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Rock Kriging With the Microscope[1]

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An idea to consider rock textures from a geostatistical viewpoint is suggested. Mineral grains are coded by indicator functions. Four metrics are shown of interest for petrographic applications. The simplest one is used to calculate covariograms of indicators for platinum-bearing gabbronorite from the Pansky rock massif (Kola Peninsula, Russia) with maximal range of 2 units. This is generalized in the concept of a minimal cluster of mineral grains for the given rock. The theory allows us to combine grain-by-grain and cluster-by-cluster considerations of rock texture. It may be used to classify monotonous lithological series using nuances of rock textures.

KEY WORDS: rock texture, kriging, geostatistics, indicator function, metrics, mineral grain, gabbronorite.

INTRODUCTION

What is the main (mathematical) idea concealed by Nature in rocks? This question has been asked, from time to time, by prominent mineralogists and petrologists for at least the last two centuries.

The most important result is that we are not allowed to use genetic interpretations when modelling rock. Probably, it was C. F. Naumann who distinctly divided genetic and structural aspects of the problem in 1859 for the first time (Naumann, 1907, p. 4). Harker emphasized in 1895 that "some fundamental principle has yet to be found in petrology . . . and any genetic classification of rocks must be regarded as one of convenience rather than of principle" (Harker, 1908, p. 20).

The concept was introduced from crystallography after the fundamentals of that science had been established by E. S. Fedorov and A. M. Schoenflies. Following this principle, some elementary cells (in respect of mineral and chemical

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compositions and texture) build rock like a macrocrystal. To our mind, there is neither physical reason for mineral grains to be joined in such a manner nor experimental evidence for such a process. Nevertheless, the hypothesis has been very popular up to the present. See a critical review of the recent viewpoints in Voytekhovsky (1998).

What we suggest in this paper is another way to understand any crystalline rock. We begin from individual mineral grains of different species obviously in contact with each other, and look for some internal principle to combine them into units of higher hierarchical levels.

METRICS

In view of prevailing pragmatic philosophy regarding rock as an industrial material, it makes sense to stress a rather simple idea. Since its origin, rock has nothing to do with our needs. Usually, we consider it contained in an ordinary Euclidean space. But, any rock can be represented in a proper space which might be Euclidean or not depending on the rules laid down. Let us assume real mineral grains to be the "points" of this space with "to be or not to be in contact" as the only inherent spatial relation between them, and try to define some natural metrics.

An intuitively clear construction is $h(a, b) = \min[\text{dist}(a, b)]$, where dist($a$,$b$) is the number of binary intergrain boundaries crossed on the continuous way from grain a to b. Let us check the axiomatics.

1. Requirements $h(a, b) \geq 0$ and $h(a, b) = 0 \Leftrightarrow a \equiv b$ follow from the sense of $h(a, b)$.
2. Let $h(a, b) = p$, then $h(b, a) \leq p$ because a path of length p from b to a exists. If $h(b, a) < p$, then $h(a, b) < p$ because the way of length less than p from a to b exists. It follows from this contradiction that $h(b, a) = p = h(a, b)$.
3. Let $h(a, b) = p$, $h(b, c) = q$, then $h(a, c) = \min \text{dist}(a, c) \leq \text{dist}(a, c) = p + q = h(a, b) + h(b, c)$ because a path of length $p + q$ from a to c via b exists.

So, $h(a, b)$ meets all the requirements of a metric . It is interesting to extend it to any aggregates of mineral grains, say A and B. It is easy to show that $h(A, B) = \min \text{dist}(a, b | a \in A, b \in B)$ is not a wanted extension of $h(a, b)$. For example, if $A \cap B \neq \emptyset$, $B \cap C \neq \emptyset$, $A \cap C = \emptyset$ then $h(A, B) = h(B, C) = 0$, $h(A, C) > 0$, and $h(A, C) > h(A, B) + h(B, C)$ is in contradiction with (3). A real extension is given by Hausdorff metric $\sigma(A, B) = \max\{\{\zeta(a, B) | a \in A\}, \{\zeta(b, A) | b \in B\}\}$, where $\zeta(a, B) = \min\{h(a, b) | b \in B\}$, $\zeta(b, A) = \min\{h(b, a) | a \in A\}$.

