

Discrete frequency inequalities for magnetotelluric impedances of one-dimensional conductors

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Abstract. For the one-dimensional magnetotelluric inverse problem the ties between the impedances at neighbouring frequencies, reflecting the analytical properties of the transfer function, are expressed in terms of inequalities between the data. After the derivation of some elementary necessary constraints for data sets with two or three frequencies, a set of necessary and sufficient conditions warranting the existence of a one-dimensional conductivity model in the general M -frequency case is given. This set of constraints characterizes a 1-D data set by the signs of $2M$ determinants derived from the data.

Key words: Magnetotellurics - Inverse problem

Introduction

The transfer functions of electromagnetic induction are analytical functions of frequency which, in principle, are completely defined for all frequencies by prescribing them only on an arbitrarily small interval. This introduces strong ties between the values of the transfer functions at neighbouring frequencies. Measured data in general do not show these strong interrelations, they are inconsistent and can be interpreted only in the least squares sense. The nature of the frequency constraints depends on the allowed class of models, being defined by the conductivity distribution and the source field. Of interest is the problem of finding both necessary and sufficient criteria which identify a given data set as belonging to a specified class of models. Necessary conditions are diagnostic if at least one of them is violated; on the other hand, sufficient conditions are diagnostic if all of them are satisfied. If the set of necessary and sufficient conditions is identical, they will provide a complete characterization of the admitted data sets.

In the present paper a complete characterization of data is given for the simple class of one-dimensional conductivity models with a quasi-uniform inducing field, which is the classical magnetotelluric case (Cagniard, 1953). The solution in terms of inequalities to be satisfied within the data set is presented in the third section. In the preceding section, some elementary necessary inequalities for two and three data sets are derived.

All inequalities also hold for the slightly extended class of spatially harmonic source fields, provided that the data belong to the same modulus of the horizontal wavenumber vector. The inequalities also apply to a spherically layered earth with a single spherical harmonic of fixed degree as source field (Weidelt, 1972).

Necessary conditions for data sets with two and three frequencies

Assuming a time factor $e^{i\omega t}$ and SI units, Schmucker's transfer function $c(\omega)$ is defined as

$$c(\omega) = \frac{E_x(\omega)}{i\omega\mu_0 H_y(\omega)} = g(\omega) - ih(\omega) = |c(\omega)|e^{-i\psi(\omega)}, \quad (1)$$

where E_x and H_y are two orthogonal horizontal components of the electric and magnetic field at the surface, and μ_0 is the magnetic permeability of free space. The relation between c and the commonly used impedance Z , apparent resistivity ρ_a , and phase φ is

$$Z = i\omega\mu_0 c, \quad \rho_a = \omega\mu_0 |c|^2, \quad \varphi = 90^\circ - \psi. \quad (2)$$

For a 1-D conductivity structure the theoretical data allow the spectral expansion (Weidelt, 1972; Parker, 1980)

$$c(\omega) = a_0 + \int_0^\infty \frac{a(\lambda)d\lambda}{\lambda + i\omega} \quad (3)$$

with $a_0 \geq 0$, $a(\lambda) \geq 0$, where $a(\lambda)$ is a generalized function to include both the discrete and continuous part of the spectrum. For sake of convenience the following discussion is confined to a fully discrete version of Eq. (3)

$$c(\omega) = a_0 + \sum_{n=1}^N \frac{a_n}{b_n + i\omega} \quad (4)$$

with $a_0 \geq 0$, $a_n > 0$, $b_n \geq 0$. The set b_n is assumed to be distinct. The extension of all results to the more general case (3) is straightforward.

