simply denoted by $\mathbf{C}_2$:

(...)

$$C_2 = C_2(m_2) . \qquad (4)$$

The diagonal elements of C_2 clearly equal the variances (square of standard deviations) previously defined:

$$C_2^{ii} = (\sigma_2^i)^2 .$$

The covariance operator in the ℓ_2 norm sense (or *ordinary* covariance operator) has the following properties (see, for instance, Pugachev 1965):

i) C_2 is symmetric:

$$C_2^{ij} = C_2^{ji} .$$

ii) C_2 is definite nonnegative: for any vector x,

$$x^t \; C_2^{-1} \; x \geq 0 .$$

iii) if C_2 is positive definite, then, for any vector x, the quantity

$$\| x \|_2 = (x^t \; C_2^{-1} \; x)^{1/2}$$

has the properties of a norm. It is termed the *weighted* ℓ_2 *norm* of the vector x.

iv) The *correlation coefficients* ρ_2^{ij} defined by

$$\rho_2^{ij} = \frac{C_2^{ij}}{\sigma_2^i \, \sigma_2^j}$$

have the property

$$-1 \leq \rho_2^{ij} \leq +1 .$$

v) The probability density

$$f(x) = ((2\pi)^N \det C_2)^{-1/2} \exp\left[-\frac{1}{2} (x - x_0)^t \; C_2^{-1} \; (x - x_0) \right] ,$$

where N is the dimension of the vector x, is normalized, with a mean value x_0, and covariance operator C_2 (e.g., Dubes, 1968). From the results of problem 1.15 it follows that among all the probability densities with given ℓ_2 norm covariance operator, the Gaussian function has (...)

minimum information content (i.e., it has maximum "spreading").
The discussion of the multidimensional spaces has been limited to the ℓ_2 norm case. It is not clear at present which is the right generalization of these concepts to the general ℓ_p norm case.

1.2.3: The state of Perfect Knowledge

If we definitely know that the true value of $\mathbf{x}$ is $\mathbf{x} = \mathbf{x}_0$, it is clear that the corresponding probability density is

$$f(\mathbf{x}) = \delta(\mathbf{x} - \mathbf{x}_0) , \tag{1.21}$$

where $\delta(.)$ represents Dirac's delta function. The probability density (1.21) gives null probability to $\mathbf{x} \neq \mathbf{x}_0$, and probability 1 to $\mathbf{x} = \mathbf{x}_0$. The use of such a state of knowledge does not make sense in itself, because all our knowledge of the real world is subjected to uncertainties, but it is often justified when a certain type of error is negligible *compared* to another type of error (see for instance section 1.5.3).

1.2.4: The state of Total Ignorance (or the reference state of information)

Given a parameter set, it is useful to define a certain state of information which represents a *reference* state of information: in some sense the state of "lowest" information. The probability representing this particular state of information is termed *non-informative*, and is represented by $M(\cdot)$. The associated probability density is denoted $\mu(\cdot)$:

$$M(A) = \int_A dx \ \mu(x) ,$$

and is termed the *non-informative probability density.*

Example 18: Assume that our problem is the estimation of the spatial location of some event. We can intuitively accept that the non-informative probability gives equal probabilitites of containing the event to all regions of the space with equal volume. Using, for instance, cartesian coordinates (x,y,z), the volume element of the space is

$$dV = dx\, dy\, dz .$$

The requirement

$$P(V) = \iiint_V dx\, dy\, dz\ \mu(x,y,z) \qquad \text{proportional to } V \tag{1.22}$$

shows that the non-informative probability density for a location is, in cartesian coordinates,

$$\mu(x,y,z) = \text{const}. \tag{1.23}$$

It is of course possible to choose other systems of coordinates to represent a spatial location. Using, for instance, spherical coordinates (r,θ,ϕ), equation (1.22) becomes

$$P(V) = \iiint_V dr\, d\theta\, d\phi\ \mu^*(r,\theta,\phi) \qquad \text{proportional to } V \tag{1.24}$$

and, as the volume element of the space is, in spherical coordinates,

$$dV = r^2 \sin\theta\, dr\, d\theta\, d\phi\,,$$

we deduce that the non-informative probability density for a location is, in spherical coordinates,

$$\mu^*(r,\theta,\phi) = \text{const}\ r^2 \sin\theta \tag{1.25}$$

(this last result can also be directly obtained from (1.23) using (1.18)). This example shows that there is no intuitive reason for assuming that a non-informative density function has to be uniform. It also shows that there may exist a particular choice of parameters for which it is uniform. ■

All situations are not so obvious, and explicit notions of invariance may have to be invoked in order to define the non-informative probability density.

Example 19: Let $\mathbf{v}$ be the velocity of a non-relativistic particle:

$$\mathbf{v} = \frac{d\mathbf{r}}{dt}\,,$$

where $\mathbf{r}$ denotes the spatial position of the particle, and t a Newtonian time. Let v denote the euclidean norm of $\mathbf{v}$:

$$v = \frac{\|d\mathbf{r}\|}{|dt|}\,.$$

Using cartesian coordinates, we have

$$v = \frac{\sqrt{dx^2+dy^2+dz^2}}{|dt|} .$$

Let $\mu(v)$ denote the non-informative probability density for v.

Assume that a second observer uses another Galilean coordinate system (x^*,y^*,z^*,t^*). It is then related with the previous one by a change of origin and of scale,

$$x^* = x_0 + a\,x , \qquad y^* = y_0 + a\,y , \qquad z^* = z_0 + a\,z ,$$

and

$$t^* = t_0 + b\,t ,$$

where a and b are some constants. Let $\mu^*(v^*)$ be the non-informative probability density for the second observer. The postulate of space-time homogeneity implies that the two coordinate systems have to be equivalent. In particular, $\mu(\cdot)$ and $\mu^*(\cdot)$ have to be the same function, i.e., for any w,

$$\mu(w) = \mu^*(w) . \tag{1.26}$$

We have

$$v^* = \frac{\sqrt{dx^{*2}+dy^{*2}+dz^{*2}}}{|dt^*|} = c\,v ,$$

where $c = |a/b|$. Using (1.18),

$$\mu(v) = \mu^*(v^*) \left| \frac{dv^*}{dv} \right| = c\ \mu^*(c\,v) .$$

Condition (1.26) then gives

$$\mu(v) = c\ \mu(c\,v) ,$$

i.e.,

$$\mu(v) = \frac{\text{const}}{v} . \tag{1.27}$$

It should be noticed that (1.27) defines a measure density which is not a probability density (it is not normalizable). ■

Example 20: Assume that an observer prefers to use slowness $n = 1/v$ instead of velocity. Which is the function $\mu^*(n)$ representing the non-infor-

mative probability density for n ?

It is possible here to follow exactly the same argument as in the previous example. More simply, using the properties of the change of variables (equation 1.18), we directly obtain

$$\mu^*(n) = \mu(v) \left| \frac{dv}{dn} \right| = \frac{\text{const}}{n} . \qquad (1.28)$$

It is interesting to note that in addition to the invariance of form of μ with respect to a change of space-time coordinates, we also have invariance of form with respect to the choice of *reciprocal parameters* (the choice $\mu(v) =$ const would not be consistent with the choice $\mu^*(n) =$ const) . ■

There is a lot of controversy in the literature as to the possibility of effectively defining non-informative probability densities. Jaynes (1968), for instance, suggests that for a given definition of the physical parameters x it is possible to find a *unique* density function $\mu(\mathbf{x})$ which has the strong property of being *form invariant* under the transform groups which leave the fundamental equations of physics invariant. He then suggests taking such a density function as the non-informative one. Additional discussion can be found in Box and Tiao (1973), Rietsch (1977), or Savage (1954, 1962).

In the rest of this book I assume that, for any parameter set, it is possible to exhibit some probability density (or measure density) which, by consensus, will be termed the *reference probability density*, and which some (as myself) will call the *non-informative probability density* .

The parameterizations for which the probability density is uniform ($\mu(\mathbf{x}) =$ const) play an important practical role. This justifies the following definition: *a parameter set* $\mathbf{x}$ *is termed* ***cartesian*** *if the corresponding non-informative probability is represented by a uniform probability density.*

Example 21: **The cartesian (in the usual sense) coordinates of example 18.** ■

Example 22: The non-informative probability density for a velocity has been obtained in example 19:

$$\mu(v) = \frac{\text{const}}{v} .$$

Introducing the "log-velocity" v^* by

$$v^* = \alpha \, \text{Log}\left(\frac{v}{v_0}\right) ,$$

where v_0 is an arbitrary fixed velocity, and α an arbitrary constant, gives the non-informative probability density

$$\mu^*(v^*) = \mu(v) \left| \frac{dv}{dv^*} \right| = \frac{\text{const}}{v} \frac{v}{\alpha} = \frac{\text{const}}{\alpha} = \text{const} ,$$

thus showing that the log-velocity is a cartesian parameter, while the velocity is not. ■

Example 23: The slowness $n = 1/v$ of example 20 is not a cartesian parameter. But the log-slowness

$$n^* = \alpha \, \text{Log}\left(\frac{n}{n_0}\right)$$

is. ■

Examples 19 and 20 suggest that the probability density

$$f(x) = 1/x$$

plays an important role in practical applications. As taking the logarithm of the parameter

$$x^* = \alpha \, \text{Log}\left(\frac{x}{x_0}\right)$$

transforms the probability density into a uniform one,

$$f^*(x^*) = \text{const} ,$$

the function $1/x$ will be termed the *log-uniform probability density* . It is shown in box 1.3 to be a particular case of the log-normal probability density. As discussed by Jeffreys (1939, 1957), parameters with a log-uniform non-informative probability density are characterized by being *positive* by definition (a temperature T , a density of matter ρ , a wave-celerity v ,...). Their reciprocal parameters ($\beta = 1/kT$, lightness of matter $\ell = 1/\rho$, slowness $n = 1/v$,...) can naturally be introduced, and also have a log-uniform non-informative probability density.

It should be mentioned that, although no coherent inverse theory can be set without the introduction of the non-informative probability, generally it does not play an important role, and, except in highly degenerated problems, numerical inverse results do not critically depend on the particular form of $\mu(\mathbf{x})$.

There are two ways of defining a physical parameter. It can be defined *operationally*, or it can be defined *mathematically* as a function of other parameters already defined. In the latter case, the equation relating the parameters is *not* a physical law. I postulate that if a parameter set contains only *independently defined* (i.e., operationally defined) parameters, the non-infor-

mative joint probability density $\mu(\mathbf{x})$ is given by

$$\mu(\mathbf{x}) = \prod_A \mu_A(x^A) \qquad (A \in \mathbf{I}_X) \tag{1.29}$$

where $\mu_A(x^A)$ is the non-informative probability density for the parameter x^A. Such a parameter set is termed *minimal*. Unless otherwise stated, I assume that this is always the case (this avoids, for instance, having, say, a velocity, *and* the corresponding slowness *defined* by $n = 1/v$ in a parameters set).

Box 1.2: Generalized Gaussian

As shown in problem 1.15, among all the normalized probability densities $f(x)$ with fixed ℓ_p norm estimator of dispersion,

$$\int_{-\infty}^{+\infty} dx \; | x - x_0 |^p \; f(x) = (\sigma_p)^p ,$$

the one with *minimum information content* (i.e., with maximum "spreading") is given by

$$f_p(x) = \frac{p^{1-1/p}}{2\,\sigma_p\,\Gamma(1/p)} \exp\left(- \frac{1}{p} \frac{| x - x_0 |^p}{(\sigma_p)^p} \right), \tag{1}$$

where $\Gamma(.)$ denotes the Gamma function.

Figure 1.2 shows some examples with p respectively equal to 1.0, 1.5, 2.0, 3.0, and 100.0. For $p = 1$,

$$f_1(x) = \frac{1}{2\,\sigma_1} \exp\left(- \frac{| x - x_0 |}{\sigma_1} \right),$$

and $f_1(x)$ is a symmetric exponential, centered at $x = x_0$ with *mean deviation* equal to σ_1. For $p = 2$,

$$f_2(x) = \frac{1}{\sqrt{2\pi}\,\sigma_2} \exp\left(- \frac{1}{2} \frac{(x - x_0)^2}{\sigma_2^2} \right),$$

and $f_2(x)$ is a Gaussian function, centered at $x = x_0$ with *standard deviation* equal to σ_2. For $p \to \infty$,

(...)

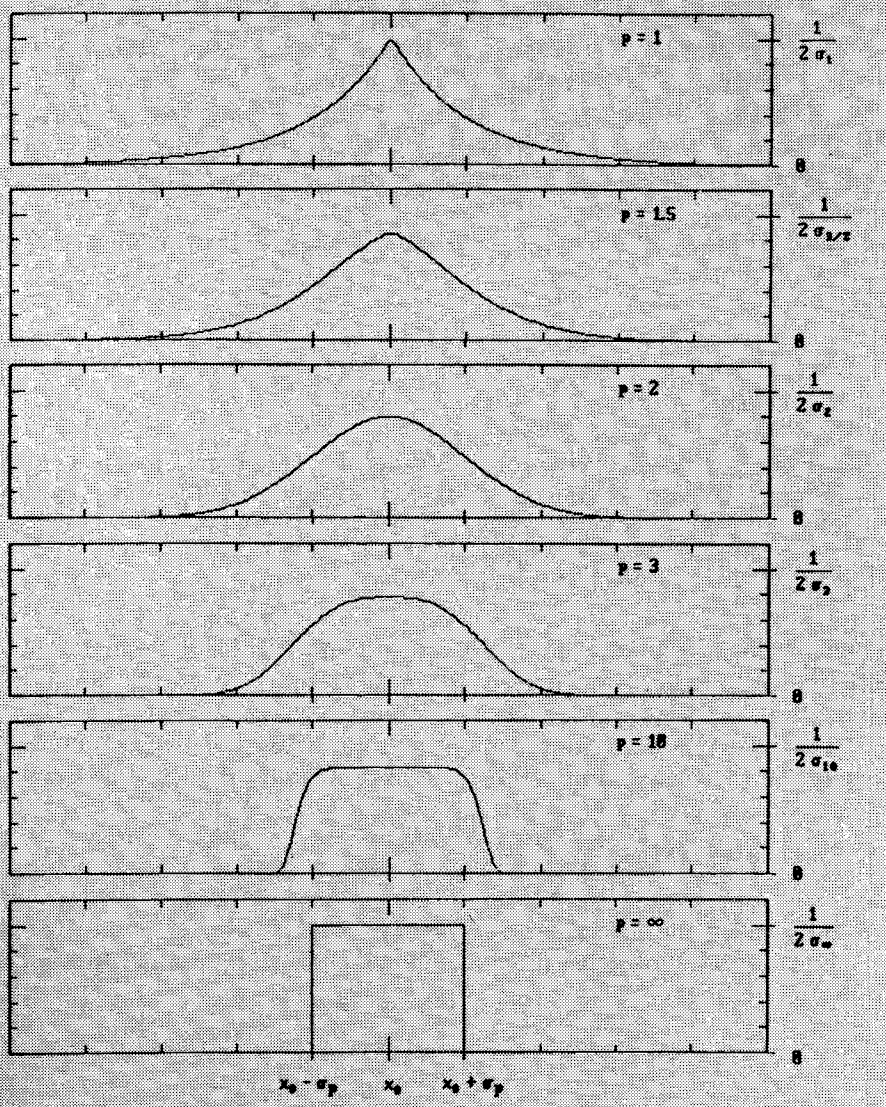


Figure 1.2: Generalized Gaussian of order p . The value p = 1 gives a double exponential, p = 2 gives an ordinary Gaussian, and p = ∞ gives a box-car.

(...)

$$f_\infty(x) = \begin{cases} 1/(2\,\sigma_\infty) & \text{for } x_0 - \sigma_\infty \le x \le x_0 + \sigma_\infty \\ 0 & \text{otherwise,} \end{cases}$$

and $f_\infty(x)$ is a box function, centered at $x = x_0$ with *mid-range* equal to σ_∞. Problem 1.21 shows that $f_p(x)$ is normalized to unity.

The function $f_p(x)$ defined in (1) can be termed *generalized Gaussian*, because it generates a family of well-behaved functions containing the Gaussian function as a particular case. Symmetric exponentials, Gaussian functions, and box-car functions are often used to model error distribution. The definition of generalized Gaussian slightly widens the possibility of choice.

1.2.5: Shannon's measure of Information Content

Given two normalized probability density functions $f_1(\mathbf{x})$ and $f_2(\mathbf{x})$, the *relative information content* of $\mathbf{f}_1$ with respect to $\mathbf{f}_2$ is defined by

$$I(f_1;f_2) = \int d\mathbf{x}\; f_1(\mathbf{x})\; \text{Log}\; \frac{f_1(\mathbf{x})}{f_2(\mathbf{x})}\,. \tag{1.30a}$$

When the logarithm base is 2, the unit of information is termed a *bit*; if the base is e=2.71828..., the unit is the *nep*; if the base is 10, the unit is the *digit*.

The relative information content of a probability density $f(\mathbf{x})$ with respect to the (normalized) non-informative probability density $\mu(\mathbf{x})$,

$$I(f;\mu) = \int d\mathbf{x}\; f(\mathbf{x})\; \text{Log}\; \frac{f(\mathbf{x})}{\mu(\mathbf{x})}\,, \tag{1.30b}$$

is simply called the *information content* of $f(\mathbf{x})$.

Equation (1.30b) generalizes Shannon's (1948) original definition for discrete probabilities

$$I(P) = \sum_i P_i\; \text{Log}\; P_i$$

to density functions. It should be noticed that the expression $\int d\mathbf{x}\; f(\mathbf{x})\; \text{Log}\; f(\mathbf{x})$ cannot be used as a definition because it is not consistent (because, besides the fact that the logarithm of a dimensional quantity is not defined, a bijective change of variables $\mathbf{x}^* = \mathbf{x}^*(\mathbf{x})$ would alter the information content, which is not the case with the right definition (1.30b) (see problem

1.13).

It can be shown (problem 1.14) that the information content is always positive

$$I(f;\mu) \geq 0 ,$$

and that it is null only if $f(x) \equiv \mu(x)$: the non-informative probability density function $\mu(x)$ represents the *state of null information.*

1.2.6: The Combination of States of Information

The classical theory of logic gives the rules human beings use to handle information. As an example, let r denote the radius of the Earth's metallic core, and let A_1 and A_2 be the propositions

A_1 : " 3300 km < r < 3500 km "

A_2 : " 3400 km < r < 3600 km " .

These two propositions can be combined to obtain new propositions. For instance, the *disjunction*, $(A_1$ *or* $A_2)$, and the *conjunction*, $(A_1$ *and* $A_2)$, are

$(A_1$ *or* $A_2)$: " 3300 km < r < 3600 km "

$(A_1$ *and* $A_2)$: " 3400 km < r < 3500 km " .

Let $P(A)$ be the "value of truth" of the proposition A , i.e., $P(A) = 1$ if A is "true", and $P(A) = 0$ if A is "false". The combination of logical propositions can be defined by their "table of truth". For instance, the propositions $(A_1$ *or* $A_2)$ and $(A_1$ *and* $A_2)$ are characterized in Table 1.1 .

$P(A_1)$	$P(A_2)$	$P(A_1$ *or* $A_2)$	$P(A_1$ *and* $A_2)$
0	0	0	0
0	1	1	0
1	0	1	0
1	1	1	1

Table 1.1: Values of truth of the logical propositions *and* and *or* .

More formally,

$$P(A_1 \textit{ or } A_2) = 0 \quad \Leftrightarrow \quad \begin{cases} P(A_1) = 0 \\ \text{and} \\ P(A_2) = 0 \end{cases} \tag{1.31}$$

$$P(A_1 \textit{ and } A_2) = 0 \quad \Leftrightarrow \quad \begin{cases} P(A_1) = 0 \\ \text{or} \\ P(A_2) = 0 \,. \end{cases} \tag{1.32}$$

The value of truth of a proposition can also be referred to its "probability": it is equal to 1 for a (certainly) true proposition, and equal to 0 for a (certainly) false proposition.

In section 1.2.2 a state of information on a parameter set X has been defined as a probability over X. Let P_1 and P_2 be two probabilities over X representing two states of information. For the development of our theory, we need to define the conjunction of two states of information; this will be a generalization of the conjunction of logical propositions. The probability representing the new state of information will be denoted $(P_1 \textit{ and } P_2)$.

The equivalent of (1.32) for states of information is as follows: for any $A \subset X$,

$$(P_1 \textit{ and } P_2)(A) = 0 \quad \Leftrightarrow \quad \begin{cases} P_1(A) = 0 \\ \text{or} \\ P_2(A) = 0 \,, \end{cases}$$

or, equivalently,

$$\left.\begin{array}{l} P_1(A) = 0 \\ \text{or} \\ P_2(A) = 0 \end{array}\right\} \Rightarrow \quad (P_1 \textit{ and } P_2)(A) = 0 \tag{1.33a}$$

$$\left.\begin{array}{l} P_1(A) \neq 0 \\ \text{and} \\ P_2(A) \neq 0 \end{array}\right\} \Rightarrow \quad (P_1 \textit{ and } P_2)(A) \neq 0. \tag{1.33b}$$

These conditions are not strong enough to define the conjunction $(P_1 \textit{ and } P_2)$ uniquely. It seems reasonable to impose that the conjunction of any state of information P with the state of null information, M, does not modify the information:

$$(P \textit{ and } M)(A) = P(A) \qquad \text{for any } A \subset X \tag{1.34}.$$

Equations (1.33a) and (1.34) now define a probability uniquely. For greater

compactness, I write the definition of the conjunction (P_1 *and* P_2) as follows:

for any P_1 and P_2 : $$(P_1 \textit{ and } P_2) = (P_2 \textit{ and } P_1) \tag{1.35a}$$

for any P_1 , P_2 , and any $A \subset X$: $P_1(A) = 0 \Rightarrow (P_1 \textit{ and } P_2)(A) = 0$ (1.35b)

for any P : $$(P \textit{ and } M) = P \ , \tag{1.35c}$$

where M represents the state of null information. In problem 1.17 it is shown that if $f_1(x)$, $f_2(x)$,and $\mu(x)$ are the probability densities representing P_1 , P_2 , and M respectively:

$$P_1(A) = \int_A dx \quad f_1(x) \ ,$$

$$P_2(A) = \int_A dx \quad f_2(x) \ ,$$

$$M(A) = \int_A dx \quad \mu(x) \ ,$$

and $\sigma(x)$ is the probability density representing (P_1 *and* P_2) ,

$$(P_1 \textit{ and } P_2)(A) = \int_A dx \quad \sigma(x) \ ,$$

then we have

$$\boxed{\sigma(x) = \frac{f_1(x)\, f_2(x)}{\mu(x)} \ .} \tag{1.36}$$

The conjunction of states of information was first defined by Tarantola and Valette (1982a).

Example 24: Let x and y be cartesian coordinates on a cathodic screen. A random device projects electrons on the screen with a known probability density $f_1(x,y)$. We are interested in the coordinates (x,y) at which a particular electron will hit the screen, and we build an experimental device for measuring them. The measuring instrument is not perfect, and in performing the experiment we can only get the information that the true

coordinates of the impact point had the probability density $f_2(x,y)$. We wish to combine this experimental information with the previous knowledge of the random device, and obtain a better estimate of the impact point. This example is developed in problem 1.12. ■

Let P_1 be a probability measure on the space $X = Y \times Z$, with probability density $f_1(y,z)$, and let P_2 be the probability measure with probability density $f_2(y,z)$, giving a probability of 1 to the event that $z = z_0$:

$$f_2(y,z) = \mu_Y(y)\, \delta(z-z_0) ,$$

where $\mu_Y(y)$ denotes the null information probability density on y. Using (1.36), the conjunction of these two states of information gives the probability density (1.36)

$$\sigma(y,z) = \frac{f_1(y,z)\, f_2(y,z)}{\mu(y,z)} = \frac{f_1(y,z)\, \delta(z-z_0)}{\mu_Z(z)} ,$$

where $\mu_Z(z)$ is the null information probability density for z (equation (1.29) has been used).

The a posteriori marginal probability density for z is

$$\sigma_Z(z) = \int_Y dy\ \sigma(y,z) = \delta(z-z_0) ,$$

in accordance with the information that the true value of z is z_0. The a posteriori marginal probability density for y is

$$\sigma_Y(y) = \int_Z dz\ \sigma(y,z) = \frac{f_1(y,z_0)}{\mu_Z(z_0)} ,$$

or, if it can be normalized,

$$\sigma_Y(y) = \frac{f_1(y,z_0)}{\int_Y dy\ f_1(y,z_0)} . \qquad (1.37)$$

This expression corresponds to the usual definition of *conditional probability density* for y, given $f_1(y,z)$ and $z = z_0$, which is usually denoted $f_1(y|z_0)$. We see that this concept is here contained in the more general concept of combination of states of information (see also box 1.4).

In section 1.5.1, the conjunction of states of information is used to combine information obtained from measurements with information obtained from a physical theory, and is shown to be the basis of the Inverse Problem Theory.

1.3: Information obtained from Physical Theories (Solving the Forward Problem)

Strictly speaking, to solve the forward problem means to predict the error-free values of data, $\mathbf{d}$, that would correspond to a given model, $\mathbf{m}$. I denote this theoretical prediction by

$$\mathbf{d}_{cal} = \mathbf{g}(\mathbf{m}) , \tag{1.38}$$

which is a short notation for the set of equations

$$d^i_{cal} = g^i(\mathbf{m}) \qquad (i \in I_D) .$$

Example 25: Some physical quantity, d , depends on time, t , through the equation

$$d = m^1 t + m^2 .$$

If the parameters m^1 and m^2 are known, for any value t^i we can estimate the corresponding value d^i by

$$d^i_{cal}(m) = g^i(\mathbf{m}) = g^i(m^1,m^2) = m^1 t^i + m^2 . \blacksquare$$

Example 26: The model parameters may represent a discretization of the Potential V(r) describing the spherically symmetric electric field created by an atomic nucleus. The observable parameters d^i may represent the flux of electrons diffused at different directions for a given incident flux. To solve the forward problem corresponds to the resolution of the Schrödinger equation. ■

The predicted values cannot, in general, be identical to the true "observed" values, for two reasons: experimental uncertainties and modelization errors. It is important to note that these two very different sources of error generally produce errors which are of the *same order of magnitude*, because, due to the continuous progress of scientific research, as soon as new experimental methods are capable of decreasing the experimental uncertainty, new theories and new models arise which allow of explaining the observations more accurately. For this reason, it is generally not possible to set inverse problems properly without a careful analysis of modelization errors.

The way of describing experimental uncertainties will be studied in section 1.4. Let us see here how to describe uncertainties due to modelization

errors. Following our postulate that the more general way of describing any state of information is to define a probability density function, we have to accept here that the most general way of describing uncertainties due to rough modelization is by defining, for given values of the model parameters $\mathbf{m}$, a probability density over $\mathbf{d}$, i.e., a *conditional probability density* which will be denoted by $\Theta(\mathbf{d}|\mathbf{m})$.

Example 27: For an exact theory

$$\Theta(\mathbf{d}|\mathbf{m}) = \delta(\mathbf{d}-\mathbf{g}(\mathbf{m})) , \tag{1.39}$$

where $\mathbf{g}(\mathbf{m})$ represents the vector function introduced in equation (1.38). ■

Example 28: Theory with independent error bars. An example can be

$$\Theta(\mathbf{d}|\mathbf{m}) = \left(\prod_{i \in I_D} \frac{1}{2\,\sigma^i(\mathbf{m})} \right) \exp\left(- \sum_{i \in I_D} \frac{| d^i - g^i(\mathbf{m}) |}{\sigma^i(\mathbf{m})} \right) , \tag{1.40}$$

where it is assumed that a double exponential function conveniently models the error distribution, and where the "error bar" of the i-th predicted data value is $\sigma^i(\mathbf{m})$ and is independent of the error bar of the j-th predicted data (null covariances), but depending on the current value of $\mathbf{m}$. ■

Example 29: Gaussian errors. Letting $\mathbf{C}_T(\mathbf{m})$ be a covariance operator (see box 1.1) describing the estimated modeling errors for a model $\mathbf{m}$, it is possible to take

$$\Theta(\mathbf{d}|\mathbf{m}) = ((2\pi)^{ND} \det \mathbf{C}_T(\mathbf{m}))^{-\frac{1}{2}} \exp\left[-\tfrac{1}{2} (\mathbf{d}-\mathbf{g}(\mathbf{m}))^t \, \mathbf{C}_T^{-1}(\mathbf{m}) \, (\mathbf{d}-\mathbf{g}(\mathbf{m})) \right], \tag{1.41}$$

where ND represents the dimension of the data space (number of data parameters). ■

Example 30: Errors due to linearization. Sometimes, the resolution of the forward problem (i.e., the computation of $\mathbf{d}_{cal} = \mathbf{g}(\mathbf{m})$) is too difficult or too expensive, and a *linearization* around a reference model is used:

$$\mathbf{g}(\mathbf{m}) \simeq \mathbf{g}(\mathbf{m}_{ref}) + \mathbf{G}_{ref} \, (\mathbf{m}-\mathbf{m}_{ref}) , \tag{1.42}$$

where

$$G^{i\alpha}_{ref} = \left(\frac{\partial g^i}{\partial m^\alpha} \right)_{m_{ref}} .$$

In this case, modelization errors are usually strongly correlated, and neglecting them may severely alter the solution of the problem. It is often difficult to give a realistic estimation of the linearization errors. ■

Example 31: Errors independent of the model value $\mathbf{m}$. A useful approximation is sometimes that the true value $\mathbf{d}$ differs from the "computed" value $\mathbf{g(m)}$ by an "error" ϵ_T :

$$\mathbf{d} = \mathbf{g(m)} + \epsilon_T , \tag{1.43}$$

where the error ϵ_T is assumed to have known statistics described by the probability density function $f_T(\epsilon_T)$. This gives

$$\Theta(\mathbf{d}|\mathbf{m}) = f_T(\epsilon_T) = f_T(\mathbf{d}-\mathbf{g(m)}) . \blacksquare \tag{1.44}$$

In section 1.2.4, the density function $\mu_M(\mathbf{m})$ describing the state of null information on model parameters was introduced. It is clear that the function defined by

$$\Theta(\mathbf{d},\mathbf{m}) = \Theta(\mathbf{d}|\mathbf{m})\, \mu_M(\mathbf{m}) \tag{1.45}$$

does not contain any information on $\mathbf{m}$ (the marginal probability density for $\mathbf{m}$ is the null information probability density), and it still describes the physical correlations between $\mathbf{d}$ and $\mathbf{m}$ that the physical theory is able to predict. So, for greater generality, I will assume that the description of the information concerning the resolution of the forward problem is not given by a conditional density function $\Theta(\mathbf{d}|\mathbf{m})$ but by a joint density function $\Theta(\mathbf{d},\mathbf{m})$ over the space $\boldsymbol{D}\times\boldsymbol{M}$. Equation (1.45) will only represent a particular (very current) case.

In fact, there exists a class of problems in which the correlations between $\mathbf{d}$ and $\mathbf{m}$ are not predicted by a formal theory, but result from an accumulation of observations. In this case, the joint density function $\Theta(\mathbf{d},\mathbf{m})$ is the natural description of the information.

Example 32: The data parameters d^i may represent the current state of a volcano (intensity of seismicity, rate of accumulation of strain, ...). The model parameters m^α may represent, for instance, the time interval to the next volcanic eruption, the magnitude of this eruption, etc. Our present knowledge of volcanoes does not allow of relating these parameters realistically using physical laws, so that, at present, the only scientific description is

statistical. Provided that in the past we were able to observe a significative number of eruptions of this volcano, we can construct a histogram in the space DxM which describes all our information correlating the parameters (see Tarantola et al., 1985, for an example). This histogram can directly be identified with $\Theta(\mathbf{d},\mathbf{m})$. ■

Briefly synthesizing the conclusions of this section: the expected physical correlations between model and observable parameters can be described using a joint density function $\Theta(\mathbf{d},\mathbf{m})$. When these correlations are predicted by a (necessarily inexact) physical theory, $\Theta(\mathbf{d},\mathbf{m})$ is given by $\Theta(\mathbf{d},\mathbf{m}) = \Theta(\mathbf{d}|\mathbf{m})\ \mu_M(\mathbf{m})$, where $\Theta(\mathbf{d}|\mathbf{m})$ represents the probability density of $\mathbf{d}$ for any given value $\mathbf{m}$. This usually corresponds to put some "error bars" around a "predicted value" $\mathbf{g}(\mathbf{m})$ (see figure 1.3).

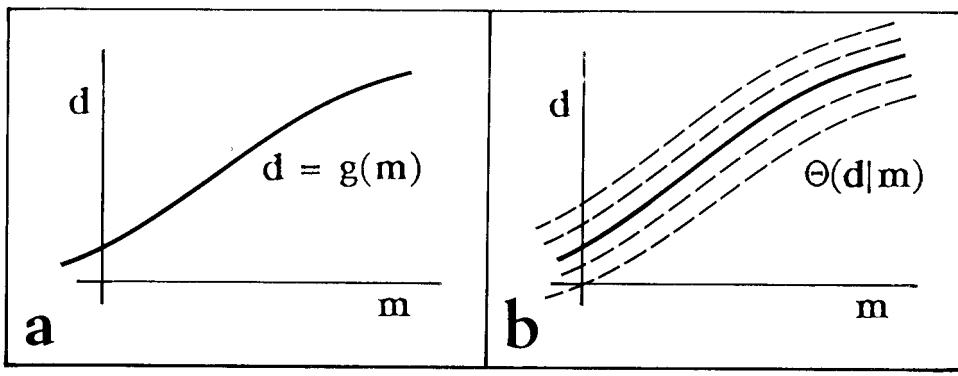


Figure 1.3: a) If uncertainties in the forward modelization can be neglected, a functional relationship $\mathbf{d} = \mathbf{g}(\mathbf{m})$ can be introduced which gives, for each model $\mathbf{m}$, the predicted (or "calculated") data values, $\mathbf{d}$. b) If forward-modeling uncertainties cannot be neglected, they can be described using a conditional probability density, $\Theta(\mathbf{d}|\mathbf{m})$, giving, for each model $\mathbf{m}$, a probability density for $\mathbf{d}$. Roughly speaking, this corresponds to putting "error bars" on the theoretical relation $\mathbf{d} = \mathbf{g}(\mathbf{m})$.

1.4: Information obtained from measurements, and a priori information

1.4.1: Results of the measurements

The measurement experiment will give a certain amount of information on the true values of the observable parameters. Let $\rho_D(\mathbf{d})$ be the probability density function describing this information.

Example 33: Observations are the output of an instrument with known statistics. To simplify the discussion, I will refer to "the instrument" as if all the measurements could result from a single reading on a large apparatus although, more realistically, we generally have some readings from several apparatuses. Assume that at each measurement the instrument delivers a given value of $\mathbf{d}$, denoted $\mathbf{d}_{out}$. Ideally, the supplier of the apparatus should provide a statistical analysis of the errors of the instrument (if he does not, we should not pay for it!). The most useful and general way of giving the results of the statistical analysis is to define the probability density for the value of the output, $\mathbf{d}_{out}$, when the actual input is $\mathbf{d}$. Let $\nu(\mathbf{d}_{out}|\mathbf{d})$ be this conditional probability density. If $f(\mathbf{d}_{out},\mathbf{d})$ denotes the joint probability density for $\mathbf{d}_{out}$ and $\mathbf{d}$, and if we don't use any information on the input, we have

$$f(\mathbf{d}_{out},\mathbf{d}) = \nu(\mathbf{d}_{out}|\mathbf{d})\, \mu_D(\mathbf{d}) .$$

If the actual result of a measurement is $\mathbf{d}_{out} = \mathbf{d}_{obs}$, then we can assimilate $\rho_D(\mathbf{d})$ to the conditional probability density for $\mathbf{d}$ given $\mathbf{d}_{out} = \mathbf{d}_{obs}$:

$$\rho_D(\mathbf{d}) = f_{D|D_{out}}(\mathbf{d}|\mathbf{d}_{out}=\mathbf{d}_{obs}) = \frac{f(\mathbf{d}_{obs},\mathbf{d})}{\int_D d\mathbf{d}\, f(\mathbf{d}_{obs},\mathbf{d})} ,$$

i.e.,

$$\rho_D(\mathbf{d}) = \frac{\nu(\mathbf{d}_{obs}|\mathbf{d})\, \mu_D(\mathbf{d})}{\int_D d\mathbf{d}\, \nu(\mathbf{d}_{obs}|\mathbf{d})\, \mu_D(\mathbf{d})} . \blacksquare \qquad (1.46)$$

Example 34: Perfect instrument. In that case,

$$\nu(\mathbf{d}_{obs}|\mathbf{d}) = \delta(\mathbf{d}-\mathbf{d}_{obs}) , \qquad (1.47)$$

thus giving

$$\rho_D(\mathbf{d}) = \delta(\mathbf{d}-\mathbf{d}_{obs}) . \tag{1.48}$$

The assumption of a perfect instrument may be made when measuring errors are negligible *compared* to modelization errors (see section 1.5.3). ■

Example 35: Gaussian uncertainties. Taking

$$\nu(\mathbf{d}_{obs}|\mathbf{d}) = ((2\pi)^{ND}\det \mathbf{C}(\mathbf{d}_{obs}))^{-1/2}\exp\left[-\frac{1}{2}(\mathbf{d}-\mathbf{d}_{obs})^t\ \mathbf{C}(\mathbf{d}_{obs})^{-1}\ (\mathbf{d}-\mathbf{d}_{obs})\right], \tag{1.49a}$$

where ND represents the number of data, corresponds to the assumption that estimated experimental errors can be described by the covariance operator $\mathbf{C}$, which may depend on the observed values $\mathbf{d}_{obs}$. Using (1.46) this gives

$$\frac{\rho_D(\mathbf{d})}{\mu_D(\mathbf{d})} = ((2\pi)^{ND}\det \mathbf{C}(\mathbf{d}_{obs}))^{-1/2}\exp\left[-\frac{1}{2}(\mathbf{d}-\mathbf{d}_{obs})^t\ \mathbf{C}(\mathbf{d}_{obs})^{-1}(\mathbf{d}-\mathbf{d}_{obs})\right]. \blacksquare \tag{1.49b}$$

Example 36: Errors of the measuring instrument are independent of the input. Assume that the output $\mathbf{d}_{obs}$ is related to the input $\mathbf{d}$ through the simple relation

$$\mathbf{d}_{obs} = \mathbf{d} + \epsilon_D , \tag{1.50}$$

where ϵ_D is an unknown error with known statistics described by the probability density function $f_D(\epsilon_D)$. In that case,

$$\nu(\mathbf{d}_{obs}|\mathbf{d}) = f_D(\epsilon_D) = f_D(\mathbf{d}_{obs}-\mathbf{d}) . \blacksquare \tag{1.51}$$

Example 37: Outliers in a data set. Some data sets contain outliers which are difficult to eliminate, in particular when the data space is highly dimensioned, because it is difficult to visualize such data sets. Problem (1.9) shows that a single outlier in a data set can lead to unacceptable inverse results if the Gaussian assumption is used. This problem suggests using "long-tailed" density functions to represent uncertainties on this kind of data sets. Examples of long-tailed density functions are the symmetric exponential (Laplace) function

$$\rho_D(\mathbf{d}) = \prod_{i \in I_D} \left(\frac{1}{2\sigma^i} \exp\left(- \frac{\left| d^i - d^i_{obs} \right|}{\sigma^i} \right) \right) = \prod_i \frac{1}{2\sigma^i} \exp\left(- \sum_i \frac{\left| d^i - d^i_{obs} \right|}{\sigma^i} \right) ,$$

or the Cauchy function

$$\rho_D(\mathbf{d}) = \prod_{i \in I_D} \left(\frac{1}{\pi \sigma^i} \frac{1}{1 + \left(\frac{d^i - d^i_{obs}}{\sigma^i} \right)^2} \right) ,$$

which has the nice particularity of having infinite standard deviations. ■

Example 38: Consider a measurement made to obtain the arrival time of a given seismic wave recorded by a seismograph. Sometimes, the seismogram is simple enough to give a simple result (Figure 1.4a). But sometimes, due to strong noise (with unknown statistics), the measurement is not trivial. Figure 1.4b shows a particular example where it is difficult to obtain a numerical value, say t_{obs} , for the arrival time. The use of a probability density function allows of describing information on the arrival time with a sufficient degree of generality (Figure 1.4c). With such kinds of data, it is clear that the subjectivity of the scientist plays a major role. It is indeed the case, *whichtever inverse method is used*, that results obtained by different scientists (for instance, for the location of a hypocenter) from such data sets are different. Objectivity can only be attained if the data redundancy is great enough that differences in data interpretation among different observers do not significantly alter the models obtained. ■

Example 39: Assume that the only instrument we have for measuring a given observable is a buzzer that responds when the true value $\mathbf{d}$ is in the range $\mathbf{d}_{inf} \leq \mathbf{d} \leq \mathbf{d}_{sup}$. We make the measurement, and the buzzer does *not* respond. The corresponding probability density is then

$$\rho_D(\mathbf{d}) = \begin{cases} 0 & \text{for } \mathbf{d}_{inf} \leq \mathbf{d} \leq \mathbf{d}_{sup} \\ \mu_D(\mathbf{d}) & \text{otherwise} , \end{cases} \tag{1.52}$$

where $\mu_D(\mathbf{d})$ is the non-informative probability density for observable parameters. ■

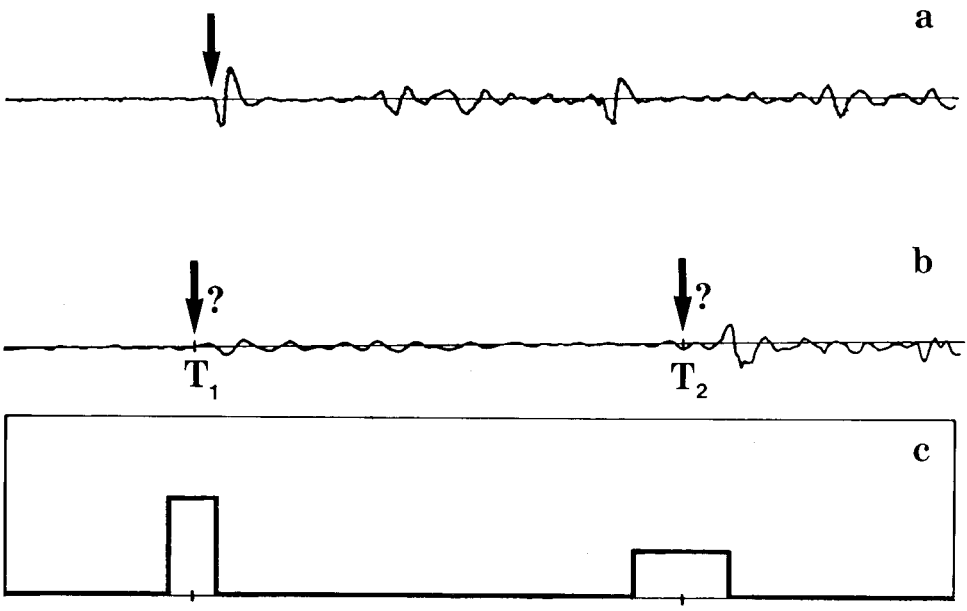


Figure 1.4: a) Seismogram corresponding to an earthquake that occurred in the south of Honshu (Japan) on April 24, 1984, recorded in Paris. The time of first arrival of the seismic wave is clearly visible. b) Seismogram corresponding to an earthquake that occurred east of New Guinea on June 27, 1974, recorded in the south of France. Due to the presence of "ambient noise", it is difficult to pick the first arrival time of the waves. In particular, one may hesitate between times T_1 and T_2. If an expert gives, say, a 50% probability of the first arrival time being in the vicinity of T_1 and a 50% probability of its being in the vicinity of T_2, it is possible to represent this information by the probability density shown in c). The width of each "peak" represents the uncertainty of the reading of each of the possible arrivals, while the separation of the peaks, represents the overall uncertainty.

1.4.2: A priori information on model parameters

By a priori information (or prior information) I mean information which is obtained independently of the results of measurements. The probability density function representing this a priori information will be denoted by $\rho_M(\mathbf{m})$.

Example 40: We have no a priori information. In that case,

$$\rho_M(\mathbf{m}) = \mu_M(\mathbf{m}) \ , \tag{1.53}$$

where $\mu_M(\mathbf{m})$ is the noninformative probability density for model parameters. ■

Example 41: For a given parameter m^α we have only the information that it is strictly bounded by the two values m^α_{inf} and m^α_{sup}. We can take

$$\rho_M(\mathbf{m}) = \prod_{\alpha \in I_M} \rho_\alpha(m^\alpha)$$

where

$$\rho_\alpha(m^\alpha) = \begin{cases} \mu_\alpha(m^\alpha) & \text{for} \quad m^\alpha_{inf} \leq m^\alpha \leq m^\alpha_{sup} . \\ 0 & \text{otherwise} \ , \end{cases}$$

and where $\mu_\alpha(m^\alpha)$ represents the non-informative probability density for m^α . ■

Example 42: The parameters m^α represent a discretization of an unknown continuous function $\Psi(t)$. Assume, for instance, that the a priori information we have on the true value of $\Psi(t)$ is that it belongs to the class of functions represented by the members shown in Figure 1.5. This means that we know that the unknown function is smooth, with a given smoothness length, and that, for each value of t , it takes a value $\Psi_{Mean}(t) \pm \sigma(t)$. In order for the discretization $m^\alpha = \Psi(t_\alpha)$ to be acceptable, we have first to assume that the discretization interval is significantly smaller than the smoothness length of the function. The family of functions in Figure 1.5 seems to be reasonably well represented by a gaussian process with given mean value $\Psi_{Mean}(t)$, and given covariance function $C(t,t')$, both of them grossly estimated from the Figure. Taking

$$m^{\alpha}_{prior} = \Psi_{Mean}(t_\alpha)$$

$$C_M{}^{\alpha\beta} = C(t_\alpha, t_\beta) ,$$

the density function representing the a priori information in the model space is

$$\rho_M(\mathbf{m}) = ((2\pi)^{NM} \det \mathbf{C}_M)^{-1/2} \exp\left(-\frac{1}{2} (\mathbf{m}-\mathbf{m}_{prior})^t \mathbf{C}_M^{-1} (\mathbf{m}-\mathbf{m}_{prior}) \right). \qquad (1.54)$$

This density function gives a high probability density to models $\mathbf{m}$ which are close to $\mathbf{m}_{prior}$ in the sense of the covariance operator $\mathbf{C}_M$, i.e., models in which the difference $\mathbf{m}-\mathbf{m}_{prior}$ is small at each point (with respect to standard deviations in $\mathbf{C}_M$) and smooth (with respect to correlations in $\mathbf{C}_M$). Covariance operators are defined in box 1.1. ■

Example 43: Let us consider a particular atomic nucleus, and let T denote its *half-life*. By definition of half-life, T is necessarily positive. A Gaussian probability density cannot be used to represent any a priori information on T, because a Gaussian function gives a non-vanishing probability for T being negative. Figure 1.6 shows a histogram of the half-lives of the first 580 atomic nuclei quoted in the 1984 CRC Handbook of Chemistry and Physics (I got tired before arriving at the end of the list!). The abscissa of the Figure is

$$T^* = \text{Log}_{10}\left(\frac{T}{1 \text{ second}} \right) . \qquad (1.55a)$$

The logarithmic scale has been chosen for the time axis because, as the half-lives span many orders of magnitude, it is difficult to show the histogram in a linear time axis. With this logarithmic scale, the histogram may conveniently be approximated by a Gaussian function:

$$f^*(T^*) = \frac{1}{(2\pi)^{1/2}\, \sigma^*} \exp\left(-\frac{1}{2} \frac{(T^*-T_0^*)^2}{(\sigma^*)^2} \right) , \qquad (1.56a)$$

with $T_0^* \simeq 3$ and $\sigma^* \simeq 3$. For greater generality, let me write (1.55a) as

$$T^* = \beta \, \text{Log}\left(\frac{T}{\tau_0} \right) \qquad T = \tau_0 \exp\left(\frac{T^*}{\beta} \right) , \qquad (1.55b)$$

where, in our example, $\tau_0 = 1$ second, $\beta = \text{Log } 10$. Using (1.18), we can then obtain the probability density for the time variable T:

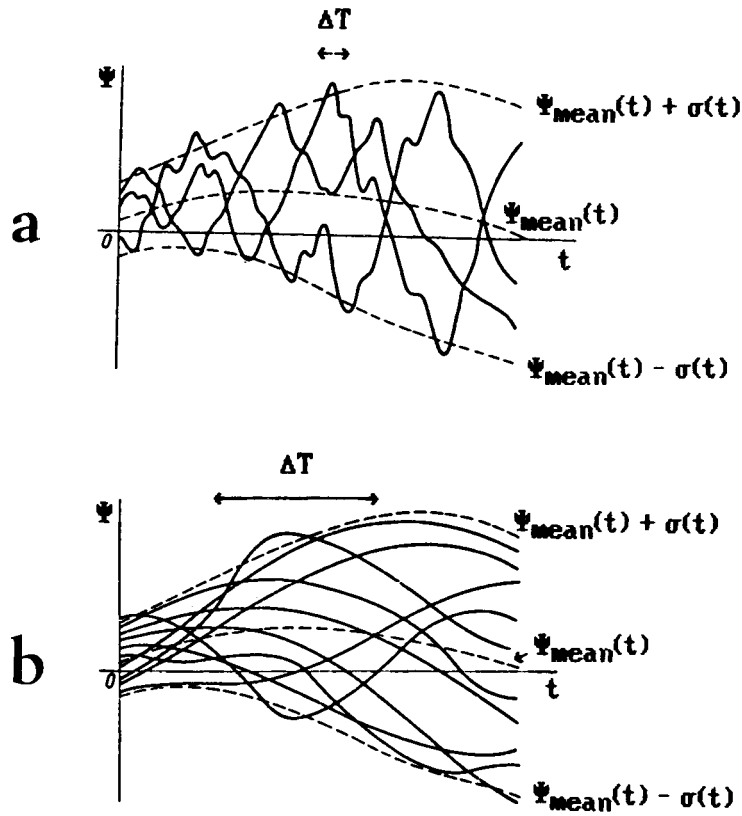


Figure 1.5: Each family of functions (a) and (b) represents some realizations of two different random functions (from Pugachev, 1965). In both cases the mean value, $\Psi_{Mean}(t)$, of the random function is the same. At a given value t , the variance $\sigma^2(t) = C(t,t)$ is also the same. But the covariance $C(t,t')$ between the value at t and the value at t' is different in the two examples. The "correlation length", ΔT , of the family (a) is shorter than the correlation length of the family (b). These two random families can be (quite simplistically) modeled by a Gaussian process (equation (1.54)) with mean $\Psi_{Mean}(t)$ and with the covariance function

$$C(t,t') = \sigma^2\left[\frac{t+t'}{2}\right] \exp\left[-\frac{1}{2}\frac{(t-t')^2}{\Delta T^2}\right],$$

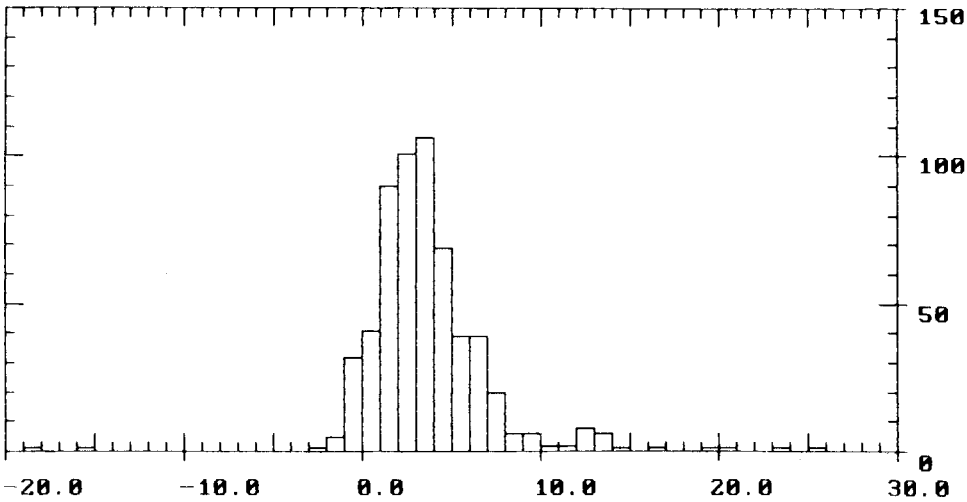


Figure 1.6: Histogram of disintegration periods (half-lives) of the first 580 atomic nuclei in the CRC Handbook of Chemistry and Physics (1984). The horizontal axis represents the logarithm of the half life: $T^* = \mathrm{Log}_{10}(\, T \,/\, 1 \text{ second} \,)$. It is very difficult to show the histogram in a linear time axis, because observed disintegration periods span 45 orders of magnitude in time. Note that the use of a logarithmic time axis allows the histogram to be approximated by a Gaussian probability density. This implies a lognormal probability density in a linear time axis.

$$f(T) = \frac{1}{(2\pi)^{1/2}\, s}\ \frac{1}{T}\ \exp\left[-\frac{1}{2\, s^2}\left(\mathrm{Log}\ \frac{T}{T_0}\right)^2\right], \qquad (1.56b)$$

with

$$T_0^* = \beta\ \mathrm{Log}\left(\frac{T_0}{\tau_0}\right) \qquad T_0 = \tau_0\ \exp\left(\frac{T_0^*}{\beta}\right)$$

and

$$s = \frac{\sigma^*}{\beta} \qquad \sigma^* = \beta\, s\ .$$

The density function (1.56b) is well known and is termed the *log-normal* probability density (because the logarithm of the variable has a normal [Gaussian] probability density). The log-normal density function is studied in box 1.3.

