COMPUTER-ASSISTED INTERPRETATION
OF
ELECTRICAL SOUNDINGS

by

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The interpretation of an electrical sounding is the estimation of the geo-electric properties of the geologic section over which the sounding has been obtained. The parameters are electrical resistivity and thickness (or combinations thereof) for assumed layers.

This interpretation can best be done in the wave-number domain. Here the function characterizing the section (the Stefanesco function) is free of any dependence on the array used to obtain the electrical sounding experimentally, and can be computed easily. The Stefanesco function is related to the sounding-curve by a Hankel transformation.

In this paper a computer program to assist in the interpretation of electrical soundings is developed. The computer-assisted interpretation of an observed electrical sounding consists of the following steps:

1. Obtaining the Stefanesco function for the field section by numerical Hankel transformation of the observed sounding-curve. The procedures for Schlumberger-type soundings are developed.

2. Employing the classical techniques of least-squares curve fitting to adjust a given first cut in order to obtain a better-and-better match. A variation of the Stefanesco function, the "Kernel," is used as a theoretical model.
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INTRODUCTION

The purpose of electrical soundings is to obtain meaningful information about the subsurface geology. This goal is reached by following two fundamental steps:

1. Obtain the direct-current electrical sounding by careful measurement on the surface. The resulting curve gives the variation of apparent resistivity as a function of a separation parameter and the electrode configuration used.

2. Obtain the variation of true layer-resistivity as a function of depth from the sounding-curve. This process constitutes the interpretation of the sounding-curve.

a) In this respect it should be noted that the principle of equivalence holds over a wide range of geo-electric sections. This means that the interpretation frequently can be done only in terms of the longitudinal conductance or transverse resistance of intermediate layers, depending on which parameter is valid.

b) Any additional information should be taken into account (well-data, known depths or resistivities, compatibility with adjacent soundings), and a geologically meaningful set of thicknesses and
resistivities selected to define the subsurface geology.

Interpretation, as outlined in step 2 above, has been studied extensively by many investigators. The most widely used method is probably that of curve matching with theoretical curves compiled in the form of master-curve albums (Compagnie Générale de Géophysique, 1963; and Orellana and Mooney, 1966).

In typical field studies, sounding-curves of four layers or more are frequently encountered. In such cases, partial curve matching is required because so few four-layer or more-layer master-curves are available. The auxiliary-point method, devised for such cases, produces excellent results when used with care and insight. For a review of this method see Zohdy (1965).

With the advent of digital computers, several investigators pursued the problem of exact calculation of master-curves (Van Dam, 1964; Mooney and others, 1966). With these powerful tools available, an unlimited number of master-curves, for any number of layers, can be computed to aid in curve matching.

These techniques were also used to compute the theoretical sounding-curve for an interpretation; this sounding curve was then compared with the observed curve. If the curves did not agree closely enough, the interpretation could be modified, and the procedure repeated. To reach a
satisfactory end-result at reasonable cost, the sound judgment and experience of the interpreter is essential.

An alternative to curve matching sounding-curves can be found in techniques which use the Stefanesco function or variations thereof. The Stefanesco function can be thought of as the wave-number domain representation of a geo-electric section, whereas the sounding-curve corresponds to the distance domain. The Stefanesco function will be described in more detail later in this text.

The Stefanesco function is that function of resistivities and thicknesses which indirectly expresses the boundary-conditions at every layer-interface in a geo-electric section. This function characterizes the section, and does not depend in any way on the electrode-configuration used to measure the corresponding sounding-curve. The Stefanesco function unfortunately cannot be measured in the field.

Interpretation techniques using the Stefanesco function were described by Slichter (1933), Pekeris (1940), Vozoff (1958), and most extensively by Koefoed (1968). A major difficulty in the methods of the first two investigators was that the Stefanesco function is not easily obtainable from the observed sounding-curve. Koefoed presented a graphical method to obtain the Stefanesco function, therefore his technique may yet find wide application.

A technique unlike either of the other two mentioned, was described by Kunetz and Rocroi (1970). The use of a
digital computer is required to implement this technique. In this approach, a series of current-pole images is obtained by the Fourier transformation of a function which depends on the observed sounding-curve. Factorization of the image-series produces the electrical reflection coefficients and, hence, resistivities. An initial requirement that all layers have the same thickness defines the section completely. Additional information, as well as the properties of the relevant Dar-Zarrouk curves, are then taken into account to produce a geologically meaningful interpretation.

The purpose of the present paper is to develop methods suitable for implementation on a digital computer, by which to assist in the interpretation of electrical soundings. In this approach, economy was considered of prime importance, and the most efficient means of arriving at the end-result was sought. It is in this context that the choice was made to do the computer-assisted interpretation in the wave-number domain. In the wave-number domain, the Stefanescu function serves as the theoretical model; efficient computational techniques by which to compute this function exist.

A function differing from the Stefanescu function by simple constants has been given the name "Kernel" by Slichter (1933). It is for the computation of this kernel that we have at least three algorithms: Vanyan's recurrence relation (Vanyan, 1967), Flathe's recurrence relation (Flathe,
1955) and Sunde's recurrence relation (Sunde, 1967). Of these recurrence relations, Sunde's lends itself most favorably to computer-applications; accordingly, it has been used throughout this study.

The well established technique of least-squares curve fitting was adapted to do the curve matching in the wave-number domain. Least-squares curve fitting has previously been used successfully in the interpretation of other kinds of potential-field data: gravity profiles (Corbató, 1965; Snyder, 1968), magnetic profiles (Hall, 1958) and magneto-telluric soundings (Wu, 1968).

In this paper, the theory underlying the least-squares curve fitting method, as adapted to direct-current electrical soundings, is studied. From the theoretical considerations, the necessary flow-charts for computer-interpretation are then developed and presented; a Fortran-IV program is the end-result.
The Potential-Distribution at the Surface of a Layered Earth

Consider a medium made up of a sequence of horizontal layers, every one homogeneous and isotropic electrically. These layers are infinite in extent, and have geo-electric parameters \( \rho_1 \) and \( h_1 \) for the surface layer, \( \rho_2 \) and \( h_2 \) for the second layer, \ldots \( \rho_{n-1} \) and \( h_{n-1} \) for the next-to-last layer, and resistivity \( \rho_n \) for the infinitely thick substratum. This model serves as an approximation to the earth, in which sedimentary beds correspond to the isotropic and homogeneous layers of the model.

When a current-source of intensity \( I \) is placed at the surface of this layered earth, a potential-field develops. The potential-field reflects the presence of these subsurface layers in the way in which it deviates from the potential-field over a homogeneous half-space.

One of the earliest and most significant papers on this subject was presented by Stefanesco and his co-workers (Stefanesco and others, 1930). They derived an expression for the potential at the surface due to current introduced at a point. Their expression is a solution of Laplace's equation, modified to reflect the cylindrical symmetry of the model. Expressed in cylindrical coordinates, this equation is:

\[
\frac{\partial^2 U}{\partial r^2} + \frac{1}{r} \frac{\partial U}{\partial r} + \frac{\partial^2 U}{\partial z^2} = 0 \tag{2.1}
\]
From the solution of Laplace's equation and the evaluation of boundary conditions, Stefanesco derived an expression for the surface-potential $U$. At a point $M$, a distance $r$ away from the current-pole, the potential is

$$
U = \frac{\rho_1 I}{2\pi r} \left\{ \frac{1}{r} + 2\int_0^\infty \frac{\Theta(\lambda)}{\lambda} J_0(\lambda r) \, d\lambda \right\},
$$

(2.2)

where

$\rho_1 = \text{electrical resistivity, of the surface-layer},$

$I = \text{the current-input},$

$J_0 = \text{the zero-order Bessel function of the first kind},$

$\Theta(\lambda) = \text{a rational fraction of exponential functions of the thicknesses and resistivities of the layers present.}$

In a discussion of Stefanesco's work, Kunetz named this function "the Stefanesco function" (Kunetz, 1966, p. 62).

When the introduction of current is by means of two electrodes, as it would be in practice, the resulting potential-field is simply the sum of the fields due to the two current-poles separately, one of intensity $I$ and the other of intensity $-I$.

The addition of a second measuring-electrode to detect the potential-difference between two points leave us with the typical four-electrode array used in direct-current electrical prospecting. When we also require that the four electrodes lie on a straight line, spaced symmetrically around a central point, we have defined the electrode-configuration of some electrical soundings. For the
Schlumberger electrode-configuration, the two current-electrodes are usually designated by the symbols A and B, the measuring-electrodes by M and N. For this configuration it is necessary that MN be small relative to AB.

The Sounding-Curve as Characterizing the Geo-Electric Section

The quantities that are measured with a Schlumberger-type array are

1) $V$, the potential-difference between M and N,
2) $I$, the total current flowing between A and B,
3) $r$, the distance from the center of the array to either A or B,
4) $b$, the distance between M and N.

When the above set of measurements is taken on the surface of a homogeneous half-space of resistivity $\rho$, the measured quantities can be combined in a certain way so that the resulting value equals the resistivity $\rho$, and has the dimensions of resistivity.

Over a layered half-space, when the measured quantities are combined in the same manner, the resulting value is called the apparent resistivity $\rho_a$. For the Schlumberger array the formula for apparent resistivity is

$$\rho_a = \pi \left( \frac{r^2}{b} - \frac{b}{4} \right) \cdot \frac{V}{I}$$

The requirement that $b \ll r$ permits this expression to be simplified into

$$\rho_a = \frac{\pi}{b} \frac{r^2}{I} \cdot \frac{V}{I} \quad (2.3)$$
When a series of measurements is obtained for increasing separations $r$, we plot the apparent resistivity $\rho_a$ versus separation $r$, and thus obtain a Schlumberger sounding-curve. This plot is usually done on a logarithmic scale (Keller, 1966, p. 120; Kunetz, 1966, p. 54).

An electrical sounding-curve obtained in the manner described above can be thought of as characterizing the geo-electric section. All the information about the subsurface section that can reasonably be derived from surface-measurements is contained in this curve. Sounding-curves are furthermore strongly affected by the geometry of the array used to obtain them; this fact must be taken into account when an interpretation is performed.

The Stefanesco Function as Characterizing the Geo-Electric Section

From an expression for the potential-field (equation 2.2), the geometric requirements for the electrode array and the expression for apparent resistivity (2.3), Koefoed (1968, p. 9) derived the following relationship for Schlumberger soundings:

$$\rho_a(r) = \rho_i \left\{ 1 + 2r^2 \int_0^\infty \Theta(\lambda) \cdot J_t(\lambda r) \cdot \lambda d\lambda \right\}$$

(2.4)

This expression shows that there is a more fundamental function, the Stefanesco function $\Theta(\lambda)$, which characterizes the geo-electric section. This function contains all the
information about the geo-electric properties of the section, and is **not** dependent on the geometry of the array used to obtain the sounding-curve.

The Stefanesco function has been the subject of many papers oriented toward interpretation techniques. Its very desirable property of being a function of the geo-electric properties only is the primary reason for this interest.

**Relationship Between the Stefanesco Function and the Sounding-Curve**

**Hankel Transformation**

Hankel transformation is defined in the following manner (Ryzhik and Gradshtein, 1965):

1) If \( g(x) \) is defined everywhere in the interval \( 0 \leq x \leq \infty \),

2) If \( g(x) \) is continuous and monotonic in every small but finite interval of \( x \),

3) If \( \int_0^\infty |g(x)| \, dx \) converges, then for \( y \geq 0 \), \( r \geq -1/2 \) and \( x > 0 \)

\[
\begin{align*}
  f(y) &= \int_0^\infty g(x) \cdot (xy)^k \cdot J_r(xy) \, dx \\
  g(x) &= \int_0^\infty f(y) \cdot (xy)^k \cdot J_r(xy) \, dy
\end{align*}
\]

In equations (2.5), \( f(y) \) and \( g(x) \) constitute a Hankel transform pair.
With slight modification, the expressions in (2.5) can be simplified:

\[
\begin{align*}
  f(y) &= \int_0^\infty g(x) \sqrt{y} x^{\frac{1}{2}} J_r(xy) \, dx, \\
  y^{-\frac{1}{2}} f(y) &= \int_0^\infty x^{-\frac{1}{2}} g(x) \times J_r(xy) \, dx, \\
  y^{\frac{1}{2}} f(y) &= \int_0^\infty x^{\frac{1}{2}} g(x) \times J_r(xy) \, dx \quad \text{or} \quad F(y) = \int_0^\infty g(x) \times J_r(xy) \, dx \\
  G(x) &= \int_0^\infty F(y) \sqrt{y} J_r(xy) \, dy
\end{align*}
\]  

(2.6)

Hankel Transformation of Sounding-Curves

The relationship in equation (2.4) can be modified to yield

\[
\frac{1}{r^2} \left[ \frac{\rho_a(r)}{P_1} - 1 \right] = \int_0^\infty 2 \tilde{\theta}(\lambda) J_r(\lambda r) \, d\lambda
\]  

(2.7)

Hankel transformation of this equation according to equation (2.6) yields for \( \lambda > 0 \):

\[
2 \tilde{\theta}(\lambda) = \int_0^1 \frac{1}{r^2} \left[ \frac{\rho_a(r)}{P_1} - 1 \right] J_r(\lambda r) \, dr .
\]  

(2.8)

Equation (2.8) shows the relationship between the Stefanesco function \( \theta(\lambda) \) and the sounding-curve \( \rho_a(r) \). We see that these functions are related through the Hankel transform-pair

\[
2 \tilde{\theta}(\lambda) \leftrightarrow \frac{1}{r^2} \left[ \frac{\rho_a(r)}{P_1} - 1 \right] .
\]  

(2.9)
THE STEFANESCO FUNCTION AND THE KERNEL

One of the earliest papers on the theory of direct-current sounding methods is that of Stefanesco and C. and M. Schlumberger (Stefanesco and others, 1930). In their paper, the significance of the Stefanesco function already was very clear. Papers on interpretation techniques using this function soon followed.

From the Lipschitz integral (Watson, 1966, p. 384) we know that

$$\int_0^\infty J_0(\lambda r) \, d\lambda = 1/r \quad (3.1)$$

This relationship permits us to write equation (2.2) as

$$U = \frac{-\rho I}{2\pi r} \int_0^\infty \left[ 1 + 2\Theta(\lambda) \right] J_0(\lambda r) \, d\lambda \quad (3.2)$$

It was from an expression in this form that Slichter (1933) designated the function

$$k(\lambda) = 1 + 2\Theta(\lambda) \quad (3.3)$$

as the "Kernel." This designation is contrary to the accepted use of the term in mathematics; in an integral-transform like equation (3.2), the Bessel function is usually called the kernel, and the function $[1 + 2\Theta(\lambda)]$ the object function. In the literature on direct-current electrical methods however, the name "Kernel" as defined by Slichter, is now well established. In this paper it will be used in that sense too.
Our understanding of the Stefanesco function and Kernel can be attributed to a great extent to papers by Slichter, Pekeris (1940), Meinardus (1967) and Koefoed (1968). Of these contributors, Pekeris and Meinardus used the name "Kernel" in the sense that Slichter defined it. The corresponding function is defined in equation (3.3). Koefoed also used the name "Kernel" but for the Stefanesco function (Koefoed, 1968, p. 10).

