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The Time-Domain Matched Filter and the Spectral-Domain Matched Filter in 1-Dimensional NMR Spectroscopy

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Abstract

A type of “matched filter” (MF), used extensively in the processing of one-dimensional spectra, is defined by multiplication of a free-induction decay (FID) by a decaying exponential with the same time constant as that of the FID. This maximizes, in a sense to be defined, the signal-to-noise ratio (SNR) in the spectrum obtained after Fourier transformation. However, a different entity known also as the matched filter was introduced by van Vleck in the context of pulse detection in the 1940's and has become widely integrated into signal processing practice. These two types of matched filters appear to be quite distinct. In the NMR case, the “filter”, that is, the exponential multiplication, is defined by the characteristics of, and applied to, a time domain signal in order to achieve improved SNR in the *spectral* domain. In signal processing, the filter is defined by the characteristics of a signal in the spectral domain, and applied in order to improve the SNR in the *temporal* (pulse) domain. We reconcile these two distinct implementations of the matched filter, demonstrating that the NMR “matched filter” is a special case of the matched filter more rigorously defined in the signal processing literature. In addition, two limitations in the use of the MF are highlighted. First, application of the MF distorts resonance ratios as defined by amplitudes, although not as defined by areas. Second, the MF maximizes SNR with respect to resonance amplitude, while intensities are often more appropriately defined by areas. Maximizing the SNR with respect to area requires a somewhat different approach to matched filtering.

Introduction

A widely used technique for improving signal-to-noise (SNR) in 1-D NMR spectroscopy is to multiply a free-induction decay signal (FID) by an exponential with the same decay time constant. This operation, which we will denote the NMR matched filter (NMR-MF), can strictly be applied only when the signal consists of a single exponential component, that is, when the corresponding spectrum consists of a single Lorentzian spectral line. It is nevertheless implemented empirically when multiple, and possibly non-Lorentzian, lines are present through multiplication by an exponential which roughly matches the decay of the FID; of course, the resulting SNR will then differ somewhat from that obtained in the ideal case. The NMR-MF can be understood intuitively by noting that SNR is greatest at the beginning of an FID and decreases over the acquisition period, so that preferential weighting of the initial part of the signal leads to an increase in spectral SNR after Fourier transformation. Multiplication by many functional forms would result in such preferential weighting; the fact that among exponentials, maximum SNR results from multiplication as described above has been demonstrated in many places (1–3). It is important to note that the

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SNR maximized in this way is defined according to maximum spectral line amplitude, rather than area.

However, the concept of an SNR-optimizing MF predates pulse NMR and has a long history in signal processing (4,5). This filter, which we denote the SP-MF, maximizes the SNR of a time domain signal and is derived by considering the FT of that signal (5,6). In contrast, the NMR-MF maximizes the SNR of a spectrum, and is derived by considering the FID, which is the inverse FT of that spectrum. At face value, then, the NMR-MF and the SP-MF are distinct constructs, although one suspects an intimate relationship. Given the fact that the ideal NMR lineshape, the Lorentzian, is the Fourier transform of a decaying exponential, it is tempting to state that the relationship between the NMR-MF and the SP-MF is trivial and follows from the convolution theorem. This is not quite the case. In fact, when queried, well-known NMR signal processing experts have stated that the NMR-MF and the SP-MF are quite different entities.

Our goal is to reconcile the SP-MF with the NMR-MF, demonstrating that contrary to appearances and common belief, they are equivalent. We demonstrate this from both a signal-domain approach and a transform-domain approach after first establishing our notation for the Fourier transform and reviewing the required concepts of convolution, the convolution theorem, and signal filtering.

Finally, we describe a modification of the MF which maximizes spectral SNR defined with respect to signal area rather than amplitude. The derivation of this modified matched filter (MMF) is based on the fact that spectral line area is proportional to the amplitude of the first point of the FID, which is also the position of maximal SNR.

The Fourier Transform (7)

The relationships between a continuous complex-valued function of time, $f(t)$, and its Fourier transform (FT) $F(\nu)$, which is a function of frequency, are

$$F(\nu) = \int_{-\infty}^{\infty} f(t)\, e^{-j2\pi\nu t}\, dt \tag{1}$$

and

$$f(t) = \int_{-\infty}^{\infty} F(\nu)\, e^{j2\pi\nu t}\, d\nu \tag{2}$$

The variables t and ν are called conjugate variables; according to these definitions, they must have reciprocal units. We will generally take $f(t)$ to be real; $F(\nu)$ will nevertheless be complex in general. $F(\nu)$ will be called the spectrum of $f(t)$; other definitions may be found in the literature. The real and imaginary parts of $F(\nu)$ define the amplitudes and phases of the frequency components comprising $f(t)$. From Eq.(2),

$$f(0) = \int_{-\infty}^{\infty} F(\nu)\, d\nu \tag{3}$$

In the case of one-dimensional NMR, in which $f(t)$ is the FID and $F(\nu)$ is the spectrum, this means that spectral line area is proportional to the initial value of the FID.

The FT is a map between function spaces and may be written

$$\Im\left[f(t)\right](\nu)=F(\nu) \tag{4}$$

with inverse mapping

$$\Im^{-1}\left[F(\nu)\right](t)=f(t) \tag{5}$$

Designating the variable labels in Eqs. (4) and (5) is not strictly necessary, but is often done for clarity to indicate functions in the domain and range of the FT. A common choice is *t* and ν, as in the above.

The FT operation, when composed with itself, does not yield the identity:

$$\Im\circ\Im\neq I \tag{6}$$

Rather,

$$\Im\left[\Im\left[f(t)\right]=f(-t)\right. \tag{7}$$

Similarly,

$$\Im^{-1}\left[\Im^{-1}\left[F(\nu)\right]=F(-\nu)\right. \tag{8}$$

The presence of the (−) signs in Eqs. (7) and (8) accounts for much of the difficulty in establishing the relationship between the NMR-MF and the SP-MF.

