Discriminating glioblastomas from metastases in a SV ^{1}H-MRS brain tumour database

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Introduction

A Feature Selection (FS) process with a simple Machine Learning method, namely the Single-Layer Perceptron (SLP), is shown to discriminate metastases from glioblastomas with high accuracy using single voxel ^{1}H-MRS from an international, multi-centre database of brain tumors. The method has low computational cost and its results are intuitively interpretable.

Subjects and methods

The available data are SV ^{1}H-MR spectra acquired in-vivo from brain tumour patients at short and long echo times (SET and LET). They include 78 *glioblastomas* (WHO 9440/3)) and 31 *metastases* (WHO 8000/6). These were extracted from the web-accessible INTERPRET project database [1]. Clinically-relevant regions of the spectra were sampled to obtain 195 frequency intensity values (data features).

The FS process is based on the hypothesis that irrelevant features produce smaller variations in the values of the predicted outputs of the SLP than relevant ones. Here, the relative relevance of two features was gauged by comparison of the absolute values of the derivatives of the output with respect to the corresponding input of the SLP. A backward selection technique was used as search procedure: starting from the complete dataset, several features were removed at every step. Saliencies were estimated using the complete datasets, and five runs of a 5-fold stratified Cross-Validation (CV) were carried out to estimate generalization performances.

Experimental results

Generalization results are reported in Table 1 for SET, LET, and a combination of both (LET+SET) by straight concatenation of the spectra [2]. SET data achieve the lowest performance. LET, instead, achieve 86.10% accuracy with a parsimonious selection of 8 frequencies and 92.12% with 18. The LET+SET combination slightly increases this performance to 89.14% with only 11 frequencies and 94.48% (an average of only 6 misclassifications) with 27. These results compare favourably with others reported in the literature, although they require further validation with independent test sets. An example of the features selected is shown in Fig.1 for LET+SET. Frequencies corresponding to metabolites such as, for instance, Creatine, mobile lipids and glycine/myoinositol can be clearly identified.

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References

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Data Set	Test	NF	Features Selected
SET	80.33%	22	3.01 3.90 3.88 3.49 2.31 2.23 2.96 3.09 2.98 2.04 2.42 2.32 3.47 2.34 3.24 4.13 4.20 3.55 1.69 0.85 2.57 0.77
SET	74.17%	11	3.90 3.01 2.34 2.98 3.88 2.23 2.31 4.13 2.57 4.20 3.49

Data Set	Test	NF	Features Selected
LET	90.10%	20	2.32 1.83 2.19 1.73 2.99 2.04 2.59 1.04 4.22 3.01 0.69 2.09 1.40 2.08 3.71 3.76 2.02 0.54 1.46 3.48
LET	86.10%	8	2.32 3.01 2.02 3.76 4.22 2.19 1.83 3.71

Data Set	Test	NF	Features Selected
SET+LET	94.48%	27	L2.32 L2.02 L3.01 L0.91 L1.04 L3.42 L2.09 S4.20 L2.55 L0.58 S1.29 S2.32 L2.29 L3.80 L3.55 L4.22 L2.40 S1.60 S3.36 S1.35 S2.17 S2.15 L3.78 L3.07 L1.75 L3.84 L1.90
SET+LET	89.14%	11	L2.02 L2.32 S4.20 L3.01 S2.32 L3.42 L1.04 L4.22 L2.40 L3.55 L3.80

Table 1: Table 1. Classification and FS results for the discrimination of metastases and glioblastomas. For all tables, first column: Data set description; second column: Average test accuracy of 5 repetitions of a a 5-fold cross-validation procedure; third column: Number of features (NF) selected by the algorithm; fourth column: Frequency (in ppm) of the selected features, ranked according to their relative relevance. For the SET+LET data set, the frequencies are preceded by a letter indicating their ascription to either SET (S) or LET (L).

