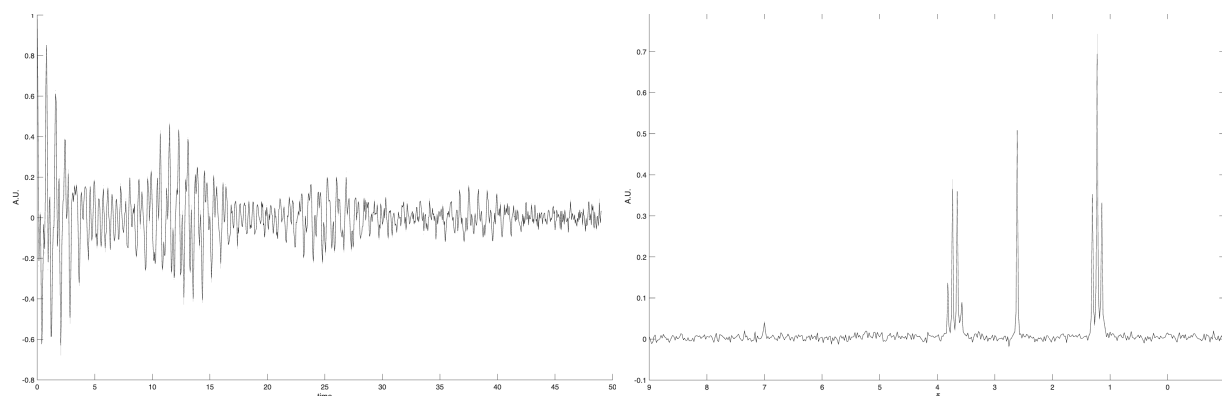


August 2025 NMR Topic of the Month: On Filters Part III

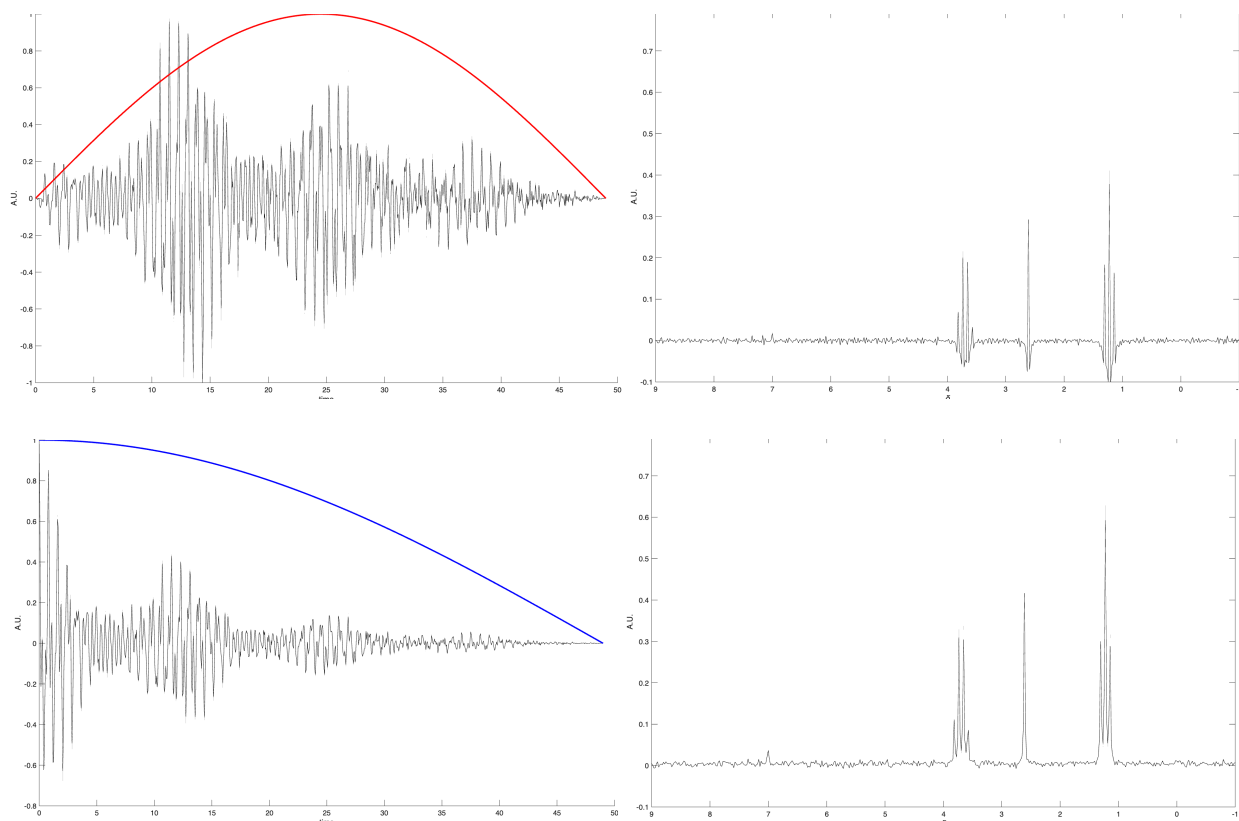
The Four Sine Filters

Amongst the available window multiplication filter parameters in TopSpin is “Sine bell shift SSB (0, 1, 2, ...)”, which is used in four different sine function related filters. As always, we start with our straight FID and its Fourier transform shown immediately below for comparison purposes.



