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4.3.1 Largest Principal Components
4.3.2 Discriminatory Principal Components; 4.3.3 Partial Least Squares Discriminatory Analysis Scores; 4.4 Strategies for Data Preprocessing; 4.4.1 Flow Charts; 4.4.2 Level 1; 4.4.3 Level 2; 4.4.4 Level 3; 4.4.5 Level 4; Bibliography; 5 Two Class Classifiers; 5.1 Introduction; 5.1.1 Two Class Classifiers; 5.1.2 Preprocessing; 5.1.3 Notation; 5.1.4 Autoprediction and Class Boundaries; 5.2 Euclidean Distance to Centroids; 5.3 Linear Discriminant Analysis; 5.4 Quadratic Discriminant Analysis; 5.5 Partial Least Squares Discriminant Analysis; 5.5.1 PLS Method
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6.4.4 Q-Statistic or Squared Prediction Error

Sommario/riassunto

Over the past decade, pattern recognition has been one of the fastest growth points in chemometrics. This has been catalysed by the increase in capabilities of automated instruments such as LCMS, GCMS, and NMR, to name a few, to obtain large quantities of data, and, in parallel, the significant growth in applications especially in biomedical analytical chemical measurements of extracts from humans and animals, together with the increased capabilities of desktop computing. The interpretation of such multivariate datasets has required the application and development of new chemometric techniques
