1.	Record Nr.	UNINA9910780000703321
	Titolo	Informatics for materials science and engineering : data-driven discovery for accelerated experimentation and application / / edited by Krishna Rajan
	Pubbl/distr/stampa	Oxford, : Butterworth-Heinemann, 2013 Oxford : , : Butterworth-Heinemann, , 2013
	ISBN	0-12-394614-X
	Edizione	[1st ed.]
	Descrizione fisica	1 online resource (xv, 525 pages) : illustrations (some color)
	Collana	Gale eBooks
	Disciplina	620.110285
	Soggetti	Materials science - Data processing
	Lingua di pubblicazione	Inglese
	Formato	Materiale a stampa
	Livello bibliografico	Monografia
	Note generali	Description based upon print version of record.
	Nota di bibliografia	Includes bibliographical references and index.
	Nota di contenuto	Front Cover; Informatics for Materials Science and Engineering; Copyright Page; Contents; Preface: A Reading Guide; Acknowledgment; 1. Materials Informatics: An Introduction; 1. The What and Why of Informatics; 2. Learning from Systems Biology: An "Omics" Approach to Mater; 3. Where Do We Get the Information?; 4. Data Mining: Data- Driven Materials Research; References; 2. Data Mining in Materials Science and Engineering; 1. Introduction; 2. Analysis Needs of Science Applications; 3. The Scientific Data-Mining Process; 4. Image Analysis; 5. Dimension Reduction; 5.1 Feature Selection Techniques Distance Filter Chi-Squared Filter; Stump Filter; Relief; 5.2 Feature Transformation Techniques; Principal Component Analysis (PCA); Isomap; Locally Linear Embedding (LLE); Laplacian Eigenmaps; 5.3 Comparison of Dimension Reduction Methods; 6. Building Predictive and Descriptive Models; 6.1 Classification and Regression; 6.2 Clustering; 7. Further Reading; Acknowledgments; References; 3. Novel Approaches to Statistical Learning in Materials Science; 1. Introduction; 2. The Supervised Binary Classification Learning Problem; 3. Incorporating Side Information; 4. Conformal Prediction 5. Optimal Learning 6. Optimal Uncertainty Quantification; 7. Clustering Including Statistical Physics Approaches; 8. Materials Science Example: The Search for New Piezoelectrics; 9. Conclusion; 10. Further Reading; Acknowledgments; References; 4. Cluster Analysis: Finding Groups in

	 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: Basic Ideas and Taxonow; 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