1. Record Nr. UNINA9910451227003321

Autore	Delamont Sara <1947-, >
Titolo	The doctoral experience : success and failure in graduate school / / Sara Delamont, Paul Atkinson and Odette Parry
Pubbl/distr/stampa	London : , : Falmer Press, , 2000
ISBN	0-203-45140-6 1-280-10616-6 1-135-70142-3 1-138-96788-2
Descrizione fisica	viii, 206 p
Altri autori (Persone)	AtkinsonPaul <1947-> ParryOdette <1954->
Disciplina	378.1550941
Soggetti	Graduate students - Great Britain College teachers - Great Britain Universities and colleges - Great Britain - Graduate work Electronic books.
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Bibliographic Level Mode of Issuance: Monograph
Nota di bibliografia	Includes bibliographic references and index.
Nota di contenuto	1. Cultures of the academy -- 2. Researching our peers -- 3. The nature of the quest -- 4. The appliance of science : laboratory scientists in the making -- 5. Fieldwork -- 6. Modelling realities -- 7. Genealogies and generations -- 8. Supervisors' narratives : Creating a delicate balance -- 9. Pedagogic continuities -- 10. Disciplines and the doctorate.

2. Record Nr. UNINA9910454316703321

Titolo	Support vector machine in chemistry [[electronic resource] /] / Nianyi Chen ... [et al.]
Pubbl/distr/stampa	Singapore ; ; Hackensack, N.J., : World Scientific, c2004
ISBN	1-281-93460-7 9786611934606 981-279-471-9
Descrizione fisica	1 online resource (344p.)
Altri autori (Persone)	ChenNianyi
Disciplina	540.285631
Soggetti	Chemistry - Data processing Chemistry, Technical - Data processing Machine learning Electronic books.
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Bibliographic Level Mode of Issuance: Monograph
Nota di bibliografia	Includes bibliographical references (p. 319-327) and index.
Nota di contenuto	1. Introduction. 1.1. Support vector machine: data processing method for problems of small sample size. 1.2. Support vector machine: data processing method for complicated data sets in chemistry. 1.3. Underfitting and overfitting: problems of machine learning. 1.4. Theory of overfitting and underfitting control, ERM and SRM principles of statistical learning theory. 1.5. Concept of large margin - a basic concept of SVM. 1.6. Kernel functions: technique for nonlinear data processing by linear algorithm. 1.7. Support vector regression: regression based on principle of statistical learning theory. 1.8. Other machine learning methods related to statistical learning theory. 1.9. Some comments on the application of SVM in chemistry -- 2. Support Vector Machine. 2.1. Margin and optimal separating plane. 2.2. Interpretation by statistical learning therory. 2.3. Support vector classification. 2.4. Support vector regression. 2.5 V-SVM -- 3. Kernel functions. 3.1. Introduction. 3.2. Mercer kernel. 3.3. Properties of kernel. 3.4. Kernel selection -- 4. Feature selection using support vector machine. 4.1. Significance and difficulty of feature selection in chemical data processing. 4.2. SVM-BFS - application of wrapper

method and floating search method. 4.3. SVM-RFE: application of optimal brain damage and recursive feature elimination. 4.4. Multitask learning. 4.5. Computer experiments: feature selection of artificially generated data set -- 5. Principle of atomic or molecular parameter-data processing method. 5.1. Two different strategies for structure-property relationship investigation. 5.2. Number of valence electrons of atoms. 5.3. Ionization potential of atoms. 5.4. Atomic radii and ionic radii. 5.5. Electronegativity. 5.6. Charge-radius ratio. 5.7. Topological parameters of molecules and 3-D molecular descriptors. 5.8. Atomic parameters for ionic systems. 5.9. Atomic parameters for covalent compounds. 5.10. Atomic parameters for metallic systems -- 6. SVM applied to phase diagram assessment and prediction. 6.1. Comprehensive assessment and computerized prediction of phase diagrams. 6.2.Atomic parameter-pattern recognition method for phase diagram prediction. 6.3. Prediction of intermediate compound formation. 6.4. Prediction of formation of extended solid solutions. 6.5. Prediction of melting types of intermediate compounds. 6.6. Modeling of melting points or decomposition temperature of intermediate compounds. 6.7. Prediction of crystal types of intermediate compounds. 6.8. Modeling of liquid-liquid immiscibility of inorganic systems. 6.9. SVM applied to intelligent database of phase diagrams. 7. SVM applied to thermodynamic property prediction. 7.1. Significance of estimation of thermodynamic properties of chemical substances. 7.2. Modeling of enthalpy of formation of compounds. 7.3. Modeling of free energy of mixing of liquid alloy systems. 7.4 Prediction of activity coefficient of concentrated electrolyte solutions. 7.5. Regularity of the solubility of C[symbol] in organic solvents -- 8. SVM applied to molecular and materials design. 8.1. concepts of molecular design and materials design. 8.2. SVM applied to new compound synthesis problems. 8.3. SVM applied to the computerized prediction of properties of materials. 8.4. SVM applied to process design for materials preparation -- 9. SVM applied to structure-activity relationships. 9.1. Concept of Structure-Activity Relationships (SAR). 9.2. Brief Introduction to some of chemometric methods used in SAR. 9.3. Brief introduction to molecular descriptors used in SAR. 9.4 SAR of N-(3-Oxo-3,4-dihydro-2H-benzo[l,4]oxazine-6-carbonyl) guanidines. 9.5. SAR of triazole-derivatives. 9.6. SAR of the 5-hydroxytryptamine receptor antagonists. 9.7. QSAR of N-phenylacetamides as herbicides -- 10. SVM applied to data of trace element analysis. 10.1. Trace element science and chemical data processing. 10.2. SVM applied to trace element analysis of human hair. 10.3. SVM applied to trace elements analysis of cigarettes. 10.4. SVM applied to trace element analysis of tea -- 11. SVM applied to archeological chemistry of ancient ceramics. 11.1. SVM applied to archeological data processing. 11.2. Identification of Jun Wares of Song Dynasty. 11.3. Modeling of official Ru Wares. 11.4. Modeling of composition of Yue Wares. 11.5. Modeling of composition of blue and white porcelain samples. 11.6. Archeological research of ancient porcelain kilns. 11.7. Period discrimination of ancient samples -- 12. SVM applied to cancer research. 12.1. SVM applied to cancer epidemiology. 12.2. Carcinogenic and environmental behaviors of polycyclic aromatic hydrocarbons. 12.3. SVM applied to cancer diagnosis -- 13. SVM applied to some topics of chemical analysis. 13.1. Multivariate calibration in chemical analysis. 13.2. Retention indices estimation in chromatography. 13.3. Detection of hidden explosives -- 14. SVM applied to chemical and metallurgical technology. 14.1. Physico-chemical basis of modeling of chemical processes. 14.2. Characteristics of data processing for industrial process modeling. 14.3. Optimal zone: strategy of large

margin search. 14.4. Application of strategy of large margin search. 14.5. Optimal control for target maximization or minimization. 14.6. Optimal control for problem of restricted response. 14.7. Materials properties estimation for production process. 14.8. Comprehensive strategy for industrial optimization.