THE USE OF LINEAR INVERSE TECHNIQUES IN GEOTHERMAL STUDIES

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ABSTRACT-The knowledge of the present day temperature distribution within a basin is important both as a constraint for thermal evolution models, and as an indication of the processes that may have governed the thermal state of the basin through time. These aspects are essential for the complete understanding of gas and oil maturation in sedimentary basins. In this paper, general ideas about inversion and an inversion method to estimate geothermal gradients from bottom-hole temperature measurements are presented. Combining the gradients with thermal conductivity information makes it possible to estimate the heat flow density that constitutes the most important thermal parameter in geothermal studies. Bottom-hole temperature measurements are generally abundant in sedimentary basins because of the high number of wells drilled for gas and oil exploration. However, they are of poor quality and in this case inversion methods have given better results than the traditional ones.

1.INTRODUCTION

In spite of the fact that the distribution of temperature inside the Earth is probably one of the most fundamental parameters needed to understand its evolution and behaviour, it remains one of the most poorly determined Earth properties. Knowledge and evaluation of the internal temperature of the Earth is obtained through measurements of geothermal gradients in wells or, equivalently, through the calculation of heat flow density (HFD) near the surface. Unfortunately, reliable geothermal gradient measurements are relatively rare due to well drilling costs and scarcity of appropriate wells. Besides, since the temperature distribution within the Earth is a continuous function and the surface measurements are discrete, the problem of its interpretation is never unique.

The problem of trying to determine the temperature distribution at a given depth is further complicated by the fact that there are uncertainties in the radiogenic heat production of rock formations and, at the same time, the heat transfer mode is generally very complicated, i.e., non steady-state conduction and convection of heat by fluid motion. Measurements of HFD at the Earth's surface provide, however, constraints on its internal temperature distribution and therefore many heat flow density studies are being performed.

Because of hydrocarbon exploration, sedimentary basins provide a great amount of temperature data that can be used to determine, analyze and interpret the temperature distribution within the Earth. These data exist in the form of bottom-hole temperatures (BHT) and, despite their quantity, their quality is generally low. Nevertheless, because of the large numbers of BHTs available for analysis, statistically significant information is contained in these data sets [2], [9],[10],[15],[18].

Several methods have been proposed to analyze BHTs measured in oil wells. There are essentially two ways of approaching this problem. In the first one [2], [7], [8], [9], [16], the calculation of geothermal gradients or heat flow density is considered a forward problem, while in the second one [10], [18], [19], it is considered a linear discrete inverse problem.

Inverse theory was developed by scientists and mathematicians who had different backgrounds and goals and, therefore, the resulting versions look different, in spite of the fact that they are fundamentally similar. There are three major approaches to inverse theory [17], The first is based on probability theory. In this version the data (measured values) and the model parameters (estimated values) are treated as random variables and the emphasis is placed on the determination of their probability distributions. The second, developed from more deterministic physical sciences, emphasizes the estimation of model parameters and associated errors rather than probabilistic distributions. The third approach was developed from the consideration that model parameters are intrinsically continuous functions rather than discrete, as considered in the two first approaches.

In this work only the Gaussian linear discrete inverse theory will be considered. A review of some of the linear inverse techniques will be presented as well as the way to apply them to the study of the temperature distribution inside the Earth using bottom-hole temperatures obtained in oil wells.

2.GENERAL IDEAS AND DESCRIPTION OF DISCRETE INVERSE PROBLEMS

Inverse theory consists of a set of mathematical techniques for reducing data to obtain information about the physical world. The inferences and numerical or statistical values obtained through the use of inverse theory, which are generally called "model parameters", are based on observations or simply "data". Of course, some relationship must exist between the data and the model parameters, usually a mathematical theory or model. Generally speaking, the phrase "inverse theory" is used in contrast to "forward theory". The latter is defined as the process of determining the results of measurements or data based on some specific model. The former is defined as the process of estimating the model parameters from a tabulation of measurements or data and a specific model. It is worthwhile to note that inverse methods do not provide any information about the model itself. However, in some cases they can give some insight on the correctness of a given model or a way of discriminating between several possible models.