Relationship Between the Kernel and the Schlumberger Sounding-Curve

When the definition of the Kernel as in equation (3.3) is accepted, equation (2.4) can be written as

\[ p^*(r) = \rho \left\{ 1 + r^2 \int_\infty^0 \left[ k(\lambda) - 1 \right] J_1(\lambda r) \lambda d\lambda \right\} \]  

(3.4)

From this relationship, we see that the Kernel and the sounding-curve are related through the Hankel transform pair

\[ \left[ k(\lambda) - 1 \right] \leftrightarrow \frac{1}{r^2} \left[ \frac{p^*_0(r)}{\rho} - 1 \right] \]  

(3.5)

A plot which shows the Schlumberger sounding-curve and the Kernel for the same section is presented in figure 1. The sounding-curve is a four-layer master-curve from the album by Orellana and Mooney (1966, sheet 51, curve KH4-Q). The corresponding Kernel was calculated by means of Sunde's algorithm (see next section). Note that the Kernel function is presented as log (k) versus log (1/\lambda). Plots of this
Figure 1

The Schlumberger sounding-curve and the Kernel for the same section.
nature show that the two functions have the same general shape and exactly the same asymptotes. (This is not true for the case of an infinitely conductive basement.)

The arbitrary choice of plotting the two functions so that the asymptotes are the same, shows that the Kernel function has less pronounced variation than the sounding-curve. This may suggest that it also has less resolution in reflecting the geo-electric parameters, which is not true. From mathematical considerations we know that the Kernel function and the sounding-curve contain exactly the same information regarding the geo-electric section.

Computational Techniques for the Kernel

Several computational techniques for the calculation of the Kernel exist. Meinardus (1967, p. 41) discussed some of them, and examined the difficulties and limitations of each method. On the basis of his work, it is evident that Sunde's recurrence relation is best suited for implementation on a digital computer.

Sunde's recurrence relation for the n-layered earth model is expressed as follows (Sunde, 1968, p. 55):

\[
k_{123\ldots n} = \frac{1 - \mu_{123\ldots n}}{1 + \mu_{123\ldots n}} e^{-2\lambda h_i}
\]

\[
\mu_{123\ldots n} = \frac{\rho_i - \rho_n}{\rho_i + \rho_n} k_{234\ldots n}
\]
The indices of a specific \( \mu \) or \( k \) identify the layers involved in the calculation of that \( \mu \) or \( k \).

In this recurrence relation, the Kernel is defined by the first equation in (3.6).

If we simplify the notation by letting \( k_1 \) denote \( k_1, 2, 3,..., n \), \( k_i \) denote \( k_{i(i+1)}...n \), and similarly \( \mu_i \) denote \( \mu_{i(i+1)}...n \), the algorithm for computing the general terms become

\[
\begin{align*}
  k_i &= \frac{1-\mu_i \Theta^{-2 \lambda h_i}}{1+\mu_i \Theta^{-2 \lambda h_i}} \\
  \mu_i &= \frac{\rho_i - \rho_{i+1} k_{i+1}}{\rho_i + \rho_{i+1} k_{i+1}}
\end{align*}
\]  

(Note that \( i \leq n-1 \) and \( k_n = 1 \))

The Kernel, \( k_1 \), is obtained by first computing \( \mu_{n-1} \) and \( k_{n-1} \) for the second-to-last layer, then \( \mu \) and \( k \) for the next shallower layer, and on upward, until the surface layer.
is reached. On the surface then, $\mu_1$ and $h_1$ are used to calculate the Kernel $k_1$.

**A Flow-Chart for the Procedure to Calculate a Kernel**

A flow-chart in which the above sequence of steps for several values of the independent variable, $\lambda$, is incorporated is presented in figure 2. This flow-chart is designed to be coded into a subprogram.

The flow-chart makes provision for special procedures when a two-layer Kernel is desired. Under such circumstances, which will be described later in this text, 80 points of the Kernel are computed. Under normal circumstances at most 40 values can be computed, and the user has the choice of having either $k$ or log $k$ computed.

**The Interval of $\lambda$ in Which the Kernel is of Interest**

In an examination of the asymptotic behavior of the Kernel function, the following results are obtained (Meinardus, 1967, p. 19):

\[
\begin{align*}
\lim_{\lambda \to \infty} k(\lambda) &= 1 \\
\lim_{\lambda \to 0} k(\lambda) &= \rho_n/\rho_1
\end{align*}
\]

The range of interest of the Kernel is that interval of $\lambda$ from an initial value where the Kernel begins to deviate from the asymptote $\rho_n/\rho_1$, to a final value where it has approached the asymptote 1 within a small percentage. In
Enter
Communicate:
\[ F_1 = \text{Kernel function} \]
\[ n_k = \text{no. of Kernel values wanted} \]
\[ \lambda_j = \text{set of } \lambda's \]
\[ n_l = \text{no. of layers} \]
\[ \rho_i = \text{resistivities}, \quad h_i = \text{thicknesses} \]
\[ \text{flag} = \text{true if log } K \text{ wanted} \]

\[ n_l = 2 \quad ? \]

- \[ R_A = \rho_i \]
- \[ R_B = \rho_{i+1} f_1 \]
- \[ G_4 = (R_A - R_B)/(R_A + R_B) \]
- \[ G_e = G_4 \exp(\text{temp} \cdot h_i) \]
- \[ f_1 = (1 - G_e)/(1 + G_e) \]

\[ j = n_l - 1 \]

\[ j = 0 \quad ? \]

- \[ F_i = f_1 \]
- \[ l = l + 1 \]

\[ l > n_k \quad ? \]

Return

Figure 2. Logical flow-chart for the computation of Kernel functions.
this range of interest, the Kernel changes from $\rho_n/\rho_1$ to 1 in a manner which reflects the presence of the intermediate layers. In terms of $1/\lambda$, the change is from 1 to $\rho_n/\rho_1$.

When we compute a Kernel for a very wide range of $1/\lambda$, it is evident that the range of interest numerically coincides with the range of $r$ in which the sounding-curve changes from $\rho_1$ to $\rho_n$. Figure 1 displays this relationship.

When the range of $r$ of the sounding-curve is $r_{\text{min}}$ to $r_{\text{max}}$, the range of $\lambda$ can be defined by

$$\lambda_{\text{min}} = 1/r_{\text{max}}$$

and

$$\lambda_{\text{max}} = 1/r_{\text{min}}$$

(3.9)

The significance of the Kernel function on a logarithmic plot (Meinardus, 1967, p. 25) makes it necessary to have the intermediate values of $\lambda$ in this interval logarithmically equi-spaced. Experience shows that an interval of $\sqrt{2}$ is small enough to produce an accurate representation of the Kernel by discrete points.

We see from equations (2.8) and (3.7) that the Kernel may be computed from field data or a mathematical model.

In the first case, the sounding-curve measurements were obtained for values of $r$ from $r_{\text{min}}$ to $r_{\text{max}}$. The corresponding range of $\lambda$ is defined directly by the use of equations (3.9).
In the second case, the procedure is more involved, and can be described as follows:

Replace all the layers overlying the basement with one "equivalent" layer so that the final asymptote of the "equivalent" two-layer sounding-curve falls on top of the original final asymptote.

The "equivalent" section will consist of two layers, for which the "surface-layer" parameters can be expressed in terms of the cumulative Dar-Zarrouk parameters of the original layers individually (Zohdy, 1965).

The parameters are:

"Equivalent" resistivity, or "pseudo" resistivity in Zohdy's notation

\[ \rho^* = \sqrt{\frac{\tau}{S}} \]

and "equivalent" thickness or "pseudo" thickness

\[ h^* = \sqrt{\tau \cdot S} \]

The cumulative Dar-Zarrouk parameters are:

\[ \tau = h_1 \cdot \rho_1 + h_2 \cdot \rho_2 + \cdots + h_{n-1} \cdot \rho_{n-1} \]

and

\[ S = h_1/\rho_1 + h_2/\rho_2 + \cdots + h_{n-1}/\rho_{n-1} \]

The basement layer of the "equivalent" section has the same resistivity as before, \( \rho_n \).

From experience with two-layer master-curves, we know that two-layer sounding-curves reach their final asymptotes for separations less than \( r = 100 \cdot h_1 \). This figure even
includes two-layer sections for which the basement is highly resistive; it is very liberal for sections with a conductive basement.

This consideration provides a limit on the maximum separation of interest:

\[ r_{\text{max}} = 100 h^* \]  \hspace{1cm} (3.10)

Considering the original n-layer section again, we know that the sounding-curve will approach \( \rho_1 \) as \( r \) becomes small. Again from the nature of two-layer curves, we know that the sounding-curve will first begin to deviate from the value \( \rho_1 \) for separations around \( r = .5 h_1 \). It is therefore reasonable to assign a minimum separation of interest as

\[ r_{\text{min}} = 0.2 h_1 \]  \hspace{1cm} (3.11)

We now have defined the range of \( r \) for the prescribed section, and through equations (3.9), the corresponding range of \( \lambda \).

A Flow-Chart for the Procedure to Calculate an Appropriate Set of \( \lambda \)'s

The procedure to define an appropriate set of \( \lambda \)'s consists of the following steps:

1) Definition of \( r_{\text{min}} \) and \( r_{\text{max}} \). When the Kernel for a prescribed section is desired, equations (3.10) and (3.11) are used.
2) Determination of \( \ell \), the number of values that will be defined. Because the values of \( \lambda \) will be logarithmically spaced at \( \sqrt{2} \), the number is

\[
\ell = \frac{(\log \lambda_{\text{max}} - \log \lambda_{\text{min}})}{\log \sqrt{2}} + 1
\]

(The maximum value of \( \lambda \) is restricted to 40.)

3) Definition of the first value \( \lambda_1 = \lambda_{\text{min}} \), then of the others, using the relationship

\[
\frac{\lambda_{i+1}}{\lambda_i} = \sqrt{2}
\]

Figure 3 is a flow-chart of the sequence of steps explained above. The flow-chart can be coded into a sub-program.
Communicate:
flag = true if section given
\( n_l = \text{no. of layers} \)
\( \rho_i = \text{resistivities} \)
\( h_i = \text{thicknesses} \)
\( s_{\text{max}} = \text{max separation} \)
\( s_{\text{min}} = \text{min separation} \)
\( n_k = \text{no. of Kernel values} \)
\( \lambda_i = \text{set of } \lambda's \)

flag = true

\[ r_{\text{min}} = s_{\text{min}} \]
\[ r_{\text{max}} = s_{\text{max}} \]

\[ \lambda_i = \frac{1}{r_{\text{max}}} \]
\[ \text{temp} = \frac{1}{r_{\text{min}}} \]
\[ n_k = 1 + \log(\text{temp} / \lambda_i) / \log(2) \]

i = 2

\[ \lambda_i = \lambda_{i-1} / 2 \]

i = i + 1

i > n_k ?

Return

Figure 3. Logical flow-chart for the computation of an appropriate set of \( \lambda's \).
NUMERICAL HANKEL TRANSFORMATION

The first step in any interpretation technique in the wave-number domain is to obtain the Kernel corresponding to the observed sounding-curve. This step requires the Hankel transformation of the observed curve.

The Hankel transformation of electrical sounding-curves is not possible by means of analytical integration. It is therefore necessary to revert to numerical integration, for which several methods exist.

The methods of Hankel transformation by series expansion and by numerical quadrature are discussed by Meinardus (1967, p. 86-106). Numerical quadrature can be executed by polynomial approximation of either the Kernel function or the entire integrand. Meinardus' work can be applied to the Hankel transformation of sounding-curves obtained with any of the electrode configurations in use today.

Two recent papers have treated the Hankel transformation of sounding-curves of the Wenner type and the general four-point type respectively. The Hankel transformation of Wenner sounding-curves is discussed in detail by Chan (1970), and that of the general four-point sounding by Szaraniec (1970).

A technique for the numerical Hankel transformation of Schlumberger soundings was described by Vanyan (1967, p. 161). Vanyan's technique is that of polynomial approximation of the non-oscillatory part of the integrand, and differs from other
approaches of this kind only in that a second-degree polynomial is used. In my opinion, Vanyan's technique takes into account the (mathematically) well-behaved character of sounding-curves, and thus produce accurate Hankel transformations at remarkably low cost.

Vanyan's Technique for Hankel Transformation

Consider the type of Hankel transformation required for Schlumberger soundings (compare with 2.8):

\[ g(y) = \int_0^\infty f(x) \times J_1(xy) \, dx. \]  \hspace{1cm} (4.1)

Vanyan's suggestion is that the product \( x \cdot f(x) \) be approximated by second-order polynomials in short sections, and the integration performed analytically. If \( x \cdot f(x) \) is represented by discrete pairs \( (f_i, x_i) \), the second-order polynomial is fitted to three points \( (f_i, x_i), (f_{i+1}, x_{i+1}) \) and \( (f_{i+2}, x_{i+2}) \) where \( i \) assumes the values 1, 3, 5, 7, ... successively. (Note that it is not necessary for \( x_i \) to be evenly spaced.)

For a polynomial approximation of the form

\[ x \cdot f(x) = l_0 + l_1 x + l_2 x^2 \]  \hspace{1cm} (4.2)

the interpolation coefficients \( l_0, l_1, \) and \( l_2 \) (La Grange three-point interpolation coefficients) are tabulated by Vanyan (1967, p. 161). In the next mathematical development, we will see that only \( l_1 \) and \( l_2 \) are needed explicitly. These coefficients are computed as follows:
where
\[
\begin{align*}
\beta_0 &= \frac{-(x_{i+1} + x_{i+2})}{(x_{i+1} - x_i)(x_{i+2} - x_i)} \\
\beta_1 &= \frac{(x_i + x_{i+2})}{(x_{i+1} - x_i)(x_{i+2} - x_{i+1})} \\
\beta_2 &= \frac{-(x_i + x_{i+2})}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})} \\
\gamma_0 &= \frac{1}{(x_{i+1} - x_i)(x_{i+2} - x_i)} \\
\gamma_1 &= \frac{-1}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})} \\
\gamma_2 &= \frac{1}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})}
\end{align*}
\]

and

If the function \( x \cdot f(x) \) is represented by \( m \) points (\( m \) must be odd), the number of panels of three points, \( p \), is

\[
p = (m-1)/2.
\]

With the polynomial approximation expressed by (4.2), equation (4.1) can be written as

\[
g(y) = \sum_{i=1}^{p} \int_{x_i}^{x_{i+2}} \left\{ l_0 + l_1 x + l_2 x^2 \right\} \int_l(x_0) \, dx
\]

For this equation to be true, the function \( x \cdot f(x) \) must be zero outside the range in which it is specified by \( x_i \), and must be accurately represented by the pairs \((f_i, x_i)\).
Broken up into three separate integrals, the previous equation yields

\[
g(y) = \sum_{i=1}^{p} \left\{ \ell_2 \int_{x_i}^{x_{i+2}} \mathcal{J}_i(xy) \, dx + \ell_1 \int_{x_i}^{x_{i+2}} x \mathcal{J}_i(xy) \, dx \right\} + \ell_2 \int_{x_1}^{x_{i+2}} x^2 \mathcal{J}_i(xy) \, dx
\]

(4.5)

The following integral expressions are developed in Appendix A. They are similar to Vanyan's expressions for the same integrals, except that incorrect signs in a few places in Vanyan's text have been changed.

\[
\int \mathcal{J}_i(xy) \, dx = -\frac{4}{y} \mathcal{J}_o(xy)
\]

(4.6)

\[
\int x \mathcal{J}_i(xy) \, dx = \frac{4}{y^2} \left[ \mathcal{J}_i(xy) - xy \mathcal{J}_o(xy) - \mathcal{J}_u(xy) \right]
\]