This example suggests that the use of a log-normal probability density is well adapted to modelling a priori information of the type $T \simeq T_0 \pm \Delta T$ for a positive parameter.

Nevertheless, as shown in box 1.3, if the "dispersion" s in (1.56b) is very small, the log-normal function tends to the normal function

$$f(T) \rightarrow \frac{1}{(2\pi)^{1/2}\,\sigma} \exp\left[-\frac{1}{2} \frac{(T-T_0)^2}{\sigma^2} \right] \qquad (\sigma = s\, T_0 << 1) , \tag{1.57}$$

and the subtleties between normal and log-normal probabilities can be neglected. This corresponds to the case where the a probability density gives negligible probabilities to the negative values of the parameter.

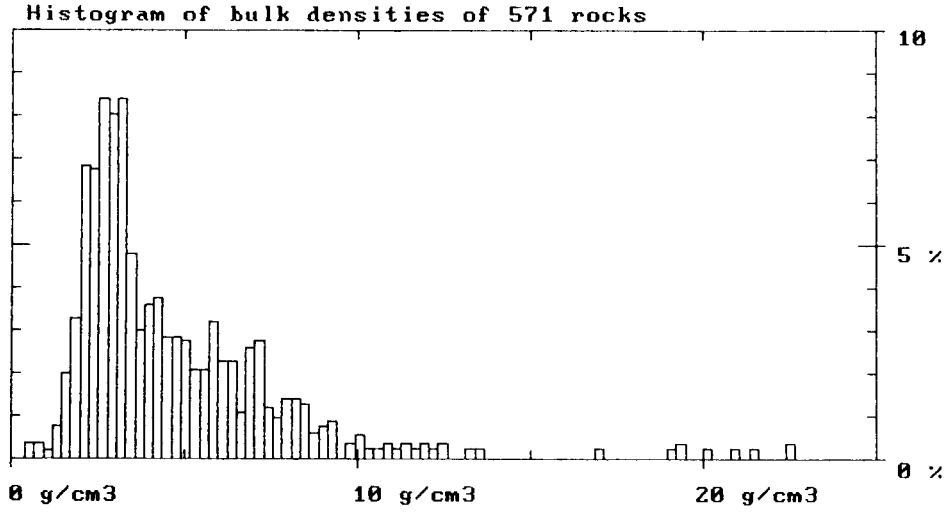
The opposite limit (σ very large) is also interesting. As seen in box 1.3, we then have

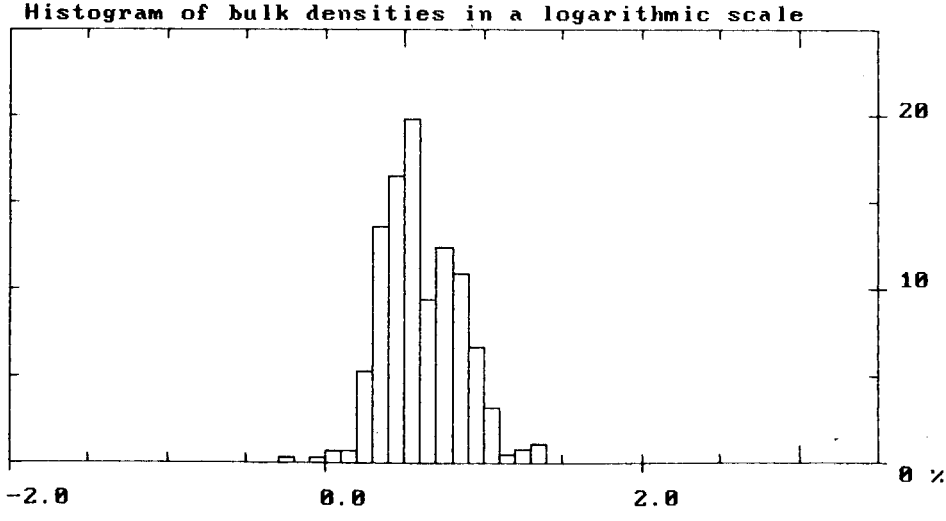
$$f(T) \rightarrow \frac{1}{(2\,\pi)^{1/2}\;s} \frac{1}{T} \qquad (s >> 1) , \tag{1.58}$$

which is the log-uniform probability density introduced in section 1.2.4. In his 1968 paper, Jaynes uses invariance arguments to obtain the non-informative probability density for the half-life of an atomic nucleus, and he obtains (1.58). It is remarkable that the experimental histogram suggests the same conclusion. ■

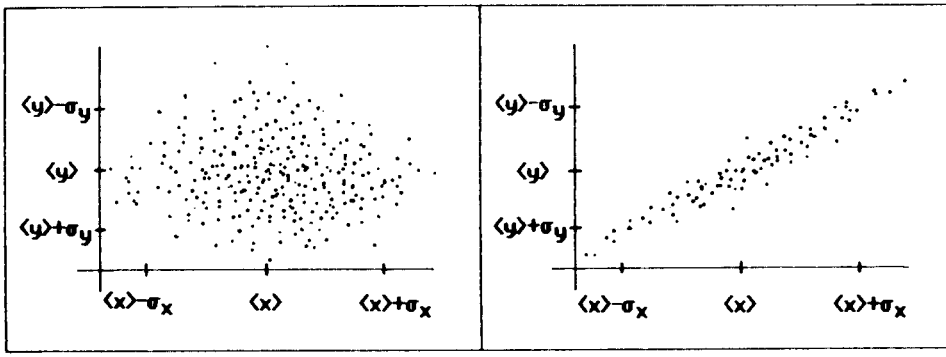
Example 44: Figure 1.7a shows the histogram of densities of different known materials in the Earth's crust (independently of their relative abundance). In 1.7b, the same histogram is shown on a logarithmic scale. If one should stumble over a stone, one may wonder (whilst falling) what the density of the stone may be. If you bear in mind Figure 1.7b, you can take this log-normal function as representing your prior state of information as to its density. If you do not have this Figure in mind, the log-uniform density function will represent your ignorance well. (If, in going to measure the actual density, you stumble over the stone again, better go to another example...). ■

The examples in this section show how it is possible to use probability densities to describe prior information. I have never found a state of information (in the intuitive sense) which cannot be very precisely stated using a probability density. On the other hand, it may seem that probability densities have too many degreees of freedom to allow a definite choice that represents a given state of information.


Histogram of bulk densities of 571 rocks
10 %
5 %
0 %
0 g/cm3
10 g/cm3
20 g/cm3


Histogram of bulk densities in a logarithmic scale
20 %
10 %
0 %
-2.0
0.0
2.0

← *Figure 1.7:* Top: histogram of bulk densities of the 571 different rock types quoted by Johnson & Olhoeft in the CRC Handbook of Physical Properties of Rocks, Vol. III, 1984. Bottom: the same histogram in a logarithmic horizontal scale $\rho^* = \mathrm{Log}_{10}(\rho/\mathrm{g\ cm^{-3}})$. The top histogram is very asymmetric, due to the existence of very heavy minerals ($\rho \simeq 20$ g cm^{-3}) . In a logarithmic scale, it is much more symmetric (bottom). A Gaussian probability density is a reasonably good approximation of the histogram in the ρ^* variable, which means that the corresponding probability density in the ρ variable is log-normal.



↑ *Figure 1.8:* The random points (x_i,y_i) of these diagrams have been generated using 2-dimensional probability densities $f_1(x,y)$ (left) and $f_2(x,y)$ (right). The two probability densities have identical mean values and standard deviations. Only the covariance C_{xy} is different. On the left, the covariance is small, on the right it is large. The probability density $f_2(x,y)$ is more "informative" than $f_1(x,y)$, because it demarcates a smaller region in the space $X \times Y$. This example suggests that if off-diagonal elements of a covariance operator are difficult to estimate, setting them to zero corresponds to neglecting information.

In fact, only a few characteristics of a density function are usually relevant, such as for instance, the position of the "center", the degree of asymmetry, the size of the "error bounds", the "correlations" between different parameters, and the behaviour of the density function "far from the center".

If hesitation exists in choosing the a priori error bars, it is of course best to be overconservative and to choose them very large. A conservative choice for correlations is to neglect them (see Figure 1.8 for an example). The behaviour of the density functions far from the center is only crucial if outliers may exist: the choice of functions tending too rapidly to zero (box-car functions or even Gaussian functions) may lead to inconsistencies; the solution to the problem (as defined in the next section) may not exist, or may be senseless.

Usually the a priori states of information have the form of "soft bounds"; the normal or log-normal density functions generally apply well to that case. If the normal function is thought to vanish too rapidly when the parameter's value tends to infinity, longer tailed functions may be used, such as for instance, the symmetric-exponential function (see box 1.2).

Box 1.3: The Log-normal probability density

It is defined by

$$f(x) = \frac{1}{(2\pi)^{1/2}\, s}\, \frac{1}{x} \exp\left[-\frac{1}{2\, s^2} \left(\mathrm{Log}\, \frac{x}{x_0} \right)^2 \right] . \qquad (1)$$

Figure 1.9 shows some examples for $x_0 = 1$ and s respectively equal to 0.1 , 0.2 , 0.4 , 0.8 , 1.6 , and 3.2 .

The mode, median, and mean of $f(x)$ are respectively

$$m_0 = x_0 \exp(-s^2) \qquad (\, f(x) \text{ maximum for } x = m_0 \,)$$

$$m_1 = x_0 \qquad (2)$$

$$m_2 = x_0 \exp(s^2/2) .$$

The mean deviation and standard deviation are respectively

$$\sigma_1 = x_0 \exp(s^2/2) \, (\mathrm{Erf}(1/s) - \mathrm{Erf}(-1/s)) \qquad (3)$$

$$\sigma_2 = x_0 \exp(s^2/2) \, (\exp(s^2) - 1)^{1/2} , \qquad (...)$$

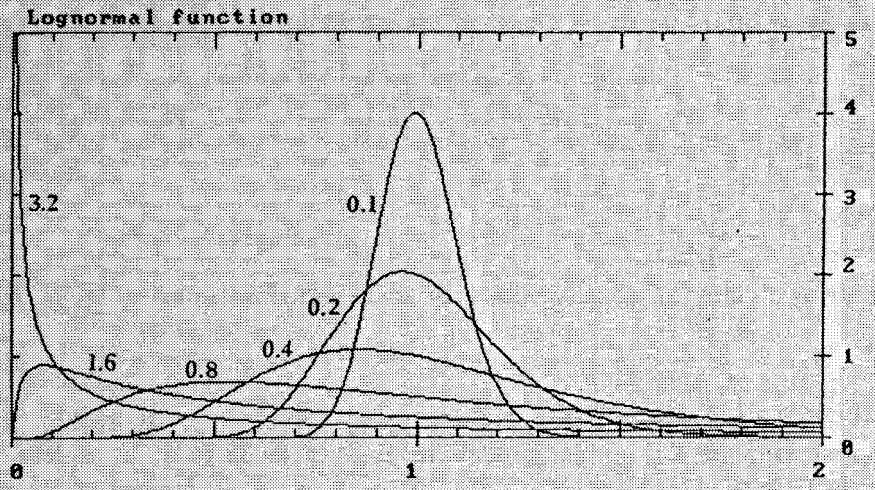


Figure 1.9: The Log-normal probability density.

where Erf(·) denotes the error function

$$\mathrm{Erf}(u) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{u} dt \, \exp\left[-\frac{t^2}{2}\right]$$

The log-normal probability density is so called because the *logarithm* of the variable has a normal (Gaussian) probability density. For the change of variables

$$x^* = \beta \, \mathrm{Log}\left[\frac{x}{\gamma}\right] \qquad x = \gamma \exp\left[\frac{x^*}{\beta}\right] \tag{4}$$

transforms f(x) into

$$f^*(x^*) = \frac{1}{(2\pi)^{1/2}\,\sigma} \exp\left[-\frac{1}{2}\,\frac{(x^*-x_0^*)^2}{\sigma^2}\right], \tag{5}$$

with

(...)

$$\sigma = s\,\beta \qquad\qquad s = \frac{\sigma}{\beta} \tag{6a}$$

and

$$x_0^* = \beta \operatorname{Log}\left(\frac{x_0}{\gamma}\right) \qquad\qquad x_0 = \gamma \exp\left(\frac{x_0^*}{\beta}\right). \tag{6b}$$

In (4), the constant β is often $\operatorname{Log}_e 10$, which corresponds to defining x^* by $x^* = \operatorname{Log}_{10}(x/\gamma)$. The constant γ often corresponds to the physical unit used for x (see example 43). Alternatively, the particular choice

$$x^* = \frac{1}{s} \operatorname{Log}\left(\frac{x}{x_0}\right) \qquad\qquad x = x_0 \exp(s\,x^*)$$

leads to a Gaussian density with zero mean and unit standard deviation:

$$f^*(x^*) = \frac{1}{(2\pi)^{1/2}} \exp\left(-\frac{(x^*)^2}{2}\right).$$

Figure 1.9 suggests that, for given x_0, when the "dispersion" s is very small, the log-normal probability density tends to a Gaussian function. This is indeed the case. For, when $s \to 0$, $f(x)$ takes significant values only in the vicinity of x_0, and

$$f(x) = \frac{1}{(2\pi)^{1/2}\, s\, x_0} \exp\left(-\frac{1}{2\,s^2}\left(-1 + \frac{x}{x_0} - \dots\right)^2\right)$$

$$\simeq \frac{1}{(2\pi)^{1/2}\,(s\,x_0)} \exp\left(-\frac{1}{2}\,\frac{(x-x_0)^2}{(s\,x_0)^2}\right). \tag{7}$$

If, for given x_0, the dispersion s is very large, the log-normal probability density tends to a log-uniform probability density (i.e., proportional to $1/x$; see section 1.2.4). For any x not too close to the origin, the argument of the exponential in (1) can be taken as null, thus showing that, at the limit $s \to \infty$,

$$f(x) \simeq \frac{1}{(2\pi)^{1/2}\, s}\,\frac{1}{x}. \tag{8}$$

The convergence of (1) into (8) is not a uniform convergence, in the sense that while the function (8) tends to infinity when x tends to 0, the log-normal (1) takes the value 0 at the origin. But for values of x of the same order of magnitude as x_0, the approximation (8) is adequate (for instance, for the values $x_0 = 1$, $s = 10.$, the log-normal function

(...)

and the log-uniform function are indistinguishable in Figure 1.9).

As suggested in section 1.2.4, the log-normal probability density is often adequate to represent probability distributions for variables which by definition are constrained to be positive.

The reader will easily verify that if a variable x has a log-normal distribution, the variable $y = 1/x$ has the same distribution.

The function

$$f(x) = \frac{p^{1-1/p}}{2\, s\, \Gamma(1/p)} \frac{1}{x} \exp\left(- \frac{1}{p\, s^p} \left| \mathrm{Log} \frac{x}{x_0} \right|^p \right) , \qquad (9)$$

transforms, under the change of variables (4), into the generalized Gaussian

$$f^*(x^*) = \frac{p^{1-1/p}}{2\, \sigma\, \Gamma(1/p)} \exp\left(- \frac{1}{p} \frac{\left| x^* - x_0^* \right|^p}{\sigma^p} \right) , \qquad (10)$$

where σ and x_0^* are given by (6). This suggests that (9) can be referred to as the "generalized log-normal in the ℓ_p norm sense".

1.4.3: Joint prior information in the $\boldsymbol{D} \times \boldsymbol{M}$ space

By definition, the a priori information on model parameters is independent of observations. The information we have in both model parameters and observable parameters can then be described in the $\boldsymbol{D} \times \boldsymbol{M}$ space by the joint density function

$$\rho(\mathbf{d},\mathbf{m}) = \rho_D(\mathbf{d})\, \rho_M(\mathbf{m}) \ . \qquad (1.59)$$

It may happen that part of the "a priori" information has been obtained from a first, rough analysis of the data set. Rigorously then, there exist correlations between $\mathbf{d}$ and $\mathbf{m}$ in $\rho(\mathbf{d},\mathbf{m})$, and equation (1.59) no longer holds. For a maximum of generality we thus have to assume the existence of a general probability density $\rho(\mathbf{d},\mathbf{m})$, not necessarily satisfying (1.59), and representing all the information we have in data and model parameters *independently* of the use of any theoretical information (which is described by the probability density $\Theta(\mathbf{d},\mathbf{m})$ introduced in section 1.3).

1.5: Defining the solution of the Inverse Problem

1.5.1: Combination of experimental, a priori, and theoretical information

We have seen in the previous section that the *prior probability density* $\rho(\mathbf{d},\mathbf{m})$, defined in the space $D \times M$, represents both information obtained on the observable parameters (data) $\mathbf{d}$, and a priori information on model parameters $\mathbf{m}$. We have also seen that the *theoretical probability density* $\Theta(\mathbf{d},\mathbf{m})$ represents the information on the physical correlations between $\mathbf{d}$ and $\mathbf{m}$, as obtained from a physical law, for instance.

These two states of information combine to produce the *a posteriori state of information*. I postulate here that the way used in the previous sections to introduce the a priori and the theoretical states of information is such that the a posteriori state of information is given by the *conjunction* of these two states of information.

From (1.36), the probability density $\sigma(\mathbf{d},\mathbf{m})$ representing the a posteriori information is then

$$\sigma(\mathbf{d},\mathbf{m}) = \frac{\rho(\mathbf{d},\mathbf{m})\ \Theta(\mathbf{d},\mathbf{m})}{\mu(\mathbf{d},\mathbf{m})} , \tag{1.60}$$

where $\mu(\mathbf{d},\mathbf{m})$ represents the state of null information.

Like all postulates, this one is justified by the correctness of its consequences. All the rest of this book is based on (1.60). It will be seen that the conclusions obtained from this equation, although more general than those obtained from more traditional approaches, reduce to them in all particular cases. Equation (1.60) first appeared in Tarantola and Valette (1982a).

Once the a posteriori information in the $D \times M$ space has been defined, the a posteriori information in the model space is given by the marginal density function

$$\sigma_M(\mathbf{m}) = \int_D d\mathbf{d}\ \ \sigma(\mathbf{d},\mathbf{m}) , \tag{1.61}$$

while the a posteriori information in the data space is given by

$$\sigma_D(\mathbf{d}) = \int_M d\mathbf{m}\ \ \sigma(\mathbf{d},\mathbf{m}) . \tag{1.62}$$

Figure 1.10 illustrates geometrically the determination of $\sigma_M(\mathbf{m})$ and $\sigma_D(\mathbf{d})$ from $\rho(\mathbf{d},\mathbf{m})$ and $\Theta(\mathbf{d},\mathbf{m})$.

1.5.2: Resolution of Inverse Problems

Equation (1.60) solves a very general problem. Inverse Problems correspond to the particular case where the spaces $\boldsymbol{D}$ and $\boldsymbol{M}$ have fundamentally different physical meaning, and where we are interested in "translating" information from the data space $\boldsymbol{D}$ into the model space $\boldsymbol{M}$. Let us make the assumptions usual in this sort of problems.

First, the theoretical information takes the form:

$$\Theta(\mathbf{d},\mathbf{m}) = \Theta(\mathbf{d}|\mathbf{m}) \ \mu_M(\mathbf{m}) \ , \tag{1.63}$$

i.e., is a conditional probability density in $\mathbf{d}$ for given $\mathbf{m}$ (see section 1.3). Second, the prior information $\rho(\mathbf{d},\mathbf{m})$ takes the form:

$$\rho(\mathbf{d},\mathbf{m}) = \rho_D(\mathbf{d}) \ \rho_M(\mathbf{m}) \ , \tag{1.64}$$

which means that information in the data space has been obtained (from measurements) independently of the prior information in the model space (see section 1.4). This gives, for the posterior information in the model space,

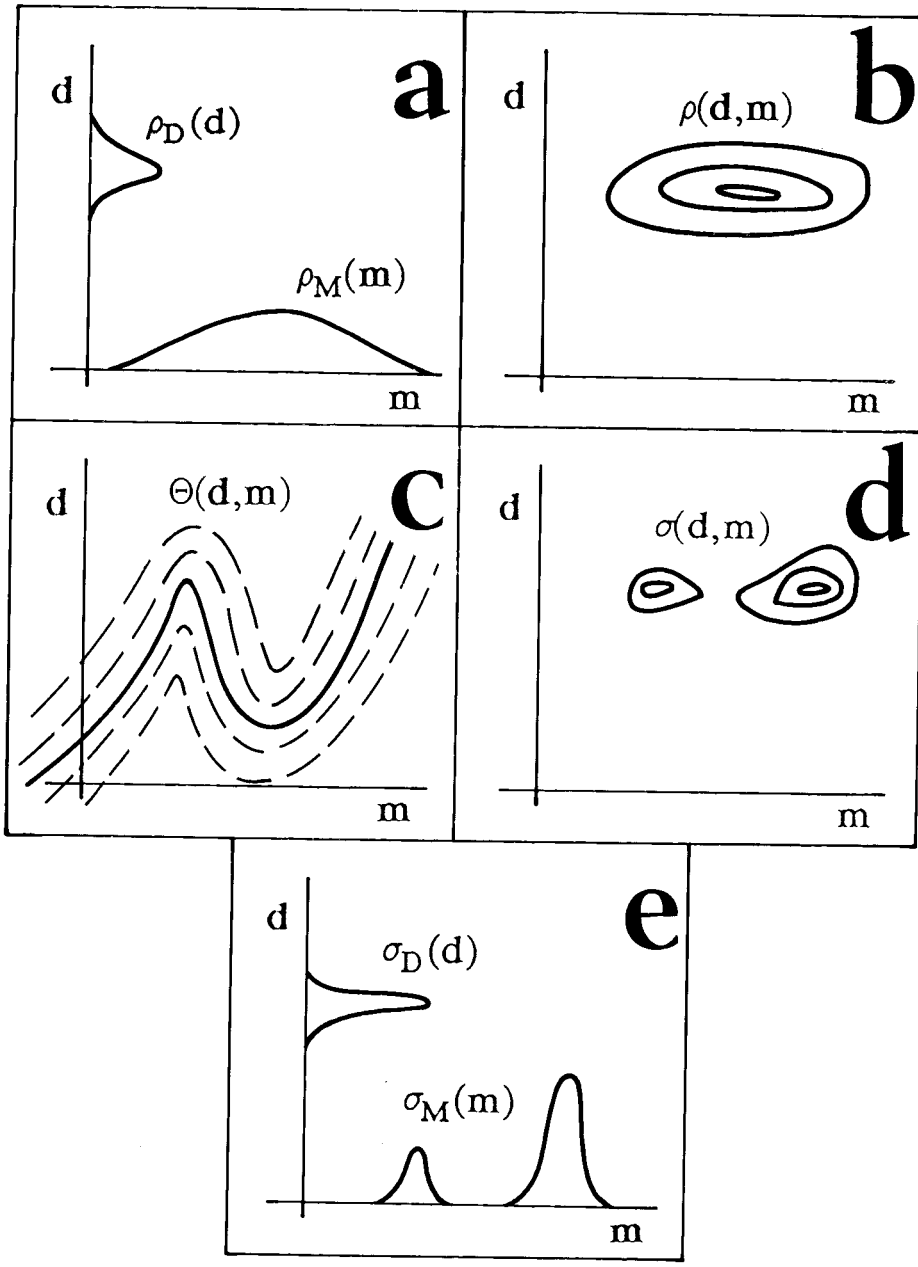
$$\sigma_M(\mathbf{m}) = \int_{\boldsymbol{D}} \mathbf{dd} \ \sigma(\mathbf{d},\mathbf{m}) = \rho_M(\mathbf{m}) \int_{\boldsymbol{D}} \mathbf{dd} \ \frac{\rho_D(\mathbf{d}) \ \Theta(\mathbf{d}|\mathbf{m})}{\mu_D(\mathbf{d})} \ , \tag{1.65}$$

where it has been assumed that $\mu(\mathbf{d},\mathbf{m}) = \mu_D(\mathbf{d}) \ \mu_M(\mathbf{m})$ (see section 1.2.4).

Equation (1.65) gives ***the*** solution of the general inverse problem. From $\sigma_M(\mathbf{m})$ is is possible to obtain any sort of information we wish on model parameters: mean values, median values, maximum likelihood values, error bars,... Section 1.6 gives a discussion.

The "existence" of the solution simply means that $\sigma_M(\mathbf{m})$, as defined by (1.65), is not identically null. If this were the case, it would indicate the incompatibility of the experimental results, the a priori hypothesis on model parameters, and the theoretical information, thus showing that some "error bars" have beeen underestimated. I have not been able to define, in the general case, a "test" that would measure the degree of compatibility of the a posteriori information with respect to the a priori one (like the χ^2 test introduced in chapter 4 for least squares problems).

The "uniqueness" of the solution is evident when by solution we mean the probability density $\sigma_M(\mathbf{m})$ itself, and is simply a consequence of the uniqueness of the conjunction of states of information. Of course, $\sigma_M(\mathbf{m})$ may be very pathological (non-normalizable, multimodal,...) but that would


a
d
$\rho_D(d)$
$\rho_M(m)$
m
b
d
$\rho(d,m)$
m
c
d
$\Theta(d,m)$
m
d
d
$\sigma(d,m)$
m
e
d
$\sigma_D(d)$
$\sigma_M(m)$
m

← *Figure 1.10:* a) The probability densities $\rho_D(\mathbf{d})$ and $\rho_M(\mathbf{m})$ respectively represent the information on observable parameters (data) and the prior information on model parameters. b) As the prior information on model parameters is, by definition, independent of the information on observable parameters (measurements), the joint probability density in the space $\boldsymbol{D} \times \boldsymbol{M}$ representing both informations is $\rho(\mathbf{d},\mathbf{m}) = \rho_D(\mathbf{d})\, \rho_M(\mathbf{m})$. c) $\Theta(\mathbf{d},\mathbf{m})$ represents the information on the physical correlations between $\mathbf{d}$ and $\mathbf{m}$, as predicted by a physical theory (usually, $\Theta(\mathbf{d},\mathbf{m}) = \Theta(\mathbf{d}|\mathbf{m})\ \mu_M(\mathbf{m})$) . d) Given the two states of information represented by $\rho(\mathbf{d},\mathbf{m})$ and $\Theta(\mathbf{d},\mathbf{m})$, their conjuction is $\sigma(\mathbf{d},\mathbf{m}) = \frac{\rho(\mathbf{d},\mathbf{m})\ \Theta(\mathbf{d},\mathbf{m})}{\mu(\mathbf{d},\mathbf{m})}$, and represents the "combination" of the two states of information. e) From $\sigma(\mathbf{d},\mathbf{m})$ it is possible to obtain the marginal probability densities $\sigma_M(\mathbf{m}) = \int d\mathbf{d}\ \sigma(\mathbf{d},\mathbf{m})$ and $\sigma_D(\mathbf{d}) = \int d\mathbf{m}\ \sigma(\mathbf{d},\mathbf{m})$. By comparison of the posterior probability density $\sigma_M(\mathbf{m})$ with the prior one, $\rho_M(\mathbf{m})$, we see that some information has been gained on the model parameters, thanks to the data $\rho_D(\mathbf{d})$ and to the theoretical information $\Theta(\mathbf{d},\mathbf{m})$.

simply mean that such is the information we possess on model parameters. The information itself is uniquely defined.

Using (1.63) and (1.64), the posterior probability density in the data space is

$$\sigma_D(\mathbf{d}) = \int_{\boldsymbol{M}} d\mathbf{m}\ \sigma(\mathbf{d},\mathbf{m}) = \frac{\rho_D(\mathbf{d})}{\mu_D(\mathbf{d})} \int_{\boldsymbol{M}} d\mathbf{m}\ \Theta(\mathbf{d}|\mathbf{m})\ \rho_M(\mathbf{m}) \ . \tag{1.66}$$

While the probability density (1.65) allows us to estimate the posterior values of the model parameters, the probability density (1.66) allows of estimating the posterior values of data parameters ("recalculated data").

1.5.3: Some special cases

a) Results of the measurements are the output of an instrument with known statistics: Example 33 has shown that if a measuring instrument del-

ivers the value $\mathbf{d}_{obs}$, then

$$\rho_D(\mathbf{d}) = \frac{\nu(\mathbf{d}_{obs}|\mathbf{d})\ \mu_D(\mathbf{d})}{\int_D d\mathbf{d}\ \nu(\mathbf{d}_{obs}|\mathbf{d})\ \mu_D(\mathbf{d})} ,$$

where $\nu(\mathbf{d}_{obs}|\mathbf{d})$ describes the statistics of the instrument, and represents the probability density of the output being $\mathbf{d}_{obs}$ when the input is $\mathbf{d}$. Equation (1.65) then gives

$$\sigma_M(\mathbf{m}) = \text{const. } \rho_M(\mathbf{m}) \int_D d\mathbf{d}\ \ \nu(\mathbf{d}_{obs}|\mathbf{d})\ \theta(\mathbf{d}|\mathbf{m}) ,$$

or, in normalized form,

$$\sigma_M(\mathbf{m}) = \frac{\rho_M(\mathbf{m}) \int_D d\mathbf{d}\ \nu(\mathbf{d}_{obs}|\mathbf{d})\ \theta(\mathbf{d}|\mathbf{m})}{\int_M d\mathbf{m}\ \rho_M(\mathbf{m}) \int_D d\mathbf{d}\ \nu(\mathbf{d}_{obs}|\mathbf{d})\ \theta(\mathbf{d}|\mathbf{m})} . \qquad (1.67)$$

This equation is identical to equation (6) of box 1.4 obtained using a strict Bayesian approach. ■

b) Errors of the measure instrument are independent of the input, and errors in the theory are independent of the model value. This case corresponds to examples 31 and 36. The output of the measure instrument is related to the input though

$$\mathbf{d}_{obs} = \mathbf{d} + \epsilon_D ,$$

where ϵ_D is un unknown error with known statistics described by the probability density function $f_D(\epsilon_D)$. Then

$$\nu(\mathbf{d}_{obs}|\mathbf{d}) = f_D(\mathbf{d}_{obs}-\mathbf{d}) .$$

If the true value $\mathbf{d}$ differs from the computed value $\mathbf{g}(\mathbf{m})$ by an error ϵ_T,

$$\mathbf{d} = \mathbf{g}(\mathbf{m}) + \epsilon_T ,$$

independent of $\mathbf{m}$, with known statistics described by the probability den-

sity function $f_T(\epsilon_T)$, then

$$\theta(\mathbf{d}|\mathbf{m}) = f_T(\mathbf{d}-\mathbf{g}(\mathbf{m})) \ .$$

Equation (1.67) then gives

$$\sigma_M(\mathbf{m}) = \frac{f(\mathbf{d}_{obs}-\mathbf{g}(\mathbf{m}))\ \rho_M(\mathbf{m})}{\int_M d\mathbf{m}\ f(\mathbf{d}_{obs}-\mathbf{g}(\mathbf{m}))\ \rho_M(\mathbf{m})} \ , \tag{1.68a}$$

where $f(\epsilon)$ is the convolution of $f_D(\epsilon)$ and $f_T(\epsilon)$,

$$f(\epsilon) = f_D(\epsilon) * f_T(\epsilon) \ , \tag{1.68b}$$

and represents the probability density of the sum of observational and theoretical errors:

$$\epsilon = \epsilon_D + \epsilon_T \ .$$

Equations (1.68) were used by Duijndam (1987) to show, in this particular example, the equivalence between the strict Bayesian approach and the approach introduced by Tarantola and Valette (1982a) (and developed in this book). ■

c) Negligible modelisation errors: If modelisation errors are negligible compared to observational errors, we can take

$$\Theta(\mathbf{d}|\mathbf{m}) = \delta(\mathbf{d}-\mathbf{g}(\mathbf{m})) \ ,$$

where $\mathbf{d} = \mathbf{g}(\mathbf{m})$ denotes the (exact) resolution of the forward problem. Equation (1.65) then gives

$$\sigma_M(\mathbf{m}) = \rho_M(\mathbf{m}) \left[\frac{\rho_D(\mathbf{d})}{\mu_D(\mathbf{d})} \right]_{\mathbf{d}=\mathbf{g}(\mathbf{m})} \ . \ \blacksquare \tag{1.69}$$

d) Negligible observational errors: Letting $\mathbf{d}_{obs}$ denote the observed data values, the hypothesis of negligible observational errors (with respect to modelization errors) is written

$$\rho_D(\mathbf{d}) = \delta(\mathbf{d}-\mathbf{d}_{obs}) \ . \tag{1.70}$$

Equation (1.65) then gives

$$\sigma_M(\mathbf{m}) = \rho_M(\mathbf{m}) \frac{\Theta(\mathbf{d}_{obs}|\mathbf{m})}{\mu_D(\mathbf{d}_{obs})}, \tag{1.71a}$$

or, more simply, if we can normalize to unity,

$$\sigma_M(\mathbf{m}) = \frac{\rho_M(\mathbf{m}) \ \Theta(\mathbf{d}_{obs}|\mathbf{m})}{\int_M d\mathbf{m} \ \rho_M(\mathbf{m}) \ \Theta(\mathbf{d}_{obs}|\mathbf{m})} . \blacksquare \tag{1.71b}$$

e) Gaussian modelisation and observational errors: This corresponds respectively to (equation (1.41) of example 29)

$$\Theta(\mathbf{d}|\mathbf{m}) = ((2\pi)^{ND} \det \mathbf{C}_T)^{-\frac{1}{2}} \exp\left[-\frac{1}{2}(\mathbf{d}-\mathbf{g}(\mathbf{m}))^t \ \mathbf{C}_T^{-1} \ (\mathbf{d}-\mathbf{g}(\mathbf{m}))\right], \tag{1.72}$$

and (equation (1.49b) of example 35)

$$\frac{\rho_D(\mathbf{d})}{\mu_D(\mathbf{d})} = ((2\pi)^{ND} \det \mathbf{C}_d)^{-\frac{1}{2}} \exp\left[-\frac{1}{2}(\mathbf{d}-\mathbf{d}_{obs})^t \ \mathbf{C}_d^{-1} \ (\mathbf{d}-\mathbf{d}_{obs})\right]. \tag{1.73}$$

As demonstrated in problem 1.20, equation (1.65) then gives

$$\sigma_M(\mathbf{m}) = \rho_M(\mathbf{m}) \exp\left[-\frac{1}{2} \ (\mathbf{g}(\mathbf{m})-\mathbf{d}_{obs})^t \ \mathbf{C}_D^{-1} \ (\mathbf{g}(\mathbf{m})-\mathbf{d}_{obs})\right], \tag{1.74}$$

where

$$\mathbf{C}_D = \mathbf{C}_d + \mathbf{C}_T . \tag{1.75}$$

Result (1.74)-(1.75) is important because it shows that, *in the Gaussian assumption, observational errors and modelization errors simply combine by addition of the respective covariance operators*, even when the forward problem is nonlinear. ■

Box 1.4: Solving Inverse Problems using the Bayesian paradigm.

Let $\mathbf{f(d,m)}$ be a joint probability density on the parameters $\mathbf{(d,m)}$. From $\mathbf{f(d,m)}$ one can ***define*** the *marginal* probability densities

(...)

$$f_M(\mathbf{m}) = \int_D d\mathbf{d}\, f(\mathbf{d},\mathbf{m}) \tag{1a}$$

and

$$f_D(\mathbf{d}) = \int_M d\mathbf{m}\, f(\mathbf{d},\mathbf{m}) \tag{1b}$$

and the *conditional* probability densities

$$f_{M|D}(\mathbf{m}|\mathbf{d}_0) = \frac{f(\mathbf{d}_0,\mathbf{m})}{\int_M d\mathbf{m}\, f(\mathbf{d}_0,\mathbf{m})}, \tag{2a}$$

and

$$f_{D|M}(\mathbf{d}|\mathbf{m}_0) = \frac{f(\mathbf{d},\mathbf{m}_0)}{\int_D d\mathbf{d}\, f(\mathbf{d},\mathbf{m}_0)}. \tag{2b}$$

It is easy to see that, for a given $\mathbf{d}_0$, $f_{M|D}(\mathbf{m}|\mathbf{d}_0)$ is a probability density in $\mathbf{m}$. Respectively, for a given $\mathbf{m}_0$, $f_{D|M}(\mathbf{d}|\mathbf{m}_0)$ is a probability density for $\mathbf{d}$. See Figure 1.11.

One can easily obtain the identities

$$f_{M|D}(\mathbf{m}|\mathbf{d}_0) = \frac{f_{D|M}(\mathbf{d}_0|\mathbf{m})\, f_M(\mathbf{m})}{\int d\mathbf{m}\, f_{D|M}(\mathbf{d}_0|\mathbf{m})\, f_M(\mathbf{m})}, \tag{3a}$$

and

$$f_{D|M}(\mathbf{d}|\mathbf{m}_0) = \frac{f_{M|D}(\mathbf{m}_0|\mathbf{d})\, f_D(\mathbf{d})}{\int d\mathbf{d}\, f_{M|D}(\mathbf{m}_0|\mathbf{d})\, f_D(\mathbf{d})}, \tag{3b}$$

which are known as the *theorem of Bayes*. Replacing $\mathbf{d}_0$ by $\mathbf{d}_{obs}$ in (4a) gives

(...)

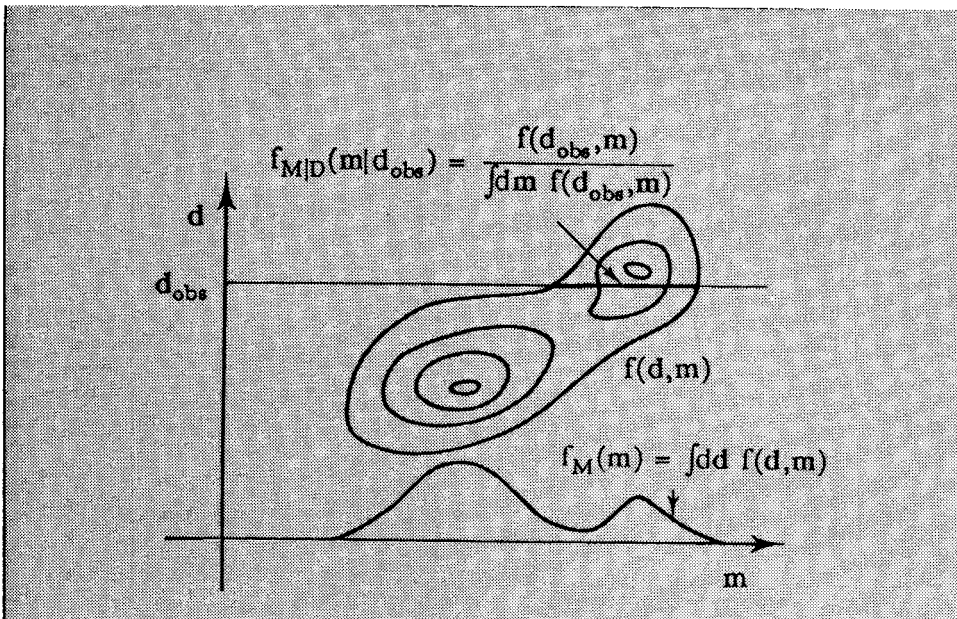


Figure 1.11: A joint probability density $f(\mathbf{d},\mathbf{m})$, the marginal (prior) probability density for $\mathbf{m}$, $f_M(\mathbf{m})$, and the conditional (posterior) probability density for $\mathbf{m}$, $f_{M|D}(\mathbf{m}|\mathbf{d}_{obs})$, given the observation $\mathbf{d} = \mathbf{d}_{obs}$.

$$f_{M|D}(\mathbf{m}|\mathbf{d}_{obs}) = \frac{f_{D|M}(\mathbf{d}_{obs}|\mathbf{m})\ f_M(\mathbf{m})}{\int d\mathbf{m}\ f_{D|M}(\mathbf{d}_{obs}|\mathbf{m})\ f_M(\mathbf{m})} \,. \qquad (4)$$

The interpretation of a probability density as representing an state of information over a parameter set is coherent with the interpretation of the conditional probability density (4) as the *posterior* probability density for $\mathbf{m}$ if an actual measurement of $\mathbf{d}$ gives unambiguosly the result $\mathbf{d} = \mathbf{d}_{obs}$. Then, $f_M(\mathbf{m})$ corresponds to the prior probability density for $\mathbf{m}$. The conditional probability density $f_{D|M}(\mathbf{d}|\mathbf{m})$ is interpreted as the probability density for the observed data value to be $\mathbf{d}$ when the true model value is $\mathbf{m}$. This describes the forward modeling of data, taking into account all sources of uncertainties in the prediction of $\mathbf{d}$ (in particular, observational uncertainties and uncertainties in the physical theory used to predict the data values). This interpretation justifies the use of (4) for the resolution of inverse problems.

(...)

Example: Let $\theta(\mathbf{d}|\mathbf{m})$ be the conditional probability density describing the theoretical relationship between $\mathbf{d}$ and $\mathbf{m}$ (as described in section 1.3), and let $\nu(\mathbf{d}_{obs}|\mathbf{d})$ be the probability density for the output of a measuring instrument to be $\mathbf{d}_{obs}$ when the input is $\mathbf{d}$ (example 33). Then, the conditional probability density $f_{D|M}(\mathbf{d}_{obs}|\mathbf{m})$ defined above is given by

$$f_{D|M}(\mathbf{d}_{obs}|\mathbf{m}) = \int_D d\mathbf{d}\ \nu(\mathbf{d}_{obs}|\mathbf{d})\ \theta(\mathbf{d}|\mathbf{m}) \ . \tag{5}$$

Then, equation (4) gives

$$f_{M|D}(\mathbf{m}|\mathbf{d}_{obs}) = \frac{f_M(\mathbf{m}) \int_D d\mathbf{d}\ \nu(\mathbf{d}_{obs}|\mathbf{d})\ \theta(\mathbf{d}|\mathbf{m})}{\int_M d\mathbf{m}\ f_M(\mathbf{m}) \int_D d\mathbf{d}\ \nu(\mathbf{d}_{obs}|\mathbf{d})\ \theta(\mathbf{d}|\mathbf{m})} \ . \tag{6}$$

Although with different notations, this equation is identical to equation (1.67), obtained from the general concept of combination of information developed in this book. Of course, equation (1.60), at the basis of this book, applies to much more general situations than (6) does. For instance, Figure (1.4) shows that situations exist such that the result of a measurement does not give a thing which can be named $\mathbf{d}_{obs}$, which is central in the concept of conditional probability, and thus, in the strict Bayesian approach.

1.6: Using the solution of the Inverse Problem

1.6.1: Describing the a posteriori information in the model space

What does it mean to "solve" an inverse problem? This depends on the sort of practical application we have in view.

Very often we are interested in the model parameters *per se*. The most general way of studying the information obtained on the parameter values is by a direct study of the probability density $\sigma_M(\mathbf{m})$. As a probability density may be quite complicated (multimodal, infinite variances,...) there is no general procedure for obtaining simple pieces of information. The most comprehensive understanding is obtained by directly discussing the *probability* that the true value of the model parameters lies in a given range (i.e., it belongs

to a given subset):

$$P(\mathbf{m}\in A) = \frac{1}{N}\int_A d\mathbf{m}\ \sigma_M(\mathbf{m}) , \tag{1.76}$$

where N is the norm of σ_M :

$$N = \int_M d\mathbf{m}\ \sigma_M(\mathbf{m}) \tag{1.77}$$

(if σ_M is not normalizable, only *relative* probabilities can be computed).

Choosing different subsets $A \subset M$ it is possible to get quite a good idea of the actual information we possess on the true values of the model parameters. If $\sigma_M(\mathbf{m})$ does not have a very complicated shape, it is possible to describe it adequately by its central estimator and estimators of dispersion (box 1.1 recalls the general definitions in norm ℓ_p for $1 \le p \le \infty$). Among the central estimators, the easiest to obtain are generally the maximum likelihood value $\mathbf{m}_{ML}$

$$\mathbf{m}_{ML} \quad : \quad \sigma_M(\mathbf{m}_{ML}) \ \text{MAX} ; \tag{1.78}$$

and the mean value (or mathematical expectation) $\langle\, \mathbf{m} \,\rangle$

$$\langle\, \mathbf{m} \,\rangle = \frac{1}{N}\int_M d\mathbf{m}\ \mathbf{m}\ \sigma_M(\mathbf{m}) . \tag{1.79}$$

Among the estimators of dispersion, the easiest to obtain is generally the posterior covariance operator $\mathbf{C}_{M'}$

$$\mathbf{C}_{M'} = \frac{1}{N}\int_M d\mathbf{m}\ (\mathbf{m}-\langle\, \mathbf{m} \,\rangle)(\mathbf{m}-\langle\, \mathbf{m} \,\rangle)^t\ \sigma_M(\mathbf{m})$$

$$= \frac{1}{N}\int_M d\mathbf{m}\ \mathbf{m}\ \mathbf{m}^t\ \sigma_M(\mathbf{m}) - \langle\, \mathbf{m} \,\rangle\ \langle\, \mathbf{m} \,\rangle^t , \tag{1.80}$$

but it has to be emphasized that the covariance operator gives understandable information only in the case when the probability density $\sigma_M(\mathbf{m})$ can be fitted reasonably well by a Gaussian function.

Sometimes the inverse problem is solved as an intermediate one in a more general decision problem in which the decision maker has to combine information obtained from the inverse problem with economic considerations such as, for instance, in operational research. As an example, consider the oil company which, in the light of the results obtained after a 1 million dollar

seismic exploration experiment has to decide on the eventual drilling of a 5 million dollar exploratory well. Unfortunately, although the present state of computer technology allows a reasonably general resolution of the inverse problem in seismic exploration, it does not yet allow a general resolution of the coupled inverse problem / decision problem in realistically complex cases. This field will certainly undergo a rapid growth in the coming years. Readers interested in Bayesian decision theory can refer to Box and Tiao (1973), Morgan (1968), Schmitt (1969), or Winkler (1972).

1.6.2: Analysis of error and resolution

When the solution of the inverse problem is given as a central estimator (such as mean, median, or maximum likelihood), it is necessary to discuss error and resolution.

By discussion of errors is usually meant the obtainment of significant "error bars". What the meaning of an error bar may be is not always evident. For instance, while the probability of the parameter being at more than 3.5 standard deviations from the mean is null for a box-car function, it is approximately 10% for a symmetric-exponential function. For multimodal density functions, the standard deviation can be completely meaningless.

In the traditional "analysis of resolution", two different concepts are involved. First, a parameter is *well resolved* by the data set if its posterior error bar is much smaller than the prior one. More generally, if its posterior marginal probability density is significantly different from the prior one. If, for instance, the prior and posterior probability densities are identical, the parameter is completely unresolved.

The second concept involved in the analysis of resolution arises when the parameters m^α represent a discretization of a function $\Psi(t)$ of a continuous variable t (representing for instance a location in time or space). Assume that the posterior covariance operator adequately represents the dispersion around the mean. Usual covariance operators (prior and posterior) are not diagonal, but are "band diagonal" (covariances between neighbouring parameters are not null). This means that neighbouring parameters have errors which are correlated. The greater the correlation length of errors, the worse is the (temporal, spatial,...) resolution attained with the data set. In Chapter 9 the different (although equivalent) point of view of Backus and Gilbert (1968) is discussed.

Stability is defined as the property of a central estimator of being insensitive to small random errors in the data values. If the a priori information in the model space has been properly introduced, stability is generally warranted.

Robustness is the property of insensitivity with respect to a small number of big errors (outliers) in the data set. For instance, the hypothesis that errors

are described by a symmetric exponential is robust; the hypothesis that errors are distributed following a Gaussian function is *not* robust (see Chapter 6).

Another important concept is that of the *importance* of a particular datum for a particular model parameter. If, for instance, the conditional probability density of the parameter m^α with respect to d^i, $\sigma(m^\alpha|d^i)$, is, in fact, independent of d^i, the datum d^i has a null importance for m^α. A possible definition of the importance of the datum d^i for the model parameter m^α is the change of information content of the posterior marginal probability density for m^α when suppressing the datum d^i from the data set. See, for instance, Chapter 4, or Minster et al. (1974), for a discussion of the importance of data in least-squares problems. The analysis of data importance may be helpful for optimizing experimental configurations.

It may happen that some of the hypotheses made are inconsistent. For instance, in least-squares problems, the posterior data residuals may be much greater than experimental or modelization uncertainties (Chapter 4), and a χ^2 test can easily detect such an inconsistency. In the general case, inconsistency is detected if the product $\rho(\mathbf{d},\mathbf{m})\,\Theta(\mathbf{d},\mathbf{m})$ is very small everywhere in the space $D \times M$, but I have not yet been able to obtain a quantitative test. Possibly, Shannon's concept of information content (section 1.2.4) should be applied for the general study of resolution, data importance, or consistency, but no general result yet exists.

Let me now review some of the numerical techniques that may be used to solve the inverse problem.

1.6.3: Analytic solutions

In some cases, it is possible to obtain a simple analytical expression for the posterior probability density. For instance, if probability densities used to describe observational uncertainties, forward modelization uncertainties, and prior uncertainties on model parameters are *Gaussian*, and if the forward equation $\mathbf{d}_{cal} = \mathbf{g}(\mathbf{m})$ is linear in $\mathbf{m}$, then it can be shown that the posterior probability density $\sigma_M(\mathbf{m})$ is also Gaussian. It can then be completely described by its central value and its covariance operator, for which it is possible to obtain explicit expressions (see section 1.7).