Convolution and the Convolution Theorem

The convolution of two functions *f*(*t*) and *g*(*t*) is defined by:

$$(f*g)(t)=\int_{-\infty}^{\infty}f(\tau)\,g(t-\tau)\,d\tau \tag{9}$$

and has the property

$$(f*g)(t)=(g*f)(t) \tag{10}$$

Convolution is of central importance because convolution in the time domain is equivalent to multiplication in the frequency domain, and conversely (7). For functions *f*(*t*) and *g*(*t*) with FT's *F*(ν) and *G*(ν) , the time convolution theorem is

$$\Im\left[(f*g)(t)\right](\nu)=F(\nu)\,G(\nu) \tag{11}$$

while the frequency convolution theorem is

$$\Im\left[f(t)\,g(t)\right](\nu)=(F*G)(\nu) \tag{12}$$

Signal Filtering

We consider a time domain signal, denoted $s(t)$, and its spectrum $S(\nu)$. Many filtering operations on $S(\nu)$ can be defined as increasing or decreasing the amplitude of $S(\nu)$ over particular frequency ranges corresponding respectively to desired or undesired frequency components. Such filtering is conveniently achieved by multiplication of $S(\nu)$ by a transfer function, $G(\nu)$, so that the filtered spectrum $S_F(\nu)$ is

$$S_F(\nu) = G(\nu)\, S(\nu). \tag{13}$$

Examples include low-pass filters designed to reduce or eliminate high-frequency noise; $G(\nu)$ is then large in the region of the frequency axis origin, that is at low frequencies, and smaller, perhaps zero, away from the origin towards higher frequencies. An ideal low-pass filter which eliminates all frequency components with $|\nu| > B$ while leaving all lower frequencies intact is the top-hat function

$$\begin{aligned} G(\nu) &= 1, |\nu| < B \\ &= 0, |\nu| > B \end{aligned} \tag{14}$$

A high-pass filter designed to emphasize rapid changes in the signal and de-emphasize slow drift, or a bandpass filter designed to emphasize the components of a signal within a certain frequency band, may be defined analogously. The SNR-maximization property used below to derive the SP-MF is an example of a design criterion more subtle than tailoring of frequency response.

Although filter characteristics are usually specified by a transfer function defined in the frequency domain, the filtering step is often applied to the time-domain signal directly so that desirable signal properties are presented to downstream processing steps. We can describe the time-domain operation corresponding to frequency filtering by using the convolution theorem. Applying the inverse FT to Eq. (13) and using Eq. (11), we find for the time-domain filtered signal $s_F(t)$:

$$\begin{aligned} s_F(t) &= \Im^{-1}\left[S_F(\nu)\right](t) \\ &= \Im^{-1}\left[G(\nu)\, S(\nu)\right](t) \\ &= (g * s)(t) \\ &= \int_{-\infty}^{\infty} g(\tau)\, s(t-\tau)\, d\tau \end{aligned} \tag{15}$$

where $g(t) = \Im^{-1}\left[G(\nu)\right](t)$. The function $g(t)$ is called the impulse response function of $G(\nu)$, since for an impulse signal $s(t) = \delta(t)$, where δ denotes the Dirac delta function, one has $s_F(t) = g(t)$.

In summary, we have described two formulations of filtering a signal $s(t)$ with spectrum $S(\nu)$. Filtering in the time domain by a filter with impulse response function $g(t)$ is defined by the convolution

$$s_F(t) = (g * s)(t) \tag{16}$$

with corresponding spectrum

$$S_F(\nu) = \Im[s_F(t)](\nu). \tag{17}$$

. Equivalently, filtering can be described in the frequency domain through multiplication by the corresponding transfer function

$$S_F(\nu) = G(\nu) S(\nu) \tag{18}$$

where the impulse response function and the transfer function are related by Fourier transformation:

$$\Im[g(t)](\nu) = G(\nu) \tag{19}$$

Derivation of the SP-MF

We now derive the SP-MF following Turin (5). Consider a waveform $x(t)$ consisting of a desired signal$s(t)$ corrupted by stationary white noise$n(t)$:

$$x(t) = s(t) + n(t) \tag{20}$$

The waveform $x_F(t)$ resulting from application of a filter with impulse response $g(t)$ to $x(t)$ will consist of components due to the desired signal and to the noise:

$$x_F(t) = s_F(t) + n_F(t) \tag{21}$$

We wish to determine the $g(t)$ that maximizes the ratio of the output power of the desired component of the filtered signal at some time $t = \Delta$, $s_F(\Delta)$, to the noise power. Let $S(n)$ denote the unfiltered spectrum of the desired signal and $G(n)$ the transfer function of the filter. $G(n)S(n)$ is the spectrum of the desired signal after filtering:

$$\Im[(g * s)(t)](\nu) = G(\nu) S(\nu) \tag{22}$$

with the amplitude of the corresponding filtered output at $t = \Delta$ given by:

$$\begin{aligned} s_F(\Delta) &= (g * s)(\Delta) \\ &= \Im^{-1}[G(\nu) S(\nu)](\Delta) \\ &= \int_{-\infty}^{\infty} G(\nu) S(\nu) e^{i2\pi\Delta\nu} d\nu \end{aligned} \tag{23}$$

The power in the filtered signal at time D is the square of this.

