



TOPSPIN

Improving Phase and Baseline Correction: An Extended Algorithm for 1D NMR Spectra in TopSpin 5

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Innovation with Integrity

Abstract

Phase and baseline correction are central processing steps in the analysis of nuclear magnetic resonance (NMR) spectra. The importance of automating these tasks has long been recognized, leading to the development of various algorithms over the years. As a part of this ongoing effort, Bruker has introduced an algorithm in 2008 designed to perform phase and baseline correction for heteronuclei. The method was optimized for liquid-state spectra and achieved good performance. A deep learning-based part was added later and optimized for unsuppressed liquid proton spectra. The extended version presented here improves the performance on heteronuclei and adds additional functionalities for handling solid-state spectra, suppressed spectra and spectra with negative peaks. The extended algorithm performs very well on diverse experimental conditions and can handle all nuclei. Overall, the performance is superior to *apk/abs* and the previous implementation of *apbk*. The updated algorithm is available in TopSpin as command *apbk* starting from version 5.0.0.

Introduction

NMR spectroscopy has been experiencing remarkable growth driven by advances in instrumentation and automation software which are transforming its applications in both industrial and academic domains [1,2]. Spectral data processing is an essential and inevitable component of reliable data analysis. Within the processing workflow, phase and baseline correction are probably the most crucial steps. Phase correction ensures that resonance peaks appear in pure absorption mode, with the imaginary part in dispersion mode, while baseline correction removes unwanted drifts and offsets, as well as background signals, resulting in a flat and stable baseline.

Phase and baseline artefacts in NMR spectra arise primarily from instrumental and processing imperfections. Phase distortions generally appear as zero-order and first-order distortions. Zero-order phase distortion is a constant phase shift applied uniformly across all frequencies in the spectrum [3]. It typically arises from a phase mismatch between the transmitter pulse and the receiver. First-order phase distortion introduces a frequency-dependent phase shift across the spectrum, often caused by different sources such as the delay between excitation and detection, or phase shifts induced by noise-reducing filters [4]. Phase distortions lead to asymmetric and dispersive peak shape

which complicates spectral interpretations and reliable data analysis. Baseline distortion in NMR is mainly caused by unwanted signals or artefacts appearing in the first few points of the FID (free induction decay). They are caused by various factors such as so-called 'dead time' inherent to pulsed NMR [5], instrumental instabilities, nonlinearities in the filter-phase response [7] and other sources. Baseline distortions offset the intensity values and result in inaccuracy in peak assignment and quantification.

Accurate phase and baseline correction is essential for applications such as quantitative NMR (qNMR), metabolomics, reaction and process monitoring, where even small deviations can significantly affect the results [8,9]. Improper phasing can cause peaks to appear asymmetric, while a distorted baseline can bias peak area measurements and generate inaccurate results in automated analysis. These artifacts can obscure weak signals, distort integrals, or lead to misinterpretation of chemical shifts. For example, when NMR spectroscopy is used as a sensor for process control and reaction monitoring, continuous spectra must be processed automatically and reliably. The reaction mixtures change rapidly leading to variations in peak intensities and chemical shifts (e.g., from pH changes), requiring robust algorithms. Accurate quantitative analysis depends heavily on proper phase and baseline correction to determine mixture composition via integration. These corrections enable accurate peak integration for quantitative experiments and reliable interpretation of NMR spectra [10,11].

Estimating the baseline in spectra with residual phase distortion or correcting the phase in spectra with baseline distortions is challenging and leads to inaccurate results. Therefore, the necessity for robust, fully automated algorithms capable of simultaneously performing phase and baseline corrections have long been recognized. As a result, various algorithms have been developed over the years [3-6]. In 2008 Bruker introduced an algorithm for phase and baseline correction of heteronuclei in liquid-state. Later, a deep learning-based method was added to handle specifically unsuppressed liquid proton spectra [12]. However, none of these algorithms is well suited to correct solid-state spectra, spectra with solvent suppression, and spectra with negative peaks.