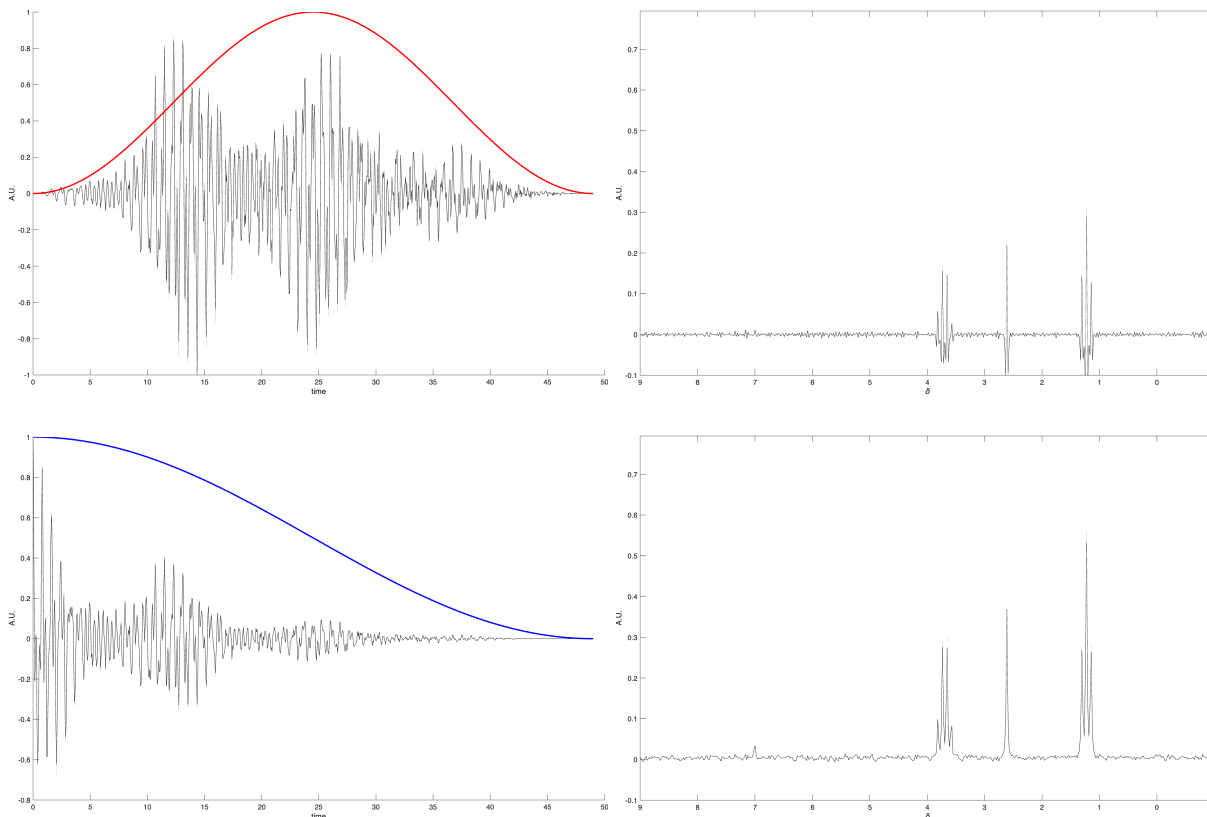
The Sine Bell

The sine bell window function is: $\sin[(\pi - \varphi)(t/AQ) + \varphi]$. Where t is the acquisition time (variable/vector), AQ is total acquisition time, and φ is defined on $[0, \pi)$ by: π/SSB where SSB is a positive integer input. The most common choices for SSB are $SSB = 1 (\rightarrow \varphi = 0)$ for a pure sine function and $SSB = 2 (\rightarrow \varphi = \pi/2)$ for a pure cosine function, with higher values offering a filter involving both trigonometric functions. Immediately below and left are figures with the straight FID above filtered with a sine ($SSB = 1$, overlaid in red) and the cosine ($SSB = 2$, overlaid in blue) and the resulting Fourier transform under each filter immediately to the right of each filtered