The discrete frequency inequalities given in this section are generalizations of a set of smoothness constraints given by Weidelt [1972, Eqs. (2.33a, b) and (2.34a, b)], which read

$$|c'| \leq h/\omega, \quad |(\omega c')'| \leq g, \quad (5a, b)$$

$$|c' + \omega c''| \leq h/\omega, \quad |(\omega c)' + \omega(\omega c)''| \leq g, \quad (6a, b)$$

where $c' := dc/d\omega$, $c'' := d^2c/d\omega^2$. These inequalities are necessary conditions for real data to be consistent with a 1-D conductivity model. Since the required differentiations are difficult to perform with real data, discrete frequency analogues are more appropriate. In the following, the abbreviations $c_j := c(\omega_j)$, etc. are used.

a) Let ω_1 and ω_2 be two distinct frequencies. Then the analogues of (5a, b) are

$$\left| \frac{c_2 - c_1}{\omega_2 - \omega_1} \right|^2 \leq \frac{h_1 h_2}{\omega_1 \omega_2}, \quad \left| \frac{\omega_2 c_2 - \omega_1 c_1}{\omega_2 - \omega_1} \right|^2 \leq g_1 g_2. \quad (7a, b)$$

b) Let ω_1, ω_2 and ω_3 be three equidistant frequencies with $\omega_1 = \omega_2 - \Delta$, $\omega_3 = \omega_2 + \Delta$, $\Delta \neq 0$ (e.g. three successive harmonics). Then the counterparts of (6a, b) are

$$\left| \frac{c_3 - c_1}{2\Delta} + \omega_2 \frac{c_3 - 2c_2 + c_1}{\Delta^2} \right|^2 \leq \frac{h_1 h_3}{\omega_1 \omega_3}, \quad (8a)$$

$$\left| \frac{\omega_3 c_3 - \omega_1 c_1}{2\Delta} + \omega_2 \frac{\omega_3 c_3 - 2\omega_2 c_2 + \omega_1 c_1}{\Delta^2} \right|^2 \leq g_1 g_3. \quad (8b)$$

The proofs follow almost immediately by inserting Eq. (4). Consider as an example the most involved inequality (8b). With the abbreviation

$$A := \frac{\omega_3 c_3 - \omega_1 c_1}{2\Delta} + \omega_2 \frac{\omega_3 c_3 - 2\omega_2 c_2 + \omega_1 c_1}{\Delta^2}$$

one finds

$$A = a_0 + \sum_{n=1}^N \frac{a_n b_n (b_n - i\omega_2)}{(b_n + i\omega_1)(b_n + i\omega_2)(b_n + i\omega_3)},$$

$$|A| \leq a_0 + \sum_{n=1}^N \frac{a_n b_n}{(b_n^2 + \omega_1^2)^{1/2} (b_n^2 + \omega_3^2)^{1/2}}.$$

The Cauchy-Schwarz inequality

$$\left(\sum_{n=0}^N p_n q_n \right)^2 \leq \sum_{n=0}^N p_n^2 \sum_{m=0}^N q_m^2$$

with $p_0 = q_0 := \sqrt{a_0}$ and

$$p_n := \left(\frac{a_n b_n}{b_n^2 + \omega_1^2} \right)^{1/2}, \quad q_n := \left(\frac{a_n b_n}{b_n^2 + \omega_3^2} \right)^{1/2}, \quad n \geq 1$$

then yields $|A|^2 \leq g_1 g_3$.

Equality holds in Eqs. (7a) and (8a) only for $N=0$ or $N=1$, equality in Eqs. (7b) and (8b) requires either $N=0$, $a_0 > 0$ or $N=1$, $a_0 = 0$. In the special case $\omega_1 = 0$, $\omega_2 = \omega$, Eq. (7b) reduces to $|c(\omega)|^2 \leq g(0)g(\omega)$, implied already in Eq. (5.6) of Parker (1972). The formulation of the above constraints in terms of apparent resistivity and phase does not lead to simple results.

Existence conditions for the general M -frequency case

The M complex data $c_j := g_j - ih_j$, $j=1, \dots, M$ are given for M distinct frequencies ω_j . The necessary and sufficient conditions, under which the data can be in-

terpreted by a 1-D model are, investigated. This problem of existence has previously been discussed by Parker (1980), who states as necessary and sufficient conditions for the consistency with a 1-D model that the data have to allow a representation of type (4). The actual consistency check then requires the solution of a quadratic programming problem with positivity constraints. In the present approach the answer to the existence problem is given in terms of $2M$ inequality constraints to be satisfied within the data set.

