Feature Selection in Proton Magnetic Resonance Spectroscopy Data of Brain Tumors

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Outline

1. **1H-MRS Spectroscopy**
   - 1H-MRS Proton Magnetic Resonance Spectroscopy

2. **Class-Separability Feature Selection**
   - A distinctive aspect
   - The Algorithm

3. **Experimental Settings**
   - The Data Set
   - The Addressed Problem
   - Experimental Conditions

4. **Results**
   - Feature Selection - XVAL
   - Visualization

5. **Conclusions**
   - Conclusions
Is a non-invasive technique that provides information about the biochemical profile of brain tissue

Figure 1: $^1$H-MRS Fundamentals. Image source:
http://www.chem.ucalgary.ca/courses/351/Carey/Carey.html
Figure 2: $^1$H-MRS example.
Metabolites

- Meningiomas NAA = ∅, Choline =↑

- Metastases Creatine =↓

- High–Grade tumors Lipids =↑
The Class-Separability Feature Selection Algorithm (CSFS)

1. Calculate distance value for each metabolite.

<table>
<thead>
<tr>
<th>Metabolites</th>
<th>1</th>
<th>…</th>
<th>m</th>
</tr>
</thead>
<tbody>
<tr>
<td>Class 1</td>
<td>$\bar{X}_{1,1}$</td>
<td>$\bar{X}_{1,\ldots}$</td>
<td>$\bar{X}_{1,m}$</td>
</tr>
<tr>
<td>Class 2</td>
<td>$\bar{X}_{2,1}$</td>
<td>$\bar{X}_{2,\ldots}$</td>
<td>$\bar{X}_{2,m}$</td>
</tr>
<tr>
<td>Class 3</td>
<td>$\bar{X}_{3,1}$</td>
<td>$\bar{X}_{3,\ldots}$</td>
<td>$\bar{X}_{3,m}$</td>
</tr>
</tbody>
</table>
The Class-Separability Feature Selection Algorithm (cont.)

2. Separability degree for each metabolite.

\[ DS_i = \sum_{j \neq k} |\bar{x}_{j,i} - \bar{x}_{k,i}| \]

3. Sort \( DS_i \) in descending order.

4. \( DS_i \) feeds a Forward-Backward Search.

5. All computations are bootstrap averages.
The Data Set

Single voxel $^1$H-MR spectra acquired *in vivo* from brain tumor patients

LTE (PRESS 135–144 ms): 195 cases with 55 meningiomas, 78 glioblastomas, 31 metastases, 20 astrocytomas grade II, 6 oligoastrocytomas grade II and 5 oligodendrogliomas grade II

STE (PRESS 30–32 ms): 217 cases with 58 meningiomas, 86 glioblastomas, 38 metastases, 22 astrocytomas grade II, 6 oligoastrocytomas grade II, and 7 oligodendrogliomas grade II

LSTE: the merged LET and SET data, with 195 cases

195 frequency intensity values, from 4.21 ppm → 0.51 ppm

International Network for Pattern Recognition of Tumors
Using Magnetic Resonance *INTERPRET*
Three Super-classes

1. High-grade Gliomas.
2. Low-grade Gliomas.
3. Meningiomas.
The LTE, STE and LSTE data. The three super-classes.

The median metric is used.

Forward-Backward selection in wrapper mode

Trained Six classifiers: NN, LDC, QDC, LR, ISVM, rSVM by 10x10 cross validation on the original data sets.
<table>
<thead>
<tr>
<th></th>
<th>NN</th>
<th>LDC</th>
<th>QDC</th>
<th>LR</th>
<th>ISVM</th>
<th>rSVM</th>
</tr>
</thead>
<tbody>
<tr>
<td>LTE</td>
<td>89.70</td>
<td>93.51</td>
<td>89.09</td>
<td>91.48</td>
<td>91.82</td>
<td>93.88</td>
</tr>
<tr>
<td>STE</td>
<td>92.21</td>
<td>93.34</td>
<td>87.40</td>
<td>90.48</td>
<td>93.14</td>
<td>94.48</td>
</tr>
<tr>
<td>LSTE</td>
<td>96.14</td>
<td><strong>98.27</strong></td>
<td>92.83</td>
<td>92.07</td>
<td>94.83</td>
<td>94.77</td>
</tr>
</tbody>
</table>

**Table 1**: CSFS Feature selection results and final performance. The number in square brackets is the final Best Spectral Subset (BSS) size. The right number is the averaged 10x10 CV accuracy in the original (continuous) $^1$H-MRS datasets.
**Figure 3**: Best Spectral Subset from LSTE-LDC model as positioned in the whole spectrum.
Figure 4: Projection of the dataset (using the final selected feature subset of the best LSTE-LDC model) onto the first two eigenvectors of the scatter matrices as coordinate system. Circles represent low-grade gliomas; filled squares high-grade malignant tumors and stars meningiomas.
The proposed algorithm takes advantage of the differential presence of certain metabolites.

It also accounts for possible redundancies.

A competitive model w.r.t. other solutions in the literature.
The “Best” Subset: It is extremely unlikely that it is found by a search process.

This study confirmed that the LSTE combination renders better subsets in classification accuracy.

Linear models are among the best suited for the task.
Most of the identified metabolites are positively defined by the medical literature.

Some concordances are found with successful recent machine learning works.