FID. In this case the signals are badly distorted by the sine filter, which would make it an unusual choice, but for other signals (like those from a COSY) the sine filter is ideal.



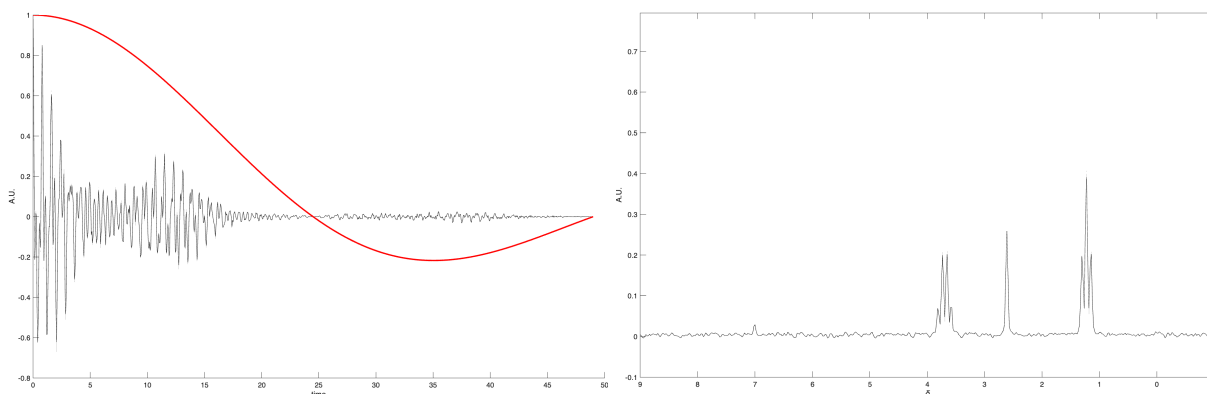
The Squared Sine Bell

The squared sine bell window function (designated as QSIN in TopSpin) is: $\sin^2[(\pi - \varphi)(t/AQ) + \varphi]$. Its variables work exactly like the sine bell window function above, this filter produces a sharper maximum and more gradual tapering to zero. Immediately below and left are figures with the straight FID above filtered with a sine squared ($SSB = 1$, overlaid in red) and the cosine squared ($SSB = 2$, overlaid in blue) and the resulting Fourier transform under each filter immediately to the right of each filtered FID.