The complete formulation of the constraints requires the distinction between a regular and a degenerate case. In the *regular* case there exists a representation of the data as an expansion (4) involving at least $2M$ positive constants. In theory this requirement is met for all physical conductors (i.e. not infinitely thin conductors), which lead to a representation with an infinite number of positive constants. The regular case also results from a conductivity structure with more than M thin sheets. For the given frequency set ω_j , $j=1, \dots, M$, any theoretical response $c(\omega)$ of the regular case can be interpolated by two different representations requiring exactly $2M$ positive constants

$$1) \quad c_j = \sum_{m=1}^M \frac{A_m}{B_m + i\omega_j}, \quad (9)$$

$$2) \quad c_j = \bar{A}_0 + \sum_{m=1}^{M-1} \frac{\bar{A}_m}{\bar{B}_m + i\omega_j} + \frac{\bar{A}_M}{i\omega_j}, \quad (10)$$

$j=1, \dots, M$ (Weidelt, 1985). These representations allow a physical interpretation as an equivalent stack of thin sheets. The $2M$ positive constants in Eqs. (9) or (10) will induce a set of $2M$ positivity constraints as consistency conditions within the data set.

In the *degenerate* case the data are represented by Eq. (4) with less than $2M$ positive constants. The existence conditions will now also involve a number of equality constraints corresponding to the number of deficient constants. Therefore, the more complicated degenerate case is of no relevance for consistency checks with real data and will be discussed in the Appendix for completeness only.

Before stating the consistency conditions, some further definitions are required. By linear combination with the weights

$$\alpha_{jk} := (-\omega_j^2)^k \prod_{\substack{l=1 \\ l \neq j}}^M (\omega_l^2 - \omega_j^2) \quad (11)$$

$k=0, \dots, M-1$, $j=1, \dots, M$ and $\alpha_{10}=1$ for $M=1$, a set of new data β_m is defined as

$$\beta_{2k} := \sum_{j=1}^M (h_j/\omega_j) \alpha_{jk}, \quad (12a)$$

$$\beta_{2k+1} := \sum_{j=1}^M g_j \alpha_{jk}, \quad (12b)$$

$k=0, \dots, M-1$. With these data we form the symmetrical $(j+1)$ -order determinants

$$\Delta_{j+1}^{(i)} = \begin{vmatrix} \beta_i & \beta_{i+1} & \cdots & \beta_{i+j} \\ \beta_{i+1} & \beta_{i+2} & \cdots & \beta_{i+j+1} \\ \vdots & \vdots & \ddots & \vdots \\ \beta_{i+j} & \beta_{i+j+1} & \cdots & \beta_{i+2j} \end{vmatrix} = \det\{\beta_{i+m+n}\} \quad (13)$$

$m, n=0, \dots, j$. The argument i indicates that β_i is the upper-left corner element. The matrices associated with $\Delta_{j+1}^{(i)}$ are Hankel matrices, i.e. the entries depend only on the sum of the indices of the rows and the columns. Since β_m is defined only up to $m=2M-1$, Eq. (13) is subject to the constraint $0 \leq i+2j \leq 2M-1$. With the above definitions the characterization theorem for the regular case reads:

The necessary and sufficient conditions, in order that the data $c_j = g_j - ih_j$ for the frequencies ω_j , $j=1, \dots, M$ can be interpreted by a regular one-dimensional conductivity model, are the $2M$ positivity constraints

$$\Delta_k(i) > 0, \quad i=0, 1 \quad \text{and} \quad k=1, \dots, M. \quad (14)$$

Necessity

It has to be shown that the response function representation of type (4) with at least $2M$ positive constants implies the inequalities (14). Using the partial fraction expansion

$$x^{2k} \left/ \prod_{j=1}^M (x^2 + \omega_j^2) \right. = \sum_{j=1}^M \frac{\alpha_{jk}}{x^2 + \omega_j^2}, \quad k=0, \dots, M-1 \quad (15)$$

with α_{jk} defined in Eq. (11) and

$$g_j = a_0 + \sum_{n=1}^N \frac{a_n b_n}{b_n^2 + \omega_j^2}, \quad (16a)$$

$$h_j / \omega_j = \sum_{n=1}^N \frac{a_n}{b_n^2 + \omega_j^2}, \quad (16b)$$

$$\sum_{j=1}^M \alpha_{jk} = \delta_{k, M-1}, \quad 0 \leq k \leq M-1,$$

where δ_{km} is the Kronecker symbol, Eqs. (4) and (12a, b) yield

$$\beta_m = a_0 \delta_{m, 2M-1} + \sum_{n=1}^N \gamma_n b_n^m, \quad m=0, \dots, 2M-1 \quad (17)$$

with

$$\gamma_n := a_n \left/ \prod_{j=1}^M (b_n^2 + \omega_j^2) \right. > 0. \quad (18)$$

