Deconvolution of NMR Spectra: A Deep Learning-Based Approach

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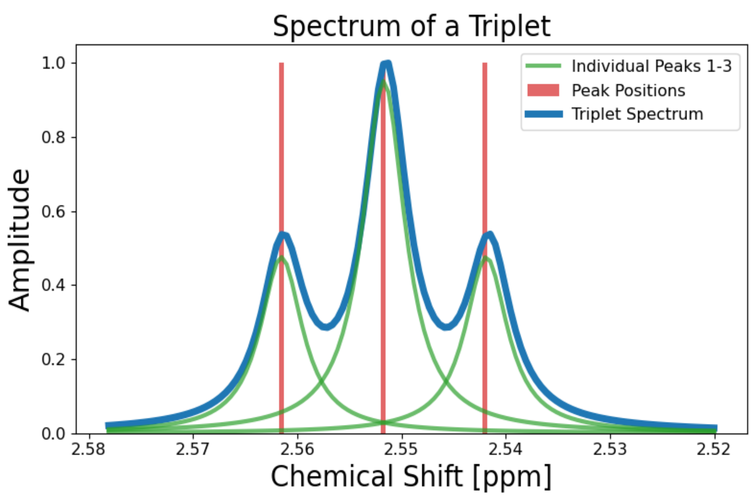
Introduction

Deconvolution of a spectrum involves several steps, from phase and baseline correction to peak picking and estimation of peak shapes. These steps are typically time-consuming and require operator supervision as well as expert knowledge to achieve a reasonable result. We present a deep learning-based approach for automated deconvolution of NMR spectra that works without any strong assumptions on the NMR spectra and performs well on spectra with strongly overlapping peak.

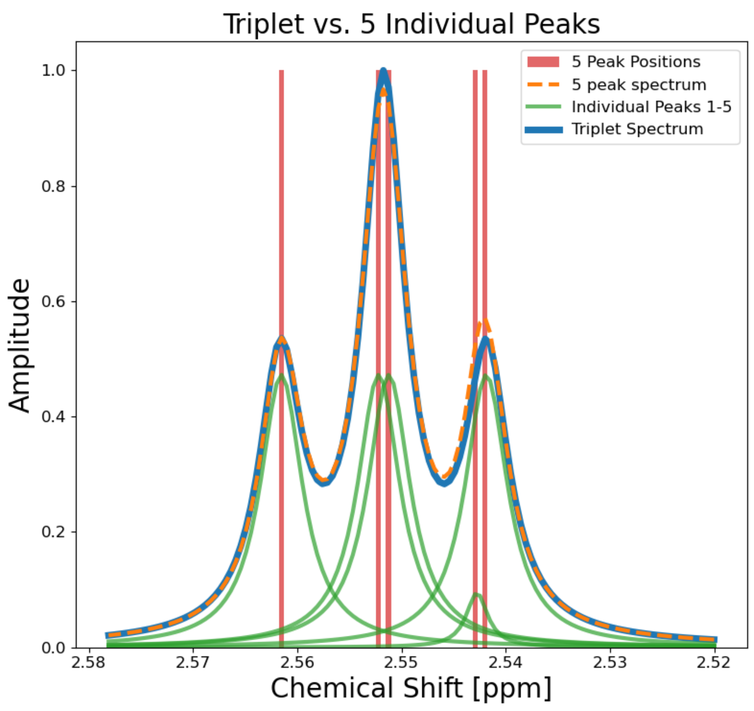
1.Deconvolution



Triplet with its three peaks

Goal: Find the peaks and their respective parameters, i.e. position, width, amplitude, lineshape.

2. Ill-Posed Problem



Spectrum of a Triplet and a spectrum of 5 individual peaks. The two spectra look identical.

Problem: Deconvolution doesn't have an unique solution.
Solution: Define which solution is favored through **regularization**.

3. Labeling-Based Regularization

Regularization: Addressed through an **automatic labeling procedure** of the synthetic spectra.