Sometimes, the forward equation $\mathbf{d}_{cal} = \mathbf{g}(\mathbf{m})$ is not linear, but it can be linearized around some *reference* model $\mathbf{m}_0$:

$$\mathbf{d}_{cal} = \mathbf{g}(\mathbf{m}) \simeq \mathbf{g}(\mathbf{m}_0) + \mathbf{G}_0\,(\mathbf{m}-\mathbf{m}_0)\,,$$

where the linear operator $\mathbf{G}_0$ represents the derivative of $\mathbf{g}$ at $\mathbf{m} = \mathbf{m}_0$. Then, the analytic advantages of linear problems are preserved (see also section 1.7 for an example).

For nonlinear forward problems, there is generally no explicit expression of the solution.

1.6.4: Systematic exploration of the model space

If the number of model parameters is very small (≤ 4), and if the computation of the numerical value of $\sigma_M(\mathbf{m})$ for an arbitrary $\mathbf{m}$ is inexpensive (i.e., not consuming too much computer-time), we can define a grid over the model space, compute $\sigma_M(\mathbf{m})$ everywhere in the grid, and directly use these results to discuss the information obtained on model parameters. This is certainly the most general way of solving the inverse problem. Problem 1.1 gives an illustration of the method.

1.6.5: Monte Carlo methods

If the number of parameters is not small, and if the computation of $\sigma_M(\mathrm{m})$ at any point $\mathbf{m}$ is not expensive, the systematic exploration of the model space can advantageously be replaced by a random (Monte Carlo) exploration. Monte Carlo methods are discussed in Chapter 3. For instance, the method of *simulated annealing* allows of obtaining the maximum likelihood point, even when the probability density $\sigma_M(\mathbf{m})$ is multimodal. Also, the computation of the mathematical expectation and of the posterior covariance operator can be made by evaluating the sums (1.79) and (1.80) by a Monte Carlo method of numerical integration.

Monte Carlo methods have the advantage of not using any linear approximation.

1.6.6: Computation of the maximum likelihood point

Usual problems do not have a small number of parameters and the computation of $\sigma_M(\mathbf{m})$ at any point $\mathbf{m}$ is expensive. The only practical approach is often to try to define an astute strategy which, in a small number of moves, will give the point $\mathbf{m}_{ML}$ maximizing $\sigma_M(\mathrm{m})$, i.e., the maximum likelihood point.

If $\sigma_M(\mathbf{m})$ is a differentiable function of $\mathbf{m}$, the maximum likelihood point can be obtained using gradient methods. The gradient of $\sigma_M(\mathbf{m})$ has components $\partial\sigma_M/\partial m^\alpha$. As discussed in Chapters 4 and 5, "gradient" is *not* synonymous with "direction of steepest ascent": to define the latter it is necessary to define a *distance* over the model space (or, more precisely, over the chosen *chart* of the model space). Except for very special cases (e.g. example 2), there is no "natural" definition of distance. The simplest choice (not

necessarily very good) is the ℓ_2 distance

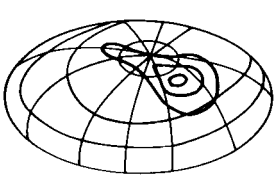
$$D(\mathbf{m}_1,\mathbf{m}_2) = \left[\sum_{\alpha \in \mathbf{I}_M} \frac{(m_1^\alpha - m_2^\alpha)^2}{(\sigma^\alpha)^2} \right]^{1/2} ,$$

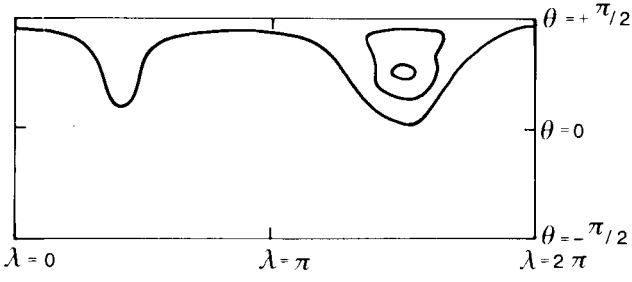
where σ^α is any characteristic length for m^α, such as for instance, the corresponding estimator of dispersion in the prior probability density, $\rho_M(\mathbf{m})$. Although any definition of distance is acceptable, astute choices may speed the convergence of a gradient method. For instance, in example 2, the parameters $(m^1,m^2) = (\lambda,\theta)$ were geographical coordinates; the best definition of distance in the map (λ,θ) between two points $\mathbf{m}_1 = (\lambda_1,\theta_1)$ and $\mathbf{m}_2 = (\lambda_2,\theta_2)$ is the length of the corresponding great circle in the sphere:

$$D(\mathbf{m}_1,\mathbf{m}_2) = \text{Arc cos}(\sin\theta_1 \sin\theta_2 + \cos\theta_1 \cos\theta_2 \cos(\lambda_2-\lambda_1)) . \quad (1.81)$$

To take this definition of distance to compute the direction of steepest descent simply correspond to the computation of the gradient "in spherical coordinates". Figure 1.12 illustrates the dependence of the direction of steepest descent on the particular choice of distance. For more details on gradient methods, see Chapters 4 and 5.

As $\sigma_M(\mathbf{m})$ is, in general, an arbitrarily complicated function of $\mathbf{m}$, there is no warranty that the maximum likelihood point is unique, or that a given point which is locally maximum, is the absolute maximum. Only a full exploration of the space would give the proof, but this is generally too expensive to make. Only a skilful blend of mathematical discussion and physical arguments usually gives some insight into the uniqueness of the maximum likelihood point.





1.7: Special cases

1.7.1: The Gaussian Hypothesis (least-squares criterion). Case $\mathbf{d} = \mathbf{g}(\mathbf{m})$.

As discussed in section 1.5, the general solution of inverse problems is

$$\sigma_M(m) = \rho_M(m) \int_D dd \, \frac{\rho_D(d) \, \Theta(d|m)}{\mu_D(d)} , \qquad \text{(1.65 again)}$$

where $\rho_D(\mathbf{d})$ represents the available information on the true values of observable parameters (data), $\mu_D(\mathbf{d})$ is the non-informative probability density on observable parameters, $\Theta(\mathbf{d}|\mathbf{m})$ is the conditional probability density representing the forward modelization, $\rho_M(\mathbf{m})$ represents the a priori information on model parameters, and $\sigma_M(\mathbf{m})$ represents the a posteriori information.

If the observations consist of the observed output, $\mathbf{d}_{obs}$, of a measuring instrument with known statistics, and if $\nu(\mathbf{d}_{obs}|\mathbf{d})$ represents the conditional probability density for the observed value to be $\mathbf{d}_{obs}$ when the true value is $\mathbf{d}$, then, as discussed in example 33,

$$\frac{\rho_D(\mathbf{d})}{\mu_D(\mathbf{d})} = \frac{\nu(\mathbf{d}_{obs}|\mathbf{d})}{\int_D dd \; \nu(\mathbf{d}_{obs}|\mathbf{d}) \; \mu_D(d)} . \qquad \text{(1.46 again)}$$

If the statistic of the instrument is Gaussian, then (equation (1.49a))

$$\nu(\mathbf{d}_{obs}|\mathbf{d}) = ((2\pi)^{ND} \det \mathbf{C}(\mathbf{d}_{obs}))^{-1/2} \exp\left[-\frac{1}{2} (\mathbf{d}-\mathbf{d}_{obs})^t \, \mathbf{C}_d^{-1} \, (\mathbf{d}-\mathbf{d}_{obs}) \right],$$

where $\mathbf{C}_d$ is the covariance operator describing "experimental uncertainties".

If the forward modelization can be written

$$\mathbf{d}_{cal} = \mathbf{g}(\mathbf{m}) , \qquad (1.82)$$

$\mathbf{g}$ represents a nonlinear operator from the model space into the data space, and if estimated modelization errors are assumed Gaussian, then

---

← *Figure 1.12:* A function $\sigma(\lambda,\theta)$ defined over the sphere has to be minimized. A naïve use of gradient methods would correspond to the choice of an euclidean distance *over the chart*. A right use of gradient methods implies the definition of a distance over the chart (equation (1.81)) which corresponds to the (geodetic) distance over the sphere.

$$\theta(\mathbf{d}|\mathbf{m}) = ((2\pi)^{ND} \det \mathbf{C}_T)^{-1/2} \exp\left[-\frac{1}{2}(\mathbf{d}-\mathbf{g}(\mathbf{m}))^t \mathbf{C}_T^{-1} (\mathbf{d}-\mathbf{g}(\mathbf{m}))\right], \quad \text{(1.41 again)}$$

where $\mathbf{C}_T$ is the covariance operator describing "forward modelization uncertainties".

With these assumptions, the sum over the data space in (1.65) can be performed analytically (problem 1.20), and we obtain

$$\sigma_M(\mathbf{m}) = \rho_M(\mathbf{m}) \exp\left[-\frac{1}{2} (\mathbf{g}(\mathbf{m})-\mathbf{d}_{obs})^t \mathbf{C}_D^{-1} (\mathbf{g}(\mathbf{m})-\mathbf{d}_{obs})\right], \quad \text{(1.75 again)}$$

where the covariance operator $\mathbf{C}_D$ combines experimental and theoretical uncertainties:

$$\mathbf{C}_D = \mathbf{C}_d + \mathbf{C}_T . \quad (1.83)$$

Thanks to the simplicity of (1.83), when using Gaussian models for uncertainties, we can forget that there are two different sources of uncertainties in the data space. All happens as if the forward modelization were exact, and $\mathbf{C}_D$ represented only experimental uncertainties (or, conversely, as if observations were exact, and $\mathbf{C}_D$ represented only forward modelization errors).

In this section we examine the case where the probability density representing the a priori information on model parameters is also Gaussian:

$$\rho_M(\mathbf{m}) = ((2\pi)^{NM} \det \mathbf{C}_M)^{-1/2} \exp\left[-\frac{1}{2} (\mathbf{m}-\mathbf{m}_{prior})^t \mathbf{C}_M^{-1} (\mathbf{m}-\mathbf{m}_{prior})\right]. \quad (1.84)$$

$\mathbf{m}_{prior}$ is the "a priori model", and $\mathbf{C}_M$ is the covariance operator describing estimated uncertainties in $\mathbf{m}_{prior}$.

We then have, up to a real (adimensional) normalizing constant,

$$\sigma_M(\mathbf{m}) = \text{const} \quad (1.85)$$
$$\exp\left[-\frac{1}{2}\left[(\mathbf{g}(\mathbf{m})-\mathbf{d}_{obs})^t \mathbf{C}_D^{-1} (\mathbf{g}(\mathbf{m})-\mathbf{d}_{obs}) + (\mathbf{m}-\mathbf{m}_{prior})^t \mathbf{C}_M^{-1} (\mathbf{m}-\mathbf{m}_{prior})\right]\right].$$

Let me discuss linear and nonlinear problems separately.

a) The forward problem is linear. Instead of writing $\mathbf{d} = \mathbf{g}(\mathbf{m})$, we then write

$$\mathbf{d} = \mathbf{G}\,\mathbf{m} , \quad (1.86)$$

where $\mathbf{G}$ represents a *linear* operator acting from the model space into the data space.

This gives

$$\sigma_M(\mathbf{m}) = \text{const. } \exp(- S(\mathbf{m})) , \tag{1.87}$$

where $S(\mathbf{m})$ is the quadratic function

$$S(\mathbf{m}) = \tag{1.88}$$
$$\frac{1}{2}\left[(\mathbf{G}\,\mathbf{m} - \mathbf{d}_{obs})^t\, \mathbf{C}_D^{-1}\, (\mathbf{G}\,\mathbf{m} - \mathbf{d}_{obs}) + (\mathbf{m}-\mathbf{m}_{prior})^t\, \mathbf{C}_M^{-1}\, (\mathbf{m}-\mathbf{m}_{prior})\right].$$

Defining

$$\boxed{\langle\, \mathbf{m}\,\rangle = \left[\mathbf{G}^t\, \mathbf{C}_D^{-1}\, \mathbf{G} + \mathbf{C}_M^{-1}\right]^{-1} \left[\mathbf{G}^t\, \mathbf{C}_D^{-1}\, \mathbf{d}_{obs} + \mathbf{C}_M^{-1}\, \mathbf{m}_{prior}\right],} \tag{1.89}$$

and

$$\boxed{\mathbf{C}_{M'} = \left[\mathbf{G}^t\, \mathbf{C}_D^{-1}\, \mathbf{G} + \mathbf{C}_M^{-1}\right]^{-1},} \tag{1.90}$$

we obtain

$$2\, S(\mathbf{m}) = (\, \mathbf{m} - \langle\, \mathbf{m}\,\rangle\,)^t\, \mathbf{C}_{M'}^{-1}\, (\, \mathbf{m} - \langle\, \mathbf{m}\,\rangle\,)$$
$$- \langle\, \mathbf{m}\,\rangle^t\, \mathbf{C}_M^{-1}\, \langle\, \mathbf{m}\,\rangle + \mathbf{d}_{obs}{}^t\, \mathbf{C}_D^{-1}\, \mathbf{d}_{obs} + \mathbf{m}_{prior}{}^t\, \mathbf{C}_M^{-1}\, \mathbf{m}_{prior} .$$

All the right-hand terms but the first are constant (independent of $\mathbf{m}$), and can be absorbed in the constant factor of (1.87). This gives

$$\sigma_M(\mathbf{m}) = \text{const. } \exp\left[-\frac{1}{2} (\, \mathbf{m} - \langle\, \mathbf{m}\,\rangle\,)^t\, \mathbf{C}_{M'}^{-1}\, (\, \mathbf{m} - \langle\, \mathbf{m}\,\rangle\,) \right],$$

or in normalized form,

$$\sigma_M(\mathbf{m}) = ((2\pi)^{NM} \det \mathbf{C}_{M'})^{-1/2}$$
$$\exp\left[-\frac{1}{2} (\, \mathbf{m} - \langle\, \mathbf{m}\,\rangle\,)^t\, \mathbf{C}_{M'}^{-1}\, (\, \mathbf{m} - \langle\, \mathbf{m}\,\rangle\,) \right]. \tag{1.91}$$

Equation (1.91) shows the important result that, when the forward problem is linear, the a posteriori probability density in the model space is Gaussian. The center of this Gaussian is given by (1.89), while its covariance

operator is given by (1.90).

We successively have

$$\langle \mathbf{m} \rangle = \mathbf{C}_{M'} \left(\mathbf{G}^t \mathbf{C}_D^{-1} \mathbf{d}_{obs} + \mathbf{C}_M^{-1} \mathbf{m}_{prior} \right)$$

$$= \mathbf{C}_{M'} \mathbf{G}^t \mathbf{C}_D^{-1} \mathbf{d}_{obs} + \mathbf{C}_{M'} \mathbf{C}_M^{-1} \mathbf{m}_{prior}$$

$$= \mathbf{C}_{M'} \mathbf{G}^t \mathbf{C}_D^{-1} \mathbf{d}_{obs} + \mathbf{C}_{M'} \left(\mathbf{G}^t \mathbf{C}_D^{-1} \mathbf{G} + \mathbf{C}_M^{-1} - \mathbf{G}^t \mathbf{C}_D^{-1} \mathbf{G} \right) \mathbf{m}_{prior}$$

$$= \mathbf{C}_{M'} \mathbf{G}^t \mathbf{C}_D^{-1} \mathbf{d}_{obs} + \mathbf{C}_{M'} \left(\mathbf{C}_{M'}^{-1} - \mathbf{G}^t \mathbf{C}_D^{-1} \mathbf{G} \right) \mathbf{m}_{prior}$$

$$= \mathbf{C}_{M'} \mathbf{G}^t \mathbf{C}_D^{-1} \mathbf{d}_{obs} + \left(\mathbf{I} - \mathbf{C}_{M'} \mathbf{G}^t \mathbf{C}_D^{-1} \mathbf{G} \right) \mathbf{m}_{prior}$$

$$= \mathbf{m}_{prior} + \mathbf{C}_{M'} \mathbf{G}^t \mathbf{C}_D^{-1} (\mathbf{d}_{obs} - \mathbf{G} \mathbf{m}_{prior}) ,$$

i.e.,

$$\boxed{\langle \mathbf{m} \rangle = \mathbf{m}_{prior} + \left(\mathbf{G}^t \mathbf{C}_D^{-1} \mathbf{G} + \mathbf{C}_M^{-1} \right)^{-1} \mathbf{G}^t \mathbf{C}_D^{-1} (\mathbf{d}_{obs} - \mathbf{G} \mathbf{m}_{prior}).} \qquad (1.92)$$

In problem 1.19 it is shown that expressions (1.90) and (1.92) can also be written:

$$\boxed{\langle \mathbf{m} \rangle = \mathbf{m}_{prior} + \mathbf{C}_M \mathbf{G}^t (\mathbf{G} \mathbf{C}_M \mathbf{G}^t + \mathbf{C}_D)^{-1} (\mathbf{d}_{obs} - \mathbf{G} \mathbf{m}_{prior}) ,} \qquad (1.93)$$

and

$$\boxed{\mathbf{C}_{M'} = \mathbf{C}_M - \mathbf{C}_M \mathbf{G}^t (\mathbf{G} \mathbf{C}_M \mathbf{G}^t + \mathbf{C}_D)^{-1} \mathbf{G} \mathbf{C}_M .} \qquad (1.94)$$

As $\langle \mathbf{m} \rangle$ clearly maximizes $\sigma_M(\mathbf{m})$, it minimizes the quadratic expression

$$S(\mathbf{m}) = \qquad (1.95)$$

$$\frac{1}{2} \left((\mathbf{G} \mathbf{m} - \mathbf{d}_{obs})^t \mathbf{C}_D^{-1} (\mathbf{G} \mathbf{m} - \mathbf{d}_{obs}) + (\mathbf{m} - \mathbf{m}_{prior})^t \mathbf{C}_M^{-1} (\mathbf{m} - \mathbf{m}_{prior}) \right),$$

thus justifying the usual terminology of a *least-squares estimator.*

From equations (1.92) and (1.93) it is clear that $\langle \mathbf{m} \rangle - \mathbf{m}_{prior}$ depends linearly on $\mathbf{d}_{obs} - \mathbf{G} \mathbf{m}_{prior}$. It can be shown (see for instance Rao

(1973)) that among all such linear estimators, the least squares estimator has the property of "minimum variance", whatever the a priori statistics in the data and model spaces may be (Gaussian or not). This result is often used as a justification of the least-squares criterion. This is a mistake, because the minimization of the variances is a *bad* criterion when dealing with non-Gaussian functions. We have thus to emphasize here that, even if data errors have $\mathbf{C}_D$ as covariance operator, if the a priori model has $\mathbf{C}_M$ as covariance operator, we should *not* accept the minimization of $S(\mathbf{m})$ defined in equation (1.95) as a good criterion *unless* these error distributions can reasonably be modeled by Gaussian functions. Problem 1.9 shows an example where this is not the case.

Numerical aspects of the use of the previous equations are given in Chapter 4.

So far we have only been interested in the posterior probability density for model parameters. For data parameters this density is:

$$\sigma_D(\mathbf{d}) = \int_M d\mathbf{m}\ \sigma(\mathbf{d},\mathbf{m}) = \frac{\rho_D(\mathbf{d})}{\mu_D(\mathbf{d})} \int_M d\mathbf{m}\ \Theta(\mathbf{d}|\mathbf{m})\ \rho_M(\mathbf{m})\ . \qquad \text{(1.66 again)}$$

Using the assumptions in this paragraph, it can be shown (see section 1.7.2 for a demontration) that $\sigma_D(\mathbf{d})$ is also Gaussian:

$$\sigma_D(\mathbf{d}) = (2\pi)^{ND} \det \mathbf{C}_{D'})^{1/2} \exp\left(-\frac{1}{2} (\mathbf{d} - \langle \mathbf{d} \rangle)^t\ \mathbf{C}_{D'}^{-1}\ (\mathbf{d} - \langle \mathbf{d} \rangle) \right) . \qquad (1.96)$$

For instance, for negligible modeling errors ($\mathbf{C}_T = \mathbf{0}$), we obtain the following simple results (see section 1.7.2):

$$\boxed{\langle \mathbf{d} \rangle = \mathbf{G} \langle \mathbf{m} \rangle\ ,} \qquad (1.97a)$$

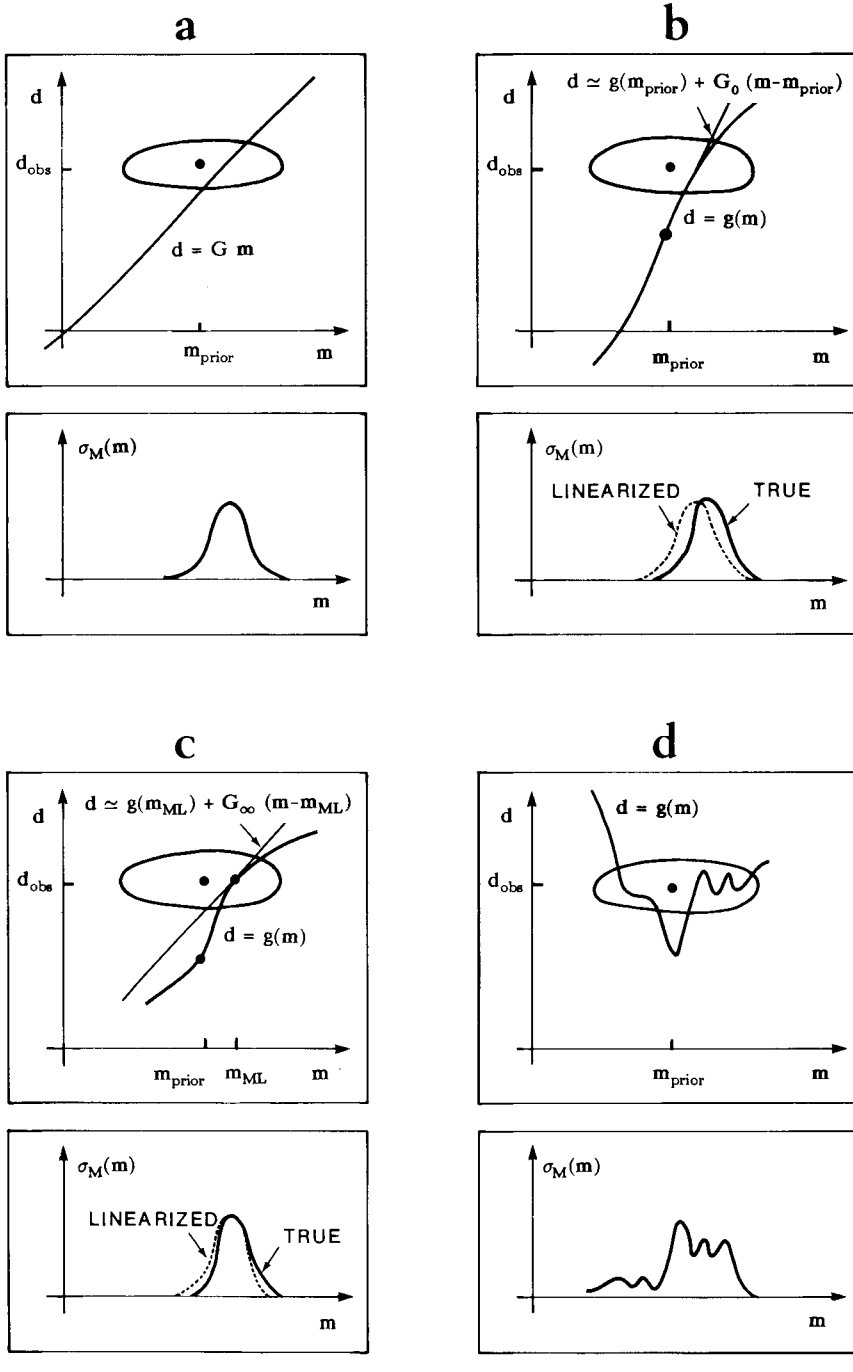
and

$$\boxed{\mathbf{C}_{D'} = \mathbf{G}\ \mathbf{C}_{M'}\ \mathbf{G}^t\ .} \qquad (1.97b)$$

b) The forward problem is nonlinear In this case, equation (1.85) cannot be further simplified:

$$\sigma_M(\mathbf{m}) = \text{const.} \qquad \text{(1.85 again)}$$

$$\exp\left(-\frac{1}{2} \left[(\mathbf{g}(\mathbf{m})-\mathbf{d}_{obs})^t\ \mathbf{C}_D^{-1}\ (\mathbf{g}(\mathbf{m})-\mathbf{d}_{obs}) + (\mathbf{m}-\mathbf{m}_{prior})^t\ \mathbf{C}_M^{-1}\ (\mathbf{m}-\mathbf{m}_{prior}) \right] \right) .$$


a
d
d_{obs}
d = G m
m_{prior}
m
$\sigma_M(m)$
m
b
$d \simeq g(m_{prior}) + G_0 (m-m_{prior})$
d
d_{obs}
d = g(m)
m_{prior}
m
$\sigma_M(m)$
LINEARIZED
TRUE
m
c
$d \simeq g(m_{ML}) + G_\infty (m-m_{ML})$
d
d_{obs}
d = g(m)
m_{prior}
m_{ML}
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$\sigma_M(m)$
LINEARIZED
TRUE
m
d
d
d_{obs}
d = g(m)
m_{prior}
m
$\sigma_M(m)$
m

← *Figure 1.13:* In sketches (a) to (d), the top is a representation of the probability density $\rho(\mathbf{d},\mathbf{m})$ and of the theoretical relationship $\mathbf{d} = \mathbf{g}(\mathbf{m})$ (resolution of the forward problem), with increasing nonlinearity from (a) to (d). The bottom is a representation of the corresponding a posteriori probability density $\sigma_M(\mathbf{m})$.

a) The forward equation $\mathbf{d} = \mathbf{G}\,\mathbf{m}$ is linear. The posterior probability density $\sigma_M(\mathbf{m})$ is Gaussian:

$$\sigma_M(\mathbf{m}) = ((2\pi)^N \det \mathbf{C}_{M'})^{-1/2} \exp\left[-\frac{1}{2}(\mathbf{m}-\langle\,\mathbf{m}\,\rangle)^t\,\mathbf{C}_{M'}^{-1}\,(\mathbf{m}-\langle\,\mathbf{m}\,\rangle)\right],$$

with

$$\langle\,\mathbf{m}\,\rangle = \mathbf{m}_{prior} + \left[\mathbf{G}^t\,\mathbf{C}_D^{-1}\,\mathbf{G} + \mathbf{C}_M^{-1}\right]^{-1}\mathbf{G}^t\,\mathbf{C}_D^{-1}\,(\mathbf{d}_{obs} - \mathbf{G}\,\mathbf{m}_{prior})$$

$$\mathbf{C}_{M'} = \left[\mathbf{G}^t\,\mathbf{C}_D^{-1}\,\mathbf{G} + \mathbf{C}_M^{-1}\right]^{-1} .$$

b) The forward equation $\mathbf{d} = \mathbf{g}(\mathbf{m})$ can be linearized around $\mathbf{m}_{prior}$:

$$\mathbf{g}(\mathbf{m}) \simeq \mathbf{g}(\mathbf{m}_{prior}) + \mathbf{G}_0\,(\mathbf{m} - \mathbf{m}_{prior}) ,$$

where $\mathbf{G}_0$ represents the derivative operator with elements

$$G_0^{i\alpha} = \left(\frac{\partial g^i}{\partial m^\alpha}\right)_{\mathbf{m}_{prior}} .$$

The posterior probability density $\sigma_M(\mathbf{m})$ is approximately Gaussian. Its maximum likelihood point is given approximately by

$$\mathbf{m}_{ML} \simeq \mathbf{m}_{prior} + \left[\mathbf{G}_0^t\,\mathbf{C}_D^{-1}\,\mathbf{G}_0 + \mathbf{C}_M^{-1}\right]^{-1}\mathbf{G}_0^t\,\mathbf{C}_D^{-1}\,(\mathbf{d}_{obs} - \mathbf{g}(\mathbf{m}_{prior})) ,$$

and the a posteriori covariance operator is approximately given by

$$\mathbf{C}_{M'} \simeq \left[\mathbf{G}_0^t\,\mathbf{C}_D^{-1}\,\mathbf{G}_0 + \mathbf{C}_M^{-1}\right]^{-1} .$$

c) The forward equation $\mathbf{d} = \mathbf{g}(\mathbf{m})$ can be linearized around the true maximum likelihood point, $\mathbf{m}_{ML}$:

$$\mathbf{g}(\mathbf{m}) \simeq \mathbf{g}(\mathbf{m}_{ML}) + \mathbf{G}_\infty\,(\mathbf{m} - \mathbf{m}_{ML}) ,$$

where $\mathbf{G}_\infty$ represents the derivative operator with elements

$$G_\infty^{i\alpha} = \left(\frac{\partial g^i}{\partial m^\alpha}\right)_{\mathbf{m}_{ML}} .$$

The point $\mathbf{m}_{ML}$ has to be obtained by the non-quadratic minimization of

$$S(\mathbf{m}) = \frac{1}{2}\left((g(\mathbf{m})-\mathbf{d}_{obs})^t\ \mathbf{C}_D^{-1}\ (g(\mathbf{m})-\mathbf{d}_{obs}) + (\mathbf{m}-\mathbf{m}_{prior})^t\ \mathbf{C}_M^{-1}\ (\mathbf{m}-\mathbf{m}_{prior})\right) .$$

This can be achieved using an iterative algorithm (see Chapter 4):

$$\mathbf{m}_{n+1} = \mathbf{m}_n + \delta\mathbf{m}_n .$$

Denote by $\mathbf{m}_\infty$ the point where we decide to stop the iterations ($\mathbf{m}_{ML} \simeq \mathbf{m}_\infty$) . The posterior covariance operator can then be estimated by

$$\mathbf{C}_{M'} \simeq \left(\mathbf{G}_\infty^t\ \mathbf{C}_D^{-1}\ \mathbf{G}_\infty + \mathbf{C}_M^{-1}\right)^{-1} .$$

d) The forward equation $\mathbf{d} = g(\mathbf{m})$ cannot be linearized. The a posteriori probability density is far from Gaussian and special methods should be used (see text).

It is clear that if $\mathbf{g}(\mathbf{m})$ is not a linear function of $\mathbf{m}$, $\sigma_M(\mathbf{m})$ is not Gaussian. The more nonlinear $\mathbf{g}(\mathbf{m})$ is, the more remote is $\sigma_M(\mathbf{m})$ from a Gaussian function.

Figure 1.13 schematically represents different degrees of nonlinearity. In 1.13a, the problem is linear. In 1.13b it can be linearized around the a priori model, $\mathbf{m}_{prior}$. In 1.13c the linearization around $\mathbf{m}_{prior}$ is no longer acceptable, but the problem is still quasi-linear. In figure 1.13d the problem is strongly nonlinear. Let us examine these cases separately.

The weakest case of nonlinearity arises when the function $\mathbf{g}(\mathbf{m})$ can be linearized around $\mathbf{m}_{prior}$:

$$\mathbf{g}(\mathbf{m}) \simeq \mathbf{g}(\mathbf{m}_{prior}) + \mathbf{G}_0\ (\mathbf{m} - \mathbf{m}_{prior}) , \tag{1.98}$$

where

$$\mathbf{G}_0^{i\alpha} = \left(\frac{\partial g^i}{\partial m^\alpha}\right)_{\mathbf{m}_{prior}} . \tag{1.99}$$

The symbol $\simeq$ in equation (1.98) means precisely that second-order terms can be neglected compared to observational and modelization errors (i.e., compared with standard deviations and correlations in $\mathbf{C}_D$). This is the sense of figure 1.13b.

Replacing (1.98) in (1.85), we see that the a posteriori probability density is then approximately Gaussian, the center being given by

$$\langle\ \mathbf{m}\ \rangle \simeq \mathbf{m}_{prior} + \left(\mathbf{G}_0^t\ \mathbf{C}_D^{-1}\ \mathbf{G} + \mathbf{C}_M^{-1}\right)^{-1}\ \mathbf{G}_0^t\ \mathbf{C}_D^{-1}\ (\mathbf{d}_{obs}-g(\mathbf{m}_{prior})) \tag{1.100}$$

$$= \mathbf{m}_{prior} + C_M\, G_0^t\, (G_0\, C_M\, G_0^t + C_D)^{-1}\, (\mathbf{d}_{obs} - \mathbf{g}(\mathbf{m}_{prior}))\ , \qquad (1.101)$$

and the a posteriori covariance operator being given by

$$C_{M'} \simeq \left(G_0^t\, C_D^{-1}\, G_0 + C_M^{-1}\right)^{-1} \qquad (1.102)$$

$$= C_M - C_M\, G_0^t\, (G_0\, C_M\, G_0^t + C_D)^{-1}\, G_0\, C_M\ . \qquad (1.103)$$

We see thus that solving linearizable problems is not more difficult than solving strictly linear problems.

In the case shown in figure 1.13c the linearization (1.98) is no longer acceptable, but the function $\mathbf{g}(\mathbf{m})$ is still quasi-linear inside the region of the $D \times M$ space of significant posterior probability density. The right strategy for these problems is to obtain (using some iterative algorithm) the maximum likelihood of $\sigma_M(\mathbf{m})$, say $\mathbf{m}_{ML}$, and to use a linearization of $\mathbf{g}(\mathbf{m})$ around $\mathbf{m}_{ML}$ for estimating the a posteriori covariance operator.

Let us see how this can work. The point maximizing $\sigma_M(\mathbf{m})$ clearly minimizes

$$S(\mathbf{m}) =$$

$$\frac{1}{2}\left[(\mathbf{g}(\mathbf{m})-\mathbf{d}_{obs})^t\, C_D^{-1}\, (\mathbf{g}(\mathbf{m})-\mathbf{d}_{obs}) + (\mathbf{m}-\mathbf{m}_{prior})^t\, C_M^{-1}\, (\mathbf{m}-\mathbf{m}_{prior})\right]\ , \qquad (1.104)$$

(the factor 1/2 is left for subsequent simplifications). As (1.104) is quadratic in data and model residuals, it justifies the name of *least-squares estimator* for $\mathbf{m}_{ML}$. The obtainment of the minimum of $S(\mathbf{m})$ corresponds to a classical problem of nonlinear optimization. Using, for instance, a quasi-Newton method, an iterative algorithm is obtained which corresponds to the three equivalent equations (see Chapter 4 for more details) :

$$\mathbf{m}_{n+1} = \mathbf{m}_n - \left(G_n^t\, C_D^{-1}\, G_n + C_M^{-1}\right)^{-1}$$

$$\left(G_n^t\, C_D^{-1}\, (\mathbf{g}(\mathbf{m}_n)-\mathbf{d}_{obs}) + C_M^{-1}\, (\mathbf{m}_n-\mathbf{m}_{prior})\right) \qquad (1.105)$$

$$= \mathbf{m}_{prior} - \left(G_n^t\, C_D^{-1}\, G_n + C_M^{-1}\right)^{-1}$$

$$G_n^t\, C_D^{-1}\, ((\mathbf{g}(\mathbf{m}_n)-\mathbf{d}_{obs}) - G_n\, (\mathbf{m}_n-\mathbf{m}_{prior})) \qquad (1.106)$$

$$= \mathbf{m}_{prior} - C_M\, G_n^t\, (C_D + G_n\, C_M\, G_n^t)^{-1}$$

$$((\mathbf{g}(\mathbf{m}_n)-\mathbf{d}_{obs}) - G_n\, (\mathbf{m}_n-\mathbf{m}_{prior})). \qquad (1.107)$$

In these equations,

$$\mathbf{G}_n = \left(\frac{\partial \mathbf{g}}{\partial \mathbf{m}} \right)_{\mathbf{m}_n} , \tag{1.108}$$

or, explicitly,

$$G_n^{i\alpha} = \left(\frac{\partial g^i}{\partial m^\alpha} \right)_{m_n} .$$

If the problem is quasi-linear (see figure 1.13c) such a method will not present convergence troubles. For more details of the numerical aspects, the reader is referred to Chapter 4.

Once the maximum likelihood point $\mathbf{m}_{ML} = \mathbf{m}_\infty$ has been conveniently approached, the a posteriori covariance operator can be estimated by

$$\mathbf{C}_{M'} \simeq \left(\mathbf{G}_\infty^t \, \mathbf{C}_D^{-1} \, \mathbf{G}_\infty + \mathbf{C}_M^{-1} \right)^{-1} \tag{1.109}$$

$$= \mathbf{C}_M - \mathbf{C}_M \, \mathbf{G}_\infty^t \, (\mathbf{G}_\infty \, \mathbf{C}_M \, \mathbf{G}_\infty^t + \mathbf{C}_D)^{-1} \, \mathbf{G}_\infty \, \mathbf{C}_M . \tag{1.110}$$

The main computational difference between this "nonlinear" solution and the linearized solution is that here, $\mathbf{g}(\mathbf{m})$, the predicted data for the current model, has to be computed at each iteration without using any linear approximation. In usual problems it is more difficult to compute $\mathbf{g}(\mathbf{m})$ than $\mathbf{g}(\mathbf{m}_0) + \mathbf{G}_0 \, (\mathbf{m}-\mathbf{m}_0)$: nonlinear problems are in general more expensive to solve than linearizable problems.

Of course, even if a problem is linearizable, it can be solved nonlinearly, but the gain in accuracy usually does not justify the computational effort.

Last, we have to discuss the strongly nonlinear problems represented by Figure 1.13d. The a posteriori probability density is then clearly non-Gaussian, and no general discussion of the solution can be made without a rather exhaustive exploration of the model space. If the number of model parameters is small, then we can use the general methods described in section 1.6.4. As, in that case, no advantage is taken of the Gaussian hypothesis, we do better to drop it and use a more realistic error modelization. If the number of parameters is large, we can always use equations (1.108)-(1.110) to obtain a local maximum likelihood point, to fix all its components except a few, and to explore the subspace thus defined.

Sometimes, the number of secondary maxima of $\sigma_M(\mathbf{m})$ (i.e., of secondary minima of $S(\mathbf{m})$) is not too large. Starting the iterative algorithms (1.105)-(1.107) at different points $\mathbf{m}_0$, we can check the existence of secondary minima in the region of interest. At the least, this strategy will allow of making a semi-quantitative discussion of the a posteriori state of information in the model space.

1.7.2: The Gaussian Hypothesis (least-squares criterion). Case $f(\mathbf{d},\mathbf{m}) = \mathbf{0}$.

In the previous section I have assumed that the equations solving the forward problem were written under the form $\mathbf{d} = \mathbf{g}(\mathbf{m})$. In fact, the distinctions between data vector and model vector do not necessarily correspond to observable parameters and model parameters, and it is the equation $\mathbf{d} = \mathbf{g}(\mathbf{m})$, expressing the theoretical correlations between all the parameters, that allows of *defining* the data and model vectors as those appearing in the left and right-hand sides of the equation $\mathbf{d} = \mathbf{g}(\mathbf{m})$, respectively.

Sometimes, it may be easy to consider the more general equation

$$\mathbf{f}(\mathbf{d},\mathbf{m}) = \mathbf{0} \ , \tag{1.111}$$

and this section gives the corresponding formulas. It is not more difficult to examine the most general problem that can be solved, within the Gaussian hypothesis, using the approach developed here.

Let $\mathbf{x} = (\mathbf{d},\mathbf{m})$ be a generic vector of the joint space $\boldsymbol{D}\times\boldsymbol{M}$ defined in section 1.1.3, containing observable and model parameters. The a priori information on $\mathbf{x}$ is assumed Gaussian,

$$\frac{\rho(\mathbf{x})}{\mu(\mathbf{x})} = \text{const. } \exp\left(-\frac{1}{2} (\mathbf{x}-\mathbf{x}_{\text{prior}})^t \, \mathbf{C}_X^{-1} \, (\mathbf{x}-\mathbf{x}_{\text{prior}}) \right) , \tag{1.112}$$

with center $\mathbf{x}_{\text{prior}}$ and covariance operator $\mathbf{C}_X$. Instead of writting the theoretical information on $\mathbf{x}$ as

$$\mathbf{f}(\mathbf{x}) = \mathbf{0} \ , \tag{1.113}$$

we allow theoretical uncertainties which, if they are assumed Gaussian, can be described using the probability density

$$\Theta(\mathbf{x}) = \text{const. } \exp\left(-\frac{1}{2} \, \mathbf{f}(\mathbf{x})^t \, \mathbf{C}_T^{-1} \, \mathbf{f}(\mathbf{x}) \right) . \tag{1.114}$$

The combination of $\rho(\mathbf{x})$ with $\Theta(\mathbf{x})$ leads to (see section 1.5)

$$\sigma(\mathbf{x}) = \frac{\rho(\mathbf{x}) \, \Theta(\mathbf{x})}{\mu(\mathbf{x})} \ , \tag{1.115}$$

i.e.,

$$\boxed{\sigma(\mathbf{x}) = \text{const. } \exp\left(-\frac{1}{2} \left(\mathbf{f}(\mathbf{x})^t \, \mathbf{C}_T^{-1} \, \mathbf{f}(\mathbf{x}) + (\mathbf{x}-\mathbf{x}_{\text{prior}})^t \, \mathbf{C}_X^{-1} \, (\mathbf{x}-\mathbf{x}_{\text{prior}}) \right) \right) .} \tag{1.116}$$

As for the explicit case, let me discuss linear and nonlinear problems separately,

a) The theoretical equation is linear. Instead of writing $\mathbf{f}(\mathbf{x}) = \mathbf{0}$, we then write

$$\mathbf{F}\,\mathbf{x} = \mathbf{0}\,, \tag{1.117}$$

where $\mathbf{F}$ represents a linear operator acting from the total space of parameters into a space of "residuals".

This gives

$$\sigma(\mathbf{x}) = \text{const}\,\exp(-S(\mathbf{x}))\,, \tag{1.118}$$

where $S(\mathbf{x})$ is the quadratic function

$$S(\mathbf{x}) = \frac{1}{2}\left[(\mathbf{F}\,\mathbf{x})^t\,\mathbf{C}_T^{-1}\,(\mathbf{F}\,\mathbf{x}) + (\mathbf{x}-\mathbf{x}_{prior})^t\,\mathbf{C}_X^{-1}\,(\mathbf{x}-\mathbf{x}_{prior})\right]. \tag{1.119}$$

Defining

$$\boxed{\langle\,\mathbf{x}\,\rangle = \left(\mathbf{F}^t\,\mathbf{C}_T^{-1}\,\mathbf{F} + \mathbf{C}_X^{-1}\right)^{-1}\,\mathbf{C}_X^{-1}\,\mathbf{x}_{prior}\,,} \tag{1.120}$$

and

$$\boxed{\mathbf{C}_{X'} = \left(\mathbf{F}^t\,\mathbf{C}_T^{-1}\,\mathbf{F} + \mathbf{C}_X^{-1}\right)^{-1}\,,} \tag{1.121}$$

we obtain

$$S(\mathbf{x}) = (\,\mathbf{x} - \langle\,\mathbf{x}\,\rangle\,)^t\,\mathbf{C}_{X'}^{-1}\,(\,\mathbf{x} - \langle\,\mathbf{x}\,\rangle\,) - \langle\,\mathbf{x}\,\rangle^t\,\mathbf{C}_X^{-1}\,\langle\,\mathbf{x}\,\rangle + \mathbf{x}_{prior}^t\,\mathbf{C}_X^{-1}\,\mathbf{x}_{prior}\,.$$

All the right-hand terms but the first are constant (independent of $\mathbf{x}$), and can be absorbed in the constant facto of (1.118). This gives

$$\sigma(\mathbf{x}) = \text{const.}\,\exp\left[-\frac{1}{2}\,(\,\mathbf{x} - \langle\,\mathbf{x}\,\rangle\,)^t\,\mathbf{C}_{X'}^{-1}\,(\,\mathbf{x} - \langle\,\mathbf{x}\,\rangle\,)\right],$$

or, in normalized form,

$$\boxed{\sigma(\mathbf{x}) = ((2\pi)^N\,\det\,\mathbf{C}_{X'})^{-1/2}\,\exp\left[-\frac{1}{2}(\mathbf{x}-\langle\,\mathbf{x}\,\rangle)^t\,\mathbf{C}_{X'}^{-1}\,(\mathbf{x}-\langle\,\mathbf{x}\,\rangle)\right].} \tag{1.122}$$

Equation (1.122) shows the important result that, when the theoretical equation is linear, the a posteriori probability density in the model space is Gaussian. The center of this Gaussian is given by (1.120), while its covari-

ance operator is given by (1.121).

Successively we have

$$\begin{aligned}
\langle \mathbf{x} \rangle &= \mathbf{C}_{X'} \mathbf{C}_X^{-1} \mathbf{m}_{prior} \\
&= \mathbf{C}_{X'} \left(\mathbf{F}^t \mathbf{C}_T^{-1} \mathbf{F} + \mathbf{C}_X^{-1} - \mathbf{F}^t \mathbf{C}_T^{-1} \mathbf{F} \right) \mathbf{x}_{prior} \\
&= \mathbf{C}_{X'} \left(\mathbf{C}_{X'}^{-1} - \mathbf{F}^t \mathbf{C}_T^{-1} \mathbf{F} \right) \mathbf{x}_{prior} \\
&= \left(\mathbf{I} - \mathbf{C}_{X'} \mathbf{F}^t \mathbf{C}_T^{-1} \mathbf{F} \right) \mathbf{x}_{prior} \\
&= \mathbf{x}_{prior} - \mathbf{C}_{X'} \mathbf{F}^t \mathbf{C}_T^{-1} \mathbf{F} \mathbf{x}_{prior} ,
\end{aligned}$$

i.e.

$$\boxed{\langle \mathbf{x} \rangle = \mathbf{x}_{prior} - \left(\mathbf{F}^t \mathbf{C}_T^{-1} \mathbf{F} + \mathbf{C}_X^{-1} \right)^{-1} \mathbf{F}^t \mathbf{C}_T^{-1} \mathbf{F} \mathbf{x}_{prior} .} \qquad (1.123)$$

In problem 1.19 it is shown that expressions (1.120) and (1.123) can also be written:

$$\boxed{\langle \mathbf{x} \rangle = \mathbf{x}_{prior} - \mathbf{C}_X \mathbf{F}^t (\mathbf{F} \mathbf{C}_X \mathbf{F}^t + \mathbf{C}_T)^{-1} \mathbf{F} \mathbf{x}_{prior} ,} \qquad (1.124)$$

and

$$\boxed{\mathbf{C}_{X'} = \mathbf{C}_X - \mathbf{C}_X \mathbf{F}^t (\mathbf{F} \mathbf{C}_X \mathbf{F}^t + \mathbf{C}_T)^{-1} \mathbf{F} \mathbf{C}_X .} \qquad (1.125)$$

As $\langle \mathbf{x} \rangle$ clearly maximizes $\sigma(\mathbf{x})$, it minimizes the quadratic expression

$$S(\mathbf{x}) = \frac{1}{2} \left((\mathbf{F} \mathbf{x})^t \mathbf{C}_T^{-1} (\mathbf{F} \mathbf{x}) + (\mathbf{x} - \mathbf{x}_{prior})^t \mathbf{C}_X^{-1} (\mathbf{x} - \mathbf{x}_{prior}) \right) , \qquad (1.126)$$

thus justifying the usual terminology of *least-squares estimator*.