The determinants $\Delta_k(i)$ defined in Eq. (13) are according to the Cauchy-Binet theorem (e.g. Smirnov, 1964, p. 28) for $i+2k < 2M+1$ given by

$$\Delta_k(i) = \sum \left\{ \prod_{m=1}^k \gamma_{n_m} b_{n_m}^i \right\} \cdot \begin{vmatrix} 1 & b_{n_1} \cdots b_{n_1}^{k-1} \\ \vdots & \vdots \\ 1 & b_{n_k} \cdots b_{n_k}^{k-1} \end{vmatrix}^2. \quad (19)$$

For $i+2k=2M+1$, the term $a_0 \delta_{m, 2M-1}$ in Eq. (17) gives rise to the additional term $a_0 \Delta_{k-1}^{(i)}$ on the right-hand side. The summation in Eq. (19) extends over all k -tuples n_m , $m=1, \dots, k$ with $1 \leq n_1 < n_2 < \dots < n_k \leq N$. This summation can equivalently be represented by

$$\frac{1}{k!} \sum_{n_1=1}^N \cdots \sum_{n_k=1}^N$$

(e.g. Smirnov, 1964, p. 23), which is immediately generalized to a k -fold integral in the case of the integral representation (3). The determinants $\Delta_k(i)$ are positive for $k < N$, so that Eq. (14) is certainly satisfied for $M < N$. Since it is assumed that Eq. (4) involves at least $2M$ positive constants, it is excluded that a_0 and $\min\{b_n\}$ vanish simultaneously in the case $M=N$. The determinant $\Delta_M(1)$ involves the additional term $a_0 \Delta_{M-1}(1)$ and, therefore, is positive even if $\min\{b_n\} = 0$.

Sufficiency

It has to be shown that the data constraints (14) are sufficient to ensure the existence of any regular 1-D response function. This may be of type (4) with $N \geq M$ or even of the simpler type (9) or (10). For ease of presentation, attention is confined to Eq. (9); identical sufficient conditions, however, are obtained when starting from Eq. (10), which is of course a necessary requirement (cf. the remark at the end of the Appendix).

Using the same procedure, which has led to Eq. (17), we infer from Eq. (9)

$$\sum_{n=1}^M G_n B_n^m = \beta_m, \quad m=0, \dots, 2M-1 \quad (20)$$

with

$$G_n := A_n \left/ \prod_{j=1}^M (B_n^2 + \omega_j^2) \right. \quad (21)$$

The conditions on the data β_m , under which the nonlinear system (20) has $2M$ positive solutions G_k (or A_k) and B_k , $k=1, \dots, M$, has to be investigated. This is just the finite moment problem, for which the existence conditions are well-known (e.g. Gantmacher, 1959, Chap. 15, §16). The main arguments are briefly repeated here in a slightly modified way. Taking the generic pair G_p, B_p , $p \in [1, M]$, a set of M variables $x_k = x_k(p)$ is defined by the expansion

$$\prod_{m=1}^M \frac{\lambda - B_m}{B_p - B_m} = \sum_{k=0}^{M-1} x_k \lambda^k, \quad (22)$$

where the prime denotes the omission of the factor $m=p$. Then Eqs. (20) and (22) yield

$$\sum_{k=0}^{M-1} \beta_{i+j+k} x_k = G_p B_p^{i+j}, \quad i+j=0, \dots, M,$$

from which the final result

$$\sum_{k=0}^{M-1} \sum_{j=0}^{M-1} \beta_{i+j+k} x_j x_k = G_p B_p^i, \quad i=0, 1 \quad (23)$$

is obtained by appealing again to Eq. (22). The left-hand side of Eq. (23) presents the M -dimensional quadratic form

$$Q(i) = \sum_{j=0}^{M-1} \sum_{k=0}^{M-1} q_{jk}(i) x_j x_k, \quad i=0, 1 \quad (24)$$

with $q_{jk} = q_{kj} = \beta_{i+j+k}$.