In most inverse problems the data are a sequence of numerical values (**d**) and therefore vectors constitute a convenient means to represent them. The same applies to the model parameters (**m**). These two quantities are generally related by one or more implicit equations such as

$$\begin{aligned} & f_1(\mathbf{d},\mathbf{m}) = 0 \\ & f_2(\mathbf{d},\mathbf{m}) = 0 \\ & \cdot \\ & \cdot \\ & \cdot \\ & f_L(\mathbf{d},\mathbf{m}) = 0 \end{aligned} \tag{1}$$

where L is the number of equations. These equations can be compactly written as a vector equation

$$\mathbf{f}(\mathbf{d},\mathbf{m}) = 0 \tag{2}$$

which summarizes what is known about how the data and the unknown model parameters are related. The main purpose of the inverse theory is to solve these equations for the model parameters. In general, the system of equations (1) consists of arbitrarily non-linear functions of the data and model parameters. Also, in most cases, it does not contain enough information to uniquely determine the model parameters. There are, however, many problems where the system of equations (1) takes one of several simple forms. If **f** is linear in both data and model parameters, equation (2) can be written as a matrix equation

$$\mathbf{f}(\mathbf{d},\mathbf{m}) = 0 = \mathbf{F}\begin{bmatrix}\mathbf{d} \\ \mathbf{m}\end{bmatrix} \tag{3}$$

where **F** is a L∗(M+N) matrix, M is the number of elements of the model parameter matrix, and N is the number of elements of the data matrix. If it is possible to separate the data from the model parameters and to form L=N equations that are linear in the data and non-linear in the model parameters, then equation (2) can be written as

$$\mathbf{f}(\mathbf{d},\mathbf{m}) = 0 = \mathbf{d} - \mathbf{g}(\mathbf{m}) \tag{4}$$

where **g(m)** represents a non-linear function of the model parameters. If in equation (4) **g** is also linear, equation (2) can be written as

$$\mathbf{f}(\mathbf{d},\mathbf{m}) = 0 = \mathbf{d}\text{-}\mathbf{G}\mathbf{m} \tag{5}$$

where **G** is a N∗M matrix.

Equation (5) corresponds to the simplest and best understood inverse problems and constitutes the foundation of the study of discrete inverse theory. Fortunately, this equation appears in many physical science problems, and even some non-linear problems can be reduced to it in certain cases. Matrix **G** is called the data kernel in analogy with continuous inverse theory where the function $G(x,\xi)$ is the kernel of an integral equation [3], [4], [5] .

The simplest solution to an inverse problem is an estimate of the model parameters, $\mathbf{m}^{est}$. This consists on a numerical sequence of values, which in certain cases can be misleading. In fact, estimates in themselves do not give any information about the quality of the solutions and therefore there is no control of the errors in the model parameters estimation. One way to partially solve the problem is to define either absolute or probabilistic bounds that allow an assessment of the degree of certainty of the solution. Absolute bounds imply that the true value of a given model parameter lies between two stated values, which is equivalent asserting an absolute error to the estimate. Probabilistic bounds imply that the estimate is likely to be between the bounds with some degree of certainty; a generalization of this consists in stating the complete probability distribution for the model parameters.

There are three points of view that can be used to study Gaussian linear inverse problems [1], [17]. The first point of view [11] that is generally called the length or stochastic method, emphasizes the data and the model parameters themselves, and the method of least squares is used to estimate the model parameters with the smallest prediction error. This approach will be detailed in the next section since it seems to be the most suitable one to apply to geothermal problems. The second point of view [13] emphasizes the relationship between the data and the model parameters. It is called the method of generalized inverses and it provides a means to tell a well designed experiment from a poor one, even without knowing the numerical values of the data and model parameters. The third point of view is called the method of maximum likelihood and it assumes that the optimum values of the model parameters maximize the probability that the observed data are in fact observed. This third point of view will not be described in this work.

Before describing in a more formal way the stochastic inversion point of view it is useful to define the concepts of underdetermined, even-determined, and overdetermined inverse problems, and *a priori* information.

