

Blind Removal of Lipids in ^1H MRSI Using Constrained Non-Negative Matrix Factorization

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Introduction

In vivo MRSI allows non-invasive characterization and quantification of molecular markers of potentially high clinical utility. However, in whole brain ^1H MRSI, incomplete suppression of intense resonances due to tissue water and lipids can often adversely affect the ability of the technique to yield diagnostic information contained in lower concentration metabolites such as N-acetyl-aspartate (NAA) and lactate. With the increasing demand for clinical MRSI scans, there is a need for MRSI spectral processing methods that can automatically rid *in vivo* MRSI of residual water and lipid resonances after acquisition to maximize the quality of the derived clinical information. Here, we describe a novel approach, based on non-negative matrix factorization (NMF)^{[1][2]}, for automated removal of residual lipids and water from human brain ^1H MRSI data. The technique assumes that each sample is as a mixture of tissue types, with individually associated basic spectral shapes, so that each spectrum is a sum of varying amounts of these basic spectra. Both the spectral shapes and their magnitudes are simultaneously determined. The results show that this technique uncovers the spectral patterns and distributions of different types of tissue, such that those that are associated with residual water and lipids can be separated and then removed from brain tissue spectra.

Methods

We seek a representation of the original data-matrix as a mixture of several constituent spectra. Let X be a spectral data-matrix, containing in its rows N voxels, L spectral points in its columns. Two matrices are desired to be determined simultaneously: A and S , such that their product reconstructs X given noise in the data. Each row of S is seen as M constituent spectra with the columns in A representing the mixing coefficients, corresponding to the concentration, or abundance of the constituent material. Our long TE MRSI protocol is such that A and S are constrained to be non-negative. Given that the noise in the data can be modeled as Gaussian, one can formulate the problem as a maximum likelihood estimation. The NMF algorithm constructs a gradient descent over the objective function of negative log-likelihood with optimizing A and S . Lee and Seung^{[1][2]} formulate multiplicative update rules for A and S , which can ensure non-negative A and S , given all spectral data X non-negative and both A and S are initialized non-negative. However, due to noise, X can have negative values and since they are used in updating A and S a possible solution may contain negative values. We have extended NMF to include a positivity constraint on the value of the recovered spectra and mixing matrices. Recovered source spectra are analyzed given prior knowledge about the spectral signatures (i.e., spectra for brain versus pericranial lipids) and their spatial distributions (location of the brain/lipids in the image and its approximate shape). A mask is generated on the spatial mapping of the brain-like spectra and only voxels through this mask are considered having brain signal, while other voxels are filtered out thus removing residual lipids and water from the original data.

Experiments and Results

cNMF is demonstrated by experimental results of 2 cases of human brain ^1H MRSI data, showing how the approach removes residual lipids and water from a 32-by-32 ^1H MRSI data set of a “whole” human brain. In the two cases source component number is set to 4 by principal component analysis (PCA), which is consistent with physiology of head having 3-4 primary tissues: brain, lipids and water. By integrated analysis of the spectra pattern and their corresponding spatial concentration distribution maps, we can find only one source component spectrum is brain-like, while the others are probably lipids and water. Thus by thresholding the spatial map corresponding to the selected brain-like spectrum, a 32-by-32 (same resolution as original dataset) mask can be generated, only voxels through the mask are thought brain signal containing, while other voxels are filtered out as residual lipids and water that should remove.

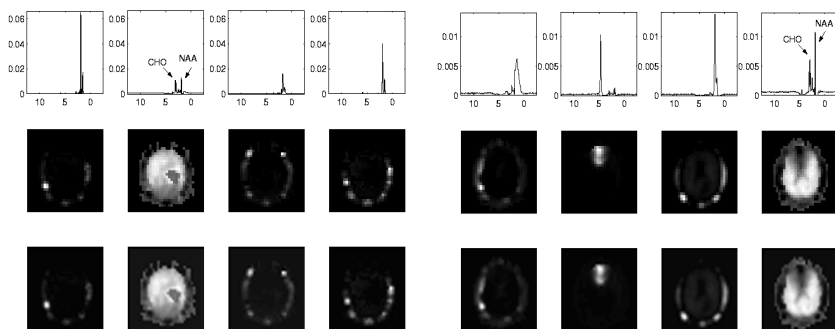


Figure 1. cNMF spectra recovery results of two ^1H MRSI cases. The first row is the recovered spectra, second row is the spatial distribution of each recovered spectra and the third row is an upscaled version of the spatial distribution for visualization. **Left Panel:** Clearly the column 2 spectrum is with biochemical markers for brain: peaks for choline (CHO, single peak at 3.22ppm) and N-acetyl-aspartate (NAA, single peak at 2.02ppm) and the column 1, 3 and 4 spectra are with biochemical markers of lipids (single peak around 0.9-1.3ppm). **Right Panel:** Column 4 spectrum is consistent with biochemical markers for brain: peaks for CHO and NAA, while column 1 and 3 spectra are probably lipids, and column 2 spectrum of water (single peak at 4.7ppm). The corresponding spatial

mappings consistently map the brain-like spectrum to the region of the brain in the center of the image, the water-like spectrum in the **Right Panel**, column 2 to the position of sinuses of head and other spectra to the region of lipids around brain like a ring.

Conclusion

We present a fast maximum likelihood algorithm, cNMF, that blindly separate source spectra in MRSI given “noisy” magnetic resonance spectra which may have negative observations. By integrating analysis of recovered source spectra and spatial distributions, a mask can be generated by thresholding the mapping of brain-like spectrum and thus to filter out residual lipids and water from head data while keeping voxels containing brain signals for further analysis.

References

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