(4.7)

\[
\int x^2 \mathcal{J}_i(xy) \, dx = -\frac{x}{y^2} \left[ xy \mathcal{J}_o(xy) - 2 \mathcal{J}_i(xy) \right]
\]

(4.8)

where

\[
\mathcal{J}_u(u) = \int_{u}^{\infty} \frac{\mathcal{J}_i(t)}{t} \, dt
\]

With the analytical expressions for the integrals in (4.5) now known, a numerical procedure for the evaluation of \( g(y) \) can be developed:
\[
g(y) = \sum_{i=1}^{p} \left\{ \epsilon_0 \left[ - \frac{J_o(y \sigma^y)}{y} \right]^2 + \epsilon_1 \left[ - \frac{1}{2} \left\{ xy J_o(x y) - J_i(x y) + J_{i+1}(x y) \right\} \right]^2 \right\} + \epsilon_2 \left[ \frac{x}{y} \left\{ xy J_o(x y) - 2 J_i(x y) \right\} \right]^2 \right\} \\
= \sum_{i=1}^{p} \left\{ - \frac{\epsilon_0}{\sigma} J_o(y x_{i+2}) - \frac{\epsilon_1}{2} \left[ y x_{i+2} J_o(y x_{i+2}) - J_i(y x_{i+2}) + J_{i+1}(y x_{i+2}) \right] - \frac{\epsilon_2}{2} \left[ y x_{i+2} J_o(x y_{i+2}) - 2 x_{i+2} J_i(x y_{i+2}) \right] \\
+ \frac{\epsilon_0}{\sigma} J_o(y x_i) + \frac{\epsilon_1}{2} \left[ y x_i J_o(y x_i) - J_i(y x_i) + J_{i+1}(y x_i) \right] + \frac{\epsilon_2}{2} \left[ y x_i^2 J_o(y x_i) - 2 x_i J_i(y x_i) \right] \right\} \\
= \sum_{i=1}^{p} \left\{ - J_o(y x_{i+2}) \left[ \frac{\epsilon_0}{\sigma} + \frac{\epsilon_1}{2} x_{i+2} + \frac{\epsilon_2}{2} x_{i+2}^2 \right] + J_i(y x_{i+2}) \left[ \frac{\epsilon_1}{2} + \frac{\epsilon_2}{2} x_{i+2} \right] - J_{i+1}(y x_{i+2}) \right\} \\
= \sum_{i=1}^{p} \left\{ - \frac{1}{\sigma} J_o(y x_{i+2}) f_{i+2} + \frac{1}{\sigma} J_i(y x_{i+2}) \left( \epsilon_1 + \epsilon_2 x_{i+2} \right) - \frac{\epsilon_2}{2} J_{i+1}(y x_{i+2}) \right\} \\
+ \frac{1}{\sigma} J_o(y x_i) f_i - \frac{1}{\sigma} J_i(y x_i) \left( \epsilon_1 + \epsilon_2 x_i \right) + \frac{\epsilon_2}{2} J_{i+1}(y x_i) \right\} \\
= \sum_{i=1}^{p} \left\{ \frac{1}{\sigma} \left[ J_o(y x_i) f_i - J_o(y x_{i+2}) f_{i+2} \right] - \frac{1}{\sigma} \left[ \epsilon_1 \left\{ J_i(y x_i) - J_i(y x_{i+2}) \right\} + 2 \epsilon_2 \left\{ x_i J_i(y x_i) - x_{i+2} J_i(y x_{i+2}) \right\} \right] \right\} \\
+ \frac{\epsilon_2}{2} \left[ J_{i+1}(y x_i) - J_{i+1}(y x_{i+2}) \right] \right\} \right\} (4.9)
The algorithm of equation (4.9), preceded by the calculation of the coefficients \( l_1 \) and \( l_2 \), can readily be coded into a computational procedure. In figure 4, the above sequence of steps is presented in a flow-chart; the flow-chart makes provision for many values of \( g(y) \) to be computed. (The flow-chart in figure 4 is developed in the general notation of \( x \) and \( y \), because it is equally useful for the computation of

\[
\int_a^b f(\lambda) \lambda J_{\lambda r} d\lambda \quad \text{and} \quad \int_a^b f(r) r J_\lambda(\lambda r) dr.
\]

A computational procedure to calculate the Bessel functions \( J_0 \), \( J_1 \) and \( J_{11} \) was obtained by combining three separate subprograms developed by Meinardus. Algorithms for the generation of the \( J_0 \) and \( J_1 \) Bessel functions can be found in Abramowitz and Stegun (1968, p. 369-370); the algorithm for \( J_{11} \) is derived from the series expansion of \( J_1 \).

The Problem of Truncation in Numerical Integration

Replacing the semi-infinite integral of (4.1) by a finite integral as in (4.4), imposes a strict requirement on the function \( x f(x) \). If the finite integral is expressed as

\[
g(y) = \int_a^b f(x) x J_{\lambda y} dx
\]

(4.10)

the requirement is that \( x f(x) \) be zero outside the interval \([a,b]\). When this requirement is not met, equation (4.10)
Figure 4. Logical flow-chart for the computation of the definite integral of the product of a given function and a first-order Bessel function.
will be incorrect due to the truncation of the non-zero function \( x \cdot f(x) \).

For the functions of interest in this study, the Hankel transformation can be expressed in the following form (from 3.5):

\[
[k(\lambda)-1] = \int_0^\infty \frac{1}{r^2} \left[ \frac{\rho_a(r)}{\rho_1} - 1 \right] r J_1(\lambda r) \, dr
\]

\[
= \int_0^\infty \frac{1}{r} \left[ \frac{\rho_a(r)}{\rho_1} - 1 \right] J_1(\lambda r) \, dr \tag{4.11}
\]

We know that apparent-resistivity curves have the following asymptotic behavior:

- at short spacing, \( \rho_a(r) \) approaches \( \rho_1 \), so that \( \frac{1}{r} \left[ \frac{\rho_a(r)}{\rho_1} - 1 \right] \to 0 \) for \( r < r_{\text{min}} \),

- at large spacing, \( \rho_a(r) \neq \rho_1 \)

except in the rare case of \( \rho_n = \rho_1 \). The multiplying factor \( \frac{1}{r} \) is not strong enough to ensure rapid convergence of \( \int_1^\infty \frac{1}{r} \left[ \frac{\rho_a(r)}{\rho_1} - 1 \right] \) for large \( r \). In practice, electrical soundings are typically obtained for values of \( r \) as great as \( 10^4 \) meters, but very seldom more.

From the foregoing considerations, it is evident that a technique must be devised to ensure rapid convergence of the integral.

**Subtracting a Two-Layer Curve**

Consider the two-layer master-curve which has the same value (\( \rho_1 \)) as the observed curve for small separations \( r \),
as well as the same asymptote (approaching $\rho_n$) for large separations $r$. Let this two-layer sounding-curve be $\rho^*(r)$ and its corresponding two-layer Kernel $k^*(\lambda)$.

Rewrite equation (4.11) as

$$[k(\lambda)-1] = \frac{i}{\rho_i} \int_0^\infty \frac{1}{r} \left[ \rho_a(r) - \rho^*_i \right] J_1(\lambda r) \, dr .$$

This equation is mathematically equivalent to

$$[k(\lambda)-1] = \frac{i}{\rho_i} \int_0^\infty \frac{1}{r} \left[ \rho_a(r) - \rho^*_1 \right] J_1(\lambda r) \, dr$$

$$+ \int_0^\infty \frac{1}{r} \left[ \rho^*_1 \right] J_1(\lambda r) \, dr$$

$$= \frac{i}{\rho_i} \int_0^\infty \frac{1}{r} \left[ \rho_a(r) - \rho^*_1 \right] J_1(\lambda r) \, dr$$

$$+ \int_0^\infty \frac{1}{r} \left[ \frac{\rho^*_1}{\rho^*_i} - 1 \right] J_1(\lambda r) \, dr$$

$$= \frac{i}{\rho_i} \int_0^\infty \frac{1}{r} \left[ \rho_a(r) - \rho^*_1 \right] J_1(\lambda r) \, dr + [k(\lambda)-1] .$$

(the last term is replaced with 4.11).

This relationship can be rewritten as

$$k(\lambda) = \frac{i}{\rho_i} \int_0^\infty \frac{1}{r} \left[ \rho_a(r) - \rho^*_1 \right] J_1(\lambda r) \, dr + k^*(\lambda)$$

It is now evident from the choice of $\rho^*(r)$ that the function $[\rho_a(r) - \rho^*(r)]$ approaches zero rapidly outside
the range of observation. The semi-infinite integral can therefore be replaced by a finite integral as follows:

\[ k(\lambda) = \frac{1}{\rho_1} \int_{r_{\min}}^{r_{\max}} \frac{1}{r} \left[ \rho_a(r) - \rho^*(r) \right] J_1(\lambda r) \, dr + k^*(\lambda). \]  

(4.12)

The calculation of the desired Kernel, \( k(\lambda) \), corresponding to the observed sounding-curve, \( \rho_a(r) \), will include the following steps, prescribed by equation (4.12):

1) By two-layer curve-matching, find a two-layer master-curve with the same asymptotes on both sides. The parameters for this curve will be \( \rho_1 \) (same as for the field curve), a fictitious \( h^* \) (equal to the separation where the two-layer theoretical cross falls), and \( \rho_n \) (basement resistivity for the field section; the interpreting geophysicist will frequently have to decide on a value for \( \rho_n \)).

2) Subtract the \( \rho^*(r) \) from \( \rho_a(r) \) point for point, and divide by \( r \) to obtain \( 1/r [\rho_a(r) - \rho^*(r)] \). This resulting function is submitted to numerical integration by Vanyan's technique.

3) By means of Sunde's algorithm, calculate \( k^*(\lambda) \) for the fictitious two-layer section with parameters \( \rho_1, h^* \) and \( \rho_n \).

4) Divide the function obtained by numerical integration by \( \rho_1 \), and add \( k^*(\lambda) \) point for point to the result to obtain \( k(\lambda) \).

The sequence of operations described above is illustrated in figures 5 and 6. The two upper curves in figure 5 are the
Figure 5
The preparation of sounding-curves for Hankel transformation.
Completing calculations to obtain the corresponding Kernel.
"observed" sounding-curve $\rho_a(r)$, and the two-layer master-curve with the same asymptotes, $\rho^*(r)$. The lower curve in figure 5 is the resulting curve $[\rho_a(r) - \rho^*(r)]$.

Figure 6 shows the wave-number domain equivalents: the lower curve is the result of numerical Hankel transformation, the two upper curves are $k^*(\lambda)$ and the desired $k(\lambda)$, respectively. (Both plots in figure 5 and 6 are presented with logarithmic scales. As is customary in plots of this kind, negative portions of a function are plotted in absolute value, but with a dashed line to indicate the negative sign.)

**Calculation of the Two-Layer Curve to Subtract**

The two-layer master-curve to be calculated can be expressed in terms of its Kernel by means of equation (3.4) as follows:

$$\rho^*(r) = \rho_1 \left\{ 1 + r^2 \int_0^\infty \left[ k^*(\lambda) - 1 \right] J_1(\lambda r) \lambda \, d\lambda \right\}. \quad (4.13)$$

From the asymptotic behavior of two-layer Kernels (Keller and Frischknecht, 1966, p. 143), we know that $k^*(\lambda) = 1$ for values $\lambda h^* > 5$; and that for $\lambda h^* = 10$, $k^*(\lambda) = 1$. This fact permits equation (4.13) to be written as:

$$\rho^*(r) = \rho_1 \left\{ 1 + r^2 \int_0^{10/h} \left[ k^*(\lambda) - 1 \right] \lambda J_1(\lambda r) \lambda \, d\lambda \right\}. \quad (4.14)$$

We see that all the computational tools to calculate $\rho^*(r)$ are available:

1) Compute $k^*(\lambda)$ by means of Sunde's algorithm.
2) Compute \([k^*(\lambda) - 1] \lambda\) and submit to numerical integration by Vanyan's technique.

3) Multiply the result by \(r^2\), add 1 and multiply the new result by \(\rho_1\) to obtain \(\rho^*(r)\).

In the case of an infinitely resistive basement, \(k^*(\lambda) \to \infty\) for \(\lambda \to 0\), generally for \(\lambda h^* < 0.1\). In the range \([0, .1/h^*]\), log \(k^*(\lambda)\) versus log \(\lambda h^*\) forms a straight line with slope \(-1\). In this range,

\[
\log k^*(\lambda) = - \log \lambda h^*,
\]

from which it follows that

\[
[k^*(\lambda) - 1] = \frac{1 - \lambda h^*}{\lambda h^*}
\]

With the above conditions taken into account, \(\rho^*(r)\) for a very resistive basement can be computed by means of the equation

\[
\rho^*_a(r) = \rho_1 \left\{ 1 + r^2 \int_0^{1/h^*} \left[ k(\lambda) - 1 \right] \lambda J_1(\lambda r) \, d\lambda + \int_{1/h^*}^{10/h^*} \left[ k(\lambda) - 1 \right] \lambda J_1(\lambda r) \, d\lambda \right\}
\]

\[
= \rho_1 \left\{ 1 + \frac{r^2}{h^*} \int_0^{1/h^*} \left[ 1 + \lambda h^* \right] J_1(\lambda r) \, d\lambda + \int_{1/h^*}^{10/h^*} \left[ k(\lambda) - 1 \right] \lambda J_1(\lambda r) \, d\lambda \right\}
\]

From equations (4.6) and (4.7) it follows then that

\[
\rho^*_a(r) = \rho_1 \left\{ 1 + r^2 \int_{10/h^*}^{100/h^*} \left[ k(\lambda) - 1 \right] \lambda J_1(\lambda r) \, d\lambda \right\}
\]

\[
+ \rho_1 \left\{ -9 \frac{r}{10 h^*} J_0 \left( \frac{r}{10 h^*} \right) + J_1 \left( \frac{r}{10 h^*} \right) + J_1 \left( \frac{r}{10 h^*} \right) + \frac{r}{h^*} - 1 \right\} \tag{4.16}
\]
In this expression, the first group of terms is evaluated in the same fashion as in the case of a finitely resistive basement; the last group of terms by the computation of the appropriate Bessel functions and constants.

The computation of two-layer curves for sections in which the basement is very conductive warrants special attention too. Two-layer sounding-curves of this type decrease in amplitude extremely rapidly at large separations. In this region, it was found that errors due to round-off accumulate, and produce erroneous results in Hankel transformation. For this reason, values of \( \rho^*(r) \) are computed only for values of \( r \) less than \( 5h^* \). If values of \( \rho^*(r) \) are required for greater separations, they are directly set equal to \( \rho_n \).

A Flow-Chart for the Preparation of a Sounding-Curve for Numerical Integration

In figure 7 a flow-chart including the sequence of steps outlined above is presented. The flow-chart also makes provision for the rare occurrence of \( \rho_1 = \rho_n \), in which case it defines all values of \( \rho^*(r) = \rho_1 \). The flow-chart furthermore includes steps to define a set of \( \lambda \)'s (79 values) for which \( k^*(\lambda) \) is to be computed. (This set of \( \lambda \)'s will be different from that used in calculating the Kernel corresponding to the observed sounding.) The final result of computation is \( 1/r \left[ \rho_a(r) - \rho^*(r) \right] \), the function required for numerical integration in (4.12).
Figure 7. Logical flow-chart of the procedure to prepare a given sounding for Hankel transformation.
Accuracy of Computation

The root-mean-square error between two discrete functions \( f_i \) and \( g_i \) is defined as

\[
E = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (f_i - g_i)^2}
\]  

(4.17)

where \( N \) = the total number of points representing \( f \) and \( g \).

