One-Class Classifier for Accurate Brain Tissue Classification from Noisy 1H-MRS Spectra

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Target audience: The target audience is those professionally concerned with multivariate signal processing in ^{1}HMRS. This includes researchers from the academic, industrial and medical communities, who are involved in building new techniques.

PURPOSE: Low signal to noise ratio (SNR), baseline distortions, large line-widths and asymmetric line-shapes caused by poor shimming, as well as contaminations caused by significant chemical shift displacement effects produce complicated MRS signals [1]. This study presents a robust soft modeling class analogy (SIMCA) for ^{1}HMRS spectra classification. Applied strategy improves performance of the SIMCA by decreasing its inherent defect characteristics in the classification of noisy measurements [2].

METHODS: Totally 139 spectra from healthy and tomure glial brains –10 healthy cases,11 grade II, 6 grade III, as well as 9 grade IV brain gliomas according to the WHO rules – were collected and used for building and evaluating the SIMCA one-class classifier. All data were acquired according to the medical ethics regulations of the Imam Khomeini Hospital, Tehran, Iran. The MRS spectrawere acquired on a 3T scanner (TimTrio, Siemens, Germany), employing the PRESS (Point-Resolved Spectroscopy) pulse sequence with a short echo-time (STE) of 30 msec, and a signal dimension of 16×16×1 (containing 256 separated spectra). Then the spectra were digitalized by jMRUIV5, and transferred to MATLAB V.7.12 (Math Works Inc.). The preprocessing steps were SNR improvement, Eddy current correction (ECC), water referencing, phase correction, normalization and baseline correction. The SIMCA, PCA, NMF algorithms were developed by in-house programs in MATLAB.

RESULTS:SIMCA was used in two directions; by application of the principal component analysis (PCA) in common rule and by using of the non-negative matrix factorization (NMF) [3]as a robust technique. For assessment of the class membership of external validation set, squared prediction error (Q statistic) was used.Results of robust SIMCA showed significant modification in percentage of correct classified samples as 93.7 vs 86.8 for the general model in an independent test set.For better visualization of samples in selected subspaces by NMF, the projected samples in subspace of each classes were illustrated in **Figure (1)**.

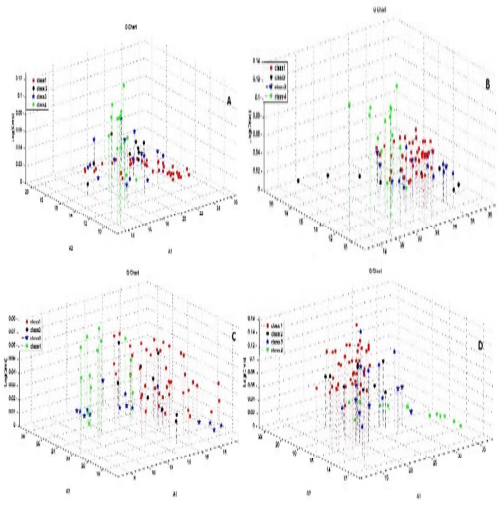

Table (1). Figures of merit of built model by using NMF in SIMCA for independent test set.

FIGURE OF MERIT IN TEST	**CONTROL**	**II**	**III**	**IV**
SENSITIVITY	83.8	66.6	83.3	100
SPECIFICITY	100	94.4	94.7	97.5
PCC(% OF CORRECT CLASSIFIED)	91	92.8	92.9	98.2

Figure (1). 3D Q plot after decomposition of samples in each class samples. The Q statistic geometrically represents the Euclidean distance between the new sample vector and its projection onto the class model.(A:healthygroup,B:grade II, C:grade III,D:grade IV)

DISCUSSION: Presence of the noise degrades the performance of the SIMCA classification algorithm and causes incorrect projection of noisy measurement to their correct sub space. Furthermore, in SIMCA based PCA, the effect of pre-processing is high and the strategies such as normalization or scaling could change data structure. NMF components do not have to be orthogonal in the initial space of data and matches more closely to local data structures. Finally, the non-negativity characteristic of NMF in this application makes it most suitable for deconvolving complex mixtures of metabolites, such as chemicals in ^{1}HMRS of Brain tumours.

CONCLUSION: Noisy characteristics of In-vivo MR spectroscopy makes it difficult to take advantage of the PCA-based classifiers such as SIMCA. In this paper, we proposed a modified and robust version of SIMCA classifier base on NMF .Results showed advantages of NMF for better decomposition of noisy measurements to true basis vectors by proposed one-class classifier. Finally, the prediction ability of the NMF-based SIMCA classifier showed suitable classification for diagnosing and grading of brain tumors.

REFRENCES: :[1] Mountford CE, Stanwell P, Lin A, Ramadan S, Ross B (2010),Chemical reviews 110 (5):3060-3086. [2]Rezghi M (2014),Expert Systems with Applications [3] Lee DD, Seung HS (1999),Nature 401 (6755):788-791