One more idea is to use any measure μ (i.e., nonnegative, monotonic, and additive function, e.g., the number of grains composing an aggregate) to define another type of metric for the aggregates. It can be shown that $\xi(A, B) =$

$\mu(A \cup B) - \mu(A \cap B)$ and $\rho(A, B) = 1 - \mu(A \cap B)/\mu(A \cup B)$ satisfy the above axiomatics. The condition (3) being the most difficult to check, is given in Appendix for the above three metrics.

COVARIANCES

Following general theory of geostatistics (Armstrong, 1998; Journel and Huijbregts, 1991; Rivoirard, 1994;) to calculate the space covariograms for mineral grains of different species, we code them by indicators:

$$\mathrm{I}[m(x) = m_i] = 1 \quad \text{if } m(x) = m_i \quad \text{and} \quad \mathrm{I}[m(x) = m_i] = 0 \quad \text{if } m(x) \neq m_i.$$

An indicator is a random function of grain, x. Its mathematical expectation and variance are

$$\begin{aligned} \mathrm{E}_i &= \mathrm{E}\{\mathrm{I}[m(x) = m_i]\} = \mathrm{P}[m(x) = m_i], \quad \mathrm{V}_i = \mathrm{V}\{\mathrm{I}[m(x) = m_i]\} \\ &= \mathrm{P}[m(x) = m_i] \times \mathrm{P}[m(x) \neq m_i]. \end{aligned}$$

Covariances of indicators are

$$\begin{aligned} \mathrm{C}_{ii}(h) &= \mathrm{P}[m(x) = m_i, m(x+h) = m_i] - \{\mathrm{P}[m(x) = m_i]\}^2, \\ &\times \text{hence } \mathrm{C}_{ii}(0) = \mathrm{V}_i, \\ C_{ij}(h) &= \mathrm{P}[m(x) = m_i, m(x+h) = m_j] - \mathrm{P}[m(x) = m_i] \times \mathrm{P}[m(x) = m_j], \\ &\times \text{hence } \mathrm{C}_{ij}(0) = -\mathrm{E}_i \mathrm{E}_j. \end{aligned}$$

EXAMPLES

The above formulae were used to calculate automatically the space covariograms of minerals in gabbronorite from the Pansky rock massif, Kola Peninsula, Russia. See a petrographical section (Fig. 1) and calculated covariograms (Fig. 2). Plagioclase, clinopyroxene, orthopyroxene are white, grey, black and indicated by 1, 2, 3, respectively. The values of $\mathrm{C}_{ii}(h)$, $\mathrm{C}_{ij}(h)$ for $h = 0, \ldots, 10$ are in Table 1.

DISCUSSION

In our case, the maximal range appears to be equal to 2 as follows from the $\mathrm{C}_{11}(h)$ covariogram. The value, $\mathrm{C}_{11}(1) = -0.0949$, visually differs from zero.

