A Visual Encoding System for Comparative Exploration of Magnetic Resonance Spectroscopy Data

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Abstract

Magnetic resonance spectroscopy (MRS) allows for assessment of tissue metabolite characteristics used often for early detection and treatment evaluation of intracranial pathologies. In particular, this non-invasive technique is important in the study of metabolic changes related to brain tumors, strokes, seizure disorders, Alzheimer's disease, depression, as well as other diseases and disorders affecting the brain. However, meaningful variations in ratios of tissue metabolites within a sample area are difficult to capture with current visualization tools. Furthermore, the learning curve to interpretation is steep and limits the more widespread adoption of MRS in clinical practice. In this work we present a novel, tiered visual encoding system for multi-dimensional MRS data to aid in the visual exploration of metabolite concentration ratios. Our system was developed in close collaboration with domain experts including detailed data and task analyses. This visual encoding system was subsequently realized as part of an interactive insight-generation tool for rapid exploration and comparison of metabolite ratio variation for deeper insights to these complex data.

CCS Concepts

• ***Human-centered computing*** → ***Scientific visualization; Information visualization;*** *User centered design;*

1. Introduction

Magnetic resonance spectroscopy (MRS) is an in vivo non-invasive biochemical imaging technique utilized for tissue metabolite characterization used often for early detection and treatment evaluation of tumors and neuropsychiatric conditions. While magnetic resonance imaging (MRI) produces a stack of high-resolution anatomical images, MRS produces a static or time-resolved spectral graph of localized metabolite concentrations. As it is extremely sensitive to subtle tissue composition changes, clinical researchers have begun to explore MRS as a tool for tracking metabolite variation over time, space, and across individuals [VDG10]. Although promising, MRS has not yet been widely implemented in clinical practice: acquisitions are highly variable with a steep learning curve to interpretation, and understanding the success of a given acquisition and subsequently extracting meaningful information requires extensive prior knowledge and is frequently time-consuming [PODA13]. The richness of these data furthermore presents challenges in a clean presentation without clutter or occlusion. In clinical research settings these challenges are unmet in current visualization tools – it is impossible to interactively compare relative metabolite concentrations across individuals or time, or to clearly see how much influence outlier data have on metabolite values in a cohort. Achieving this degree of insight is critical to understanding what each piece of the data contribute to the entire study. Visualization research in MRS data is a largely unexplored area – the few applications developed in this area have relatively narrow focus, utilizing basic scatterplots and parallel coordinate plots to show patterns in the data. Options for visualizing metabolite ratios on both an aggregate and individual basis are furthermore limited in these systems [NLK*14]. In developing our visual system we drew inspiration from table visualization techniques such as PivotTable [STH02] and the Atom unit visualization grammar [PDFE17] to represent key dimensions in MRS data. In this work we propose a taxonomy of visual encodings to represent the range of different metabolite concentration ratios at different dimensional tiers. We subsequently used this system to realize a novel MRS visualization tool, developed iteratively in close coordination with domain experts, and validated with two case studies to provide early evidence for the utility of our visual system in MRS data analysis.

2. Visual Encoding System

Our visual taxonomy for MRS data attributes is framed around spectral metabolite concentration ratios. Because spatial resolution of metabolic spectra is low, we opt for an abstract visual presentation of metabolite spectra, effectively trading spatial resolution for a higher resolution abstract data space. To visualize metabolite concentrations as ratios, we orient spectra along an x- and y-axis and discretize each continuous spectrum to produce a 20 by 20 cell table. Each cell corresponds to the ratio of averaged spectral

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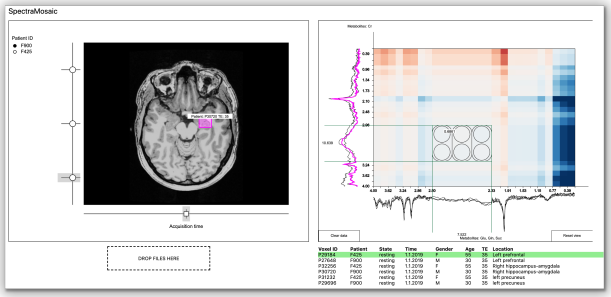

Figure 1: *SpectraMosaic supports exploration and comparison of magnetic resonance spectroscopy (MRS) metabolite ratios within a cohort between different voxel positions, over time, and between different brain stimulation states. The tool utilizes a two-panel view; the left panel allows for loading and selection of spectral voxels, while the right permits rapid visual comparison of mean metabolite concentration ratios as a heatmap. Interesting areas may be expanded for more detailed exploration of individual voxel ratio values.*

Case	patient	voxel	time pt	state	encoding
1	single	single	single	single	
2	single	single	single	dual	
3	single	single	multiple	single	
4	single	single	multiple	dual	
5	single	multiple	single	single	
6	single	multiple	single	dual	
7	single	multiple	multiple	single	
8	single	multiple	multiple	dual	

Case	patient	voxel	time pt	state	encoding
9	multiple	single	single	single	
10	multiple	single	single	dual	
11	multiple	single	multiple	single	
12	multiple	single	multiple	dual	
13	multiple	multiple	single	single	
14	multiple	multiple	single	dual	
15	multiple	multiple	multiple	single	
16	multiple	multiple	multiple	dual	

