

**Título:** ON THE USE OF ADVANCED PATTERN RECOGNITION TECHNIQUES FOR THE ANALYSIS OF MRS AND MRSI DATA IN NEURO-ONCOLOGY

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**Resumen:** Cancer is a leading cause of death worldwide. Tumours of the Central Nervous System and, among them, brain tumours have a relatively low incidence as compared to other more widespread cancer pathologies, but the prognosis of some of them is very poor, contributing significantly to morbidity. The clinical management of an abnormal mass in the brain is sensitive and difficult, making experts to rely on non-invasive indirect measurements of the tumour characteristics and growth. In current radiological practice, these data measurements are often provided by magnetic resonance (MR) techniques, such as imaging (MRI) and spectroscopy (MRS). The rich information contained in MR signals makes them ideally suited to the application

of pattern recognition (PR) techniques. Over the last two decades, these techniques have been successfully used to address the problem of knowledge extraction from human brain tumour data, for their diagnosis and prognosis. Nevertheless, the discrimination of some tumour types and subtypes, along with the accurate delimitation of the tumour area, remained challenging.

In this thesis, we approach these challenges using a set of advanced PR techniques. A variety of common and well-known dimensionality reduction (DR), classification, and evaluation methods are first gathered in a software tool, used for the development of classifiers that are suitable for the analysis of MRS data. We then delve into the feature extraction (FE) family of DR methods to propose a method that is robust in the presence of noise, not prone to overfitting, and which also provides interpretation of the extracted MRS signal prototypes. Two spectral decomposition techniques, in different algorithmic variants, are subsequently used to extract the sources of the MRS signals and identify the one that provides better results in the context of neuro-oncology, using single-voxel (SV) MRS data. The best and most adequate source extraction method is then used to derive sources correlated with the mean spectra of known tissue types. Its accuracy for class assignment when sources are used directly for classification is assessed, as well as when used for DR prior to classification. The former, an unsupervised approach, is also applied in this thesis in the multi-voxel (MV) context, where we propose a mechanism for delimiting the pathological area of the tumour.

The contributions of this thesis can be summarised as follows. First, the development of a software tool allowed us to reproduce previously published MRS-based classifiers, and test new hypotheses that led to new publications. We also contributed a FE method, whose performance is comparable to its most commonly used counterpart in MRS data analysis, while improving on the interpretability. Moreover, we identified, after an exhaustive evaluation, the spectral decomposition variant that best suits the analysis of SV MRS data, namely Convex Non-negative Matrix Factorisation (NMF), and showed its ability to discriminate between healthy tissue, necrosis, and actively proliferating tumour, with results that are comparable to those obtained in fully supervised mode. The use of the extracted sources for DR leads to simple classifiers with independent test performances that are comparable with, and are often better than, previously described strategies. For MV data, we successfully benchmarked alternative spectral decomposition methods, and provided evidence supporting that very accurate delimitation can be achieved through the application of Convex-NMF.

With this thesis, we provide spectroscopists with a tool that facilitates the development of classifiers for the analysis of MRS data, for a large group of tumour types; allowing them to concentrate on the interpretation of the results, without requiring a specialised mathematical expertise for testing their hypotheses. We also provide an unsupervised alternative to improve the discrimination between tumour types and subtypes, placing this approach one step ahead of classical label-requiring supervised methods for detection of the increasingly recognised molecular subtype heterogeneity within human brain tumours. This also allowed us to accurately tackle one of the main sources of uncertainty in the clinical management of brain tumours, which is the difficulty of appropriately delimiting the pathological area.