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How; 4.2. Description Language for Optimisation Tasks in Catalysis; 4.3. Tackling Constrained Mixed Optimisation; 4.4. A Prototype Implementation; Bibliography; Chapter 5. Analysis and Mining of Data Collected in Catalytic Experiments (M. Holena); 5.1. Similarity and Difference Between Data Analysis and Mining; 5.2. Survey of Existing Methods; 5.2.1. Statistical Methods; 5.2.2. Extraction of Logical Rules from Data; 5.3. Case Study with the Synthesis of HCN BibliographyChapter 6. Artificial Neural Networks in the Development of Catalytic Materials (M. Holena); 6.1. What are Artificial Neural Networks?; 6.1.1. Network Architecture; 6.1.2. Important Kinds of Neural Networks; 6.1.3. Activity of Neurons; 6.1.4. What do Neural Networks Compute?; 6.2. Approximation Capability of Neural Networks; 6.3. Training Neural Networks; 6.4. Knowledge Obtainable from a Trained Network; Bibliography; Chapter 7. Tuning Evolutionary Algorithms with Artificial Neural Networks (M. Holena); 7.1. Heuristic Parameters of Genetic Algorithms
7.2. Parameter Tuning Based on Virtual Experiments7.3. Case Study with the Oxidative Dehydrogenation of Propane; Bibliography; Chapter 8. Improving Neural Network Approximations (M. Holena); 8.1. Importance of Choosing the Right Network Architecture; 8.2. Influence of the Distribution of Training Data; 8.3. Boosting Neural Networks; 8.4. Case Study with HCN Synthesis Continued; Bibliography; Chapter 9. Applications of Combinatorial Catalyst Development and An Outlook on Future Work (M. Baerns); 9.1. Introduction; 9.2. Experimental Applications of Combinatorial Catalyst Development
9.3. Methodology

Sommario/riassunto

The book provides a comprehensive treatment of combinatorial development of heterogeneous catalysts. In particular, two computer-aided approaches that have played a key role in combinatorial catalysis and high-throughput experimentation during the last decade - evolutionary optimization and artificial neural networks - are described. The book is unique in that it describes evolutionary optimization in a broader context of methods of searching for optimal catalytic materials, including statistical design of experiments, as well as presents neural networks in a broader context of data analysis.