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Joe Bible, Susmita Datta, Somnath Datta

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Cluster analysis is a useful technique in finding natural groups in data. In this chapter, we describe a number of popular statistical clustering techniques and their R implementations. We also introduce a number of cluster analysis tools (R packages) developed by our group in the past for statistical mining of biological data, such as microarray gene expression data and mass-spectrometry proteomic data that are perhaps equally applicable to materials data. We illustrate these techniques by grouping materials with properties of a semiconducting chalcopyrite compounds using certain properties (descriptors) such as the melting point of the constituting elements.

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