

Application of interactive regularised discriminant analysis to wine data

U. Römisch¹, D. Vandev² and K. Zur¹

¹ TU Berlin, Fak. III, Gustav- Meyer- Allee 25, D- 13355 Berlin

² Univ. of Sofia, Blvd. Bourchier 5, B- 1164 Sofia

Project Steering Committee: R. Wittkowski BfR, Germany, P. Brereton CSL, United Kingdom, E. Jamin Eurofins, France, X. Capron VUB, Belgium, C. Guillou JRC, Italy, M. Forina UGOA, Italy, U. Römisch TUB, Germany, V. Cotea UIASI.VPWT.LO, Romania, E. Kocsi NIWQ, Hungary, R. Schoula CTL, Czech Republic.

Testing the possibility of determination the geographical origin (country) of wines on the base of chemico-analytical parameters was the aim of the European project "Establishing of a wine data bank for analytical parameters for wines from Third countries (G6RD-CT-2001-00646-WINE DB)" supported by the European Commission. Therefore a data base containing 400 samples of commercial and authentic wines from Hungary, Czech Republic, Romania and South Africa has been created. For each of those samples around 100 analytical parameters, among them rare earth elements and isotopic ratios were measured.

Besides other multivariate statistical methods of discrimination and classification the method of regularised discriminant analysis (RDA) was used to distinguish the wines of the different countries on the base of a minimal number of the most important parameters. A MATLAB-program developed by Vandev, which allows an interactive stepwise discriminant model building on the base of an optimal choice of the "nonlinearity" parameter alpha was used. The program will be described shortly and models for authentic and commercial wines with corresponding classification and prediction error rates will be given.

As a result of using RDA the number of analytical parameters could be reduced to the most important necessary parameters (8-9) for recognising the geographical origin of commercial as well as for authentic wines.