Let us now direct our interest to the special case where we can divide the parameter set X into two subsets D and M such that the theoretical equation $\mathbf{F} \mathbf{x} = \mathbf{0}$ simplifies to

$$\mathbf{F} \mathbf{x} = \mathbf{G} \mathbf{m} - \mathbf{d} = \mathbf{0} , \qquad (1.127)$$

i.e.,

$$\mathbf{d} = \mathbf{G} \mathbf{m} , \qquad (1.128)$$

where $\mathbf{G}$ is a linear operator from M into D. Formally,

$$\mathbf{F} \mathbf{x} = \begin{bmatrix} -\mathbf{I} & \mathbf{G} \end{bmatrix} \begin{bmatrix} \mathbf{d} \\ \mathbf{m} \end{bmatrix} = \mathbf{0} ,$$

i.e.,

$$\mathbf{F} = [\, -\mathbf{I} \quad \mathbf{G} \,]\,. \tag{1.129}$$

Using the notations

$$\mathbf{x} = \begin{bmatrix} \mathbf{d} \\ \mathbf{m} \end{bmatrix} \qquad \mathbf{x}_{prior} = \begin{bmatrix} \mathbf{d}_{prior} \\ \mathbf{m}_{prior} \end{bmatrix} \qquad \langle\, \mathbf{x} \,\rangle = \begin{bmatrix} \langle\, \mathbf{d} \,\rangle \\ \langle\, \mathbf{m} \,\rangle \end{bmatrix}, \tag{1.130a}$$

and

$$\mathbf{C}_X = \begin{bmatrix} \mathbf{C}_{DD} & \mathbf{C}_{MD} \\ \mathbf{C}_{DM} & \mathbf{C}_{MM} \end{bmatrix} \qquad \mathbf{C}_{X'} = \begin{bmatrix} \mathbf{C}_{DD'} & \mathbf{C}_{MD'} \\ \mathbf{C}_{DM'} & \mathbf{C}_{MM'} \end{bmatrix}, \tag{1.130b}$$

and using (1.124) and (1.125) we easily obtain

$$\langle\, \mathbf{m} \,\rangle = \mathbf{m}_{prior} - (\mathbf{C}_{MM}\, \mathbf{G}^t - \mathbf{C}_{MD}) \tag{1.131}$$
$$(\mathbf{C}_T + \mathbf{C}_{DD} + \mathbf{G}\, \mathbf{C}_{MM}\, \mathbf{G}^t - \mathbf{C}_{DM}\, \mathbf{G}^t - \mathbf{G}\, \mathbf{C}_{MD})^{-1}\, (\mathbf{G}\, \mathbf{m}_{prior} - \mathbf{d}_{obs})\,,$$

$$\langle\, \mathbf{d} \,\rangle = \mathbf{G}\, \mathbf{m}_{prior} - (\mathbf{C}_T + \mathbf{G}\, (\mathbf{C}_{MM}\, \mathbf{G}^t - \mathbf{C}_{MD})) \tag{1.132}$$
$$(\mathbf{C}_T + \mathbf{C}_{DD} + \mathbf{G}\, \mathbf{C}_{MM}\, \mathbf{G}^t - \mathbf{C}_{DM}\, \mathbf{G}^t - \mathbf{G}\, \mathbf{C}_{MD})^{-1}\, (\mathbf{G}\, \mathbf{m}_{prior} - \mathbf{d}_{obs})\,,$$

$$\mathbf{C}_{MM'} = \mathbf{C}_{MM} - (\mathbf{C}_{MM}\, \mathbf{G}^t - \mathbf{C}_{MD}) \tag{1.133}$$
$$(\mathbf{C}_T + \mathbf{C}_{DD} + \mathbf{G}\, \mathbf{C}_{MM}\, \mathbf{G}^t - \mathbf{C}_{DM}\, \mathbf{G}^t - \mathbf{G}\, \mathbf{C}_{MD})^{-1}\, (\mathbf{G}\, \mathbf{C}_{MM} - \mathbf{C}_{DM})\,,$$

$$\mathbf{C}_{DD'} = \mathbf{C}_{DD} - (\mathbf{C}_{DM}\, \mathbf{G}^t - \mathbf{C}_{DD}) \tag{1.134a}$$
$$(\mathbf{C}_T + \mathbf{C}_{DD} + \mathbf{G}\, \mathbf{C}_{MM}\, \mathbf{G}^t - \mathbf{C}_{DM}\, \mathbf{G}^t - \mathbf{G}\, \mathbf{C}_{MD})^{-1}\, (\mathbf{G}\, \mathbf{C}_{MD} - \mathbf{C}_{DD})\,,$$

$$\mathbf{C}_{DM'} = \mathbf{C}_{DM} - (\mathbf{C}_{DM}\, \mathbf{G}^t - \mathbf{C}_{DD}) \tag{1.135a}$$
$$(\mathbf{C}_T + \mathbf{C}_{DD} + \mathbf{G}\, \mathbf{C}_{MM}\, \mathbf{G}^t - \mathbf{C}_{DM}\, \mathbf{G}^t - \mathbf{G}\, \mathbf{C}_{MD})^{-1}\, (\mathbf{G}\, \mathbf{C}_{MM} - \mathbf{C}_{DM})\,,$$

and

$$\mathbf{C}_{MD'} = \mathbf{C}_{MD} - (\mathbf{C}_{MM}\, \mathbf{G}^t - \mathbf{C}_{MD})\, (\mathbf{C}_T + \mathbf{C}_{DD} + \mathbf{G}\, \mathbf{C}_{MM}\, \mathbf{G}^t - \mathbf{C}_{DM}\, \mathbf{G}^t - \mathbf{G}\, \mathbf{C}_{MD})^{-1}\, (\mathbf{G}\, \mathbf{C}_{MD} - \mathbf{C}_{DD}) = \mathbf{C}_{DM'}{}^t\,.$$

Using some algebra, many equivalent expressions may be obtained. Among them, we will need the following:

$$\mathbf{C}_{DD'} = \mathbf{C}_T + \mathbf{G}\, \mathbf{C}_{MM}\, \mathbf{G}^t - (\mathbf{C}_T + \mathbf{G}\, (\mathbf{C}_{MM}\, \mathbf{G}^t - \mathbf{C}_{MD}))$$

$$(\mathbf{C}_T + \mathbf{C}_{DD} + \mathbf{G}\,\mathbf{C}_{MM}\,\mathbf{G}^t - \mathbf{C}_{DM}\,\mathbf{G}^t - \mathbf{G}\,\mathbf{C}_{MD})^{-1}$$

$$(\mathbf{C}_T + (\mathbf{G}\,\mathbf{C}_{MM} - \mathbf{C}_{DM})\,\mathbf{G}^t)\,, \tag{1.134b}$$

and

$$\mathbf{C}_{DM'} = \mathbf{G}\,\mathbf{C}_{MM} - (\mathbf{C}_T + \mathbf{G}\,(\mathbf{C}_{MM}\,\mathbf{G}^t - \mathbf{C}_{MD}))$$
$$(\mathbf{C}_T + \mathbf{C}_{DD} + \mathbf{G}\,\mathbf{C}_{MM}\,\mathbf{G}^t - \mathbf{C}_{DM}\,\mathbf{G}^t - \mathbf{G}\,\mathbf{C}_{MD})^{-1}$$

$$(\mathbf{G}\,\mathbf{C}_{MM} - \mathbf{C}_{DM})\,. \tag{1.135b}$$

In the particular case where errors in the theoretical relationship $\mathbf{d} = \mathbf{G}\,\mathbf{m}$ can be neglected,

$$\mathbf{C}_T = \mathbf{0}\,,$$

and equations (1.131)-(1.135) reduce to the simple expressions

$$\langle\,\mathbf{m}\,\rangle = \mathbf{m}_{prior} - (\mathbf{C}_{MM}\,\mathbf{G}^t - \mathbf{C}_{MD}) \tag{1.136}$$
$$(\mathbf{C}_{DD} + \mathbf{G}\,\mathbf{C}_{MM}\,\mathbf{G}^t - \mathbf{C}_{DM}\,\mathbf{G}^t - \mathbf{G}\,\mathbf{C}_{MD})^{-1}\,(\mathbf{G}\,\mathbf{m}_{prior} - \mathbf{d}_{obs})\,,$$

$$\langle\,\mathbf{d}\,\rangle = \mathbf{G}\,\langle\,\mathbf{m}\,\rangle\,, \tag{1.137}$$

$$\mathbf{C}_{MM'} = \mathbf{C}_{MM} - (\mathbf{C}_{MM}\,\mathbf{G}^t - \mathbf{C}_{MD}) \tag{1.138}$$
$$(\mathbf{C}_{DD} + \mathbf{G}\,\mathbf{C}_{MM}\,\mathbf{G}^t - \mathbf{C}_{DM}\,\mathbf{G}^t - \mathbf{G}\,\mathbf{C}_{MD})^{-1}\,(\mathbf{G}\,\mathbf{C}_{MM} - \mathbf{C}_{DM})\,,$$

$$\mathbf{C}_{DD'} = \mathbf{G}\,\mathbf{C}_{MM'}\,\mathbf{G}^t\,, \tag{1.139}$$

$$\mathbf{C}_{DM'} = \mathbf{G}\,\mathbf{C}_{MM'}\,, \tag{1.140}$$

and

$$\mathbf{C}_{MD'} = \mathbf{C}_{MM'}\,\mathbf{G}^t\,. \tag{1.141}$$

It should be noticed that, in the particular case where a priori information on $\mathbf{m}$ is uncorrelated with the a priori information on $\mathbf{d}$,

$$\mathbf{C}_{DM} = \mathbf{C}_{MD}{}^t = \mathbf{0}\,,$$

and all the above equations reduce to those shown in the previous section.

b) The theoretical equation is nonlinear. The point maximizing $\sigma(\mathbf{x})$ (the maximum likelihood point) will minimize the exponent in (1.116), i.e.,

$$S(\mathbf{x}) = \frac{1}{2} \left(\mathbf{f}(\mathbf{x})^t \, \mathbf{C}_T^{-1} \, \mathbf{f}(\mathbf{x}) + (\mathbf{x}-\mathbf{x}_{prior})^t \, \mathbf{C}_X^{-1} \, (\mathbf{x}-\mathbf{x}_{prior}) \right), \tag{1.142}$$

which intuitively means that the maximum likelihood point will approximately satisfy the theoretical equations ($\mathbf{f}(\mathbf{x}) \simeq \mathbf{0}$) and will be close to the a priori point $\mathbf{x}_{prior}$, the appropriate trade-off being imposed by the relative values of $\mathbf{C}_T$ and $\mathbf{C}_X$.

Using a quasi-Newton method (see Chapter 4 for more details) to obtain the maximum likelihood point leads to the algorithm

$$\mathbf{x}_{n+1} = \mathbf{x}_n - \left(\mathbf{F}_n^t \, \mathbf{C}_T^{-1} \, \mathbf{F}_n + \mathbf{C}_X^{-1} \right)^{-1} \left(\mathbf{F}_n^t \, \mathbf{C}_T^{-1} \, \mathbf{f}(\mathbf{x}_n) + \mathbf{C}_X^{-1} \, (\mathbf{x}_n-\mathbf{x}_{prior}) \right) \tag{1.143}$$

$$= \mathbf{x}_{prior} - \left(\mathbf{F}_n^t \, \mathbf{C}_T^{-1} \, \mathbf{F}_n + \mathbf{C}_X^{-1} \right)^{-1} \mathbf{F}_n^t \, \mathbf{C}_T^{-1} \, (\mathbf{f}(\mathbf{x}_n) - \mathbf{F}_n \, (\mathbf{x}_n-\mathbf{x}_{prior})) \tag{1.144}$$

$$= \mathbf{x}_{prior} - \mathbf{C}_X \, \mathbf{F}_n^t \, (\mathbf{C}_T + \mathbf{F}_n \, \mathbf{C}_X \, \mathbf{F}_n^t)^{-1} \, (\mathbf{f}(\mathbf{x}_n) - \mathbf{F}_n \, (\mathbf{x}_n-\mathbf{x}_{prior})) \, . \tag{1.145}$$

In these equations,

$$\mathbf{F}_n = \left(\frac{\partial \mathbf{f}}{\partial \mathbf{x}} \right)_{\mathbf{x}_n} , \tag{1.146}$$

or, explicitly,

$$\mathbf{F}_n^{iA} = \left(\frac{\partial f^i}{\partial x^A} \right)_{\mathbf{x}_n} .$$

Once the maximum likelihood point $\mathbf{x}_{ML} = \mathbf{x}_\infty$ has been conveniently approached, the a posteriori covariance operator can be estimated by

$$\mathbf{C}_{X'} \simeq \left(\mathbf{F}_\infty^t \, \mathbf{C}_T^{-1} \, \mathbf{F}_\infty + \mathbf{C}_X^{-1} \right)^{-1} \tag{1.147}$$

$$= \mathbf{C}_X - \mathbf{C}_X \, \mathbf{F}_\infty^t \, (\mathbf{F}_\infty \, \mathbf{C}_X \, \mathbf{F}_\infty^t + \mathbf{C}_T)^{-1} \, \mathbf{F}_\infty \, \mathbf{C}_X \, . \tag{1.148}$$

The solution of the formulas (1.143)-(1.145) for the case $\mathbf{f}(\mathbf{x}) = \mathbf{f}(\mathbf{d},\mathbf{m}) = \mathbf{g}(\mathbf{m}) - \mathbf{d} = \mathbf{0}$ is left as an exercise for the reader.

1.7.3: Generalized Gaussian (least-absolute-values criterion, minimax criterion)

In this section we explore the implications of assuming that experimental uncertainties on observations, or uncertainties in the a priori model, can be described using the Generalized Gaussian functions introduced in box 1.2.

Let d^i_{obs} represent the observed data values. We assume that errors are uncorrelated, that they can be estimated by the values σ^i_D, and that the density function describing uncertainties can be modeled by the Generalized Gaussian of order p

$$\frac{\rho_D(\mathbf{d})}{\mu_D(\mathbf{d})} = \text{const.} \prod_{i \in I_D} \exp \left(-\frac{1}{p} \frac{\left| d^i - d^i_{obs} \right|^p}{\left(\sigma^i_D \right)^p} \right) . \tag{1.149}$$

Similarly, let m^α_{prior} represent the a priori model values, and σ^α_M the estimated errors. We represent the a priori density function in the model space by

$$\rho_M(\mathbf{m}) = \text{const.} \prod_{\alpha \in I_M} \exp \left(-\frac{1}{p} \frac{\left| m^\alpha - m^\alpha_{prior} \right|^p}{\left(\sigma^\alpha_M \right)^p} \right) . \tag{1.150}$$

Simple results are obtained only when modelization errors are neglected. Thus, let us assume here that the forward modelization can be written

$$\mathbf{d} = \mathbf{g}(\mathbf{m}) ,$$

and that observational errors are predominant with respect to errors in the modelization. From equation (1.72) we obtain the a posteriori density function in the model space:

$$\sigma_M(\mathbf{m}) = \exp\left[-\frac{1}{p}\left(\sum_{i\in I_D}\frac{\left|g^i(\mathbf{m})-d^i_{obs}\right|^p}{\left(\sigma^i_D\right)^p}+\sum_{\alpha\in I_M}\frac{\left|m^\alpha-m^\alpha_{prior}\right|^p}{\left(\sigma^\alpha_M\right)^p}\right)\right]. \qquad (1.151)$$

The maximum likelihood $\mathbf{m}_{ML}$ maximizes $\sigma_M(\mathbf{m})$, i.e., minimizes

$$S(\mathbf{m}) = \frac{1}{p}\left(\sum_{i\in I_D}\frac{\left|g^i(\mathbf{m})-d^i_{obs}\right|^p}{\left(\sigma^i_D\right)^p}+\sum_{\alpha\in I_M}\frac{\left|m^\alpha-m^\alpha_{prior}\right|^p}{\left(\sigma^\alpha_M\right)^p}\right), \qquad (1.152)$$

which clearly corresponds to the minimization of an ℓ_p norm. We see thus how ℓ_p norm minimization problems arise in Inverse Problem Theory.

Two important particular cases are usually considered, namely, the ℓ_1 norm and the ℓ_∞ norm problems (in addition, of course, to the ℓ_2 norm already considered). For $p=1$ we have to minimize the quantity

$$S(\mathbf{m}) = \sum_{i\in I_D}\frac{\left|g^i(\mathbf{m})-d^i_{obs}\right|}{\sigma^i_D}+\sum_{\alpha\in I_M}\frac{\left|m^\alpha-m^\alpha_{prior}\right|}{\sigma^\alpha_M}, \qquad (1.153)$$

which corresponds to a *minimum-absolute-values criterion*. See Chapter 5 for more details.

For $p\to\infty$ it can be shown (see Chapter 5) that the minimization of $S(\mathbf{m})$ is equivalent to the *minimization of the maximum* of

$$\left\{\frac{\left|g^{i(\mathbf{m})}-d^i_{obs}\right|}{\sigma^i_D}\quad(i\in I_D)\quad;\quad\frac{\left|m^\alpha-m^\alpha_{prior}\right|}{\sigma^\alpha_M}\qquad(\alpha\in I_M)\right\}. \qquad (1.154)$$

This is the reason why the case $p\to\infty$ is known as the *minimax* criterion.

Techniques for solving intermediate cases ($1 < p < \infty$) are also described in Chapter 5.

Sometimes the following question arises: Which is the best criterion to use for the resolution of inverse problems, the least-absolute-values criterion, the least-squares criterion, or the minimax criterion? We have seen in this section that each of these criteria can be considered as implied by a particular assumption about the probability densities under consideration. It is thus clear that, depending on the particular form of these probability densities, any one of the criteria can be better than the other two. As an illustration

see problems 1.5, 1.9, and 1.11.

Problems for chapter 1:

Problem 1.1: Estimation of the epicentral coordinates of a seismic event: A nuclear explosion took place at time T=0 in an unknown location at the surface of the Earth. The seismic waves produced by the explosion have been recorded at a network of six seismic stations whose coordinates in a rectangular system are

$$\begin{aligned}
(x^1,y^1) &= (3 \text{ km} , 15 \text{ km}) \\
(x^2,y^2) &= (3 \text{ km} , 16 \text{ km}) \\
(x^3,y^3) &= (4 \text{ km} , 15 \text{ km}) \\
(x^4,y^4) &= (4 \text{ km} , 16 \text{ km}) \\
(x^5,y^5) &= (5 \text{ km} , 15 \text{ km}) \\
(x^6,y^6) &= (5 \text{ km} , 16 \text{ km}) .
\end{aligned} \tag{1}$$

The observed arrival times of the seismic waves at these stations are

$$\begin{aligned}
d^1_{obs} &= 3.12 \text{ s} \pm \sigma \\
d^2_{obs} &= 3.26 \text{ s} \pm \sigma \\
d^3_{obs} &= 2.98 \text{ s} \pm \sigma \\
d^4_{obs} &= 3.12 \text{ s} \pm \sigma \\
d^5_{obs} &= 2.84 \text{ s} \pm \sigma \\
d^6_{obs} &= 2.98 \text{ s} \pm \sigma ,
\end{aligned} \tag{2}$$

where

$$\sigma = 0.10 \text{ s} , \tag{3}$$

and where $\pm \sigma$ is a short notation indicating that experimental uncertainties are independent and can be modeled using a Gaussian probability density with a standard deviation equal to σ.

Estimate the epicentral coordinates (X,Y) of the explosion, assuming a velocity of

$$v = 5 \text{ km/s} \tag{4}$$

for the seismic waves. Use the approximation of a flat Earth's surface, and consider that the coordinates in (1) are cartesian.

Discuss the generalization of the problem to the case where the time of the explosion, the locations of the seismic observatories, or the velocity of the seismic waves is not perfectly known, and to the case of a realistic Earth.

Solution: The model parameters are the coordinates of the epicenter of the explosion:

$$\mathbf{m} = (X,Y) , \tag{5}$$

and the data parameters are the arrival times at the seismic network:

$$\mathbf{d} = (d^1,d^2,d^3,d^4,d^5,d^6) , \tag{6}$$

while the coordinates of the seismic stations and the velocity of seismic waves are assumed perfectly known (i.e., known with errors which are negligible with respect to errors in the observed arrival times).

The probability density representing the state of null information on the epicentral coordinates is

$$\mu_M(X,Y) = \text{const} , \tag{7}$$

because, as we use cartesian coordinates, (7) assigns equal probabilities to identical volumes (see example 18). Let $\rho_M(X,Y)$ be the probability density representing the a priori information on the epicentral location. As the statement of the problem does not give any a priori information,

$$\rho_M(X,Y) = \mu_M(X,Y) = \text{const} . \tag{8}$$

As data uncertainties are Gaussian and independent, the probability density representing the information we have on the true values of the arrival times is

$$\rho_D(d^1,d^2,d^3,d^4,d^5,d^6) = \text{const} \exp\left(-\frac{1}{2} \sum_{i=1}^{6} \frac{\left(d^i - d^i_{obs}\right)^2}{\sigma^2} \right) . \tag{9}$$

As d^i are Newtonian times, the null information probability density in the data space is (see section 1.2.4)

$$\mu_D(d^1,d^2,d^3,d^4,d^5,d^6) = \text{const} . \tag{10}$$

For a given (X,Y), the arrival times of the seismic wave at the seismic stations can be computed using the (exact) equation

$$d^i = g^i(X,Y) = \frac{1}{v}\sqrt{(x^i-X)^2 + (y^i-Y)^2} \qquad (i=1,...,6) , \tag{11}$$

which solves the forward problem. As the theoretical relationship between data and model parameters is assumed to be error free, the probability density representing this theoretical information is the conditional probability density

$$\theta(\mathbf{d}|(X,Y)) = \delta(\mathbf{d}-\mathbf{g}(X,Y)) , \tag{12}$$

where $\delta(\mathbf{d})$ is the delta function in the data space, and where $g(X,Y)$ denotes the (vector) function (11).

The posterior information resulting from the combination of $\rho_D(\mathbf{d})$, $\rho_M(X,Y)$, and $\theta(\mathbf{d}|(X,Y))$ is (equations (1.60), (1.63), and (1.64)):

$$\sigma(\mathbf{d},X,Y) = \frac{\rho(\mathbf{d},X,Y)\ \theta(\mathbf{d},X,Y)}{\mu(\mathbf{d},X,Y)} = \frac{\rho_D(\mathbf{d})}{\mu_D(\mathbf{d})}\ \rho_M(X,Y)\ \theta(\mathbf{d}|(X,Y)) . \tag{13}$$

The marginal a posteriori information for the model parameters is

$$\sigma_M(X,Y) = \int_D d\mathbf{d}\ \ \sigma(\mathbf{d},X,Y) , \tag{14}$$

which, using (12) and (13), gives

$$\sigma_M(X,Y) = \rho_M(X,Y) \left(\frac{\rho_D(\mathbf{d})}{\mu_D(\mathbf{d})} \right)_{\mathbf{d}=\mathbf{g}(X,Y)} . \tag{15}$$

Using equations (8) to (11) gives

$$\sigma_M(X,Y) = \text{const}\ \exp\left(-\frac{1}{2\sigma^2} \sum_{i=1}^{6} \left(d^i_{cal} - d^i_{obs} \right)^2 \right) , \tag{16}$$

where

$$d^i_{cal} = \frac{1}{v}\sqrt{(x^i-X)^2 + (y^i-Y)^2} . \tag{17}$$

The probability density $\sigma_M(X,Y)$ describes all the a posteriori information we have on the epicentral coordinates. As we only have two parameters, the simplest (and more general) way of studying this information is to plot the values of $\sigma_M(X,Y)$ directly in the region of the plane where it takes significant values. Figure 1.14 shows the corresponding result.

We see that the zone of non-vanishing probability density is crescent-shaped. This can be interpreted as follows. The arrival times of the seismic wave at the seismic network (top left of the figure) is of the order of 3 s , and as we know that the explosion took place at time T = 0. , and the velocity of the seismic wave is 5 km/s , this gives the reliable information that

the explosion took place at a distance of approximately 15 km from the seismic network. But as the observational errors (±0.1 s) in the arrival times are of the order of the travel times of the seismic wave between the stations, the azimuth of the epicenter is not well resolved. As the distance is well determined but not the azimuth, it is natural to obtain a probability density with a crescent shape.

From the values shown in Figure 1.14 it is possible to obtain any estimator of the epicentral coordinates we wish, such as, for instance, the median values, the mean values, the maximum likelihood values, and so on. But the general solution of the inverse problem is the probability density itself. Notice in particular that a computation of the covariance between X and Y will miss the circular aspect of the correlation.

If the time of the explosion was not known, or the coordinates of the seismic stations were not perfectly known, or if the velocity of the seismic waves was only imperfectly known, the model vector would contain all these parameters:

$$\mathbf{m} = (X,Y,T,x^1,y^1,...,x^6,y^6,v) . \tag{18}$$

After properly introducing the a priori information on T (if any), on (x^i,y^i) , and on v , the posterior probability density $\sigma_M(X,Y,T, x^1,y^1,...,x^6,y^6,v)$ should be defined as before, from where the marginal probability density on the epicentral coordinates (X,Y) could be obtained through

$$\sigma_{X,Y}(X,Y) = \int_{-\infty}^{\infty} dT \int_{-\infty}^{\infty} dx^1 ... \int_{-\infty}^{\infty} dy^6 \int_0^{\infty} dv\ \sigma_M(X,Y,T,x^1,y^1,...,x^6,y^6,v), \tag{19}$$

while the posterior probability density on the time T of the explosion is

$$\sigma_T(T) = \int_{-\infty}^{\infty} dX \int_{-\infty}^{\infty} dY \int_{-\infty}^{\infty} dx^1 ... \int_{-\infty}^{\infty} dy^6 \int_0^{\infty} dv\ \sigma_M(X,Y,T,x^1,y^1,...,x^6,y^6,v). \tag{20}$$

As computations rapidly become expensive, it may be necessary to make some simplifying assumptions. The most drastic one is to neglect uncertainties on (x^i,y^i) and v , and to increase the estimated error in the observed arrival times artificially, to compensate approximately for the simplification.

A realistic Earth is tridimensional and heterogeneous. It is generally simpler to use spherical coordinates (R,Θ,Φ) . Then the null information probability density is no longer uniform (see example 18). Also, for a realistic Earth, errors made in computing the travel times of seismic waves are not negligible compared to errors in the observation of arrival times at the seismic stations. Equation (12) should then be replaced, for instance, by the

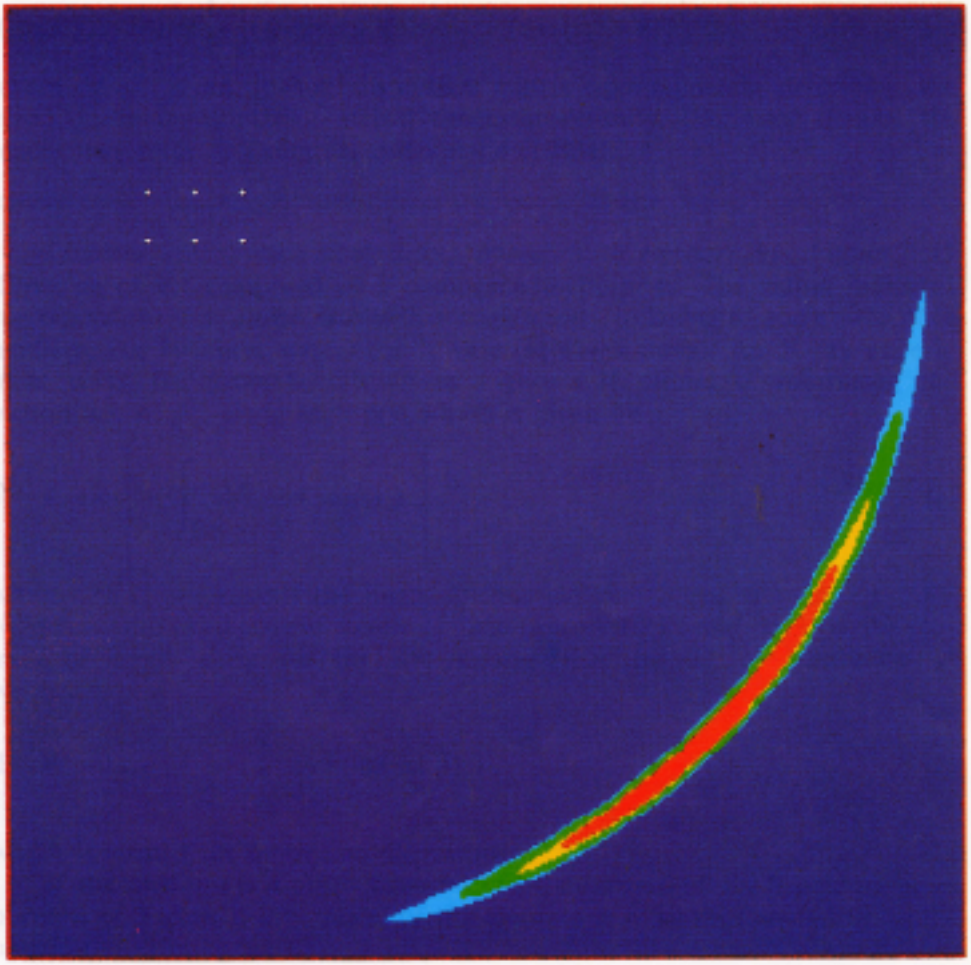


Figure 1.14: Probability density for the true epicentral coordinates of the seismic event, obtained using as data the arrival times of the seismic wave at six seismic stations (points in the top of the figure). The color scale is linear, between zero and the maximum value of the probability density. The crescent-shape of the region of significant probability density cannot be described using a few numbers (mathematical expectation, variances, covariances,...) as in usual solutions to inverse problems.

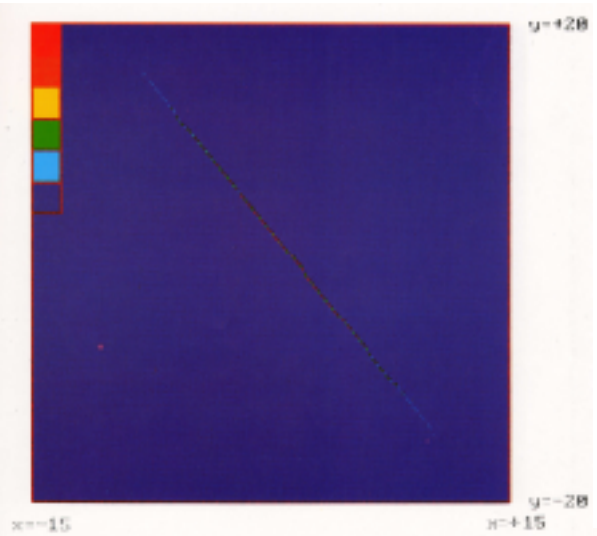


Figure 1.35 (from problem 1.10): Marginal probability density for the parameters m^1 and m^2. Uncertainties are so strongly correlated that it is difficult to distinguish the ellipsoid of errors from a segment. Although the standard deviations for each of the parameters are large, we have much information on these parameters, because their true values must lie on the "line". The resolution of the plotting device (300 pixel x 300 pixel) is not fine enough for a good representation, so that the colors obtained for the ellipsoid are aliased. The next figure shows a zoom of the central region.

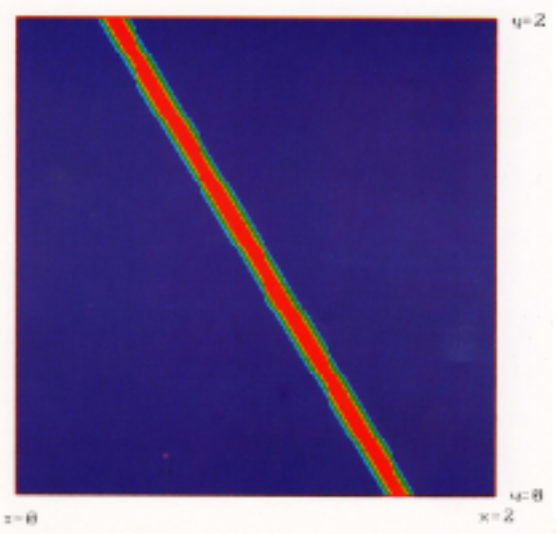


Figure 1.36 (from problem 1.10): Same as the previous figure, with finer detail.

equation

$$\theta(\mathbf{d}|r,\theta,\phi,T) = \exp\left[-\frac{1}{2}(\mathbf{d}-\mathbf{g}(r,\theta,\phi,T))^t\ \mathbf{C}_T^{-1}\ (\mathbf{d}-\mathbf{g}(r,\theta,\phi,T))\right], \tag{21}$$

where $\mathbf{C}_T$ is an ad-hoc covariance matrix approximately describing the errors made in estimating arrival times theoretically. For more details, the reader may refer to Tarantola and Valette (1982a).

Problem 1.2: First (elementary) approach to tomography. Figure 1.15 shows an object composed of 9 homogeneous portions. The values indicated correspond to the *linear attenuation coefficients* (relative to some reference medium, for instance, water) for X-rays (in given units). An X-ray experiment using the geometry shown in Figure 1.16 allows of measuring the *transmittance* ρ^{ij} along each ray, which is given by

$$\rho^{ij} = \exp\left[- \int_{R^{ij}} ds^{ij}\ m(\ \mathbf{x}(s^{ij})\ )\ \right], \tag{1}$$

where $m(\mathbf{x})$ represents the linear attenuation coefficient at point $\mathbf{x}$, R^{ij} represents the ray between source i and receiver j, and ds^{ij} is the element of length along the ray R^{ij}. Assume that instead of measuring ρ^{ij} we measure

$$d^{ij} = - \text{Log}\ \rho^{ij} = \int_{R^{ij}} ds^{ij}\ m(\ \mathbf{x}(s^{ij})\ )\ , \tag{2}$$

which is termed the *integrated attenuation.*

If the medium is a priori assumed to be composed of the 9 homogeneous portions of Figure 1, any model of the medium may be represented using the notation

$$\mathbf{m} = \begin{bmatrix} m^{11} & m^{12} & m^{13} \\ m^{21} & m^{22} & m^{23} \\ m^{31} & m^{32} & m^{33} \end{bmatrix}, \tag{3}$$

where the first index represents the column and the second index represents the row. Any possible set of numerical values in (3) is a *model vector.* For instance, the true model is (Figure 1)

$$\begin{bmatrix} m^{11} & m^{12} & m^{13} \\ m^{21} & m^{22} & m^{23} \\ m^{31} & m^{32} & m^{33} \end{bmatrix} = \begin{bmatrix} 50 & 60 & 50 \\ 60 & 58 & 60 \\ 50 & 60 & 50 \end{bmatrix}. \tag{4}$$

A *data vector* is represented by

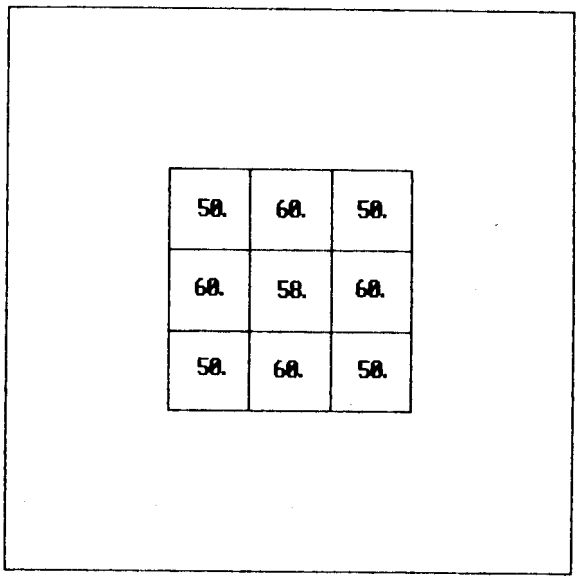


Figure 1.15: A bidimensional medium is composed of 3×3 homogeneous blocks. Indicated are the "true values" of the linear attenuation coefficient for X-rays (with respect to the surrounding medium).

$$\mathbf{d} = \begin{bmatrix} d^{11} & d^{12} & d^{13} & d^{14} & d^{15} & d^{16} \\ d^{21} & d^{22} & d^{23} & d^{24} & d^{25} & d^{26} \end{bmatrix}, \tag{5}$$

where the first index denotes the source number, and the second index denotes the receiver number. Equation (2) then simplifies to the discrete equation

$$d^{ij} = \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} G^{ij\alpha\beta} \, m^{\alpha\beta} \qquad \text{for } i=1,2 \qquad j=1,2,3,4,5,6 \ , \tag{6}$$

where $G^{ij\alpha\beta}$ represents the length of the ray ij inside the block $\alpha\beta$. An actual measurement of the integrated attenuation gives the values

$$\begin{bmatrix} d^{11} & d^{12} & d^{13} & d^{14} & d^{15} & d^{16} \\ d^{21} & d^{22} & d^{23} & d^{24} & d^{25} & d^{26} \end{bmatrix} =$$

$$\begin{bmatrix} 341.9\pm0.1 & 353.1\pm0.1 & 356.2\pm0.1 & 356.2\pm0.1 & 353.1\pm0.1 & 341.9\pm0.1 \\ 341.9\pm0.1 & 353.1\pm0.1 & 356.2\pm0.1 & 356.2\pm0.1 & 353.1\pm0.1 & 341.9\pm0.1 \end{bmatrix}, \tag{7}$$

where ±0.1 indicates the standard deviation of the estimated (Gaussian) error.

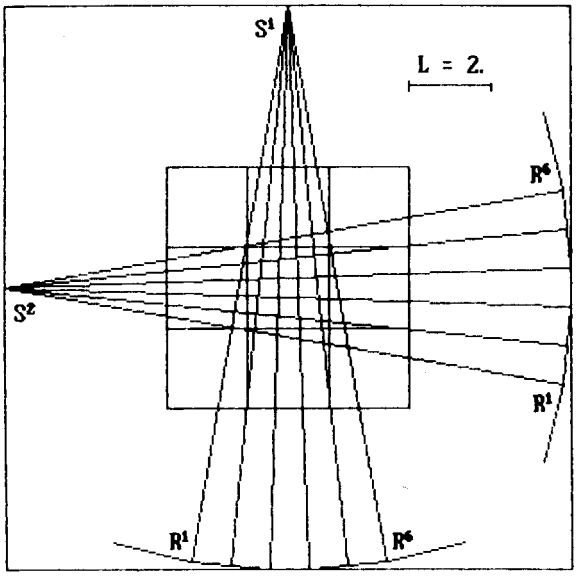


Figure 1.16: In order to infer the true (unknown) values of the linear attenuation coefficient, an X-ray transmission tomographic experiment is performed. Each block measures $L = 2$ units of length, and the figure is to scale (the angular separation between rays is 4 degrees). S^1 and S^2 represent the two source locations, and $R^1,...,R^6$ the six receivers used. Let $m(\mathbf{x})$ represent the linear attenuation coefficient at point $\mathbf{x}$ of the medium under study, R^{ij} the ray between source 1 and receiver j , s^{ij} the position along ray R^{ij} ,and d^{ij} the integrated attenuation along ray R^{ij} : $d^{ij} = \int ds^{ij}\ m(\mathbf{x}(s^{ij}))$ (along R^{ij}) . The measured values of the integrated attenuation along each ray are, in order for each receiver, 341.9±0.1, 353.1±0.1, 356.2±0.1 356.2±0.1 , 353.1±0.1, and 341.9±9±0.1 for source 1 , and 341.9±0.1, 353.1±0.1, 356.2±0.1 356.2±0.1 , 353.1±0.1, and 341.9±9±0.1 for source 2 (these values correspond in fact to the actual values as they can be computed from the true linear attenuation values of Figure 1, plus a Gaussian noise with standard deviation 0.1, and are rounded to the first decimal). These values are assumed to be corrected for the effect of the propagation outside the 3×3 model, so that the linear attenuation coefficient outside the model can be taken as null. The inverse problem consists in using these "observed" values of integrated attenuation to infer the actual model values. Remark that the upper-left block is explored with very short ray lengths, and owing to the relatively high noise in the data, the actual value of this block will probably be poorly resolved.

Assume that you have the a priori information that the model values of the linear attenuation coefficients equal 55 ± 15 (Figure 1.17). Give a better estimation of them using the data (7) and the least squares theory. Discuss.

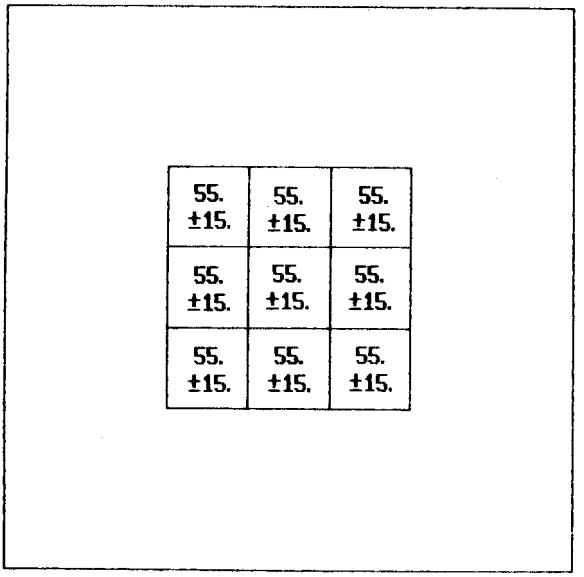


Figure 1.17: We have the a priori information that the true linear attenuation coeffients are 55±15 . It is assumed that a Gaussian probability density well represents this a priori information (in particular, ±15 represent "soft limits", which can be outpassed with a probability corresponding to the Gaussian density function).

Solution: We wish here to obtain the model $\mathbf{m}$ minimizing

$$S(\mathbf{m}) = \frac{1}{2}\left[(\mathbf{Gm}-\mathbf{d}_{obs})^t\, \mathbf{C}_D^{-1}\, (\mathbf{Gm}-\mathbf{d}_{obs}) + (\mathbf{m}-\mathbf{m}_{prior})^t\, \mathbf{C}_M^{-1}\, (\mathbf{m}-\mathbf{m}_{prior})\right], \tag{8}$$

where

$$\mathbf{d}_{obs} = \begin{bmatrix} 341.9 & 353.1 & 356.2 & 356.2 & 353.1 & 341.9 \\ 341.9 & 353.1 & 356.2 & 356.2 & 353.1 & 341.9 \end{bmatrix}, \tag{9}$$

$$(C_D)^{ijkl} = 0.1^2\, \delta^{ik}\, \delta^{jl}\,, \tag{10}$$

$$\mathbf{m}_{\text{prior}} = \begin{bmatrix} 55 & 55 & 55 \\ 55 & 55 & 55 \\ 55 & 55 & 55 \end{bmatrix}, \tag{11}$$

$$(C_M)^{\alpha\beta\gamma\delta} = 15^2 \, \delta^{\alpha\gamma} \, \delta^{\beta\delta} , \tag{12}$$

and where the elements of the kernel of the linear operator $\mathbf{G}$ can be obtained from Figure 1.16 using a simple geometrical computation:

$$\begin{bmatrix} G^{1111} & G^{1112} & G^{1113} \\ G^{1121} & G^{1122} & G^{1123} \\ G^{1131} & G^{1132} & G^{1133} \end{bmatrix} = \begin{bmatrix} 0.3338 & 1.6971 & 0.0000 \\ 2.0309 & 0.0000 & 0.0000 \\ 2.0309 & 0.0000 & 0.0000 \end{bmatrix}, \tag{13a}$$

$$\begin{bmatrix} G^{1211} & G^{1212} & G^{1213} \\ G^{1221} & G^{1222} & G^{1223} \\ G^{1231} & G^{1232} & G^{1233} \end{bmatrix} = \begin{bmatrix} 0.0000 & 2.0110 & 0.0000 \\ 0.0000 & 2.0110 & 0.0000 \\ 0.4883 & 1.5227 & 0.0000 \end{bmatrix}, \tag{13b}$$

$$\begin{bmatrix} G^{1311} & G^{1312} & G^{1313} \\ G^{1321} & G^{1322} & G^{1323} \\ G^{1331} & G^{1332} & G^{1333} \end{bmatrix} = \begin{bmatrix} 0.0000 & 2.0012 & 0.0000 \\ 0.0000 & 2.0012 & 0.0000 \\ 0.0000 & 2.0012 & 0.0000 \end{bmatrix}, \tag{13c}$$

$$\begin{bmatrix} G^{1411} & G^{1412} & G^{1413} \\ G^{1421} & G^{1422} & G^{1423} \\ G^{1431} & G^{1432} & G^{1433} \end{bmatrix} = \begin{bmatrix} 0.0000 & 2.0012 & 0.0000 \\ 0.0000 & 2.0012 & 0.0000 \\ 0.0000 & 2.0012 & 0.0000 \end{bmatrix}, \tag{13d}$$

$$\begin{bmatrix} G^{1511} & G^{1512} & G^{1513} \\ G^{1521} & G^{1522} & G^{1523} \\ G^{1531} & G^{1532} & G^{1533} \end{bmatrix} = \begin{bmatrix} 0.0000 & 2.0110 & 0.0000 \\ 0.0000 & 2.0110 & 0.0000 \\ 0.0000 & 1.5227 & 0.4883 \end{bmatrix}, \tag{13e}$$

$$\begin{bmatrix} G^{1611} & G^{1612} & G^{1613} \\ G^{1621} & G^{1622} & G^{1623} \\ G^{1631} & G^{1632} & G^{1633} \end{bmatrix} = \begin{bmatrix} 0.0000 & 1.6971 & 0.3338 \\ 0.0000 & 0.0000 & 2.0309 \\ 0.0000 & 0.0000 & 2.0309 \end{bmatrix}, \tag{13f}$$

$$\begin{bmatrix} G^{2111} & G^{2112} & G^{2113} \\ G^{2121} & G^{2122} & G^{2123} \\ G^{2131} & G^{2132} & G^{2133} \end{bmatrix} = \begin{bmatrix} 0.0000 & 0.0000 & 0.0000 \\ 1.6971 & 0.0000 & 0.0000 \\ 0.3338 & 2.0309 & 2.0309 \end{bmatrix}, \tag{13g}$$

$$\begin{bmatrix} G^{2211} & G^{2212} & G^{2213} \\ G^{2221} & G^{2222} & G^{2223} \\ G^{2231} & G^{2232} & G^{2233} \end{bmatrix} = \begin{bmatrix} 0.0000 & 0.0000 & 0.0000 \\ 2.0110 & 2.0110 & 1.5227 \\ 0.0000 & 0.0000 & 0.4883 \end{bmatrix}, \tag{13h}$$

$$\begin{bmatrix} G^{2311} & G^{2312} & G^{2313} \\ G^{2321} & G^{2322} & G^{2323} \\ G^{2331} & G^{2332} & G^{2333} \end{bmatrix} = \begin{bmatrix} 0.0000 & 0.0000 & 0.0000 \\ 2.0012 & 2.0012 & 2.0012 \\ 0.0000 & 0.0000 & 0.0000 \end{bmatrix}, \tag{13i}$$

$$\begin{bmatrix} G^{2411} & G^{2412} & G^{2413} \\ G^{2421} & G^{2422} & G^{2423} \\ G^{2431} & G^{2432} & G^{2433} \end{bmatrix} = \begin{bmatrix} 0.0000 & 0.0000 & 0.0000 \\ 2.0012 & 2.0012 & 2.0012 \\ 0.0000 & 0.0000 & 0.0000 \end{bmatrix}, \quad (13j)$$

$$\begin{bmatrix} G^{2511} & G^{2512} & G^{2513} \\ G^{2521} & G^{2522} & G^{2523} \\ G^{2531} & G^{2532} & G^{2533} \end{bmatrix} = \begin{bmatrix} 0.0000 & 0.0000 & 0.4883 \\ 2.0110 & 2.0110 & 1.5227 \\ 0.0000 & 0.0000 & 0.0000 \end{bmatrix}, \quad (13k)$$

and

$$\begin{bmatrix} G^{2611} & G^{2612} & G^{2613} \\ G^{2621} & G^{2622} & G^{2623} \\ G^{2631} & G^{2632} & G^{2633} \end{bmatrix} = \begin{bmatrix} 0.3338 & 2.0309 & 2.0309 \\ 1.6971 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 \end{bmatrix}. \quad (13l)$$

The minimum of expression (8) can, for instance, be obtained using equation (1.92) of the text:

$$\mathbf{m} = \mathbf{m}_{prior} + \left(\mathbf{G}^t \mathbf{C}_D^{-1} \mathbf{G} + \mathbf{C}_M^{-1} \right)^{-1} \mathbf{G}^t \mathbf{C}_D^{-1} (\mathbf{d}_{obs} - \mathbf{G}\, \mathbf{m}_{prior}) . \quad (14)$$

This gives

$$\mathbf{m} = \begin{bmatrix} 55.9 & 59.3 & 50.3 \\ 59.3 & 58.4 & 60.2 \\ 50.3 & 60.2 & 50.3 \end{bmatrix}. \quad (15)$$

The covariance operator describing a posteriori uncertainties in the model parameters is (equation 1.90 of the text)

$$\mathbf{C}_{M'} = \left(\mathbf{G}^t \mathbf{C}_D^{-1} \mathbf{G} + \mathbf{C}_M^{-1} \right)^{-1} . \quad (16)$$

Instead of representing variances and covariances of $\mathbf{C}_{M'}$, it is more useful to represent standard deviations and correlations (see box 1.1). This gives the standard deviations

$$\sigma_{M'} = \begin{bmatrix} 14.7 & 1.7 & 0.7 \\ 1.7 & 1.0 & 0.7 \\ 0.7 & 0.7 & 0.6 \end{bmatrix}, \quad (17)$$

and the coefficients of correlation

$$\begin{bmatrix} R^{1111} & R^{1112} & R^{1113} \\ R^{1121} & R^{1122} & R^{1123} \\ R^{1131} & R^{1132} & R^{1133} \end{bmatrix} = \begin{bmatrix} 1.0000 & -0.9977 & 0.9536 \\ -0.9977 & 0.9958 & 0.9874 \\ 0.9536 & 0.9874 & 0.9901 \end{bmatrix}, \quad (18a)$$

$$\begin{bmatrix} R^{1211} & R^{1212} & R^{1213} \\ R^{1221} & R^{1222} & R^{1223} \\ R^{1231} & R^{1232} & R^{1233} \end{bmatrix} = \begin{bmatrix} -0.9977 & 1.0000 & -0.9710 \\ 0.9997 & -0.9972 & -0.9897 \\ -0.9708 & -0.9902 & -0.9896 \end{bmatrix}, \quad (18b)$$

$$\begin{bmatrix} R^{1311} & R^{1312} & R^{1313} \\ R^{1321} & R^{1322} & R^{1323} \\ R^{1331} & R^{1332} & R^{1333} \end{bmatrix} = \begin{bmatrix} 0.9536 & -0.9710 & 1.0000 \\ -0.9708 & 0.9657 & 0.9624 \\ 0.9948 & 0.9632 & 0.9515 \end{bmatrix}, \quad (18c)$$

$$\begin{bmatrix} R^{2111} & R^{2112} & R^{2113} \\ R^{2121} & R^{2122} & R^{2123} \\ R^{2131} & R^{2132} & R^{2133} \end{bmatrix} = \begin{bmatrix} -0.9977 & 0.9997 & -0.9708 \\ 1.0000 & -0.9972 & -0.9902 \\ -0.9710 & -0.9897 & -0.9896 \end{bmatrix}, \quad (18d)$$

$$\begin{bmatrix} R^{2211} & R^{2212} & R^{2213} \\ R^{2221} & R^{2222} & R^{2223} \\ R^{2231} & R^{2232} & R^{2233} \end{bmatrix} = \begin{bmatrix} 0.9958 & -0.9972 & 0.9657 \\ -0.9972 & 1.0000 & 0.9776 \\ 0.9657 & 0.9776 & 0.9963 \end{bmatrix}, \quad (18e)$$

$$\begin{bmatrix} R^{2311} & R^{2312} & R^{2313} \\ R^{2321} & R^{2322} & R^{2323} \\ R^{2331} & R^{2332} & R^{2333} \end{bmatrix} = \begin{bmatrix} 0.9874 & -0.9897 & 0.9624 \\ -0.9902 & 0.9776 & 1.0000 \\ 0.9632 & 0.9977 & 0.9622 \end{bmatrix}, \quad (18f)$$

$$\begin{bmatrix} R^{3111} & R^{3112} & R^{3113} \\ R^{3121} & R^{3122} & R^{3123} \\ R^{3131} & R^{3132} & R^{3133} \end{bmatrix} = \begin{bmatrix} 0.9536 & -0.9708 & 0.9948 \\ -0.9710 & 0.9657 & 0.9632 \\ 1.0000 & 0.9624 & 0.9515 \end{bmatrix}, \quad (18g)$$

$$\begin{bmatrix} R^{3211} & R^{3212} & R^{3213} \\ R^{3221} & R^{3222} & R^{3223} \\ R^{3231} & R^{3232} & R^{3233} \end{bmatrix} = \begin{bmatrix} 0.9874 & -0.9902 & 0.9632 \\ -0.9897 & 0.9776 & 0.9977 \\ 0.9624 & 1.0000 & 0.9622 \end{bmatrix}, \quad (18h)$$

and

$$\begin{bmatrix} R^{3311} & R^{3312} & R^{3313} \\ R^{3321} & R^{3322} & R^{3323} \\ R^{3331} & R^{3332} & R^{3333} \end{bmatrix} = \begin{bmatrix} 0.9901 & -0.9896 & 0.9515 \\ -0.9896 & 0.9963 & 0.9622 \\ 0.9515 & 0.9622 & 1.0000 \end{bmatrix}. \quad (18i)$$

The solution (15) with the errors (17) is represented in Figure 1.18 (to be compared with Figure 1.15 and Figure 1.17). The a priori information was that the values in each block were 55 ± 15 . We see that the a posteriori errors are much smaller except in block (1 1) , where the solution, 55.9 ± 14.7 , practically coincides with the a priori solution. As can be seen in Figure 1.16, this block contains very short lengths of rays, so that it has practically not been explored by our data; the value of the attenuation coefficient is practically not resolved by the data set used. If a least squares inversion was performed with the data (7) but without using a priori information, that block would certainly take very arbitrary values, thus polluting the values of the attenuation coefficient in all the other blocks. More dramatically, numerical instabilities could arise (because the the operator $\mathbf{G}^t \mathbf{C}_D^{-1} \mathbf{G}$ could become numerically not positive definite due to computer rounding errors) and the used computer code would clash with a "zero divide" diagnostic

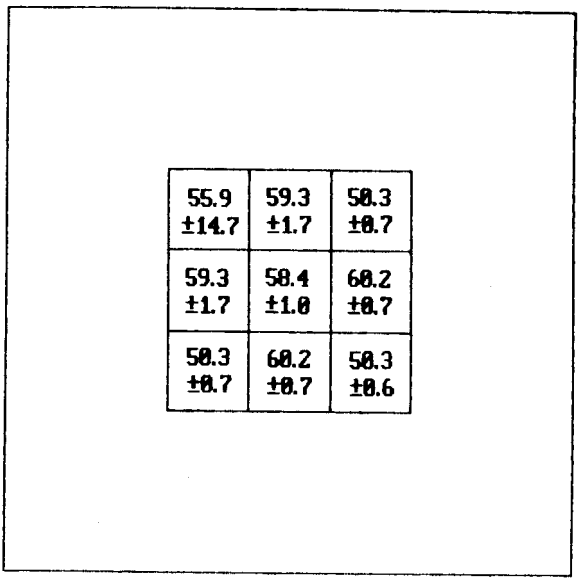


Figure 1.18: The a posteriori solution obtained by inversion of the available data. Remark that the value of the upper-left block has not been resolved (a posteriori value and estimated error almost identical to the a priori values). The values of all other blocks have been estimated with a relative error of less than 3%.

