

AXIOMATIC CHARACTERIZATION OF THE GENERAL MIXTURE RULE

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ABSTRACT

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The paper is addressed to the following problem, frequently occurring in geophysics, rock physics and solid state physics.

Suppose we are given a composite material of volume V consisting of two phases of the respective volume fractions P , Q ; $P + Q = V$, and suppose these constituents are uniformly distributed within the total volume. Suppose g is some physically measurable property that assumes the values g_1 and g_2 , respectively, for the two constituents, and a value \bar{g} for the composite. Suppose, further, that the value of \bar{g} is unambiguously determined by the volume fractions P , Q and the specific properties g_1 , g_2 :

$$\bar{g} = M(g_1, g_2, P, Q)$$

It is shown that, if a set of physically plausible conditions are met, the only possible functional form of $M(g_1, g_2, P, Q)$ is the “general mixture rule”:

$$M(g_1, g_2, P, Q) = [\Phi g_1^t + (1 - \Phi) g_2^t]^{1/t}$$

for some real t , $t \neq 0$, or:

$$M(g_1, g_2, P, Q) = g_1^\Phi g_2^{1-\Phi}$$

where Φ is porosity, defined as $\Phi = P/(P + Q)$.

Examples are given where some of the conditions are violated, indicating that the physical property of the composite cannot be expressed by simple mixture rules.

In applied geophysics, rock physics and solid state physics we are frequently faced with the following problem:

Suppose we are given a composite material of volume V consisting of N phases of the respective volume fractions V_i , $V_1 + V_2 + \dots + V_N = V$, and suppose all these constituents are uniformly distributed within the total volume. Suppose g is some physically measurable property that assumes the value g_i for the i -th constituent, and some value \bar{g} for the composite material. In many cases, the value of \bar{g} only depends on the volume fractions V_i and individual parameters g_i :

$$\bar{g} = M(g_1, g_2, \dots, g_N, V_1, V_2, \dots, V_N) \quad (1)$$

In what follows it will be shown that in case of two-component materials (as e.g. porous rocks) a simple set of physically plausible axioms can be given that completely determine the functional form of eq. (1). Namely, by introducing porosity as

$$\Phi = \frac{V_1}{V_1 + V_2}, 1 - \Phi = \frac{V_2}{V_1 + V_2} \quad (2)$$

it will be shown that if a set of conditions are satisfied, eq. (1) can be written as:

$$\bar{g} = [\Phi g_1^t + (1 - \Phi) g_2^t]^{1/t} \quad (3)$$

where t , $t \neq 0$, is some arbitrary real value in $(-\infty, \infty)$, or:

$$\bar{g} = g_1^\Phi g_2^{1-\Phi} \quad (4)$$

which is of course, by l'Hôpital's rule the limit of expression (3) for $t \rightarrow 0$.

The paper is a sequel of Korvin (1978), where some important properties of the generalized mean values of eq. (3) are pointed out and specific references to geophysical-physical applications are given.

The main reason for my returning once more to this problem is that since 1978 I have succeeded in completing the set of axioms proposed in my previous paper by a further condition so that the conditions to be given below will already unambiguously determine the expressions (3) and (4). Also, I have collected a few examples where some of the conditions are violated indicating that the physical property of the composite cannot be expressed by simple formulae like (3) and (4).

I hope these results will be useful in deciding, in any given case, whether formulae like Wyllie's "time-average equation" (Wyllie et al., 1956):

$$\frac{1}{\bar{V}} = \frac{\Phi}{V_1} + \frac{1 - \Phi}{V_2} \quad (5)$$

Meese and Walther's (1967) "vugular carbonate formula"

$$\bar{V} = V_1^\Phi V_2^{1-\Phi} \quad (6)$$

and many other similar expressions, proposed in the theory of elasticity (Shermergor, 1977), for the sound speed and effective attenuation in an alternating sequence of sand shale layers (Tegland, 1970; Mateker, 1971), or for the estimation of thermal- and electric conductivity of fluid-filled sedimentary rocks (Beck, 1976; Rzhovsky and Novik, 1971; Schön, 1971; Woodside and Messmer, 1961; Grant and West, 1965; Pearce et al., 1973; etc.) should be considered as approximate "empirical rules" or they do have a sound physical meaning.