If the noise power density is P_0, the power density Y of the filtered noise is (8)

$$\Psi(\nu) = P_0 |G(\nu)|^2 \tag{24}$$

so that the total output noise power across all frequencies is

$$\int_{-\infty}^{\infty}\Psi(\nu)\,d\nu = P_0\int_{-\infty}^{\infty}|G(\nu)|^2 d\nu \tag{25}$$

Therefore, the SNR ratio we wish to maximize is

$$\rho = \frac{\left[\int_{-\infty}^{\infty} G(\nu)\,S(\nu)\,e^{i2\pi\Delta\nu}d\nu\right]^2}{P_0\int_{-\infty}^{\infty}|G(\nu)|^2 d\nu} \tag{26}$$

This can be accomplished through the Schwarz inequality (9), which states that for two complex-valued functions f_1 and f_2

$$\left|\int f_1(x)\,(f_2(x))^* dx\right|^2 \le \int|f_1(x)|^2 dx\int|f_2(x)|^2 dx \tag{27}$$

with equality holding if and only if $f_2(x) = kf_1^*(x)$, for k an arbitrary constant and with the asterisk denoting complex conjugate.

We identify $G(\nu)$ and $S(\nu)e^{i2\pi\Delta\nu}$ with $f_1(x)$ and $f_2(x)$, respectively, obtaining for the numerator of Eq. (26):

$$\left[\int_{-\infty}^{\infty} G(\nu)\,S(\nu)\,e^{i2\pi\Delta\nu}d\nu\right]^2 \le \int_{-\infty}^{\infty}|G(\nu)|^2 d\nu\int_{-\infty}^{\infty}|S(\nu)|^2 d\nu \tag{28}$$

Eq. (26) then becomes

$$\rho \le \frac{1}{P_0}\int_{-\infty}^{\infty}|S(\nu)|^2 d\nu \tag{29}$$

By inspection, equality in Eq. (28), maximizing the SNR ρ, holds for

$$G(\nu) = k(S(\nu))^* e^{-i2\pi\Delta\nu}. \tag{30}$$

Here and in the following, multiplicative constants in the definitions of filters and transfer functions represent arbitrary scaling and are of no significance.

Thus, the transfer function of the SP-MF, Eq. (30), is, except for an arbitrary multiplicative constant, equal to the complex conjugate of the spectrum of the desired signal, multiplied by an adjustable phase factor which defines the time, D, at which the filtered signal maximum is to occur. The designation “matched filter” refers to the fact that $G(\nu)$ is just a scaled and phase-shifted version of$(S(\nu))^*$. Eq. (30) also accounts for another common name for the SP-MF, namely the Fourier conjugate filter. It is of central importance that $G(\nu)$ is independent of $n(t)$, depending solely upon $s(t)$.

Eq. (30) defines the SP-MF in the frequency domain. We now wish to derive the equivalent time-domain representation, in accordance with Eq. (16), through signal convolution with the inverse FT of Eq. (30). We make use of the following relations. Denoting as usual Á[$f(t)$] (n) ° $F(n)$ for a real-valued function f, we have

$$\acute{\mathrm{A}}\left[f(-t)\right](n)=\left[F(n)\right]^{*} \tag{31}$$

and, if we define

$$\widehat{f}(t)=f(\mathrm{D}+t), \tag{32}$$

then

$$\acute{\mathrm{A}}\left[\widehat{f}(t)\right](n)^{\circ}\widehat{F}(n)=F(n)\,e^{i2p n\mathrm{D}} \tag{33}$$

The impulse response function corresponding to $G(\nu)$ defined in Eq. (30) is then

$$\begin{aligned} g(t) = {} & \acute{\mathrm{A}}^{-1}\left[k(S(n))^{*}e^{-i2p\mathrm{D}n}\right](t) \\ = {} & k\acute{\mathrm{A}}^{-1}\left\{\left[S(n)\,e^{+i2p\mathrm{D}n}\right]*\right\}(t) \\ = {} & k s(\mathrm{D}-t) \end{aligned} \tag{34}$$

that is, $g(t)$ is a shifted and time-reversed version of $s(t)$. Therefore, the filtered signal in the time domain is

$$\begin{aligned} s_{F}(t) &= (s*g)(t) \\ &= \acute{\mathbf{O}}\, s(t)\,g(t-t)\,dt \\ &= k\,\acute{\mathbf{O}}\, s(t)\,s(t-[t-\mathrm{D}])\,dt \\ &= k\mathrm{F}_{ss}(t-\mathrm{D}) \end{aligned} \tag{35}$$

with $\mathrm{F}_{ss}(t)$ denoting the autocorrelation function of $s(t)$.

It might be thought that application of this time-domain filtering to the special case of the FID will provide the NMR-MF. However, the above calculation was based on maximizing the SNR of a time-domain signal, not a spectrum, and calculations were performed in the frequency domain only for convenience in obtaining the final expression, Eq. (30), or equivalently, Eq. (34).

In summary, application of the SP-MF to the waveform$x(t) = s(t) + n(t)$ is accomplished by convolving it with a filter function $g(t)$ constructed from$s(t)$ as specified in Eq. (34). The SNR of the time-domain filtered signal is thereby maximized, as appropriate for detection and characterization of a pulse, such as a radar signal. The calculations leading to Eq. (30) were performed in the frequency domain, but otherwise the spectrum of the signal was not of independent interest. This is in contrast to NMR spectroscopy, where it is the SNR of the spectrum of a time-domain signal that is to be maximized. In effect, in NMR, the “pulse” which is to have its SNR maximized is on the frequency, rather than the time, axis. Before showing that the NMR-MF and the SP-MF are equivalent, we briefly review the effect of exponential multiplication of the FID in one-dimensional NMR and then discuss the derivation of the NMR-MF.