Linear inverse problems are said to be underdetermined when equation (5) does not provide enough information to uniquely determine all the model parameters or, in a simpler manner, when there are more unknown model parameters than data. This case generally happens when there are several solutions to the problem that have zero prediction error (by definition the prediction error is given by $e_i = d_i^{obs} - d_i^{pre}$, where d_i^{obs} is the measured data and d_i^{pre} is the predicted data obtained using the estimated model parameters).

Even-determined problems appear when there is just enough information to determine the model parameters. In this case there is only one solution to the problem and the prediction error is zero.

Overdetermined problems happen when there is too much information contained in equation (5). In this case there are several solutions and the method of least squares is used to obtain the best approximate solution. Overdetermined problems have typically more data than unknown model parameters.

To obtain a solution to an inverse problem it is necessary to choose one solution from the great number of solutions generally available. This is particularly true in the underestimated problem. To achieve that, information that is not contained in equation (5) must be given. This extra information is called *a priori* information [12] and generally quantifies expectations about the character of the solution that are not based on the actual data.

3. THE LENGTH OR STOCHASTIC INVERSION METHOD

In this method the main idea is to determine the model parameters so that the predicted data are as close as possible to the observed data. The predicted data are calculated using the estimated model parameters and, therefore, for each observation it is possible to define the above-mentioned prediction error, e_i. The best solution will then be that which makes the overall error E, defined as

$$E=\sum_{i=1}^{N} e_i^2 \tag{6}$$

a minimum. In vector terms this can be written

$$E = \mathbf{e}^T \mathbf{e} \tag{7}$$

where T means transpose and $\mathbf{e}$ is the vector column formed by the values of e_i. Using the least squares method it is then possible to find the model parameters that minimize a particular measure of the length of the estimated data, $\mathbf{d}^{est}$, from the observations, $\mathbf{d}^{obs}$.

The term norm is generally used to refer to some measure of length and is indicated by a set of vertical bars. Several norms can be used but the most common is the L_2 norm defined as

$$\|\mathbf{e}\|_2 = \left(\sum_i |e_i|^2\right)^{\frac{1}{2}}. \tag{8}$$

This norm is used in the method of least squares to quantify length and implies that the data obey Gaussian statistics [17]. Using equation (7), it is possible to calculate the least squares solution to the linear inverse problem defined by equation (5):

$$\begin{aligned} E &= \mathbf{e}^T\mathbf{e} = (\mathbf{d} - \mathbf{Gm})^T(\mathbf{d} - \mathbf{Gm}) \\ &= \sum_i^N \left(d_i - \sum_j^M G_{ij} m_j\right)\left(d_i - \sum_k^M G_{ik} m_k\right) \end{aligned} \tag{9}$$

Multiplying and reversing the order of the summations leads to

$$E = \sum_j^M \sum_k^M m_j m_k \sum_i^M G_{ij} G_{ik} - 2\sum_j^M m_j \sum_i^N G_{ij} d_i + \sum_i^N d_i d_i \tag{10}$$

The derivatives $\partial E/\partial m_q$ should now be computed. Performing this differentiation term by term gives for the first term

$$\frac{\partial}{\partial m_q}\left[\sum_j^M \sum_k^M m_j m_k \sum_i^N G_{ij} G_{ik}\right] =$$

$$\sum_{j}^{M} \sum_{k}^{M} [\delta_{jq} m_k + m_j \delta_{kq}] \sum_{i}^{N} G_{ij} G_{ik} =$$
$$2 \sum_{k}^{M} m_k \sum_{i}^{N} G_{iq} G_{ik} \qquad (11)$$

The second term gives

$$-2 \frac{\partial}{\partial m_q} \left[\sum_{j}^{M} m_j \sum_{i}^{N} G_{ij} d_i \right] = -2 \sum_{j}^{M} \delta_{jq} \sum_{i}^{N} G_{ij} d_i =$$
$$-2 \sum_{i}^{N} G_{iq} d_i \qquad (12)$$

