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Cardinal series to sort out defective samples in magnetic resonance data sets

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ABSTRACT

NMR signals are unavoidably impaired with noise stemming from the electronic circuits of the spectrometer. This noise is most often white and Gaussian and can be greatly reduced by applying low pass analogue and digital filters. Nevertheless, extra noise with other statistics than Gaussian may interfere with the signal, e.g. when auxiliary electrical devices are placed near the magnet of the NMR spectrometer. This paper reports on how one can make use of this difference in statistics to remove the noise caused by electrical devices before any further data processing. The algorithm is based on the use of a new linear low pass filter, which consists in fitting NMR data in the time domain with a cardinal series and whose spectral width can be controlled. Over other filtering methods such filter has the advantage of not distorting the signal neither at the beginning nor the end of the acquisition period. The performance of the method is demonstrated by applying it to a data set collected in a flow PGSE experiment and impaired with noise emanated from a brushed DC electric motor.

1. Introduction

NMR signals are inevitably corrupted by noise stemming from electronic circuits of the spectrometer. Within the spectrometer's bandwidth, this noise can most often be viewed as white and Gaussian. As the spectrum of the signal emanating from the sample is, contrariwise, limited to a rather restricted zone of the frequency domain, most noise can be efficiently eliminated with the benefit of low pass filters. For this purpose, most commercial spectrometers are now equipped with either finite (FIR) or infinite (IIR) impulse response analogue and digital filters with often a limited number of fixed bandwidths.

After its frequency has been scaled down from radio to audio range, the continuous physical signal emitted by the NMR sample is fed into analogue filters. The digital filters are fed with discrete data points of the signal sampled by analogue-to-digital converters (ADC) at a much higher frequency than required by the Nyquist criterion to accurately record all the harmonics in the spectrum of the signal. The output of the filters of either type is a signal from which high frequency noise was removed and whose frequency band width and sampling frequency, as far as digital filters are concerned, correspond to the Bruker acquisition parameter *swh* set by the spectroscopist. One can also deliberately acquire an oversampled signal by increasing *swh* and using an analogue filter with a broader passband and process it with one of the digital convolution filter described in literature.

Unfortunately, most known analogue and digital convolution filters are designed to optimise the filtering of signals in the frequency domain and tend to severely distort them in the time domain when applied to truncated signals. In this manuscript we outline the principles of a new linear low pass filtering method that preserves all the features of the signal in both time and frequency domain. The filtering method is an example of using the Bayesian approach to solving inverse problem [1] and consists in fitting raw NMR data with a finite sum of cardinal sine functions. A thorough description of the 'cardinal series filter' and rules for setting its parameters will be discussed in detail elsewhere. Instead, we introduce herein one of possible applications of this filter and demonstrate its usefulness in processing data collected in a PGSE experiment for determining velocity field in a fluid flowing in a porous medium.

Certain experiments require that auxiliary electric devices should be placed near or inside the magnet of the NMR spectrometer, which may bring about severe extra distortions of measured NMR signals [2–9]. In rheological and fluid mechanics studies by NMR in particular, electric motors and various monitoring units are put underneath the magnet of the NMR tomographer. Such distortions often obey statistics rather different from that of above-mentioned electronic noise. Unlike Gaussian noise, they often appear as a limited number of chaotically dispersed sharp spikes in the time domain, have hardly identifiable spectrum patterns and thus are difficult to remove by using a linear low pass filter. Noise caused by a brushed DC electric engine, which we have

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observed in our rheological studies [6–9], has a significantly higher covariance than Gaussian electronic noise; and even though only about one of ten NMR data samples were thus affected, it greatly reduced the overall signal-to-noise ratio, while Gaussian noise level was very reasonable.