The FID and the Spectrum

We review well-known facts to establish our framework and notation. The FID for uncoupled spins is given by a superposition of damped sinusoids:

$$FID(t) = \sum_i 2M_{0i} e^{-t/T_{2,i}} \mathrm{COS} 2\pi\nu_{0,i} t \tag{36}$$

where i labels the $i-th$ signal component, with FID amplitude $2M_{0i}$, offset frequency $\nu_{0,i}$, and decay time constant $T_{2,i}$. Eq. (36) is written for single-phase detection; for quadrature detection, $\cos 2\pi\nu_{0,i}t$ is replaced by $e^{-2\pi\nu 0,it}$.

The signal for a single-component on-resonance FID is:

$$s(t) = 2M_0 e^{-t/T_2} \tag{37}$$

with corresponding spectral line

$$S(\nu) = 2M_0 \int_0^\infty e^{-t/T_2} e^{-i2\pi\nu t} dt \tag{38}$$

having real and imaginary parts:

$$S_{\mathrm{Re}}(\nu) = 2M_0 \frac{\left(\frac{1}{T_2}\right)}{\left(\frac{1}{T_2}\right)^2 + 4\pi^2\nu^2} \tag{39}$$

and

$$S_{\mathrm{Im}}(\nu) = -i2M_0 \frac{2\pi\nu}{\left(\frac{1}{T_2}\right)^2 + 4\pi^2\nu^2} \tag{40}$$

The spectral lineshape described by Eq. (39) is the Lorentzian line with area M_0. For a line with frequency offsetν_0,ν in Eqs. (39) and (40) is replaced by $\Delta\nu \equiv -\nu_0$. The maximum amplitude of $S_{\mathrm{Re}}(\nu)$ occurs at $\nu = 0$ and is

$$S_{\mathrm{Re,max}} = S_{\mathrm{Re}}(0) = 2M_0 T_2 \tag{41}$$

The full-width at half-maximum (FWHM) is

$$FWHM = \frac{1}{\pi T_2} \tag{42}$$

Exponential Multiplication of the FID

The signal after exponential multiplication (EM) by $r(t) = e^{-t/\tau}$ is:

$$s_{EM}(t) \equiv s(t)\, r(t) = 2M_0 e^{-t/T_2} e^{-t/\tau} \tag{43}$$

Comparison of Eq. (43) with Eq. (37) shows that we can obtain the spectrum and FWHM of $s_{EM}(t)$ by replacing $1/T_2$ in Eqs. (39) – (42) with $\left(\frac{1}{T_2}+\frac{1}{\tau}\right)$. Thus,

$$S_{EM,\mathrm{Re}}(\nu) = 2M_0 \frac{\left(\frac{1}{T_2}+\frac{1}{\tau}\right)}{\left(\frac{1}{T_2}+\frac{1}{\tau}\right)^2 + 4\pi^2\nu^2} \tag{44}$$

$$S_{EM,\mathrm{Im}}(\nu) = -i2M_0 \frac{2\pi\nu}{\left(\frac{1}{T_2}+\frac{1}{\tau}\right)^2 + 4\pi^2\nu^2} \tag{45}$$

$$S_{EM,\mathrm{Re,max}} = S_{EM,\mathrm{Re}}(\nu=0) = 2M_0 \frac{1}{\left(\frac{1}{T_2}+\frac{1}{\tau}\right)} \tag{46}$$

and

$$FWHM_{EM} = \frac{1}{\pi}\left(\frac{1}{T_2}+\frac{1}{\tau}\right) \tag{47}$$

Derivation of the NMR-MF

Since SNR is the main consideration in deriving the NMR-MF, the above approach must be modified to account for noise; data acquired after the FID has largely decayed is predominantly noise, so that SNR analysis must incorporate acquisition time.

Following Lindon and Ferrige (3), the spectral line resulting from acquisition of the FID over a time T is:

$$S_T(\nu) = 2M_0 \int_0^T e^{-t/T_2} e^{-i2\pi\nu t} dt \tag{48}$$

It can be shown either through direct calculation or using the convolution theorem that the spectral line maximum is attained at $n = 0$, as for Eq. (38). The maximum line amplitude is therefore

$$\begin{aligned} S_T(0) &= 2M_0 \int_0^T e^{-t/T_2} dt \\ &= 2M_0 T_2 \left(1 - e^{-T/T_2}\right) \end{aligned} \tag{49}$$

The RMS noise amplitude $\bar{n}$ is given in terms of the time-domain noise fluctuations by:

$$\bar{n} = \left\{ \frac{1}{T} \int_0^T [n(t)]^2 dt \right\}^{1/2} \tag{50}$$

Clearly, spectral domain noise will be proportional to time domain noise, as well as to a factor of $\sqrt{T}$, coming about from addition of random noise over time T. In the spectral domain, the RMS noise therefore becomes (8)

$$Noise = \sqrt{T}\,\bar{n} \tag{51}$$

so that the SNR, the ratio of Eq. (49) to Eq.(51), is:

$$SNR = \frac{2M_0}{\sqrt{T}\,\bar{n}} T_2 \left(1 - e^{-T/T_2}\right) \tag{52}$$

This is maximized as a function of T for T ; 1.25 T_2; additional signal acquired beyond this time is outweighed by additional noise, leading to a decrease in SNR. In fact, Eq. (52) shows that in the limit of $T \rightarrow \infty$, $SNR = 0$

