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Support Vector Machines and Their Application in Chemistry and Biotechnology

Yizeng Liang, Qing-Song Xu, Hong-Dong Li, Dong-Sheng Cao

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Support vector machines (SVMs) are used in a range of applications, including drug design, food quality control, metabolic fingerprint analysis, and microarray data-based cancer classification. While most mathematicians are well-versed in the distinctive features and empirical performance of SVMs, many chemists and biologists are not as familiar with what they are and how they work. Presenting a clear bridge between theory and application, **Support Vector Machines and Their Application in Chemistry and Biotechnology** provides a thorough description of the mechanism of SVMs from the point of view of chemists and biologists, enabling them to solve difficult problems with the help of these powerful tools.

Topics discussed include:

- Background and key elements of support vector machines and applications in chemistry and biotechnology
- Elements and algorithms of support vector classification (SVC) and support vector regression (SVR) machines, along with discussion of simulated datasets
- The kernel function for solving nonlinear problems by using a simple linear transformation method
- Ensemble learning of support vector machines
- Applications of support vector machines to near-infrared data
- Support vector machines and quantitative structure-activity/property relationship (QSAR/QSPR)
- Quality control of traditional Chinese medicine by means of the chromatography fingerprint technique
- The use of support vector machines in exploring the biological data produced in OMICS study

Beneficial for chemical data analysis and the modeling of complex physic-chemical and biological systems, support vector machines show promise in a myriad of areas. This book enables non-mathematicians to understand the potential of SVMs and utilize them in a host of applications.

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