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Evaluation of Classification Criteria in the 4M Method Applied to Ordinary Chondrites

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In 2019, our group introduced a new method for the classification of ordinary chondrites based on Mössbauer spectroscopy results. In 2026, this method was further developed. In the original version, the classification criterion was the level of similarity determined on the basis of the Mahalanobis distance, whereas in the updated version a Bayesian approach based on maximum *a posteriori* probability was proposed. The aim of the study is to evaluate the effectiveness of the new approach used in the revised 4M method, with particular emphasis on the role of *a priori* probability in the classification procedure. Three classification variants were compared.

topics: ordinary chondrites, Mössbauer spectroscopy, Bayesian classification, Mahalanobis distance

1. Introduction

Ordinary chondrites (OCs) constitute the most abundant group of meteorites found on Earth. They contain significant amounts of iron (18–28 wt%).

Three main groups of ordinary chondrites are distinguished: H (high iron), L (low iron), and LL (low total iron and low metallic iron). In the classical classification, based on electron microprobe results, the assignment to individual groups is determined on the basis of the fayalite content in olivines and the ferrosilite content in pyroxenes.

In 2019, our group proposed the 4M method (the name is derived from the terms Meteorites, Mössbauer spectroscopy, Mahalanobis distance, and Multidimensional discriminant analysis), which enables the classification of ordinary chondrites based on Mössbauer spectra [1]. This method was subsequently developed and improved [2].

A typical Mössbauer spectrum of an ordinary chondrite contains signals originating from four main mineral phases: olivine, pyroxene, metallic phase, and troilite. Additionally, subspectra related to weathering products, i.e., Fe^{3+} compounds, may be present in the spectra.

The analysis of spectra of different ordinary chondrites indicates the existence of relationships between the abundances of individual mineral phases and the meteorite type. The first research group to investigate this issue was the Mössbauer spectroscopy group from Kanpur [3–5]. A review of subsequent studies is presented in [6]. However, these relationships are not sufficiently unambiguous to constitute the basis for classification based on a single parameter. Therefore, the 4M method simultaneously uses information concerning all four main mineral phases.

The method is based on a database comprising 59 Mössbauer spectra of ordinary chondrites with known types (Table I). Each sample is represented as a point in a four-dimensional space, whose dimensions correspond to the distribution of iron among the main mineral phases (olivine, pyroxene, metallic phase, and troilite) present in the Mössbauer spectrum. These points form three clusters corresponding to the H, L, and LL groups.

Classification of an unknown sample involves determining its position in this space and calculating the Mahalanobis distance [7] between the investigated sample and the centers of individual reference clusters. In the original version of the method,

TABLE I

The mean values of subspectral areas as percentages, related to four main mineral phases, obtained from a collected database of 59 Mössbauer measurements of OCs of H, L, and LL types.

Mineral phases	Type and cluster size n		
	Type H $n = 22$	Type L $n = 20$	Type LL $n = 17$
Olivine	39.2 ± 5.1	51.3 ± 5.7	61.7 ± 4.1
Pyroxene	24.3 ± 4.0	22.0 ± 2.5	24.2 ± 3.5
Metallic phase	17.3 ± 7.1	8.4 ± 3.5	1.2 ± 1.7
Troilite	16.5 ± 2.6	15.7 ± 3.5	10.6 ± 3.5

this distance was used to determine the similarity level (S_{clust}). In the modified version of the method, proposed in 2026 [2], the Mahalanobis distance constitutes the basis for the determination of posterior probabilities, and the final classification is performed according to the maximum *a posteriori* (MAP) rule.

2. Fundamentals of the Bayesian approach

In the Bayesian approach, probability is interpreted as a measure of uncertainty associated with the phenomenon under investigation [8]. In contrast to classical statistics, model parameters are treated as random variables described by probability distributions [9].

Bayesian inference is based on three fundamental elements [10]: (i) the prior distribution, describing the knowledge about model parameters before taking the current data into account; (ii) the likelihood function, containing information derived from the analyzed data; (iii) the posterior distribution, obtained by combining prior knowledge with the information contained in the data.

In the 4M method, the likelihood function is related to the position of a sample in the four-dimensional Mössbauer parameter space and to the Mahalanobis distance from each reference class.

The classification is based on the maximum *a posteriori* (MAP) rule. For each sample, the probabilities of belonging to the H, L, and LL classes are determined, and the sample is then assigned to the class corresponding to the highest posterior probability

$$P(\pi_k \,|\boldsymbol{x}\,) = \frac{p_k \, f(\boldsymbol{x}\,|\pi_k\,)}{\sum\limits_{l=1}^{K} p_l \, f(\boldsymbol{x}\,|\pi_l\,)}, \tag{1}$$

where $P(\pi_k|\boldsymbol{x})$ denotes the posterior probability that the observed vector (x) belongs to subpopulation π_k. Here, p_k denotes the prior probability that an observation belongs to subpopulation π_k, $f(x|\pi_k)$ is the conditional probability density function of the vector $(\boldsymbol{x})$ in subpopulation π_k, and K is the number of subpopulations.

After substituting the probability density function and the expression for the Mahalanobis distance (d_M), the discriminant function can be written as

$$g_k\,(\boldsymbol{x}) = -\frac{1}{2}\,(d_M)^2 - \frac{1}{2}\log\,(\Sigma_k) + \log(p_k), \tag{2}$$

where Σ_k is the covariance matrix.