Because this error criterion will be used frequently in the rest of this text, the abbreviation "rms error" will be used for convenience. This error will be expressed as a percentage, with the meaning that 100% represents the distance equal to one decade of the usual logarithmic scale. This means that an rms error of 1% will correspond to a distance of 0.625 mm on the frequently-used scale of 62.5 mm per decade.

Figure 8 is a logical flow-chart of the procedure to calculate the rms error between two given functions.

Test cases of four sections were computed to determine the accuracy achieved in the calculation of two-layer sounding-curves. The parameters for two cases were chosen to be the same as those for master-curves tabulated by Orellana and Mooney (1966, p. T2-T3). The other two cases were approximations of the two conditions of an infinitely resistive basement and an infinitely conductive basement respectively. Actual values of \( \rho_n = 1000 \) and \( \rho_n = .001 \) were used in the numerical calculations.
Communicate:
\( F_i = \) first function
\( G_i = \) second function
\( n = \) no. of points in \( F \) and \( G \)
\( e = \) rms error returned

\[
e \leftarrow 0
\]

\[
i \leftarrow 1
\]

\[
\text{term} \leftarrow F_i - G_i
\]

\[
e \leftarrow e + \text{term}
\]

\[
i \leftarrow i + 1
\]

\[
i > n ?
\]

\[
e \leftarrow \sqrt{e/n}
\]

Return

Figure 8. Logical flow-chart of the procedure to compute the root-mean-square error.
The results of the test cases, relative to Orellana's tables, are given below:

1) Basement resistivity $\rho_n \rightarrow \infty$ : $e = 0.26\%$
2) Basement resistivity $\rho_n = 20$ : $e = 0.05\%$
3) Basement resistivity $\rho_n = 0.05$ : $e = 2.7\%$
4) Basement resistivity $\rho_n \rightarrow 0$ : $e = 3.0\%$

The computational procedure for numerical integration (see equation 4.1) was tested individually with a test function $x \cdot f(x) = e^{-x}$.

According to Watson (1966, p. 386),

$$\int_0^\infty e^{-x} J_1(xy) \, dx = \frac{(\sqrt{1+y^2} - 1)}{y \sqrt{1+y^2}} \quad (4.18)$$

The test function was represented by 120 discrete points, linearly equi-spaced in the interval $[0, 12]$. For this test case, the rms error between the numerical results and the closed-form expression of (4.18) was found to be $0.01\%$ for 12 values computed.

The entire string of operations involved in finding the Kernel corresponding to a given sounding-curve was tested by using the four-layer master-curve of figure 1 as a test function.

Numerical values for the test function were obtained from the master tables (Orellana and Mooney, 1966, p. T94-T95); results of the numerical Hankel transformation were checked against the Kernel calculated by means of Sunde's
algorithm. The rms error was found to be 0.10% for 25 values computed.

The error-considerations discussed above provide evidence that the approximate numerical methods employed yield results accurate to fractions of 1%. Accuracy of this order is considered sufficient for the treatment of real data where individual points may scatter by as much as 5%.
LEAST-SQUARES CURVE FITTING

Least-Squares Curve Fitting in General

The problem of fitting a theoretically calculated curve to a given set of points is well known in mathematical physics. The solution to this problem of curve fitting has been the objective of many studies, and because of that is now reasonably well understood.

A study of non-linear curve fitting from a geophysical point of view was done by Snyder (1968, p. 100). His discussion was aimed at the curve fitting of gravity data specifically, but provides a great deal of insight into the problem in general.

When a theoretical model \( (M_i) \) is calculated at \( n \) discrete points, the desired result is that the points \( M_i \) should fall as close as possible to an observed set of points \( O_i \). The most frequently used criterion of how well two curves agree, is that of least-squares. If

\[
S = \sum_{i=1}^{n} \left[ M_i - O_i \right]^2 ,
\]

the objective is to find that set of \( M_i \) for which \( s \) will be a minimum. A prerequisite for the least-squares method is that the number of observation points be greater than the number of parameters to be determined (the system is overdetermined).
From the mathematical development of the requirements stated above, a set of simultaneous equations, the normal equations, is obtained. The normal equations are set up in terms of the changes required in each parameter to bring the new model $M_i$ closer to the observed set $O_i$. If the model $M$ is a function of $k$ parameters $p$ and the parameter of observation $x$, we can write

$$M_i = M(p_1, p_2, \ldots, p_k, x_i).$$

In terms of the notation above, there are $k$ simultaneous equations, for which the unknowns are $\Delta p_1, \Delta p_2, \ldots, \Delta p_k$. Also in terms of the notation above, the requirement for a best fit is expressed as

$$\frac{\delta s}{\delta (\Delta p_j)} = 0.$$

The normal equations of least-squares curve fitting may be expressed in matrix notation:

$$[p^T p] R = [p^T D]. \tag{5.2}$$

A development of the normal equations in this form was given by Forsythe and Moler (1967, p. 16). In this form, $p^T p$ is a $k \times k$ matrix containing the coefficients of the simultaneous equations, $D$ is a column vector containing the residuals $M_i - O_i$, and $R$ is the desired small-changes vector $\Delta p_j$.

In equation (5.2) $P$ is a matrix of $n$ rows x $k$ columns. The elements of column $l$ of this matrix is obtained as follows:
According to this definition, the elements of column \( \ell \) are found by evaluating the partial derivative of the model with respect to the \( \ell \)-th parameter. The partial derivative is calculated for every value of the observation parameter, the results are stored in consecutive rows. \( P^T \) is the transpose of matrix \( P \).

The solution of the matrix equation (5.2) presents a numerical problem of considerable proportions. For this reason, it has received a considerable amount of attention from distinguished investigators. In a book devoted entirely to this problem, Forsythe and Moler (1967) discussed the mathematics involved, as well as the problems encountered in solving such an equation by computer.

An equally intensive study of this problem was presented by J. H. Wilkinson in Ralston and Wilf (1967, p. 65). As an end-result of this development, Wilkinson presented a logical flow-chart for the computational procedure involved in solving equation (5.2). In the present study, the author used a FORTRAN-4 subprogram based on this flow-chart. This FORTRAN subprogram was coded by Snyder, and is available upon request from the Department of Geophysics, Colorado School of Mines.
Least-Squares Curve Fitting of Kernel Functions

The Log Kernel as Theoretical Model

In the least-squares curve fitting of electrical data, the logarithm of the Kernel function serves as theoretical model. The same reasons by which we attach a special significance to the logarithmic function of the sounding-curve (Kunetz, 1966, p. 54) prescribe that we use the logarithm of the Kernel rather than the Kernel as theoretical model.

The Principle of Equivalence

In the distance domain, we are very familiar with the limitations brought about by the principle of equivalence. The effect of the principle of equivalence is that two different geo-electric sections may produce sounding-curves which are practically indistinguishable from each other. An extensive study of the effects of this principle on three-layer sounding-curves was presented by Keller and Frischknecht (1966, p. 158-177). Their development clearly shows the complexity of the problem even in a simple three-layer case. For more layers, the validity of the principle of equivalence for a particular layer depends on the geo-electric parameters of all the layers present in the section (Kunetz, 1966, p. 58). In summary it can be said that a layer will be equivalent if its thickness is not many times that of the adjacent layers, and it has a resistivity contrast of more than about 2:1 to those layers.
From experience in electrical prospecting methods, we know that equivalent conditions are frequently encountered. This is especially true if four or more layers are present in a sounding-curve which extends over three or four decades in the separation parameter. The range of validity of the principle of equivalence becomes ever wider as the number of layers increase.

The principle of equivalence in the wave-number domain is valid to the same degree as in the distance domain (Koefoed, 1968, p. 33).

The Number of Parameters Upon Which the Kernel Depends

In the case of an equivalent layer, the Kernel function (like the sounding-curve) does not depend on the resistivity and thickness of that layer individually. The Kernel does depend on either the transverse resistance $T$ or longitudinal conductance $S$ of that layer, whichever is applicable. The parameters $T$ and $S$, called the Dar-Zarrouk parameters, are defined as

$$\begin{align*}
T &= h \cdot \rho \\
S &= h / \rho
\end{align*} \quad (5.4)$$

To simplify the computational procedures involved in this approach of computer-assisted interpretation, it was decided that all intermediate layers will be considered equivalent. This decision was made in anticipation of the fact that the computer's assistance will be most useful in the interpretation of four- or more-layer curves. In such
cases the range of validity of the principle of equivalence is indeed wide. It was also anticipated that when non-equivalent cases are encountered, they will be recognized as such when the interpreting geophysicist studies graphs of the "field" Kernel and the program's best interpretation. Extension of the curve fitting methods to non-equivalent cases is straightforward.

The above mentioned simplifying assumptions have proven to be very useful, as will be shown later in the results of test cases.

In a recent paper, Meinardus (1970) treats the problem of least-squares fitting of Kernel functions on the assumption that no intermediate layer is equivalent. The curve fitting technique described in the above mentioned paper can be used for the interpretation of non-equivalent cases encountered.

In the simplifying approach which regards every intermediate layer as equivalent, the Kernel function depends on the following parameters:

1) The first-layer thickness $h_1$.

2) The parameter $T$ or $S$ of every intermediate layer, depending on which one is valid. (The "intermediate" layers are those between the surface layer and the semi-infinite basement.)

Note that the surface-resistivity and basement-resistivity are determined prior to Hankel transformation. The parameters
\( \rho_1 \) and \( \rho_n \) are thus not included among those to be adjusted by the least-squares curve fitting technique.

For an \( n \)-layer section, we see that there are \( n-1 \) parameters on which the Kernel depends. The parameters are \( h^1, T^2 \) or \( S^2, T^3 \) or \( S^3 \).... and \( T^{n-1} \) or \( S^{n-1} \).

The "main" direction of current-flow in the layer in question (Zohdy, 1965) relative to that in the layer below, frequently is enough indication of whether \( S \) or \( T \) is the parameter of interest. This phenomenon can be likened to the "refraction" of current-lines emanating from a point-source on the surface. When the current lines leaving the layer of interest are convergent in the next-deeper layer, the "main" direction of current-flow in the layer of interest is considered to be horizontal, and for that layer the parameter of interest is the longitudinal conductance (S). This condition occurs when the next-deeper layer is more resistive than the layer in question.

The decision on whether the parameter T or S is of importance for layer \( i \), can thus be made on the basis of the following conditions:

if \( \rho_{i+1} > \rho_i \), the parameter is S;

if \( \rho_{i+1} < \rho_i \), the parameter is T.

The procedure involved in deciding upon T or S for all the intermediate layers, is included in the flow-chart of figure 9. The sequence of T's or S's defined by this
Communicate:
\( n_l = \text{no. of layers} \)
\( n_p = \text{no. of parameters} \)
\( \rho_i = \text{resistivities} \)
\( h_i = \text{thicknesses} \)
\( \text{type}_i = \text{Symbol S or T} \)

Figure 9. Logical flow-chart for the determination of the "type" of section regarding T or S.
The procedure is considered to be a label of the "type" of section present.

**The Partial Derivatives of the Kernel Function**

In setting up the matrix equation (5.2), the matrix $P$ has to be defined. In terms of using the logarithm of the Kernel as theoretical model, the elements of column $\lambda$ of this matrix are defined as

$$
\Theta_{i\lambda} = \frac{\partial}{\partial p_{i\lambda}} \log k(\lambda_i), \quad i = 1, 2, \ldots, m
$$

(5.5)

In this expression

$m =$ the number of values of $\lambda$ for which the "field" Kernel was obtained,

$p_{i\lambda} = T_\lambda$ or $S_\lambda$,

and $p_1 = h_1$.

The partial derivatives required to define matrix $P$ can be computed by means of algorithms based on Sunde's recurrence relation. Analytic expressions for the partial derivatives required in this approach are given by Meinardus (1970, p. 424-427).

An alternative method of obtaining the partial derivatives is that of finite differences. In this approach, the partial derivative is calculated by computing two theoretical Kernels for which all but one of the parameters are exactly the same. The parameter with respect to which the partial derivative is wanted is the one which is different. This parameter is defined by incrementing the original one by a
small amount (0.5% was found to be small enough). The difference between the two Kernels divided by the small increment is the desired partial derivative. The above sequence of steps can be expressed in the following form:

$$\frac{\partial}{\partial p_k} \log k(\lambda) \approx \frac{1}{\Delta p_k} \left[ \log k(p_1, p_2, \ldots, p_k + \Delta p_k, \ldots, p_{n-1}) - \log k(p_1, p_2, \ldots, p_k, \ldots, p_{n-1}) \right]$$ (5.6)

A logical flow-chart for the computation of partial derivatives is presented in figure 10. The partial derivatives are computed according to (5.6). The partial derivative with respect to $T_3$, for example, is computed by making small changes to both $p_3$ and $h_3$, from which it follows that

$$\Delta T_3 = (h_3 + \Delta h_3) \cdot (p_3 + \Delta p_3) - h_3 \cdot p_3$$

Examples of partial derivatives are shown in figure 11. The Kernel function in this figure corresponds to the sounding-curve $K_{H4}(Q)$ (Orellana and Mooney, 1966, sheet 51), and is the same as that in figure 1. For the section in question, the Dar-Zarrouk parameters to be considered are $T_2$ and $S_3$.

**Iterative Matching of Kernel Functions**

In the least-squares curve fitting of Kernel functions, the objective is to determine the parameters of the theoretically computed Kernel which matches the "observed" data to a pre-defined degree. The "observed" data in this case correspond to the log Kernel function obtained by Hankel
Figure 10. Logical flow-chart for the computation of the partial derivatives of log Kernel with respect to $h_1$ and the Dar-Zarrouk parameters of the intermediate layers.
Figure 11

The Kernel for KH4(Q) and the partial derivatives with respect to $h_2$, $T_2$, and $S_3$. 
transformation of the experimentally-determined sounding-curve.

The sequence of repeated steps involved in arriving at an end-result is the following:

1) Calculation of the log Kernel for the present set of geo-electric parameters or "cut".

2) Calculation of the rms error between this theoretical model and the "observed" data.

3) Testing the rms error to see whether the agreement is good enough; if it is, the procedure is discontinued.

4) Definition and solution of the matrix equation to determine the new set of parameters for which the error will hopefully be smaller. Go back to step 1.

In some cases the error of the present "cut" will be larger than that of the previous "cut" - over-correction has taken place. When such a condition is encountered, the specified amounts of change to the parameters of the previous cut are reduced and the sequence restarted at step 1.

The procedure of steps 1-4 is permitted to run through 30 iterations. Experience has shown that under normal conditions, the theoretical curve has converged as much as it will to the "observed" curve after 8 to 10 iterations. If it has not converged after 30 iterations, a poor first cut is indicated, and human intervention is needed.

The least-squares criterion is satisfied when the error has reached a minimum, irrespective of whether this minimum
is small or not. In order to make sure that a minimum has been reached, the procedure checks for the possibility of overcorrection, and if indeed it cannot improve the degree of fit after 10 attempts, the process is discontinued.

The flow-chart in figure 12 contains the steps involved in executing the iterative procedures of steps 1-4, as well as for the other stop-conditions.

**Definition and Solution of the Normal Equations**

The first step in defining the normal equations

\[(P^TP)R = P^TD\] (5.7)

is the calculation of the matrix of partial derivatives, \(P\).