At this point it is necessary to recall some properties of quadratic forms (e.g. Smirnov, 1964, pp. 125–130). A quadratic form Q is called *positive definite* if it assigns a positive value to any real M -tuple x_0, \dots, x_{M-1} with $\sum x_m^2 > 0$. Criteria for the positive definite character of Q can be formulated in terms of the signs of certain determinants derived from the elements q_{jk} . A *principal minor* of order k of the M -dimensional quadratic form Q is the determinant of the remainder of the quadratic array q_{jk} after deleting *any* $(M-k)$ rows and columns intersecting at the main diagonal. A subset of these principal minors are the *corner minors* Δ_k obtained by deleting the *last* $(M-k)$ rows and columns. Then Q is positive definite if (and only if) $\Delta_k > 0$, $k=1, \dots, M$. This result is proved by Jacobi's theorem (Smirnov, 1964, p. 130), which reduces Q to a sum of squares on using a triangular transformation

$$\xi_k = x_k + \sum_{l=k+1}^{M-1} a_{kl} x_l, \quad k=0, \dots, M-1, \quad (25)$$

and leads under the conditions $\Delta_k > 0$ to

$$Q = \sum_{k=0}^{M-1} (\Delta_{k+1}/\Delta_k) \xi_k^2, \quad \Delta_0 = 1. \quad (26)$$

Since the determinant of the transformation (25) is non-zero, all ξ_k vanish only if all x_k vanish. Therefore, the conditions $\Delta_k > 0$ are sufficient to ensure that Eq. (26) assigns a positive value to any set x_k with $\sum x_k^2 > 0$, i.e. that Q is positive definite.

The positive definite character of Q does not change by renumbering the variables x_k . However, the corner minors will change and a set of different but equivalent conditions is obtained. By a suitable renumbering each principal minor can serve as corner minor. Hence, all principal minors of a positive definite quadratic form are positive.

The conditions (14) ensure, in view of Eq. (26), that $Q(0)$ and $Q(1)$ are positive definite. From $Q(0)$ it then follows, via Eq. (23), that G_p is positive. This result, in conjunction with $Q(1) > 0$, shows also that B_p is positive and completes the proof for the regular case. From the principal minors of $Q(0)$ and $Q(1)$ one may obtain $2(2^M - 1)$ inequalities from which, however, only $2M$ are independent.

The evaluation of the conditions (14) yields

a) for $M=1$:

$$\beta_0 > 0, \quad \beta_1 > 0 \quad \text{or} \quad h_1 > 0, \quad g_1 > 0,$$

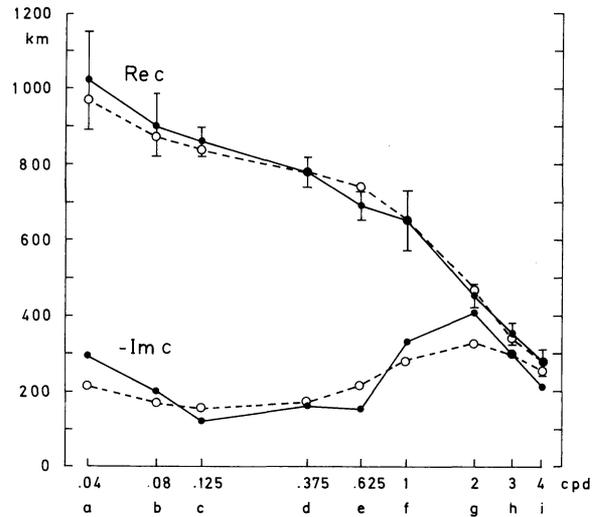
b) for $M=2$:

$$\beta_0 > 0, \quad \beta_1 > 0, \\ \beta_0 \beta_2 - \beta_1^2 > 0, \quad \beta_1 \beta_3 - \beta_2^2 > 0$$