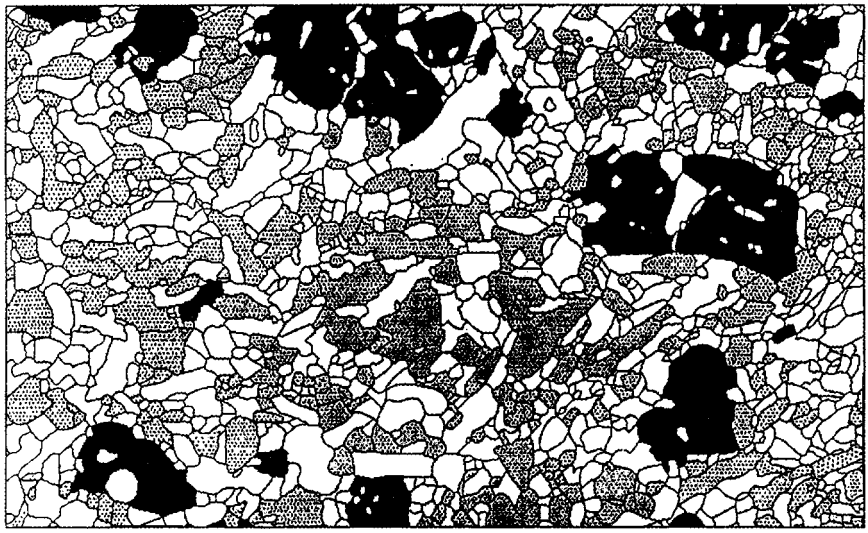

Figure 1. Gabbronorite from the Pansky rock massif.

But, the situation is not so definite for $C_{11}(2) = 0.0293$. We obviously need a more precise criterion to solve this dilemma. This is especially important when considering covariograms for minor minerals. In this case, the absolute $C_{ij}(h)$ values are negligible if compared with those of the main rock-forming minerals. The appropriate covariograms should be analysed in their proper scale.

It is conspicuous that some covariograms are systematically positive (e.g., C_{12}, C_{13}, C_{23}) and tend not to zero but to some small positive value while others (C_{22})

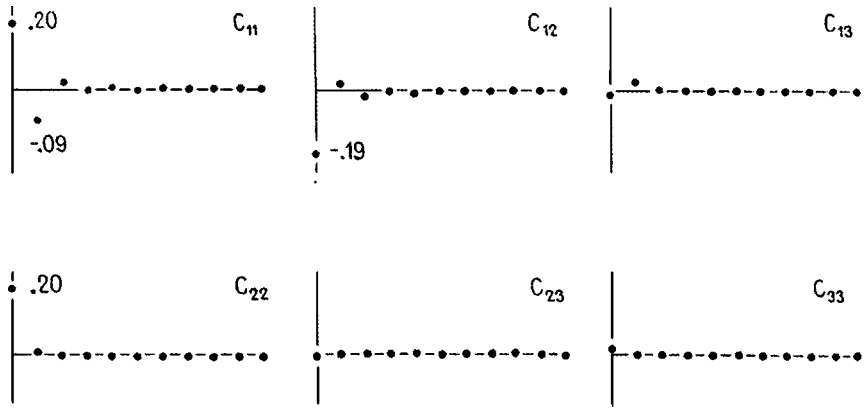

Figure 2. Covariograms for the gabbronorite-forming minerals.

Table 1. Covariances for the Gabbronorite-Forming Minerals

h	C_{11}	C_{12}	C_{13}	C_{22}	C_{23}	C_{33}
0	1.98E−1	−1.86E−1	−1.21E−2	1.90E−1	−4.22E−3	1.63E−2
1	−9.49E−2	2.12E−1	6.65E−2	1.12E−2	7.14E−3	3.27E−5
2	2.93E−2	1.53E−1	1.66E−2	−6.03E−3	8.06E−3	6.35E−4
3	−4.31E−3	1.83E−1	1.90E−2	−1.05E−3	4.79E−3	3.12E−5
4	9.11E−3	1.78E−1	1.13E−2	−1.90E−3	5.06E−3	1.38E−4
5	−3.02E−3	1.92E−1	1.23E−2	−3.13E−3	4.32E−3	−1.42E−4
6	9.68E−3	1.81E−1	9.60E−3	−2.51E−3	4.11E−3	3.02E−5
7	7.05E−3	1.79E−1	1.22E−2	−3.96E−5	3.94E−3	−1.57E−4
8	4.85E−3	1.87E−1	9.05E−3	−1.60E−3	3.11E−3	−9.38E−5
9	2.80E−3	1.86E−1	1.13E−2	−1.76E−3	3.46E−3	−4.82E−8
10	5.02E−3	1.81E−1	1.06E−2	1.78E−3	3.65E−3	−4.29E−5

tend to a small negative value. Probably, this fact may result from the mathematical properties of the closed number system:

$$\sum_i \mathrm{I}[m(x) = m_i] = 1.$$

So, one more problem to bear in mind for the future geostatistical investigations of rock texture, is to find criteria for the sills in case of the closed number system.