The matrix \(P\) is defined in accordance with equation (5.5), using the appropriate Dar-Zarrouk parameters as the characteristic parameters of the intermediate layers.

The vector \(D\) is defined by the equation

\[D_i = \log k_f - \log k_c\]

where \(k_f\) = the "observed" Kernel

\(k_c\) = the Kernel of the present "cut".

The other steps prescribed by equation (5.7) are the multiplications \(P^TD\) and \(P^TP\), and a call to one of the existing procedures to solve the simultaneous equations.

Figure 13 is a flow-chart of the procedures outlined above. The steps include: definition of \(P\) and \(D\), calculation of \(P^TD\) and \(P^TP\), a call to a subprogram that solves simultaneous equations, and a forced exit when a singular matrix is encountered.
Figure 12. Logical flow-chart of the procedure to curve match Kernel functions.
Communicate:

- \( n_k \) = no. of Kernel values
- \( K_{ref_i} \) = 'field' Kernel
- \( K_{try_i} \) = Kernel for the present cut
- \( n_p \) = no. of parameters to adjust
- \( r_i \) = results returned

Compute the matrix of partial derivatives, result is \( P_{ij} \)

\[
\begin{align*}
    &i-1 \\
    \text{Compute } &d_i = K_{ref_i} - K_{try_i} \\
    \text{Compute } &i ightarrow i + 1 \\
    \text{Compute } i &> n_k ? \text{ N, otherwise Y} \\
    \text{Compute } &P^T \cdot d, \text{ result stored over } d_i \\
    \text{Compute } &P^T \cdot P, \text{ result stored over } P_{ij} \\
    \text{Solve the matrix equation } &P \cdot r = d, \text{ result is } r_i \\
    \text{Singular matrix} \? \text{ Y, otherwise N} \\
    \text{STOP} \\
\end{align*}
\]

Figure 13. Logical flow-chart of the procedure to define and solve the normal equations in matrix form.
The Matrix Multiplications: A separate subprogram to perform the matrix multiplications was developed. This subprogram uses the matrix P as starting-point, and by proper choice of column entries of P, uses them as row entries of PT.

In the calculation of the product PT·D, the result is a column vector, and is defined in a straightforward manner. In the calculation of PT·P, it is profitable to note that the result is a square symmetric matrix. The procedures are therefore organized to define one half of the result matrix only, and the other half is obtained by simple replacement.

The logical flow-chart in figure 14 includes the sequence of steps outlined above.

Definition of the Parameters of a New "Cut"

The curve matching of Kernel function in terms of the Dar-Zarrouk parameters produces a slight complication at intermediate stages. The solution of the normal equations is in terms of required changes in the Dar-Zarrouk parameters; the theoretical model, the log Kernel, requires the definition of resistivities and thicknesses as its parameters. It is therefore necessary to redistribute a specified amount of change in S, say, to the resistivity and thickness in such a way that the specified ΔS is preserved. This requirement can be formulated as follows:

S-equivalence: find Δρ, Δh such that

\[(h + Δh)/(ρ +Δρ) - h/ρ = ΔS;\]
Communicate:

- \( a_i \) = left matrix
- \( b_j \) = right matrix
- \( n_a \) = no. of columns in \( a \)
- \( n_b \) = no. of columns in \( b \)
- \( n_r \) = no. of rows in \( a \) and \( b \)

Double-precision accuracy required.

Figure 14. Logical flow-chart for the efficient multiplication of the matrices involved.
T-equivalence: find Δρ, Δh such that

\[(h + Δh) \cdot (ρ + Δρ) - h \cdot ρ = ΔT.\]

With the further requirement that for S-equivalence

\[Δh = -Δρ,\]

and for T-equivalence \[Δh = Δρ,\]
it follows that for

S-equivalence: \[Δh = -Δρ = \frac{ρ \cdot ΔS}{2h + ρ \cdot ΔS}\]

and for T-equivalence: \[Δh = Δρ = [1 + \frac{ΔT}{h \cdot ρ}]^{1/2} - 1.\] (5.8)

In the above expressions, ΔS and ΔT are the specified small changes obtained from the solution of equation (5.7); h and ρ are the old values of the thickness and resistivity respectively.

The flow-chart for the computational procedures to define the parameters for a new "cut" is presented in figure 15. The procedures include steps by which the amounts of change Δh and Δρ are restricted so that positive resistivities and thicknesses are returned under all circumstances. The flow-chart also includes a step for the definition of a new \[h_1\], positive under all circumstances.

Computer Interpretation from Sounding-Curve to Geo-Electric Parameters

A master program to coordinate all the procedures described until now is developed next. This master program will handle input and output of data, and will start execution
Communicate:

- $n_i$ = no. of layers
- $\rho_i$ = resistivities
- $h_i$ = thicknesses
- type$_i$ = Dar-Zarrouk symbol
- $r_i$ = specified changes in parameters

\[ \Delta h_i = \text{minimum of } (r_i, 95) \]
\[ \Delta h_i = \text{maximum of } (\Delta h_i, -95) \]
\[ h_i = (1 + \Delta h_i) \cdot h_i \]

$i = 2$

\[ \Delta p = \rho_i \cdot r_i / (2 h_i \cdot \rho_i \cdot r_i) \]
\[ \Delta p = \text{minimum of } (\Delta p, 75) \]
\[ \Delta p = \text{maximum of } (\Delta p, -75) \]
\[ \rho_i = (1 - \Delta p) \cdot \rho_i \]
\[ h_i = (1 + \Delta p) \cdot h_i \]

\[ \Delta p = \text{maximum of } (r_i, -9h_i \cdot \rho_i) \]
\[ \Delta p = \sqrt{1 + (\Delta p / h_i \cdot \rho_i)} \]
\[ \rho_i = \Delta p \cdot \rho_i \]
\[ h_i = \Delta p \cdot h_i \]

$i = i + 1$

\[ i > n_i - 1 \]

Return

Figure 15. Logical flow-chart for the definition of the parameters for a new cut.
of the subprograms at the appropriate times. A general outline of the steps required to do this is as follows:

1) Reading data for the observed sounding.
2) Reading the three parameters of the two-layer curve to subtract.
3) Preparation of the observed sounding for Hankel transformation.
4) Definition of an appropriate set of $\lambda$'s for the section.
5) The numerical integration.
6) Computations to complete the "field" Kernel or reference Kernel.
7) Reading data for the first cut interpretation.
8) Definition of the appropriate Dar-Zarrouk parameter for every intermediate layer.
9) Iterative matching of the theoretical model to the field Kernel.
10) Computation of the parameters which define the best interpretation.
11) Printing of results.

A logical flow-chart of the coordinating master program is presented in figure 16. The flow-chart includes the sequence of steps outlined above; the numbered sections of the flow-chart correspond to the numbers of the individual steps in this outline.
Figure 16. Logical flow-chart for the coordinating master program.
EXAMPLES

The computer program developed in this study was submitted to test-runs of various kinds. The test runs serve to illustrate the operation of the program, and in the cases where theoretical data are used, give an indication of the accuracy attained.

All test cases were run on a Digital Equipment Corporation Model PDP-10 computer, a 1 μ sec cycle-time machine.

The following test cases were treated:
1) A theoretically computed Kernel function.
2) The Kernel of case 1 with random noise added.
3) The sounding-curve of case 1.
4) Two field sounding-curves.

The geo-electric parameters for cases 1 and 2 were chosen to be the same as that of the master-curve KH4(Q) (Orellana and Mooney, 1966, sheet 51). By this choice, an accurately-computed sounding-curve for case 3 was available in the master-tables (Orellana and Mooney, 1966, p. T94-T95).

Test Case 1

The operation of the curve fitting section of the program was tested by using a Kernel function as input. In this case the numerical Hankel transformation was not executed.

The reference function for the curve fitting procedure thus consisted of a Kernel for which the parameters were known.
It was furthermore noise-free, and calculated to a high degree of accuracy. The parameters of this Kernel function are:

<table>
<thead>
<tr>
<th>layer</th>
<th>( \rho )</th>
<th>( h )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1:</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>2:</td>
<td>20</td>
<td>1</td>
</tr>
<tr>
<td>3:</td>
<td>.1</td>
<td>25</td>
</tr>
<tr>
<td>4:</td>
<td>1000</td>
<td></td>
</tr>
</tbody>
</table>

(Units of resistivity in ohm-meters; of thickness, in meters throughout)

Parameters for the first cut were chosen to be:

<table>
<thead>
<tr>
<th>layer</th>
<th>( \rho )</th>
<th>( h )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1:</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>2:</td>
<td>30</td>
<td>.2</td>
</tr>
<tr>
<td>3:</td>
<td>.05</td>
<td>20</td>
</tr>
<tr>
<td>4:</td>
<td>1000</td>
<td></td>
</tr>
</tbody>
</table>

The program needed 4 iterations to reach an error of less than 1%, and took 3.8 seconds of central-processor time.

The error was reduced in the following way: first cut error 26%, next 8.8%, 1.08% and finally 0.24%.

A best interpretation was returned as:

- layer 1: \( h = 1.02 \)
- layer 2: \( T = 19.8 \)
- layer 3: \( S = 248 \)

The Kernel functions for this test case are plotted in the usual logarithmic fashion in figure 17. In this figure,
Figure 17
Test Case 1. Curve-fitting a theoretical Kernel.
the reference Kernel and the Kernel for the best fit (cut 4) fall on top of each other within plotting accuracy.

Test Case 2

Electrical sounding-data are never noise-free - a typical good field sounding may contain as much as 5% scatter due to experimental errors and geologic inhomogeneities on the surface. A comparable amount of noise will be present in the Kernel obtained from that sounding.

A test run to study the operation of the computer program for Kernels that contain some scatter was devised by the addition of random noise to the theoretical Kernel of case 1. The set of numbers representing the random noise was normalized to lie between -0.1 and 0.1, and the resulting fraction used to add a small amount to every value of the theoretical Kernel. The new Kernel was computed as

\[ k'_i = k_i (1 + r_i) \]

where \( r_i \) = the set of random numbers in the range (-0.1,0.1).

Parameters for the first cut were chosen to be the same as for case 1.

Six iterations were needed to reduce the error to a minimum; the minimum of 2.7% was reached in 5.1 seconds (central-processor time). Sequential values of the rms error were 28% for the first cut, then 9.3%, 2.9%, 2.71%, 2.70% and finally 2.70%. The difference between the last two numbers was lost in rounding to three significant figures.
The program's best interpretation was:

layer 1:  h = 1.01
2:  T = 20.2
3:  S = 247

The curves plotted in figure 18 represent the Kernel functions calculated for cuts 1, 2, and 6. The curves for cuts 3, 4, and 5 are closer together than can be plotted, and fall on top of the curve for cut 6. The reference Kernel is indicated by the discrete symbols.

We see that in spite of a fair amount of scatter in the points representing the "field" Kernel, the final interpretation comes very close to the true set of parameters. This is a characteristic of the least-squares approach since a redundant amount of information is used for the determination of only a few parameters.

It should be noted that this test case is not an attempt to simulate the conditions that would be encountered with a sounding-curve containing a high degree of scatter. Random noise in the distance domain will be transmitted via Hankel transformation into the wave-number domain, but will appear in a different form. In this test case the step of Hankel transformation was not executed.

Test Case 3

The entire sequence of operations involved in the computer-assisted interpretation of a sounding-curve includes Hankel
Figure 18. A theoretical Kernel with random noise added.
transformation and least-squares curve fitting. For the third test case, a sounding-curve was used as input so that both steps could be tested.

The numerical values of the sounding-curve were obtained from the master tables of Orellana and Mooney. Parameters for the first cut were chosen to be the same as those for test cases 1 and 2.

The program required 5 iterations to reduce the error to less than 1%; the entire operation was executed in 6.0 seconds of central-processor time. Reduction of the error was achieved in the order 26% (first cut), 11%, 2.8%, 1.1%, and finally 0.24%.

The Kernel functions of interest in this test case are very close to those plotted in figure 17. A separate figure for this test case was consequently not included.

It is important to note that this test case included every step of the interpretation procedure, and produced an excellent end-result at the cost of $1.70. (Cost was computed for charges to outside persons using the PDP-10 computer at the Colorado School of Mines.)

Test Case 4

The operation of the program under practical conditions was checked with the use of a field sounding-curve as input. The sounding-curve for this test case (as for test case 5) was kindly provided by Dr. Jan van Zijl of the National
Physical Research Laboratory, Pretoria. Great care was taken with the acquisition of field data, with the result that a sounding-curve of excellent quality was obtained.

The numerical values representing the sounding-curve are plotted on the upper part of the plot in figure 19. The Kernel function corresponding to this field sounding is plotted by the discrete symbols on the lower part of the graph.

Parameters for the first cut in this case were those obtained by Van Zijl after preliminary curve matching. The Kernel function for this first cut is seen to be in close agreement with the observed data; the rms error was 3.6%.

The first-cut parameters were:

<table>
<thead>
<tr>
<th>layer</th>
<th>( \rho )</th>
<th>( h )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1:</td>
<td>100</td>
<td>10</td>
</tr>
<tr>
<td>2:</td>
<td>300</td>
<td>40</td>
</tr>
<tr>
<td>3:</td>
<td>76</td>
<td>380</td>
</tr>
<tr>
<td>4:</td>
<td>550</td>
<td>3300</td>
</tr>
<tr>
<td>5:</td>
<td>10000</td>
<td></td>
</tr>
</tbody>
</table>

After 8 iterations of the curve fitting process, the program returned its best interpretation for which the rms error was 1.42%. The curve corresponding to this interpretation is also included in figure 19.

Interpretation returned:

layer 1: \( h = 9.8 \)

2: \( T = 16,130 \)
Figure 19. Test Case 4. Field sounding AW-N.
3: $ S = 5.23$
4: $ S = 6.24$

Execution time for this test run was 9 seconds of central-processor time; cost amounted to $2.66.

**Test Case 5**

A sounding-curve obtained in a different geologic environment was used for the next test run. This sounding-curve shows evidence of a very conductive basement, as can be seen in the upper portion of figure 20.

By Hankel transformation the corresponding Kernel was computed, and is plotted by the discrete points in the lower portion of figure 20.

First-cut parameters for this test run was defined by the author after cursory inspection of the graph. The parameters were

<table>
<thead>
<tr>
<th>layer</th>
<th>$\rho$</th>
<th>$h$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1:</td>
<td>260</td>
<td>12</td>
</tr>
<tr>
<td>2:</td>
<td>150</td>
<td>10</td>
</tr>
<tr>
<td>3:</td>
<td>460</td>
<td>380</td>
</tr>
<tr>
<td>4:</td>
<td>600</td>
<td>2100</td>
</tr>
<tr>
<td>5:</td>
<td>0.0001</td>
<td></td>
</tr>
</tbody>
</table>

The Kernel function for this first cut is shown in figure 20; the rms error was 7.3%.

Parameters for the program's best interpretation were returned after 7 iterations (8.9 seconds central-processor
time), when the rms error reached 1.4%. Total cost for this test-run again amounted to $2.66. Best interpretation parameters were:

1. Layer 1: \( h = 8.5 \)
2. \( S = 0.115 \)
3. \( S = 0.892 \)
4. \( T = 1.91 \times 10^6 \)

The Kernel function for the final interpretation is also plotted in figure 20, and we see that it agrees excellently with the "field" Kernel.

The sounding-curve used for this test case calls attention to an additional responsibility of the interpreting geophysicist. The solid circles in this figure represent the data points obtained in the field; open circles represent points that were graphically added.