or

$$\frac{h_2/\omega_2 - h_1/\omega_1}{\omega_2 - \omega_1} < 0, \quad \frac{g_2 - g_1}{\omega_2 - \omega_1} < 0, \quad (27a, b)$$

$$\left| \frac{c_2 - c_1}{\omega_2 - \omega_1} \right|^2 < \frac{h_1 h_2}{\omega_1 \omega_2}, \quad \left| \frac{\omega_2 c_2 - \omega_1 c_1}{\omega_2 - \omega_1} \right|^2 < g_1 g_2. \quad (27c, d)$$



	a	b	c	d	e	f	g	h
b	+							
c	-	-						
d	+	+	+					
e	+	+	+	-				
f	+	+	+	-	-			
g	+	+	+	-	-	-		
h	+	+	+	-	-	-	-	
i	+	+	+	-	-	-	-	-

Fig. 1. Pairwise existence checks for a real data set (full lines). A “+” (or “-”) in the table at the bottom indicates that the particular frequency pair can (or cannot) be interpreted by a 1-D conductivity model. The best 1-D fit is shown by dashed lines

There exist equivalent constraint sets in which $\beta_0 > 0$ and/or $\beta_1 > 0$ are replaced by $\beta_2 > 0$ and/or $\beta_3 > 0$, i.e.

$$\frac{h_2 \omega_2 - h_1 \omega_1}{\omega_2 - \omega_1} > 0 \quad \text{and/or} \quad \frac{g_2 \omega_2^2 - g_1 \omega_1^2}{\omega_2 - \omega_1} > 0.$$

Explicit expressions of the constraints (14) for $M > 2$ are lengthy and not particularly illuminating. The inequalities (27c, d) agree with (7a, b). Therefore, one might expect that in the equidistant three-frequency case the conditions $\Delta_2(i) > 0$, $i=0, 1$ would reproduce (8a, b). However, $\Delta_2(i) > 0$ yields the different inequalities

$$\left| \frac{F_3 - F_1}{2\Delta} - \omega_2 \frac{F_3 - 2F_2 + F_1}{\Delta^2} \right|^2 < f_1 f_3 - \omega_2 f_2 \frac{f_3 - f_1}{\Delta} \\ + 2\omega_2^2 \frac{f_1 f_2 - 2f_1 f_3 + f_2 f_3}{\Delta^2} = f_1 f_3 - \omega_2 f_2 \frac{f_3 - f_1}{\Delta} \\ + 2\omega_2^2 \left[2 \frac{f_2 - f_1}{\Delta} \cdot \frac{f_3 - f_2}{\Delta} - f_2 \frac{f_3 - 2f_2 + f_1}{\Delta^2} \right]$$

with $F_j = c_j$, $f_j = h_j/\omega_j$ for $i=0$ and $F_j = \omega_j c_j$, $f_j = g_j$ for $i=1$.

For moderate M the signs of the determinants (14) can be obtained by counting the negative signs in the nontrivial diagonal after an LU-decomposition of the associated matrix, allowing for the possible interchange of rows by pivoting. Since consistency depends only on the relative amplitudes of data and frequencies, these quantities can be scaled to avoid large or small numbers.

Figure 1 shows an application of Eq. (27a-d) to a

set of real data, consisting of nine low-frequency response estimates for Europe (U. Schmucker, personal communication). The data (connected by full lines) are of good quality, as is seen by comparing them with the best-fitting 1-D model (dashed lines). This best fit to a representation (4) is obtained by quadratic programming, using a least-squares norm with the inverse variances as weights (Parker, 1980). The residuals generally lie within one standard deviation (given in Fig. 1 only for $g = \text{Re } c$; the same error estimate, however, applies also to $h = -\text{Re } c$). The table at the bottom shows the results of consistency checks for all pairs of frequencies. The diagonal indicates that, despite the good data quality, the response estimates for successive frequencies are generally inconsistent. On the other hand, the ties between data with a wide frequency separation are weak and no consistency problems arise.