The SNR of the exponentially multiplied signal is derived similarly, with the integrands in Eqs. (49) and (50) being multiplied by $e^{-t/\tau}$. One finds for the maximum line amplitude:

$$S_{T,EM,\max} = 2M_0 \frac{1}{\left(\frac{1}{T_2} + \frac{1}{\tau}\right)} \left(1 - e^{-T\left(\frac{1}{T_2} + \frac{1}{\tau}\right)}\right) \tag{53}$$

and for the RMS noise amplitude:

$$Noise_{EM} = \bar{n} \sqrt{\frac{\tau}{2}\left(1 - e^{-2T/\tau}\right)} \tag{54}$$

so that the resulting SNR is:

$$SNR_{EM} = \frac{2M_0}{\bar{n}} \frac{\left(1 - e^{-T\left(\frac{1}{T_2} + \frac{1}{\tau}\right)}\right)}{\sqrt{\frac{\tau}{2}\left(1 - e^{-2T/\tau}\right)}\left(\frac{1}{T_2} + \frac{1}{\tau}\right)} \tag{55}$$

Maximizing with respect to τ rsults in $\tau = T_2$, thus deriving the NMR-MF. Substituting $t = T_2$, the resulting SNR is:

$$SNR_{NMR-MF} = \frac{\sqrt{2}M_0}{\bar{n}} \sqrt{T_2}\left(1 - e^{-2T/T_2}\right)^{1/2} \tag{56}$$

In contrast to Eq. (52), SNR_{NMR-MF} increases as a function of T, although it is bounded as $T \rightarrow \infty$, reflecting the fact that the desired signal component diminishes with time.

Similarly, from Eqs. (44) and (47) the line shape and linewidth resulting from application of the NMR-MF are:

$$S_{MF,\mathrm{Re}}(\nu) = 2M_0 \frac{\left(\frac{2}{T_2}\right)}{\left(\frac{2}{T_2}\right)^2 + 4\pi^2\nu^2} \tag{57}$$

and

$$FWHM_{MF} = \frac{1}{\pi}\left(\frac{2}{T_2}\right) \tag{58}$$

These formulas are those that would be obtained directly from an FID decaying at twice the rate of that in Eq. (37), that is, from

$$s(t) = 2M_0 e^{-2t/T_2} \tag{59}$$

Strictly, the NMR-MF can only be derived for and applied to a single, Lorentzian, spectral line. In a multiple-line spectrum, one could apply the filter corresponding to the linewidth of the line for which maximizing the SNR is most critical. More commonly, the time constant of the multiplying exponential, τ, is estimated from the overall decay time constant of the FID envelope. This leads to a substantial increase in SNR for all spectral lines including those for which $T_{2,i} \neq \tau$ (3).

Relationship between the NMR-MF and the SP-MF

We can now consider the relationship between the NMR-MF and the SP-MF. We will make use of the following FT relationships.

$$\Im\left[e^{-\alpha|t|}\right](\nu) = \frac{2\alpha}{\alpha^2 + 4\pi^2\nu^2} \tag{60}$$

and, from symmetry,

$$\Im\left[\frac{2\alpha}{\alpha^2 + 4\pi^2 t^2}\right](\nu) = e^{-\alpha|\nu|} \tag{61}$$

These expressions have been written for the conventional case in which the FT is applied to a function of time, *t*, and produces a function of frequency, ν. Since conjugate variables must have reciprocal units, the FT of functions of frequency will be functions of a variable with dimensions of time. However, due to Eqs. (7) and (8), this variable must be distinguished from that of Eq. (1) and will be denoted $\tilde{t}$. The relationships between the variable labels we are using is:

$$g(t) \xrightarrow{\Im} G(\nu) \xrightarrow{\Im} \Gamma\left(\tilde{t}\right) \tag{62}$$

where $\Gamma\left(\tilde{t}\right)$, a function of a variable with the dimensions of time, is the FT of a function of frequency. Functions of ν are in the conjugate FT domain of functions of *t*, and functions of $\tilde{t}$ are in the conjugate FT domain of functions of ν. With this notation, Eq. (61) becomes:

$$\Im\left[\frac{2\alpha}{\alpha^2+4\pi^2\nu^2}\right]\left(\tilde{t}\right)=e^{-\alpha|\tilde{t}|} \tag{63}$$

so that we also have, using Eq. (39),

$$\begin{aligned}\Im\left[S_{\mathrm{Re}}(\nu)\right]\left(\tilde{t}\right) &= \Im\left(2M_0\frac{\left(\frac{1}{T_2}\right)}{\left(\frac{1}{T_2}\right)^2+4\pi^2\nu^2}\right)\left(\tilde{t}\right)\\ &= M_0e^{-|\tilde{t}|/T_2}\end{aligned} \tag{64}$$

Given the Fourier transform pair

$$\Im\left[G(\nu)\right]\left(\tilde{t}\right)=\Gamma\left(\tilde{t}\right) \tag{65}$$

we note for later use that Eq. (33) may be written

$$\Im\left[G(\nu-\Delta)\right]\left(\tilde{t}\right)=\Gamma\left(\tilde{t}\right)e^{-i2\pi\tilde{t}\Delta} \tag{66}$$

so that

$$\Im^{-1}\left[\Gamma\left(\tilde{t}\right)e^{-i2\pi\tilde{t}\Delta}\right](\nu)=G(\nu-\Delta) \tag{67}$$

The equivalence of the NMR-MF and the SP-MF can now be demonstrated in both the $\tilde{t}$ -domain and the ν -domain.

I. Maximizing the SNR of a spectral “pulse”: conjugate domain approach

As noted, the SP-MF is designed to maximize the SNR of a time-domain pulse signal, although the calculations are carried out in the frequency domain. In NMR, the desire is to maximize the SNR of a spectral line, and the analogous calculation must again take place in the conjugate FT domain, that is, in the $\tilde{t}$ domain.