To observe the requirements for accurate Hankel transformation, the input data must extend over a wide enough range of \( r \) so that a two-layer sounding-curve falls on top of the left- and rightmost points. Considering the field-obtained points only, we see that the two-layer master-curve with \( \rho_1 = 260, \rho_2 = 0 \) cannot be made to fall on the final asymptote of the field curve.

To circumvent this problem the interpreting geophysicist has decided on a basement resistivity, and by means of the two-layer master-curve \( \rho_1 = 600, h_1 = 4,000, \rho_2 = 0 \) graphically "completed" the sounding. The five data points for
values of $r > 8$ km were obtained from this graphically added final asymptote. The sounding-curve now has two points (at $r = 16$ km and $r = 18$ km) that fall on the two-layer curve $\rho_1 = 260$, $h_1 = 4800$, $\rho_2 = 0$ (two more points for $r < 10$).

The test cases presented in this section demonstrate that the least-squares technique of curve fitting can be applied to Kernel functions with confidence. For the two real-data cases, the author has not attempted to complete the process of interpretation by specifying thicknesses and resistivities explicity. This is due primarily to the lack of additional information and inexperience regarding the geologic setting of the sounding-curves. The excellent degree of fit between the computer's interpretation and field data, however, requires that the resistivities and thicknesses be chosen in agreement with the values of $S$ and $T$ returned.
CONCLUSIONS

The least-squares technique of curve fitting can be applied with great success to electrical sounding-data, provided that the Hankel inversion of field data succeeds. The curve fitting is executed most economically in the wave-number domain, where the Kernel function serves as theoretical model. An efficient computational algorithm for the Kernel exists in the form of Sunde's recurrence relation.

Numerical integration is required to obtain the Kernel function from a measured sounding-curve. A simplified technique suggested by Vanyan performs this numerical integration with sufficient accuracy, and at remarkably low cost.

The least-squares technique requires that the smallest number of parameters upon which the model depends be treated in the curve fitting procedure. The minimum number of parameters for any condition is \( n-1 \) in the case of an \( n \)-layer model. These parameters are first-layer thickness and the appropriate Dar-Zarrouk parameter for intermediate layers. This simplification was used in this study, and produced excellent results for a variety of real-data cases treated.

Interpretation in terms of the Dar-Zarrouk parameters only is indeed an oversimplification, and may in the rare case be a severe limitation of the usefulness of this method.
Fortunately, with sophisticated techniques of matrix-manipulation available (Marquardt, 1963), interpretation in terms of thickness and resistivity individually is possible at increased but still reasonable cost (Meindardus, 1970).

A successful execution of the computer-assisted interpretation of a sounding-curve depends on the insight and skill of the interpreting geophysicist. His responsibilities are the following:

1) Careful determination of the field data.
2) A decision on the number of layers present in the geo-electric section.
3) Definition of the parameters of the first-cut interpretation. This first cut is used to define the "type" of section present, in terms of which Dar-Zarrouk parameter to consider for every intermediate layer. The program tolerates a wide range of first-cut parameters as long as the "type" is correct.
4) An evaluation of the computer's best interpretation. With the use of additional information (well-data, adjacent soundings, experience), the interpreting geophysicist must define the geo-electric section in terms of thicknesses and resistivities individually. The end-result must be geologically meaningful!

The techniques employed in this approach to interpretation are affected by the same assumptions and limitations as
conventional curve matching. Horizontal layering is assumed, and no provision is made for the recognition of the effects of lateral inhomogeneities. In spite of the limitations involved, the computer program developed in this study can serve a useful purpose in the routine interpretation of electrical soundings.
APPENDIX A

Integrals involving Bessel functions

Consider the function

\[ J_{i\lambda}(u) = \int_u^\infty \frac{J_i(x)}{x} \, dx \]

\[ = \left[ \int \frac{J_i(x)}{x} \, dx \right]_{x=u}^{x=\infty} \]

For \( a < b \), we have:

\[ J_{i\lambda}(y) \bigg|_{y=a}^{y=b} = \left[ \int \frac{J_i(x)}{x} \, dx \right]_a^b - \left[ \int \frac{J_i(x)}{x} \, dx \right]_a^\infty \]

\[ = -\int_a^b \frac{J_i(x)}{x} \, dx \bigg|_{x=a}^{x=b} + \int_a^b \frac{J_i(x)}{x} \, dx \bigg|_{x=a}^{x=b} \]

\[ = \int_a^b \frac{J_i(x)}{x} \, dx , \]

or \( \int_a^b \frac{J_i(x)}{x} \, dx = -J_{i\lambda}(y) \bigg|_{y=a}^{y=b} \) \hspace{1cm} (A.1)

From Magnus and others (1966, p. 68) we have:

\[ \int J_\nu(z) \, dz = 2 J_{\nu+1}(z) + \int J_{\nu+2}(z) \, dz . \]

For \( \nu = 0 \):

\[ \int J_0(z) \, dz = 2 J_1(z) + \int J_2(z) \, dz . \]

From Dwight (1966, p. 205) we have:

\[ J_2(z) = \frac{2J_1(z)}{z} - J_0(z) \] \hspace{1cm} (A.2)

so that

\[ \int J_0(z) \, dz = 2 J_0(z) + 2 \int \frac{J_1(z)}{z} \, dz - \int J_0(z) \, dz \]

or

\[ \int J_0(z) \, dz = J_1(z) + \int \frac{J_1(z)}{z} \, dz \]
Using relationship (A.1), this equation can be written as:
\[ a \int J_i(z) \, dz = J_i(z) \bigg|_a^b - J_0(z) \bigg|_a^b \]  \hspace{1cm} (A.3)

From Magnus and others (1966, p. 86) we have:
\[ \int z^{-\nu+1} J_\nu(z) \, dz = -z^{-\nu} J_{\nu+1}(z). \]

Taking \( \nu = 1 \) and substituting \( z = xy \), \( dz = y \, dx \) \((y = \text{constant})\), yields:
\[ \int J_i(xy) \, y \, dx = -J_i(xy), \]
or
\[ \int J_i(xy) \, dx = -\frac{1}{y} J_o(xy) \] \hspace{1cm} (A.4)

From Dwight (1966, p. 205) we have:
\[ \int z^n J_{n-1}(z) \, dz = z^n J_n(z), \]
so for \( n = 2 \):
\[ \int z^2 J_i(z) \, dz = z^2 J_2(z). \]

Using equation (A.2):
\[ \int z^2 J_i(z) \, dz = z^2 \left\{ \frac{2 J_i(z)}{z} - J_0(z) \right\}, \]
or
\[ \int z^2 J_i(z) \, dz = 2 z J_i(z) - z^2 J_0(z) \] \hspace{1cm} (A.5)

With the substitution \( z = xy \), \( dz = y \, dx \) \((y = \text{constant})\), equation (A.5) becomes:
\[ \int x^2 y^2 J_i(xy) \, y \, dx = 2xy J_i(xy) - x^2 y^2 J_0(xy), \]
or
\[ \int x^2 J_i(xy) \, dx = \frac{2x}{y^2} J_i(xy) - \frac{x^2}{y} J_0(xy), \]
or
\[ \int x^2 J_i(xy) \, dx = -\frac{x}{y} \left[ xy J_0(xy) - 2xy J_0(xy) \right] \] \hspace{1cm} (A.6)
Consider the expression
\[ \int_a^b z J_n(z) \, dz = \int_a^b \frac{1}{z} \cdot z^2 J_n(z) \, dz. \]

Using the product rule of integration, we obtain:
\[ \int_a^b z J_n(z) \, dz = \left[ \frac{1}{z} \int z^2 J_n(z) \, dz \right]_a^b + \int_a^b \left[ z^2 J_n(z) \, dz \right] \cdot \frac{1}{z^2} \, dz. \]

With the use of (A.5) this becomes:
\[ \int_a^b z J_n(z) \, dz = \left[ \frac{1}{z} \{ 2z J_n(z) - z^2 J_0(z) \} \right]_a^b + \int_a^b \frac{1}{z^2} \{ 2z J_n(z) - z^2 J_0(z) \} \, dz. \]

By using (A.1) and (A.3), this expression becomes:
\[ \int_a^b z J_n(z) \, dz = \left[ 2 J_n(z) - z J_0(z) \right]_a^b + \int_a^b \frac{J_n(z)}{z} \, dz - \int_a^b J_0(z) \, dz. \]

With the substitution \( z = xy \), \( dz = y \, dx \) (\( y \) is constant), this equation becomes:
\[ \int_c^d xy J_n(xy) \, dx = \left[ J_n(xy) - xy J_0(xy) - J_i(xy) \right]_c^d. \]

or
\[ \int_c^d x J_n(xy) \, dx = \frac{1}{y^2} \left[ J_n(xy) - xy J_0(xy) - J_i(xy) \right]_c^d. \] (A.7)
APPENDIX B

FORTRAN-4 LISTING OF THE COMPUTER PROGRAM.
PROGRAM CAIES EXECUTES A COMPUTER-ASSISTED INTERPRETATION OF SCHLUMBERGER-TYPE ELECTRICAL SOUNDINGS (ES). THE PROGRAM USES THE PRINCIPLE OF LEAST-Squares NON-LINEAR CURVE FITTING. THE PROGRAM IS WRITTEN IN THE FORTRAN-4 LANGUAGE, AND IS MODULAR IN FORM. SUBPROGRAMS ARE USED EXTENSIVELY, AS WELL AS LABELED COMMON BLOCKS TO FACILITATE FAST TRANSFER OF VARIABLES BETWEEN PROGRAM SUBSECTIONS.

PROGRAM CAIES WAS DEVELOPED ON A DIGITAL COMPUTER CORPORATION MODEL PDP-10 COMPUTER, A TIME-SHARING SYSTEM. THE INPUT/OUTPUT STATEMENTS BELOW REFLECT THIS FACT: INPUT REQUESTS ARE PRECEDED BY INSTRUCTIONS OF HOW AND WHAT TO TYPE. THIS FORM OF I/O IS CERTAINLY NOT ESSENTIAL, AND MAY BE CHANGED TO MORE CONVENTIONAL FORMS FOR TYPICAL BATCH-TYPE OPERATIONS.

THE PROGRAM REQUIRE A TOTAL OF 10K WORDS OF STORAGE.

THE PROGRAM-INPUT IS IN THE FOLLOWING FORM AND SEQUENCE:
1) NUMBER OF OBSERVATION POINTS FOR THE OBSERVED ES.
2) PAIRS OF (DISTANCE, APPARENT RESISTIVITY) FOR THE OBSERVED DATA. (UNITS ARE METERS, OHM-METERS RESPECTIVELY.)
3) THE PARAMETERS FOR THE TWO-LAYER CURVE WITH THE SAME ASYMPTOTES AS THE OBSERVED CURVE. (THESE PARAMETERS, SURFACE RESISTIVITY, A THICKNESS (DISTANCE), AND BASEMENT RESISTIVITY MUST BE OBTAINED THROUGH CURVE MATCHING WITH THE COLLECTION OF TWO-LAYER CURVES IN A MASTER-CURVE ALBUM.)
4) THE PARAMETERS FOR THE 1ST CUT INTERPRETATION
   A) NUMBER OF LAYERS.
   B) PAIRS OF (RESISTIVITY, THICKNESS) FOR EACH LAYER SEQUENTIALLY. (UNITS ARE METERS, OHM-METERS.)
   C) THE BASEMENT RESISTIVITY.

THE PROGRAM'S BEST INTERPRETATION IS RETURNED AS
1) FIRST-LAYER THICKNESS. (FIRST-LAYER RESISTIVITY REMAINS UNCHANGED THROUGHOUT.)
2) THE LONGITUDINAL CONDUCTANCE S OR TRANSVERSE RESISTANCE T OF EVERY INTERMEDIATE LAYER. (THE PROGRAM USES THE 1ST CUT PARAMETERS TO DECIDE WHICH OF T OR S IS SIGNIFICANT.)
3) THE BASEMENT RESISTIVITY REMAINS UNCHANGED THROUGHOUT.
   THE PROGRAM ALSO RETURNS A MEASURE OF HOW WELL ITS INTERPRETATION FITS THE OBSERVED DATA (RMS ERROR), AND A TABLE OF VALUES FOR THE THEORETICALLY COMPUTED MODEL.

PROGRAM CAIES WAS DEVELOPED AT THE COLORADO SCHOOL OF MINES AS PART OF A THESIS-RESEARCH STUDY FOR THE DEGREE OF MASTER OF SCIENCE IN GEOPHYSICAL ENGINEERING. FOR FURTHER INFORMATION SEE CSM THESIS T-1363, "COMPUTER-ASSISTED INTERPRETATION OF ELECTRICAL SOUNDINGS" BY CHRISTIAN M. CROUS.

C. M. CROUS JANUARY 1971
COLORADO SCHOOL OF MINES
C PROGRAM CAIES, PAGE 2

C

REAL LMDA
COMMON /SKFUNC/ NSK,LMDA(40),SKREF(40),F(40),D(40)
COMMON /PARA/ NLAY,NPARA,RHOC1(0),THC1(0),TYPEC(9)
COMMON /SCRCH/ TMP(40),ES(40),DIST(40)

C INPUT/OUTPUT DEVICE ASSIGNMENT ...

C

IN = 1
IOUT = 2

C READ DATA FOR THE OBSERVED ES ...

C

WRITE(IOUT,10)
10 FORMAT(' READY TO ACCEPT REDUCED FIELD DATA. ',/,' TYPE NO. OF OBSERVATION POINTS: ',$)
READ(IN,20) NES
20 FORMAT(I)
NES = MIN0(NES,40)
WRITE(IOUT,30)
30 FORMAT(' TYPE PAIRS OF (DISTANCE,RESISTIVITY) ',/,' FOR THE OBSERVED SOUNDING CURVE: '/)
READ(IN,40) (DIST(I),ES(I),I=1,NES)
40 FORMAT(2F)

C READ THE PARAMETERS FOR THE TWO-LAYER CURVE TO SUBTRACT ...

C

WRITE(IOUT,60)
60 FORMAT(' TYPE THE PARAMETERS OF THE TWO-LAYER CURVE ',/,' WITH THE SAME ASYMPTOTES LEFT AND RIGHT: ',/,'% RH01, H1, RH02'/)
READ(IN,70) RH01,TH1,RH0B
70 FORMAT(3F)
NLAY = 2
RH0(1) = RH01
TH(1) = TH1
RH0(2) = RH0B
RH01 = 1. / RH01

C PREPARE THE OBSERVED ES FOR HANKEL TRANSFORMATION ...

C

CALL PREPHT(NES)
TH(1) = DIST(1)
TH(2) = DIST(NES)
LMDA(1) = -1.

C DEFINE THE APPROPRIATE SET OF LMDA'S FOR THE SECTION ...