From the argument above, we may define a "minimal cluster" of rock as any maximal aggregate of grains being at a distance less than the range from each other. If the range equals 1, we have common grain-by-grain consideration of rock. An example of such rock was shown by Kretz (1969). A pyroxene–scapolite–sphene granulite from the Grenville terrain, Quebec, Canada, was found to be a pure mosaic by the crystal density, area fraction, point-sample, quadrat, nearest-neighbor, random-point, contact-area, contact frequency, and line-transect methods. We have obtained the same result from the covariogram analysis.

If the range exceeds 1, there appears to be intrinsic reason to consider rock as built from minimal clusters also. As they are identical only in a statistical sense, clusters may be of the same or different mineral/chemical composition. And this phenomenon may be also investigated geostatistically with the metrics $\sigma(A, B)$, $\xi(A, B)$, and $\rho(A, B)$ derived especially to operate with mineral aggregates. As a result, any grain/cluster may be effectively estimated by a kriging procedure given the species/composition of some neighbors.

CONCLUSION

So, what is the main idea concealed by Nature in rocks? A century-old mathematical crystallography affirms that an ideal crystal may be described, in principle, within the framework of a deterministic theory. Any real crystal is already more or

less nonideal and needs more complicated probabilistic methods to be described. By comparison, rock is a stochastic system even in the best approximation. We suppose the range may exceed 2 for some equigranular magmatic rocks. But it is unlikely to be very high. Rock is a type of locally ordered system.

This fundamental property may be used in applied geology, for example, to classify monotonous lithological series by range value. This is just what we do for the platinum-bearing Pansky rock massif to correlate its tectonic units.

Another idea is to use noneuclidean metrics when modelling rock textures. The first step is to build the space partition with a noneuclidean range needed. The second is to add euclidean granulometric distributions of the rock-forming minerals.

A more profound idea is to correlate the nuances of textures with petrogenesis. An apparent problem is that recent petrology does not use parameters calculated with noneuclidean metrics. Nevertheless, some relations can be seen even in Figures 1 and 2. Plagioclase crystallized first of the three rock-forming minerals. And it is the covariogram of plagioclase C_{11} that shows the maximal range. The reason is that plagioclase created the original matrix in the holes of which other minerals appeared one by one from the extracted melt. And the question is whether is it possible to get some more detailed information from the covariograms or not. We believe it is.

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APPENDIX

Derivation of condition (3) for the three metrics described.

Metric 1

Let us take such a and c that $h(a, c) = \sigma(A, C)$. Without loss of generality, $h(a, c) = \zeta(a, C)$. Let us take such $b \in B$ and $c' \in C$ that $h(a, b) = \zeta(a, B)$ and $h(b, c') = \zeta(b, C)$. Then $h(a, b) \le \sigma(A, B)$ and $h(b, c') \le \sigma(B, C)$. By definition of $\zeta(a, C)$, $h(a, c) \le h(a, c')$. Because of $h(a, c')$ property, $h(a, c') \le h(a, b) + h(b, c')$. Hence, $\sigma(A, C) = h(a, c) \le h(a, c') \le h(a, b) + h(b, c') \le \sigma(A, B) + \sigma(B, C)$.

Metric 2

Let us denote the mutually disjointed sets of mineral grains as follows: $(A \cap C)\backslash B = 1$, $(A \cap B)\backslash C = 2$, $A \cap B \cap C = 3$, $(B \cap C)\backslash A = 4$, $A\backslash(B \cup C) = 5$, $B\backslash(A \cup C) = 6$, $C\backslash(A \cup B) = 7$. Required is $\xi(A, B) + \xi(B, C) \ge \xi(A, C)$, i.e., $\mu(A \cup B) - \mu(A \cap B) + \mu(B \cup C) - \mu(B \cap C) \ge \mu(A \cup C) - \mu(\mathrm{A} \cap \mathrm{C})$, i.e., $\mu 1 + \mu 2 + \mu 3 + \mu 4 + \mu 5 + \mu 6 - \mu 2 - \mu 3 + \mu 1 + \mu 2 + \mu 3 + \mu 4 + \mu 6 + \mu 7 - \mu 3 - \mu 4 \ge \mu 1 + \mu 2 + \mu 3 + \mu 4 + \mu 5 + \mu 7 - \mu 1 - \mu 3$, i.e., $\mu 1 + \mu 6 \ge 0$. The latter results from the nonnegativity of $\mu 1$ and $\mu 6$.