Conclusion

The present study establishes necessary and sufficient data constraints for the existence of a 1-D conductivity model. It complements a previous result of Parker (1980), who characterizes the data by a representation (4). Although the results are mostly of theoretical interest, quick pairwise existence checks can be performed by (27a-d).

The approach does not shed any light on the extremely difficult problem of how to characterize the data when two- or even three-dimensional conductivity models are allowed. It is generally assumed that the necessary requirements for the lower dimensional counterpart of the transfer function are relaxed when the class of conductivity models is widened. However, in two and three dimensions the response function is tensorial and the relaxation of constraints for the frequency dependence of individual tensor elements will be counteracted by additional constraints between the elements, which might be even more severe. Nevertheless, it would be useful to study the relaxation of necessary constraints in an extended class of models because it could be concluded from a violated relaxed constraint that, even in the extended class, no satisfactory model exists.

Appendix

Existence conditions for the degenerate case

In the degenerate case the data are represented by an expansion of type (4) with less than $2M$ (positive) constants, i.e.

$$c(\omega_j) = a_0 + \sum_{n=1}^r \frac{a_n}{b_n + i\omega_j} + \frac{a_{r+1}}{i\omega_j}, \quad j=1, \dots, M \quad (28)$$

with $0 \leq r \leq M-1$, $a_n > 0$, $b_n > 0$ for $n=1, \dots, r$, $a_0 \geq 0$, $a_{r+1} \geq 0$. In addition, for $r=0$ the sum in Eq. (28) is omitted and for $r=M-1$ there is the extra condition $a_0 \cdot a_M = 0$ (in order to have less than $2M$ positive constants). The response function of the degenerate case can be interpreted by only one conductivity profile, and this lies in the class of thin sheets (Parker, 1980; Weidelt, 1985). The structure of Eq. (28) will also be re-

flected in the existence conditions. There will be $2r$ positivity constraints, 2 non-negativity constraints and $2(M-r-1)$ equality constraints. The latter refer to the $2(M-r-1)$ deficient constants.

A degenerate data set is characterized as follows:

There exists an integer r with $0 \leq r \leq M-1$ such that

$$\Delta_k(i) > 0, \quad i=0, 1 \quad \text{and} \quad k=1, \dots, r, \quad (29)$$

but

$$\Delta_{r+1}(0) \cdot \Delta_{r+1}(1) = 0. \quad (30)$$

For this number r holds

$$\Delta_{r+1}(0) \geq 0, \quad \Delta_{r+1}(2M-2r-1) \geq 0. \quad (31)$$

For $r < M-1$ there are the $2(M-r-1)$ equality constraints

$$\Delta_{r+1}(i) = 0, \quad i=1, \dots, 2(M-r-1). \quad (32)$$

The necessity of the above conditions is easily inferred from the explicit expression of $\Delta_k(i)$ in Eq. (19). Considering the sufficient conditions on the data β_m to ensure a representation (28), we first find as analogues of Eq. (20) [or Eq. (17), since the data set does not permit an alternative representation]

$$\sum_{n=1}^r \gamma_n b_n^m = \bar{\beta}_m, \quad m=0, \dots, 2M-1 \quad (33)$$

with

$$\begin{aligned} \bar{\beta}_0 &= \beta_0 - \gamma_{r+1}, & \bar{\beta}_{2M-1} &= \beta_{2M-1} - a_0, \\ \bar{\beta}_m &= \beta_m, & m &= 1, \dots, 2M-2, \end{aligned} \quad (34)$$

and β_m and γ_n defined in Eqs. (12a, b) and (18), respectively. Absorbing for the moment the constants a_0 and γ_{r+1} in the data $\bar{\beta}_m$, Eq. (33) is a system of $2M$ equations for the $2r$ unknowns b_n and γ_n . The existence of a solution requires $2M-2r$ consistency conditions between the $\bar{\beta}_m$. Defining a set of r variables y_k by the expansion

$$\prod_{m=1}^r (\lambda - b_m) = \sum_{k=0}^r y_k \lambda^k, \quad y_r = 1, \quad (35)$$