C

CALL DEFLMD
C------ PROGR\-AM CAIES, PAGE 3 -----------------------------
C
C PERFORM THE NUMERICAL INTEGRATION ...
C--------------------------------------------
CALL J1NT(ES,DIST,NE,SKREF,LMDA,NSK)
C-----------
C COMPUTE THE TWO-LAYER KERNEL TO ADD BACK IN ...
C---------------------------------------------
TH(1) = TH1
CALL SUNDEC(.TRUE.)
C--------------
C COMPLETE COMPUTATIONS FOR THE REFERENCE KERNEL ...
C-----------------------------------------------
DO 80 I = 1,NSK
SKREF(I) = SKREF(I) * RH01 + F(I)
80 F(I) = 1. / LMDAC(I)
WRITE(10UT,90) (F(I),SKREF(I),I=NSK,1,-1)
90 FORMAT('"KERNEL\" CORRESPONDING TO THE GIVEN ES.\"
& '"1/LAM\-DA KERNEL',/,(5X,2(PE9.2)))
C-------------------
C READ PARAMETERS FOR THE FIRST CUT INTERPRETATION ...
C------------------------------------------------
95 WRITE(IOUT,100)
100 FORMAT('READY TO ACCEPT YOUR FIRST CUT AT INTERPRETATION.\"
& '"TYPE NO. OF LAYERS: 'S) READ(I\-N,110) N\-LAY
110 FORMAT(I)
IF(NLAY.LE.10) GO TO 120
WRITE(IOUT,112)
112 FORMAT('MAXIMUM NO. OF LAYERS IS 10! TRY AGAIN.\")
G0 TO 95
120 WRITE(IOUT,130)
130 FORMAT('TYPE PAIRS OF (RESISTIVITY,THICKNESS)\",
& '"FOR THE FIRST CUT INTERPRETATION:\")
READ(IN,140) (RH0(I),TH(I),I=1,NLAY)
140 FORMAT(2F)
RH0(I) = 1. / RH01
RH0(NLAY) = RH0B
DO 145 I = 1,NSK
145 SKREF(I) = ALOG10(SKREF(I))
C-------------------
C DEFINE THE TYPE OF SECTION PRESENTED (REGARDING T OR S) ...
C--------------------------------------
CALL TYPER
C---------------------
C PERFORM THE CURVE MATCHING ...
C--------------------------------
CALL MATCH(CERMS)
CALL SUNDEC(.TRUE.)
C------- PRORAM CAIES, PAGE 4 -----------------------------------
C
C-----------------
C COMPUTE T'S OR S'S FOR THE INTERPRETATION • • •
C-----------------

 DO 160 I=2,NPARA
  IF(TYPE(I).EQ.1HT) GO TO 150
  D(I) = TH(I) / RHO(I)
  GO TO 160
150 D(I) = TH(I) * RHO(I)
160 CONTINUE
C-----------------
C PRINT RESULTS • •
C-----------------
WRITE(IOUT,170) NLAY
170 FORMAT('1*************** BEST INTERPRETATION ','
          ' ***************','/
          ' NUMBER OF LAYERS = ',I2,'/
          WRITE(IOUT,180) RHO(1),TH(1)
180 FORMAT(' LAYER 1: RHO =','1PE10.3,' H =','1PE10.3)
 WRITE(IOUT,190) (I,TYPE(I),D(I),I=2,NPARA)
190 FORMAT(' LAYER ',I2,'; ',A1,' =','1PE10.3)
 WRITE(IOUT,200) RHO(NLAY)
200 FORMAT(' BASEMENT: RHO =','1PE10.3)
 ERMS = ERMS * 100.
 WRITE(IOUT,205) ERMS
205 FORMAT(' RMS ERROR = ','F6.2,'%')
 DO 208 I=1,NSK
208 LMDA(I) = 1. / LMDA(I)
 WRITE(IOUT,210) (LMDA(I),F(I),I=NSK,1,-1)
210 FORMAT(' "KERNEL" FUNCTION FOR THIS INTERPRETATION. ','
          ' 1/LAMBDA KERNEL'/(SX,2(1PE9.2)))
 WRITE(IOUT,220)
220 FORMAT(1H1)
 STOP
END
SUBROUTINE SUNDE

This subroutine computes the kernel function for a given geo-electric section. The independent variable (LMDA) must be defined beforehand, and is communicated via the COMMON block /SKFUNC/. The parameters for the geo-electric section are communicated via COMMON /PARA/.

Special procedures are followed for the two-layer case: when this subroutine is called by PREPHT, 80 values of the kernel are returned into the last 80 locations of /SKFUNC/. The 80 values for the independent variable must be presented in locations 2 thru 81 of /SKFUNC/.

ARGUMENT DEFINITION...

NOLOG = a LOGICAL flag signifying whether LOGK or K is to be computed. NOLOG=.TRUE. - compute K
NOLOG=.FALSE. - compute LOGK


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SUBROUTINE SUNDE(NOLOG)
REAL LMDA, LMDA2(80), F2(80)
LOGICAL NOLOG
EQUIVALENCE (F2(1), F), (F2(41), D)
EQUIVALENCE (LMDA2(1), LMDA), (LMDA2(41), SKREF)
COMMON /SKFUNC/ NSK, LMDA(40), SKREF(40), F(40), D(40)
COMMON /PARA/ NLAY, NPARA, RH0(10), TH(10), TYPE(9)
IF(NLAY.EQ.2) GO TO 40
D0 20 L=1, NSK
F1 = 1.
TMP = -2. * LMDA(L)
D0 10 J=NLAY-1, 1, -1
RH0A = RH0(J)
RH0B = RH0(J+1) * F1
G1 = (RH0A - RH0B) / (RH0A + RH0B)
GEXP = G1 * EXP(TMP * TH(J))
10 F1 = (1. - GEXP) / (1. + GEXP)
20 F(L) = F1
C------- SUBROUTINE SUNDE, PAGE 2. ---------------------
C
C-----------------------------------------------------------------
C  WHEN INFORMATION ABOUT THE INTERMEDIATE STAGES
C  OF CURVE FITTING IS DESIRED, THE FOLLOWING SEQUENCE
C  OF STATEMENTS CAN BE USED. IN THAT CASE IT WILL BE
C  NECESSARY TO REMOVE THE C*'S FROM COLUMNS 1 AND 2,
C  AND PROVIDE THE PROPER OUTPUT-DEVICE ASSIGNMENT.
C*    IOUT = 2
C*    WRITE(IOUT,22) (RH0(I),TH(I),I=1,NLAY-1),RH0(NLAY)
C* 22 FORMAT(/, 'INTERMEDIATE INTERPRETATION:/',
C*       & 8X,'RH0',H'(3X,2(1PE11.3))
C*    WRITE(IOUT,24) (F(I),I=NSK,1,-1)
C* 24 FORMAT(/, 'CORRESPONDING KERNEL:/',(1X,5E11.3))
C
C  THE ABOVE SEQUENCE OF STATEMENTS WILL CAUSE PRINTING
C  OF THE GEOMETRIC PARAMETERS AND THE KERNEL FUNCTION
C  OF THE PRESENT "CUT".
C (KERNEL-VALUES FROM SMALLEST TO LARGEST 1/LMDA.)
C-----------------------------------------------------------------
        IF(N0L0G) RETURN
    D0 30 L=1,NSK
30    FL(L) = ALOG10(F(L))
    RETURN
40    RH0A = RH0(1)
    RH0B = RH0(2)
    G1 = (RH0A - RH0B) / (RH0A + RH0B)
    TMP = -2. * TH(1)
    D0 50 I=1,NSK
        GE1X = G1 * EXP(TMP * LMDA(I))
50    F2(I) = (1. - GE1X) / (1. + GE1X)
    RETURN
END
SUBROUTINE DEFLMD

C THIS SUBROUTINE DEFINES THE SET OF VALUES OF THE INDEPENDENT VARIABLE (LMDA) FOR WHICH THE KERNEL IS OF INTEREST.
C A FLAG INDICATING THAT THE LMDA-VALUES MUST BE COMPUTED FROM DATA OF AN OBSERVED SOUNDING, IS OBTAINED BY SETTING LMDA(1) = -1. IN THIS CASE, MAXIMUM LMDA = 1/MINIMUM DISTANCE AND MINIMUM LMDA = 1/MAXIMUM DISTANCE.
C INTERMEDIATE VALUES ARE LOGARITHMICALLY SPACED AT SQRT(2).
C
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SUBROUTINE DEFLMD
REAL LMDA, LMIN, LMAX
COMMON /SKFUNC/ NSK, LMDA(40), SKREF(40), F(40), D(40)
COMMON /PARA/ NLAY, NPARA, RH0(10), TH(10), TYPE(9)
DATA FCTR/1.414214/
IF(LMDA(1) .GT. -1.) GO TO 5
RMIN = TH(1)
RMAX = TH(2)
GO TO 15
5 RT = 0.
CT = 0.
DO 10 I=1,NLAY-1
RT = RT + TH(I) * RH0(I)
10 CT = CT + TH(I) / RH0(I)
HEQ = SQRT(RT * CT)
RMAX = 100. * HEQ
RMIN = 0.2 * TH(1)
15 LMIN = 1. / RMAX
LMAX = 1. / RMIN
NSK = INT(ALOG10(LMAX/LMIN) / LOG10(FCTR)) + 1
NSK = MIN(40, NSK)
LMDA(1) = LMIN
DO 20 I=2,NSK
20 LMDA(I) = LMDA(I-1) * FCTR
RETURN
END
SUBROUTINE J1INT

THIS SUBROUTINE EVALUATES THE DEFINITE INTEGRAL OF THE
PRODUCT F(X) • J1(YX).
(J1(YX) IS THE FIRST-ORDER BESSEL FUNCTION OF THE FIRST KIND.)
THE SUBROUTINE RETURNS

G(Y) = \int_{A}^{B} F(X) • J1(YX) • DX

FÖR ACCURATE RESULTS, IT IS ESSENTIAL THAT F(X) BE ZERO (OR
NEGLIGIBLY SMALL) OUTSIDE THE RANGE X=A TO X=B.
INTEGRATION IS PERFORMED BY FITTING A 2ND-ORDER POLYNOMIAL
TO EVERY 3 SUCCESSIVE POINTS OF THE DISCRETE F(X), DOING THE
INTEGRATION ANALYTICALLY, AND SUMMING THE TERMS FOR ALL POSSIBLE
PANELS OF 3 POINTS. (NOTE THAT THE "PANELS" LIE END-TO-END
AND DO NOT OVERLAP.)

ARGUMENT DEFINITIONS . . .

F = ARRAY CONTAINING THE DISCRETE VALUES OF F(X).
X = ARRAY CONTAINING THE VALUES OF X FOR WHICH F IS
SPECIFIED.
NF = NUMBER OF F(X) PAIRS SUPPLIED.
G = ARRAY INTO WHICH THE SUBROUTINE OUTPUT IS RETURNED.
Y = ARRAY CONTAINING THE VALUES OF Y FOR WHICH G(Y) ARE TO
BE COMPUTED.
NG = NUMBER OF VALUES OF G REQUIRED.

REFERENCE: VANYAN, L. L., 1967, ELECTROMAGNETIC DEPTH
SOUNDINGS: NEW YORK, CONSULTANTS BUREAU, P161.

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SUBROUTINE J1INT(F, X, NF, G, Y, NG)
REAL F(NF), X(NF), G(NG), Y(NG), J00, J10, J110, J02, J12, J112
REAL L1(40), L2(40)
NLS = (NF - 1) / 2
I = -1
DO 1 K=1, NLS
   I = I + 2
   I1 = I + 1
   I2 = I + 2
   BETAO = -((X(I1)+X(I2)) / ((X(I1)-X(I1))*(X(I2)-X(I1)))
   BETAI = (X(I)+X(I2)) / ((X(I1)-X(I1))*(X(I2)-X(I1)))
   BETAI = -(X(I1)+X(I2)) / ((X(I2)-X(I1))*(X(I2)-X(I1)))
   GAMMA0 = 1. / ((X(I1)-X(I1))*(X(I2)-X(I1)))
   GAMMA1 = -1. / ((X(I1)-X(I1))*(X(I2)-X(I1)))
   GAMMA2 = 1. / ((X(I2)-X(I1))*(X(I2)-X(I1)))
   L1(K) = BETAO*F(I) + BETAI*F(I1) + BETAI*F(I2)
   L2(K) = GAMMA0*F(I) + GAMMA1*F(I1) + GAMMA2*F(I2)
1
C------ SUBROUTINE J1INT, PAGE 2 ----------------------------
C
DO 4 K=1,NG
GY = 0.
YTEMP = Y(K)
ARG = X(1) * YTEMP
CALL BESSEL(ARG,J00,J10,J110)
TEMPR = 1./YTEMP
TEMPI = TEMPR * TEMPR
DO 3 I=1,NLS
II = I + 1
ARG = X(II+1) * YTEMP
CALL BESSEL(ARG,J02,J12,J112)
GY = GY + TEMPR * (J00 * F(II-1) - J02 * F(II+1)) - 
& TEMPI * (L1(I) * (J10-J12) + 2. * L2(I) * X(II-1) * 
& J10 - X(II+1) * J12)) + L1(I) * TEMPI * (J110-J112)
J00 = J02
J10 = J12
3 J110 = J112
4 G(K) = GY
RETURN
END
SUBROUTINE BESSEL

THIS SUBROUTINE CALCULATES THE BESSEL FUNCTIONS JO, J1 AND JI1 FOR A GIVEN ARGUMENT.
(JO, J1 AND JI1 ARE FLOATING POINT NUMBERS.)

ARGUMENT DEFINITIONS...

ARG = ARGUMENT FOR WHICH BESSEL FUNCTIONS ARE TO BE CALCULATED.

JO = ZERO-ORDER BESSEL FUNCTION OF THE FIRST KIND.

J1 = FIRST-ORDER BESSEL FUNCTION OF THE FIRST KIND.

JI1 = FIRST-ORDER BESSEL INTEGRAL FUNCTION OF THE FIRST KIND.