Since the mathematics to be applied heavily relies on the theory of func-

tional equations, detailed proofs would be outside the scope of the paper. Interested readers are referred to the monographs Aczél (1961) and Hardy et al. (1934).

Consider a composite material consisting of a volume fraction P of some material of physical property g_1 , and of a fraction Q of another material of physical property g_2 . Denote the measured physical property of the composite by $\bar{g} = M(g_1, g_2, P, Q)$. Suppose the function $M(g_1, g_2, P, Q)$ satisfies the following set of conditions:

Cond. 1: reflexivity

$$M(g_1, g_1, P, Q) = g_1 \text{ for all } P, Q (P + Q > 0) \quad (7a)$$

Cond. 2: idempotency (Fuchs, 1950)

$$M(g_1, g_2, P, Q) = g_1 \text{ for all } P > 0 \quad (7b)$$

$$M(g_1, g_2, 0, Q) = g_2 \text{ for all } Q > 0 \quad (7c)$$

Cond. 3: homogeneity (of 0-th order) with respect to the volume fractions. The physical property \bar{g} of the composite does not depend on the actual values of the volume fractions, only on their ratio:

$$M(g_1, g_2, P, Q) = M(g_1, g_2, \lambda P, \lambda Q) \quad (7d)$$

for all P, Q, λ such that $P + Q > 0, \lambda > 0$

Cond. 4: internity. The property g measured on the composite lies between the specific values g_1, g_2 of the constituents; if $g_1 < g_2$, say, then for $P + Q > 0$:

$$M(g_1, g_2, 1, 0) \leq M(g_1, g_2, P, Q) \leq M(g_1, g_2, 0, 1) \quad (7e)$$

Cond. 5: bi-symmetry (this concept is due to Aczél, 1946). Given two composites, the first consisting of P_1 resp. Q_1 parts of materials of g_1 resp. g_2 properties, the second of P_2 resp. Q_2 parts of materials of G_1 resp. G_2 properties, the following two expressions for the measured property \bar{g} of the four-component aggregate must be equal:

$$M(M(g_1, g_2, P_1, Q_1); M(G_1, G_2, P_2, Q_2); P_1 + Q_1; P_2 + Q_2) = M(M(g_1, G_1, P_1, P_2);$$

$$M(g_2, G_2, Q_1, Q_2); P_1 + P_2; Q_1 + Q_2) \quad (7f)$$

Cond. 6: monotonicity with respect to the volume fractions.

If $g_1 < g_2$, say, $P + Q_1 > 0, Q_2 > Q_1$ then

$$M(g_1, g_2, P, Q_1) < M(g_1, g_2, P, Q_2) \quad (7g)$$

Cond. 7: monotonicity with respect to the physical properties.

If $P + Q > 0, g_2 < g_3$ then

$$M(g_1, g_2, P, Q) < M(g_1, g_3, P, Q) \quad (7h)$$

Cond. 8: homogeneity (of first order) with respect to the physical properties.

$$M(\lambda g_1, \lambda g_2, P, Q) = \lambda M(g_1, g_2, P, Q)$$

$$\text{for all } P, Q, \lambda \text{ such that } P + Q > 0, \lambda > 0 \quad (7i)$$

Some of the above conditions (7a, 7b, 7c, 7e) have already been introduced — in a slightly different form — in a previous work (Korvin and Lux, 1971). Conditions (7a)–(7h) are all contained in Korvin (1978), while condition (7i), stating the simple fact that the property of the composite is measured in the same physical units as those of the individual constituents, is new. Interestingly, this apparently slight addendum to the set of conditions will have a crucial role in unambiguously fixing the functional form of $M(g_1, g_2, P, Q)$.