Herein we suggest how the above-mentioned difference in noise statistics can be used to eliminate those highly defective samples from each individual FID record of an experiment, before adding them together to implement further noise averaging and phase cycling. The proposed algorithm applies to oversampled band-limited NMR signals and relies on a recursive use of the cardinal series filter for estimating noise levels. Over the last ten months we have processed all the NMR data that we acquired at the presence of a brushed DC electric motor. The method has proved invaluable for our rheological studies and we believe it could be also useful for damping noise generated by other electric devices.

2. Theory

In NMR spectroscopic or imaging experiments, data, which we shall call 'total data set' hereafter, are often acquired in several steps. Data recorded at each step, e.g. FIDs, which we shall call 'individual data sets' or simply 'data sets', are stored separately and made into linear combinations to damp noise or select particular coherence pathways. Each individual data set will be digitised to give complex numbers, which we shall call 'samples'. By the word 'signal' we shall mean either an FID or echo recorded as a function of time and by 'spectrum' a Fourier transformation (FT) of the signal.

If an NMR signal $z(t)$ corrupted by an electronic noise $\delta z(t)$ was acquired during a time interval $[t_1,t_N]$ and sampled at a frequency $\Omega_s = 2\pi/(t_{n+1} - t_n)$, the resultant data set $z(t_n) + \delta z(t_n)$ $(1 \leqslant n \leqslant N)$ can be viewed as a sum of N complex samples $z(t_n) = x(t_n) + i \cdot y(t_n)$ of the noise-free signal and N corresponding complex samples $\delta z(t_n) = \delta x(t_n) + i \cdot \delta y(t_n)$ of white electronic noise. If, furthermore, we suppose that noise has zero mean value

$$\mu = \langle \delta z(t_n) \rangle = 0, \quad \text{for} \quad 1 \leqslant n \leqslant N, \tag{1}$$

standard deviation

$$\sigma = \sqrt{\frac{\langle |\delta z^2| \rangle}{2}} = \sqrt{\langle |\delta x^2| \rangle} = \sqrt{\langle |\delta y^2| \rangle}, \tag{2}$$

and Gaussian probability density distribution (solid line in Fig. 1)

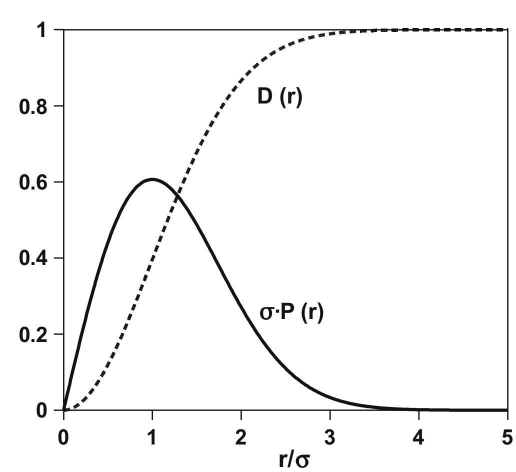

Fig. 1. Product (solid line) of Gaussian probability density $P(r)$ and standard deviation σ as well as probability (dashed line) $D(r)$ as a function of r/σ, where σ stands for a standard deviation.

$$P(|\delta z|) = \frac{|\delta z|}{\sigma^2} \exp\left(-\frac{|\delta z|^2}{2\sigma^2}\right), \tag{3}$$

and, thus, probability (dashed line in Fig. 1)

$$D(|\delta z|) = \int_{r=0}^{|\delta z|} P(r)dr = 1 - \exp\left(-\frac{|\delta z^2|}{2\sigma^2}\right), \tag{4}$$

then about 99 per cent of such noise-impaired samples $z(t_n) + \delta z(t_n)$ will fall not further than 3σ from their noise-free values $z(t_n)$.