Metric 3

Required is $\rho(A, B) + \rho(B, C) \ge \rho(A, C)$, i.e., $1\text{-}\mu(A \cap B)/\mu(A \cup B) + 1 - \mu(B \cap C)/\mu(B \cup C) \ge 1\text{-}\mu(A \cap C)/\mu(A \cup C)$, i.e., $\sum = \mu(A \cap B)/\mu(A \cup B) + \mu(B \cap C)/\mu(B \cup C) - \mu(A \cap C)/\mu(A \cup C) \le 1$. In above notation, $\sum$ is majorized by $\sum^* = (\mu 2 + \mu 3)/(\mu A + \mu 4) + (\mu 3 + \mu 4)/(\mu C + \mu 2) - \mu 3/(\mu A + \mu C - \mu 3)$. It may be shown that $\sum^* \le 1$.

Consider the function $F(\mu 2) = (\mu 2 + \mu 3)/(\mu A + \mu 4) + (\mu 3 + \mu 4)/(\mu C + \mu 2)$ on the segment $[0, \mu A - \mu 3]$. $dF/d\mu 2 = 1/(\mu A + \mu 4) - (\mu 3 + \mu 4)/(\mu C + \mu 2)^2 = 0$ if $\mu 2^* = [(\mu A + \mu 4)(\mu 3 + \mu 4)]^{1/2} - \mu C$. In this point $d^2F/d(\mu 2)^2|_{\mu 2*} = 2(\mu 3 + \mu 4)/(\mu C + \mu 2^*)^3 = 2(\mu A + \mu 4)^{-3/2}(\mu 3 + \mu 4)^{-1/2} > 0$. So, $F(\mu 2)$ has a maximum at one of the bounds.

In the same way, $F(\mu 4) = (\mu 2 + \mu 3)/(\mu A + \mu 4) + (\mu 3 + \mu 4)/(\mu C + \mu 2)$ has a maximum at one of the bounds of the segment $[0, \mu C - \mu 3]$.

In three cases we immediately get the result $\sum^* \le F(0, \mu C - \mu 3) = F(\mu A - \mu 3, 0) = F(\mu A - \mu 3, \mu C - \mu 3) = 1$. In the fourth case we have $\sum^* \le F(0, 0) = \mu 3/\mu A + \mu 3/\mu C - \mu 3/(\mu A + \mu C - \mu 3) = F(\mu 3)$. Consider $F(\mu 3)$

on the segment $[0, \min(\mu A, \mu C)]$. $dF/d\mu 3 = 1/\mu A + 1/\mu C - (\mu A + \mu C)/(\mu A + \mu C - \mu 3)^2 = 0$ if $\mu 3^* = \mu A + \mu C - (\mu A \mu C)^{1/2}$. As $\min(\mu A, \mu C) \leq (\mu A \mu C)^{1/2} \leq \max(\mu A, \mu C)$, the value of $\mu 3^* \geq \min(\mu A, \mu C)$ is located, at least, at the right bound of the segment. In this point, $d^2F/d(\mu 3)^2|_{\mu 3*} = -2(\mu A + \mu C)/(\mu A + \mu C - \mu 3^*)^3 = -2(\mu A + \mu C)/(\mu A \mu C)^{3/2} < 0$, i.e., $F(\mu 3)$ has a maximum at the right bound. Without loss of generality, assume $\min(\mu A, \mu C) = \mu A$. Hence, $\sum^* \leq F(\mu A) = 1$.