

Title [Título]

Multivariate approach using bootstrapping for the inference of distributional parameters of samples containing compositional values below detection limit

Summary (1000 characters) [Resumen del trabajo (máximo 1000 caracteres)].

Two important characteristics of geochemical data complicating their analysis are its compositional nature and the presence of values that laboratories have not been able to measure because of concentrations below the detection limit of the instruments. Logratio transformations are used to convert any compositional data in the simplex to samples in real space, thus allowing the practitioner to apply classical statistical techniques valid in real space. Nondetects can be regarded as a special case of missing values with a lower and upper bound. Recent works have proposed dealing with compositional values below detection limit using a multiplicative replacement, a modified expectation maximization (EM) algorithm, or a univariate bootstrap approach. Here we revise these techniques and propose a novel multivariate approach combining bootstrap simulation and the EM modified algorithm for the purpose of inferring distributional parameters for compositional data with nondetects.

2 Key words [2 palabras clave].

Detection limit, Simplex

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Multivariate analysis