Conditional VAE for Single-Voxel MRS Data Generation

Dennis van de Sande[1], Sina Amirrajab[1], Mitko Veta[1], Marcel Breeuwer[1,2]

[1]Biomedical Engineering Department – Medical Image Analysis Group, Eindhoven University of Technology
[2]MR R&D - Clinical Science, Philips Healthcare

Introduction

Deep Learning (DL) has become a prominent tool to process and analyze single-voxel magnetic resonance spectroscopy (MRS) data[1,2]. However, training DL models usually requires large datasets which are not always available. Therefore, we propose a conditional variational autoencoder (cVAE) to synthesize single-voxel MRS data for the purpose of enriching existing in-vivo MRS datasets for training DL applications.

Data

We simulate single-voxel MRS data using the basis set from the ISMRM MRS fitting challenge 2016[3] and the FSL-MRS Python package[4]. We simulate two different metabolites (Phosphocreatine (PCr) and N-Acetylaspartic acid (NAA)) and the parameters for line broadening, phase/frequency shifts and the 4th order baseline are sampled from a uniform distribution. In total, 6,000 spectra are generated for training and 2,000 for validation. A test set of four spectra is generated for the latent space evaluation.

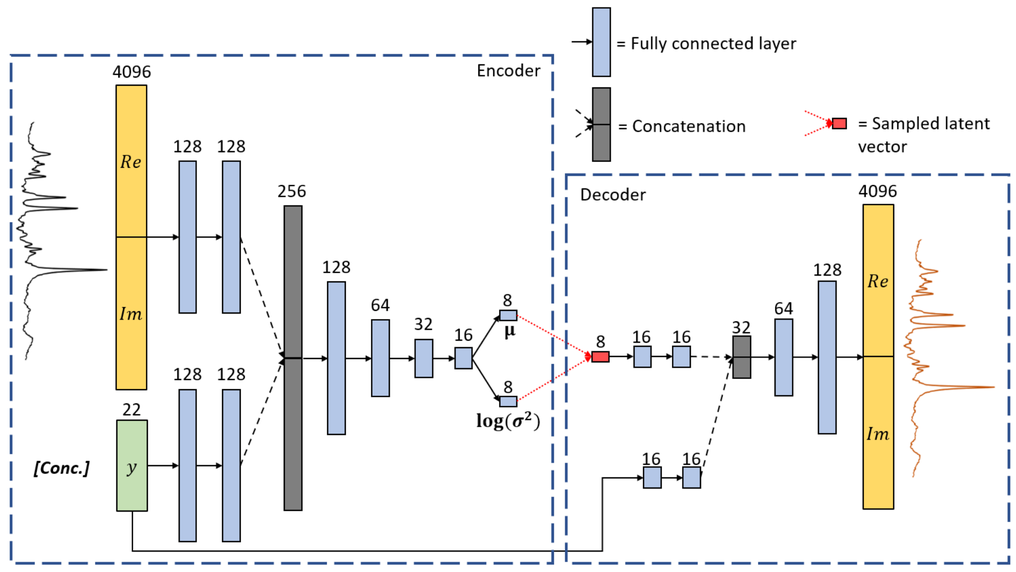

Figure 1: Architecture of the cVAE model. The Real (Re) and imaginary (Im) part of the spectra are concatenated and used as input. The label vector y contains the metabolite concentrations and is used in the encoder and decoder.

Method

The proposed cVAE model is shown in Figure 1. The model is trained using a mean squared error (MSE) reconstruction loss and the Kullback–Leibler (KL)-divergence of the latent space distribution with a standard Gaussian prior. To evaluate the generative part of the cVAE, a latent space evaluation is done to check whether the spectral parameters are captured in the latent space. This evaluation is done for the zero-order phase shift (ϕ_0) and the line broadening parameters (γ and σ) using latent space interpolation. The test set is used to interpolate between different parameter values (from $\phi_{0,1}$ to $\phi_{0,2}$ and from γ_1,σ_1 to γ_2,σ_2). This procedure is visualized in Figure 2.