According to the theorem of Finetti, Kitagawa and Aczél (Aczél, 1961) any function $M(g_1, g_2, P, Q)$ satisfying the conditions 1–7 (i.e., eqs. 7a–7i) can be described in the general form:

$$\bar{g} = M(g_1, g_2, P, Q) = f^{-1} \left[\frac{Pf(g_1) + Qf(g_2)}{P + Q} \right] \quad (8)$$

i.e., by eq. 2 as:

$$\bar{g} = f^{-1} [\Phi f(g_1) + (1 - \Phi) f(g_2)]$$

where f is some arbitrary, continuous, strictly monotone function (f is the so-called Kolmogorov-Nagumo function corresponding to the given mean $M(g_1, g_2, P, Q)$).

It should be noted that the Kolmogorov-Nagumo function f corresponding to $M(g_1, g_2, P, Q)$ is only determined up to constant factors. If we introduce the notation:

$$\mathcal{M}_f(g_1, g_2, \Phi, 1-\Phi) = f^{-1} [\Phi f(g_1) + (1-\Phi)f(g_2)] \quad (9)$$

we have the following theorem of Jessen (Hardy et al., 1934):

In order that:

$$\mathcal{M}_\phi(g_1, g_2, \Phi, 1-\Phi) = \mathcal{M}_\psi(g_1, g_2, \Phi, 1-\Phi) \quad (10)$$

for all g_1, g_2 and $\Phi \in [0, 1]$ it is necessary and sufficient that:

$$\psi = a\phi + b \quad (11)$$

where a and b are constant and $a \neq 0$.

We introduce a further notation:

$$M_t(g_1, g_2, \Phi, 1-\Phi) = \mathcal{M}_{\chi t}(g_1, g_2, \Phi, 1-\Phi) = [\Phi g_1^t + (1-\Phi)g_2^t]^{1/t},$$

$$g_1, g_2 > 0, t \neq 0 \quad (12)$$

$$M_0(g_1, g_2, \Phi, 1-\Phi) = g_1^\Phi g_2^{1-\Phi}, g_1, g_2 > 0 \quad (13)$$

The following important characterization of the means M_t is due to Nagumo, Finetti and Jessen (Finetti, 1931; Hardy et al., 1934).

Suppose that $\phi(\mathbf{x})$ is continuous in the open interval $(0, \infty)$ and that:

$$\mathcal{M}_\phi(\lambda g_1, \lambda g_2, \Phi, 1-\Phi) = \lambda \mathcal{M}_\phi(g_1, g_2, \Phi, 1-\Phi) \quad (14)$$

for all positive λ, g_1, g_2 and for all $\Phi, \Phi \in [0, 1]$.

Then:

$$\mathcal{M}_\phi(g_1, g_2, \Phi, 1-\Phi) = M_t(g_1, g_2, \Phi, 1-\Phi) \quad (15)$$

for some real t .

The expression $M_t(g_1, g_2, \Phi, 1-\Phi)$ is sometimes called *the generalized weighted mean of t -th order of g_1 and g_2* (Beckenbach and Bellman, 1961).

On strength of the above-stated three theorems the basic result of the present paper can be summarized as follows.

If the expression $M(g_1, g_2, P, Q)$ defining the effective physical parameter \bar{g} of a two-phase composite satisfies the conditions 1–8 (i.e. eqs. 7a–7i), $P + Q > 0, g_1, g_2 > 0$, then $M(g_1, g_2, P, Q) = M_t(g_1, g_2, \Phi, 1-\Phi)$ for some real t , i.e.:

$$\bar{g} = M(g_1, g_2, P, Q) = [\Phi g_1^t + (1-\Phi)g_2^t]^{1/t} \quad (t \neq 0)$$

$$\text{or: } \bar{g} = g_1^\Phi g_2^{1-\Phi}$$

In case of sound speeds in fluid-filled sedimentary rocks the above general rule contains, in particular, the following widely used velocity formulae:

- for $t = -2$ approximate Wood equation (Watermann and Truell, 1961; Korvin, 1977, 1978);
- for $t = -1$ time-average equation (Wyllie et al., 1956);
- for $t = 0$ “vugular carbonate” formula (of Meese and Walther, 1967);
- for $t = 1$ average velocity formula (Berry, 1959).