a linear combination of the equations (33) yields

$$\sum_{k=0}^r \bar{\beta}_{j+k} y_k = 0, \quad j=0, \dots, 2M-r-1. \quad (36)$$

In order that a solution of these $2M-r$ linear equations for r unknowns exists, any $r+1$ equations have to be linearly dependent. Taking the equations from $j=i$ to $j=i+r$, $i=0, \dots, 2M-2r-1$, the $2M-2r$ consistency conditions are $\bar{\Delta}_{r+1}(i) = 0$, where $\bar{\Delta}$ is built as Δ in Eq. (13) with β_m replaced by $\bar{\beta}_m$. For the original data this implies

$$\Delta_{r+1}(0) = \gamma_{r+1} \Delta_r(2), \quad (37a)$$

$$\Delta_{r+1}(i) = 0, \quad i=1, \dots, 2(M-r-1), \quad (37b)$$

$$\Delta_{r+1}(q) = a_0 \Delta_r(q) = a_0 \Delta_r(1) \prod_{n=1}^r b_n^{q-1} \quad (37c)$$

with $q = 2M - 2r - 1$. In Eq. (37c) use was made of the recurrence relation following from Eq. (19)

$$\Delta_r(l+1) = \Delta_r(l) \cdot \prod_{n=1}^r b_n, \quad l \geq 1.$$

Before evaluating Eq. (37a-c), the conditions warranting the positivity of a_p and b_p , $p \in [1, r]$ are derived by defining another set of variables, z_k , by

$$\prod_{m=1}^r \frac{\lambda - b_m}{b_p - b_m} = \sum_{k=0}^{r-1} z_k \lambda^k,$$

where the prime again denotes the omission of the factor $m = p$. Then Eq. (33) yields (cf. the regular case)

$$\sum_{j=0}^{r-1} \sum_{k=0}^{r-1} \beta_{i+j+k} z_j z_k = \gamma_p b_p^i, \quad i = 1, 2, \quad (38)$$

where it has been noted that in the required range of subscripts $\beta_m = \bar{\beta}_m$. With a new appeal to quadratic forms, sufficient conditions for $a_p > 0$ and $b_p > 0$ are

$$\Delta_k(i) > 0, \quad i = 1, 2 \quad \text{and} \quad k = 1, \dots, r. \quad (39)$$

Now we are in a position to identify Eqs. (29) to (32) as sufficient conditions for the degenerate case. The inequalities (39) almost agree with (29), except that they involve $\Delta_k(2)$ rather than $\Delta_k(0)$. The conditions (29), $\Delta_k(0) > 0$, $k = 1, \dots, r$ imply that the r -dimensional quadratic form $Q_r(0)$ is positive definite. Hence, also the principal minors $\Delta_k(2)$, $k = 1, \dots, r-1$ of the associated determinant are positive. To prove the positivity of $\Delta_r(2)$, the cases $\Delta_{r+1}(0) > 0$ and $\Delta_{r+1}(0) = 0$ have to be distinguished. In the former case also $Q_{r+1}(0)$ is positive and therefore the same holds for the principal minor $\Delta_r(2)$ of the associated determinant. However, if $\Delta_{r+1}(0) = 0$ then it follows from Eq. (37a) that $\gamma_{r+1} = 0$, because

$$\Delta_r(2) = \Delta_r(1) \prod_{i=1}^r b_i$$

[from Eq. (19)] is non-zero since $\gamma_p b_p > 0$ as a consequence of $\Delta_k(1) > 0$, $k = 1, \dots, r$. For $\gamma_{r+1} = 0$, Eq. (19) shows that

$$\Delta_r(2) = \Delta_r(0) \prod_{i=1}^r b_i^2 > 0.$$

The conditions (31) ensure, according to (37a) and (37c) that a_{r+1} and a_0 are non-negative. Finally, in the case $r < M - 1$ the conditions (32) grant, according to (37b), the existence of a solution. The condition (30) in conjunction with (29) defines the integer r .

The regular representation (10) can be considered as a special case of Eq. (28) with $r = M - 1$ and $a_i = \bar{A}_i$, $b_i = \bar{B}_i$, $\bar{A}_0 \cdot \bar{A}_M > 0$. Then the remaining conditions (29) and (31) lead to the regular conditions (14).

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