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Data; 1. Introduction; 2. Unsupervised Learning; 2.1 Principal Components Analysis; 2.2 Clustering; 3. Different Clustering Algorithms and their Implementations in R; 3.1 Agglomerative Hierarchical; 3.2 K-Means; 3.3 Divisive Hierarchical; 3.4 Partitioning Around Medoids (PAM); 3.5 Fuzzy Analysis (FANNY)
4. Validations of Clustering Results 4.1 Dunn Index; 4.2 Silhouette Width; 4.3 Connectivity; 5. Rank Aggregation of Clustering Results; 6. Further Reading; Acknowledgments; References; 5. Evolutionary Data-Driven Modeling; 1. Preamble; 2. The Concept of Pareto Tradeoff; 3. Evolutionary Neural Net and Pareto Tradeoff; 4. Selecting the Appropriate Model in EvoNN; 5. Conventional Genetic Programming; 6. Bi-Objective Genetic Programming; 6.1 BioGP Code; 7. Analyzing the Variable Response in EvoNN and BioGP; 8. An Application in the Materials Area; 9. Further Reading; References
6. Data Dimensionality Reduction in Materials Science 1. Introduction; 2. Dimensionality Reduction: Basic Ideas and Taxonomy; 3. Dimensionality Reduction Methods: Algorithms, Advantages, and Disadvantages; 3.1 Principal Component Analysis (PCA); PCA Algorithm; 3.2 Isomap; Isomap Algorithm; 3.3 Locally Linear Embedding; LLE Algorithm; 3.4 Hessian LLE; hLLE Algorithm; 4. Dimensionality Estimators; 5. Software; 5.1 Core Functionality; 5.2 User Interface; 6. Analyzing Two Material Science Data Sets: Apatites and Organic Solar Cells; 6.1 Apatite Data; Dimensionality Estimation
6.2 Unraveling Process-Morphology Pathways of Organic Solar Cells using SETDiR

Sommario/riassunto

Materials informatics: a 'hot topic' area in materials science, aims to combine traditionally bio-led informatics with computational methodologies, supporting more efficient research by identifying strategies for time- and cost-effective analysis. The discovery and maturation of new materials has been outpaced by the thicket of data created by new combinatorial and high throughput analytical techniques. The elaboration of this ""quantitative avalanche""-and the resulting complex, multi-factor analyses required to understand it-means that interest, investment, and research are revisi