The third term is of course zero because

$$\frac{\partial}{\partial m_q} \left[\sum_{i}^{N} d_i d_i \right] = 0 \ . \qquad (13)$$

Combining equations (11), (12) and (13) gives

$$\partial E / \partial m_q = 0 = 2 \sum_{k}^{M} m_k \sum_{i}^{N} G_{iq} G_{ik} - 2 \sum_{i}^{N} G_{iq} d_i \qquad (14)$$

which in matrix notation can be written as

$$\mathbf{G}^T \mathbf{G} \mathbf{m} - \mathbf{G}^T \mathbf{d} = 0 \ . \qquad (15)$$

Assuming that $[\mathbf{G}^T\mathbf{G}]^{-1}$ exists, the solution for the model parameters estimate is

$$\mathbf{m}^{est} = [\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{G}^T\mathbf{d}. \qquad (16)$$

When dealing with an inverse problem the question that always arises is if there is a solution to it and, in the affirmative case, if the solution is exact.Equation (16) implicitly assumes that there is only one "best" solution. However, it can be proved that least squares fails if the number of solutions that give the same minimum prediction error is greater than one [17]. That is the case, for instance, when a straight line must be chosen to pass through only one data point. Of course, in this situation the solution is non-unique and many possible straight lines can pass through the data point, each solution presenting zero prediction error.

Data always contain noise that causes errors in the estimated model parameters. Since the formulas to determine the model parameters are linear functions of the data ($\mathbf{m}^{est} = \mathbf{Md} + \mathbf{v}$, where $\mathbf{M}$ is a matrix and $\mathbf{v}$ is a vector), it is possible to calculate how the measurement errors influence the errors in the estimated model parameters. If the data have a distribution characterized by some covariance matrix [cov $\mathbf{d}$], the estimates of the model parameters have a distribution characterized by [cov $\mathbf{m}$] = $\mathbf{M}$[cov $\mathbf{d}$]$\mathbf{M}^T$ .If it is possible to assume that the data are uncorrelated and all of equal variance σ_d^2, simple formulas are obtained for the simple inverse problem solutions. The simpler least squares solution represented by equation (16) has covariance

$$[\mathrm{cov}\ \mathbf{m}] = \sigma_d^2 \, [\mathbf{G}^T\mathbf{G}]^{-1} \ . \qquad (17)$$

that shows that the covariance matrix of the model parameters depends on the variance of the data [17].

4.THE USE OF INVERSE THEORY IN HEAT FLOW STUDIES

When analyzing the thermal state in sedimentary basins, one of the limiting factors is the quantity and quality of the temperature data available. Accurate temperature measurements are rare. However, for most basins, a great amount of data exists in the form of bottom-hole temperatures (BHTs) obtained during geophysical logging operations. Unfortunately, the quality of the BHT measurements is low.

Numerous recent studies of basins have used BHTs for different types of geothermal analysis to try to find which gives the best results. One of the methods that has recently received attention is the linear inversion method which was first applied to the Michigan Basin [18]. In this method, the area under study is divided into m discrete layers that may be formations or lithologic units. Each of these layers is assumed to have constant thermal conductivity, K_j (j=1,2,...,m); heat flow density is assumed to be constant throughout the entire area. This implies that the geothermal gradients, g_j, are constant in each layer or formation. Using the thermal resistance method proposed in reference [6], the temperature at any depth can be obtained by

$$T = T_0 + q \sum_j (z_j / k_j) \qquad (18)$$

where T_0 is the temperature at the surface of the Earth, q is the heat flow density, z_j is the thickness of the jth layer, and K_j is the thermal conductivity of the same layer. After correcting BHTs by one of the available methods (the Horner plot technique, for instance [14]), equation (18) can be modified to:

$$(BHT - T_0)_i = \Delta T_i = \sum_j z_{ij}\, g_j \qquad (19)$$

where z_{ij} is the thickness of the jth formation at the ith well. If the number of BHTs, n, is greater than the number of unknown formation geothermal gradients, m, an overdetermined system of n equations in m unknowns exists and the BHT data can be inverted for the geothermal gradients, g_j, in each formation. These estimated gradients may then be used in a forward sense to calculate the best temperature field or, combined with thermal conductivity data, to estimate the heat flow density.