Here we introduce a machine learning based approach for automatic phase and baseline correction of 1D NMR spectra. The method is available as of TopSpin (TS) 5.0.0 using the command *apbk*. The results show that the improved *apbk* approach achieves substantially better performance compared to other phase and baseline correction algorithms available in TopSpin. The new functionalities of the algorithm improve its reliability across a broad range of nuclei and spectra including solid-state spectra, solvent-suppressed spectra, and spectra with negative peaks.

Methods

When the *apbk* command is run, the type of the 1D spectrum is obtained using the pulse program name. In the case of a proton spectra without solvent suppression, the previous *apbk* is employed and the baseline correction is performed using a deep learning algorithm, as implemented previously [12]. For solid-state spectra, spectra with solvent suppression, spectra with negative peaks and heteronuclear spectra the improved algorithm, described in this paper, is triggered. This algorithm uses a machine learning approach to correct the spectrum. The correction process is done in two steps. First, a rough phase and baseline adjustment is applied using classical algorithms. Then, a refined correction is carried out where the solution is iteratively improved through the simultaneous adjustment of phase and baseline. This two-step algorithm is based on previous literature on phase and baseline correction [13-17].

A diverse set of experimental NMR datasets from Bruker internal sources has been collected to evaluate the improved algorithm and its new functionalities. The dataset covers a broad range of spectra including solid-state spectra, solvent-suppression experiments and spectra with negative peaks. Since the updated algorithm supports all nuclei, we ensured that the test set includes a diverse range of nuclei as well. For solution-state the method was evaluated on ^1H , ^{11}B , ^{13}C , ^{15}N , ^{19}F , ^{29}Si , and ^{31}P . In addition, testing was performed on ^1H , ^{13}C , ^{15}N , and ^{29}Si spectra in solid-state. This comprehensive selection was chosen to validate the general applicability of the method across different nuclei and experimental conditions. The data set contains 676 experimental spectra recorded at base frequencies between 80 and 900 MHz.

The spectra corrected using the improved method have been compared against their respective manual corrections from Bruker NMR experts. To assess the quality of the algorithm, we have introduced custom metrics to quantify the deviation from the ground-truth, based on the phase score and baseline score described in [12]. The **phase deviation** is defined as the mean absolute phase difference to the ground truth over each peak in the spectrum. The **baseline deviation** is computed as the mean absolute deviation between the corrected and reference spectra, normalized by the noise level after adjusting the phase of the corrected spectrum to the ground truth value.

Correcting the phase of spectra with a low signal-to-noise ratio may lead to a range of phase relationships being considered correct. This arises from the bases of the peaks in such spectra vanishing into the noise, which hinders the visual estimation of the phase of the peaks. To account for this ambiguity, we have introduced a threshold for the phase deviation of a peak with respect to the ground-truth that depends on the signal-to-noise ratio of that peak, below which we consider the phase deviation to be zero. This threshold is defined as the maximum phase deviation where the base of the peak remains within the noise level.

To evaluate algorithm performance across the dataset, we computed the cumulative fraction of spectra with deviations below a given threshold. While the phase and baseline deviations quantify the correction quality for individual spectra, the cumulative fraction summarizes the overall performance of the algorithm. This representation allows not only a comparison of average correction quality, but also an assessment of the consistency and robustness of the applied methods across all spectra.

Results and Discussion

The improved *apbk* implementation presented here was compared to the two commands commonly used to correct the phase and baseline of 1D spectra in TopSpin: *apk*; *abs* and the previous version of the *apbk* command (TopSpin version < 5). The *apk* command is the default TopSpin command to apply a linear correction to the phase of a 1D spectrum. The *abs* command is then used to remove the residual baseline of the spectrum, by subtracting a polynomial of degree 5. In contrast, both the previous and the improved *apbk* implementations combine the phase and baseline corrections in a single process, reflecting the close relationship between phase and baseline in experimental spectra. In addition, a model-free baseline is used in *apbk*, which improves the flexibility of the baseline, resulting in an improved correction compared to *abs*.

In TopSpin 5, the existing deep learning-based algorithm is called for non-suppressed, liquid state ^1H spectra, whose implementation and analysis are described in [12]. Here, we focus on other spectra beyond this case, which use the improved method presented herein.