To reduce noise, a convolution low pass filter can be applied to the raw data in the time domain. This consists in calculating new samples $z_{\text{filtered}}(t_n) + \delta z_{\text{filtered}}(t_n)$ as a linear combination of the samples $z(t_n) + \delta z(t_n)$ of an experimentally acquired data set, i.e.

$$z_{\text{filtered}}(t_n) + \delta z_{\text{filtered}}(t_n) = \frac{2\pi}{\Omega_s} \sum_{m=1}^{N} (z(t_m) + \delta z(t_m)) f(t_n - t_m). \tag{5}$$

This amounts to the multiplication of the spectrum of the signal by the FT $\tilde{f}(\omega)$ of the kernel function $f(t)$ in the frequency domain. The linear transformation of Eq. (5) with a properly chosen $f(t)$ will preserve all the low frequency harmonics of which consists the noise-free signal $z(t_n)$, while partially removing harmonics whose frequencies exceed the bandwidth of the signal and which, therefore, pertain exclusively to high frequency noise.

Kernels most often used in convolution low pass filters are cardinal sine and functions similar to it. The FT of the normalised cardinal sine function, i.e.

$$f(t) = \frac{\Omega}{2\pi} \text{sinc}\left(\frac{\Omega}{2} t\right), \quad \text{where} \quad \text{sinc}(\alpha) = \frac{\sin(\alpha)}{\alpha} \tag{6}$$

is a rectangular function, i.e. $\tilde{f}(\omega) = 1$ for $|\omega| < \Omega/2$ and $\tilde{f}(\omega) = 0$ elsewhere. When applied to a signal acquired during a period of time long enough to achieve high spectral resolution and sampled at a frequency higher than required by the Nyquist criterion, the sinc convolution filter has negligible roll-off and allows to reduce the overall noise level in the time domain by a factor

$$R = \sqrt{\Omega_s/\Omega}. \tag{7}$$

However, the convolution filters distort the noise-free data set $z(t_n)$ at the beginning and end of the record, as the sum in Eq. (5) cannot be extended for t_m smaller than t_1 and larger than t_N. These distortions are particularly severe and widespread when the signal is truncated to narrower $[t_1,t_N]$. In the frequency domain, this failure can be explained by the spectral resolution $\delta\omega = 2\pi/(t_N - t_1)$ of the signal being rather poor compared to the filter bandwidth.

We propose a new low pass filter suitable for processing truncated signals. It consists in fitting the N available raw data samples $z(t_n) + \delta z(t_n)$ of a data set with a truncated cardinal series

$$z(t_n) + \delta z(t_n) \approx \sum_{m=M_{inf}}^{M_{sup}} a_m \text{sinc} \frac{\Omega}{2}(t_n - \tau_m) \quad \text{for} \quad 1 \leqslant n \leqslant N, \tag{8}$$

where the bandwidth of the cardinal sine functions Ω is set to just over that of the signal Ω_o and locations of their maxima τ_m are regularly spaced at $\delta\tau = \tau_{m+1} - \tau_m = 2\pi/\Omega$ within an interval $[t_1 - 12\pi/\Omega, t_N + 12\pi/\Omega]$. The complex coefficients a_m are sought for to achieve the best least square agreement in Eq. (8). Thus found optimum coefficients a_m can be used to calculate the complex signal $s(t)$ at an arbitrary moment t as

$$s(t) = \sum_{m=M_{inf}}^{M_{sup}} a_m sinc \frac{\Omega}{2}(t - \tau_m) \tag{9}$$

and, in particular, at the moments t_n at which the signal was originally sampled by the ADC of the spectrometer. And the ensemble of these $s(t_n)$ are considered as a filtered data set.

In theory, the series on the right hand side of Eq. (9) is a band-limited function with a bandwidth Ω. In practice, the Fourier transformation of the series within the finite interval $[t_1,t_N]$ may prove to have a bandwidth somewhat broader than Ω, owing to this truncation. Like its infinite analogue [10], it gives an excellent approximation to any band-limited signal with a bandwidth narrower than or equal to Ω in the finite interval $[t_1,t_N]$. On the other hand, it can't account for the harmonics whose frequencies appear outside its own bandwidth. This makes of the truncated cardinal series and excellent low pass filter.