To maximize the SNR of a frequency “pulse”, i.e., a spectral line, we proceed by analogy to the development starting with Eq. (20). The frequency domain waveform is denoted

$$x(n)=S_{Re}(n)+n(n) \tag{68}$$

with $S_{\mathrm{Re}}(\nu)$ given by Eq. (39). By direct analogy with Eq. (30), the SP-MF is implemented by multiplying the FT of $S_{\mathrm{Re}}(\nu)$ by the transfer function

$$G\left(\tilde{t}\right)=k\left(\Im\left[S_{\mathrm{Re}}(\nu)\right]\left(\tilde{t}\right)\right)^{*}e^{-i2\pi\Delta\tilde{t}} \tag{69}$$

so that the transform-domain representation of the filtered signal is

$$\begin{aligned} S_{SP-MF}\left(\tilde{t}\right) &= k\left|\Im\left[S_{\mathrm{Re}}(\nu)\right]\left(\tilde{t}\right)\right|^{2}e^{-i2\pi\Delta\tilde{t}} \\ &= kM_0{}^2e^{-2|\tilde{t}|/T_2}e^{-i2\pi\Delta\tilde{t}} \end{aligned} \tag{70}$$

where we have used Eq. (64). We take the inverse FT to recover the form of the spectral line after matched filtering:

$$\begin{aligned} S_{SP-MF}(\nu) &= \Im^{-1}\left[kM_0{}^2e^{-2|\tilde{t}|/T_2}e^{-i2\pi\Delta\tilde{t}}\right](\nu) \\ &= kM_0{}^2\Im^{-1}\left[e^{-2|\tilde{t}|/T_2}\right](\nu-\Delta) \\ &= 2kM_0^2\frac{\left(\frac{2}{T_2}\right)}{\left(\frac{2}{T_2}\right)^2+4\pi^2(\nu-\Delta)^2} \end{aligned} \tag{71}$$

As stated, Δ is an arbitrary offset that permits shifting the position of the signal maximum; it can be set to zero. The identical form of Eq. (71) and Eq. (57) is the desired result, demonstrating that the SP-MF is equivalent to the NMR-MF.

II. Maximizing the SNR of a spectral “pulse”: spectral domain approach

The equivalence of the SP-MF and the NMR-MF can also be demonstrated in the pulse domain. In the classic treatment of the SP-MF, this is the time domain; in our case, for maximizing the SNR of a spectral line, it is the frequency domain. The pulse shape is given by Eq. (39), so that

$$\begin{aligned} S_{SP-MF}(\nu) &= 2M_0\frac{\left(\frac{1}{T_2}\right)}{\left(\frac{1}{T_2}\right)^2+4\pi^2\nu^2} * 2kM_0\frac{\left(\frac{1}{T_2}\right)}{\left(\frac{1}{T_2}\right)^2+4\pi^2(\nu-\Delta_\nu)^2} \\ &= 4kM_0^2\int\frac{\left(\frac{1}{T_2}\right)}{\left(\frac{1}{T_2}\right)^2+4\pi^2\nu'^2}\frac{\left(\frac{1}{T_2}\right)}{\left(\frac{1}{T_2}\right)^2+4\pi^2(\nu-\nu')^2}d\nu' \\ &= 4kM_0^2\frac{\left(\frac{1}{T_2}\right)}{\left(\frac{2}{T_2}\right)^2+4\pi^2\nu^2} \end{aligned} \tag{72}$$

where we have set the arbitrary frequency offset $\Delta_\nu = 0$ for simplicity. This is the form of the filtered “pulse”, that is, the spectral lineshape, and is equivalent to Eqs. (57) and (72)..

III. Equivalence of SNR resulting from the SP-MF and the NMR-MF

The equivalence of the functional forms of the filtered signal resulting from application of the SP-MF and the NMR-MF has been established; we now demonstrate the equality of the SNR of the filtered signals.

The SNR of the spectrum obtained from the SP-MF follows from Eq. (29). We use Parseval's theorem, stating that the energy in a signal $s(t)$ is equal to the energy in its Fourier transform $S(\nu)$ (7):

$$\int_{-\infty}^{\infty}[s(t)]^2 dt = \int_{-\infty}^{\infty}[S(\nu)]^2 d\nu \tag{73}$$

For $s(t)$ given by Eq.(37) and for acquisition over a time T, the equality in Eq. (29), achieved under matched filtering, may therefore be written

$$\begin{aligned}\rho &= \frac{1}{P_0}\int_{-\infty}^{\infty}|s(t)|^2 dt \\ &= \frac{4}{P_0}\int_0^T |M_0 e^{-t/T_2}|^2 dt \\ &= \frac{2M_0^2}{P_0}T_2\left(1-e^{-2T/T_2}\right)\end{aligned} \tag{74}$$

This is the ratio of the signal power to the noise power $P_o = \bar{n}^2$, so that in terms of the amplitude-based SNR:

$$SNR_{SP-MF} = \frac{\sqrt{2}M_0}{\bar{n}}\sqrt{T_2}\left(1-e^{-2T/T_2}\right)^{1/2} \tag{75}$$

in agreement with Eq. (56).

To summarize, the equivalence of the NMR-MF and the SP-MF has now been established through calculations both in the domain of the NMR spectral line and in its conjugate domain.

