Journal of Magnetic Resonance 233 (2013) 64–73

Contents lists available at SciVerse ScienceDirect

Journal of Magnetic Resonance

journal homepage: www.elsevier.com/locate/jmr

Extrapolation and phase correction of non-uniformly broadened signals

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ARTICLE INFO

Article history:
Received 6 February 2013
Revised 2 May 2013
Available online 18 May 2013

Keywords:
Extrapolation
Phase-correction
Cardinal series
Bayesian
Oversampling
Porous
MRI

ABSTRACT

The initial part of FID-signals cannot always be acquired experimentally. This is particularly true for signals characterised by strong inhomogeneous broadening, such as those in porous materials, e.g. cements, soils and rocks, those measured by portable NMR-apparatus, or EPR-signals. Here we report on a numerical method we designed to extrapolate those initial missing parts, i.e. to retrieve their amplitude and phase. Should the entire signal be available from an experiment, the algorithm can still be used as an automatic phase-corrector and a low-pass filter. The method is based on the use of cardinal series, applies to any oversampled signals and requires no prior knowledge of the system under study. We show that the method can also be used to restore entire one-dimensional MRI-data sets from those in which less than half of the *k*-space was sampled, thus not only potentially allowing to speed up data acquisition – when extended to two or three dimensions, but also to circumvent phase-distortions usually encountered when exploring the *k*-space near its origin.

1. Introduction

In magnetic resonance spectroscopy and imaging, signals, experimentally acquired as a function of the time, are usually Fourier- or Laplace-transformed [1–5] to obtain precession or relaxation spectra, or images. Quite often, though, physically or chemically relevant information is extracted from the signal direct in the time domain [6–10]. Recording of the FID-signal can effectively start a short while after the end of the last RF-pulse to avoid burning the receiver by feeding into it intense RF-field generated by the transmitter. Furthermore a few first samples of the FID-signal was sometimes found to have much lower signal-to-noise ratio than in the rest of the signal and should be rejected [11]. This is of rather limited importance when studying systems characterised by slow spin–spin relaxation and uniform magnetic susceptibility [11,12–15] and can, if necessary, easily be avoided by using more sophisticated acquisition protocols rather than a single-pulse sequence [7,15]. On the contrary, this becomes a real problem when a system with great intrinsic heterogeneity of magnetic susceptibility, such as interstitial fluids in porous materials, should be studied, as then a significant part of its FID-signal turns out to be irreversibly lost because of its fast defocusing combined with molecular diffusion. Similar problems can arise when using mobile NMR-spectrometers or -imagers [17–19], whose magnetic field is rather inhomogeneous.

Depending on the system and purpose of its investigation, various approaches have been taken to process incomplete signals. There are methods that rely on comparison of experimental signals with those in data bases [20]. Those are of little use for processing signals of heterogeneous systems, for which there are no data bases. Other methods, e. g. maximum entropy [21,22], multi-way decomposition [23,24], periodgrams [25], base cosine fitting [26] and some others [27], are intended for calculating spectra rather than the signal in the time domain. Signals in the time domain can be recalculated by methods such as linear prediction [28–34] and Lagrange interpolation [35,36]. Nevertheless linear prediction algorithms assume that the FID-signal can be approximated by a sum of complex exponentials and so can hardly be applicable to the extremely narrow FID-signals of heterogeneous systems, such as porous materials, known to have no particular shape. Moreover, having proved themselves suitable for restoring FID-signals at long times, both methods fail to recalculate the signals at short times owing to their extreme sensitivity to noise [39]. Yet signals of porous media are characterised by relatively low signal-to-noise ratio. Finally, there are techniques provided by the non-uniform sampling theory [37,38], which deals with the problem of reconstruction of band-limited functions from sets of their non-uniform samples. To do so, the function is periodically copied and thus constructed periodic function approximated by a series of trigonometric polynomials in the least-square sense [39]. If these techniques happened to be numerically stable enough [39,40], they could possibly be applied to processing heterogeneously broadened

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http://dx.doi.org/10.1016/j.jmr.2013.05.003

NMR-signals. Here we report on a numerical method based on the use of cardinal series for extrapolation of both the amplitude and phase of the missing initial parts of such FID-signals. In the past we already used cardinal series to design a low pass filter [41], an algorithm to identify and remove strong sporadic noise [42] and an interpolation technique [36] for such NMR-signals and so could convince ourselves with their low sensitivity to noise.

2. Theory

2.1. Interpolation of echo signals

According to the sampling theorem [43–45], any band-limited signal with a band width Ω_0 can be expressed as an infinite cardinal series:

$$x(t) = \sum_{p=-\infty}^{+\infty} a_p \mathrm{sinc}\frac{\Omega}{2}(\tau_p - t), \tag{1}$$

where the cardinal sine function *sinc* is defined as

$$\mathrm{sinc}(\alpha) = \frac{\sin\alpha}{\alpha}, \tag{2}$$

the positions of the maxima of the cardinal sine functions τ_p's are regularly spaced by $\delta\tau = \tau_{p+1} - \tau_p = 2\pi/\Omega$ and the band width of the series Ω has to be equal to or greater than that of the signal Ω_0 to satisfy the Nyquist condition. Here we defined the band width Ω_x so that $\Omega_x/2\pi$ corresponds to the band width in Hertz in the common usage of NMR-spectroscopists.

