

Unsupervised anomaly detection using generative adversarial networks in 1H-MRS of the brain

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Introduction

The potential applicability of deep learning in ¹H-MRS(I) has been well demonstrated for quality management^{1,2} as well as quantification^{3,7}. For supervised deep learning-based binary classification of spectral quality^{1,2}, the training sets for the two classes need to be prepared with precise labels and a sufficient amount of examples, and in comparable amounts for optimal training^{1,8}. Given the broad ranges of spectral abnormalities³, therefore, the binary classification of spectral quality in a supervised manner could become challenging as one extends the regime of abnormal spectra. We investigated the potential applicability of generative adversarial networks (GANs⁹) capable of unsupervised anomaly detection (AnoGAN¹⁰) in the management of quality of human brain spectra at 3.0T. The AnoGAN was trained in an unsupervised manner solely on simulated normal brain spectra and used for filtering out abnormal spectra with diverse abnormalities including abnormal SNR, linewidth and metabolite concentrations and spectral artifacts such as ghost, residual water, and lipid.

Methods

Brain Spectra Simulation: The brain spectra were simulated using 17 metabolite basis spectra obtained in phantom and spectral baselines modeled with 9 resonance groups^{6,11-16}. Normal brain spectra were simulated for training (Spec_{train}, N = 100,000) by randomly varying the relative metabolite concentrations and baseline resonances, SNR, and linewidth within the predefined normal ranges. In addition, 2,000 normal spectra (Spec_{norm}) were simulated and used as a validation and a test sets (N = 1000 for each set). For abnormal spectra, various groups of spectra were simulated, which were abnormal due to: (A) low SNR (Spec_{ano.SNR}), (B) broad linewidth (Spec_{ano.LW}), (C-F) high and low concentrations of (C) GABA (Spec_{ano.GABA}), (D) ml (Spec_{ano.ml}), (E) NAA (Spec_{ano.NAA}), (F) 9 metabolites of Cr, GABA, Gln, Glu, GSH, Lac, ml, NAA, and Tau (Spec_{ano.multimeta}), and (G) low SNR, broad linewidth, and high and low concentrations of the 9 metabolites (Spec_{ano.all}). For each of these 7 abnormal spectra groups (A) through (G), 1000 spectra were simulated and used as a test set. For Spec_{ano.all}, additional 1000 spectra were simulated and used as a validation set. Finally, abnormal spectra contaminated with (H) ghost, (I) residual water, or (J) lipid were simulated (N = 1000, 500, and 1000, respectively).

AnoGAN: We employed an AnoGAN, which is capable of detecting unseen abnormalities in each of the input data based on a reference data obtained from AnoGAN by latent space mapping¹⁰. The AnoGAN was designed and trained solely on Spec_{train} using Matlab deep learning toolbox.

Anomaly Detection: Assuming that a given query spectrum is abnormal, the AnoGAN tries to generate a spectrum that is as close to the query spectrum as possible, but is still belonging to normal spectra, because the AnoGAN was trained solely on normal spectra. Therefore, as the deviation of the query spectrum from the normal regime is large, so is the difference between the query and the AnoGAN-generated spectra. The actual binary classification of a query spectrum into either normal or abnormal is achieved quantitatively based on the normalized mean squared error (NMSE) between the query and the AnoGAN-generated spectra and the 2 x standard deviation (2SD) of the noise measured from the query spectrum. The optimal threshold values of the NMSE and 2SD that differentiate best between normal and abnormal spectra were predetermined from the validation sets of Spec_{norm} and Spec_{ano.all}, and then used for the test sets of Spec_{norm} and all abnormal spectra groups for the evaluation of the performance of the AnoGAN. The abnormality of the query spectrum is directly visualized by the residual spectrum between the query and the AnoGAN-generated spectra¹⁰.

Results

The classification accuracy was over 80% for Spec_{ano.SNR}, Spec_{ano.NAA}, Spec_{ano.multimeta}, and Spec_{ano.all}. Despite the fact that they have never been involved in the training or optimization of the AnoGAN, those spectra contaminated with ghost, residual water or lipid can be correctly classified as abnormal regardless of the types of the artifacts, depending solely on their intensity. The proposed method was not sensitive enough to precisely detect abnormal linewidth and abnormal levels of a single metabolite such as GABA and ml. Nonetheless, the observation that it can detect Spec_{ano.SNR}, Spec_{ano.NAA}, Spec_{ano.multimeta}, and Spec_{ano.all} with more than 80% accuracy supports its potential applicability in the spectral quality management. The advantage of our unsupervised learning approach may be seen best in the detection of the spectra contaminated with artifacts. In the case of supervised learning, the artifact detection may require far more thorough preparation of the training data, considering the diverse types of the artifacts and their variable shapes and locations for a given type, in addition to their variable intensity. In our approach, the intensity of the artifacts would be the only factor that influences the detectability.

Conclusion

Our unsupervised deep learning-based approach could be an option in addition to supervised deep learning-based approaches in the binary classification of spectral quality with an extended abnormal spectra regime.

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