Except for the unresolved block m^{11}, the values obtained are close to the true values, and within the estimated error bar. Of course, as the data used were noise-corrupted, the obtained values cannot be identical to the true values. Using more rays would give a more precise solution.

The data values recalculated from the solution (15) are

$$\mathbf{d}_{obs} = \begin{bmatrix} 341.92 & 353.10 & 356.20 & 356.20 & 353.10 & 341.90 \\ 341.89 & 353.10 & 356.20 & 356.20 & 353.10 & 341.92 \end{bmatrix}, \qquad (19)$$

which are almost identical to the observed values (9).

The coefficients of correlation as shown in (18) are all very close to unity. This is due to the fact that there is no independent information (all rays traverse at least three blocks), and there is not much data redundancy.

Remark number 1: Assume that a new experiment produces one new datum, corresponding to a new ray (equal to or different from the previous rays). In order to incorporate this new information, we can either take the a priori model (11)-(12) and perform an inversion using 13 data, or, more simply, we can take the a posteriori solution (15)-(17)-(18) as a priori solu-

tion for an inverse problem with a single datum (the new one). As demonstrated in Chapter 4, this gives exactly the same solution (thus showing the coherence of the "a priori information" approach).

Remark number 2: Usual computer codes consider that vectors (i.e., elements of a linear space) are necessarily represented using column matrices, and that the kernels of linear operators are then represented using two-dimensional matrices. It may then be simpler for numerical computations to replace the previous notations by the matricial notations

$$\mathbf{d}_{obs} = \begin{bmatrix} 341.9 \\ 353.1 \\ 356.2 \\ 356.2 \\ 353.1 \\ 341.9 \\ 341.9 \\ 353.1 \\ 356.2 \\ 356.2 \\ 353.1 \\ 341.9 \end{bmatrix}, \tag{20}$$

$$(C_D)^{ij} = 0.1^2 \, \delta^{ij}, \tag{21}$$

$$\mathbf{m}_{prior} = \begin{bmatrix} 55 \\ 55 \\ 55 \\ 55 \\ 55 \\ 55 \\ 55 \\ 55 \\ 55 \end{bmatrix}, \tag{22}$$

$$(C_M)^{\alpha\beta} = 15^2 \, \delta^{\alpha\beta}, \tag{23}$$

and

$$G = \begin{bmatrix}
0.3338 & 1.6971 & 0.0000 & 2.0309 & 0.0000 & 0.0000 & 2.0309 & 0.0000 & 0.0000 \\
0.0000 & 2.0110 & 0.0000 & 0.0000 & 2.0110 & 0.0000 & 0.4883 & 1.5227 & 0.0000 \\
0.0000 & 2.0012 & 0.0000 & 0.0000 & 2.0012 & 0.0000 & 0.0000 & 2.0012 & 0.0000 \\
0.0000 & 2.0012 & 0.0000 & 0.0000 & 2.0012 & 0.0000 & 0.0000 & 2.0012 & 0.0000 \\
0.0000 & 2.0110 & 0.0000 & 0.0000 & 2.0110 & 0.0000 & 0.0000 & 1.5227 & 0.4883 \\
0.0000 & 1.6971 & 0.3338 & 0.0000 & 0.0000 & 2.0309 & 0.0000 & 0.0000 & 2.0309 \\
0.0000 & 0.0000 & 0.0000 & 1.6971 & 0.0000 & 0.0000 & 0.3338 & 2.0309 & 2.0309 \\
0.0000 & 0.0000 & 0.0000 & 2.0110 & 2.0110 & 1.5227 & 0.0000 & 0.0000 & 0.4883 \\
0.0000 & 0.0000 & 0.0000 & 2.0012 & 2.0012 & 2.0012 & 0.0000 & 0.0000 & 0.0000 \\
0.0000 & 0.0000 & 0.0000 & 2.0012 & 2.0012 & 2.0012 & 0.0000 & 0.0000 & 0.0000 \\
0.0000 & 0.0000 & 0.4883 & 2.0110 & 2.0110 & 1.5227 & 0.0000 & 0.0000 & 0.0000 \\
0.3338 & 2.0309 & 2.0309 & 1.6971 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000
\end{bmatrix} . \quad (24)$$

Equations (8) and (14) are then usual matricial equations.

Problem 1.3: Formulas for inverse problems when the (discrete) parameters can take only discrete values. The theory developed in this chapter applies to the case where each of the discrete parameters $d^1,d^2,...$ and $m^1,m^2,...$ can take continuous values. In some problems, the data parameters and/or the model parameters can only take some discrete values. Obtain the corresponding formulas for the resolution of inverse problems.

Solution: Let $\mathbf{x} = \{x^A\} = (x^1,x^2,...)$ denote a discrete (and finite) parameter set. In the text it has been assumed that each of the parameters x^A $(A=1,2,...)$ takes its values on some continuous set. The vector $\mathbf{x}$ then takes its values on some "volume" V. We have seen that the most general way of describing a *state of information* on the true values of the parameters is by defining a ***probability density*** $\rho(\mathbf{x})$ $(\mathbf{x}\in V)$ over the parameter space.

If each of the parameters x^A $(A=1,2,...)$ take its values on some discrete set, $x^A \in (x^A{}_1,x^A{}_2,...)$, then the vector $\mathbf{x}$ can only take some discrete values $\mathbf{x}_1$, $\mathbf{x}_2$, ..., and a state of information is then described by a ***probability*** $\tilde{\rho}(\mathbf{x}_u)$ $(u=1,2,...)$: the probability of each of the discrete values $\mathbf{x}_1$, $\mathbf{x}_2$, ...

The formulas corresponding to an inverse problem where the (discrete) parameters can only take discrete values should be obtained from a theory more general than the one developed in the text, or from an ad-hoc discrete theory. Instead, although less rigorous, it is simpler to formally consider a probability as a special case of a probability density:

$$\rho(\mathbf{x}) = \sum_{u} \tilde{\rho}(\mathbf{x}_u)\, \delta(\mathbf{x}-\mathbf{x}_u) , \tag{1}$$

where, if $\rho(\mathbf{x})$ is a probability density and $\delta(\mathbf{x})$ is Dirac's delta "function", then $\tilde{\rho}(\mathbf{x}_u)$ clearly corresponds to the probability of the point $\mathbf{x}_u$.

I consider here that the model vector $\mathbf{m}$ can only take discrete values $\mathbf{m}_1,\mathbf{m}_2,\ldots$, and for any value $\mathbf{m}_w$, the data vector $\mathbf{d}$ can only take discrete values $\mathbf{d}_1,\mathbf{d}_2,\ldots$ As discussed in the text, the a posteriori probability density in the space DxM is (equations 1.60, 1.63, and 1.64)

$$\sigma(\mathbf{d},\mathbf{m}) = \frac{\rho(\mathbf{d},\mathbf{m})\, \theta(\mathbf{d},\mathbf{m})}{\mu(\mathbf{d},\mathbf{m})} = \frac{\rho_D(\mathbf{d})\, \rho_M(\mathbf{m})\, \mu_M(\mathbf{m})}{\mu_D(\mathbf{d})\, \mu_M(\mathbf{m})}\, \theta(\mathbf{d}|\mathbf{m}) , \tag{2}$$

i.e.,

$$\sigma(\mathbf{d},\mathbf{m}) = \frac{\rho_D(\mathbf{d})\, \rho_M(\mathbf{m})}{\mu_D(\mathbf{d})}\, \theta(\mathbf{d}|\mathbf{m}) . \tag{3}$$

In equation (3), $\rho_D(\mathbf{d})$ is the probability density representing the knowledge obtained on the true values of $\mathbf{d}$ through our experiments (measurements), $\rho_M(\mathbf{m})$ is the probability density representing our a priori information on the model parameters, $\theta(\mathbf{d}|\mathbf{m})$ is the conditional probability density for $\mathbf{d}$, given $\mathbf{m}$, representing our knowledge on the theoretical correlations existing between $\mathbf{m}$ and $\mathbf{d}$, and where $\mu_D(\mathbf{d})$ is the non-informative probability density in the data space.

If $\mathbf{d}$ and $\mathbf{m}$ can only take discrete values, then

$$\rho_D(\mathbf{d}) = \sum_{v} \tilde{\rho}_D(\mathbf{d}_v)\, \delta(\mathbf{d}-\mathbf{d}_v) , \tag{4a}$$

$$\mu_D(\mathbf{d}) = \sum_{v} \tilde{\mu}_D(\mathbf{d}_v)\, \delta(\mathbf{d}-\mathbf{d}_v) , \tag{4b}$$

$$\rho_M(\mathbf{m}) = \sum_{w} \tilde{\rho}_M(\mathbf{m}_w)\, \delta(\mathbf{m}-\mathbf{m}_w) , \tag{4c}$$

and

$$\theta(\mathbf{d}|\mathbf{m}_w) = \sum_{v} \tilde{\theta}(\mathbf{d}_v|\mathbf{m}_w)\, \delta(\mathbf{d}-\mathbf{d}_v) , \tag{4d}$$

where $\tilde{\rho}_D(\mathbf{d}_v)$ is the probability that we assing of $\mathbf{d}_v$ being the true value of $\mathbf{d}$ which has been realized in our measurement (ambiguous results of the measurements), $\tilde{\mu}_D(\mathbf{d}_v)$ is the non-informative probability on $\mathbf{d}$ (usually uniform), $\tilde{\rho}_M(\mathbf{m}_w)$ is the a priori probability of the true value of $\mathbf{m}$ being $\mathbf{m}_w$, and $\theta(\mathbf{d}_v|\mathbf{m}_w)$ is the conditional probability of the true value of $\mathbf{d}$ being $\mathbf{d}_v$, if the true value of $\mathbf{m}$ was $\mathbf{m}_w$. Introducing the a posteriori probability $\tilde{\sigma}(\mathbf{d}_v,\mathbf{m}_w)$ by

$$\sigma(\mathbf{d},\mathbf{m}) = \sum_v \sum_w \tilde{\sigma}(\mathbf{d}_v,\mathbf{m}_w)\, \delta(\mathbf{d}-\mathbf{d}_v)\, \delta(\mathbf{m}-\mathbf{m}_w)\,, \tag{4e}$$

we obtain, *at each point* $(\mathbf{d}_v,\mathbf{m}_w)$,

$$\tilde{\sigma}(\mathbf{d}_v,\mathbf{m}_w) = \frac{\tilde{\rho}_D(\mathbf{d}_v)\, \tilde{\rho}_M(\mathbf{m}_w)\, \tilde{\theta}(\mathbf{d}_v|\mathbf{m}_w)}{\tilde{\mu}_D(\mathbf{d}_v)}\,. \tag{5}$$

where the symbol $\delta(\mathbf{0})$ has been formally manipulated as an ordinary (finite) constant.

The (marginal) a posteriori probability in the model space is then

$$\tilde{\sigma}_M(\mathbf{m}_w) = \sum_v \tilde{\sigma}(\mathbf{d}_v,\mathbf{m}_w)\,, \tag{6}$$

i.e.,

$$\tilde{\sigma}_M(\mathbf{m}_w) = \tilde{\rho}_M(\mathbf{m}_w) \sum_v \frac{\tilde{\rho}_D(\mathbf{d}_v)}{\tilde{\mu}_D(\mathbf{d}_v)}\, \tilde{\theta}(\mathbf{d}_v|\mathbf{m}_w)\,, \tag{7}$$

or, if the probability is normalized,

$$\tilde{\sigma}_M(\mathbf{m}_w) = \frac{\tilde{\rho}_M(\mathbf{m}_w) \sum_v \dfrac{\tilde{\rho}_D(\mathbf{d}_v)\, \tilde{\theta}(\mathbf{d}_v|\mathbf{m}_w)}{\tilde{\mu}_D(\mathbf{d}_v)}}{\sum_w \tilde{\rho}_M(\mathbf{m}_w) \sum_v \dfrac{\tilde{\rho}_D(\mathbf{d}_v)\, \tilde{\theta}(\mathbf{d}_v|\mathbf{m}_w)}{\tilde{\mu}_D(\mathbf{d}_v)}}\,. \tag{8}$$

The (marginal) a posteriori probability in the data space is

$$\tilde{\sigma}_D(\mathbf{d}_v) = \sum_w \tilde{\sigma}(\mathbf{d}_v,\mathbf{m}_w) , \tag{9}$$

i.e.,

$$\tilde{\sigma}_D(\mathbf{d}_v) = \frac{\tilde{\rho}_D(\mathbf{d}_v)}{\tilde{\mu}_D(\mathbf{d}_v)} \sum_w \tilde{\rho}_M(\mathbf{m}_w)\, \tilde{\theta}(\mathbf{d}_v|\mathbf{m}_w) , \tag{10}$$

or, if the probability is normalized,

$$\tilde{\sigma}_D(\mathbf{d}_v) = \frac{\dfrac{\tilde{\rho}_D(\mathbf{d}_v)}{\tilde{\mu}_D(\mathbf{d}_v)} \displaystyle\sum_w \tilde{\rho}_M(\mathbf{m}_w)\, \tilde{\theta}(\mathbf{d}_v|\mathbf{m}_w)}{\displaystyle\sum_v \frac{\tilde{\rho}_D(\mathbf{d}_v)}{\tilde{\mu}_D(\mathbf{d}_v)} \sum_w \tilde{\rho}_M(\mathbf{m}_w)\, \tilde{\theta}(\mathbf{d}_v|\mathbf{m}_w)} . \tag{11}$$

In the particular case where the measurement is perfect and gives an unambiguous result, $\mathbf{d} = \mathbf{d}_{obs}$;

$$\tilde{\rho}_D(\mathbf{d}_v) = \delta_{vv_{obs}} = \begin{cases} 1 & \text{for } v = v_{obs} \\ 0 & \text{for } v \neq v_{obs} . \end{cases} \tag{12}$$

Equation (8) then becomes

$$\tilde{\sigma}_M(\mathbf{m}_w) = \frac{\tilde{\theta}(\mathbf{d}_{obs}|\mathbf{m}_w)\, \tilde{\rho}_M(\mathbf{m}_w)}{\displaystyle\sum_w \tilde{\theta}(\mathbf{d}_{obs}|\mathbf{m}_w)\, \tilde{\rho}_M(\mathbf{m}_w)} , \tag{13}$$

while equation (11) degenerates into

$$\tilde{\sigma}_D(\mathbf{d}_v) = \tilde{\rho}_D(\mathbf{d}_v) . \tag{14}$$

Formula (13) encounters a large domain of application. Let us recall the sense of each of the terms. $\tilde{\rho}_M(\mathbf{m}_w)$, for w=1,2,..., is the a priori

(subjective) probability we assign of each of the $\mathbf{m}_w$ being the true model vector, $\tilde{\theta}(\mathbf{d}_v|\mathbf{m}_w)$, for v=1,2,..., is the probability we assign of each of the $\mathbf{d}_v$ being the true data vector if the true model vector is $\mathbf{m}_v$, and $\tilde{\sigma}_M(\mathbf{m}_w)$ is the a posteriori (subjective) probability we assign to each of the $\mathbf{m}_w$, after a measurement of the true value of the data vector which has given the unambiguous result that the true value is $\mathbf{d}_{v_{obs}}$.

For the sake of completeness, let me give the formulas corresponding to (8), (11), and (13) in the case where only one of the data vector or the model vector is discrete.

If only the model vector $\mathbf{m}$ takes discrete values, equation (8) becomes

$$\tilde{\sigma}_M(\mathbf{m}_w) = \frac{\tilde{\rho}_M(\mathbf{m}_w) \int_D d\mathbf{d} \, \frac{\rho(\mathbf{d}) \, \theta(\mathbf{d}|\mathbf{m}_w)}{\mu_D(\mathbf{d})}}{\sum_w \tilde{\rho}_M(\mathbf{m}_w) \int_D d\mathbf{d} \, \frac{\rho_D(\mathbf{d}) \, \theta(\mathbf{d}|\mathbf{m}_w)}{\mu_D(\mathbf{d}_v)}} , \tag{15}$$

equation (11) becomes

$$\sigma_D(\mathbf{d}) = \frac{\frac{\rho_D(\mathbf{d})}{\mu_D(\mathbf{d})} \sum_w \tilde{\rho}_M(\mathbf{m}_w) \, \theta(\mathbf{d}|\mathbf{m}_w)}{\int_D d\mathbf{d} \, \frac{\rho_D(\mathbf{d})}{\mu_D(\mathbf{d})} \sum_w \tilde{\rho}_M(\mathbf{m}_w) \, \theta(\mathbf{d}|\mathbf{m}_w)} , \tag{16}$$

and equation (13) becomes

$$\tilde{\sigma}_M(\mathbf{m}_w) = \frac{\theta(\mathbf{d}_{obs}|\mathbf{m}_w) \, \tilde{\rho}_M(\mathbf{m}_w)}{\sum_w \theta(\mathbf{d}_{obs}|\mathbf{m}_w) \, \tilde{\rho}_M(\mathbf{m}_w)} . \tag{17}$$

If only the data vector $\mathbf{d}$ takes discrete values, equation (8) becomes

$$\sigma_M(\mathbf{m}) = \frac{\rho_M(\mathbf{m}) \sum_v \frac{\tilde{\rho}_D(\mathbf{d}_v)\, \tilde{\theta}(\mathbf{d}_v|\mathbf{m})}{\tilde{\mu}_D(\mathbf{d}_v)}}{\int_M d\mathbf{m}\, \rho_M(\mathbf{m}) \sum_v \frac{\tilde{\rho}_D(\mathbf{d}_v)\, \tilde{\theta}(\mathbf{d}_v|\mathbf{m})}{\tilde{\mu}_D(\mathbf{d}_v)}}, \tag{18}$$

equation (11) becomes

$$\tilde{\sigma}_D(\mathbf{d}_v) = \frac{\frac{\tilde{\rho}_D(\mathbf{d}_v)}{\tilde{\mu}_D(\mathbf{d}_v)} \int_M d\mathbf{m}\ \rho_M(\mathbf{m})\, \tilde{\theta}(\mathbf{d}_v|\mathbf{m})}{\sum_v \frac{\tilde{\rho}_D(\mathbf{d}_v)}{\tilde{\mu}_D(\mathbf{d}_v)} \int_M d\mathbf{m}\ \rho_M(\mathbf{m})\, \tilde{\theta}(\mathbf{d}_v|\mathbf{m})}, \tag{19}$$

and equation (13) becomes

$$\sigma_M(\mathbf{m}) = \frac{\tilde{\theta}(\mathbf{d}_{obs}|\mathbf{m})\, \rho_M(\mathbf{m})}{\int_M d\mathbf{m}\, \tilde{\theta}(\mathbf{d}_{obs}|\mathbf{m})\, \rho_M(\mathbf{m})}. \tag{20}$$

Problem 1.4: Approximately one in each 100,000 individuals of a given population is affected by a very dangerous disease, which is only apparent in the final stages. A medical test has been designed to indicate if a given individual is affected by the disease. If that person is affected, the response of the test is always positive, but if not, it gives a positive (erroneous) response in one per cent of the cases. I have been submitted to the test and have obtained a positive response. Am I affected by the disease?

Solution: Let $\mathbf{m}_1$ and $\mathbf{m}_2$ be defined as follows

$$\mathbf{m}_1 = \text{I am affected by the disease}, \tag{1a}$$

m_2 = I am not affected by the disease , (1b)

and let d_1 and d_2 be defined as follows

d_1 = The test gives a positive response , (2a)
d_2 = The test gives a negative response . (2b)

As approximately one of every 100,000 individuals is affected by the disease, the a priori information I have on the value of m is described by the probability

$\tilde{\rho}_M(m_1) = 0.000\,01$, (3a)
$\tilde{\rho}_M(m_2) = 0.999\,99$. (3b)

Let $\tilde{\theta}(d_v|m_w)$ be the probability of the result of the test being d_v if the value of m is m_w . As, if an individual is affected, the response of the test is always positive,

$\tilde{\theta}(d_1|m_1) = 1.$, (4a)
$\tilde{\theta}(d_2|m_1) = 0.$, (4b)

and as if the individual is not affected, the test gives a positive (erroneous) response in one percent of the cases,

$\tilde{\theta}(d_1|m_2) = 0.01$, (5a)
$\tilde{\theta}(d_2|m_2) = 0.99$. (5b)

The application of the test in my case has unambiguously given the value

$d_{obs} = d_1$, (6)

so that the information I have on the true value of d is represented by the probability

$\tilde{\rho}_D(d_1) = 1.$, (7a)
$\tilde{\rho}_D(d_2) = 0.$. (7b)

The a posteriori information on the true value value of m can then be computed using equation (8) of the previous problem:

$$\tilde{\sigma}_M(m_w) = \frac{\tilde{\rho}_M(m_w) \sum_v \frac{\tilde{\rho}_D(d_v)\,\tilde{\theta}(d_v|m_w)}{\tilde{\mu}_D(d_v)}}{\sum_w \tilde{\rho}_M(m_w) \sum_v \frac{\tilde{\rho}_D(d_v)\,\tilde{\theta}(d_v|m_w)}{\tilde{\mu}_D(d_v)}}, \tag{8}$$

which, using (7), becomes

$$\tilde{\sigma}_M(m_w) = \frac{\tilde{\theta}(d_{obs}|m_w)\,\tilde{\rho}_M(m_w)}{\sum_w \tilde{\theta}(d_{obs}|m_w)\,\tilde{\rho}_M(m_w)}. \tag{9}$$

This gives

$$\tilde{\sigma}_M(m_1) = \frac{\tilde{\theta}(d_1|m_1)\,\tilde{\rho}_M(m_1)}{\tilde{\theta}(d_1|m_1)\,\tilde{\rho}_M(m_1) + \tilde{\theta}(d_1|m_2)\,\tilde{\rho}_M(m_2)}$$

$$= \frac{1. \cdot 0.000\,01}{1. \cdot 0.000\,01 + 0.01 \cdot 0.999\,99} \simeq 0.000\,999\,0$$

$$\simeq 10^{-3}, \tag{10a}$$

and

$$\tilde{\sigma}_M(m_2) = \frac{\tilde{\theta}(d_1|m_2)\,\tilde{\rho}_M(m_2)}{\tilde{\theta}(d_1|m_1)\,\tilde{\rho}_M(m_1) + \tilde{\theta}(d_1|m_2)\,\tilde{\rho}_M(m_2)}$$

$$= \frac{0.01 \cdot 0.999\,99}{1. \cdot 0.000\,01 + 0.01 \cdot 0.999\,99} \simeq 0.999\,001\,0$$

$$\simeq 1\text{-}10^{-3}, \tag{10b}$$

i.e., in spite of the fact that the response of the test (which makes only one per cent of errors) has been positive, I only have one chance per thousand of being affected by the disease. The intuitive interpretation is as follows: although the test makes very few errors, the percentage of

diseased individuals in the population is so low that the test may make many errors before it is used with a diseased individual. As the a priori probability of my having the disease was of one in 100,000 , and the a posteriori probability is 100 times greater, the test effectively generates information, although I do not yet have to worry very much about it, because a probability of one per thousand is still very low. However, further health checks are justified.

Assume now that the response to the test had not been unambiguous (Hi, Pr. Tarantola, here is Dr. Jekyll. My assistant just gave me the response of the test, and she says that the result was positive. Nevertheless, I have to inform you that my assistant is not a very reliable woman: each time she has a result, she throws a dice, and if she obtains a six, she lies to me about the result...).

As the probability $\tilde{\rho}_D(d_v)$ is the (a priori) probability that the true value of d is d_v , instead of (7) I should now take

$$\tilde{\rho}_D(d_1) = 5/6 , \tag{11a}$$

$$\tilde{\rho}_D(d_2) = 1/6 , \tag{11b}$$

and representing the null information by the probability

$$\tilde{\mu}_D(d_1) = \tilde{\mu}_D(d_2) = 0.5 , \tag{12}$$

the a posteriori probability for m can be obtained from equation (8), which gives

$$\tilde{\sigma}_M(m_1) \simeq 4.8\ 10^{-5} . \tag{13}$$

The a posteriori probability for the true result of the test can be computed using equation (11) of the previous problem:

$$\tilde{\sigma}_D(d_v) = \frac{\dfrac{\tilde{\rho}_D(d_v)}{\tilde{\mu}_D(d_v)} \displaystyle\sum_w \tilde{\rho}_M(m_w)\, \tilde{\theta}(d_v|m_w)}{\displaystyle\sum_v \frac{\tilde{\rho}_D(d_v)}{\tilde{\mu}_D(d_v)} \sum_w \tilde{\rho}_M(m_w)\, \tilde{\theta}(d_v|m_w)} , \tag{14}$$

which gives

$$\tilde{\sigma}_D(d_1) \simeq 4.8\ 10^{-2} . \tag{15}$$

Result (13) shows that the a posteriori probability of being affected by the disease is only five times greater than the a priori one, despite the fact that the assistant says the response was positive. Result (15) explains this result by the fact that the a posteriori probability of the assistant of telling the untruth is very high.

Should the assistant tell the truth only if she throws a six, then

$$\tilde{\rho}_D(d_1) = 1/6 \,, \tag{16a}$$

$$\tilde{\rho}_D(d_2) = 5/6 \,, \tag{16b}$$

which gives

$$\tilde{\sigma}_M(m_1) \simeq 2.0\ 10^{-6} \,. \tag{17}$$

If she always lies, then

$$\tilde{\rho}_D(d_1) = 0. \,, \tag{18a}$$

$$\tilde{\rho}_D(d_2) = 1. \,, \tag{18b}$$

and

$$\tilde{\sigma}_M(m_1) = 0. \,. \tag{19}$$

Problem 1.5: Some physical quantity d is related with the physical quantity x through the equation

$$d = m^1 + m^2 x \,, \tag{1}$$

where m^1 and m^2 are unknown parameters. Equation (1) represents a straight line on the plane (d,x). In order to estimate m^1 and m^2, the parameter d has been experimentally measured for some selected values of x, and the following results have been obtained (Figure 1.19):

$$\begin{array}{lll} x^1 = 03.500 & d^1_{obs} = 2.0 & \pm 0.5 \\ x^2 = 05.000 & d^2_{obs} = 2.0 & \pm 0.5 \\ x^3 = 07.000 & d^3_{obs} = 3.0 & \pm 0.5 \\ x^4 = 07.500 & d^4_{obs} = 3.0 & \pm 0.5 \\ x^5 = 10.000 & d^5_{obs} = 4.0 & \pm 0.5 \,, \end{array} \tag{2}$$

where ± 0.5 denotes *rounding* errors (to the nearest integer). Estimate m^1 and m^2 . (Note: this problem is nonclasical in the sense that experimental errors are not Gaussian, and the usual least squares regression is not adapted).

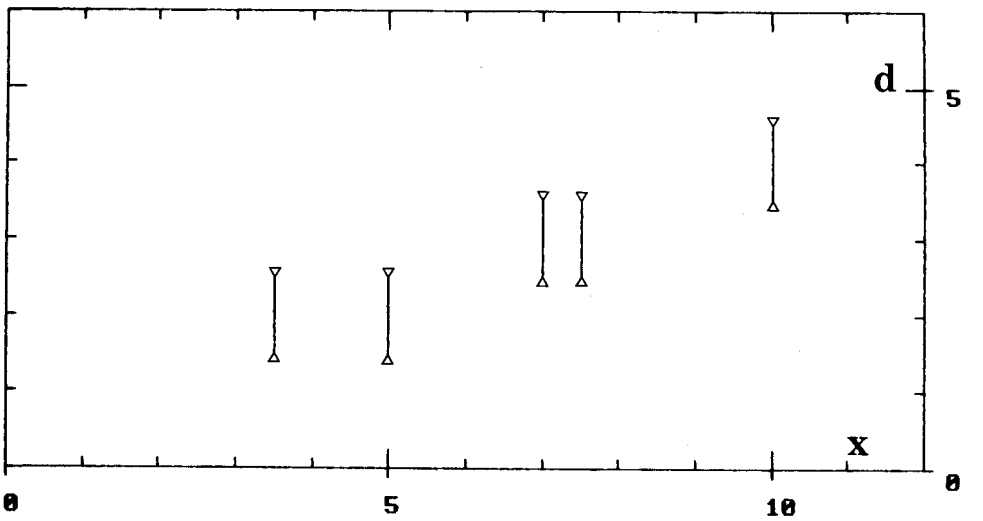


Figure 1.19: Some experimental points. Error "bars" represent *rounding* errors to the nearest integer. Solve the general problem of estimating a regression line.

Solution: Let an arbitrary set $(d^1, d^2, d^3, d^4, d^5)$ be called a data vector and be denoted by $\mathbf{d}$, let an arbitrary set (m^1, m^2) be called a parameter vector and be denoted by $\mathbf{m}$. Let

$$\mathbf{d} = \mathbf{g}(\mathbf{m}) \tag{3}$$

denote the (linear) relationship

$$\begin{aligned} d^1 &= m^1 + m^2 x^1 \\ d^2 &= m^1 + m^2 x^2 \\ d^3 &= m^1 + m^2 x^3 \\ d^4 &= m^1 + m^2 x^4 \\ d^5 &= m^1 + m^2 x^5 . \end{aligned} \tag{4}$$

Let

$$\rho_M(\mathbf{m}) = \rho_M(m^1,m^2) \tag{5}$$

be the probability density representing the a priori information (if any) on model parameters. Let

$$\rho_D(\mathbf{d}) = \rho_D(d^1,d^2,d^3,d^4,d^5) \tag{6}$$

be the probability density describing the "experimental" uncertainties (see text). As rounding errors are mutually independent,

$$\rho_D(\mathbf{d}) = \rho_D(d^1,d^2,d^3,d^4,d^5) = \rho^1{}_D(d^1)\,\rho^2{}_D(d^2)\,\rho^3{}_D(d^3)\,\rho^4{}_D(d^4)\,\rho^5{}_D(d^5)\,, \tag{7}$$

where $\rho^i_D(d^i)$ denotes the probability density describing the "experimental" uncertainty for the observed data d^i. As the errors are only rounding errors, they can be conveniently modeled using box-car probability density functions:

$$\rho^i_D(d^i) = \begin{cases} \text{const} & \text{if} \quad d^i_{obs} - 0.5 < d^i < d^i_{obs} + 0.5 \\ 0 & \text{otherwise}\,. \end{cases} \tag{8}$$

This gives

$$\rho_D(\mathbf{d}) = \begin{cases} \text{const} & \text{if} \quad \begin{cases} 1.5 < d^1 < 2.5 \\ \text{and} \\ 1.5 < d^2 < 2.5 \\ \text{and} \\ 2.5 < d^3 < 3.5 \\ \text{and} \\ 2.5 < d^4 < 3.5 \\ \text{and} \\ 3.5 < d^5 < 4.5 \end{cases} \\ 0 & \text{otherwise.} \end{cases} \tag{9}$$

The general solution of an inverse problem is obtained when the posterior probability density in the model space has been defined. It is given by equation (1.65) of the text:

$$\sigma_M(\mathbf{m}) = \rho_M(\mathbf{m}) \int_D d\mathbf{d} \; \frac{\rho_D(\mathbf{d})}{\mu_D(\mathbf{d})} \Theta(\mathbf{d}|\mathbf{m}) \,, \tag{10}$$

or more particularly, as the relationship between $\mathbf{d}$ and $\mathbf{m}$ is exact, by equation (1.69) of the text:

$$\sigma_M(\mathbf{m}) = \rho_M(\mathbf{m}) \; \frac{\rho_D(\mathbf{g}(\mathbf{m}))}{\mu_D(\mathbf{g}(\mathbf{m}))} \,, \tag{11}$$

where $\mu_D(\mathbf{d})$ represents the non-informative probability density on data parameters. Equations (9) and (11) solve the problem.

For instance, if we take as non-informative prior in the data space:

$$\mu_D(\mathbf{d}) = \mu_D(d^1,d^2,d^3,d^4,d^5) = \text{const} \,, \tag{12}$$

and if we accept a priori all pairs (m^1,m^2) as equally probable:

$$\rho_M(\mathbf{m}) = \rho_M(m^1,m^2) = \text{const} \,, \tag{13}$$

then we obtain

$$\sigma_M(\mathbf{m}) = \sigma_M(m^1,m^2) = \begin{cases} \text{const} & \text{if} \begin{cases} 1.5 < m^1 + m^2\, x^1 < 2.5 \\ \text{and} \\ 1.5 < m^1 + m^2\, x^2 < 2.5 \\ \text{and} \\ 2.5 < m^1 + m^2\, x^3 < 3.5 \\ \text{and} \\ 2.5 < m^1 + m^2\, x^4 < 3.5 \\ \text{and} \\ 3.5 < m^1 + m^2\, x^5 < 4.5 \end{cases} \\ 0 & \text{otherwise.} \end{cases} \tag{14}$$

This result is represented graphically in figure 1.20. The dark region has a positive (constant) probability density. All pairs (m^1,m^2) inside this region have equal probability density, and all pairs (m^1,m^2) outside it are impossible, so that this region represents the "domain of admissible solutions". Which is *the best* "regression line"? There is no such a thing: all lines inside the domain are equally good. Figure 1.21 shows two particular solutions (giving extremal values for m^1 and m^2).

Figure 1.22 shows the computer code effectively used for obtaining the general solution shown in Figure 1.20. For problems with few model parameters (2 in this example), the full exploration of the model space is, in general, the easiest strategy (it takes approximately 2 minutes to go from the statement of the problem to the result in figure 1.20.

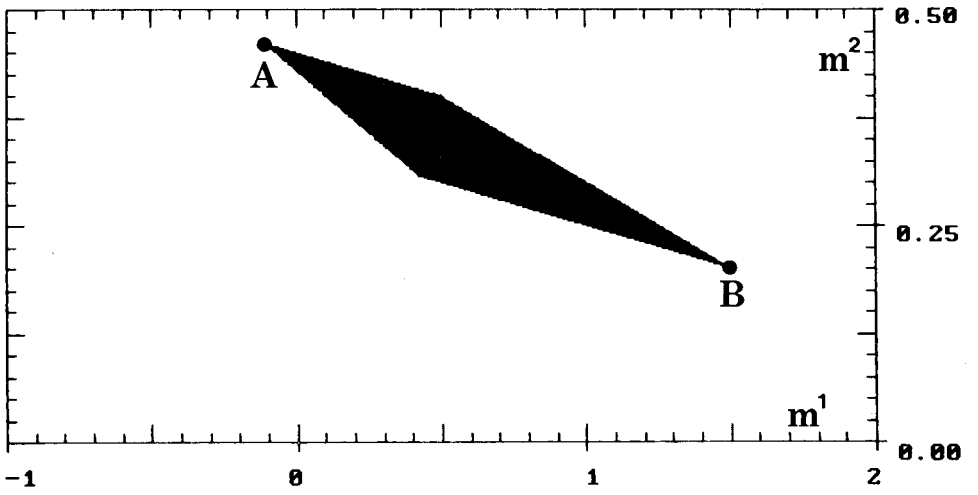


Figure 1.20: The general solution of the problem is given by the probability density $\sigma_M(m^1,m^2)$ for the parameters of the regression line. It is constant inside the dark region and null outside. The dark region represents the domain of admissible solutions. There is not any "best line": all pairs (m^1,m^2) inside the region are equally likely.

Problem 1.6 (Usual least-squares regression): Find the best regression line for the experimental points in figure 1.23, assuming Gaussian uncertainties.

Solution: Figure 1.23 suggests that errors in the t^i are negligible, while errors in the y^i are uncorrelated. Let us introduce

$$\mathbf{m} = \begin{bmatrix} a \\ b \end{bmatrix} \qquad \mathbf{d} = \begin{bmatrix} y^1 \\ y^2 \\ \cdots \\ y^n \end{bmatrix} \qquad \mathbf{G} = \begin{bmatrix} t^1 & 1 \\ t^2 & 1 \\ \cdots & \cdots \\ t^n & 1 \end{bmatrix} \tag{1}$$

($y^1,y^2,...,t^1,t^2,...$ are indexes, not powers). The equations

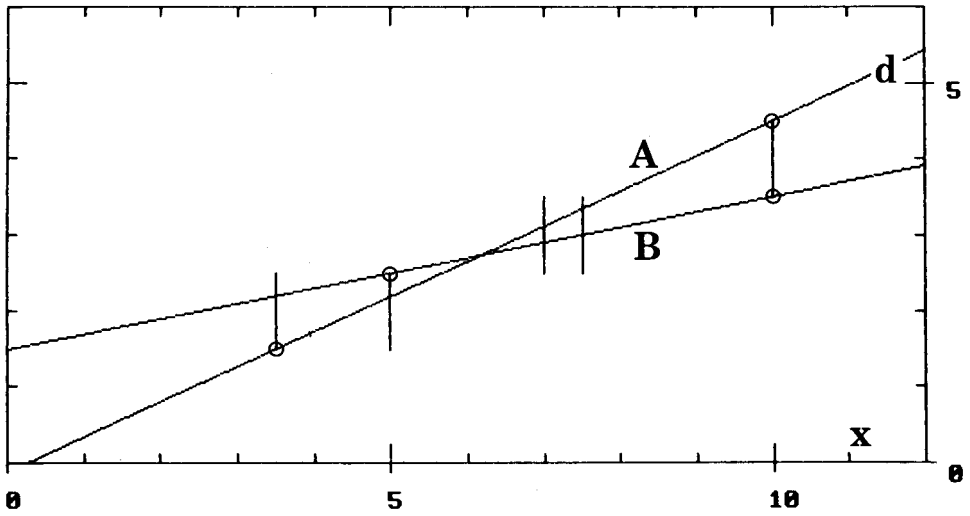


Figure 1.21: Two particular solutions (A and B in figure 1.20), corresponding to extremal values of m^1 and m^2. Notice that they touch the extremities of the error bars (circles).

$$y^1 = a\, t^i + b \qquad (i=1,2,...,n) \tag{2}$$

can be written

$$\mathbf{d} = \mathbf{G}\,\mathbf{m}\,. \tag{3}$$

The matrix $\mathbf{G}$ is assumed perfectly known. We have some information on the true values of $\mathbf{d}$, and we wish to estimate the true value of $\mathbf{m}$.

As it is assumed that errors in the y^i are uncorrelated Gaussian, the information we have on the true value of $\mathbf{d}$ can be represented using a Gaussian probability density with mathematical expectation

$$\mathbf{d}_{obs} = \begin{bmatrix} y_0^1 \\ y_0^2 \\ \cdots \\ y_0^n \end{bmatrix}, \tag{4}$$

and covariance matrix

```
110 FOR M1 = -1 TO 2 STEP .005
120 FOR M2 = 0 TO .5 STEP .002
130 D1 = M1 + 3.5 * M2
140 IF ( D1 < 1.5 ) OR ( D1 > 2.5 ) THEN GOTO 300
150 D2 = M1 + 5 * M2
160 IF ( D2 < 1.5 ) OR ( D2 > 2.5 ) THEN GOTO 300
170 D3 = M1 + 7 * M2
180 IF ( D3 < 2.5 ) OR ( D3 > 3.5 ) THEN GOTO 300
190 D4 = M1+ 7.5 * M2
200 IF ( D4 < 2.5 ) OR ( D4 > 3.5 ) THEN GOTO 300
210 D5 = M1 + 10 * M2
220 IF ( D5 < 3.5 ) OR ( D5 > 4.5 ) THEN GOTO 300
250 DRAW POINT (M1,M2)
300 NEXT M2
310 NEXT M1
```

Figure 1.22: Computer code in BASIC-like notation effectively used for obtaining the result in figure 1.20. The limits for m^1 and m^2 in lines 110-120 have been chosen after trial and error. The steps 0.005 and 0.002 in lines 110-120 have been chosen small enough not to be visible on the graphic device used to generate figure 1.20. The command DRAW POINT (X,Y) in line 250 simply plots a point on the graphic device at coordinates (X,Y).

$$\mathbf{C}_D = \begin{bmatrix} (\sigma^1)^2 & 0 & 0 & \dots \\ 0 & (\sigma^2)^2 & 0 & \dots \\ 0 & 0 & (\sigma^3)^2 & \dots \\ \dots & \dots & \dots & \dots \end{bmatrix} . \tag{5}$$

We now need to introduce the a priori information (if any) on the parameters $\mathbf{m}$. The simplest results are obtained when using a Gaussian probability density in the model space with mathematical expectation

$$\mathbf{m}_{prior} = \begin{bmatrix} a_0 \\ b_0 \end{bmatrix} , \tag{6}$$

and covariance matrix

$$\mathbf{C}_M = \begin{bmatrix} \sigma^2_a & \rho\, \sigma_a\, \sigma_b \\ \rho\, \sigma_a\, \sigma_b & \sigma^2_b \end{bmatrix} . \tag{7}$$

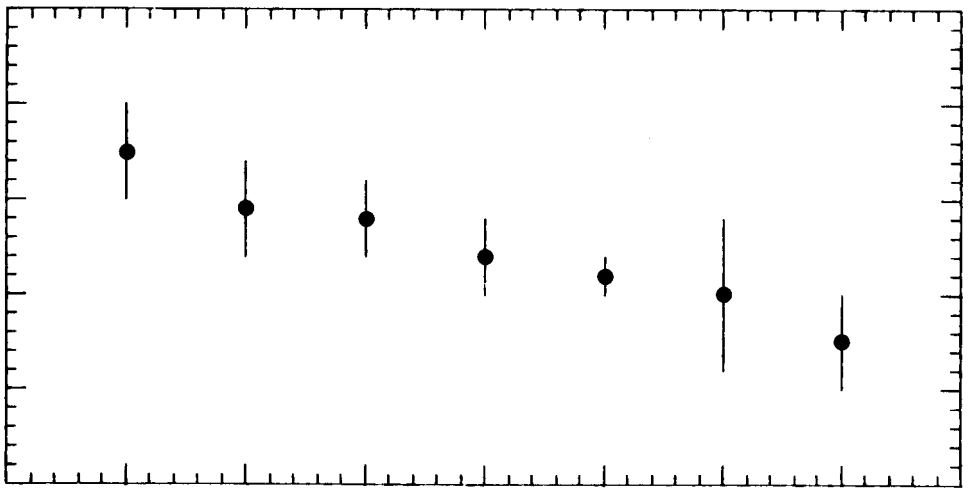


Figure 1.23: The physical parameter y (ordinate) is related with the physical parameter t (abscissa) through the equation $y = a\,t + b$, where the parameters a and b are unknown. The experimental points in the figure have to be used to estimate the best values for a and b, in the least squares sense.

As the information on both data and model parameters is Gaussian, we are in the hypothesis of section (1.7.1). The a posteriori information on the model parameters is then also Gaussian, with mathematical expectation given by

$$\mathbf{m}_{post} = \mathbf{m}_{prior} + \left(\mathbf{G}^t \mathbf{C}_D^{-1} \mathbf{G} + \mathbf{C}_M^{-1} \right)^{-1} \mathbf{G}^t \mathbf{C}_D^{-1} (\mathbf{d}_{obs} - \mathbf{G}\,\mathbf{m}_{prior}) \qquad (8)$$

$$= \mathbf{m}_{prior} + \mathbf{C}_M \mathbf{G}^t (\mathbf{G}\,\mathbf{C}_M\,\mathbf{G}^t + \mathbf{C}_D)^{-1} (\mathbf{d}_{obs} - \mathbf{G}\,\mathbf{m}_{prior}) , \qquad (9)$$

and covariance matrix given by

$$\mathbf{C}_{M'} = \left(\mathbf{G}^t \mathbf{C}_D^{-1} \mathbf{G} + \mathbf{C}_M^{-1} \right)^{-1} \qquad (10)$$

$$= \mathbf{C}_M - \mathbf{C}_M \mathbf{G}^t (\mathbf{G}\,\mathbf{C}_M\,\mathbf{G}^t + \mathbf{C}_D)^{-1} \mathbf{G}\,\mathbf{C}_M . \qquad (11)$$

The a posteriori (i.e., recalculated) data values are then (equation 1.97a)

$$\mathbf{d}_{post} = \mathbf{G}\,\mathbf{m}_{post} , \tag{12}$$

and the a posteriori data errors are given by (equation 1.97b)

$$\mathbf{C}_{D'} = \mathbf{G}\,\mathbf{C}_{M'}\,\mathbf{G}^t . \tag{13}$$

As we have only two model parameters, expressions (8) and (10) should be preferred to (9) and (11). An easy computation gives the a posteriori values of a and b :

$$a = a_0 + \frac{A\,P - C\,Q}{A\,B - C^2} \tag{14}$$

$$b = b_0 + \frac{B\,Q - C\,P}{A\,B - C^2} , \tag{15}$$

and the posteriori standard deviations and correlation:

$$\sigma_{a'} = \frac{1}{\sqrt{B - C^2/A}} , \tag{16a}$$

$$\sigma_{b'} = \frac{1}{\sqrt{A - C^2/B}} , \tag{16b}$$

$$\rho' = \frac{-1}{\sqrt{AB/C^2}} , \tag{16c}$$

where

$$A = \sum_i \frac{1}{(\sigma^i)^2} + \frac{1}{(1-\rho^2)\,\sigma_b{}^2} , \tag{17a}$$

$$B = \sum_i \frac{(t^i)^2}{(\sigma^i)^2} + \frac{1}{(1-\rho^2)\,\sigma_a{}^2} , \tag{17b}$$

$$C = \sum_i \frac{t^i}{(\sigma^i)^2} - \frac{\rho}{(1-\rho^2)\,\sigma_a\,\sigma_b} , \tag{17c}$$

$$P = \sum_i \frac{t^i}{(\sigma^i)^2} [y_0{}^i - (a_0\,t^i + b_0)] , \tag{17d}$$

and

$$Q = \sum_i \frac{1}{(\sigma^i)^2} [y_0^i - (a_0 t^i + b_0)] . \tag{17e}$$

Usually, a priori errors on model parameters are uncorrelated. Then

$$\rho = 0 . \tag{18}$$

This gives

$$A = \sum_i \frac{1}{(\sigma^i)^2} + \frac{1}{\sigma_b^2} , \tag{19a}$$

$$B = \sum_i \frac{(t^i)^2}{(\sigma^i)^2} + \frac{1}{\sigma_a^2} , \tag{19b}$$

and

$$C = \sum_i \frac{t^i}{(\sigma^i)^2} . \tag{19c}$$

If there is no a priori information on model parameters,

$$\sigma_a \rightarrow \infty \tag{20}$$

and

$$\sigma_b \rightarrow \infty . \tag{21}$$

Instead of taking the limits (20)-(21) in the last equations, it is simpler to use

$$\mathbf{C_M}^{-1} = \mathbf{0} \tag{22}$$

in equations (8) and (10). This gives

$$\mathbf{m_{post}} = \left[\mathbf{G}^t \mathbf{C_D}^{-1} \mathbf{G}\right]^{-1} \mathbf{G}^t \mathbf{C_D}^{-1} \mathbf{d_{obs}} \tag{23}$$

and

$$\mathbf{C_{M'}} = \left[\mathbf{G}^t \mathbf{C_D}^{-1} \mathbf{G}\right]^{-1} . \tag{24}$$

Equations (14) and (15) then become

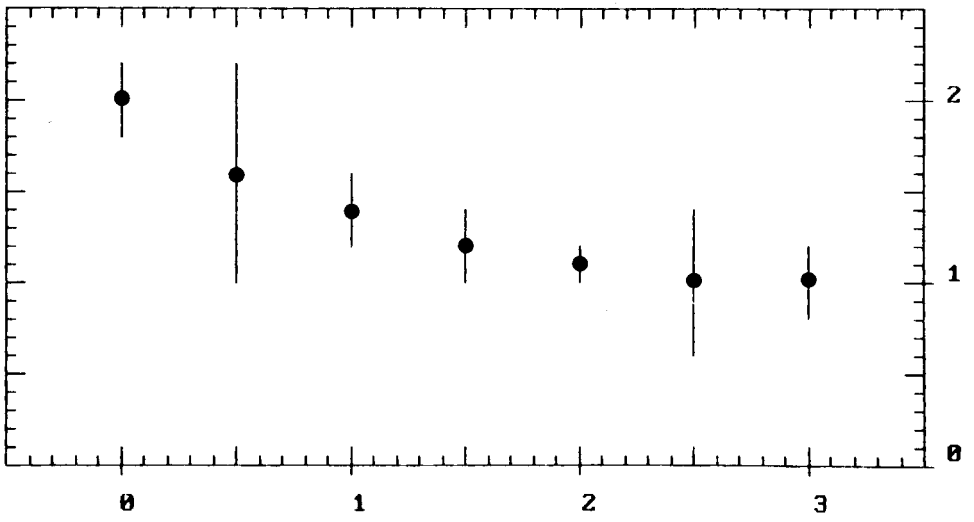


Figure 1.24: See text.

$$a = \frac{A\,P - C\,Q}{A\,B - C^2} \tag{25}$$

and

$$b = \frac{B\,Q - C\,P}{A\,B - C^2}\,, \tag{26}$$

while the constants A , B , C , P , and Q simplify to

$$A = \sum_i \frac{1}{(\sigma^i)^2} \qquad B = \sum_i \frac{(t^i)^2}{(\sigma^i)^2} \qquad C = \sum_i \frac{t^i}{(\sigma^i)^2}$$

$$P = \sum_i \frac{t^i\, y_0{}^i}{(\sigma^i)^2} \qquad Q = \sum_i \frac{y_0{}^i}{(\sigma^i)^2}\,. \tag{27}$$

If all data uncertainties are identical,

$$\sigma^i = \sigma\,, \tag{28}$$

then

$$A = \frac{n}{\sigma^2} \qquad B = \frac{1}{\sigma^2} \sum_i (t^i)^2 \qquad C = \frac{1}{\sigma^2} \sum_i t^i$$

$$P = \frac{1}{\sigma^2} \sum_i t^i \, y_0^i \qquad Q = \frac{1}{\sigma^2} \sum_i y_0^i \, . \tag{29}$$

Problem 1.7: The two variables y and t are related through the parabolic relationship

$$y = a\, t^2 + b\, t + c \, . \tag{1}$$

The points (y^i, t^i) shown in Figure 1.24 have been obtained experimentally. Error bars denote Gaussian errors. Estimate the parameters a, b, and c, and analyze uncertainties.

Answer the same question if the assumed relationship between y and t is

$$y = a\, e^{-bt} + c \, . \tag{2}$$

Problem 1.8 (Two-axes least-squares regression): Find the best regression line for the experimental points in figure 1.25, assuming Gaussian uncertainties.

Solution: There are some equivalent ways of properly setting this problem. The approach followed here has the advantage of giving a symmetrical treatment to both axes.

As the statement of the problem refers to a regression *line*, a linear relationship has to be assumed between the variables y and t :

$$\alpha\, y + \beta\, t = 1 \, . \tag{1}$$

We have measured some pairs (x^i, y^i) and wish to estimate the true values of α and β .