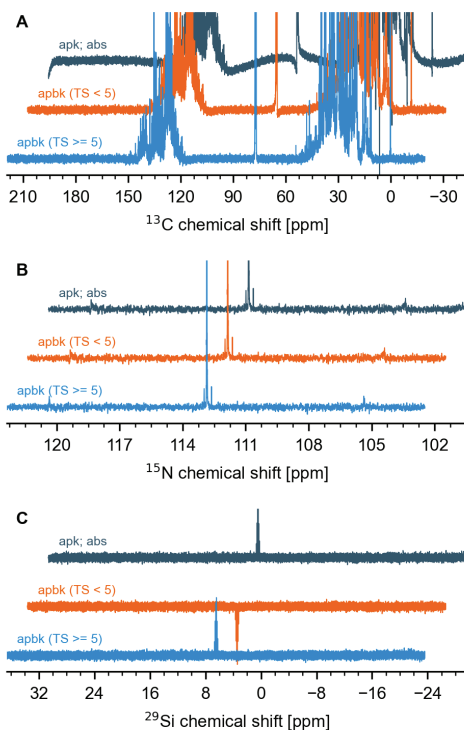


Figure 1: Example of phase- and baseline-corrected (A) ^{13}C , (B) ^{15}N , and (C) ^{29}Si spectra obtained using *apbk* in TopSpin 5 (light blue), *apbk* before TopSpin 5 (orange), and *apk*; *abs* (dark blue). The spectra are offset horizontally and vertically for the sake of clarity.

Figure 1 shows the comparison between three spectra from common heteronuclei corrected using the *apk*; *abs* command, the *apbk* command implemented in TopSpin before version 5.0.0, as well as the improved *apbk* implementation presented here. Overall, the updated command provides higher quality phase and baseline correction compared to the two other methods for these example spectra. The improved correction is reflected by the absence of signal dips below the baseline at the base of peaks and by a flat baseline in spectral regions that do not contain signal. In particular, the updated *apbk* implementation outperforms both *apk*; *abs* and the previous method in correcting the phase of the ^{13}C spectrum in **Fig. 1A**. In addition, it properly corrects the weak peaks around 105 and 120 ppm in the ^{15}N spectrum shown in **Fig. 1B**, and remedies the inability of the previous method to phase the ^{29}Si spectrum in **Fig. 1C**.

While **Fig. 1** showcases the improvements brought to the *apbk* command, a more thorough evaluation was performed by running the three commands on datasets of 116 ^{13}C spectra, and 67 spectra of other heteronuclei (^{11}B , ^{15}N , ^{29}Si , ^{31}P) for which the phase and baseline correction was performed manually to use as a ground-truth.

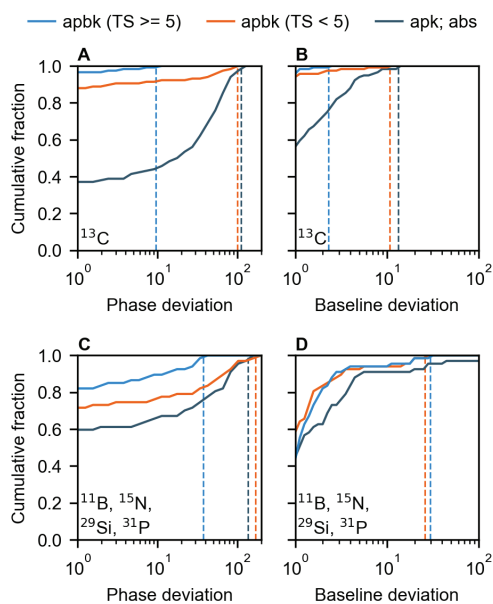


Figure 2: Cumulative distributions of (A, C) phase and (B, D) baseline deviations in the experimental datasets of (A, B) ^{13}C , and (C, D) other heteronuclei (^{11}B , ^{15}N , ^{29}Si , ^{31}P) spectra. The solid lines show the fraction of spectra with deviations below a given threshold. The light blue and orange lines correspond to *apbk* in and before TopSpin 5, respectively, and the dark blue lines to *apk; abs*. The dashed vertical lines indicate the largest deviation in each cumulative distribution.

