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PII: S0375-6742(17)30365-5
DOI: doi: 10.1016/j.gexplo.2017.05.006
Reference: GEXPLO 5923

To appear in: *Journal of Geochemical Exploration*

Received date: 23 March 2017
Revised date: 13 May 2017
Accepted date: 25 May 2017

Please cite this article as: A. Buccianti, A. Lima, S. Albanese, B. De Vivo , Measuring the change under compositional data analysis (CoDA): Insight on the dynamics of geochemical systems, *Journal of Geochemical Exploration* (2017), doi: 10.1016/j.gexplo.2017.05.006

Measuring the change under Compositional Data Analysis (CoDA): insight on the dynamics of geochemical systems

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Abstract

Geochemical systems are complex and the analysis of the shape of the frequency distribution of elements and chemical species often informs about the variability and dispersion related to the underlying dynamics. However, when compositional data are used it is incorrect to investigate concentrations in the Euclidean space. Distribution analysis is aimed at focussing on real coordinates, which can be obtained by applying some appropriate log-ratio transformation. In particular, distributional analysis for compositional data can be applied to isometric coordinates, called balances, obtained through partition of a multi-element data set. As an alternative the same investigation can be performed on indices such as the robust Mahalanobis distance after having ranked log-ratio compositions with respect to some reference composition (i.e. average Earth crust) and having obtained a sort of "measure of change". By considering this second new perspective, the chemical composition of topsoils of the Campania Region (Southern Italy) was investigated by analysing the concentrations of Al, As, B, Ba, Ca, Co, Cr, Cu, Fe, K, La, Mg, Mn, Mo, Na, Ni, P, Pb, Sr, Th, Ti, V and Zn, in mg/kg, determined on more than 3500 samples. Results reveal the presence of complex processes governed by interaction-dominant dynamics where self-organisation appears to play some role.

Keywords: compositional data, power laws, multifractals, dissipative systems, distributional analysis, robust Mahalanobis distance, compositional changes

1. Introduction

In this contribution the regionalised structure of geochemical processes will be investigated by considering the joint behaviour of several elements constituting for each sample its whole composition. The approach is based on the CoDA (Compositional Data Analysis) theory so that the proportionality features of abundance data are fully taken into account enhancing their relative multivariate behaviour (Aitchison, 1986). The work is motivated by the fact that the shape of a probability distribution of chemical variables reveals information about the dynamics governing the system under investigation (van Rooij et al., 2013). However, whenever the sample space is not the real space, some change of

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