I introduce a parameter vector $\mathbf{m}$ which contains the y^i , the t^i , α , and β :

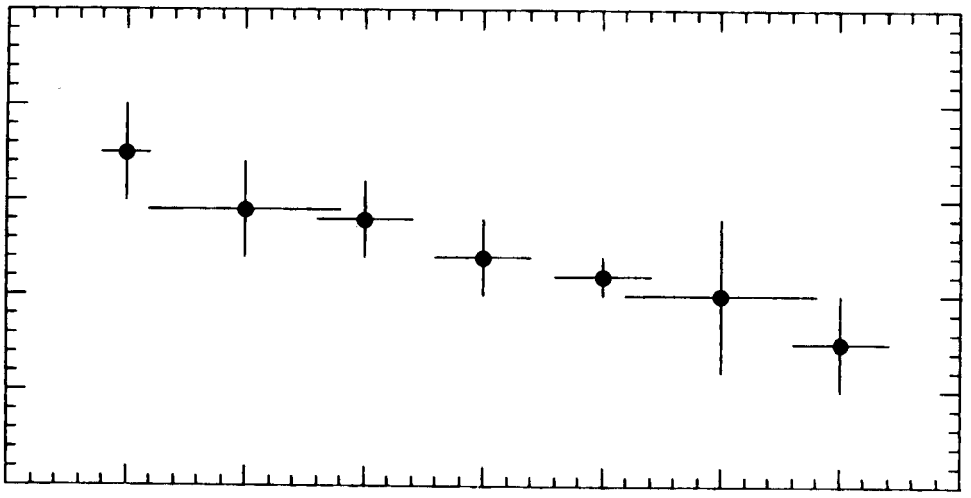


Figure 1.25: The physical parameter y (ordinate) is related to the physical parameter t (abscissa) through the equation $y = a\,t + b$, where the parameters a and b are unknown. The experimental points in the figure have to be used to estimate the best values for a and b, in the least squares sense. This problem is nonclassical in the sense that uncertainties are present in both coordinates.

$$\mathbf{m} = \begin{bmatrix} \mathbf{y} \\ \mathbf{t} \\ \mathbf{u} \end{bmatrix} = \begin{bmatrix} y^1 \\ y^2 \\ \cdots \\ t^1 \\ t^2 \\ \cdots \\ \alpha \\ \beta \end{bmatrix}, \tag{2}$$

and, for each conceivable value of $\mathbf{m}$, I define a vector

$$\mathbf{d} = \begin{bmatrix} d^1 \\ d^2 \\ \cdots \end{bmatrix} \tag{3}$$

by

$$d^i = g^i(\mathbf{m}) = \alpha\, y^i + \beta\, t^i \qquad (i=1,2,...) \,. \tag{4}$$

Defining the "observed value" of $\mathbf{d}$ by

$$\mathbf{d}_{obs} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ \dots \end{bmatrix}, \tag{5}$$

and the "a priori" value of $\mathbf{m}$ by

$$\mathbf{m}_{prior} = \begin{bmatrix} y^1{}_0 \\ y^2{}_0 \\ \dots \\ t^1{}_0 \\ t^2{}_0 \\ \dots \\ \alpha_0 \\ \beta_0 \end{bmatrix}, \tag{6}$$

where $\mathbf{y}_0$ and $\mathbf{t}_0$ are the experimental values, and α_0 and β_0 the a priori values of α and β, the inverse problem can now be set as the problem of obtaining a vector $\mathbf{m}$ such that $\mathbf{g}(\mathbf{m})$ is close (or identical) to $\mathbf{d}_{obs}$, and such that $\mathbf{m}$ is close to $\mathbf{m}_{prior}$. We see thus that this "relabeling" of the variables allows an immediate use of the standard equations. Nevertheless, this problem is less simple than the previous problem of one-axis regression, because here we have twice the number of points + 2 "unknowns" instead of 2, and the forward equation $\mathbf{d} = \mathbf{g}(\mathbf{m})$ is nonlinear (because it contains the mutual product of parameters).

More precisely, I assume that the a priori information on $\mathbf{m}$ can be described using a Gaussian probability density with mathematical expectation $\mathbf{m}_{prior}$ and covariance matrix

$$\mathbf{C}_M = \begin{bmatrix} \mathbf{C}_y & \mathbf{0} & 0 & 0 \\ \mathbf{0} & \mathbf{C}_t & 0 & 0 \\ 0 & 0 & \sigma^2{}_\alpha & 0 \\ 0 & 0 & 0 & \sigma^2{}_\beta \end{bmatrix}, \tag{7}$$

where independence of errors has been assumed only to simplify the notations. The a priori information on $\mathbf{d}$ is also assumed to be Gaussian, with mathematical expectation $\mathbf{d}_{obs}$ and covariance matrix $\mathbf{C}_D$. Later, we may take $\mathbf{C}_D = \mathbf{0}$, so that the observed values (5) may be fitted exactly by the a posteriori solution. Instead, we may keep $\mathbf{C}_D$ finite to allow for errors in the hypothesis of a strictly linear relationship between y and t.

Now we are exactly in the hypothesis of section 1.7.1. The a posteriori probability density for $\mathbf{m}$ is (equation 1.85):

$$\sigma_M(\mathbf{m}) = \text{const.} \cdot \exp\left[-\frac{1}{2}\left[(\mathbf{g}(\mathbf{m})-\mathbf{d}_{obs})^t\, \mathbf{C}_D^{-1}\, (\mathbf{g}(\mathbf{m})-\mathbf{d}_{obs}) + (\mathbf{m}-\mathbf{m}_{prior})^t\, \mathbf{C}_M^{-1}\, (\mathbf{m}-\mathbf{m}_{prior})\right]\right], \tag{8}$$

which, owing to the nonlinearity of $\mathbf{g}(\mathbf{m})$, is not Gaussian. The maximum likelihood value of $\mathbf{m}$ can be obtained using, for instance, the iterative algorithm suggested in equation (1.107):

$$\mathbf{m}_{n+1} = \mathbf{m}_{prior} - \mathbf{C}_M\, \mathbf{G}_n^t\, (\mathbf{G}_n\, \mathbf{C}_M\, \mathbf{G}_n^t + \mathbf{C}_D)^{-1}\, [(\mathbf{g}(\mathbf{m}_n)-\mathbf{d}_{obs}) - \mathbf{G}_n\, (\mathbf{m}_n-\mathbf{m}_{prior})]\,. \tag{9}$$

We have

$$\mathbf{G}_n = \left[\left(\frac{\partial \mathbf{g}}{\partial y}\right)_{\mathbf{m}_n} \quad \left(\frac{\partial \mathbf{g}}{\partial t}\right)_{\mathbf{m}_n} \quad \left(\frac{\partial \mathbf{g}}{\partial \alpha}\right)_{\mathbf{m}_n} \quad \left(\frac{\partial \mathbf{g}}{\partial \beta}\right)_{\mathbf{m}_n}\right], \tag{10}$$

which gives

$$\mathbf{G}_n = [\, \alpha_n \mathbf{I} \quad \beta_n \mathbf{I} \quad \mathbf{y}_n \quad \mathbf{t}_n \,], \tag{11}$$

$$\mathbf{C}_M\, \mathbf{G}_n^t = \begin{bmatrix} \alpha_n \mathbf{C}_y \\ \beta_{n_2} \mathbf{C}_t \\ \sigma_{a_2}\, \mathbf{y}_n^t \\ \sigma_\beta\, \mathbf{t}_n^t \end{bmatrix}, \tag{12}$$

$$\mathbf{G}_n\, \mathbf{C}_M\, \mathbf{G}_n^t + \mathbf{C}_D = \sigma_a^2\, \mathbf{y}_n\, \mathbf{y}_n^t + \sigma_b^2\, \mathbf{t}_n\, \mathbf{t}_n^t + \alpha_n^2\, \mathbf{C}_y + \beta_n^2\, \mathbf{C}_t + \mathbf{C}_D\,, \tag{13}$$

and

$$\mathbf{g}(\mathbf{m}_n)-\mathbf{d}_{obs} - \mathbf{G}_n\, (\mathbf{m}_n-\mathbf{m}_{prior}) = (\alpha_0-\alpha_n)\, \mathbf{y}_n + (\beta_0-\beta_n)\, \mathbf{t}_n - \mathbf{d}_{obs} + \alpha_n\, \mathbf{y}_0 + \beta_n\, \mathbf{t}_0\,. \tag{14}$$

Denoting

$$\delta\hat{\mathbf{d}}_n = (\, \mathbf{G}_n\, \mathbf{C}_M\, \mathbf{G}_n^t + \mathbf{C}_D)^{-1}\, [\, (\mathbf{g}(\mathbf{m}_n)-\mathbf{d}_{obs}) - \mathbf{G}_n\, (\mathbf{m}_n-\mathbf{m}_{prior})], \tag{15}$$

the iterative algorithm (9) can be written

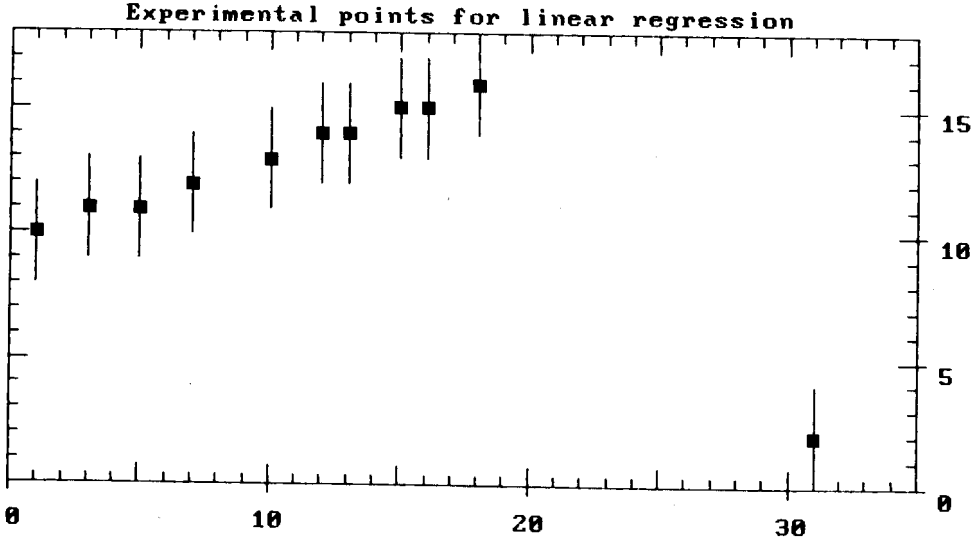


Figure 1.26: Two variables y (ordinate) and t (abscissa) are related by the relationship $y = a\,t + b$, where a and b are unknown parameters. In order to estimate a and b, an experiment has been performed which has furnished the 11 experimental points shown in the figure. The exact meaning of the "error bars" is not indicated.

$$\mathbf{y}_{n+1} = \mathbf{y}_0 - \alpha_n \, \mathbf{C}_y \, \delta\hat{\mathbf{d}}_n \,, \tag{16a}$$

$$\mathbf{t}_{n+1} = \mathbf{t}_0 - \beta_n \, \mathbf{C}_t \, \delta\hat{\mathbf{d}}_n \,, \tag{16b}$$

$$\alpha_{n+1} = \alpha_0 - \sigma_\alpha^{\,2} \, \mathbf{y}_n^{\,t} \, \delta\hat{\mathbf{d}}_n \,, \tag{16c}$$

and

$$\beta_{n+1} = \beta_0 - \sigma_\beta^{\,2} \, \mathbf{t}_n^{\,t} \, \delta\hat{\mathbf{d}}_n \,. \tag{16d}$$

The algorithm usually converges in a few iterations ($\simeq 3$). The values α_∞ and β_∞ are the estimated values of the parameters defining the regression

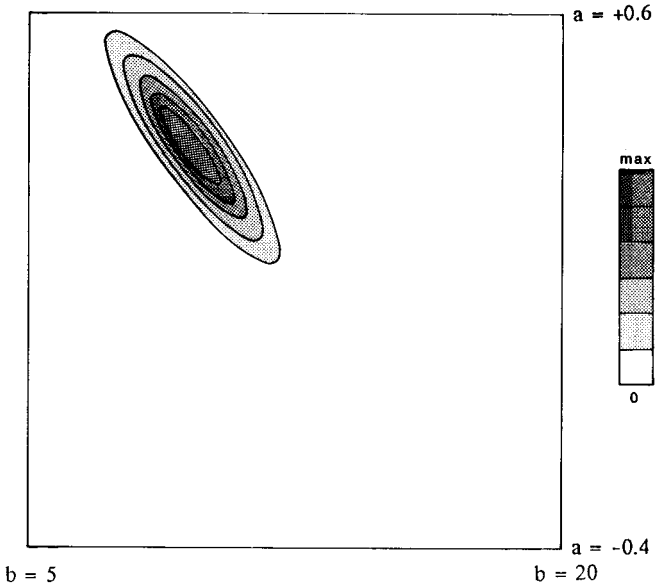


Figure 1.27: The probability density for the parameters (a,b) obtained using the Gaussian hypothesis for experimental uncertainties, and without using the blunder.

line, and the values (t^i_∞, y^i_∞) (i=1,2,...) are the a posteriori values of the experimental points. If $\mathbf{C_D} = \mathbf{0}$, the a posteriori points belong to the straight line.

Problem 1.9: Two variables y and t are related through a linear relationship

$$y = a\,t + b\,. \qquad (1)$$

In order to estimate the parameters a and b, the 11 experimental points (y^i, t^i) shown in Figure 1.26 have been obtained.

It is clear that if the linear relationship (1) applies, then the point indicated with an arrow must be an outlier. Suppress that point and solve the problem of estimating a and b, under the hypothesis of Gaussian errors. Does the solution change very much if the outlier is included?

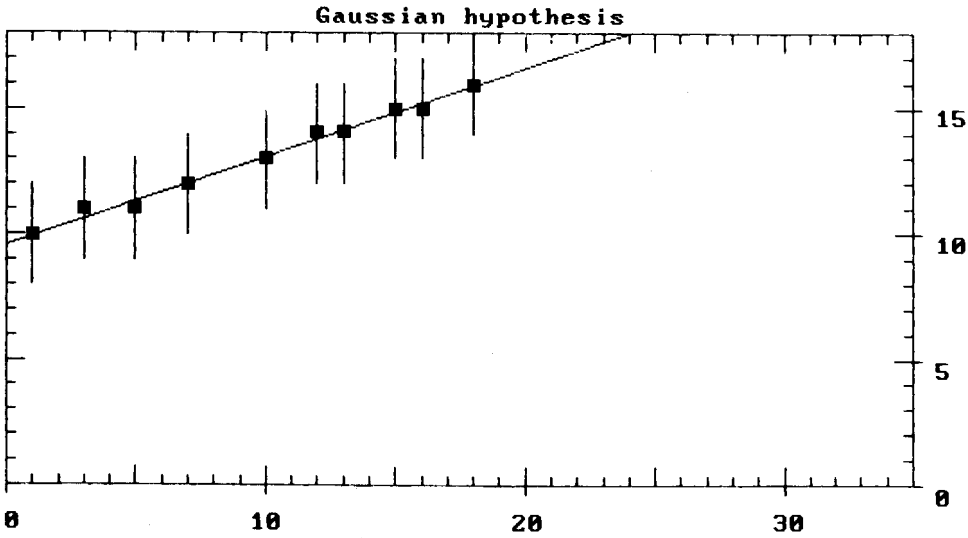


Figure 1.28: The maximum likelihood line for the probability density in figure 1.27.

Assume now that errors can be modeled using an exponential probability density, and solve the problem again. Discuss the relative robustness of the Gaussian and exponential hypotheses with respect to the existence of outliers on a data set.

Solution: Let

$$\mathbf{m} = (a,b) \tag{2}$$

denote a model vector, and

$$\mathbf{d} = (d^1,d^2,...) \tag{3}$$

a data vector. The (exact) theoretical relationship between $\mathbf{d}$ and $\mathbf{m}$ is linear:

$$d^i = a\, t^i + b\,, \tag{4a}$$

or, for short,

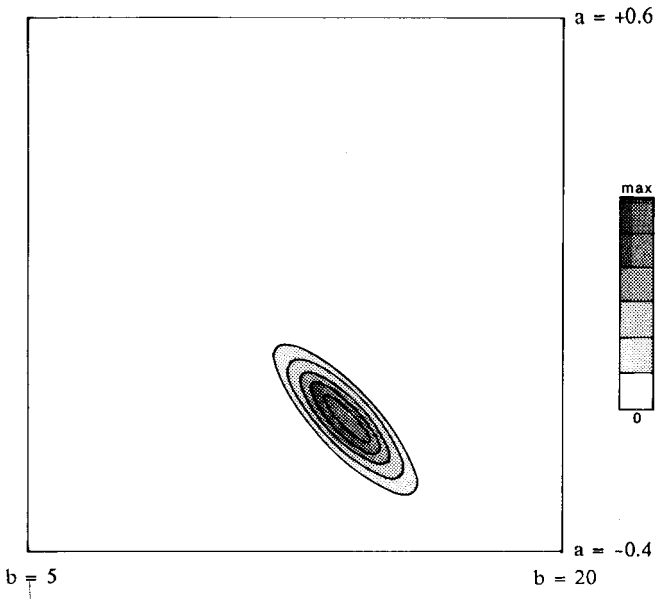


Figure 1.29: Same as Figure 1.27, but the 11 experimental points have been used. The blunder has "translated" the probability density. This shows that the Gaussian hypothesis is not very robust with respect to the existence of a small number of blunders in a data set.

$$\mathbf{d} = \mathbf{G}\,\mathbf{m}\ , \tag{4b}$$

where $\mathbf{G}$ is a linear operator.

Assume that the null information probability density on model parameters is

$$\mu_M(a,b) = \text{const}\ , \tag{5}$$

and that we do not have a priori information on model parameters:

$$\rho_M(a,b) = \mu_M(a,b) = \text{const.}\ . \tag{6}$$

Assume that the null information probability density on data parameters is

$$\mu_D(d^1,d^2,...) = \text{const}\ . \tag{7}$$

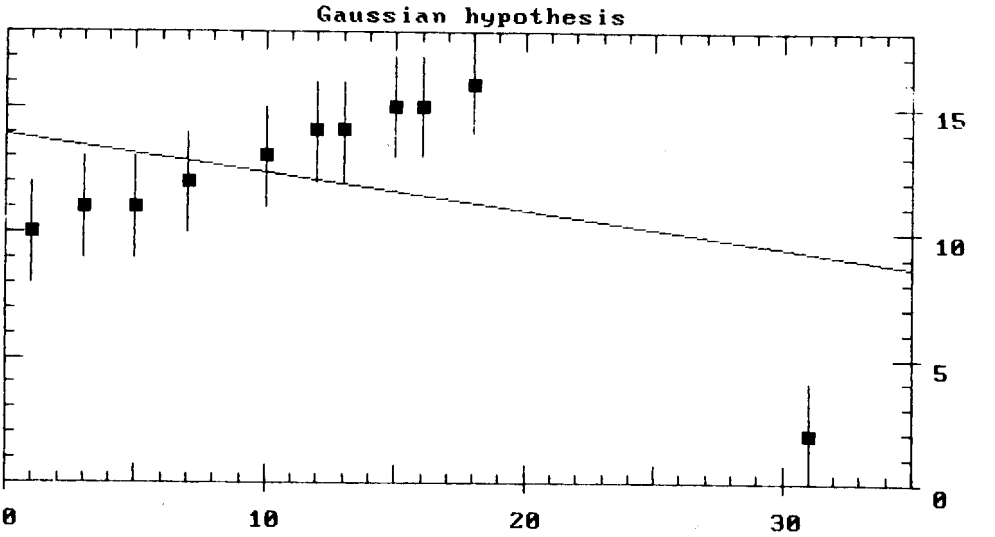


Figure 1.30: The maximum likelihood line for the probability density in figure 1.29.

If $\rho_D(d^1,d^2,...)$ is the probability density representing the information on the true values of $(d^1,d^2,...)$ as obtained through the measurements, then the Gaussian hypothesis gives (for independent uncertainties)

$$\rho_D(d^1,d^2,...) = \exp\left(-\frac{1}{2} \sum_i \frac{\left(d^i - d^i_{obs} \right)^2}{\sigma^2} \right), \tag{8}$$

where $\mathbf{d}_{obs}$ is the vector of observed values

$$\mathbf{d}_{obs} = (10. , 11. , 11. , 12. , 13. , 14. , 14. , 15. , 15. , 16. , 2.) , \tag{9}$$

and where, if we interpret the error bars in Figure 1 as standard deviations,

$$\sigma = 2. \tag{10}$$

Let $\theta(\mathbf{d},\mathbf{m})$ be the probability density representing the information we have on the theoretical relationship between $\mathbf{d}$ and $\mathbf{m}$. As (4) is an exact relationship

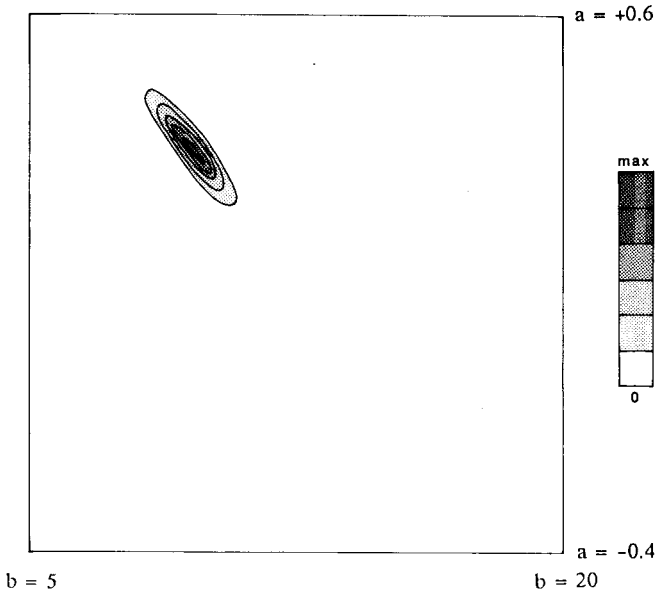


Figure 1.31: The exponential hypothesis for data uncertainties has been used instead of the Gaussian hypothesis. Here the blunder has not been used. The solution looks similar to the solution corresponding to the Gaussian hypothesis in Figure 1.27.

$$\theta(\mathbf{d},\mathbf{m}) = \theta(\mathbf{d}|\mathbf{m})\, \mu_M(\mathbf{m}) = \delta(\mathbf{d}-\mathbf{G}\,\mathbf{m})\, \mu_M(\mathbf{m}) \,. \tag{11}$$

The posterior information on the parameters $(\mathbf{d},\mathbf{m})$ is given by (equation 1.60)

$$\sigma(\mathbf{d},\mathbf{m}) = \frac{\rho(\mathbf{d},\mathbf{m})\, \theta(\mathbf{d},\mathbf{m})}{\mu(\mathbf{d},\mathbf{m})} = \frac{\rho_D(\mathbf{d})\, \rho_M(\mathbf{m})}{\mu_D(\mathbf{d})}\, \theta(\mathbf{d}|\mathbf{m}) \,, \tag{12}$$

and the posterior information on model parameters alone is given by the marginal probability density

$$\sigma_M(\mathbf{m}) = \int_D \mathrm{d}\mathbf{d}\ \sigma(\mathbf{d},\mathbf{m}) \,. \tag{13}$$

Using (4), (6), (7), (8), and (11) easily gives

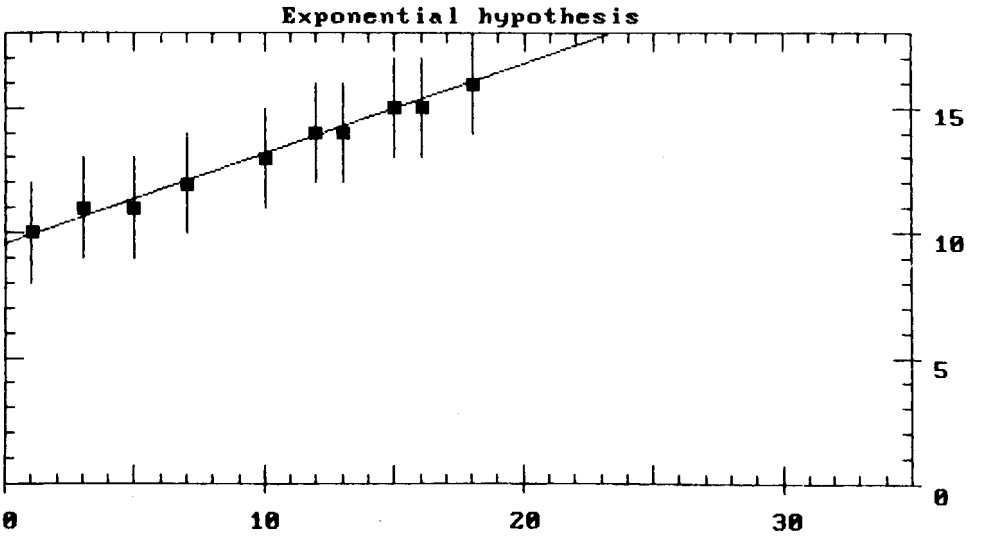


Figure 1.32: The maximum likelihood line for the probability density in Figure 1.31.

$$\sigma_M(a,b) = \exp\left(-\frac{1}{2} \sum_i \frac{\left(d^i_{obs} - d^i_{cal}(a,b) \right)^2}{\sigma^2} \right), \qquad (14)$$

where

$$d^i_{cal}(a,b) = a\, t^i + b\,. \qquad (15)$$

As this problem only has two model parameters, the simplest way to analyze the a posteriori information we have on model parameters is to directly compute the values $\sigma_M(a,b)$ in a given grid, and to plot the results. Figure 1.27 shows the corresponding result, if the outlier is suppressed from the data set (only 10 points have been used). This probability density is Gaussian, and the line corresponding to its center is shown in Figure 1.28. If the outlier is not suppressed, so that the 11 points are used, the probability density $\sigma_M(a,b)$ obtained is shown in figure 1.29. The probability density has been essentially "translated" by the outlier. The line corresponding to the

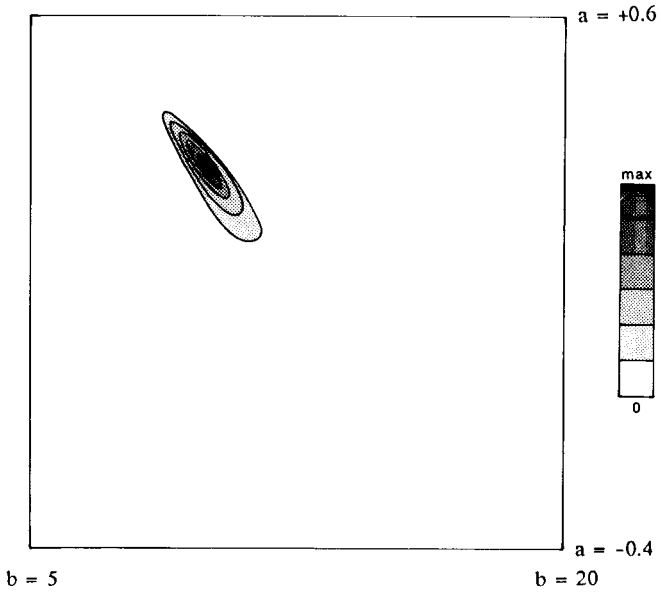


Figure 1.33: The probability density using all 11 experimental points in the exponential hypothesis. By comparison with Figure 1.31, we see that the introduction of the blunder does not completely distort the solution. This shows that the exponential hypothesis is more robust than the Gaussian hypothesis with respect to the existence of a few blunders in a data set.

center of the probability density is shown in figure 1.30. Figures 1.29 and 1.30 show that the Gaussian assumption gives results which are not robust with respect to the existence of outliers in a data set. This may be annoying, because in multidimensional problems it is not always easy to detect outliers.

If instead of assuming uncorrelated Gaussian, we assume uncorrelated exponential uncertainties, equation (8) is replaced by

$$\rho_D(d^1,d^2,\ldots) = \exp\left(- \sum_i \frac{\left| d^i - d^i_{obs} \right|}{\sigma} \right) . \qquad (16)$$

The a posteriori probability density is then

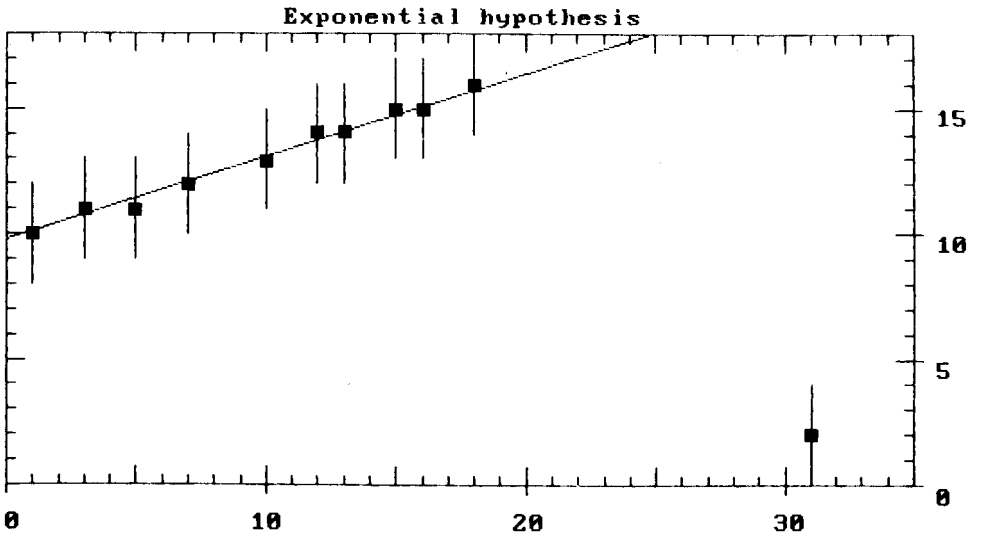


Figure 1.34: The maximum likelihood line for the probability density in Figure 1.33.

$$\sigma_M(a,b) = \exp\left(- \sum_i \frac{\left| d^i_{obs} - d^i_{cal}(a,b) \right|}{\sigma} \right) . \qquad (17)$$

This probability density is shown in Figure 1.31 for all points but the outlier, and in Figure 1.33 for all 11 points. The corresponding maximum likelihood lines are shown in Figures 1.32 and 1.34. We see that the introduction of the outlier "deforms" the posterior probability density, but it does not "translate" it. The exponential hypothesis for data uncertainties is more robust than the Gaussian hypothesis.

It should be noticed that the question of which probability density may truly represent the experimental uncertainties for the data in Figure 1.26 has not been adressed. Obviously, it is not Gaussian, because the probability of a outlier like the one present in the figure is extremely low. But the probability of such an outlier is also very low in the exponential hypothesis. A careful examination of the experimental conditions can, in principle, suggest a realistic choice of probability density for representing uncertainties, but this is not always easy. The conclusion of this numerical example is that if a pro-

bability density adequately representing experimental uncertainties is unknown, but we suspect a small number of large errors, we should not take the Gaussian probability density, but a more long-tailed one.

Problem 1.10: Condition number and a posteriori errors. The (Cramer's) solution of the system

$$\begin{bmatrix} 10 & 7 & 8 & 7 \\ 7 & 5 & 6 & 5 \\ 8 & 6 & 10 & 9 \\ 7 & 5 & 9 & 10 \end{bmatrix} \begin{bmatrix} m^1 \\ m^2 \\ m^3 \\ m^4 \end{bmatrix} = \begin{bmatrix} 32.0 \\ 23.0 \\ 33.0 \\ 31.0 \end{bmatrix} \tag{1}$$

is

$$\begin{bmatrix} m^1 \\ m^2 \\ m^3 \\ m^4 \end{bmatrix} = \begin{bmatrix} 1.0 \\ 1.0 \\ 1.0 \\ 1.0 \end{bmatrix}, \tag{2}$$

while the solution of the system

$$\begin{bmatrix} 10 & 7 & 8 & 7 \\ 7 & 5 & 6 & 5 \\ 8 & 6 & 10 & 9 \\ 7 & 5 & 9 & 10 \end{bmatrix} \begin{bmatrix} m^1 \\ m^2 \\ m^3 \\ m^4 \end{bmatrix} = \begin{bmatrix} 32.1 \\ 22.9 \\ 33.1 \\ 30.9 \end{bmatrix}, \tag{3}$$

where the right hand member has been slightly modified, is completely different:

$$\begin{bmatrix} m^1 \\ m^2 \\ m^3 \\ m^4 \end{bmatrix} = \begin{bmatrix} 9.2 \\ -12.6 \\ 4.5 \\ -1.1 \end{bmatrix}. \tag{4}$$

This result may be surprising, because the determinant of the matrix of the system is not "small" (it equals one), and the inverse matrix looks as ordinary as the original one:

$$\begin{bmatrix} 10 & 7 & 8 & 7 \\ 7 & 5 & 6 & 5 \\ 8 & 6 & 10 & 9 \\ 7 & 5 & 9 & 10 \end{bmatrix}^{-1} = \begin{bmatrix} 25 & -41 & 10 & -6 \\ -41 & 68 & -17 & 10 \\ 10 & -17 & 5 & -3 \\ -6 & 10 & -3 & 2 \end{bmatrix} . \tag{5}$$

This nice example is due to R.S. Wilson, and is quoted by Ciarlet (1982). Clearly, the matrix in the example has some special property, which it is important to identify. In classical numerical analysis it is usual to introduce the concept of "condition number" of a matrix. It is defined by

$$\text{cond}(\mathbf{A}) = \| \mathbf{A} \| \, \| \mathbf{A}^{-1} \| , \tag{6}$$

where $\| \mathbf{A} \|$ denotes a given matricial norm. For instance, the ℓ_p matricial norms can be defined by

$$\| \mathbf{A} \|_1 = \sup \frac{\| \mathbf{A v} \|_1}{\| \mathbf{v} \|_1} , \tag{7a}$$

$$\| \mathbf{A} \|_2 = \sup \frac{\| \mathbf{A v} \|_2}{\| \mathbf{v} \|_2} , \tag{7b}$$

$$\| \mathbf{A} \|_\infty = \sup \frac{\| \mathbf{A v} \|_\infty}{\| \mathbf{v} \|_\infty} , \tag{7c}$$

and verify (e.g. Ciarlet, 1982):

$$\| \mathbf{A} \|_1 = \max \sum_i | A^{ij} | , \tag{8a}$$

$$\| \mathbf{A} \|_2 = \sqrt{\max \lambda_i(\mathbf{A}^* \mathbf{A})} , \tag{8b}$$

$$\| \mathbf{A} \|_\infty = \max \sum_j | A^{ij} | , \tag{8c}$$

where $\lambda_i(\mathbf{B})$ denotes the eigenvalues of the matrix $\mathbf{B}$, and where $\mathbf{A}^*$ denotes the adjoint of $\mathbf{A}$ (in chapter 4 the difference between adjoint and transpose will be explained; for the while, let us simply admit that we only consider euclidean scalar products, and adjoint and transpose coincide).

The interpretation of the condition number is obtained as follows. Let $\mathbf{A}$ and $\mathbf{d}$ respectively represent a given regular matrix and a given vector, and let $\mathbf{m}$ represent the solution of

$$\mathbf{A m} = \mathbf{d} , \tag{9}$$

i.e.,

$$\mathbf{m} = \mathbf{A}^{-1}\,\mathbf{d} \quad . \tag{10}$$

Let now $\mathbf{m} + \delta\mathbf{m}$ represent the solution of the "perturbed system"

$$\mathbf{A}\,(\,\mathbf{m} + \delta\mathbf{m}\,) = \mathbf{d} + \delta\mathbf{d} \quad . \tag{11}$$

From $\mathbf{d} = \mathbf{A}\,\mathbf{m}$ and $\delta\mathbf{m} = \mathbf{A}^{-1}\,\delta\mathbf{d}$ it can be deduced that

$$\| \mathbf{d} \| \leq \| \mathbf{A} \| \; \| \mathbf{m} \| \tag{12a}$$

$$\| \delta\mathbf{m} \| \leq \| \mathbf{A}^{-1} \| \; \| \delta\mathbf{d} \| \quad , \tag{12b}$$

i.e.,

$$\frac{\| \delta\mathbf{m} \|}{\| \mathbf{m} \|} \leq \| \mathbf{A} \| \; \| \mathbf{A}^{-1} \| \; \frac{\| \delta\mathbf{d} \|}{\| \mathbf{d} \|} \quad , \tag{13}$$

which, using the definition of condition number, can be written

$$\frac{\| \delta\mathbf{m} \|}{\| \mathbf{m} \|} \leq \mathrm{cond}(\,\mathbf{A}\,) \; \frac{\| \delta\mathbf{d} \|}{\| \mathbf{d} \|} \quad . \tag{14}$$

This shows that for given "relative data error" $\| \delta\mathbf{d} \| / \| \mathbf{d} \|$, the "relative solution error" $\| \delta\mathbf{m} \| / \| \mathbf{m} \|$ may be large if the condition number is large. As it can be shown that

$$1 \leq \mathrm{cond}(\,\mathbf{A}\,) \leq \infty \quad , \tag{15}$$

a linear system for which $\mathrm{cond}(\,\mathbf{A}\,) \simeq 1$ is called *well conditioned*; a linear system for which $\mathrm{cond}(\,\mathbf{A}\,) >> 1$ is called *ill conditioned*.

The following properties which are sometimes useful can be demonstrated (Ciarlet, 1982):

$$\mathrm{cond}(\,\mathbf{A}\,) = \mathrm{cond}(\,\mathbf{A}^{-1}\,) \tag{16}$$

$$\mathrm{cond}_2(\,\mathbf{A}\,) = \frac{\sqrt{\max\ \lambda_i(\,\mathbf{A}^{*}\,\mathbf{A}\,)}}{\sqrt{\min\ \lambda_i(\,\mathbf{A}^{*}\,\mathbf{A}\,)}} \tag{17}$$

$$\mathbf{A}^* \mathbf{A} = \mathbf{M}^2 \qquad \Longrightarrow \qquad \mathrm{cond}_2(\mathbf{A}) = \frac{\max |\lambda_i(\mathbf{M})|}{\min |\lambda_i(\mathbf{M})|} \tag{18}$$

Coming back to the numerical example, the eigenvalues of $\mathbf{A}$ are

$$\begin{aligned} \lambda_1 &\simeq 0.010 \\ \lambda_2 &\simeq 0.843 \\ \lambda_3 &\simeq 3.858 \\ \lambda_4 &\simeq 30.289 \end{aligned} \tag{19}$$

and using, for instance, (18) gives

$$\mathrm{cond}_2(\mathbf{A}) = \frac{\lambda_4}{\lambda_1} \simeq 3\ 10^3 \ , \tag{20}$$

which shows that the system is ill conditioned, and the relative error of the solution may amount to $\simeq 3\ 10^3$ times the relative data error (as is almost the case in the example).

In fact, the introduction of the concept of condition number is only useful when a simplistic approach is used for the resolution of "linear systems". More generally, the reader is asked to solve the following problem:

The observable values $\mathbf{d} = (d^1, d^2, d^3, d^4)$ are known to depend on the model values $\mathbf{m} = (m^1, m^2, m^3, m^4)$ through the (exact) equation

$$\begin{bmatrix} d^1 \\ d^2 \\ d^3 \\ d^4 \end{bmatrix} = \begin{bmatrix} 10 & 7 & 8 & 7 \\ 7 & 5 & 6 & 5 \\ 8 & 6 & 10 & 9 \\ 7 & 5 & 9 & 10 \end{bmatrix} \begin{bmatrix} m^1 \\ m^2 \\ m^3 \\ m^3 \end{bmatrix} , \tag{21}$$

or, for short,

$$\mathbf{d} = \mathbf{G}\,\mathbf{m} \ . \tag{22}$$

A measurement of the observable values gives

$$\begin{bmatrix} d^1 \\ d^2 \\ d^3 \\ d^4 \end{bmatrix} = \begin{bmatrix} 32.0 \pm 0.1 \\ 23.0 \pm 0.1 \\ 33.0 \pm 0.1 \\ 31.0 \pm 0.1 \end{bmatrix} . \tag{23}$$

Use the least squares theory to solve the inverse problem and *discuss error and resolution*

Solution: The best solution (in the least squares sense) for a linear problem is (equations 1.90 and 1.92):

$$\langle \mathbf{m} \rangle = \mathbf{m}_{prior} + \left[\mathbf{G}^t \mathbf{C}_D^{-1} \mathbf{G} + \mathbf{C}_M^{-1}\right]^{-1} \mathbf{G}^t \mathbf{C}_D^{-1} [\mathbf{d}_{obs} - \mathbf{G}\, \mathbf{m}_{prior}] , \quad (24)$$

$$\mathbf{C}_{M'} = \left[\mathbf{G}^t \mathbf{C}_D^{-1} \mathbf{G} + \mathbf{C}_M^{-1}\right]^{-1} . \quad (25)$$

If there is no a priori information, $\mathbf{C}_M \to \infty \mathbf{I}$, and

$$\langle \mathbf{m} \rangle = \left[\mathbf{G}^t \mathbf{C}_D^{-1} \mathbf{G}\right]^{-1} \mathbf{G}^t \mathbf{C}_D^{-1} \mathbf{d}_{obs} \quad (26)$$

$$\mathbf{C}_{M'} = \left[\mathbf{G}^t \mathbf{C}_D^{-1} \mathbf{G}\right]^{-1} . \quad (27)$$

In our numerical example,

$$\mathbf{d}_{obs} = \begin{bmatrix} 32.0 \\ 23.0 \\ 33.0 \\ 31.0 \end{bmatrix} \quad (28)$$

$$\mathbf{C}_D = \sigma^2 \mathbf{I} = 0.01\, \mathbf{I} = \begin{bmatrix} 0.01 & 0 & 0 & 0 \\ 0 & 0.01 & 0 & 0 \\ 0 & 0 & 0.01 & 0 \\ 0 & 0 & 0 & 0.01 \end{bmatrix} \quad (29)$$

$$\mathbf{G} = \begin{bmatrix} 10 & 7 & 8 & 7 \\ 7 & 5 & 6 & 5 \\ 8 & 6 & 10 & 9 \\ 7 & 5 & 9 & 10 \end{bmatrix} . \quad (30)$$

As, in this particular example, $\mathbf{G}$ is squared and regular, we successively have

$$\langle \mathbf{m} \rangle = \left[\mathbf{G}^t \mathbf{C}_D^{-1} \mathbf{G}\right]^{-1} \mathbf{G}^t \mathbf{C}_D^{-1} \mathbf{d}_{obs}$$

$$= \mathbf{G}^{-1} \mathbf{C}_D (\mathbf{G}^t)^{-1} \mathbf{G}^t \mathbf{C}_D^{-1} \mathbf{d}_{obs} = \mathbf{G}^{-1} \mathbf{d}_{obs} , \quad (31)$$

i.e.,

$$\langle \mathbf{m} \rangle = \begin{bmatrix} \langle m^1 \rangle \\ \langle m^2 \rangle \\ \langle m^3 \rangle \\ \langle m^4 \rangle \end{bmatrix} = \begin{bmatrix} 1.0 \\ 1.0 \\ 1.0 \\ 1.0 \end{bmatrix} . \quad (32)$$

The posterior covariance operator is given by

$$\mathbf{C}_{M'} = \left[\mathbf{G}^t \mathbf{C}_D^{-1} \mathbf{G}\right]^{-1} = \mathbf{G}^{-1} \mathbf{C}_D (\mathbf{G}^t)^{-1} = \sigma^2 \mathbf{G}^{-1} (\mathbf{G}^t)^{-1} , \tag{33}$$

and, as $\mathbf{G}$ is symmetric,

$$\mathbf{C}_{M'} = \sigma^2 \mathbf{G}^{-1} \mathbf{G}^{-1} , \tag{34}$$

i.e.,

$$\mathbf{C}_{M'} = 0.01 \begin{bmatrix} 2442 & -4043 & 1015 & -602 \\ -4043 & 6694 & -1681 & 997 \\ 1015 & -1681 & 423 & -251 \\ -602 & 997 & -251 & 149 \end{bmatrix} . \tag{35}$$

From $\mathbf{C}_{M'}$ it is easy to obtain the standard deviations of model parameters

$$\begin{aligned} \sigma^1_M &= 4.94 \\ \sigma^2_M &= 8.18 \\ \sigma^3_M &= 2.06 \\ \sigma^4_M &= 1.22 , \end{aligned} \tag{36}$$

and the correlation matrix (see box 1.1)

$$\mathbf{R} = \begin{bmatrix} 1 & -0.99997 & +0.99867 & -0.99800 \\ -0.99997 & 1 & -0.99898 & +0.99830 \\ +0.99867 & -0.99898 & 1 & -0.99979 \\ -0.99800 & +0.99830 & -0.99979 & 1 \end{bmatrix} . \tag{37}$$

The overall information on the solution can thus be expressed by this correlation matrix and the short notation

$$\langle \mathrm{m} \rangle = \begin{bmatrix} \langle \mathrm{m}^1 \rangle \\ \langle \mathrm{m}^2 \rangle \\ \langle \mathrm{m}^3 \rangle \\ \langle \mathrm{m}^4 \rangle \end{bmatrix} = \begin{bmatrix} 1.00 \pm 4.94 \\ 1.00 \pm 8.18 \\ 1.00 \pm 2.06 \\ 1.00 \pm 1.22 \end{bmatrix} . \tag{38}$$

The interpretation of these results is as follows.

The least-squares approach is only fully justified if errors (in this example, data errors) are modeled using Gaussian probability densities. For a linear problem, as discussed in section 1.7, the a posteriori errors are then also Gaussian. Taking, for instance, twice the standard deviation, the probability of the true value of the parameter $\mathrm{m}^1_{\mathrm{true}}$ verifying the inequality

$$-8.88 \leq \mathrm{m}^1_{\mathrm{true}} \leq +10.88 \tag{39a}$$

is about 95% , *independently of the respective values of* $\mathrm{m}^2_{\mathrm{true}}$, $\mathrm{m}^3_{\mathrm{true}}$, *and* $\mathrm{m}^4_{\mathrm{true}}$. Similarly, the probability of the true values of each of the

parameters m^2_{true} , m^3_{true} , and m^4_{true} verifying the inequalities

$$\begin{array}{rcl} -15.36 & \leq & m^2_{true} \leq +17.36 \\ -3.12 & \leq & m^3_{true} \leq +5.12 \\ -1.44 & \leq & m^4_{true} \leq +3.44 \end{array} \qquad (39b)$$

is also about 95% .

This gives information on the true value of each parameter, considered independently, but the correlation matrix gives additional information on error correlation. For instance, the correlation of m^1 with m^2 is -0.99997 . This means that if the estimated value for m^1 , $\langle m^1 \rangle$, is in error (with respect to the true unknown value) it is *almost certain* that the the estimated value for m^2 , $\langle m^2 \rangle$, will also be in error (because the absolute value of the correlation is close to 1), and the the sign of the error will be opposite to the error in $\langle m^1 \rangle$ (because the correlation is negative). For instance, if the true value of m^1 was $m^1_{true} = \langle m^1 \rangle + 2\,\sigma^1_M$ it is almost certain that the true value of m^2 will be $m^2_{true} = \langle m^2 \rangle - 2\,\sigma^2_M$.

The easiest way to understand this is to consider the a posteriori probability density in the parameter space (equation 1.91):

$$\sigma_M(\mathbf{m}) = \left((2\pi)^2 \det \mathbf{C}_{M'} \right)^{-1/2} \exp\left(-\frac{1}{2} \left(\mathbf{m} - \langle \mathbf{m} \rangle \right)^t \mathbf{C}_{M'}^{-1} \left(\mathbf{m} - \langle \mathbf{m} \rangle \right) \right) . \qquad (40)$$

To simplify the discussion, let us first analyze the two parameters m^1 and m^2 . Their marginal probability density is

$$\sigma_{12}(m^1,m^2) = \left(2\pi \det \mathbf{C}_{12} \right)^{-1/2} \exp\left(-\frac{1}{2} \begin{bmatrix} m^1-1.0 \\ m^2-1.0 \end{bmatrix}^t \begin{bmatrix} 24.42 & -40.43 \\ -40.43 & 66.94 \end{bmatrix}^{-1} \begin{bmatrix} m^1-1.0 \\ m^2-1.0 \end{bmatrix} \right) \qquad (41)$$

(it is well known [e.g. Dubes, 1968] that marginal probability densities corresponding to a mutidimensional Gaussian are simply obtained by "picking" the corresponding covariances in the joint covariance operator). Figures 1.35 and 1.36 illustrate this probability density. The correlation between m^1 and m^2 is so strong in this numerical example, that the 95% confidence ellipsoid is undistinguishable from a segment. This means that, although the data set used in this example is not able to give an accurate location for the true values of m^1 or m^2 independently, it imposes that these true values must lie on the segment of the figure. As the volume of the allowed region is almost null, this gives, in fact, a lot of information.

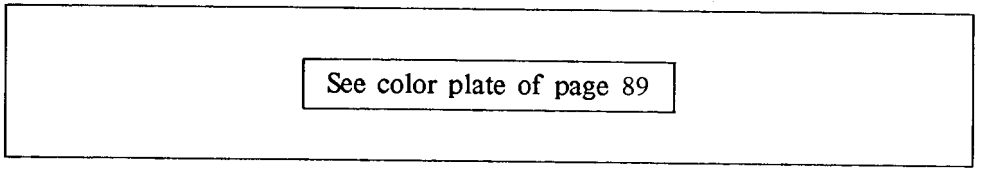


Figure 1.35: Marginal probability density for the parameters m^1 and m^2 . Uncertainties are so strongly correlated that it is difficult to distinguish the ellipsoid of errors from a segment. Although the standard deviations for each of the parameters are large, we have much information on these parameters, because their true values must lie on the "line". The resolution of the plotting device (300 pixel x 300 pixel) is not fine enough for a good representation, so that the colors obtained for the ellipsoid are aliased. The next figure shows a zoom of the central region.

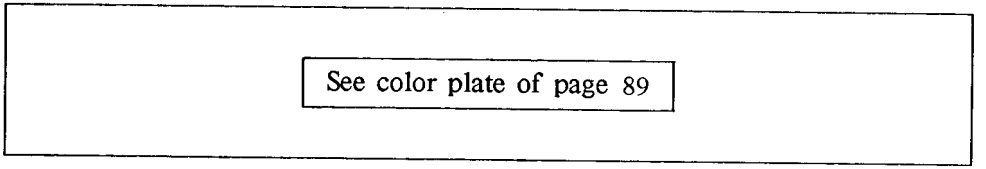


Figure 1.36: Same as the previous figure, with finer detail.

Similarly, the four-dimensional probability density $\sigma_M(\mathbf{m})$ defines a 95% confidence "ellipsoid" on the parameter space which corresponds to the extra-long "cigar" joining the point (-8.88 , +17.36 , -3.12 , +3.44) to the point (+10.88 , -15.36 , +5.12 , -1.44) . The reader will easily verify that the two "solutions" of the linear system obtained using Cramer's method for two slightly different data vectors correspond to two points on the cigar.

It should be noticed that if a further experiment gives accurate information on the true value of one of the parameters, the values of the other three parameters can readily be deduced, with very small uncertainties.

This example has shown that:

i) a careful analysis of the a posteriori covariance operator always has to be made when solving least-squares inverse problems,

ii) the information given by the "condition number" is very rough compared with the information given by the covariance operator (it only gives information about the ratio between the largest and shortest diameters of the ellipsoid of errors in the model space).

