

Statistical methods for diagnosis and pattern classification for proteomics mass spectra

B. J. A. Mertens¹

¹ Department of Medical Statistics and Bioinformatics, Leiden University Medical Center, The Netherlands

There is an urgent need in medical science to develop new diagnostic tools for the detection of pathological state, particularly for diseases where either no diagnostic methods are available or when the reliability of existing methods is poor. Research in metabolomic and proteomic science seeks to address this problem by evaluating advanced methods of spectrometry on serum, plasma or urine samples, such as mass spectrometry, nuclear magnetic resonance and other novel forms of spectrometry for the construction of diagnostic procedures. In this presentation, we describe statistical methods for the evaluation of diagnostic potential in early stage case-control feasibility studies using mass spectrometry. As examples, we discuss two studies on the evaluation of serum samples for detection of colon carcinoma which have been run in sequence at the Leiden University Medical Hospital. We present data analysis based on double cross-validatory likelihood estimation for logistic modelling. Extension of the logistic model is presented to take the functional nature of the spectra into account. Results are compared and discussed.