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Multivariate data analysis of biochemical markers of oncological patients

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Computer data handling of the results from laboratory tests creates new opportunities to support the process of diagnosis in laboratory medicine and clinical chemistry. This is an area of laboratory measurements that has brought new elements to the theory of analytical chemistry. Multivariate Data Analysis (MDA) is interdisciplinary branch between chemistry, mathematics and computer science, which deals with an exploratory analysis of the measured data, the classification of measured objects or multivariate calibration. It provides a guideline for chemo-informatics, the way from data to knowledge. More widespread and more used chemo-metrics tools allow to reveal important relations and information in the data, as well as to obtain the data necessary to carry out the decisions, that solve the problem. All outlined statistical methods of MDA applied in data processing to the results from biochemical tests in clinical practice can be generally used to the evaluation of any analytical measurements. The analytically determined biochemical parameters used in the study are: the onco-marker CSI (Carcinoma Serum Index), the inflammation markers CRP (C-Reactive Protein) and PCT (Procalcitonin) as well as further, routine laboratory parameters resolved in the serum. Altogether, 300 samples were gained from 106 patients and were analyzed by a fully automated biochemical analyzer Cobas 6000, Roche Diagnostics, Mannheim, Deutschland, and by hematological analyzer CELLTAC F, Nihon Kohden Corporation, Tokyo, Japan. Principal component analysis and cluster analysis belong to the unsupervised methods, because there is no supervisor in the sense of known membership of objects to classes. Classification methods - linear and quadratic discriminant analysis are supervised methods because the membership of objects to particular cluster is known in advance. All mentioned methods were used for assess the interaction of some markers of inflammation (CRP, Procalcitonin, Leukocyte, etc.) in cancer patients and the grade of malignancies, that were evaluated according to carcinoma serum index (ratio of Orosomuroid and Prealbumin). For the study of inflammatory markers of oncological patients by MDA, following statistical software packages were used: Statgraphics Plus 5.1, Systat 12.0, SPSS 15 and Microsoft Excel 2010. Studied data set consists of 268 cancer patients, 168 men and 100 women who were depending on the extent and severity of disease hospitalized at National Oncological Institute in Bratislava, Department of Surgical Oncology, Internal Medicine Department, Transplantation Unit and Department of Anesthesia and Intensive Care. Diagnostic efficiency was evaluated by means of MDA methods and mutual correlations between observed parameters in patients and suspected illness was specified. For the training data sets and for the validation sets the classification of patients into classes according to extent of disease had good span values (67-94%) for men and women category. After reduction to six variables (Thromb, Prea, Ca, Na, K and Hgb) the most prosperous model with a success rate of 96.0% for classification and cross-validation of 89.0% was obtained by quadratic discriminant analysis for women dataset. The objective of the chemo-metrical data processing, applying mathematical and statistical techniques realized by means of modern software packages, was to discover information, hidden in the measured data series, in order to better understanding of inflammatory processes of oncological patients. The developed multidimensional models based on inflammatory markers enable to predict the category, to which the given patient's sample belongs which help in patient's treatment.

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