In what follows, the variables that are generally used in heat flow density studies will be substituted into the equations described in the previous paragraph.

To apply inverse theory to geothermal studies two assumptions are usually made: first, heat transfer only occurs in the vertical direction and is purely conductive; second, the average geothermal gradients are constant over each formation. Given these assumptions, equation (19) can be written in matrix form as

$$\underset{\sim}{T_\Delta} = \underset{\approx}{Z}\, \underset{\sim}{g} \qquad (20)$$

where $\underset{\sim}{T}_\Delta$ is the vector of n temperature differences, $\underset{\approx}{Z}$ is a (n*m) matrix of formation thicknesses, and $\underset{\sim}{g}$ is the vector of m unknown geothermal formation gradients. Because $\underset{\sim}{T}_\Delta$ contains noise, and the model generally used is only an approximation to physical reality, it is unlikely that an exact solution exists. The inverse problem then becomes one of finding a set of formation gradients that minimizes the error

$$\underset{\sim}{r} = \underset{\sim}{T}_\Delta - \underset{\approx}{Z}\, \underset{\sim}{g}_{est} \qquad (21)$$

where g_{est} is the best estimate of the true formation gradient. Therefore, for the ith well there is a residual, r_i, given by

$$r_i = \Delta T_i - \sum_{j=1}^{m} z_{ij}\, g_{est\, j} \qquad (22)$$

where ΔT_i is the measured temperature difference, and the second term on the right hand side of the equation is the estimated temperature difference calculated using the inverse solution. Applying the least squares approach, the solution will be the one that makes the sum of the squares of the residuals, r_i, a minimum. In terms of the variables common to heat flow studies, equation (16) takes the form

$$\underset{\sim}{g}_{est} = \left(\underset{\approx}{Z}^T \underset{\approx}{Z}\right)^{-1} \underset{\approx}{Z}^T \underset{\sim}{T}_\Delta \ . \qquad (23)$$

Since this equation does not preclude negative geothermal gradients as solutions and they are geologically unreasonable, the solution must be constrained to be non-negative. This condition constitutes *a priori* information.

The variance σ_d^2 of the temperature is estimated by

$$\sigma_d^2 = \sum_{i=1}^{n} r_i^2 / (n - m) \qquad (24)$$

and the variance σ_m^2 of the jth estimated geothermal gradient is the jth diagonal element of the covariance matrix [10]

$$\sigma_m^2 = \sigma_d^2 \left(\underset{\approx}{Z}^T \underset{\approx}{Z}\right)^{-1}_{jj} \ . \qquad (25)$$

5. CONCLUSIONS

Compared to other methods for processing BHT data sets, the linear inverse method described in the previous paragraphs has several advantages. An easy linear solution is generally obtained and the theory provides methods to deal with data error. Furthermore, insufficient data and non-uniqueness of the solution are explicitly dealt with. It also allows all the available data to be included in the calculation, specifying how data of different quality should be weighted. Finally, it provides the means to estimate the variance of the error in each model parameter, giving a relative and absolute measure of the quality of the solution [19].

In the length point of view of the Gaussian linear inverse problem, the data and model parameters are treated as random variables and it is assumed that they have a certain probability distribution, which in fact constitutes *a priori* information. The inverse methodology then returns the minimum variance solution, that is, the solution that best fits within the probable ranges of the data and model parameters and minimizes the variance of the error in that solution.

ACKNOWLEDGEMENTS

This review was originally suggested by Dr. E. Kanasewich, who also gave suggestions which greatly improved the first draft of the manuscript. Dr. M. Victor and Dr. F. W. Jones are also thanked for their constructive comments and revision of the paper. This review was prepared while the author was at the Department of Physics of the University of Alberta, Canada, under a leave of absence from the Physics Department of the University of Évora, Portugal. The author received financial support by the University of Évora, the Junta Nacional de Investigação Científica e Tecnológica, Portugal, and the University of Alberta through a teacher assistantship.

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