Figure 2 shows the cumulative distributions of phase and baseline deviations in each dataset for the three methods investigated. The phase and baseline deviations are displayed starting from a value of 1. A phase deviation lower than 1 corresponds to an average phase difference between the corrected spectrum and the ground-truth below 1° . Similarly, a baseline deviation below 1 corresponds to an amplitude difference between the corrected spectrum and the ground-truth below the noise level of the spectrum. We thus consider that results yielding deviations below 1 are indistinguishable from the ground-truth. The deviation threshold for which the cumulative distribution reaches 1 represents the algorithm's worst case prediction, indicated by a dashed vertical line. The value of the cumulative distribution at a deviation of 1 (left limit of the plot) corresponds to the fraction of data sets for which the algorithm achieved a "perfect" solution. **Figure 2A, C** highlights the better phase-correction performance of the improved *apbk* implementation compared to the two previously available commands. This is indicated by a reduction of the maximum phase deviation from over 100° to below 20° in the ^{13}C dataset, and to below 40° in the heteronuclei dataset. In addition, 97% of ^{13}C spectra were considered perfectly corrected by the improved *apbk* command, against 88% for the previous *apbk* implementation and 37% for *apk; abs*. For other heteronuclei, the percentages of perfectly corrected spectra were 82%, 72%, and 60% for the updated *apbk* command, the previous *apbk* implementation and *apk; abs*, respectively. This improvement in the phase correction is achieved without sacrificing the quality of the baseline model (see **Fig. 2B, D**). For ^{13}C , the improved *apbk* command generally produces a better baseline, as seen in **Fig. 2B**. In comparison, the *apk; abs* command generally gives poorer results for both phase and baseline, especially for the ^{13}C dataset. These statistical results confirm the behaviour seen in **Fig. 1**: the updated *apbk* implementation improves the accuracy of the phase correction and is less prone to result in unrealistic phase relationship, such as *apk; abs* in **Fig. 1A** and the previous *apbk* implementation in **Fig. 1C**.

In addition to improving performance, we also extended the features of *apbk* to be able to handle a wider range of spectra. **Figure 3** highlights the three main features added to the command: the ability to correct suppressed spectra, handling of negative peaks, and support for solid-state spectra.

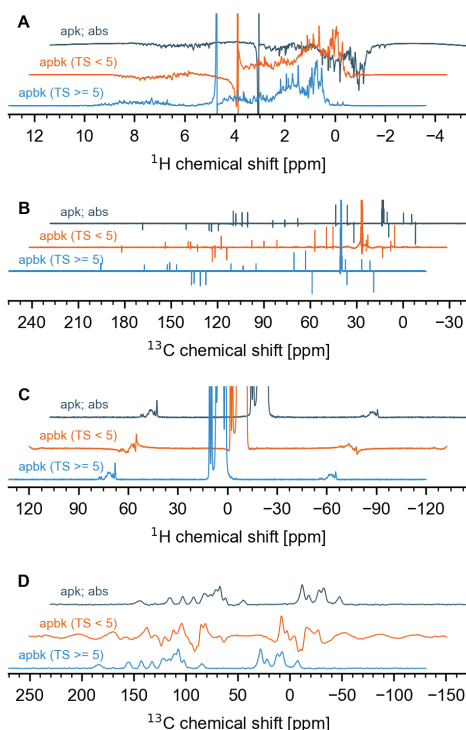


Figure 3: Example of phase- and baseline-corrected (A) suppressed ^1H , (B) ^{13}C DEPT, (C) ^1H 60 kHz MAS [19], and (D) ^{13}C 22 kHz MAS [20] spectra obtained using *apbk* in TopSpin 5 (light blue), *apbk* before TopSpin 5 (orange), and *apk; abs* (dark blue). The spectra are offset horizontally and vertically for the sake of clarity.