Tegland’s (1970) method of sand-shale ratio-determination also assumes a $t = -1$ time average equation, while Mateker’s (1971) effective attenuation factor in an alternating sequence of (thick) sand-shale layers is a linear (weighted) combination (i.e., $t = 1$) of the specific attenuations. In case of electric or thermal conductivities the meaning of the $t = -1$ and $t = +1$ rules should be clear. It can be shown that the $t = 0$ rule, i.e.:

$$\bar{\sigma} = \sigma_1^\Phi \sigma_2^{1-\Phi} \quad (16)$$

is the limiting case for $\Phi \ll 1$ and $\sigma_2/\sigma_1 \approx 1$ of the well-known Maxwell

formula:

$$\bar{\sigma} = \frac{2\sigma_2 + \sigma_1 + 2\Phi(\sigma_2 - \sigma_1)}{2\sigma_2 + \sigma_1 - \Phi(\sigma_1 - \sigma_2)} \quad (17)$$

describing the case when a small fraction $\Phi \ll 1$ of a homogeneous medium of conductivity σ_2 is filled by small-sized, randomly distributed spheres of conductivity σ_1 (Maxwell, 1892; Grant and West, 1965). For the derivation of eq. (16) from eq. (17) see Beck (1976), Korvin (1978), Woodside and Messmer (1961). Another application of a $t = 0$ type law is due to Aleksandrov and Aisenberg (1966) who express the effective elastic constants of composite materials as:

$$\left. \begin{aligned} \log \bar{K} &= \sum v_i \log K_i \\ \log \bar{M} &= \sum v_i \log M_i \end{aligned} \right\} (v_i = \text{volume fractions}) \quad (18)$$

Another kind of mean value formula is given in Korvin (1978), where it is shown that the velocity-porosity dependence for the PAGE sandstone data of Meese and Walther (1967) can be approximated by a $t = -0.65$ rule.

From the point of view of geophysical—physical applications the following property of the generalized mean M_t could be important:

If g_1 and g_2 are positive, $\Phi \neq 0$, $\Phi \neq 1$ and $g_1 \neq g_2$ then $M_t(g_1, g_2, \Phi, 1-\Phi)$ is a strictly monotone function of t in $(-\infty, \infty)$.

(The assertion easily follows from Jensen's inequality, cf. Beckenbach and Bellman, 1961, § 1.16.)

For the above-quoted velocity rules, e.g., this theorem implies that:

$$v_{\text{Wood}} < v_{\text{Wyllie}} < v_{\text{Meese-Walther}} < v_{\text{average}}$$

Finally, a few particular cases will be pointed out where some of the conditions 1–8 are violated so that no simple mixture rules of the form (3) or (4) could be expected.

First, observe that reflexivity (7a), idempotency (7b, 7c) and bi-symmetry (7f) together imply *interchangability* or *symmetry* in the sense that:

$$\text{for } P + Q > 0 \quad M(g_1, g_2, P, Q) = M(g_2, g_1, Q, P) \quad (19)$$

Indeed, by applying in turn idempotency, bi-symmetry and then reflexivity, we have:

$$\begin{aligned} M(g_2, g_1, Q, P) &= M[M(g_1, g_2, 0, Q); M(g_1, g_2, P, 0); Q, P] = M[M(g_1, g_1, 0, P); \\ M(g_2, g_2, Q, 0); P, Q] &= M(g_1, g_2, P, Q) \end{aligned}$$

As an example that the roles of the two constituents cannot be always interchanged recall Maxwell's rule (eq. 17) provided Φ is not sufficiently

small or there is a substantial conductivity contrast. Another, generally non-symmetric, case is connected to the Takayanagi model of the elasticity of compounds (Takayanagi et al., 1965; Baresova, 1969), here, e.g. the Young modulus is expressed as:

$$\frac{1}{\bar{E}} = \frac{a}{b E_1 + (1-b)E_2} + \frac{1-a}{E_2} \quad (20)$$

$$E = \left[\frac{a}{E_1} + \frac{1-a}{E_2} \right]^{-1} + (1-b)E_2 \quad (21)$$

where $ab = V_1$, the volume fraction of the first constituent, a and b give the relative amounts of the elements connected in series and parallel, respectively.