= \int_{ARG}^{\infty} \frac{(J1(X)}{X} DX

REFERENCE:


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SUBROUTINE BESSEL(ARG,JO,J1,JI1)
REAL JO,J1,JI1,A0(5),B0(5),C0(5),A1(5),B1(5),C1(5)
REAL A11(9),B11(6),C11(6)
DATA & A0/- .00394440, .04444790, -.31636660, 1.2656208, -2.499997/,
& B0/- .00072805, .00137237, -.0009512, -.00552740, -.0000077/,
& C0/- .00029333, -.00054125, -.00262573, -.00003954, -.04166397/,
& A1/- .00031761, .00443319, -.03954289, -.21093573, -.56249885/,
& B1/- .00113653, -.00249511, -.00017105, .01659667, .0000156/,
& C1/- .00079824, .00074348, -.00637879, .00005650, .12499612/,
& A11/- .18673710E 00, .12014677E 01, .56024572E 01,
& .19898386E 02, .52952437E 02, .10113454E 03,
& .13003159E 03, .10239999E 03, .42666666E 02/,
& B11/- .11072990E-03, .25439550E-03, .41006760E-03,
& .67401480E-03, .17870944E-02, .12564241E-01/,
& C11/- .12700390E-03, .27550370E-03, .39928250E-03,
& .53661690E-03, .1008972 E-02, .40403539E-02/,

ARG = ABS(ARG)
SQRA = ARG * ARG
IF(ARG.GT.3.) G0 T0 20
X = SQRA / 9.
J0 = .0002100
J1 = .00001109
D0 10 I=1,5
J0 = J0 * X + A0(I)
10 J1 = J1 * X + A1(I)
J0 = J0 * X + 1.
J1 = ARG * (J1*X + .5)
G0 T0 40
SRTA = 1. / SQRT(ARG)
X = 3. / ARG
T0 = .00013558
T1 = -.00029166
F0 = -.00014476
F1 = -.00020033
DO 30 I=1,5
T0 = T0 * X + C0(I)
F0 = F0 * X + B0(I)
T1 = T1 * X + C1(I)
F1 = F1 * X + B1(I)
30
TO = TO * X + ARG - .78539816
T1 = T1 * X + ARG - 2.3561945
F0 = F0 * X + .79788456
F1 = F1 * X + .79788456
JO = F0 * COS(T0) * SRTA
J1 = F1 * COS(T1) * SRTA
IF(ARG.GT.8.) GO TO 60
40 X = SQRA * .01562500
JI1 = .16247546E-01
DO 50 I=1,9
50 JI1 = JI1 * X + AI1(I)
JI1 = ARG * (JI1 * X + 7.9999999) * .125
JI1 = 1. - JI1 + J1
RETURN
60 X = 64. / SQRA
P = -.22623800E-04
Q = .26848200E-04
DO 70 I=1,6
70 P = P * X + BI1(I)
Q = (Q * X - .06233473) * 8. / ARG
ANG = ARG - .78539816
JI1 = 1. + (P*SIN(ANG) + Q*COS(ANG)) * SRTA
JI1 = 1. - JI1 + J1
RETURN
END
SUBROUTINE PREPHT(NES)
REAL LMDA
COMMON /SKFUNC/ NSK,LMDA(80),F(80)
COMMON /PARA/ NLAY,NPARA,RH0(10),TH(10),TYPE(C9)
COMMON /SCRTCH/ ESPC(40),ES(40),DIST(40)
RH01 = RH0(1)
C = RH0(2) / RH01
IF(C.NE.1.) GO TO 20
DO 10 I=1,NES
  10 ESP(I) = RH01
  G0 T0 90
20 XMAX = 10. / TH(1)
LMDA(1) = 0.
  IF(C.GT.100.) LMDA(1) = .1 / TH(1)
  XI = LMDA(1)
  LMDA(2) = LMDA(1) + .0001
  NSK = 79
  DX = EXP(AL0G(XMAX/LMDA(2)) / 77.)
  DO 30 I=3,NSK
  30 LMDA(I) = LMDA(I-1) * DX
  CALL SUNDE(.TRUE.)
  D0 40 I=1,NSK
40 F(I) = (F(I)-1.) * LMDA(1)
C--------- SUBROUTINE PREPHT, PAGE 2 ----------------------------------
C
K = NES
IF(C.GE.0.05) GO TO 60
H = 5. * TH(1)
DO 50 I=K,1,-1
IF(DIST(I).*LE.H) GO TO 60
K = K - 1
50 ESP(I) = RH(2)
60 CALL JINT(F,LMDA,NSK,ESP,DIST,K)
DO 70 I=1,K
DTMP = DIST(I)
70 ESP(I) = RH(1) * (DTMP * DTMP * ESP(I) + 1.)
IF(C.LE.100.) GO TO 90
DO 80 I=1,NES
ARG = XI * DIST(I)
CALL BESSEL(ARG,BJO,BJ1,BJ1)
80 ESP(I) = ESP(I) + RH(1)*(-9.*ARG*BJO+BJ1+BJ1+10.*ARG-1.)
90 DO 100 I=1,NES
100 ES(I) = (ES(I) - ESP(I)) / DIST(I)
RETURN
END
FUNCTION ERROR

THIS SUBPROGRAM COMPUTES THE RMS ERROR BETWEEN TWO FUNCTIONS F AND G.

ARGUMENT DEFINITIONS...

F = ARRAY CONTAINING THE REFERENCE FUNCTION.
G = ARRAY CONTAINING THE SECOND FUNCTION.
N = NUMBER OF ELEMENTS IN BOTH ARRAYS F AND G.

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FUNCTION ERROR(F,G,N)
DIMENSION F(N), G(N)
ERROR = 0.
DO 10 I=1,N
TERM = F(I) - G(I)
10 ERROR = ERROR + TERM * TERM
ERROR = SQRT(ERROR / FLOAT(N))

THE FOLLOWING STATEMENTS MAY BE USED TO HAVE THE RMS ERROR PRINTED AT INTERMEDIATE STAGES OF CURVE MATCHING. IF THIS IS DESIRED, THE C* S WILL HAVE TO BE REMOVED FROM COLUMNS 1 AND 2, AND THE PROPER OUTPUT-DEVICE ASSIGNMENT MADE.
THE INTERMEDIATE INTERPRETATION AND CORRESPONDING KERNEL PRINTED IMMEDIATELY ABOVE THIS RMS ERROR WILL BE THE "CUT" TO WHICH THE ERROR PERTAINS. THE RMS ERROR IS PRINTED AS A FRACTION. (MULTIPLY BY 100 TO GET %)

IOUT = 2
WRITE(IOUT,20) ERROR
20 FORMAT(9, ' INTERMEDIATE RMS ERROR = ',1PE9.2, '///')

RETURN
END
SUBROUTINE TYPER

COMMON /PARA/ NLAY, NPARA, RH0(10), TH(10), TYPE(9)
DATA T/1HT/, S/IHS/
DO 20 I=2, NLAY-1
IF(RH0(I+1) .GE. RH0(I)) GO TO 10
TYPE(I) = T
GO TO 20
10 TYPE(I) = S
20 CONTINUE
NPARA = NLAY - 1
RETURN
END
SUBROUTINE PARTED

C THIS SUBROUTINE COMPUTES THE PARTIAL DERIVATIVES OF THE LOGARITHM OF A THEORETICAL KERNEL WITH RESPECT TO 1) FIRST-LAYER THICKNESS, AND 2) THE T- OR S-PARAMETER OF EVERY INTERMEDIATE LAYER. THE PARTIAL DERIVATIVES ARE COMPUTED BY FINITE-DIFFERENCE METHODS.

RESULTS ARE STORED IN THE TWO-DIMENSIONAL ARRAY PDM, EVERY COLUMN OF PDM CONTAINS THE PARTIAL DERIVATIVE WITH RESPECT TO ONE PARAMETER. SEQUENTIAL POINTS ON EVERY PARTIAL DERIVATIVE CURVE ARE STORED IN THE DIFFERENT ROWS OF THAT COLUMN.

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SUBROUTINE PARTLD

COMMON /PDMAT / PDM(40,9)
COMMON /SKFUNC/ NSK,XC(40),SKREF(40),SKTRY(40),SKTMP(40)
COMMON /PARA / NLAY,NPARA,RH0(10),TH(10),TYPE(9)
DATA T/1HT/
DO 1 = 1 ,NSK
1 SKTMP(I) = SKTRY(I)
THTMP = TH(I)
TH(I) = TH(I) * 1.005
CALL SUNDEC(.FALSE.)
DO 5 I=1,NSK
5 PDM(I,1) = (SKTRY(I) - SKTMP(I)) * 200.
TH(I) = THTMP
DO 10 IL=2,NLAY-1
RHOTMP = RH0(IL)
THTMP = TH(IL)
TH(IL) = TH(IL) * 1.005
IF(TYPE(IL).EQ.T) GO TO 20
RH0(IL) = RH0(IL) * .995
CALL SUNDEC(.FALSE.)
DS = 1. / (TH(IL) / RH0(IL) - THTMP / RHOTMP)
DO 10 I=1,NSK
10 PDM(I,IL) = (SKTRY(I) - SKTMP(I)) * DS
GO TO 40
20 RH0(IL) = RH0(IL) * 1.005
CALL SUNDEC(.FALSE.)
DT = 1. / (TH(IL) / RH0(IL) - THTMP * RHOTMP)
DO 30 I=1,NSK
30 PDM(I,IL) = (SKTRY(I) - SKTMP(I)) * DT
40 RH0(IL) = RHOTMP
TH(IL) = THTMP
GO TO 1
50 CONTINUE
RETURN
END
This subroutine determines that theoretically computed kernel (SKTRY) for which the deviation from a given kernel (SKREF) is a minimum in a least-squares sense. The subroutine starts with the given first "try", and by least-squares curve fitting techniques, compute models which match the reference kernel better and better. The subroutine returns a measure of how well the two kernels match (RMS error) and the geoelectric parameters of the curve that matches closest. Parameters are returned in arrays RH0 and TH. Computations are stopped when
1) the RMS error < 1%,
2) 30 tries have been made,
3) 10 attempts to get out of a local minimum has been made.

Argument definition ...

ERMS = the root-mean-square error between the given kernel and the computed model.

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SUBROUTINE MATCH(ERMS)
REAL LMDA
COMMON /SKFUNC/ NSK, LMDA(40), SKREF(40), SKTRY(40), D(40)
COMMON /PARA/ NLAY, NPARA, RH0(10), TH(10), TYPE(9)
COMMON /SCRTCH/ RESULT(9), RH0NOW(10), THNOW(10), X(91)
KOUNT = 0
CALL SUNDEC(.FALSE.)
ERMS = ERROR(SKREF, SKTRY, NSK)
10 IF(ERMS.LT.0.01) RETURN
   D0 20 I=2,NLAY-1
   RH0NOW(I) = RH0(I)
   20 THNOW(I-1) = TH(I-1)
   KOUNT = KOUNT + 1
   KOUNT1 = 0
   CALL SOLVE
   30 CALL NEWCUT
   CALL SUNDEC(.FALSE.)
   ERMS2 = ERROR(SKREF, SKTRY, NSK)
   IF(ERMS2.LT.ERMS) G0 T0 60
   KOUNT1 = KOUNT1 + 1
   IF(KOUNT1.EQ.10) G0 T0 70
   D0 50 I=1,NPARA
50 RESULT(I) = RESULT(I) * .6667
   G0 T0 30
   60 ERMS = ERMS2
   IF(KOUNT.EQ.30) RETURN
   G0 T0 10
   70 D0 80 I=2,NLAY-1
      RH0(I) = RH0NOW(I)
   80 TH(I-1) = THNOW(I-1)
   RETURN
END
SUBROUTINE SOLVE

This subroutine sets up the normal equations of the least-squares non-linear curve fitting problem. The matrix equation is

\[(PT \times P) \times R = CPI \times D\]

Where \(P\) = the matrix of partial derivatives of the theoretical model with respect to every parameter.

The theoretical model is \(L0GCK0REL\).

\(CP\) is stored in array PDM.

\(PT\) = the transpose of \(P\) (not stored; product PT\(P\) stored in array PDM.)

\(D\) = the difference between observed and calculated curves at every observation point.

\(L0G(K0BS)\) - \(L0G(K0M)\) (stored in array D.)

\(R\) = the result vector, i.e. the amount & direction in which to change every parameter to obtain a better match. (stored in array RESULT.)


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SUBROUTINE SOLVE
COMMON /PDMAT / PDM(40,9)
COMMON /SKFUNC/ NSK,X(40),SKREF(40),SKTRY(40),D(40)
COMMON /PARA / NLAY,NPARA,RHO(10),TH(10),TYPE(9)
COMMON /SCRATCH/ RESULT(9),TMP(111)
CALL PARTLD
DO 10 I=1,NSK
   10 D(I) = SKREF(I) - SKTRY(I)
CALL MATMUL(PDM,NPARA,D,1,NSK)
CALL MATMUL(PDM,NPARA,PDM,NPARA,NSK)

THE NEXT STATEMENT IS A CALL TO A SUBROUTINE WHICH
Solves the matrix equation
\(PDM \times RESULT = D\)
For the vector result.

SUBROUTINE DSOL was coded from a flow-chart presented in:

A collection of subroutines to achieve the same result is presented in FORTRAN-4 code in:

CALL DSOL(PDM,D,RESULT,40,NPARA, 001,10,KIT,1,IS)
IF(IS.EQ.2) CALL EXIT
RETURN
END
SUBROUTINE MATMUL

THIS SUBROUTINE CALCULATES THE MATRIX PRODUCT (AT*B) AND STORES THE RESULT ON TOP OF B. (AT IS THE TRANSPOSE OF A.)

THE TWO DIFFERENT TYPES OF CALLS TO THIS SUBROUTINE ARE WITH
1) B=A AND 2) B=D, A COLUMN VECTOR.

IN CASE 1, THE RESULTING PRODUCT IS A SYMMETRIC MATRIX. THE SUBROUTINE THEREFORE COMPUTES ONLY THE ELEMENTS OF THE LOWER TRIANGULAR SUBMATRIX, AND DEFINES THE ELEMENTS OF THE UPPER TRIANGLE BY SIMPLE REPLACEMENT.

IN CASE 2, THE RESULTING PRODUCT IS A COLUMN VECTOR, IN WHICH CASE ALL ITS ELEMENTS ARE COMPUTED.

THIS SUBROUTINE MINIMIZES ERRORS DUE TO ROUND-OFF BY DOUBLE-PRECISION ACCUMULATION OF PRODUCT (SEE STATEMENT 10.)

ARGUMENT DEFINITIONS . . .

A = THE MATRIX A, THE TRANSPOSE OF WHICH MUST BE USED IN (AT*B)
NCA = THE NUMBER OF COLUMNS IN MATRIX A.
B = THE SECOND MATRIX (OR VECTOR) IN (AT*B)
NCB = THE NUMBER OF COLUMNS IN B.
NRANB= THE NUMBER OF ROWS IN BOTH MATRICES A AND B.

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SUBROUTINE MATMUL(A,NCA,B,NCB,NRANB)
DIMENSION TEMP(40),A(40,NCA),B(40,NCB)
DOUBLE PRECISION SUM
DO 40 J=1,NCB
  DO 20 I=J,NCA
    SUM = 0.
    DO 10 K=1,NRANB
    SUM = SUM + A(K,I) * B(K,J)
10   TEMP(I) = SNGL(SUM)
    DO 30 I=1,NCA
30   B(I,J) = TEMP(I)
40 CONTINUE
IF(NCB.EQ.1) RETURN
DO 50 I=1,NCB-1
DO 50 J=I+1,NCB
50   B(I,J) = B(J,I)
RETURN
END
THIS SUBROUTINE TAKES THE SPECIFIED AMOUNT OF CHANGE IN EITHER LONGITUDINAL CONDUCTANCE (DS) OR TRANSVERSE RESISTANCE (DT) FOR THE INTERMEDIATE LAYERS, AND FROM IT CALCULATES NEW RESISTIVITIES AND THICKNESSES INDIVIDUALLY. THE NEW SET OF RESISTIVITIES AND THICKNESSES WILL REFLECT THE SPECIFIED DS'S OR DT'S.

THIS SUBROUTINE ALSO INTRODUCES RESTRICTIONS ON THE AMOUNTS OF CHANGE, SO THAT POSITIVE THICKNESSES AND RESISTIVITIES ARE RETURNED UNDER ALL CIRCUMSTANCES.

SUBROUTINE INPUT IS IN ARRAY RESULT, OUTPUT IS RETURNED IN COMMON BLOCK /PARA/.

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SUBROUTINE NEWCUT
COMMON /PARA/ NLAY,NPARA,RH0(10),TH(10),TYPE(9)
COMMON /SCRATCH/ RESULT(9),TMP(111)
DATA T/HT/
TH(1) = (1. + AMAX1(AMIN1(RESULT(1),.95),-.95)) * TH(1)
DO 20 I=2,NLAY-1
IF(TYPE(I).EQ.1) GOTO 10
DP = RH0(I) * RESULT(I) / (2.*TH(I) + RH0(I)*RESULT(I))
DP = AMAX1(AMIN1(DP,.75),-.75)
RH0(I) = (1. - DP) * RH0(I)
TH(I) = (1. + DP) * TH(I)
GOTO 20
10 DP = AMAX1(RESULT(I),-.9*TH(I)*RH0(I))
DP = SQRT(1. + DP / (TH(I) * RH0(I)))
RH0(I) = DP * RH0(I)
TH(I) = DP * TH(I)
20 CONTINUE
RETURN
END
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