The Matched Filter in Continuous-wave NMR

It is worth mentioning as a historical note that interpretation of the MF in continuous wave (CW) NMR with field sweeping poses no difficulties (2,10) because the spectral line is acquired directly as a time domain signal. The absorption of a radio frequency wave is measured as a function of field strength, with maximum absorption occurring at resonance and decreasing absorption being observed away from that maximum. For a Lorentzian spectral line, the signal is of the form

$$S_{CW}(t) = 2M_0\frac{\left(\frac{1}{T_2}\right)}{\left(\frac{1}{T_2}\right)^2 + 4\pi^2\alpha^2 t^2} \tag{76}$$

where α is the sweep rate in Hz/s. The MF is then given by Eq. (34) and the filtered signal by Eq. (35):

$$\begin{aligned} S_{CW-MF}(t) &= 2M_0 \frac{\left(\frac{1}{T_2}\right)}{\left(\frac{1}{T_2}\right)^2 + 4\pi^2\alpha^2 t^2} * 2kM_0 \frac{\left(\frac{1}{T_2}\right)}{\left(\frac{1}{T_2}\right)^2 + 4\pi^2\alpha^2(\Delta - t)^2} \\ &= 4kM_0^2 \int_{-\infty}^{\infty} \frac{\left(\frac{1}{T_2}\right)}{\left(\frac{1}{T_2}\right)^2 + 4\pi^2\alpha^2\tau^2} \frac{\left(\frac{1}{T_2}\right)}{\left(\frac{1}{T_2}\right)^2 + 4\pi^2\alpha^2(\Delta - t + \tau)^2} d\tau \\ &= \frac{4kM_0^2}{\alpha} \frac{\left(\frac{1}{T_2}\right)}{\left(\frac{2}{T_2}\right)^2 + 4\pi^2\alpha^2 t^2} \end{aligned} \quad (77)$$

where we have again set the arbitrary delay $\Delta = 0$. Thus, the spectral line after MF is again of the same form as the non-filtered line, but with twice the linewidth. This calculation follows that of Ernst (10).

Maximizing SNR With Respect to Area Rather than Amplitude

I. Distortion of line amplitude ratios, but not area ratios, by exponential multiplication

The MF as described maximizes SNR when the signal is defined in terms of *amplitude*; this is peak height in the case of NMR. However, signal *area* is the preferred measure of resonance intensity in NMR. Perhaps the most important reason for this is that lineshape can vary widely between spectral lines within a spectrum, so that quantification by amplitudes may not accurately reflect underlying concentration ratios. Another less well-known reason is that spectral line area ratios, but not amplitude ratios, are invariant under exponential filtering; concentration ratios can therefore be distorted.

Consider two spectral lines with amplitudes $S_{A,\max} = 2M_{0A}T_2\,(A)$ and $S_{B,\max} = 2M_{0B}T_2\,(B)$ (Eq.(41)) and therefore line amplitude ratio

$$\frac{S_{A,\max}}{S_{B,\max}} = \frac{M_{0A}T_2\,(A)}{M_{0B}T_2\,(B)} \quad (78)$$

After exponential multiplication with a decaying exponential of time constant τ, the ratio of peak amplitudes is instead (Eq. (46))

$$\frac{S^{EM}_{A,\max}}{S^{EM}_{B,\max}} = \frac{M_{0A}\left(\frac{1}{T_2(B)} + \frac{1}{\tau}\right)}{M_{0B}\left(\frac{1}{T_2(A)} + \frac{1}{\tau}\right)} \quad (79)$$

yielding an incorrect value except in the special case $T_2(A) = T_2(B)$. Therefore, line amplitude ratios are invariant under exponential multiplication only for lines with equal intrinsic linewidths. Of course this is also the only case in which the MF can be unambiguously defined for two lines simultaneously.

Consider instead the area of a spectral line after exponential multiplication. Using Eq. (44), one finds

$$\begin{aligned} Area &= \int_{-\infty}^{\infty} S_{EM,\mathrm{Re}}(\nu)\, d\nu \\ &= M_0 \end{aligned} \quad (80)$$

independent of linewidth and of τ. Thus, line areas and area ratios are not distorted by exponential multiplication, including application of the NMR-MF, in contrast to the distortion that occurs when line amplitudes are used for quantification.

II. The Modified Matched Filter

It is evident from the above that it can be important to maximize SNR based not on line amplitude, as achieved by the SP-MF and NMR-MF, but rather based on line area. This leads us to a modified matched filter (MMF).

Derivation of the MMF—We can readily modify the approach of Lindon and Ferrige outlined above. Using Eq. (80) rather than Eq. (53) as the numerator in the SNR ratio but retaining Eq. (54) as the denominator, we find, instead of Eq. (55), that

$$SNR_{MMF} = M_0 \frac{1}{\bar{n}\sqrt{\frac{\tau}{2}\left(1 - e^{-2T/\tau}\right)}} \tag{81}$$

The units of SNR as defined by Eq. (81) are different from those in Eq. (55), but maximization with respect to τ may nevertheless be performed. It is clear from inspection of Eq. (81) that SNR increases monotonically and without bound as $\tau \rightarrow 0$, that is, for an infinitely rapidly decaying exponential function. Further, SNR as defined by line area will be greater than that obtained by use of the NMR-MF whenever $\tau > T_2$. These properties define the NMR-modified matched filter, denoted as the NMR-MMF.

The behavior in the limit $\tau \rightarrow 0$ can be expected. A weighting function

$$w(t;\tau) = e^{-t/\tau} \tag{82}$$

with $\tau \rightarrow 0$ weights the FID maximally at the first point of the FID, where time-domain SNR is greatest, and de-emphasizes all subsequent times, while preserving line area (Eq. (3)).

The line shape resulting from application of the NMR-MMF is given by

$$S_{NMR-MMF,\mathrm{Re}}(\nu) = \lim_{\tau\rightarrow 0} 2M_0 \frac{\left(\frac{1}{T_2}+\frac{1}{\tau}\right)}{\left(\frac{1}{T_2}+\frac{1}{\tau}\right)^2 + 4\pi^2\nu^2} \tag{83}$$

with amplitude

$$S_{NMR-MMF,Max}(0) = \lim_{\tau\rightarrow 0} 2M_0 \frac{\left(\frac{1}{T_2}+\frac{1}{\tau}\right)}{\left(\frac{1}{T_2}+\frac{1}{\tau}\right)^2} = \lim_{\tau\rightarrow 0} 2\tau M_0 = 0 \tag{84}$$

The NMR-MMF therefore produces a spectral line with infinite SNR, zero amplitude, and infinite linewidth (Eq. (47)). This is clearly unacceptable. In fact, the amount of line broadening permissible in a particular experiment is defined primarily by the requirement to resolve spectral lines. A more appropriate implementation of the MMF approach is then to line broaden beyond the usual NMR-MF, but only to the point of maintaining required spectral resolution.

