A spectral approach for the clustering of source rocks

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ABSTRACT

The identification of family affiliation of samples emerging from oils and source rocks is a topic of primary importance in the field of exploration geoscience. We demonstrate how spectral clustering can be applied in the context of chemometrics on a set of rock extracts from Western Greece, using quantitative information of normal alkane (nC15 - nC35) concentrations. The developed method is based on the creation of a graph Laplacian matrix, that represents the latent graphical structure of the samples, and the subsequent estimation of the underlying clusters based on the eigenvectors of this matrix. The number of clusters is determined by optimizing the modularity of the resulting graph, thus ensuring high intra-cluster and low inter-cluster similarity. Our results highlight that the proposed approach partitions the geological samples in "natural" groups, with distinct concentration profiles of n-alkanes. Using this example, the reliability of this technique to support source rock classification is proved, while it provides a way to facilitate geochemical interpretations.