Note that the term containing the Mahalanobis distance appears in squared form and therefore provides the dominant contribution to the final result.

It should be emphasized that the introduction of the MAP rule does not change the assumptions of the 4M method or the experimental data used. Only the decision criterion has been modified. Consequently, the 4M method has acquired a formal probabilistic basis while preserving its original structure and physical interpretation.

3. Materials and methods

3.1. Mössbauer studies of the investigated samples

The analysis was based on Mössbauer spectroscopy results obtained for a reference group consisting of 20 ordinary chondrites that were not included in the 4M database. These spectra — similarly to the spectra included in our database — originated both from literature sources [11–13] and from measurements performed at the Mössbauer Spectroscopy Laboratory at the Faculty of Physics, Warsaw University of Technology.

The samples investigated in our laboratory were ground in an agate mortar in the presence of alcohol. The powdered material was then placed in a dedicated absorber holder and measured in transmission geometry using a Mössbauer spectrometer equipped with a ^{57}Co source.

The spectra were fitted with Lorentzian line shapes in the Full Static Hamiltonian mode using the Recoil software [14].

3.2. Bayesian approach

Each sample from the reference database was described by the distribution of iron among the four main mineral phases: olivine, pyroxene, metallic phase, and troilite. Based on these data, the samples were placed in a four-dimensional space, and the Mahalanobis distances to the centers of individual clusters were determined.

In the subsequent analysis, three variants of prior probabilities were considered:

- Neutral variant — equal prior probabilities were assumed for all groups, i.e., $p_j(\text{H}) = p_j(\text{L}) = p_j(\text{LL}) = 1/3$;

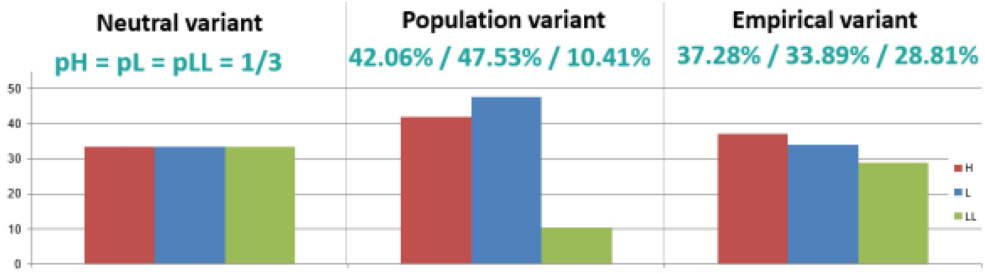


Fig. 1. Prior probability distributions for the H, L, and LL groups in three analyzed variants.

TABLE II

Results obtained using the original 4M method ('Original') compared with those obtained using the modified 4M method: with equal prior probabilities ('Neutral'), with prior probabilities based on falls and finds ('Population'), and with prior probabilities based on the database distribution ('Empirical').

Type (n)	Original	Neutral	Population	Empirical
H (8)	100%	100%	100%	100%
L (7)	71%	86%	86%	86%
LL (5)	40%	100%	40%	80%
All (20)	75%	95%	80%	90%

- Population variant — prior probabilities corresponded to the occurrence frequencies of H, L, and LL chondrites among falls and finds, i.e., $p_j(\mathrm{H}) = 42.06\%$, $p_j(\mathrm{L}) = 47.53\%$, $p_j(\mathrm{LL}) = 10.41\%$;
- Empirical variant — the prior distribution was determined from the relative abundances of individual groups in the 4M database, i.e., $p_j(\mathrm{H}) = 37.28\%$, $p_j(\mathrm{L}) = 33.89\%$, $p_j(\mathrm{LL}) = 28.81\%$.

These three prior probability variants are depicted in Fig. 1. The effectiveness of the 4M method was examined for each of the considered prior probability variants.

4. Results

For each prior probability variant, the Mahalanobis distance and the MAP parameter were determined for the reference group, and the classification using the 4M method was subsequently performed [15].

For all analyzed prior probability variants, a very high classification accuracy was obtained for the H group (Table II). Larger differences were observed for LL-type chondrites, for which the influence of the adopted prior probability distribution was more pronounced. This result is consistent with expectations, since the largest differences between the considered prior probability distributions occurred for this group.

The original version of the 4M method provided a 75% agreement with the classical classification (15 out of 20 samples). The introduction of the MAP rule improved the results in all analyzed cases [2]. The highest accuracy was obtained for the neutral variant, reaching an agreement of 95% (19 out of 20 samples). The population-based variant provided an agreement of 80%, whereas the variant based on the 4M database distribution resulted in an agreement of 90%.

5. Conclusions

The obtained results indicate that the classification performed using the 4M method is determined primarily by the information contained in Mössbauer spectra, whereas the influence of prior probabilities remains limited.

The best results were obtained for the neutral variant. This solution appears to be particularly well justified from the methodological point of view, since it does not favor any group before the analysis of the data and remains consistent with the diagnostic character of the 4M method.

The application of the maximum *a posteriori* rule provided the method with a formal probabilistic basis and made it possible to replace the intuitive similarity criterion with a procedure derived directly from Bayesian decision theory.

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