Using numerical simulations [41,42], we showed that many band-limited analogue signals within an interval $[t_{\mathrm{inf}}, t_{\mathrm{sup}}]$ can be approximated by a finite cardinal series determined within the finite interval $[t_{\mathrm{inf}} - 6\delta\tau, t_{\mathrm{sup}} + 6\delta\tau]$ with a bias that does not exceed the computer double precision round-off error:

$$x(t_{\mathrm{inf}} < t < t_{\mathrm{sup}}) \approx \sum_{t_{\mathrm{inf}}-6\delta\tau<\tau_p<t_{\mathrm{sup}}+6\delta\tau} a_p \mathrm{sinc}\frac{\Omega}{2}(\tau_p - t), \tag{3}$$

This permits to describe the analogue signal by means of solely a finite number of coefficients a_p's. Here a_p's will usually differ from $x(t_p)$'s outside the interval $[t_{\mathrm{inf}}, t_{\mathrm{sup}}]$.

To reconstruct the continuous function from a finite number of samples randomly placed in the interval $[t_{\mathrm{inf}}, t_{\mathrm{sup}}]$, these coefficients can be determined from the least-square minimisation of the difference between samples' values and the right hand side of Eq. (3). Once the a_p's have been found, they can be fed back in to Eq. (3) to calculate $x(t)$ at an arbitrary moment of the time t within $[t_{\mathrm{inf}}, t_{\mathrm{sup}}]$ and thus restore the continuous signal. Should the data set lack samples within broad intervals inside $[t_{\mathrm{inf}}, t_{\mathrm{sup}}]$, the band width of the series Ω should be set as narrow as possible, while making sure to satisfy the Nyquist criterion, to maximise performance of the interpolation. The optimal value we found numerically and suggest here is $\Omega = 1.1\Omega_0$.

We showed [36] that this can be used as an extremely accurate interpolation method for restoration of the signal over intervals as large as several times its Nyquist period, provided the rest of the signal was oversampled. Moreover, when applied to noise-impaired samples, this reconstruction method was shown to act as an efficient low pass filter as well [41,42]. However, this approach failed utterly when used for extrapolation of the signal outside $[t_{\mathrm{inf}}, t_{\mathrm{sup}}]$.

The extrapolation method described below consists in using certain symmetry of NMR-signals to generate additional samples of it on the opposite side of the extrapolation area and thus convert the problem of extrapolation into that of interpolation. The latter can safely be conferred to the cardinal series. All necessary information on the setting parameters of the cardinal series will be given in due time. For more detail on modelling NMR-signals by cardinal series the reader is referred to our previous works [42].

2.2. Restoration of the initial part of FID-signals

The complex band-limited FID-signal $x(t)$ refocused at $t = 0$ can be expressed in the rotating frame as a function of its, real-valued, pure absorption spectrum $\tilde{x}(\omega)$

$$x(t) = e^{i\phi}\int_{-\frac{\Omega_0}{2}}^{\frac{\Omega_0}{2}} \tilde{x}(\omega)e^{i\omega t}d\omega, \tag{4}$$

where the phase ϕ depends on numerous factors, such as model of the spectrometer, capacitance of the resonant circuit of the probe, receiver gain, sweep width, phase of the reading RF-pulse and so is usually unknown. Here we associated the genuine beginning $t = 0$ of the FID-signal, as it is usually done, with the middle of the last pulse in the pulse sequence. The spectrum $\tilde{x}(\omega)$ will usually be positive all over its domain of definition. However the method proposed herein can deal with any band-limited function whatever the sign its spectrum assumes. Let us now assume that the analogue-to-digital convertor (ADC) of the spectrometer provided us with N samples $\{x_n = x(t_n)\}_{n=1}^{N}$ of the FID-signal of Eq. (4) within the interval $[t_1, t_N]$, which we shall arrange in a column vector X_+ of the length $2N$

$$X_+ = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ x_1 \\ \vdots \\ x_N \end{pmatrix}, \tag{5}$$

where N zeros were added for convenience of writing the expressions below. The strictly positive t_1 corresponds to the moment when the acquisition can actually start, which depends on the length of what is sometimes called the spectrometer's dead time. Note also that the last sample x_N is not necessary equal to zero, as the acquisition may, deliberately or not, be ended prematurely. The algorithm described below aims at reconstructing the missing initial part of signal within the interval $[0, t_1]$.

Let us now imagine the FID-signal of Eq. (4) as a right-hand part of an echo with its summit at $t = 0$. In doing so, we do not imply that such an echo can be generated experimentally. According to Eq. (4), the left-hand part of the echo can then be expressed as a function of its right-hand part as

$$x(-t) = e^{2i\phi}x(t)^*, \tag{6}$$

where the asterisk stands for the complex conjugate. The symmetry expressed by Eq. (6) allows to construct an echo data set within the interval $[-t_N, -t_1] \cup [t_1, t_N]$ from the FID data set of Eq. (5), which we shall also arrange in a column vector, X, of the length $2N$:

$$X = X_+ + e^{2i\phi}X_-, \tag{7}$$

where

$$X_- = \begin{pmatrix} x_N^* \\ \vdots \\ x_1^* \\ 0 \\ \vdots \\ 0 \end{pmatrix} \tag{8}$$