



Clustering by search-and-find of density peak: a cheap and unsupervised approach to map complex data landscapes

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Abstract: Cluster analysis is aimed at classifying elements into categories on the basis of their similarity. Its applications range from bioinformatics and material science to economy and social sciences. We propose an approach based on the idea that cluster centers are characterized by a higher density than their neighbors and by a relatively large distance from points with higher densities. This idea forms the basis of a clustering procedure in which the number of clusters arises intuitively, outliers are automatically spotted and excluded from the analysis, and clusters are recognized regardless of their shape and of the dimensionality of the space in which they are embedded [Science, vol 344, p. 1492 (2014)]. We will describe applications of this approach to molecular modeling, bioinformatics and neuroimaging.