Problem 1.11: We wish to measure a single quantity x_{true} . To do this we have a digital instrument which delivers 5-digit decimal results. We have performed a great number (101) of measurements, and because the instrument has some intrinsic uncertainty, we obtain a different value at each measurement:

$x_{000} = 21.738$ $x_{001} = 21.273$ $x_{002} = 21.300$ $x_{003} = 21.540$ $x_{004} = 21.878$
$x_{005} = 21.052$ $x_{006} = 21.066$ $x_{007} = 21.894$ $x_{008} = 21.922$ $x_{009} = 21.536$
$x_{010} = 21.575$ $x_{011} = 21.990$ $x_{012} = 21.013$ $x_{013} = 21.488$ $x_{014} = 21.421$
$x_{015} = 21.296$ $x_{016} = 21.951$ $x_{017} = 21.717$ $x_{018} = 21.675$ $x_{019} = 21.136$
$x_{020} = 21.029$ $x_{021} = 21.515$ $x_{022} = 21.104$ $x_{023} = 21.872$ $x_{024} = 21.789$
$x_{025} = 21.191$ $x_{026} = 21.882$ $x_{027} = 21.578$ $x_{028} = 21.658$ $x_{029} = 21.069$
$x_{030} = 21.030$ $x_{031} = 21.217$ $x_{032} = 21.651$ $x_{033} = 21.285$ $x_{034} = 21.659$
$x_{035} = 21.965$ $x_{036} = 21.816$ $x_{037} = 21.535$ $x_{038} = 21.715$ $x_{039} = 21.104$
$x_{040} = 21.044$ $x_{041} = 21.977$ $x_{042} = 21.711$ $x_{043} = 21.758$ $x_{044} = 21.751$
$x_{045} = 21.489$ $x_{046} = 21.087$ $x_{047} = 21.814$ $x_{048} = 21.104$ $x_{049} = 21.971$
$x_{050} = 21.625$ $x_{051} = 21.581$ $x_{052} = 21.076$ $x_{053} = 21.648$ $x_{054} = 21.983$
$x_{055} = 21.888$ $x_{056} = 21.121$ $x_{057} = 21.239$ $x_{058} = 21.474$ $x_{059} = 21.788$
$x_{060} = 21.414$ $x_{061} = 21.930$ $x_{062} = 21.353$ $x_{063} = 21.001$ $x_{064} = 21.863$
$x_{065} = 21.087$ $x_{066} = 21.931$ $x_{067} = 21.776$ $x_{068} = 21.065$ $x_{069} = 21.664$
$x_{070} = 21.421$ $x_{071} = 21.127$ $x_{072} = 21.746$ $x_{073} = 21.110$ $x_{074} = 21.102$
$x_{075} = 21.947$ $x_{076} = 21.128$ $x_{077} = 21.610$ $x_{078} = 21.465$ $x_{079} = 21.822$
$x_{080} = 21.617$ $x_{081} = 21.675$ $x_{082} = 21.898$ $x_{083} = 21.573$ $x_{084} = 21.397$
$x_{085} = 21.309$ $x_{086} = 21.485$ $x_{087} = 21.018$ $x_{088} = 21.132$ $x_{089} = 21.462$
$x_{090} = 21.146$ $x_{091} = 21.391$ $x_{092} = 21.222$ $x_{093} = 21.034$ $x_{094} = 21.977$
$x_{095} = 21.079$ $x_{096} = 21.713$ $x_{097} = 21.028$ $x_{098} = 21.598$ $x_{099} = 21.105$
$x_{100} = 21.333$.

The uncertainty ϵ of the instrument has an unknown probability density function $f(\epsilon)$ which is known to be symmetric and centered at $\epsilon = 0$. Under these conditions, the median m_1 , the mean m_2 , and the mid-range m_∞ are unbiased central estimators. They are given by

$m_1 = 21.422$
$m_2 = 21.482$
$m_\infty = 21.492$.

Which of these is to be preferred for estimating x_{true} ?.

Solution: One response to the question is that it has no response. The median m_1 minimizes the mean deviation of the residuals, the mean m_2 minimizes the standard deviation, and the mid-range m_∞ minimizes the maximum deviation. So the "best" central estimator will depend on which criterion we use to measure "goodness".

That is not the good response, because with the experimental results in the previous table we can do better than computing a central estimator: we can estimate the probability density function $f(\epsilon)$ itself. Figure 1.37 shows a histogram of the results. It has the striking feature of taking strictly null values outside a given range where the values are rather uniform. As $f(\epsilon)$ is known to be symmetric, we can try to fit a Generalized Gaussian to that histogram (see box 1.2). The value $p = \infty$ (box-car function) seems not too bad a candidate (in any case is clearly better than $p = 1$ or $p = 2$). It is clear that to estimate the center of a generalized Gaussian of order p , we should use the central estimator in norm ℓ_p . The value $m_\infty = 21.492$ then is to be preferred for estimating x_{true} .

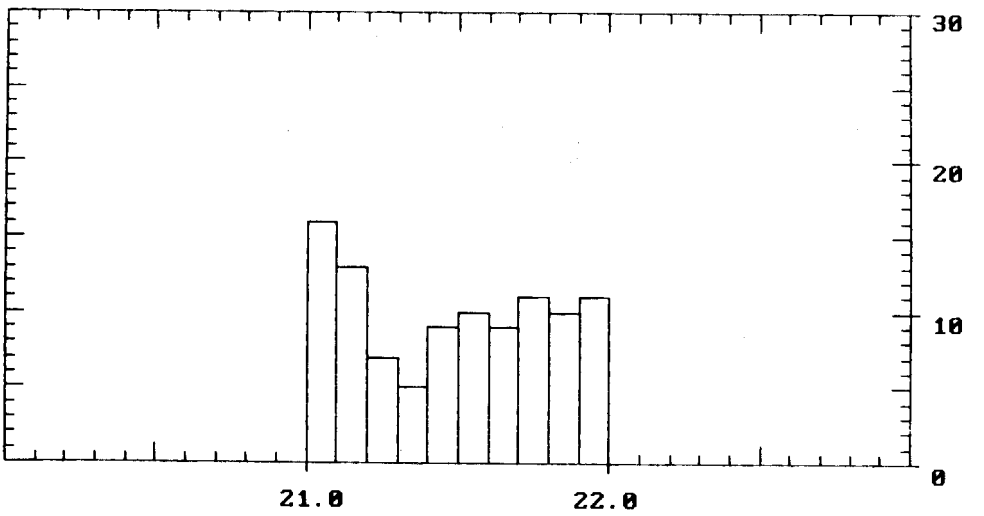


Figure 1.37: Histogram of the 101 values obtained when measuring x_{true} . The statistics of the errors are unknown, but the probability density is known to be unbiased (centered on x_{true}). Which is the best estimator of x_{true} ?

Actually, the 101 numbers used as data have been generated using the pseudo-random computer code

$$x_i = 21. + \text{RND} ,$$

where RND is a routine generating numbers with a theoretically uniform probability density over (0,1) . That m_∞ is a better estimator than m_1 or m_2 in some absolute sense can be seen by a simple numerical test. The previous experiment can be repeated a great number of times ($\simeq$100), and we can make histograms of the values thus obtained for m_1 , m_2 , and m_∞ in each experiment. They are shown in Figure 1.38. We clearly see that m_∞ is *less scattered* around the true value x_{true} than m_1 or m_2 *independently of the criterion used to measure the scatter.*

Problem 1.12: Let x and y be cartesian coordinates on a cathodic screen. A random device projects electrons on the screen with a known probability density:

$$\Theta(x,y) = \begin{cases} \text{const.} \;\; r \;\; (2-r) & \text{if} \;\; 0 \leq r \leq 2 \\ 0 & \text{if} \;\; r > 2 , \end{cases} \tag{1}$$

where $r = \sqrt{x^2+y^2}$.

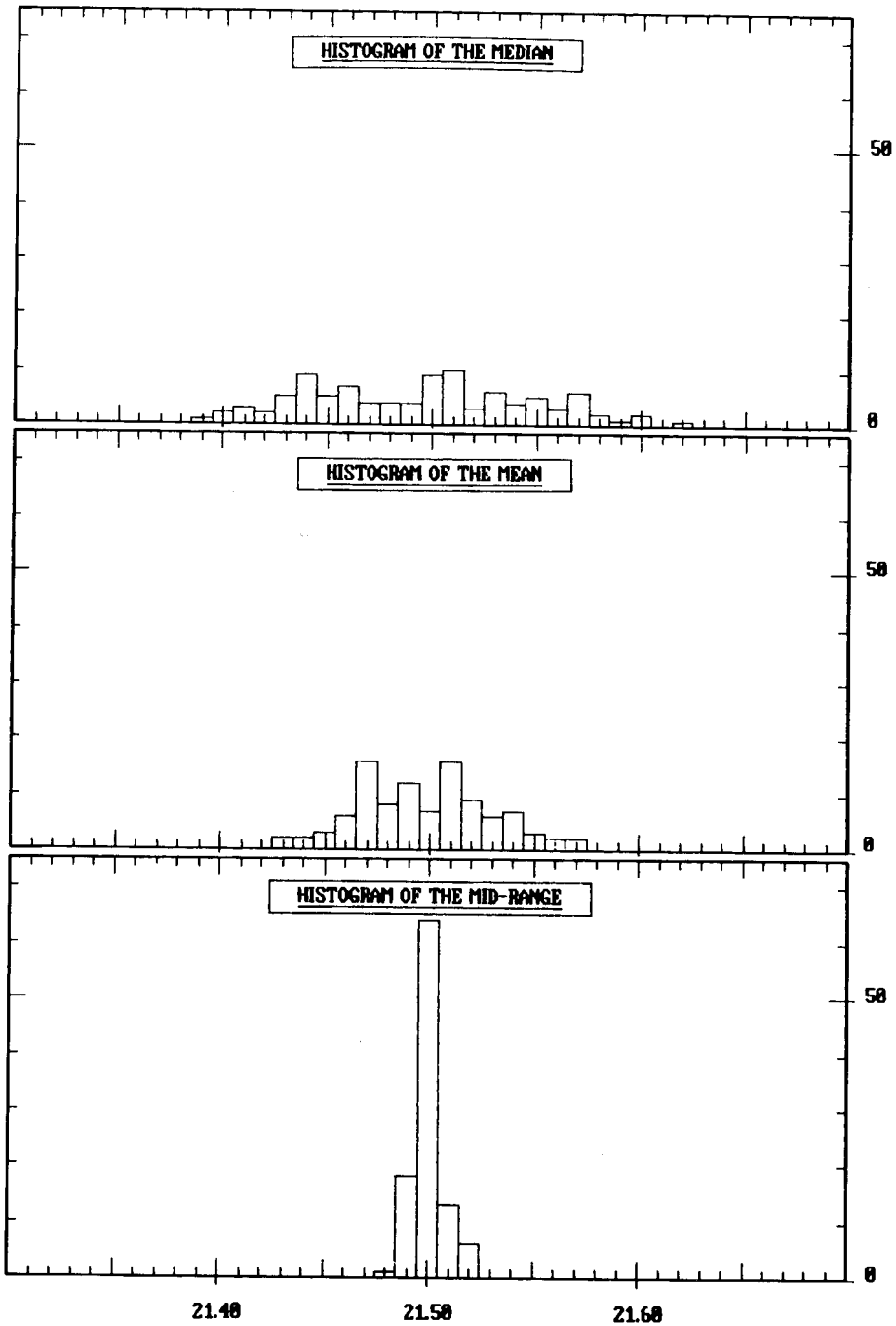
We are interested in the coordinates (x,y) at which a particular electron will hit the screen, and we build an experimental device to measure them. The measuring instrument is not perfect, and when we perform the experiment we can only get the information that the true coordinates of the impact point had the probability density

$$\rho(x,y) = \text{const.} \exp\left[-\frac{1}{2} \begin{bmatrix} x-x_0 \\ y-y_0 \end{bmatrix} \begin{bmatrix} \sigma^2 & \rho\sigma^2 \\ \rho\sigma^2 & \sigma^2 \end{bmatrix}^{-1} \begin{bmatrix} x-x_0 \\ y-y_0 \end{bmatrix} \right] \tag{2}$$

with $(x_0,y_0) = (0,0)$, $\sigma = 2$, and $\rho = 0.99$. Combine this experimental information with the previous knowledge of the random device, and obtain a better estimate of the impact point.

Solve the problem again, using everywhere polar coordinates instead of cartesian coordinates.

Solution: As x and y are cartesian coordinates, the null information probability density for the impact point is


HISTOGRAM OF THE MEDIAN
50
0
HISTOGRAM OF THE MEAN
50
0
HISTOGRAM OF THE MID-RANGE
50
0
21.48
21.58
21.68

← *Figure 1.38:* The histogram in Figure 1.37 suggests that the statistics of errors correspond to a box-car probability density. In that case the best estimator of x_{true} is the mid-range of the 101 values. These values were, in fact, generated using a computer code simulating a box-car probability density. This figure shows the histograms obtained for the median (top), mean (middle), and mid-range (bottom) when repeating the whole experiment (generation of the 101 random points) a large number of times. Undoubtedly, the mid-range is (in this example) the best estimator, whatever criterion of goodness we may use.

$$\mu(x,y) = \text{const.} \tag{3}$$

The information represented by $\Theta(x,y)$ and $\rho(x,y)$ are independent in the sense discussed in section 1.2.6 . Combination of these data then corresponds to the conjunction

$$\sigma(x,y) = \frac{\rho(x,y)\,\Theta(x,y)}{\mu(x,y)} , \tag{4}$$

which is plotted in Figure 1.39.

The polar coordinates verify

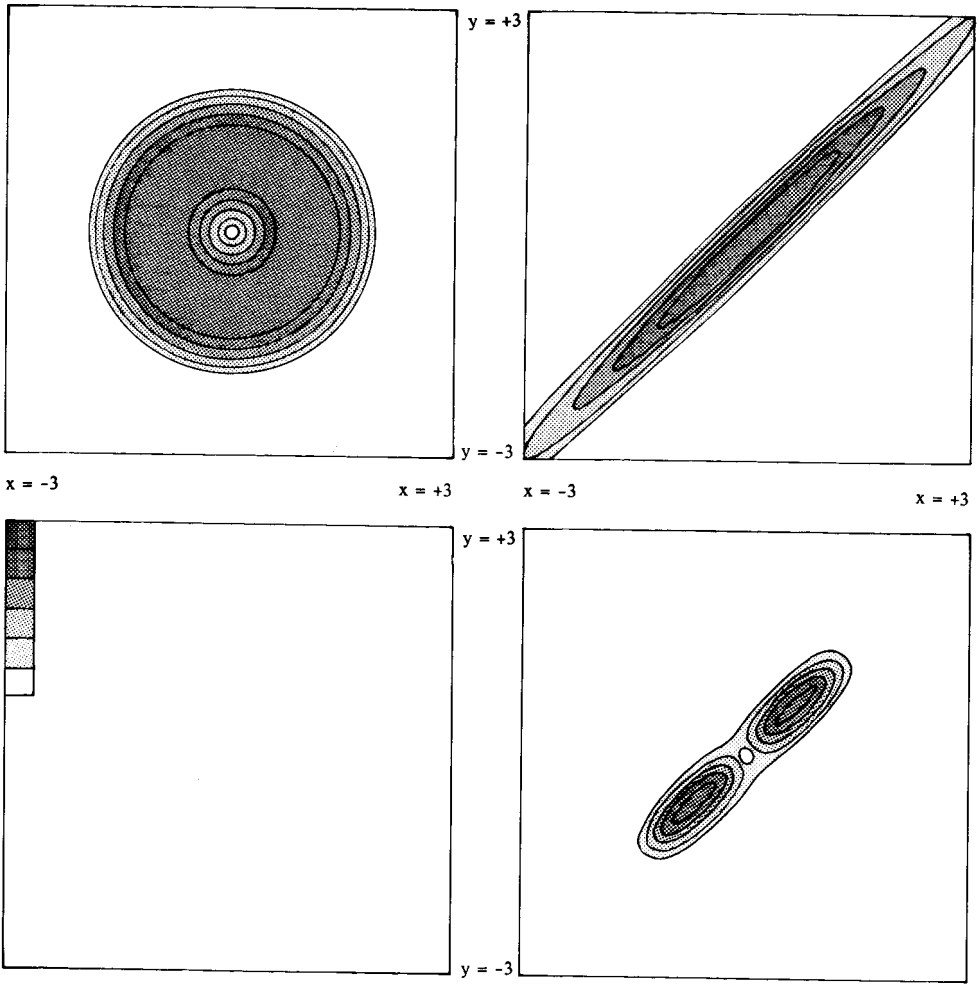
$$r = (x^2+y^2)^{1/2} \qquad \text{tg}\,\phi = \frac{x}{y} , \tag{5}$$

so that the Jacobian of the transformation is

$$J(r,\phi) = \begin{vmatrix} \frac{\partial r}{\partial x} & \frac{\partial r}{\partial y} \\ \frac{\partial \phi}{\partial x} & \frac{\partial \phi}{\partial y} \end{vmatrix} = \frac{1}{r} . \tag{6}$$

Let $f(x,y)$ be a probability density in cartesian coordinates. To any surface S of the plane it assigns the probability

$$P(S) = \iint_S dx\, dy\, f(x,y) . \tag{7}$$



Let $\tilde{f}(r,\phi)$ be a probability density in polar coordinates. If we wish $\tilde{f}(r,\phi)$ to assign to $\mathbf{S}$ the same probability as $f(x,y)$,

$$P(S) = \iint_{\mathbf{S}} dr\, d\phi\, f(r,\phi) , \tag{8}$$

then necessarily

← *Figure 1.39:* A random device has been built which projects electrons on a cathodic screen with the probability density shown in the top-left. Coordinates are cartesian. Independently of this probability, a measurement of the impact point of a particular electron gives the information represented by the probability density shown in the top right. The null information probability density (which is uniform, and has been represented in arbitrary color) is shown in the bottom left. It is then possible to combine all these states of information to obtain the posterior probability density, shown in ther bottom right.

$$\tilde{f}(r,\phi) = f(\, x(r,\phi)\, ,\, y(r,\phi)\,)\ \left|J(r,\phi)\right| . \tag{9}$$

This is the usual formula for the change of variables in a probability density. In our case

$$\tilde{f}(r,\phi) = r\, f(r \sin\phi\, ,\, r\cos\phi) . \tag{10}$$

This gives

$$\tilde{\Theta}(x,y) = \begin{cases} \text{const.}\ r^2\ (1-r) & \text{if}\ \ 0 \le r \le 2 \\ 0 & \text{if}\ \ r > 2\ , \end{cases} \tag{11}$$

$$\tilde{\rho}(r,\phi) = \text{const.}\ r\ \exp\left[- \frac{r^2\,(\,1 - 2\,\rho\,\sin\phi\,\cos\phi\,)}{2\,\sigma^2\,(1-\rho^2)} \right] , \tag{12}$$

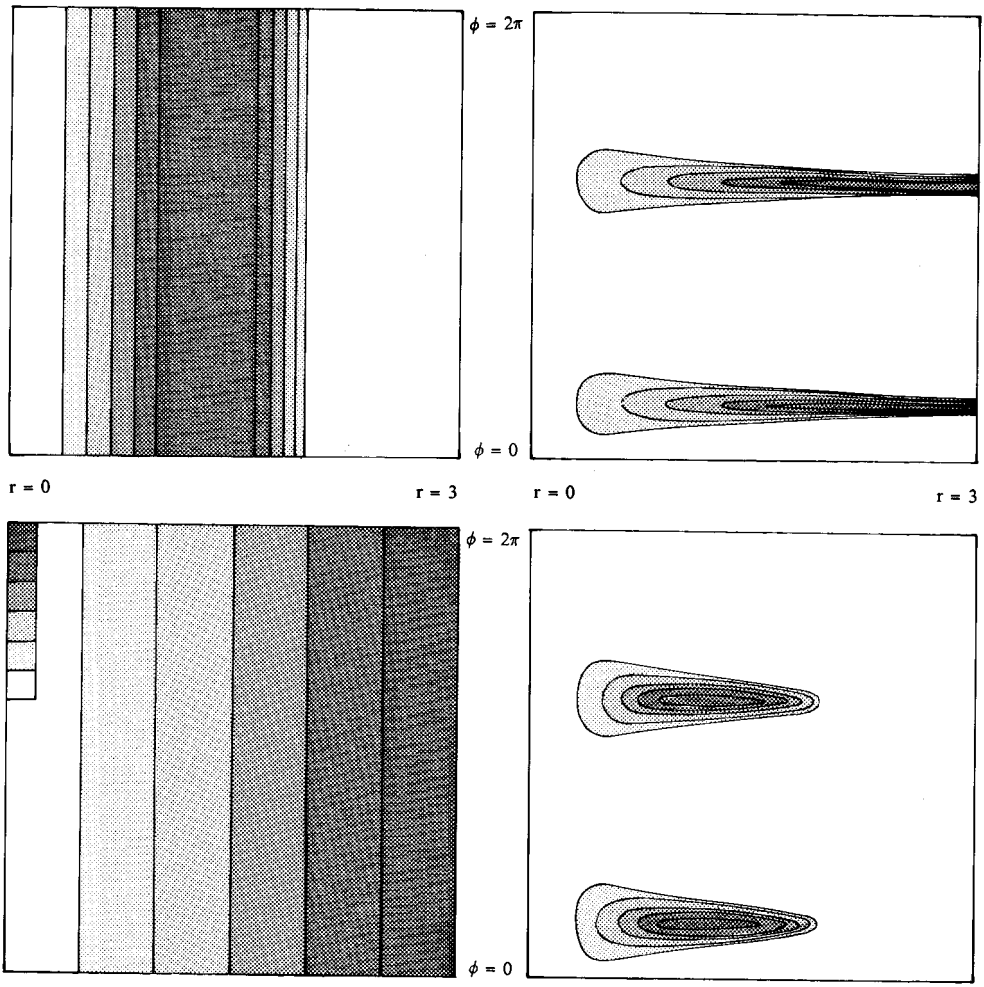
and

$$\tilde{\mu}(r,\phi) = \text{const}\ \ r . \tag{13}$$

The combination of $\Theta(r,\phi)$ with $\tilde{\rho}(r,\phi)$ is given by the conjunction

$$\tilde{\sigma}(r,\phi) = \frac{\tilde{\rho}(r,\phi)\ \tilde{\Theta}(r,\phi)}{\tilde{\mu}(r,\phi)} , \tag{14}$$

and is shown in Figure 1.40.



It should be noticed that the probability density representing the null information probability is not uniform in polar coordinates: the probability density (13) assigns equal probabilities to equal "volumes", as it must.

The solution obtained for this problem using cartesian coordinates (Figure 1.39) , and the solution obtained using polar coordinates (figure 1.40) are coherent: Figure 1.39 can be deduced from Figure 1.40 using (9) , and viceversa.

← *Figure 1.40:* It is also possible to solve the problem using polar coordinates throughout. The top-left represents the probability density of an impact on the screen, as imposed by the experimantal device. The probability density is constant for given r. The top-right shows the result of the measurement. In the bottom-left, the noninformative probability density in polar coordinates is shown. It assigns equal probability to equal surfaces of the screen. The combination of these states of information gives the posterior probability density shown in the bottom-right. This probability is completely equivalent to the probability density in the bottom-right of the previous figure, as they can be deduced one from another through the usual formula of change of variables between cartesian and polar coordinates $\tilde{\sigma}(\theta,\phi) = r\, \sigma(x,y)$.

Using more elementary approaches, this problem may present some pathologies. In particular, the result cannot be expressed using a single estimator of the impact point, because the probability density is bimodal. The mean value and median value are meaningless, and only the two maximum likelihood points make clear sense. But we should be aware that the maximum likelihood points obtained using cartesian coordinates and using polar coordinates are not identical.

It should be mentioned that the usual Bayesian approach does not apply directly to this problem.

Problem 1.13: Demonstrate that the relative information of two probabity densisities is invariant under a bijective change of variables.

Solution: Let $f(\mathbf{x})$ be a probability density function representing a given state of information on the parameters $\mathbf{x}$. The information content of $f(\mathbf{x})$ has been defined by

$$I(f;\mu) = \int d\mathbf{x}\ f(\mathbf{x})\ \text{Log}\ \frac{f(\mathbf{x})}{\mu(\mathbf{x})}\,, \tag{1}$$

where $\mu(\mathbf{x})$ represents the reference state of information. If instead of the parameters $\mathbf{x}$ we decide to use the parameters

$$\mathbf{x}^* = \mathbf{x}^*(\mathbf{x})\,, \tag{2}$$

the same state of information is described in the new variables by

$$f^*(x^*) = f(x) \left| \frac{\partial x}{\partial x^*} \right| , \tag{3}$$

while the reference state of information is described by

$$\mu^*(x^*) = \mu(x) \left| \frac{\partial x}{\partial x^*} \right| , \tag{4}$$

where $|\partial x/\partial x^*|$ denotes the absolute value of the Jacobian of the transformation. A computation of the information content in the new variables gives

$$I(f^*;\mu^*) = \int dx^* \; f^*(x^*) \; \text{Log} \; \frac{f^*(x^*)}{\mu^*(x^*)}$$

$$= \int dx^* \left| \frac{\partial x}{\partial x^*} \right| f(x) \; \text{Log} \; \frac{f(x)}{\mu(x)} , \tag{5}$$

and, using

$$dx^* \left| \frac{\partial x}{\partial x^*} \right| = dx , \tag{6}$$

we directly obtain

$$I(f^*;\mu^*) = I(f;\mu) . \tag{7}$$

Problem 1.14: Demonstrate the equivalence

$$I(f;\mu) = 0 \quad \Leftrightarrow \quad f(x) \equiv \mu(x) . \tag{1}$$

Solution: If $f(x) = \mu(x)$, it is evident that $I(f;\mu) = 0$. To demonstrate the reciprocal, let us, for given $\mu(x)$, search the minimumof $S(f) = \int dx \; f(x) \; \text{Log} \; f(x)/\mu(x)$ under the constraint $\int dx \; f(x) = 1$. Using the method of Lagrange's multipliers (see Chapter 4), we can introduce the function

$$S(f,\lambda) = \int dx \; f(x) \; \text{Log} \; \frac{f(x)}{\mu(x)} - \lambda \left[1 - \int dx \; f(x) \right] , \tag{2}$$

to be minimized with respect to the function $f(x)$ and the parameter λ . We have first

$$\frac{\partial S}{\partial \lambda} = 0 \quad \Leftrightarrow \quad \int dx \; f(x) = 1 \; , \tag{3}$$

which simply is the normalization condition. The definition of functional derivative is written (see, for instance, Chapter 7) , for arbitrary $\delta \mathbf{f}$,

$$S(\mathbf{f}+\delta\mathbf{f};\lambda) - S(\mathbf{f};\lambda) = \frac{\partial S}{\partial \mathbf{f}} \; \delta\mathbf{f} + O(||\delta\mathbf{f}||^2) \; . \tag{4}$$

We have successively

$$\begin{aligned} S(\mathbf{f}+\delta\mathbf{f};\lambda) - S(\mathbf{f};\lambda) &= \\ &= \int dx \; (f(x) + \delta f(x)) \; \text{Log} \; \frac{f(x) + \delta f(x)}{\mu(x)} - \lambda \; (\; 1 - \int dx \; (f(x) + \delta f(x)) \;) \\ &- \int dx \; f(x) \; \text{Log} \; \frac{f(x)}{\mu(x)} + \lambda \; (\; 1 - \int dx \; f(x) \;) \\ &= \int dx \left[\text{Log} \; \frac{f(x)}{\mu(x)} + 1 + \lambda \right] \delta f(x) + O(||\delta f||^2). \end{aligned} \tag{5}$$

The condition $\partial S / \partial \mathbf{f} = \mathbf{0}$ then gives successively

$$\text{Log} \; \frac{f(x)}{\mu(x)} \equiv - \lambda - 1 \; , \tag{6}$$

$$f(x) \equiv e^{-\lambda - 1} \; \mu(x) \; , \tag{7}$$

and, as the information content is only defined if $\mu(x)$ is normalized, this gives $\lambda = -1$ and

$$f(x) \equiv \mu(x) \; . \tag{8}$$

Problem 1.15: Maximum entropy probability density. Let $\mathbf{V}(x)$ be an arbitrary given vector function of x . Demonstrate that among all probability densities $f(x)$ for which the mathematical expectation for $\mathbf{V}(x)$ equals $\mathbf{V}_0$,

$$\int dx \; \mathbf{V}(x) \; f(x) = \mathbf{V}_0 \; , \tag{1}$$

the one which has ***minimum information*** (maximum extropy) with respect to a given probability density $\mu(x)$,

$$\int dx \; f(x) \; \text{Log} \left[\frac{f(x)}{\mu(x)} \right] \quad \text{MINIMUM} \; , \tag{2}$$

necessarily has the form

$$f(\mathbf{x}) = k\,\mu(\mathbf{x})\,\exp(-\mathbf{W}^t\,\mathbf{V}(\mathbf{x}))\,, \tag{3}$$

where k and $\mathbf{W}$ are constants (independent of $\mathbf{x}$).

Solution: The problem is:

Minimize
$$S'(f(\cdot)) = \int d\mathbf{x}\, f(\mathbf{x})\ \mathrm{Log}\left[\frac{f(\mathbf{x})}{\mu(\mathbf{x})}\right] \tag{4a}$$

Under the constraints
$$\begin{cases} \int d\mathbf{x}\, f(\mathbf{x}) = 1 & (4b) \\ \int d\mathbf{x}\, \mathbf{V}(\mathbf{x})\, f(\mathbf{x}) = \mathbf{V}_0\,, & (4c) \end{cases}$$

i.e., a problem of constrained minimization, which is non-typical in the sense that the variable is a function (i.e., a variable in an infinite dimensional space). Nevertheless, the problem can be solved using the classical method of Lagrange's parameters (see Chapter 4). The problem of minimization of S' under the constraints (4b)-(4c) is equivalent to the problem of unconstrained minimization of

$$S(f(\cdot), U, \mathbf{W}) = \int d\mathbf{x}\, f(\mathbf{x})\ \mathrm{Log}\left[\frac{f(\mathbf{x})}{\mu(\mathbf{x})}\right] - U\,(1 - \int d\mathbf{x}\, f(\mathbf{x})) - \mathbf{W}^t\,(\mathbf{V}_0 - \int d\mathbf{x}\, \mathbf{V}(\mathbf{x})\, f(\mathbf{x})) \tag{5}$$

because the conditions $\partial S/\partial U = 0$ and $\partial S/\partial \mathbf{W} = 0$ directly impose the constraints (4b)-(4c). We have

$$S(f(\cdot)+\delta f(\cdot), U, \mathbf{W}) - S(f(\cdot), U, \mathbf{W}) = \int d\mathbf{x}\,(f(\mathbf{x}) + \delta f(\mathbf{x}))\ \mathrm{Log}\left[\frac{f(\mathbf{x})+\delta f(\mathbf{x})}{\mu(\mathbf{x})}\right] - \int d\mathbf{x}\, f(\mathbf{x})\ \mathrm{Log}\left[\frac{f(\mathbf{x})}{\mu(\mathbf{x})}\right] + U \int d\mathbf{x}\, \delta f(\mathbf{x}) + \mathbf{W}^t \int d\mathbf{x}\, \mathbf{V}(\mathbf{x})\, \delta f(\mathbf{x})\,, \tag{6}$$

and using the first order development

$$\mathrm{Log}(1+u) = u + O(u^2)\,, \tag{7}$$

gives, everywhere $f(\mathbf{x}) \neq 0$,

$$\text{Log}\left[\frac{f(x)+\delta f(x)}{\mu(x)} \right] = \text{Log}\left[\frac{f(x)}{\mu(x)} \right] + \frac{\delta f(x)}{f(x)} + O(\delta f^2) , \tag{8}$$

and then,

$$S(f(\cdot)+\delta f(\cdot) , U , W) - S(f(\cdot) , U , W) =$$

$$= \int dx \left[\text{Log}\left[\frac{f(x)}{\mu(x)} \right] + 1 + U + W^t V(x) \right] \delta f(x) + O(\delta f^2) . \tag{9}$$

The condition of minimum of S with respect to $f(x)$ causes the factor of $\delta f(x)$ in the right hand of (9) to vanish, from which result (3) follows.

Problem 1.16: Let $f_1(x)$ and $f_0(x)$ represent two normalized probability density functions. The *relative information* on f_1 with respect to f_0 is defined by

$$I(f_1;f_0) = \int dx \; f_1(x) \; \text{Log}\left[\frac{f_1(x)}{f_0(x)} \right] . \tag{1}$$

Demonstrate that if f_1 and f_0 are Gaussian probability densities with mathematical expectations respectively equal to x_1 and x_0 and covariance operators respectively equal to C_1 and C_0, then

$$I(f_1;f_0) = \text{Log}\left[\frac{\det^{1/2} C_0}{\det^{1/2} C_1} \right] + \frac{1}{2} (x_1-x_0)^t \; C_0^{-1} \; (x_1-x_0)$$

$$+ \frac{1}{2} \text{Trace}\left[C_1 \; C_0^{-1} - I \right] . \tag{2}$$

Solution: By definition,

$$f_1(x) = \frac{1}{(2\pi)^{n/2} \; \det^{1/2} C_1} \exp\left[-\frac{1}{2} \; (x-x_1)^t \; C_1^{-1} \; (x-x_1) \right] \tag{3a}$$

and

$$f_0(x) = \frac{1}{(2\pi)^{n/2} \; \det^{1/2} C_0} \exp\left[-\frac{1}{2} \; (x-x_0)^t \; C_0^{-1} \; (x-x_0) \right] . \tag{3b}$$

Replacing (3) in (1) gives

$$I(f_1;f_0) = \text{Log}\left[\frac{\det^{1/2} C_0}{\det^{1/2} C_1} \right]$$

$$- \frac{1}{2} E_1\Big((\mathbf{x}-\mathbf{x}_1)^t \, \mathbf{C}_1^{-1} \, (\mathbf{x}-\mathbf{x}_1) \Big) + \frac{1}{2} E_1\Big((\mathbf{x}-\mathbf{x}_0)^t \, \mathbf{C}_0^{-1} \, (\mathbf{x}-\mathbf{x}_0) \Big) , \quad (4)$$

where $E_1(\cdot)$ denotes the mathematical expectation with respect to f_1 :

$$E_1(\Psi(\mathbf{x})) = \int d\mathbf{x} \; f_1(\mathbf{x}) \; \Psi(\mathbf{x}) . \quad (5)$$

From the definition of covariance operator, and using the linearity of the mathematical expection, we obtain

$$\mathbf{C}_1 = E_1((\mathbf{x}-\mathbf{x}_1) (\mathbf{x}-\mathbf{x}_1)^t) = E_1(\mathbf{x}\,\mathbf{x}^t - 2\,\mathbf{x}_1\,\mathbf{x}^t + \mathbf{x}_1\,\mathbf{x}_1^t) \quad (6)$$

$$= E_1(\mathbf{x}\,\mathbf{x}^t) - 2\,\mathbf{x}_1\,E_1(\mathbf{x}^t) + \mathbf{x}_1\,\mathbf{x}_1^t = E_1(\mathbf{x}\,\mathbf{x}^t) - \mathbf{x}_1\,\mathbf{x}_1^t ,$$

whence, using a tensor notation we deduce

$$E_1(x^\alpha \, x^\beta) = C_1^{\alpha\beta} + x_1^\alpha \, x_1^\beta . \quad (7)$$

We have

$$E_1\Big((\mathbf{x}-\mathbf{x}_1)^t \, \mathbf{C}_1^{-1} \, (\mathbf{x}-\mathbf{x}_1) \Big) = \ldots = E_1\Big(\mathbf{x}^t \, \mathbf{C}_1^{-1} \, \mathbf{x} \Big) - \mathbf{x}_1^t \, \mathbf{C}_1^{-1} \, \mathbf{x}_1$$

$$= (\mathbf{C}_1^{-1})^{\alpha\beta} \, E_1(x^\alpha \, x^\beta) - (\mathbf{C}_1^{-1})^{\alpha\beta} \, x_1^\alpha \, x_1^\beta , \quad (8)$$

whence, using (7), we deduce

$$E_1\Big((\mathbf{x}-\mathbf{x}_1)^t \, \mathbf{C}_1^{-1} \, (\mathbf{x}-\mathbf{x}_1) \Big) = (\mathbf{C}_1^{-1})^{\alpha\beta} \, C_1^{\alpha\beta} = \text{Trace } \mathbf{I} . \quad (9)$$

We also have

$$E_1\Big((\mathbf{x}-\mathbf{x}_0)^t \, \mathbf{C}_0^{-1} \, (\mathbf{x}-\mathbf{x}_0) \Big)$$

$$= \ldots = E_1\Big(\mathbf{x}^t \, \mathbf{C}_0^{-1} \, \mathbf{x} \Big) - 2\,\mathbf{x}_0^t \, \mathbf{C}_0^{-1} \, \mathbf{x}_1 + \mathbf{x}_0^t \, \mathbf{C}_0^{-1} \, \mathbf{x}_0$$

$$= (\mathbf{C}_0^{-1})^{\alpha\beta} \, E_1(x^\alpha \, x^\beta) - 2\,(\mathbf{C}_0^{-1})^{\alpha\beta} \, x_0^\alpha \, x_1^\beta + (\mathbf{C}_0^{-1})^{\alpha\beta} \, x_0^\alpha \, x_0^\beta , \quad (10)$$

whence, using (7), we deduce

$$E_1\Big((\mathbf{x}-\mathbf{x}_0)^t \, \mathbf{C}_0^{-1} \, (\mathbf{x}-\mathbf{x}_0) \Big)$$

$$= (\mathbf{C}_0^{-1})^{\alpha\beta}\ \mathbf{C}_1^{\alpha\beta} + (\mathbf{C}_0^{-1})^{\alpha\beta}\ (x_1^{\alpha}-x_0^{\alpha})\ (x_1^{\beta}-x_0^{\beta})$$

$$= \text{Trace}\left[\ \mathbf{C}_0^{-1}\ \mathbf{C}_1\ \right] + (\mathbf{x}_1-\mathbf{x}_0)^t\ \mathbf{C}_0^{-1}\ (\mathbf{x}_1-\mathbf{x}_0)\ . \qquad (11)$$

Inserting (9) and (11) in (4), result (2) follows. Notice that the factor $\det^{1/2}\mathbf{C}$ represents the (hyper) volume of the hyper-ellipsoid representing the covariance operator $\mathbf{C}$.

Problem 1.17: Let X be a parameter space, and P_1 , P_2 ,... probability distributions representing different states of information on X. In section 1.2.6, the conjunction $(P_1$ *and* $P_2)$ has been defined by

$$(P_1 \textit{ and } P_2) = (P_2 \textit{ and } P_1) \qquad \text{for any } P_1 \text{ and } P_2 \qquad (1)$$

$$P_1(A) = 0 \Rightarrow (P_1 \textit{ and } P_2)(A) = 0 \qquad \text{for any } P_1 \text{ , } P_2 \text{ , and any } A \subset X \qquad (2)$$

$$(P \textit{ and } M) = P \qquad \text{for any } P \text{ ,} \qquad (3)$$

where M represents the state of null information. If the probability densities representing P_1 , P_2 , and M , are respectively $f_1(\mathbf{x})$, $f_2(\mathbf{x})$, and $\mu(\mathbf{x})$, show that the probability density representing $(P_1$ *and* $P_2)$ is $\dfrac{f_1(\mathbf{x})\ f_2(\mathbf{x})}{\mu(\mathbf{x})}$

Solution: In mathematical terminology, the condition (2) means that the measure $(P_1$ *and* $P_2)$ is "absolutely continuous" with respect to the measure P_1. The Radon-Nikodym theorem (e.g., Taylor, 1966) states that there then exists a unique function $\phi_2(\mathbf{x})$ such that, for any $A \subset X$,

$$(P_1 \textit{ and } P_2)\ (A) = \int_A d\mathbf{x}\ \phi_2(\mathbf{x})\ f_1(\mathbf{x}) \,. \qquad (4)$$

Using conditions (1) and (2) and the Radon-Nikodym theorem again, we see that there also exists a unique function $\phi_1(\mathbf{x})$ such that, for any $A \subset X$,

$$(P_1 \textit{ and } P_2)\ (A) = \int_A d\mathbf{x}\ \phi_1(\mathbf{x})\ f_2(\mathbf{x}) \,. \qquad (5)$$

At any point $\mathbf{x}$ where the product $f_1(\mathbf{x})\ f_2(\mathbf{x})$ is non-vanishing, I define

$$\omega_1(\mathbf{x}) = \frac{f_1(\mathbf{x})}{\phi_1(\mathbf{x})} \qquad (6a)$$

$$\omega_2(\mathbf{x}) = \frac{f_2(\mathbf{x})}{\phi_2(\mathbf{x})} . \tag{6b}$$

For any $A \subset X$ we then have

$$(P_1 \textit{ and } P_2)(A) = \int_A d\mathbf{x} \; \frac{f_1(\mathbf{x}) \; f_2(\mathbf{x})}{\omega_2(\mathbf{x})} = \int_A d\mathbf{x} \; \frac{f_1(\mathbf{x}) \; f_2(\mathbf{x})}{\omega_1(\mathbf{x})} . \tag{7}$$

This gives

$$\omega_1(\mathbf{x}) = \omega_2(\mathbf{x}) = \omega(\mathbf{x}) \tag{8}$$

and

$$(P_1 \textit{ and } P_2)(A) = \int_A d\mathbf{x} \; \frac{f_1(\mathbf{x}) \; f_2(\mathbf{x})}{\omega(\mathbf{x})} . \tag{9}$$

Condition (3) then gives

$$\int_A d\mathbf{x} \; \frac{f(\mathbf{x}) \; \mu(\mathbf{x})}{\omega(\mathbf{x})} = \int_A d\mathbf{x} \; f(\mathbf{x}) , \tag{10}$$

i.e.,

$$\omega(\mathbf{x}) = \mu(\mathbf{x}) . \tag{11}$$

We finally obtain

$$(P_1 \textit{ and } P_2)(A) = \int_A d\mathbf{x} \; \frac{f_1(\mathbf{x}) \; f_2(\mathbf{x})}{\mu(\mathbf{x})} . \tag{12}$$

Equation (11) has been obtained only for the points $\mathbf{x}$ where the product $f_1(\mathbf{x}) \; f_2(\mathbf{x})$ is not vanishing. But as elsewhere the probability density vanishes, the result (12) is valid for the whole space X.

Problem 1.18: Assume the very particular case where the *exact* relationship $\mathbf{d} = \mathbf{g}(\mathbf{m})$ between model parameters and observable parameters is a bijection (i.e., we can also write $\mathbf{m} = \mathbf{g}^{-1}(\mathbf{d})$). In that case, find the relationship between the a posteriori p.d.f. in the model space, $\sigma_M(\mathbf{m})$, and the a posteriori p.d.f. in the data space $\sigma_D(\mathbf{d})$.

Solution: We start from the general solution

$$\sigma(\mathbf{d},\mathbf{m}) = \frac{\rho(\mathbf{d},\mathbf{m})\ \Theta(\mathbf{d},\mathbf{m})}{\mu(\mathbf{d},\mathbf{m})} \ . \tag{1}$$

The assumption of an exact theory is written

$$\Theta(\mathbf{d},\mathbf{m}) = \Theta(\mathbf{d}|\mathbf{m})\ \mu_M(\mathbf{m}) = \delta(\mathbf{d} - \mathbf{g}(\mathbf{m}))\ \mu_M(\mathbf{m}) \ , \tag{2}$$

where $\mu_M(\mathbf{m})$ is the marginal reference p.d.f. for $\mathbf{m}$.

The a posteriori p.d.f. in the model space is

$$\sigma_M(\mathbf{m}) = \int d\mathbf{d}\ \ \sigma(\mathbf{d},\mathbf{m}) = \frac{\rho(\mathbf{g}(\mathbf{m}),\mathbf{m})}{\mu(\mathbf{g}(\mathbf{m}),\mathbf{m})}\ \mu_M(\mathbf{m}) \ , \tag{3}$$

while the a posteriori p.d.f. in the data space is

$$\sigma_D(\mathbf{d}) = \int d\mathbf{m}\ \ \sigma(\mathbf{d},\mathbf{m}) = \int d\mathbf{m}\ \frac{\rho(\mathbf{d},\mathbf{m})}{\mu(\mathbf{d},\mathbf{m})}\ \delta(\mathbf{d}-\mathbf{g}(\mathbf{m}))\ \mu_M(\mathbf{m}) \ . \tag{4}$$

Using the bijection, the last sum can be transformed on a sum over a variable $\mathbf{d}' = \mathbf{g}(\mathbf{m})$:

$$\sigma_D(\mathbf{d}) = \int d\mathbf{d}'\ \frac{1}{\left| \frac{\partial \mathbf{g}}{\partial \mathbf{m}} \right|}\ \frac{\rho(\mathbf{d},\mathbf{g}^{-1}(\mathbf{d}'))}{\mu(\mathbf{d},\mathbf{g}^{-1}(\mathbf{d}'))}\ \delta(\mathbf{d}-\mathbf{d}')\ \ \mu_M(\mathbf{g}^{-1}(\mathbf{d}'))$$

$$= \frac{1}{\left| \frac{\partial \mathbf{g}}{\partial \mathbf{m}} \right|}\ \frac{\rho(\mathbf{d},\mathbf{g}^{-1}(\mathbf{d}))}{\mu(\mathbf{d},\mathbf{g}^{-1}(\mathbf{d}))}\ \mu_M(\mathbf{g}^{-1}(\mathbf{d})) \ . \tag{5}$$

In particular, we have

$$\sigma_D(\mathbf{g}(\mathbf{m})) = \frac{1}{\left| \frac{\partial \mathbf{g}}{\partial \mathbf{m}} \right|}\ \frac{\rho(\mathbf{g}(\mathbf{m}),\mathbf{m})}{\mu(\mathbf{g}(\mathbf{m}),\mathbf{m})}\ \mu_M(\mathbf{m}) \ , \tag{6}$$

and, by comparison with (eq1) we deduce

$$\sigma_M(\mathbf{m}) = \sigma_D(\mathbf{g}(\mathbf{m}))\ \left| \frac{\partial \mathbf{g}}{\partial \mathbf{m}} \right| \ , \tag{7}$$

which is the usual formula relating information in variables related through an exact bijection.

It should be noticed that $\rho_D(\mathbf{g}(\mathbf{m}))$ and $\sigma_M(\mathbf{m}))$ are **not** related by such an equation, as can be expected using more naïve approaches to inverse problem theory.

Problem 1.19: Letting $\mathbf{G}$ be an arbitrary linear operator from a vector space $\boldsymbol{M}$ into a vector space $\boldsymbol{D}$, and $\mathbf{C_M}$ and $\mathbf{C_D}$ two covariance operators acting respectively on $\boldsymbol{M}$ and $\boldsymbol{D}$ (i.e., two linear, symmetric, positive definite operators), demonstrate the following identities:

$$\boxed{(\mathbf{G}^t\,\mathbf{C_D}^{-1}\,\mathbf{G} + \mathbf{C_M}^{-1})^{-1}\,\mathbf{G}^t\,\mathbf{C_D}^{-1} = \mathbf{C_M}\,\mathbf{G}^t\,(\mathbf{C_D} + \mathbf{G}\,\mathbf{C_M}\,\mathbf{G}^t)^{-1}\,,} \tag{1}$$

$$\boxed{(\mathbf{G}^t\,\mathbf{C_D}^{-1}\,\mathbf{G} + \mathbf{C_M}^{-1})^{-1} = \mathbf{C_M} - \mathbf{C_M}\,\mathbf{G}^t\,(\mathbf{C_D} + \mathbf{G}\,\mathbf{C_M}\,\mathbf{G}^t)^{-1}\,\mathbf{G}\,\mathbf{C_M}\,.} \tag{2}$$

Solution: The first equation follows from the following obvious identities

$$\begin{aligned}\mathbf{G}^t + \mathbf{G}^t\,\mathbf{C_D}^{-1}\,\mathbf{G}\,\mathbf{C_M}\,\mathbf{G}^t &= \mathbf{G}^t\,\mathbf{C_D}^{-1}\,(\mathbf{C_D} + \mathbf{G}\,\mathbf{C_M}\,\mathbf{G}^t)\\ &= (\mathbf{G}^t\,\mathbf{C_D}^{-1}\,\mathbf{G} + \mathbf{C_M}^{-1})\,\mathbf{C_M}\,\mathbf{G}^t\end{aligned} \tag{3}$$

since $\mathbf{G}^t\,\mathbf{C_D}^{-1}\,\mathbf{G} + \mathbf{C_M}^{-1}$ and $\mathbf{C_D} + \mathbf{G}\,\mathbf{C_M}\,\mathbf{G}^t$ are positive definite and, thus, regular matrices. Furthermore,

$$\begin{aligned}&\mathbf{C_M} - \mathbf{C_M}\,\mathbf{G}^t\,(\mathbf{C_D} + \mathbf{G}\,\mathbf{C_M}\,\mathbf{G}^t)^{-1}\,\mathbf{G}\,\mathbf{C_M}\\ &= \mathbf{C_M} - (\mathbf{G}^t\,\mathbf{C_D}^{-1}\,\mathbf{G} + \mathbf{C_M}^{-1})^{-1}\,\mathbf{G}^t\,\mathbf{C_D}^{-1}\,\mathbf{G}\,\mathbf{C_M}\\ &= (\mathbf{G}^t\,\mathbf{C_D}^{-1}\,\mathbf{G} + \mathbf{C_M}^{-1})^{-1}\,((\mathbf{G}^t\,\mathbf{C_D}^{-1}\,\mathbf{G} + \mathbf{C_M}^{-1})\,\mathbf{C_M} - \mathbf{G}^t\,\mathbf{C_D}^{-1}\,\mathbf{G}\,\mathbf{C_M})\\ &= (\mathbf{G}^t\,\mathbf{C_D}^{-1}\,\mathbf{G} + \mathbf{C_M}^{-1})^{-1}\,.\end{aligned} \tag{4}$$

Problem 1.20 (the convolution of two Gaussians is Gaussian): Evaluate the sum

$$I = \int \mathbf{dd}\,\exp\left[-\frac{1}{2}\left[(\mathbf{d}-\mathbf{d_0})^t\,\mathbf{C_d}^{-1}\,(\mathbf{d}-\mathbf{d_0}) + (\mathbf{d}-\mathbf{g}(\mathbf{m}))^t\,\mathbf{C_T}^{-1}\,(\mathbf{d}-\mathbf{g}(\mathbf{m}))\right]\right]. \tag{1}$$

Solution: The separation of the quadratic terms from the linear terms leads to:

$$I = \int dd \exp\left(-\frac{1}{2}(d^t\ A\ d - 2\ b^t\ d + c)\right), \tag{2}$$

where

$$A = C_d^{-1} + C_T^{-1} \tag{3a}$$

$$b^t = d_0^t\ C_d^{-1} + g(m)^t\ C_T^{-1} \tag{3b}$$

$$c = d_0^t\ C_T^{-1}\ d_0 + g(m)^t\ C_T^{-1}\ g(m)\ . \tag{3c}$$

Since A is positive definite, it follows:

$$I = \int dd \exp\left(-\frac{1}{2}((d-A^{-1}\ b)^t\ A\ (d-A^{-1}\ b) + (c-b^t\ A^{-1}\ b))\right)$$

$$= \exp\left(-\frac{1}{2}(c-b^t\ A^{-1}\ b)\right) \int dd \exp\left(-\frac{1}{2}(d-A^{-1}\ b)^t\ A\ (d-A^{-1}\ b)\right)$$

$$= (2\pi)^{n/2}\ (\det A)^{-1/2} \exp\left(-\frac{1}{2}\ (c - b^t\ A^{-1}\ b)\right). \tag{4}$$

By substitution we obtain

$$\begin{aligned} c - b^t\ A^{-1}\ b = {} & d_0^t \left(C_d^{-1} - C_d^{-1} \left(C_d^{-1} + C_T^{-1} \right) C_d^{-1} \right) d_0 \\ & + g(m)^t \left(C_T^{-1} - C_T^{-1} \left(C_d^{-1} + C_T^{-1} \right) C_T^{-1} \right) g(m) \\ & - 2\ g(m)^t\ C_T^{-1} \left(C_d^{-1} + C_T^{-1} \right) C_d^{-1}\ d_0\ . \end{aligned} \tag{5}$$

Thus, by using the two identities demonstrated in the previous problem, we get

$$\begin{aligned} c - b^t\ A^{-1}\ b = {} & d_0\ (\ C_d + C_T\ )^{-1}\ d_0 + g(m)^t\ (\ C_d + C_T\ )^{-1}\ g(m) \\ & - 2\ g(m)^t\ (\ C_d + C_T\ )^{-1}\ d_0 \end{aligned}$$

$$= (d_0 - g(m))^t (C_d + C_T)^{-1} (d_0 - g(m)) . \quad (6)$$

Finally, we obtain:

$$I = (2\pi)^{n/2} \det(C_D^{-1}+C_T^{-1})^{-1/2} \exp\left[-\frac{1}{2}(d_0-g(m))^t (C_D+C_T)^{-1} (d_0-g(m))\right]. \quad (7)$$

Problem 1.21: The Generalized Gaussian of order p is defined by

$$f_p(x) = \frac{p^{1-1/p}}{2 \sigma \Gamma(1/p)} \exp\left[- \frac{1}{p} \frac{| x - x_0 |^p}{\sigma^p} \right]. \quad (1)$$

Demonstrate that it is normalized. Give a direct computation of its ℓ_p norm estimator of dispersion.