As expected, it is also possible to derive the MMF filter using the signal processing approach. The area of the filtered pulse is obtained from integrating Eq. (23) over Δ, with this then divided by the total output noise to obtain the SNR. We use the following representation of the Dirac delta function:

$$\delta(\nu) = \int_{-\infty}^{\infty} e^{i2\pi\Delta\nu} d\Delta \tag{85}$$

so that

$$\begin{aligned} \int_{-\infty}^{\infty} s_F(\Delta)\, d\Delta &= \int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} G(\nu)\, S(\nu)\, e^{i2\pi\Delta\nu} d\nu \right] d\Delta \\ &= \int_{-\infty}^{\infty} G(\nu)\, S(\nu)\, \delta(\nu)\, d\nu \\ &= G(0)\, S(0) \end{aligned} \tag{86}$$

We therefore wish to determine the function $G(\nu)$ that maximizes:

$$SNR = \frac{G(0)\, S(0)}{P_0 \int_{-\infty}^{\infty} |G(\nu)|^2 d\nu} \tag{87}$$

$G(0)$ can be taken as any non-zero value, which we will choose as $G(0) = 1$. By inspection, SNR is maximized when $G(\nu)$ is as small as possible for $|\nu| > 0$. A convenient form is

$$G(\nu) = e^{-|\nu|/\tau} \tag{88}$$

with $\tau \to 0$.

Eq. (87) was derived for the conventional case of a filter applied to a time-domain function, with conjugate domain variable *n*. In NMR, with the pulse waveform in the *n* domain and the conjugate domain variable $\tilde{t}$, the transfer function is

$$G\left(\tilde{t}\right) = e^{-|\tilde{t}|/\tau} \tag{89}$$

The filtered signal in the $\tilde{t}$ -domain is therefore:

$$\begin{aligned} S_{SP-MMF}\left(\tilde{t}\right) &= k\Im\left[S_{\mathrm{Re}}(\nu)\right]\left(\tilde{t}\right) e^{-|\tilde{t}|/\tau} \\ &= kM_0 e^{-|\tilde{t}|/T_2} e^{-|\tilde{t}|/\tau} \\ &= kM_0 e^{-(1/T_2 + 1/\tau)|\tilde{t}|} \end{aligned} \tag{90}$$

so that the filtered spectral line is

$$\begin{aligned} S_{SP-MMF}(\nu) &= \Im^{-1}\left[kM_0 e^{-(1/T_2 + 1/\tau)|\tilde{t}|} \right](\nu) \\ &= 2kM_0 \frac{\left(\frac{1}{T_2} + \frac{1}{\tau}\right)}{\left(\frac{1}{T_2} + \frac{1}{\tau}\right)^2 + 4\pi^2\nu^2} \end{aligned} \tag{91}$$

As $\tau \to 0$, as required for the MMF, this is Eq. (83) up to a multiplicative constant.

As always, one can instead start from the transfer function in the conjugate $\tilde{t}$ domain and calculate the ν -domain filter which is to be convolved with the spectral line to implement the SP-MMF. The transfer function is Eq.(89), so that filtering in theν -domain is accomplished by:

$$\begin{aligned} S_{SP-MMF}(\nu) &= S_{\mathrm{Re}}(\nu) * \Im^{-1}\left[e^{-|\tilde{t}|/\tau}\right] \\ &= 2M_0 \frac{\left(\frac{1}{T_2}\right)}{\left(\frac{1}{T_2}\right)^2 + 4\pi^2\nu^2} * \frac{2\left(\frac{1}{\tau}\right)}{\left(\frac{1}{\tau}\right)^2 + 4\pi^2\nu^2} \\ &= 2M_0 \int \frac{\left(\frac{1}{T_2}\right)}{\left(\frac{1}{T_2}\right)^2 + 4\pi^2\nu'^2} \frac{2\left(\frac{1}{\tau}\right)}{\left(\frac{1}{\tau}\right)^2 + 4\pi^2(\nu-\nu')^2} d\nu \\ &= M_0 \frac{\left(\frac{1}{T_2} + \frac{1}{\tau}\right)}{\left(\frac{1}{T_2} + \frac{1}{\tau}\right)^2 + 4\pi^2\nu^2} \end{aligned} \tag{92}$$

which is equivalent to Eq. (91).

The discussion of the MMF highlights the tradeoff between improving SNR and avoiding excessive line broadening in the application of an apodization function (2). An important advance in this area has been the introduction of the TRAF functions (11), which are effective in increasing spectral SNR without significantly increasing linewidth.

Conclusion

The NMR-MF is equivalent to the SP-MF as applied to an FID, but this equivalence does not follow trivially from the convolution theorem. Derivation requires careful attention to the definition of the signal domain. In the case of the SP-MF, this is time, with frequency as the conjugate domain. For the NMR-MF, the signal domain is frequency, with a conjugate domain variable having units of time, but being distinct from the acquisition time domain. In addition, although calculation of spectral line areas, rather than amplitudes, is the preferred method of quantification in NMR, the SP-MF and the NMR-MF maximize SNR according to amplitude. SNR maximization according to line area requires a slight modification of the usual MF.

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