Figure 2: *All 16 possible permutations of MRS case studies handled by our visual encoding system. Key attributes fall under four main categories: cohort size, number of voxels sampled, number of acquisition runs, and number of states under which spectroscopy was acquired. Each case shows a sample cell visualization using our system.*

tile integrals along the respective axes and color coded with a diverging color map (Figure 1). Within each cell we define a nesting structure for spectral concentration ratios, inspired by dimensional stacking visualization techniques pioneered in Xmdvtool and N-land by Ward et al. [War94, WLT94]. Given the importance of location in spectral samples we consider the voxel as the outermost contextual layer, followed by patient, then state, and finally time point, as shown in Figure 2. Each MRS attribute receives a consistent visual encoding in the form a simple glyph. We represent voxels as pill box glyphs, and in each unit cell evenly divide the space vertically. Patients are presented as filled disks when only shown in a single time acquisition (e.g., case 1), but expand into rounded squares when time series data are incorporated (e.g., case 3). This shape change is to permit a time spark line to move evenly across a space, rather than extend past or be cropped out by the fully rounded disk shape. Disks resize automatically to fill space optimally within their voxel frame to maximize pixel screen space. In instances where different brain states (active versus resting) are analyzed we break the patient disk/square horizontally in half, and for further clarity use an analogous color to encode this attribute (e.g., case 2). We choose an analogous color rather than continuing with the same hue in an effort to differentiate state as a unique attribute from patient or voxel, since the shapes used for those two attributes are quite similar. Finally, we encode time steps as points connected via a spark line nested into the relevant glyph (e.g., case 7). The remaining 16 cases comprise different permutations of these patient, voxel, state, and time arrangements.

We realized this visual encoding system in a novel web-based visualization tool for the interactive exploration of MRS metabolite concentration ratios using HTML, CSS, p5.js and gridster.js. The tool utilizes a two-panel view, one for upload and selection of study voxels and a second for analysis of metabolite ratios using the previously described system of encodings. Study data are loaded as file packages using a drag and drop interface, then image data are read and converted to p5 images displayed in the left view panel (Figure 1). Clicking and dragging voxel(s) of interest to the right panel generates a spectral heatmap cell table showing calculated mean metabolite concentration ratios for all 20 by 20 spectral tile segments. Expanding a cell (Figure 1, right panel) allows for detailed exploration of contributing metabolite ratio values for that cell. We use a D3 diverging color mapping function to map color to ratio values at both overview and detail view levels.

We tested this application in two case studies with a small pool of domain experts: the first study compared ratio differences in spectral acquisitions with different echo times for a single patient, while the second study allowed for similarity assessment of ratios for voxels collected from different sample locations in the brain for two patients. Study feedback was positive and encouraging for continued work – users found the tool intuitive and useful for comparing spectra, especially in instances of small differences.

3. Conclusions

We have developed a novel visual encoding system for selected MRS data attributes using simple glyph shapes with diverging color maps to represent variation. We have implemented this system in a spectral visual analysis tool, and plan to continue working with domain experts to extend our visual system to address larger cohorts with possibilities for automatic or user-created groupings. We furthermore plan to explore explicit visual encodings for additional data attributes, as well as implementing uncertainty into our visual idioms.

4. Acknowledgements

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References

[NLK*14] NUNES M., LARUELO A., KEN S., LAPRIE A., BÜHLER K.: A survey on visualizing magnetic resonance spectroscopy data. In *Proceedings of the Eurographics Workshop on Visual Computing for Biology and Medicine* (2014), pp. 21–30. doi:10.2312/vcbm.20141180. 1

[PDFE17] PARK D., DRUCKER S., FERNANDEZ R., ELMQVIST N.: Atom: A grammar for unit visualizations. *IEEE Transactions on Visualization and Computer Graphics 24*, 12 (2017), 3032 – 3043. doi:10.1109/TVCG.2017.2785807. 1

[PODA13] POSSE S., OTAZO R., DAGER S. R., ALGER J.: MR spectroscopic imaging: Principles and recent advances. *Journal of Magnetic Resonance Imaging 37* (2013), 1301–1325. doi:10.1002/jmri.23945. 1

[STH02] STOLTE C., TANG D., HANRAHAN P.: Polaris: A system for query, analysis, and visualization of multidimensional relational databases. *IEEE Transactions on Visualization and Computer Graphics 8*, 1 (2002), 52–65. doi:10.1145/1400214.1400234. 1

[VDG10] VAN DER GRAAF M.: In vivo magnetic resonance spectroscopy: Basic methodology and clinical applications. *European Biophysics Journal 39*, 4 (2010), 527–540. doi:10.1002/9780470882221. 1

[War94] WARD M. O.: Xmdvtool: integrating multiple methods for visualizing multivariate data. In *Proceedings of the Conference on Visualization* (1994), IEEE Computer Society Press, pp. 326–333. doi:10.1109/visual.1994.346302. 2

[WLT94] WARD M., LEBLANC J. T., TIPNIS R.: N-land: a graphical tool for exploring n-dimensional data. In *Proceedings of Computer Graphics International Conference* (1994), pp. 131–141. 2