Suppressed spectra: Protonated solvent in NMR samples can significantly hinder the interpretation of ^1H NMR experiments due to the strong signal from the solvent (typically water), which can be orders of magnitude more intense than the signal of the analyte. A variety of pulse sequences have thus been developed to suppress strong solvent signals, e.g. through phase cycling or gradient pulses [18]. However, experimental imperfections may lead to residual signal from the solvent, which can have a different phase compared to the rest of the spectrum. To address this issue, we implemented a mechanism to ignore the residual signal at the suppression frequency during the phase correction. **Figure 3A** shows a suppressed ^1H spectrum containing a strong, out-of-phase residual water signal at 4.7 ppm. As a result, both the *apk; abs* and the previous *apbk* implementation fail to correct the spectrum. By ignoring the region around 4.7 ppm, the improved *apbk* command is able to correctly phase the spectrum. We note that multiple suppression frequencies can also be handled by our algorithm (see **Practical Tips**).

Spectra containing negative peaks: Some spectral editing experiments such as DEPT and CPPI leverage the difference in coupling between different pairs of nuclei to separate distinct atomic environments. This can produce spectra containing both positive and negative peaks, indicative of different atomic environments [21, 22]. Since *apk; abs* and the previous *apbk* expect all peaks to be positive, such spectra cannot be properly phased using these commands. In contrast, the improved *apbk* command is able to handle spectra containing both positive and negative peaks, as shown in **Fig. 3B**. In the first step of the algorithm, the negative peaks are identified and then accounted for during the refined phase correction.

Solid-state spectra: Solid-state NMR spectra display broader linewidths compared to their liquid-state counterparts, mainly due to dipolar interactions that are not averaged out by molecular motion. While magic-angle spinning (MAS) significantly reduces these anisotropic interactions through coherent averaging, lines typically remain significantly broader in solid-state NMR spectra [23]. In addition, MAS can result in spinning sidebands, which arise at frequency offsets equal to integer multiples of the MAS rate in the spectrum. While the spectrum is not fundamentally different in solid-state NMR, an algorithm adjusted for liquid-like lineshapes may not properly correct a solid-state spectrum. We thus introduced settings dedicated to solid-state spectra, which better reflect the typical lineshapes observed. In addition, the MAS rate is used to better identify and properly phase spinning sidebands. **Figure 3C-D** shows example solid-state ^1H and ^{13}C spectra corrected by the three algorithms investigated here. The updated *apbk* displays a marked improvement over the previous version, which failed to correct both the ^1H 60 kHz as well as the ^{13}C 22 kHz MAS spectra.

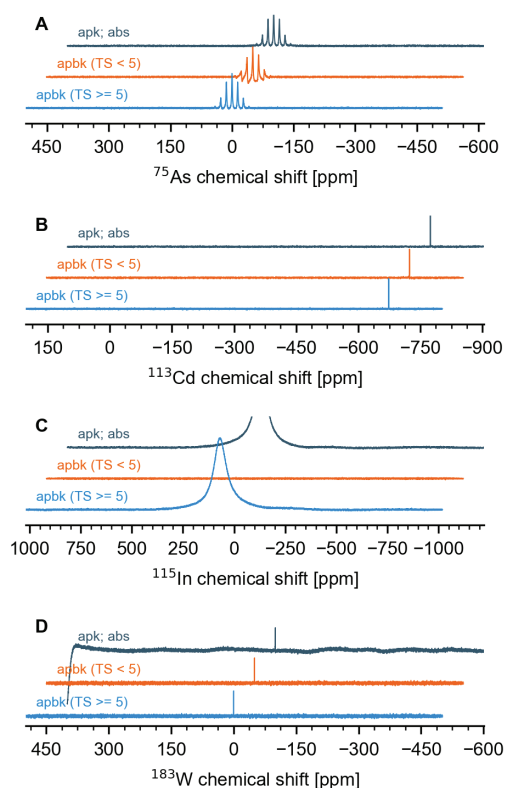


Figure 4: Example of phase- and baseline-corrected (A) ^{75}As , (B) ^{113}Cd , (C) ^{115}In , and (D) ^{183}W spectra obtained using *apbk* in TopSpin 5 (light blue), *apbk* before TopSpin 5 (orange), and *apk; abs* (dark blue). The spectra are offset horizontally and vertically for the sake of clarity.

Conclusion

We have updated the command *apbk* in TopSpin to improve phase and baseline correction for 1D NMR spectra. The algorithm is using a machine learning approach to correct the spectra and the correction process is done in two steps. Initially a rough phase and baseline adjustment is applied, which is followed by a refined correction where the solution is iteratively improved through the simultaneous adjustment of phase and baseline. The improved method is fully automated and does not require any user input. It is available as TopSpin command *apbk* starting from TopSpin 5.0.0.