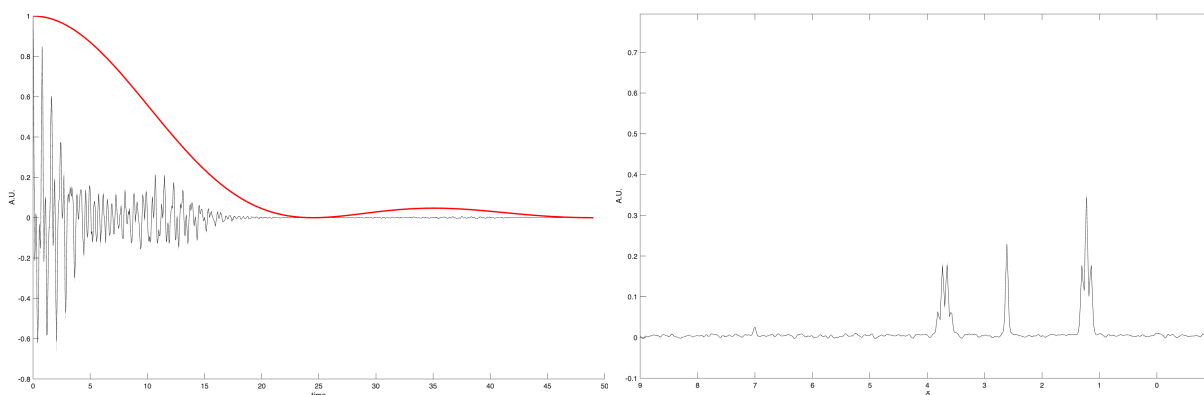
The Sinc

The sinc window function is based off the normalized sinc function ($\sin(\pi x)/\pi x$), which is the Fourier transform of a rectangular function. Specifically, the filter takes the form: $\frac{\sin[2\pi \cdot SSB \cdot (t/AQ - GB)]}{2\pi \cdot SSB \cdot (t/AQ - GB)}$. Where t is the acquisition time (variable/vector), AQ is total acquisition time, GB is defined on $[0, 1]$ to shift the peak of the filter as a fraction of AQ , and SSB is a non-zero integer that indicates the number of 2π intervals the filter has during AQ . Immediately below and left are figures with the straight FID above filtered with a sinc ($GB = 0$ and $SSB = 1$, overlaid in red) and the resulting Fourier transform immediately to the right.



The Squared Sinc

Not surprisingly, the squared sinc window function (designated QSINC in TopSpin) is the square of the sinc window function above and its variables work exactly like the sinc window function. This filter produces a sharper global maximum (at $t = GB \cdot AQ$) with a more gradual tapering to zero than the sinc window function and smaller maxima away from the global maximum. Immediately below and left is the figure with the straight FID above filtered with a sinc squared ($GB = 0$ and $SSB = 1$, overlaid in red) and the resulting Fourier transform immediately to the right.



Follow the Signs

“So, which sine function is ‘correct’?” You might ask. Well, really the answer is: “All of them and none of them.” Just like all such filters, they all have roles and can help you identify features in your spectrum. Use whichever one accomplishes the goal of elucidating the content of the spectrum, and be sure to disclose which filter(s) you used on a given spectrum whenever you present/publish it. However, there are some guidelines that will help:

1. A filter that has the same general shape as the unfiltered signal tends to distort the integral (usually Fourier) transform less than a filter that does not.
2. In the same vein as 1, the best sensitivity enhancement is accomplished by a matched filter.
3. For resolution enhancement, pick a filter that emphasizes times of less signal (but still have signal in them).
4. To reduce artifacts from abrupt signal changes (like truncation), use a filter that tapers and smoothes those instances out.

An example that demonstrates the last two points may be helpful. Suppose that on a simple pulse-acquire experiment the signal you acquired was completely lost in the noise long before the receiver was switched off. (Try not to do this, acquire properly). Do not blow up the end of the FID trying to improve the resolution, since there’s ‘no’ signal there you’d just be lowering your signal-to-noise. Instead, chop down the acquired FID, apply a matched filter that smoothly guides the FID to zero, and then zero-fill (which will be covered later) the FID before doing the Fourier transform.

Setting up the parameters for a filter can often be done in three steps: 1- look at the FID and determine which filter(s) would be best suited, 2- look at the unfiltered spectrum and note values from peaks of interest (like linewidth), and 3- use the interactive apodization in the software to finish the process. The interactive apodization shows both the FID and its Fourier transform under a set of filter choices that you can change right there. In TopSpin, if you open the “Window function” interface (wm command) and check the “Manual window adjustment” box it will open such an interface. In VnmrJ on the Process tab’s Weighting page there is an “Interactive weighting” button that will open the interface, once you have the filter(s) set to your liking hit the “Transform” button to exit and keep those values.

References

1. TopSpin: Processing Commands and Parameters User Manual Version 007 (H9776SA4_007), 57-58 (2023).
2. J.C. Hoch and A.S. Stern, *NMR Data Processing*, Section 3.10 & 3.11, Wiley-Liss, New York (1996).
3. R.N. McDonough and A.D. Whalen, *Detection of Signals in Noise*, 2nd ed., Academic Press, San Diego (1995).
4. https://en.wikipedia.org/wiki/Sinc_function