Sparse, expert-like deconvolution by differentiating which peaks are possible or reasonable to detect and which not.

Acknowledgement

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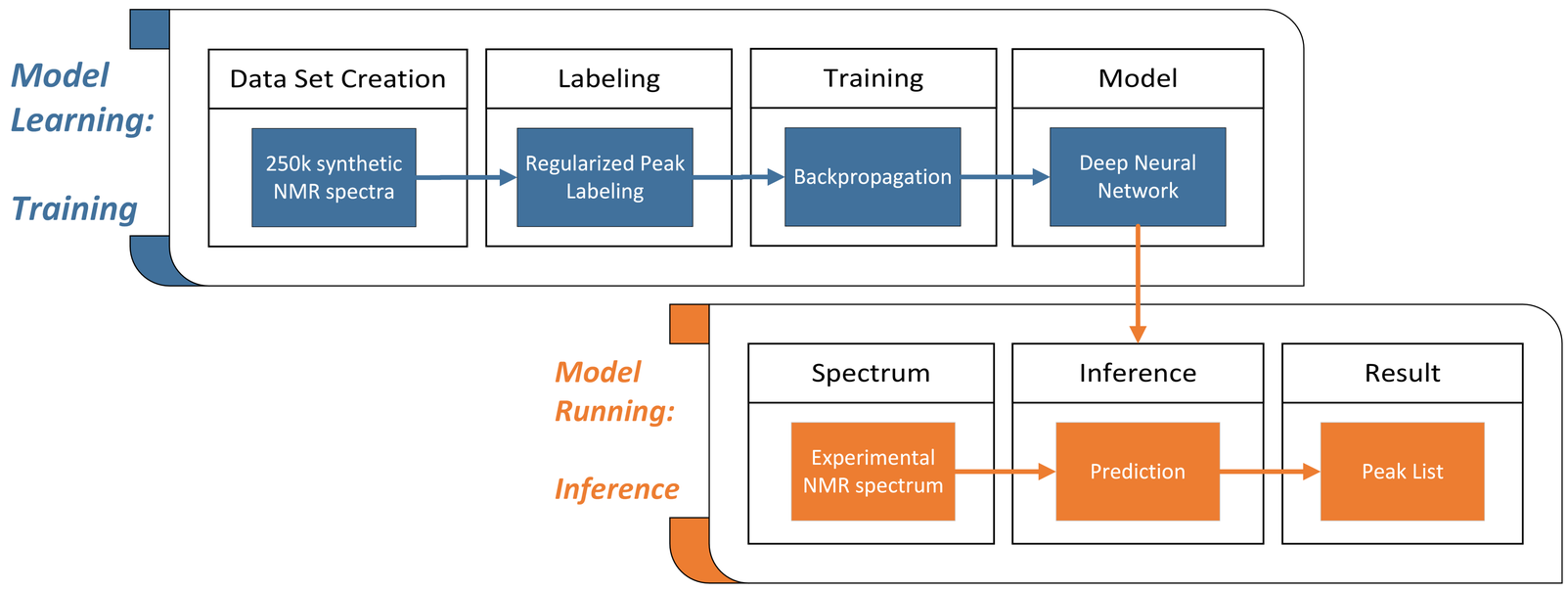
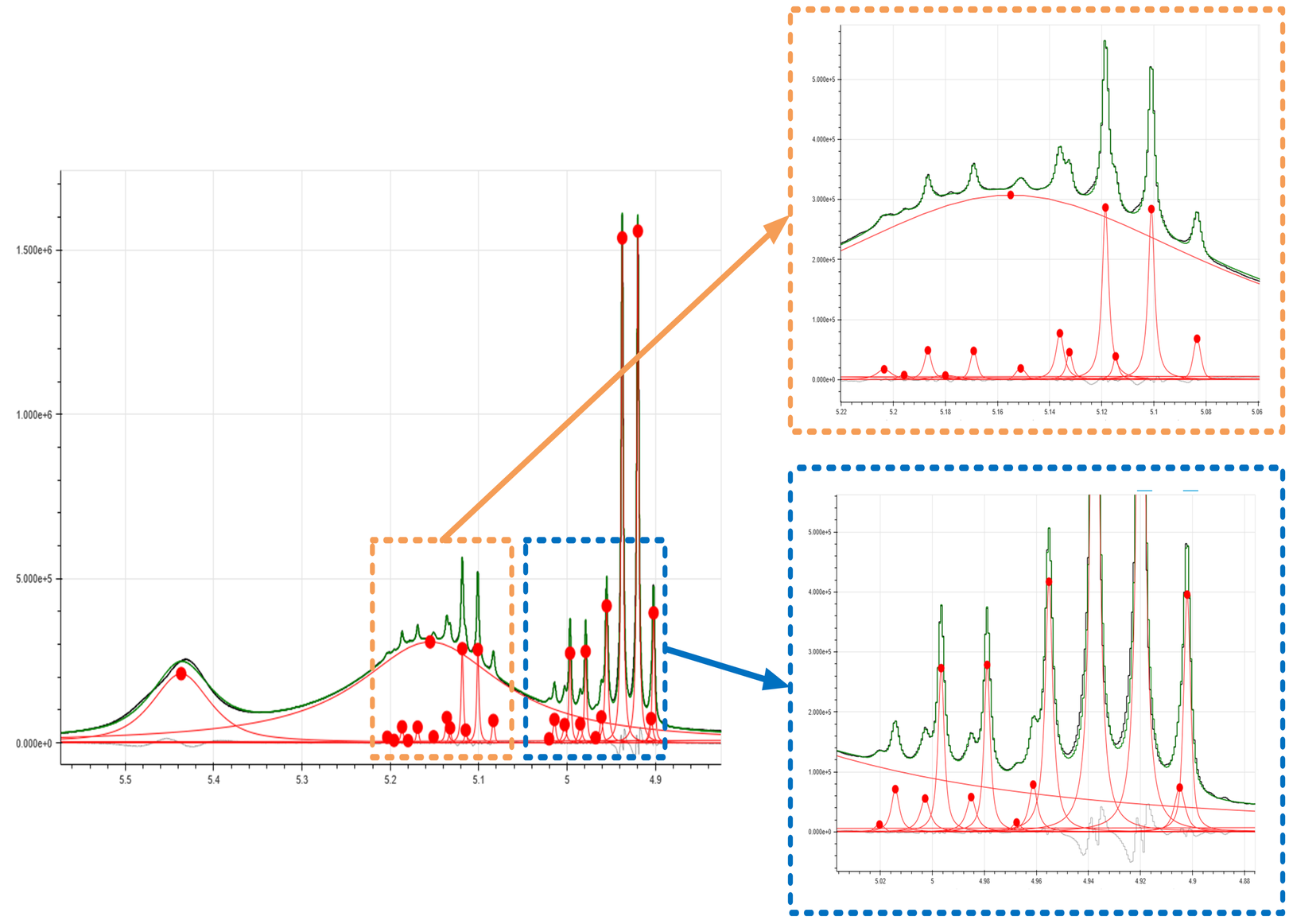
4. Model Learning and Deployment



This workflow diagram displays the different steps of the algorithmic pipeline. First the **model is learned** from synthetic data and custom labels. Second the **model is deployed** and infers a peak list from an experimental NMR spectrum.

5. Results: Deconvolution in a Crowded Spectral Region



The deconvolution works well for very **broad lines** overlapping with **narrow lines** (orange box) as well as for strongly **crowded regions** of peaks with intensities orders of magnitude apart, i.e. **high dynamic range regions** (blue box).

6. Conclusions

- We present a **deep learning-based method** for deconvolution of NMR spectra.
- The algorithm handles **strongly overlapping peaks** and **high dynamic range spectra**.
- The pipeline is **fully automated** from the **spectrum** to a **peak list**.
- The method will end up in a **commercial product** from Bruker Biospin.