From among the conditions assuring the validity of the mixture rules (3)–(4), *internity* (eq. 7e) deserves a special attention. It is well-known, that for high-porosity ($\Phi \geq 0.6$) marine sediments the velocity of sound waves might be less than that measured in water (Hamilton, 1956; Officer, 1958; Shumway, 1960; Levin, 1962), so that any kind of mixture rules are necessarily of an approximate nature, restricted to low- and medium-porosity consolidated rocks. A more drastic violation of the internity condition (7e) is encountered in liquid–gas mixtures where, for example, sound speed is about 1440–1480 m s⁻¹ in water and about 340 m s⁻¹ in air, but in air–water mixtures it falls to about 20 m s⁻¹. Since even very small concentrations of gas dramatically reduce the sound speed, we have reason to suppose that $M(g_1, g_2, \Phi, 1-\Phi)$, where Φ is gas concentration, is a discontinuous function of Φ for $\Phi \rightarrow +0$ (McWilliams and Douglas, 1969; Kiefer, 1977).

Another example for the violation of condition (7e) is provided by the absorption measurements at sufficiently low frequencies. While Tegland (1970) reports a linearly varying absorption factor for seismic wavelengths and sufficiently thick sand-shale sequences, the ultrasonic absorption in aggregates is generally higher than in any of the individual constituents (Shumway, 1960; Bradley and Fort, 1966).

A recent model experiment of Neumann and Schiel (1977) suggests an interesting counter-example where the homogeneity condition (7d) is not met. Their finding, that in highly heterogeneous materials the logarithmic amplitude fluctuation of the sound waves is not simply proportional to the path travelled, implies – due to the intimate relationship between the Nikolaev (1973) turbidity factor and the absorption coefficient, see Korvin (1972) – that in such materials the absorption coefficient possibly depends on specimen dimension, i.e. on the actual values of the volume fractions as well. I do not know of any cases in petrophysics where the scaling law (7i) were not valid.

In many cases the main reason that some of the conditions 1–8 are not met is that the effective property \bar{g} of the composite cannot be expressed in terms

of the individual properties g_1, g_2 and the volume fractions V_1, V_2 alone. An example for this has already been provided by the Takayanagi model of composite elasticity (eqs. 20, 21), as another simple example, recall the original form of Wood's (1955) equation for the sound speed in two-component media:

$$c^2 = \frac{1}{[\Phi \rho_1 + (1-\Phi)\rho_2] [\Phi M_1^{-1} + (1-\Phi)M_2^{-1}]} \quad (22)$$

where ρ_i, M_i are the respective densities and compressibilities.

Finally, it should be noted, that the value of t to be used for the computation of the mean M_t is not determined by the conditions 1–8 (eqs. 7a–7i). In any actual case the appropriate t should be determined by computer search, as indicated in Korvin (1978).

A notable exception is suggested by the following theorem (Aczél, 1961, §§ 3.1.3. and 5.3.1.):

If we suppose that $f(x)$ is a continuous, monotone function in $(-\infty, \infty)$ and the mean

$$\mathcal{M}_f(g_1, g_2, \Phi, 1-\Phi) = f^{-1} [\Phi f(g_1) + (1-\Phi) f(g_2)]$$

is translatable in the sense that

$$\mathcal{M}_f(g_1 + \tau, g_2 + \tau, \Phi, 1-\Phi) = \mathcal{M}_f(g_1, g_2, \Phi, 1-\Phi) + \tau \quad (23)$$

for all real τ , then

$$f = x, \text{ or } f = e^{\gamma x} \quad (\gamma \neq 0, \gamma \text{ arbitrary real}) \quad (24)$$

apart from the constant factors (of eq. 11).

This theorem implies that if we supplement the set of conditions by a further one:

Cond. 9: translatability ("Verschiebbarkeit") with respect to the physical properties:

$$M(g_1 + \tau, g_2 + \tau, P, Q) = M(g_1, g_2, P, Q) + \tau \quad (7h)$$

there is one and only one mean satisfying all the conditions 1–9 (i.e. eqs. 7a–7h), viz.:

$$M(g_1, g_2, P, Q) = M_1(g_1, g_2, \Phi, 1-\Phi) = \Phi g_1 + (1-\Phi)g_2 \quad (25)$$

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