The updated command now supports all nuclei and introduces extended functionalities enabling the correction of solid-state NMR spectra, solvent-suppressed spectra, and spectra containing negative peaks. The results show that the updated *apbk* performs substantially better than phase and baseline correction methods previously available in TopSpin. These capabilities broaden the applicability of the algorithm beyond solution-state NMR, making it suitable for a wider range of research and industrial applications.

Uncommon heteronuclei: NMR can access a wide variety of nuclei, each with their own frequency range and typical linewidth. A flexible and adaptive phase and baseline correction method is thus required to obtain reasonable results. For common nuclei, our improved *apbk* implementation uses pre-defined sets of parameters that describe typical spectral features for a given nucleus. However, a large and diverse enough set of spectra is required to estimate these parameters. For most heteronuclei, the available data is insufficient to confidently establish a set of parameters to use. In order to enable the use of *apbk* for nuclei for which no pre-defined parameters are available, we implemented a parameter estimation from the input spectrum. This process is independent of the initial phase of the spectrum and provides reasonable parameters to perform the phase and baseline correction.

Figure 4 shows four example spectra corrected using the improved *apbk* implementation with automatic parameter estimation, compared to the results from the previous *apbk* command and *apk; abs*. We note that by default, the previous *apbk* would fallback to *apk; abs*. Here, it was forced to run without falling back using the *-f* option. Strikingly, the improved algorithm was able to properly correct the phase and baseline of all four spectra, regardless of their spectral range and linewidth. While *apk; abs* did correctly phase all spectra, residual baseline was found in **Fig. 4D**, due to the input spectrum displaying a baseline several times larger than the signal.

Overall, these results indicate that the updated *apbk* command provides a significant improvement over the previous implementations of phase and baseline correction algorithms. In addition, the new features enable the use of the command on a broader class of spectra, including solvent suppression experiment, spectral editing methods, and solid-state spectra. Since the improved algorithm is more robust it can be applied in automation to any 1D spectrum of any nucleus. The improved *apbk* command is available in TopSpin 5.0.0 and above.

Practical Tips

The TopSpin manual, accessible by typing `"help apbk"` in the TopSpin command line, provides a detailed description of all options available to the command. This section describes example use-cases for some of the options available.

- The improved method uses different modes depending on whether the spectrum is solid-state, solvent suppressed or contains negative peaks. The selected modes are recorded in the audit trail. Although the method tries to adjust the modes automatically, it can be beneficial to set or disable them manually. For further customization, a Python script `tsapbk.py` is provided in the `python/examples` folder.
- The slope of the phase relation (first order phase) is usually small and should be close to 0, if the BASEOPT digital filter is selected in the acquisition parameters. The improved `apbk` internally restricts the first order phase values. This restriction can be modified with the `-phc1max` option. Alternatively, first order phase fitting can be completely switched off using the option `-apk0`.
- For suppressed spectra or spectra with peaks that do not follow a linear phase relation, the parameter `-supp` can be used to provide peak frequencies which should be excluded from phase fitting.
- The method internally uses signal regions that can be saved by setting the `-w` option. The user can also use integral regions with the `-intrng` option (see manual). These regions are treated as signals and thus used for phase fitting, while everything else will be considered as baseline. If the method does not automatically find the expected signals, manually provided signal regions can improve the results.
- The subtracted baseline from the spectrum by the method presented here can be stored using the `-storeb` option to a different procno within the same experiment. A typical workflow to use this option is to first apply `"apbk -storeb=999"`, then reprocess the spectrum and apply the phase correction (e.g. with `"efp"`). Finally visualize the phase corrected spectrum together with the baseline in the multiple display mode (`".md"`).
- The method used to estimate spectral parameters for uncommon nuclei can also be used for spectra with predefined parameters using the option `-estimate -f` (see **Results and Discussion**). This may provide better results when the spectrum deviates from the spectra used to tailor the algorithm.
- In older datasets, the MAS rate (acquisition parameter MASR) might be incorrect and can be provided manually using the `-solid` option.

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