Solution: We have

$$I_p = \int_{-\infty}^{+\infty} dx \; f_p(x) = \int_{-\infty}^{+\infty} dx \; f_p(x+x_0) = 2 \int_0^{\infty} dx \; f_p(x+x_0) =$$

$$= \frac{p^{1-1/p}}{\sigma \Gamma(1/p)} \int_0^{\infty} dx \; \exp\left[- \frac{1}{p} \frac{x^p}{\sigma^p} \right]. \quad (2)$$

Introducing the variable

$$u = \frac{x^p}{p \, x^{p-1}}, \quad (3)$$

we successively have

$$du = \frac{x^{p-1} \, dx}{\sigma^p}, \quad (4)$$

$$dx = \frac{\sigma^p}{x^{p-1}} du = \frac{\sigma \, u^{1-1/p}}{p^{1-1/p}} du, \quad cc(5)$$

and

$$I_p = \frac{1}{\Gamma(1/p)} \int_0^{\infty} du \; u^{1-1/p} \; e^{-u} . \quad (6)$$

Using the definition of the Gamma function

$$\Gamma(t) = \int_0^{\infty} du \; u^{1-t} \; e^{-u} \; , \tag{7}$$

we directly obtain

$$I_p = \int_{-\infty}^{+\infty} dx \; f_p(x) = 1 \; . \tag{8}$$

By definition, the estimator of dispersion in norm ℓ_p is (see Box 1.2)

$$\sigma_p = \left(\int_{-\infty}^{+\infty} dx \; | \; x - x_0 \; |^p \; f_p(x) \right)^{1/p} \; . \tag{9}$$

We successively have

$$\sigma_p = \left(\int_{-\infty}^{+\infty} dx \; | \; x \; |^p \; f_p(x+x_0) \right)^{1/p} = \left(2 \int_0^{\infty} dx \; | \; x \; |^p \; f_p(x+x_0) \right)^{1/p}$$

$$= \left(\frac{p^{1-1/p}}{\sigma \, \Gamma(1/p)} \int_0^{\infty} dx \; x^p \; \exp\left(- \frac{1}{p} \frac{x^p}{\sigma^p} \right) \right)^{1/p} \; , \tag{10}$$

and, again using the change of variables previously defined

$$\sigma_p = \left(\frac{p \, \sigma^p}{\Gamma(1/p)} \int_0^{\infty} du \; u^{1-(1+1/p)} \; e^{-u} \right)^{1/p} = \left(\frac{p \, \sigma^p \, \Gamma(1+1/p)}{\Gamma(1/p)} \right)^{1/p} \; . \tag{11}$$

Finally, using the property $\Gamma(1+t) = t \, \Gamma(t)$, we obtain

$$\sigma_p = \sigma \; . \tag{12}$$

CHAPTER 2

THE TRIAL AND ERROR METHOD

Would you tell me, please, which way I ought to go from here?,
said Alice,
That depends a good deal on where you want to get to,
said the Cat,
I don't much care where,
said Alice,
Then it doesn't matter which way you go,
said the Cat.

Lewis Carroll, 1865.

Let $\mathbf{m}$ represent an arbitrary model, $\mathbf{d}_{obs}$ the observed data values, and

$$\mathbf{d}_{cal} = \mathbf{g}(\mathbf{m})$$

the predicted data values for the model $\mathbf{m}$. *Trial and* (correction of) *error* is a method in which a user starts from some initial model $\mathbf{m}_0$, computes $\mathbf{d}_{cal} = \mathbf{g}(\mathbf{m}_0)$, compares $\mathbf{d}_{cal}$ with $\mathbf{d}_{obs}$, and appeals to his physical intuition to guess a new model $\mathbf{m}_1$ for which $\mathbf{g}(\mathbf{m}_1)$ fits the observed data values better than $\mathbf{g}(\mathbf{m}_0)$. The procedure is iterated until successive updatings of the model do not significantly improve the fit between observed and computed data values.

Usually, the method is worked interactively on a computer terminal which allows a convenient display of the data. The misfit between observed and computed data values may be measured through some "cost function" (such as, for instance, equation (1.104)), or may simply be qualitatively estimated. Only model updatings are considered which are compatible with the user's a priori information on model parameters.

CHAPTER 3

MONTE CARLO METHODS

Dans l'ordre biologique établi par la sélection,
le hasard vient de temps en temps semer le désordre.
Il secoue périodiquement ces barrières trop contraignantes
et permet à l'évolution de changer de cap.
Le hasard est anti-conservateur.

Jacques Ruffié, 1982

We have seen in Chapter 1 that the most general method for solving nonlinear inverse problems needs a complete exploration of the model space. For problems other than academic, the method is in general too computer intensive to be useful. This is why usual methods limit their scope to obtaining some "best" model, i.e., a model maximizing the probability density $\sigma_M(\mathbf{m})$ or minimizing some misfit function $S(\mathbf{m})$.

If the forward problem is not excessively nonlinear, the functions $\sigma_M(\mathbf{m})$ and/or $S(\mathbf{m})$ are well behaved and usually have a single extremum, which can be obtained, for instance, using gradient methods, i.e., methods that use the local properties of the function at a current point $\mathbf{m}_n$ to decide on a direction of search for the updated model $\mathbf{m}_{n+1}$. For highly nonlinear problems, there is a considerable risk that gradient methods will converge to secondary solutions. It happens that, for model spaces with more than a few parameters, it is dramatically more economical to select points in the model space randomly, than to define a regular grid dense enough to ensure that at least one point will be in the optimal area.

Any method which uses a random (or pseudo-random) generator at any stage is named *Monte Carlo*, in homage to the famous casino. For instance, we can use a Monte Carlo method for computing the number π: on a regular floor, made of strips of equal width w, we throw needles of length $l = w/2$. The probability that a needle will intersect a groove in the floor equals $1/\pi$ (Georges Louis Leclerc, Comte de Buffon (1707-1788)). Deltheil (1926)

CHAPTER 4

THE LEAST-SQUARES (ℓ_2-norm) CRITERION

If we know that our individual errors and fluctuations
follow the magic bell-shaped curve *exactly*,
then the resulting estimates are known to have
almost all the nice properties that people have been able to think of.

John W. Tukey, 1965.

Least squares are so popular for solving inverse problems because they lead to the easiest computations. Their only drawback is their lack of robustness, i.e., their strong sensitivity to a small number of large errors (outliers) in a data set.

In this book, the least-squares criterion is justified by the hypothesis that all sources of errors present in the problem can be modeled using Gaussian functions. Covariance operators play a central role in the method. The underlying mathematics are simple and beautiful.

The methods of resolution suggested in this chapter are based on the classical optimization theory. Gradient and Newton methods for the resolution of nonlinear problems are introduced. The approach followed in this chapter is fully nonlinear, and linear or linearized problems are treated as special cases.

4.1: Introducing least squares

Let $\mathbf{d}$ denote a generic data vector, $\mathbf{m}$ a generic model vector, and $\mathbf{d} = \mathbf{g}(\mathbf{m})$ the theoretical relationship between data and model parameters. A measurement of the true value of $\mathbf{d}$ gives $\mathbf{d}_{obs}$, with Gaussian uncertainties described by the covariance operator $\mathbf{C}_d$. The a priori information on $\mathbf{m}$ may be described by the a priori value $\mathbf{m}_{prior}$, with Gaussian uncertainties described by the covariance operator $\mathbf{C}_M$. Finally, the theoretical relationship $\mathbf{d} = \mathbf{g}(\mathbf{m})$ holds only approximately, and the corresponding uncertainties are Gaussian and are described by the covariance operator $\mathbf{C}_T$. As demonstrated in Chapter 1, the probability density representing the posterior information in the model space is then given by (equation 1.85):

$$\sigma_M(m) = \text{const} \times \tag{4.1}$$
$$\times \exp\left(-\frac{1}{2}\left((\mathbf{g}(\mathbf{m})-\mathbf{d}_{obs})^t\, \mathbf{C}_D^{-1}\, (\mathbf{g}(\mathbf{m})-\mathbf{d}_{obs}) + (\mathbf{m}-\mathbf{m}_{prior})^t\, \mathbf{C}_M^{-1}\, (\mathbf{m}-\mathbf{m}_{prior})\right)\right).$$

where

$$\mathbf{C}_D = \mathbf{C}_d + \mathbf{C}_T\,. \tag{4.2}$$

If the equation solving the forward problem is linear

$$d^i_{cal} = g^i(m) = \sum_{\alpha \in I_M} G^{i\alpha}\, m^\alpha \qquad (i \in I_D)\,, \tag{4.3a}$$

or, for short,

$$\mathbf{d}_{cal} = \mathbf{G}\,\mathbf{m}\,, \tag{4.3b}$$

the posterior probability density $\sigma_M(\mathbf{m})$ *is then Gaussian* (equations (1.89) to (1.94)):

$$\sigma_M(m) = ((2\pi)^{NM} \det \mathbf{C}_{M'})^{1/2} \exp\left(-\frac{1}{2}\,(\mathbf{m}-\langle\, \mathbf{m}\,\rangle)^t\, \mathbf{C}_{M'}^{-1}\, (\mathbf{m}-\langle\, \mathbf{m}\,\rangle)\right), \tag{4.4}$$

with center

$$\langle\, \mathbf{m}\,\rangle = \left(\mathbf{G}^t\, \mathbf{C}_D^{-1}\, \mathbf{G} + \mathbf{C}_M^{-1}\right)^{-1} \left(\mathbf{G}^t\, \mathbf{C}_D^{-1}\, \mathbf{d}_{obs} + \mathbf{C}_M^{-1}\, \mathbf{m}_{prior}\right), \tag{4.5a}$$

$$= \mathbf{m}_{prior} + \left(\mathbf{G}^t\, \mathbf{C}_D^{-1}\, \mathbf{G} + \mathbf{C}_M^{-1}\right)^{-1} \mathbf{G}^t\, \mathbf{C}_D^{-1}\, (\mathbf{d}_{obs} - \mathbf{G}\,\mathbf{m}_{prior})\,, \tag{4.5b}$$

$$= \mathbf{m}_{prior} + \mathbf{C}_M \mathbf{G}^t \left(\mathbf{G} \mathbf{C}_M \mathbf{G}^t + \mathbf{C}_D \right)^{-1} (\mathbf{d}_{obs} - \mathbf{G} \mathbf{m}_{prior}) , \qquad (4.5c)$$

and covariance operator

$$\mathbf{C}_{M'} = \left(\mathbf{G}^t \mathbf{C}_D^{-1} \mathbf{G} + \mathbf{C}_M^{-1} \right)^{-1} , \qquad (4.6a)$$

$$= \mathbf{C}_M - \mathbf{C}_M \mathbf{G}^t \left(\mathbf{G} \mathbf{C}_M \mathbf{G}^t + \mathbf{C}_D \right)^{-1} \mathbf{G} \mathbf{C}_M . \qquad (4.6b)$$

The value $\langle \mathbf{m} \rangle$, center of the Gaussian, is both the mean value of $\sigma_M(\mathbf{m})$ and its maximum likelihood point. It is abusively referred to as *the* solution of the inverse problem. We see thus that, for linear problems, we have explicit expressions for the solution and for the posterior covariance operator.

If the forward problem is nonlinear, the posterior probability density $\sigma_M(\mathbf{m})$ is not Gaussian, and the analysis of the solution is not so straightforward. For strongly nonlinear problems, $\sigma_M(\mathbf{m})$ may be quite chaotic (multimodal, with infinite dispersions, etc.), and the general methods described in Chapter 1 should be used to analyse the solution. If $\sigma_M(\mathbf{m})$ is reasonably well behaved, the a posteriori information in the model space may be well represented by a central estimator of $\sigma_M(\mathbf{m})$ and a properly defined covariance operator. Among all the central estimators, the easiest to compute is generally the maximum likelihood point $\mathbf{m}_{ML}$:

$$\sigma_M(\mathbf{m}) \qquad \textit{MAXIMUM} \qquad \text{for} \qquad \mathbf{m} = \mathbf{m}_{ML} , \qquad (4.7a)$$

because the obtainment of $\mathbf{m}_{ML}$ corresponds to a problem of optimization of a scalar function, and many methods exist allowing an economical resolution of that problem.

Defining the *misfit* function (or *cost* function, or *objective* function, or *least-squares* function, or *chi-squared* function) by

$$\boxed{S(\mathbf{m}) = \frac{1}{2} \left((\mathbf{g}(\mathbf{m}) - \mathbf{d}_{obs})^t \mathbf{C}_D^{-1} (\mathbf{g}(\mathbf{m}) - \mathbf{d}_{obs}) + (\mathbf{m} - \mathbf{m}_{prior})^t \mathbf{C}_M^{-1} (\mathbf{m} - \mathbf{m}_{prior}) \right) ,} \qquad (4.8)$$

the maximum likelihood point is clearly defined by

$$S(\mathbf{m}) \qquad \textit{MINIMUM} \qquad \text{for} \qquad \mathbf{m} = \mathbf{m}_{ML} . \qquad (4.7b)$$

For uncorrelated errors,

$$(C_D)^{ij} = (\sigma_D^i)^2 \, \delta^{ij},$$

$$(C_M)^{\alpha\beta} = (\sigma_M^\alpha)^2 \, \delta^{\alpha\beta},$$

the misfit function $S(\mathbf{m})$ becomes

$$S(\mathbf{m}) = \frac{1}{2} \left(\sum_{i \in I_D} \frac{\left(g^i(\mathbf{m}) - d^i_{obs} \right)^2}{\left(\sigma_D^i \right)^2} + \sum_{\alpha \in I_M} \frac{\left(m^\alpha - m^\alpha_{prior} \right)^2}{\left(\sigma_M^\alpha \right)^2} \right),$$

which justifies the name of *least-squares* for the criterion (4.7b).

As introduced here, the least-squares criterion is intimately related with the Gaussian probability assumption. Many people like to justify least squares from a statistical point of view. They deal almost exclusively with linear problems. For them, $\mathbf{d}$ and $\mathbf{m}$ are random variables with known covariance operators C_D and C_M, and unknown mathematical expectations $\mathbf{d}_{true}$ and $\mathbf{m}_{true}$. $\mathbf{d}_{obs}$ and $\mathbf{m}_{prior}$ are then interpreted as two particular *realizations* of the random variables $\mathbf{d}$ and $\mathbf{m}$. The problem is then to obtain an estimator of $\mathbf{m}_{true}$, $\mathbf{m}_{est}$, which is, in some sense, optimum. The Gauss-Markoff theorem (see, for instance, Plackett, 1949, or Rao, 1973) shows that, *for linear problems*, the least-squares estimator has *minimum variance* among all the estimators which are linear functions of $\mathbf{d}_{obs}$ and $\mathbf{m}_{prior}$, *irrespectively of the particular form of the probability density functions of the random variables* $\mathbf{d}$ *and* $\mathbf{m}$. This is why the least-squares criterion is sometimes used even if the form of the density functions is not Gaussian. The trouble is that the criterion of minimum variance is not magic, and, in fact, it may be a *very bad* criterion in some cases, such as, for instance, when a small number of large, uncontrolled errors are present in a data set (see problem 1.9). As the general approach developed in Chapter 1 justifies the least-squares criterion only when all errors (modelization errors, observational errors, errors in the a priori model) are Gaussian, I urge the reader to limit the use of the techniques described in this chapter to the cases where this assumption is not too strongly violated.

It often happens that some model parameters are, by definition, positive. To take a Gaussian function to model the a priori information is not coherent because a Gaussian function gives a non-nul probability to negative values. Sometimes, a least-squares criterion is used for such parameters, completed with a positivity constraint. This is not the most rigorous nor the easiest way to attack this sort of problem. As suggested in section 1.2.4, these parameters usually accept a log-normal function as a prior probability density. Taking the *logarithm* of the positive parameter defines a new

(unbounded) parameter whose a priori probability density is Gaussian, and for which standard least-squares techniques apply.

4.2: Methods of resolution (I)

We have just seen that the central problem in general least squares consists in the minimization of the misfit function

$$S(\mathbf{m}) = \frac{1}{2}\left[(\mathbf{g}(\mathbf{m})-\mathbf{d}_{obs})^t\ \mathbf{C}_D^{-1}\ (\mathbf{g}(\mathbf{m})-\mathbf{d}_{obs}) + (\mathbf{m}-\mathbf{m}_{prior})^t\ \mathbf{C}_M^{-1}\ (\mathbf{m}-\mathbf{m}_{prior})\right].$$

This section reviews the simplest (although not necessarily the more economical) methods for the resolution of this minimization problem. After a few mathematics, section 4.5 will deal with more sophisticated methods.

4.2.1: Systematic exploration of the model space

A regular grid is defined over the model space $\mathcal{M}$, and the value $S(\mathbf{m})$ is computed at each point. Taking a dense enough grid, the point minimizing $S(\mathbf{m})$ can be approached with arbitrary accuracy. The method can only be used if the model space has a small number of dimensions.

If this method has to be used, instead of plotting $S(\mathbf{m})$ I recommend dealing directly with

$$\sigma_M(\mathbf{m}) = \text{const}\ \exp(-S(\mathbf{m}))\ ,$$

because, after proper normalization, the results obtained are directly interpretable in terms of probabilities.

4.2.2: Trial and error

If the number of dimensions of the model space is small, it is also possible to work interactively with a computer terminal, modifying the current point on an intuitive basis, until a point $\mathbf{m}$ which gives an acceptably low value for the misfit $S(\mathbf{m})$ is found. See Chapter 2 for more details.

4.2.3: Relaxation

Let $\mathbf{m}_0$ represent the "starting point". To obtain the updated point $\mathbf{m}_1$, all the components of $\mathbf{m}$ but one are fixed, and the value of the free component for which $S(\mathbf{m})$ has a minimum is obtained using an arbitrary

method (trial and error, interpolation,...). All the components of $\mathbf{m}$ are chosen in turn, and the procedure is iterated until subsequent updatings alter the result only negligibly. Figure 4.1 illustrates the method. The convergence rate is, in general, poor.

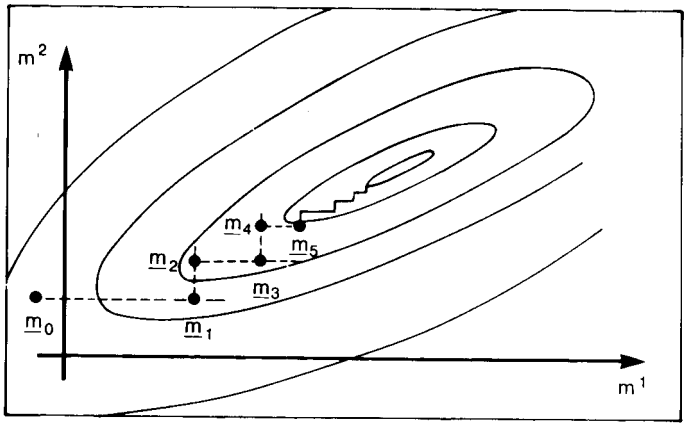


Figure 4.1: The path obtained using the relaxation method of minimization in a schematic problem with two variables.

4.2.4: Monte Carlo methods

As explained in Chapter 3, a Monte Carlo method is any method using a random generator at any stage. These methods are particularly useful for highly nonlinear problems. In its simplest formulation, a threshold value of S is fixed. Any model $\mathbf{m}$ for which $S(\mathbf{m})$ is less than the threshold value is named an *acceptable* model. Random points are generated over the model space $\boldsymbol{M}$ until a sufficient number of acceptable models has been obtained as being representative of the acceptable domain of the model space (see Chapter 3 for more details).

4.2.5: The Gauss-Newton method

If the functions $g^i(\mathbf{m})$ solving the forward problem are differentiable, i.e., if the derivatives

$$G_n^{i\alpha} = \left[\frac{\partial g^i}{\partial m^\alpha}\right]_{\mathbf{m}_n} \tag{4.9}$$

can be defined at any point $\mathbf{m}_n$ (or at "almost" any point), and if they can easily be computed, then the derivatives of $S(\mathbf{m})$ can also be easily obtained, and the very powerful gradient and Newton methods can be used for minimizing $S(\mathbf{m})$. Although their detailed study is left for section 4.5, the Gauss-Newton method is introduced here in an elementary way.

Equation (4.8) can be written explicitly as

$$S(\mathbf{m}) = \frac{1}{2}\left\{ \sum_{i\in I_D} \sum_{j\in I_D} \left(g^i(\mathbf{m})-d^i_{obs}\right) \left(C_D^{-1}\right)^{ij} \left(g^j(\mathbf{m})-d^j_{obs}\right) + \sum_{\alpha\in I_M} \sum_{\beta\in I_M} \left(m^\alpha-m^\alpha_{prior}\right) \left(C_M^{-1}\right)^{\alpha\beta} \left(m^\beta-m^\beta_{prior}\right) \right\}, \tag{4.10}$$

We obtain easily

$$\left(\frac{\partial S}{\partial m^\alpha}\right)_{m_n} = \sum_{i\in I_D} \sum_{j\in I_D} G_n^{i\alpha} \left(C_D^{-1}\right)^{ij} \left(g^j(\mathbf{m}_n)-d^j_{obs}\right) + \sum_{\beta\in I_M} \left(C_M^{-1}\right)^{\alpha\beta} \left(m^\beta-m^\beta_{prior}\right), \tag{4.11}$$

or, in more compact notation,

$$\left(\frac{\partial S}{\partial \mathbf{m}}\right)_n = \mathbf{G}_n^t \, \mathbf{C}_D^{-1} \left(g(\mathbf{m}_n)-\mathbf{d}_{obs}\right) + \mathbf{C}_M^{-1} \left(\mathbf{m}_n-\mathbf{m}_{prior}\right) . \tag{4.12}$$

The vector defined in (4.11) and (4.12) is named the *gradient* of $S(\mathbf{m})$ at $\mathbf{m} = \mathbf{m}_n$ (see Box 4.7 for more details). At the minimum of S , the gradient will vanish:

$$S(\mathbf{m}) \quad \text{minimum} \quad \text{for} \quad \mathbf{m} = \mathbf{m}_n \quad \Rightarrow \quad \left(\frac{\partial S}{\partial \mathbf{m}}\right)_{m_n} = 0 ,$$

the reciprocal of course not necessarily being true. In practical applications, once we get a point at which the gradient vanishes, in general it is easy to verify that it is not a maximum of S or a saddle point, because when any iterative method provides a sequence of points $\mathbf{m}_1$, $\mathbf{m}_2$, ..., it is easy to verify that the sequence $S(\mathbf{m}_1)$, $S(\mathbf{m}_2)$,..., is decreasing. Saddle points are in general not obtained with iterative methods because the path leading to them is very unstable (the only possible way for a drop of rain to reach the saddle point of a horse saddle is just to fall on that point).

Another more difficult question is to know whether the point reached is *the* absolute minimum, or if it only is a secondary minimum. As no local test can answer the question, the only possibility is to start iterating at different

points and to check if we converge into the same point.

A traditional way of obtaining the minimum of a function (i.e., the zero of its gradient) is to use the Newton method:

$$\mathbf{m}_{n+1} = \mathbf{m}_n - \left(\frac{\partial^2 S}{\partial \mathbf{m}^2}\right)^{-1}_{\mathbf{m}_n} \left(\frac{\partial S}{\partial \mathbf{m}}\right)_{\mathbf{m}_n} , \tag{4.13}$$

where the operator $\partial S^2/\partial \mathbf{m}^2$ is named the *Hessian* of S, and is here defined by its components:

$$\left(\frac{\partial S^2}{\partial \mathbf{m}^2}\right)^{\alpha\beta} = \frac{\partial}{\partial m^\beta} \frac{\partial S}{\partial m^\alpha} = \frac{\partial^2 S}{\partial m^\alpha \partial m^\beta} . \tag{4.14}$$

From equation (4.11) we readily obtain

$$\left(\frac{\partial^2 S}{\partial \mathbf{m}^2}\right)^{\alpha\beta}_{\mathbf{m}_n} = \sum_{i\in I_D} \sum_{j\in I_D} G_n^{i\alpha} \left(C_D^{-1}\right)^{ij} G_n^{j\beta} + \left(C_M^{-1}\right)^{\alpha\beta}$$

$$+ \sum_{i\in I_D} \sum_{j\in I_D} \left(\frac{\partial G^{i\alpha}}{\partial m^\beta}\right)_n \left(C_D^{-1}\right)^{ij} \left(g^j(\mathbf{m}_n) - d^j_{obs}\right) . \tag{4.15}$$

The last term is small if: i) the residuals are small, or ii) the forward equation is quasi linear. As in Newton methods we never need to know the Hessian with great accuracy, and as the last term in equation (4.15) is, in general, difficult to handle, it is generally dropped off, thus giving the approximation

$$\left(\frac{\partial^2 S}{\partial \mathbf{m}^2}\right)^{\alpha\beta}_{\mathbf{m}_n} \simeq \sum_{i\in I_D} \sum_{j\in I_D} G_n^{i\alpha} \left(C_D^{-1}\right)^{ij} G_n^{j\beta} + \left(C_M^{-1}\right)^{\alpha\beta} , \tag{4.16}$$

or, in compact form,

$$\left(\frac{\partial S^2}{\partial \mathbf{m}^2}\right)_n \simeq G_n^t \, C_D^{-1} \, G_n + C_M^{-1} . \tag{4.17}$$

Using equations (4.11), (4.13), and (4.17), we arrive at the following algorithm

$$\mathbf{m}_{n+1} = \mathbf{m}_n - \left(G_n^t \, C_D^{-1} \, G_n + C_M^{-1}\right)^{-1} \left(G_n^t \, C_D^{-1} \, (g(\mathbf{m}_n) - \mathbf{d}_{obs}) + C_M^{-1} \, (\mathbf{m}_n - \mathbf{m}_{prior})\right). \tag{4.18}$$

If the components of the data and model vectors have been ordered in a column matrix, this equation can then be interpreted as an ordinary matricial

equation.

As covariance operators are, by definition, positive definite (if they do not contain null variances or perfect correlations), the matrix $\mathbf{G}_n^t \mathbf{C}_D^{-1} \mathbf{G}_n + \mathbf{C}_M^{-1}$ is symmetric and positive definite, so that Cholesky's decomposition methods can be used (see Appendix 4.5). It should be noticed that, given a regular matrix $\mathbf{A}$ and a vector $\mathbf{y}$, the most economical way of computing the vector $\mathbf{x} = \mathbf{A}^{-1} \mathbf{y}$, is *not* to compute the inverse matrix $\mathbf{A}^{-1}$, and then to multiply $\mathbf{A}^{-1}$ by $\mathbf{y}$, but to use an algorithm allowing the direct resolution of the matricial equation $\mathbf{A} \mathbf{x} = \mathbf{y}$, which can be done much more economically (see, for instance, Appendices 4.4 and 4.5).

If the functions $g^i(\mathbf{m})$ are linear, then the function $S(\mathbf{m})$ is a quadratic function of $\mathbf{m}$, in which case the Newton algorithm converges in only one iteration. For nonlinear functionals $g^i(\mathbf{m})$, not only do we need to iterate, but we cannot be sure that the Newton algorithm will converge. Thus, at each iteration we have to compute $S_{n+1} = S(\mathbf{m}_{n+1})$, and check if the condition

$$S_{n+1} \leq S_n ,$$

is fulfilled. If not, equation (4.18) has to be replaced by

$$\mathbf{m}_{n+1} = \mathbf{m}_n + \epsilon_n \left(\mathbf{G}_n^t \mathbf{C}_D^{-1} \mathbf{G}_n + \mathbf{C}_M^{-1} \right)^{-1} \left(\mathbf{G}_n^t \mathbf{C}_D^{-1} (\mathbf{g}(\mathbf{m}_n) - \mathbf{d}_{obs}) + \mathbf{C}_M^{-1} (\mathbf{m}_n - \mathbf{m}_{prior}) \right) , \qquad (4.19)$$

where ϵ_n is an ad-hoc constant less than unity. Alternatively, it is also possible to dump the Newton updates by artificially diminishing the a priori variances in $\mathbf{C}_M$. This last method is almost equivalent to the method proposed by Levenberg (1944), or Marquardt (1963). See section 4.5 for more details.

4.2.6: Characterization of the solution.

At the minimum of the misfit function, the gradient must vanish. This gives, using (4.12),

$$\mathbf{C}_M^{-1} (\mathbf{m} - \mathbf{m}_{prior}) = - \mathbf{G}^t \mathbf{C}_D^{-1} (\mathbf{g}(\mathbf{m}) - \mathbf{d}_{obs}) .$$

Adding $\mathbf{G}^t \mathbf{C}_D^{-1} \mathbf{G} (\mathbf{m} - \mathbf{m}_{prior})$ to both sides we obtain

$$\left(\mathbf{G}^t\,\mathbf{C}_D^{-1}\,\mathbf{G} + \mathbf{C}_M^{-1}\right)(\mathbf{m}-\mathbf{m}_{prior}) = -\,\mathbf{G}^t\,\mathbf{C}_D^{-1}\,(\mathbf{g}(\mathbf{m})-\mathbf{d}_{obs}-\mathbf{G}\,(\mathbf{m}-\mathbf{m}_{prior})),$$

i.e.,

$$\mathbf{m} = \mathbf{m}_{prior} - \left(\mathbf{G}^t\,\mathbf{C}_D^{-1}\,\mathbf{G} + \mathbf{C}_M^{-1}\right)^{-1}\,\mathbf{G}^t\,\mathbf{C}_D^{-1}\,(\mathbf{g}(\mathbf{m})-\mathbf{d}_{obs}-\mathbf{G}\,(\mathbf{m}-\mathbf{m}_{prior}))\,, \tag{4.20a}$$

or, using the identity demonstrated in problem 1.19,

$$\mathbf{m} = \mathbf{m}_{prior} - \mathbf{C}_M\,\mathbf{G}^t\left(\mathbf{C}_D + \mathbf{G}\,\mathbf{C}_M\,\mathbf{G}\right)^{-1}(\mathbf{g}(\mathbf{m})-\mathbf{d}_{obs}-\mathbf{G}\,(\mathbf{m}-\mathbf{m}_{prior}))\,. \tag{4.20b}$$

Equations (4.20) characterize the solution. Notice that these are implicit equations (the unknown $\mathbf{m}$ appears at both sides). In fact it is possible to obtain the solution from (4.20) using a fixed point algorithm:

$$\mathbf{m}_{n+1} = \mathbf{m}_{prior} - \left(\mathbf{G}_n^t\,\mathbf{C}_D^{-1}\,\mathbf{G}_n + \mathbf{C}_M^{-1}\right)^{-1}\,\mathbf{G}_n^t\,\mathbf{C}_D^{-1}\,(\mathbf{g}(\mathbf{m}_n)-\mathbf{d}_{obs}-\mathbf{G}_n\,(\mathbf{m}_n-\mathbf{m}_{prior}))\,, \tag{4.21a}$$

$$\mathbf{m}_{n+1} = \mathbf{m}_{prior} - \mathbf{C}_M\,\mathbf{G}_n^t\left(\mathbf{C}_D + \mathbf{G}_n\,\mathbf{C}_M\,\mathbf{G}_n\right)^{-1}(\mathbf{g}(\mathbf{m}_n)-\mathbf{d}_{obs}-\mathbf{G}_n\,(\mathbf{m}_n-\mathbf{m}_{prior}))\,. \tag{4.21b}$$

4.3: Analysis of error and resolution

4.3.1: Computation of the posterior covariance operator

We have seen in section 4.1 that if the equation solving the forward problem is linear,

$$\mathbf{g}(\mathbf{m}) = \mathbf{G}\,\mathbf{m}\,,$$

the posterior probability density is then Gaussian (equation (4.4)), with center given by (4.5), and with covariance operator given by

$$\mathbf{C}_{M'} = \left(\mathbf{G}^t\,\mathbf{C}_D^{-1}\,\mathbf{G} + \mathbf{C}_M^{-1}\right)^{-1} \tag{4.22a}$$

$$= \mathbf{C}_M - \mathbf{C}_M \mathbf{G}^t \left(\mathbf{G} \mathbf{C}_M \mathbf{G}^t + \mathbf{C}_D \right)^{-1} \mathbf{G} \mathbf{C}_M \,. \tag{4.22b}$$

A problem is "linearizable around $\mathbf{m}_{ref}$ " if, for any $\mathbf{m}$ of interest,

$$\mathbf{g}(\mathbf{m}) \simeq \mathbf{g}(\mathbf{m}_{ref}) + \mathbf{G}_{ref} (\mathbf{m} - \mathbf{m}_{ref}) \tag{4.23}$$

where

$$\mathbf{G}_{ref} = \left(\frac{\partial \mathbf{g}}{\partial \mathbf{m}} \right)_{\mathbf{m}_{ref}} \,. \tag{4.24}$$

$\mathbf{m}_{ref}$ is named the reference model and usually (but not necessarily) corresponds to the a priori model

$$\mathbf{m}_{ref} = \mathbf{m}_{prior} \,. \tag{4.25}$$

It is easy to see that within the approximation (4.23), the a posteriori probability density in the model space is approximately Gaussian, with center

$$\langle \mathbf{m} \rangle = \mathbf{m}_{prior} - \left(\mathbf{G}_{ref}^t \mathbf{C}_D^{-1} \mathbf{G}_{ref} + \mathbf{C}_M^{-1} \right)^{-1} \mathbf{G}_{ref}^t \mathbf{C}_D^{-1} (\mathbf{g}(\mathbf{m}_{prior}) - \mathbf{d}_{obs}) \tag{4.26a}$$

$$= \mathbf{m}_{prior} - \mathbf{C}_M \mathbf{G}_{ref}^t \left(\mathbf{G}_{ref} \mathbf{C}_M \mathbf{G}_{ref}^t + \mathbf{C}_D \right)^{-1} (\mathbf{g}(\mathbf{m}_{prior}) - \mathbf{d}_{obs}) \,, \tag{4.26b}$$

and covariance operator

$$\mathbf{C}_{M'} = \left(\mathbf{G}_{ref}^t \mathbf{C}_D^{-1} \mathbf{G}_{ref} + \mathbf{C}_M^{-1} \right)^{-1} \tag{4.27a}$$

$$= \mathbf{C}_M - \mathbf{C}_M \mathbf{G}_{ref}^t \left(\mathbf{G}_{ref} \mathbf{C}_M \mathbf{G}_{ref}^t + \mathbf{C}_D \right)^{-1} \mathbf{G}_{ref} \mathbf{C}_M \,. \tag{4.28b}$$

For true nonlinear problems, the approximation (4.23) is no longer acceptable. As explained in Figure 1.13, least squares can only be applied to problems where the nonlinearity is not too strong, i.e., in problems where the function $\mathbf{g}(\mathbf{m})$ is linearizable in the region of significant posterior probability density. Let $\mathbf{m}_\infty$ be the maximum likelihood of $\sigma_M(\mathbf{m})$ obtained by any of the methods described in this chapter, *without* linearizing $\mathbf{g}(\mathbf{m})$ (the index "∞" stands because the maximum likelihood point is always obtained as the limit point of an iterative algorithm). That $\mathbf{g}(\mathbf{m})$ is linearizable in the region of significant posterior probability density means that, once the point

$\mathbf{m}_\infty$ has been obtained using a nonlinear algorithm, for evaluating $\sigma_M(\mathbf{m})$ we can use the linear approximation

$$\mathbf{g}(\mathbf{m}) \simeq \mathbf{g}(\mathbf{m}_\infty) + \mathbf{G}_\infty (\mathbf{m} - \mathbf{m}_\infty) , \tag{4.29}$$

where

$$\mathbf{G}_\infty = \left(\frac{\partial \mathbf{g}}{\partial \mathbf{m}} \right)_{\mathbf{m}_\infty} \tag{4.30}$$

Inserting (4.29) in (4.1) gives

$$\sigma_M(\mathbf{m}) \simeq \text{const} \exp\left[-\frac{1}{2} (\mathbf{m}-\mathbf{m}_\infty)^t \, \mathbf{C}_{M'}^{-1} \, (\mathbf{m}-\mathbf{m}_\infty) \right] , \tag{4.31}$$

where $\mathbf{m}_\infty$ has been obtained by a nonlinear computation, and where

$$\mathbf{C}_{M'} = \left[\mathbf{G}_\infty^t \, \mathbf{C}_D^{-1} \, \mathbf{G}_\infty + \mathbf{C}_M^{-1} \right]^{-1} \tag{4.32a}$$

$$= \mathbf{C}_M - \mathbf{C}_M \, \mathbf{G}_\infty^t \left[\mathbf{G}_\infty \, \mathbf{C}_M \, \mathbf{G}_\infty^t + \mathbf{C}_D \right]^{-1} \mathbf{G}_\infty \, \mathbf{C}_M . \tag{4.32b}$$

Kennett (1978) studied the first-order modification of the posterior covariance operator due to non linearity.

If you are not sure of the validity of the linearized estimation of posterior errors, you can solve the inverse problem a few times, with different values of $\mathbf{d}_{obs}$ and of $\mathbf{m}_{prior}$, and make a rough statistics of the results. If you have more time, generate Gaussian random data vectors with mean $\mathbf{d}_{obs}$ and covariance operator $\mathbf{C}_D$ and Gaussian random model vectors with mean $\mathbf{m}_{prior}$ and covariance operator $\mathbf{C}_M$, solve the nonlinear inverse problem for each realization, and make a proper computation of the mean value and covariance operator of the results.

4.3.2: Interpretation of the posterior covariance operator

The most trivial use of the posterior covariance operator $\mathbf{C}_{M'}$ is to interpret the square roots of the diagonal elements (variances) as "error bars" describing the uncertainities on the posterior values of the model parameters.

A direct examination of the off-diagonal elements (covariances) of a covariance operator is not easy, and it is much better to introduce the *correlations*

$$\rho^{\alpha\beta} = \frac{C^{\alpha\beta}}{(C^{\alpha\alpha})^{1/2} \, (C^{\beta\beta})^{1/2}} ,$$

which have the well known property

$$-1 \leq \rho^{\alpha\beta} \leq +1 \ .$$

If the posterior correlation between parameters m^α and m^β is close to zero, the posterior uncertainties are uncorrelated (in the intuitive sense). If the correlation is close to $+1$ (resp. -1), the uncertainties are highly correlated (resp. anticorrelated). A strong correlation on uncertainties means that the two parameters have not been independently resolved by the data set, and that only some linear combination of the parameters is resolved.

Sometimes the parameters m^1, m^2, ... represent the discretized values of some spatial (or temporal) function. Each row (or column) of the posterior covariance operator can then directly be interpreted in terms of spatial (or temporal) resolution power of the data set. See the color plate in Chapter 7 for a nice example.

It should not be forgotten that a covariance operator over the model space can be represented by its "ellipsoid of error". For instance, if $\mathbf{m}_\infty$ is the maximum likelihood posterior point, and $\mathbf{C}_{M'}$ is the posterior covariance operator, then we know that the posterior probability density in the model space is Gaussian (or approximately Gaussian), as given by (4.31). We can then represent the iso-density values corresponding, for instance, to probabilities of 10% , 20% , etc.

In all usual examples, the prior covariance operators $\mathbf{C}_D$ and $\mathbf{C}_M$ are chosen regular (no null or infinite variances, no perfect correlations), so that their inverse exists. But it is possible to give more general sense to the obtained results. For instance, in equation (4.22b) the prior covariance operator $\mathbf{C}_D$ may well be singular, if $\mathbf{G}\,\mathbf{C}_M\,\mathbf{G}^t$ is not. If in equation (4.22a) the operator $\mathbf{W}_{M'} = (\mathbf{G}^t\,\mathbf{C}_D^{-1}\,\mathbf{G} + \mathbf{C}_M^{-1})$ was singular, the posterior covariance operator $\mathbf{C}_{M'} = \mathbf{W}_{M'}^{-1}$ would not be defined, but all useful information could be extracted from the weighting operator $\mathbf{W}_{M'}$. From a geometrical point of view, a regular covariance operator defines a probability density which takes its maximum at a single point. If the covariance operator is singular, the maximum corresponds to a subspace of dimension ≥ 1 .

4.3.3: The resolution operator

In the approaches to inversion not directly based on probabilistic concepts, it is usual to introduce the "resolution operator". In order to make the link with these methods, let me briefly introduce this concept.

Let $\mathbf{m}_{true}$ represent "the true" model (which is known only by the gods). The observed data values $\mathbf{d}_{obs}$ generally do not equal the computed values $\mathbf{g}(\mathbf{m}_{true})$ because of observational errors and of modelization errors. The concept of resolution operator arises when the relationship is sought between the least-squares solution $\langle\, \mathbf{m} \,\rangle$ and the true model $\mathbf{m}_{true}$,

$$\langle \mathbf{m} \rangle = \mathbf{r}(\mathbf{m}_{true}) \tag{4.33}$$

in the optimum case where, by chance, data are error free:

$$\mathbf{d}_{obs} = \mathbf{g}(\mathbf{m}_{true}) .$$

Equation (4.33) defines $\mathbf{r}(\cdot)$, the *nonlinear resolution operator*. Using equation (4.20a) and linearizing around $\langle \mathbf{m} \rangle$ we obtain

$$\langle \mathbf{m} \rangle - \mathbf{m}_{prior} = \mathbf{R} (\mathbf{m}_{true} - \mathbf{m}_{prior}) , \tag{4.34}$$

where

$$\mathbf{R} = \left[\mathbf{G}^t \mathbf{C}_D^{-1} \mathbf{G} + \mathbf{C}_M^{-1}\right]^{-1} \mathbf{G}^t \mathbf{C}_D^{-1} \mathbf{G} \tag{4.35a}$$

$$= \mathbf{C}_M \mathbf{G}^t \left[\mathbf{G} \mathbf{C}_M \mathbf{G}^t + \mathbf{C}_D\right]^{-1} \mathbf{G} , \tag{4.35b}$$

thus defining the *linearized resolution operator*, $\mathbf{R}$. From the last expression we obtain

$$\mathbf{R} = \mathbf{I} - \left[\mathbf{C}_M - \mathbf{C}_M \mathbf{G}^t \left[\mathbf{G} \mathbf{C}_M \mathbf{G}^t + \mathbf{C}_D\right]^{-1} \mathbf{G} \mathbf{C}_M\right] \mathbf{C}_M^{-1} ,$$

and, using the expression (4.6b) for the posterior covariance operator,

$$\mathbf{R} = \mathbf{I} - \mathbf{C}_{M'} \mathbf{C}_M^{-1} . \tag{4.36}$$

If the resolution operator is the identity operator, equations (4.33) or (4.34) show that $\langle \mathbf{m} \rangle = \mathbf{m}_{true}$, and the model is perfectly resolved. The farther the resolution operator is from the identity, the worse the resolution is. Following Backus and Gilbert (1968), we can consider the resolution operator as a filter: the computed a posteriori model equals the true model filtered by the resolution operator. We cannot see the real world; we can only see a filtered version. For more details (in linearized problems), the reader is referred to Backus and Gilbert (1968). Interesting examples are also given by Aki and Lee (1976) or by Aki, Christofferson and Husebye (1977).

Usually, we do not wish to examine the whole kernel $R^{\alpha\beta}$ of $\mathbf{R}$. We only wish to analyze $R^{\alpha\alpha_0}$ for some selected index α_0 (a "column" of $\mathbf{R}$, if using matrix notations). We have

$$R^{\alpha\alpha_0} = \sum_{\beta} R^{\alpha\beta} \delta^{\beta\alpha_0} .$$

Introducing the vectors $\rho_0^{\alpha} = R^{\alpha\alpha_0}$ and $u_0^{\alpha} = \delta^{\alpha\alpha_0}$,we have

$$\rho_0 = \mathbf{R}\, \mathbf{u}_0 ,$$

i.e.,

$$\rho_0 = \left[\mathbf{G}^t \mathbf{C}_D^{-1} \mathbf{G} + \mathbf{C}_M^{-1}\right]^{-1} \mathbf{G}^t \mathbf{C}_D^{-1} \mathbf{G}\, \mathbf{u}_0$$

$$= \mathbf{C}_M \mathbf{G}^t \left[\mathbf{G}\, \mathbf{C}_M\, \mathbf{G}^t + \mathbf{C}_D\right]^{-1} \mathbf{G}\, \mathbf{u}_0 .$$

As noticed by Hirahara (1986) the computation of ρ_0 will need the same operations as the computation of the solution of a linear (or linearized) problem (see for instance equations (4.5)). It follows that all the gradient methods developed in sections 4.5 to 4.7 for computing $\langle\, m \,\rangle$, can also be used to compute the resolution vector ρ_0 .

Taking the trace of equation (4.36) gives

$$\text{Trace}(\, \mathbf{I} \,) = \text{Trace}(\, \mathbf{R} \,) + \text{Trace}\left[\, \mathbf{C}_{M'}\, \mathbf{C}_M^{-1} \,\right], \qquad (4.37a)$$

an equation that that can be interpreted as follows:

$$\left[\begin{array}{c}\text{TOTAL}\\ \text{NUMBER}\\ \text{OF}\\ \text{MODEL}\\ \text{PARAMETERS}\end{array}\right] = \left[\begin{array}{c}\text{NUMBER OF}\\ \text{PARAMETERS}\\ \text{RESOLVED}\\ \text{BY THE DATA}\\ \text{SET}\end{array}\right] + \left[\begin{array}{c}\text{NUMBER OF}\\ \text{PARAMETERS}\\ \text{RESOLVED BY}\\ \text{THE A PRIORI}\\ \text{INFORMATION}\end{array}\right]. \qquad (4.37b)$$

4.3.4: Eigenvector analysis

CHAPTER 5

THE LEAST-ABSOLUTE-VALUES (ℓ_1-norm) CRITERION AND THE MINIMAX (ℓ_∞-norm) CRITERION

When a traveler reaches a fork in the road,
the ℓ_1-norm tells him to take either one way or the other,
but the ℓ_2-norm instructs him to head off into the bushes.

John F. Claerbout and Francis Muir, 1973.

Because of its simplicity, the least-squares criterion (ℓ_2-norm criterion) is widely used for the resolution of inverse problems. We have seen that least squares is intimately related with the hypothesis of Gaussian uncertainties. For other types of uncertainties, better criteria exist. Among them, those based on an ℓ_p norm ($1 \leq p \leq \infty$) have the advantage of allowing an easy mathematical formulation.

As suggested in Chapter 1, when outliers are suspected in a data set, long-tailed probability density functions should be used to model uncertainties. "Long tailed" means, in fact, functions tending to zero less rapidly than the Gaussian function, when the distance between the variable and any of its central estimators tends to infinity. Two typical long-tailed probability densities are: the Cauchy function $1/(1+x^2)$ and the symmetric exponential function $\exp(-|x|)$. The former is a very tempting function to use because, although being nicely bell-shaped, it has infinite variance, which seems to be adequate for modeling suspected outliers by an unknown amount. The symmetric exponential function, on the other hand, has the advantage of leading to results intimately related with the concept of the ℓ_1 norm, so that a lot of mathematics are already available for solving the problem. The results obtained using the minimum ℓ_1-norm (least-absolute-values) criterion are known to be sufficiently insensitive to outliers (i.e., to be *robust*).

The ℓ_1-norm criterion was already used by Laplace and Gauss. In the words of Gauss (1809), quoted by Plackett (1972), "Laplace made use of another principle for the solution of linear equations, the number of which is

CHAPTER 6

THE GENERAL PROBLEM

When in doubt, smooth.

Sir Harold Jeffreys (Quoted by Moritz, 1980)

Many inverse problems involve functions: the data set sometimes consists in recordings as a function of time or space, and the main unknown in the parameter set sometimes consist in a function of the spatial coordinates and/or of time. Nevertheless, there are two kinds of arguments suggesting that the Inverse Theory could be limited to finite-dimensional problems:

i) The "technological" argument: data "functions" are recorded digitally (or, if they are recorded analogically, they have a finite bandwidth and, thus, a finite amount of information (Shannon, 1948)). The "functions" used to describe the model are handled by digital computers which can only consider a finite amount of information.

ii) The "mathematical" argument: central in the theory of inverse problems is the concept of probability. We will see in this chapter that the concept of probability density function, so essential for finite-dimensional spaces, cannot be generalized to infinite-dimensional spaces. Also, in a function space, a probability can only be defined over certain subsets, named cylinder sets, whose elements have, in fact, a finite number of degrees of freedom.

For the general inverse problem, these arguments prevail. From both the technological and mathematical points of view, after a proper understanding of all the subtleties of infinite-dimensional spaces, practical applications can only be developed over discretized problems (with finite numbers of degrees of freedom). It is only for particular cases (e.g., Gaussian assumption) that the functional approach reveals itself to be tremendously more powerful (both practically and intellectually) than the discretized approach, as demonstrated in Chapter 7.

CHAPTER 7

THE LEAST-SQUARES CRITERION IN FUNCTIONAL SPACES

Tu quoque, fili!.

Caius Julius Caesar
(when he saw that even Brutus discretized least-squares problems).

Many objects in the physical world are "fields", i.e., functions defined over spatial coordinates and/or time and taking values in an arbitrary space. For instance, seismologists describe an Earth model using the fields $\rho(\mathbf{x})$, $\kappa(\mathbf{x})$, $\mu(\mathbf{x})$,... (density, bulk modulus, shear modulus,...) as functions of the spatial coordinates $\mathbf{x} = (x^1,x^2,x^3)$, and describe a seismic wave as the field $\mathbf{u}(\mathbf{x},t)$ (displacement at the point $\mathbf{x}$ at time t). Given the boundary and initial conditions, the (macroscopic) relationships between a wavefield and an Earth model are described by a differential equation (the wave equation). As analytic solutions of the wave equation are usually not known (except for some trivial nonrealistic examples), the problem of obtaining the wavefield corresponding to a given Earth model is solved numerically, for instance, by *discretizing* the fields representing the Earth and the wavefield, and by replacing the differential equation by the corresponding finite-difference equation. But even if all the computations of wavefields that we might perform in our whole life were discretized, the functional language would remain useful, because of its compactness.

The same thing happens in least-squares inversion for problems involving fields. A theory can be built up which is essentially functional, and which considers the fields as abstract elements of a conveniently defined infinite-dimensional space. The resolution of the problem implies the use of differential and integral operators. Nevertheless, for all non-trivial applications, numerical results are always obtained after discretization. As the theory of least squares is considerably more abstract in infinite-dimensional spaces, the question arises whether we could limit ourselves to the consideration of discrete least squares. Unambiguously, the response is **no**, as, again, the

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