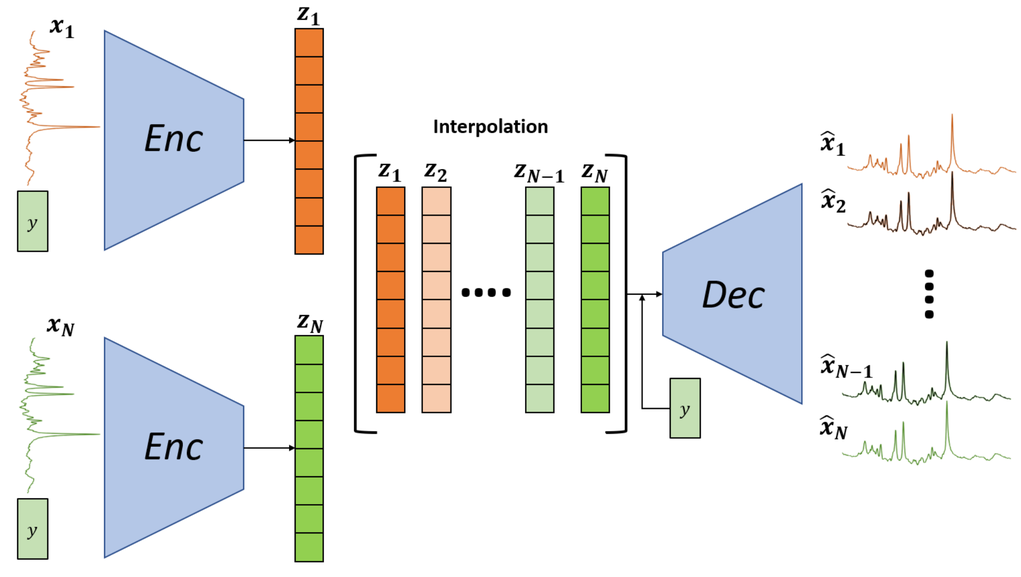

Figure 2: Procedure of latent space evaluation. Two different spectra are encoded to latent vectors z_1 and z_N and linearly interpolated to create a total of N reconstructions.

Results

The interpolation results in Figure 3 show smooth transitions between the different spectra from the test set. This indicates that ϕ_0, and γ and σ are captured well in the latent space.

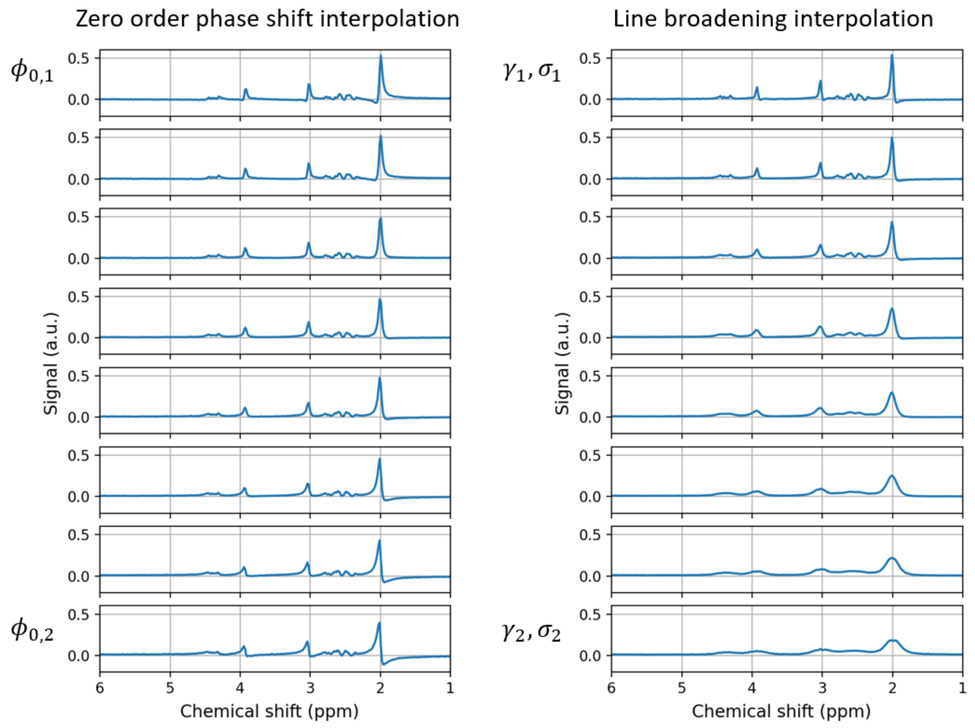

Figure 3: Results of interpolated reconstructions. Smooth transitions are observed for different values for ϕ_0 and γ and σ.

Conclusion

We conclude that our proposed cVAE model can generate new spectra that are similar to the initial dataset and that spectral properties can be encoded in the latent space. This study can be seen as a first step towards a generative model to enrich in-vivo datasets for training DL applications that can boost the clinical utility of MRS.

Correspondence:
Dennis van de Sande
✉d.m.j.v.d.sande@tue.nl
Dept. of Biomedical Engineering
PO Box 513
5600 MB Eindhoven, The Netherlands

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[1] Chen et al. (2020)
[2] Rajeev et al. (2021)
[3] Marjanska et al. (2021)
[4] Clarke et al. (2021)