TopSpin AI Algorithms

mldcon: AI-based Deconvolution in TopSpin

Application Note

Innovation with Integrity

Here we introduce *mldcon*, the latest addition to the TopSpin AI algorithms landscape. *mldcon* offers a novel approach to deconvolution that combines the flexibility of machine learning approaches with the accuracy of classical algorithms.

mldcon enhances the analytical capabilities of our software TopSpin and enables more accurate interpretation of NMR data by adding a fully automatic, parameter-free, deconvolution for 1D NMR spectra.

Introduction

Retrieving the list of peaks and peak parameters from an NMR spectrum – a process commonly known as deconvolution – is an essential step in many NMR applications and in the analysis of NMR spectra with overlapping signals. While this is a task typically carried out with the help of a computer due to its combinatorial complexity, many algorithms still struggle to provide satisfactory results in a fully automatic fashion. This is mostly due to the fact that deconvolution is an ill-posed problem, which makes it particularly challenging for an algorithm to find a solution that satisfies human needs.

At Bruker we are committed to providing innovative solutions that enhance the analytical capabilities of NMR. To support our customers' rising interest in the automation of spectroscopic workflows, including the automatic analysis of NMR spectra, we have developed *mldcon*: an Artificial Intelligence (AI) based algorithm to deconvolve 1D NMR spectra.

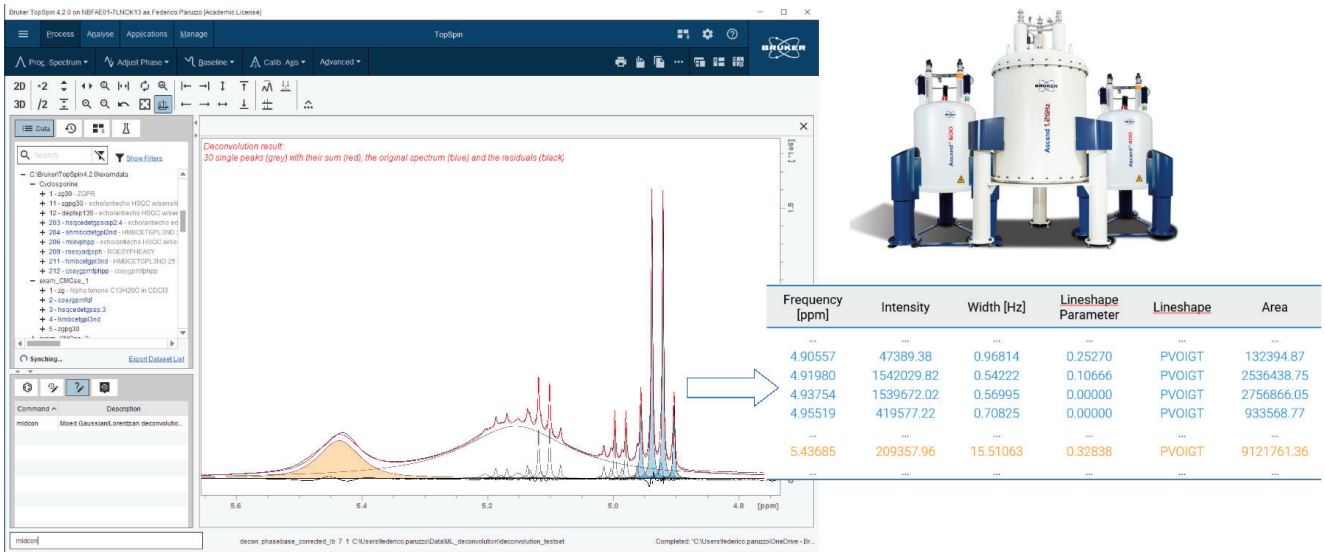
mldcon uses AI to drive the splitting of the spectrum into peaks that are meaningful for our customers' needs, combined with classical algorithms to obtain an accurate estimation of peak parameters. The algorithm can be used in our software TopSpin starting from version 4.2.0, either by typing *mldcon* in the command line or by clicking *Line Shapes > Deconvolution* (*Machine Learning Algorithm*) in the *Analyse* tab. More details on technical aspects and performances are available in ref. [1].

Quantification of Overlapping Signals

It is quite common for NMR users to calculate areas of the signals in an NMR spectrum. This is one of the steps required in applications such as structure verification and elucidation, analytes quantification using internal standards, or the evaluation of e.g., reaction yields in organic chemistry or ratios between different sites in polymer analysis. When the signals are isolated, this can be done simply by integrating the region of interest in the spectrum. Deconvolution becomes necessary if the signals of interest overlap with other signals.

With *mldcon*, analyzing spectra with overlapping signals has never been easier.

The algorithm is available in our software TopSpin starting from version 4.2.0. It will take only a few seconds to run and can be used by typing *mldcon* in the command line.



Frequency [ppm]	Intensity	Width [Hz]	Lineshape Parameter	Lineshape	Area
...	...	...	...	...	...
4.90557	47389.38	0.96814	0.25270	PVOIGT	132394.87
4.91980	1542029.82	0.54222	0.10666	PVOIGT	2536438.75
4.93754	1539672.02	0.56995	0.00000	PVOIGT	2756866.05
4.95519	419577.22	0.70825	0.00000	PVOIGT	933568.77
...	...	...	...	...	...
5.43685	209357.96	15.51063	0.32838	PVOIGT	9121761.36
...	...	...	...	...	...