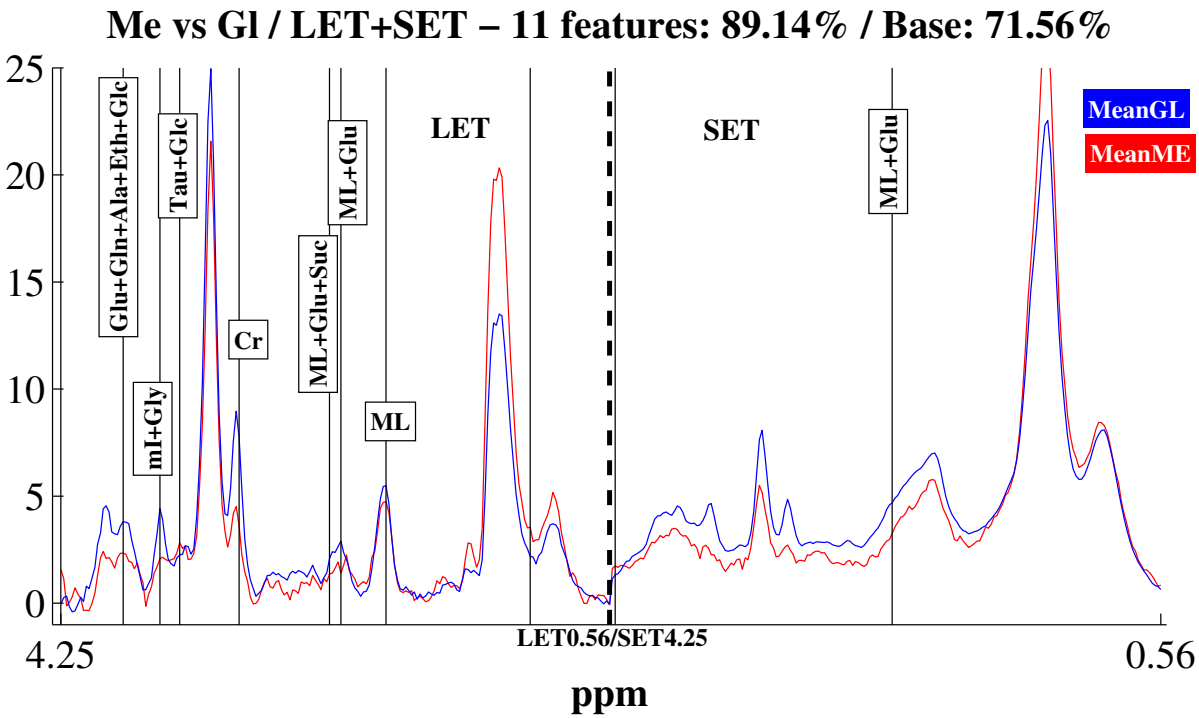

Figure 1: Illustrative representation, as vertical lines, of the subset of 11 selected spectral frequencies from the LET+ SET data set (see Table 1). Some of these have a metabolic interpretation and are labelled in the figure as: Glu+Gln+Ala+Eth+Glc (glutamate, glutamine, alanine, ethanolamine, glucose); mI+Gly (glycine/myoinositol); Tau+Glc (Taurine, glucose); Cr (creatine+Phosphocreatine); and different combinations of ML (mobile lipids) with Glu (Glutamate) and Suc (Succinate). They are superimposed to the mean spectra of glioblastomas (blue) and metastases (red). LET data are displayed on the left and are divided from SET by a thick dashed vertical line. The baseline accuracy on the title corresponds to the prevalence of glioblastomas. The average accuracy of around 89% is slightly unbalanced and corresponds to approximately an average of 93% for glioblastomas and 80% for metastases. This unbalance is much less noticeable for the accuracy for the selection of 27 frequencies described in Table 1, which corresponds to around 96% of glioblastomas and 91% of metastases (an average of 3.3 glioblastomas and 2.7 metastases misclassified).