MRSight: Ratio-Weighted Complete and Visibility Graphs for MRS Data Visualization and Assessment

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Abstract

Magnetic resonance spectroscopy (MRS) is a non-invasive technique that offers crucial biochemical insights into tissue health, particularly with 31P-MRS, which is vital for studying cellular metabolism. Despite its clinical value, interpreting MRS data is challenging due to its complexity and the limitations of current visualization tools. This paper presents MRSight, an interactive visualization tool that addresses these challenges by transforming 31P-MRS data into graph-theoretic models where nodes, edge, and weights represent metabolites, their interactions, and the relative intensity ratio values, respectively. Three model types are explored: complete metabolite graphs, horizontal visibility graphs, and natural visibility graphs. Visualizing these models enables intuitive exploration of metabolite relationships and ratio values. Interactive features, such as subject comparison and dynamic filtering, are integrated to facilitate a more efficient and insightful analysis. Moreover, global and local graph features are computed to provide further insights into MRS analysis. This tool collectively provides a clearer, network-based view of 31P-MRS, augmenting traditional workflows for both research and clinical applications.

Index Terms: Magnetic resonance spectroscopy, visibility graph, information visualization, network science, user centered design.

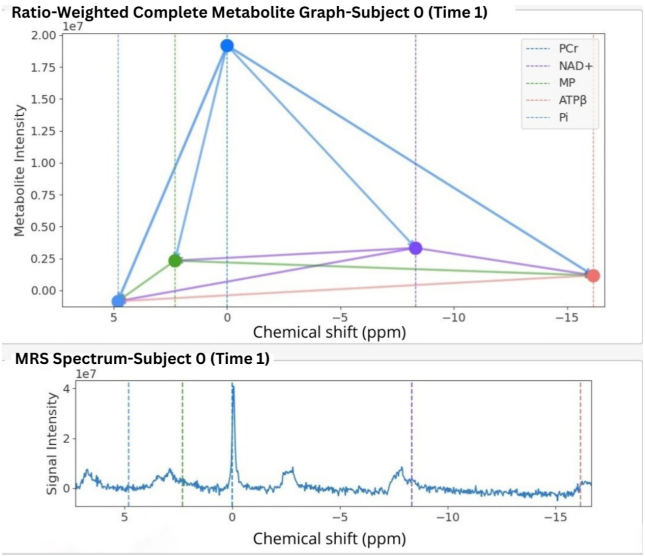

Figure 1: A ratio-weighted metabolite graph of a MRS signal.

1 Introduction

Neurological conditions are a leading cause of global disability, and early detection of these conditions is crucial for better patient outcomes. Magnetic resonance spectroscopy (MRS) is a noninvasive technique that provides biochemical information about tissues that may not be visible in standard MRI scans. Specifically, 31P-MRS is valuable for its ability to measure biomarkers related to cellular metabolism and oxidative stress [2].

The main barrier to widespread clinical adoption of MRS is the difficulty of interpreting its data. An MRS scan produces a complex spectral signal with multiple peaks representing different metabolites. Current clinical tools offer limited visualizations, making it hard to identify metabolites and understand their relationships or compare data across subjects [1]. This paper presents MRSight, a new tool that applies network science principles to visualize 31P-MRS data, addressing key challenges in analysis and interpretation.

2 Related Work

Prior research has attempted to tackle MRS visualization challenges. Nunes et al. [3] surveyed the field, highlighting the limitations of existing clinical tools that often rely on simple visualizations like histograms and overlaid maps. Garrison et al. [1] introduced SpectraMosaic for 1H-MRS, a tool that uses a heatmap with nested glyphs to compare metabolite ratios across cohorts. While effective for cohort-based analysis, this method focuses on aggregated data rather than the direct structure of the spectral signal. Our work is inspired by network science, particularly the use of complete graphs and visibility graphs (VG) for time series analysis. For visibility graphs, a linear sequence of data points is transformed into a network, where nodes represent data points and edges are determined by a visibility criterion. Variations like the natural visibility graph (NVG) and the horizontal visibility graph (HVG) capture different aspects of the topological and temporal data properties [6]. We adapt this powerful approach to create three types of novel graph-theoretic visualizations for 31P-MRS data.

3 Methods: The MRSight Tool

MRSight [1] is a Python-based tool built with PyQt5 and Matplotlib for the user interface and visualization components. It processes 31P-MRS data to create interactive network visualizations based on a novel application of visibility graphs.

3.1 Visibility Graph Construction

The core of our visualization approach is the representation of MRS data as a graph. We treat the spectral peaks, which correspond to metabolites, as nodes in a network. The connections between these nodes (edges) and their weights are determined by a visibility algorithm, where the height of each "bar" in the time series is the

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[1] https://github.com/Ahmed-Hajhamed/MRSight-public

metabolite's signal intensity. The tool provides three distinct types of graphs to cater to different analytical needs.