Figure 1 *mldcon* result on a 400 MHz ^{1}H spectrum. The table on the right side of the figure shows an example of the peak parameters determined by *mldcon*. *mldcon* result is visualized in the TopSpin *mldcon* visualization window, which displays the input spectrum (in blue), the detected peaks (in grey), their sum (reconstructed spectrum, in red), and the difference between the input and the reconstructed spectrum (residuals, in black). The algorithm stores the result as a .csv file, reporting peak position, intensity, linewidth, lineshape type and parameters, and the area of each detected peak.

In these cases, *mldcon* obtains fast and accurate reconstruction of overlapping regions. Figure 1 illustrates the result of the algorithm on a challenging region of a ^{1}H 1D spectrum acquired on a Bruker 400 MHz NMR spectrometer. The algorithm runs in full automation and is successfully able to recognize both broad and narrow components in the region. In this case, using *mldcon* we can calculate the ratio between the broad peak shown in orange in Figure 1 and the quartet shown in light blue to be 1.4:1.

Results on Fourier 80 Spectra

Figure 2 shows an example of a *mldcon* result on an 80 MHz ^{1}H NMR spectrum acquired using our benchtop spectrometer: the Bruker Fourier 80. These spectra typically benefit from deconvolution even more than high-field NMR data, due to the intrinsic lower resolution of benchtop systems and the resulting higher degree of signal overlapping.

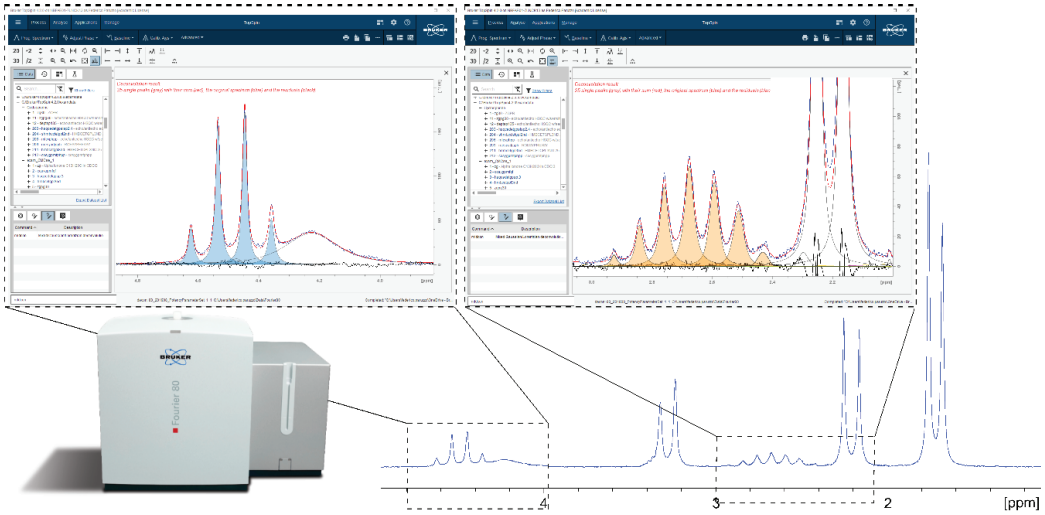


Figure 2: *mldcon* result on an 80 MHz ^{1}H spectrum acquired with the Bruker Fourier 80.

In the example of Figure 2, we used *mldcon* to quantify the 1:1 ratio between the quartet highlighted in blue and the septet in orange.

Usage information

mldcon requires phase and baseline corrected spectra as input. For a full automatic correction, try out our AI-based phase and baseline corrector *apbk*, available in TopSpin starting from version 4.1.4 [2].

While *mldcon* was developed to work in a fully automatic fashion, at times the user needs to tailor their results. We have many options that can be used to influence the deconvolution outcome. Examples are changes in the number of deconvolved peaks, constraints of peak parameter values, or a full custom initial guess for the peak fitting routine.

More information on these and other options that can be used to tailor *mldcon* results are available in the TopSpin processing user manual [3] and can be accessed by typing *help mldcon* in the TopSpin command line.

References:

1. Schmid, N., Bruderer, S., Paruzzo, F., Fischetti, G., Toscano, G., Graf, D., Fey, M., Henrici, A., Ziebart, V., Heitmann, B. and Grabner, H., Wegner J.D., Sigel R.K.O., Wilhelm D.; Deconvolution of 1D NMR Spectra: A Deep Learning-Based Approach. Journal of Magnetic Resonance, p.107357, 2022.
2. Bruderer, S., Paruzzo, F., and Bolliger, C.; Deep learning-based phase and baseline correction of 1D 1H NMR Spectra, Bruker, URL: https://www.bruker.com/en/products-andsolutions/mr/nmr-software/topspin.html, 2021.
3. Processing Commands and Parameters - TopSpin User Manual, Bruker, 2022. Available in the TopSpin installation folder, at the path TopSpin4.2.0\prog\docu\English\topspin\pdf\processing-reference.pdf

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info@bruker.com

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