3.1.1 Complete Metabolite Graphs

In a complete metabolite graph, every metabolite node is connected to every other metabolite node. The presence of other non-metabolite peaks is ignored, and each edge weight is simply the ratio of the signal intensities of the two connected metabolites. This view allows for a raw, unfiltered comparison of all possible metabolite pairs (Figure 1).

3.1.2 Natural and Horizontal Visibility Graphs

For a natural visibility graph (NVG), an edge exists between two nodes only if a line of sight can be drawn between their corresponding peaks without being intersected by any intermediate peak [6]. This approach captures both local and global relationships in the spectrum. A horizontal visibility graph (HVG) is a more constrained variant where a connection is only established if a horizontal line can be drawn between two peaks without being blocked by an intermediate peak of greater height [6]. Since the x-axis for chemical shifts runs in reverse (from higher to lower ppm values), the implementation connects nodes from right to left, stopping when an obstacle is encountered. This focuses the analysis on localized relationships. The weight of each edge is again set as the ratio of the signal intensities of the two connected metabolites. This provides an intuitive measure of their relative ratios.

3.1.3 Representational and Biological Significance

The visibility graphs (VGs) offer several representational advantages. First of all, VGs preserve the spectral ordering and the local geometry of the MRS signals [6]. Second, VGs are invariant under affine transformations, and this makes them suitable for comparing MRS signals across different subjects, sessions, and conditions. Moreover, the horizontal VGs are particularly robust to noise. Third, the expressiveness of the VG representations can be captured via different graph metrics [4].

From a biological perspective, VG metrics can be correlated with clinical insights on MRS data [2]. For example, degree distribution can be used to differentiate between regular and chaotic metabolite behavior. A clustering coefficient can indicate co-occurrences of metabolite shifts. Graph entropy can reflect the MRS signal complexity in neurodegeneration. Also, community detection can be used to group metabolite states and transitions. Indeed, VGs have been already exploited in the analysis of some types of medical data, e.g., fMRI [5].

3.2 Interactive Features

For comprehensive and flexible analysis, the MRSight tool includes the following interactive features.

Dynamic Comparison: Users can compare the metabolic profiles of two subjects by overlaying their respective graphs in a dedicated visualization panel. This allows for easy identification of differences in metabolite concentrations and network topology.

Node and Edge Highlighting: Double-clicking on a node (metabolite) highlights all its connected edges and hides all others, providing a focused view of its relationships within the network. Conversely, a double-click on an edge highlights or unhighlights that specific connection, enabling a deeper look into a particular metabolite-ratio pair.

Metadata Integration: Hovering the mouse over an edge displays a tooltip showing the ratio value, and the source and target metabolites. We have also integrated a "brain connectivity" feature using the *bctpy* library [4]. When a checkbox is enabled, hovering over a node displays its local features, and a global feature summary is shown for both the primary and secondary subjects.

Customization and Filtering: A list of all metabolites with corresponding checkboxes allows users to dynamically include or exclude metabolites from the network. This is useful for refining hypotheses and focusing on metabolites of specific clinical interest.

4 Results and Discussion

We evaluated MRSight with a synthetic 31P-MRS dataset of 18 spectral outputs from 9 subjects, each with two time points. The tool's network-based approach immediately provided a clear and intuitive data representation, surpassing what conventional spectral plots typically offer. By representing metabolites as nodes and ratios as edge weights, the tool bypasses the steep learning curve of interpreting raw spectral peaks and allows researchers to directly engage with the relationships between metabolites. For instance, a clinician interested in changes in phosphocreatine (PCr) relative to other metabolites could use the tool to select PCr as a central node. The resulting star-like graph would immediately visualize the ratios of PCr to all other metabolites, with edge thickness representing the weight (ratio value). By switching between the different visibility graph types, the user can filter out noise and focus on more significant relationships. A comparison of the graphs of two subjects quickly reveals differences in metabolite ratios. The ability to overlay graphs of two subjects further enhances this comparison, making it easy to spot discrepancies that might be indicative of a pathological state or treatment response. The integration of the brain connectivity features within the MRSight interface also allows researchers to contextualize metabolic changes with global and local network properties, a functionality that is currently not available in most clinical tools. This provides a more holistic data view, linking biochemical changes to higher-level network metrics.

5 Conclusion and Future Work

We have demonstrated a novel approach for visualizing 31P-MRS data using weighted visibility graphs. The MRSight tool provides an intuitive, interactive platform for clinicians and researchers to explore metabolite relationships and ratios, addressing the key challenges of data interpretation and comparison. By transforming spectral signals into network structures, this method facilitates a new level of analysis that can augment traditional workflows and accelerate the process of identifying key biomarkers for neurological conditions. Future work will focus on expanding this approach to other MRS modalities and incorporating features for longitudinal analysis and statistical validation.

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