Given linear character of the cardinal series filter and linear independence of at least those of the cardinal sine functions in the sum of Eq. (9) whose maxima τ_m appear within the interval $[t_1,t_N]$, the deviation σ' of the raw samples $z(t_n)+\delta z(t_n)$ from those delivered by the cardinal series filter $s(t_n)$ is proportional to their standard deviation σ from the noise-free signal $z(t_n)$ and obeys an inequality

$$\sqrt{1-\frac{M-12}{N}} \leqslant \frac{\sigma'}{\sigma} \leqslant \sqrt{1-\frac{M}{N}}, \tag{10}$$

where M stands for a total number of cardinal sine functions in the series $M = M_{sup} - M_{inf} + 1$, and σ' is defined as a root mean square (RMS) value:

$$\sigma' = \sqrt{\frac{1}{2N}\sum_{n=1}^{N}|s(t_n) - z(t_n) - \delta z(t_n)|^2} \tag{11}$$

When signals are oversampled and so $N \gg M$, σ' tends to σ and becomes a good estimate of the latter. Thus, cardinal series filters can be applied for estimating noise levels.

When extra non Gaussian noise with larger standard deviation or even non zero mean value interfered with some of the samples $z(t_n)+\delta z(t_n)$, they are likely to fall further than $3\sigma'$ from $s(t_n)$ produced by the cardinal filter. This can be used as a basis for an algorithm for filtering non Gaussian noise as follows:

(a) A raw data set is processed with a cardinal series filter and the standard deviation σ' is calculated as stated in Eq. (11).
(b) Those of the raw samples that fell less than three times the standard deviation from corresponding output samples of the filter are retained, while the others are set aside.
(c) Thus restricted data set is processed with the cardinal series filter and its standard deviation is calculated.
(d) Then the whole raw data set is sorted out again, as in the step b, but now using the filter's output samples and standard deviation as determined in the step c. The steps c and d are repeated until two sequentially retained subsets of samples turn out to be the same.
(e) One can then either keep the lastly retained subset of raw samples, which is free of non Gaussian noise, or rather the last output samples of the cardinal series filter to enjoy further noise reduction due to high frequency Gaussian noise filtering.

Should the non Gaussian noise have a non zero mean value μ, this method can still be applied successfully. Nevertheless, to streamline the method, one had better replace the definition of σ' as an RMS in Eq. (11) by

$$\sigma' = \frac{1}{c}\left(\frac{1}{N}\sum_{n=1}^{N}|s(t_n) - z(t_n) - \delta z(t_n)|^{\nu}\right)^{\frac{1}{\nu}},$$
$$\text{where} \quad c = \sqrt{2}(\Gamma(1+\nu/2))^{\frac{1}{\nu}} \tag{12}$$

Γ is a gamma function and ν a constant parameter that can be set arbitrarily within $0 < \nu < 2$, smaller values of ν giving more weight to the samples that fell near to the noise-free values $z(t_n)$ rather than $z(t_n)+\mu$.

In practice, an experiment is repeated several times, and individual data records added together to either choose a desired coherence pathway by cycling phases of RF pulses and the receiver or simply to improve on signal-to-noise ratio. To avoid that distortions due to non Gaussian noise in individual data sets spread over virtually all the moments t_n in the total data set, the records made in different scans should be stored and freed from non Gaussian noise separately from one another before they can be added together to form a total data set.

3. Results and discussion

Success in application of a convolutions filter to band-limited signal with a bandwidth Ω_o is known to depend crucially on its spectral resolution $\delta\omega$. To ensure this, the signal must be sampled long enough for $t_N - t_1 \gg 2\pi/\Omega_o$. Lowering the resolution worsens greatly the performance of the filter and it fails utterly when applied to truncated signals, i.e. $t_N - t_1 \leqslant 2\pi/\Omega_o$. To illustrate this, we applied a cardinal sine convolution filter with rectangular-shaped spectrum of unit height to signals (empty squares in Fig. 2a–c), modelled as 128 equally spaced samples of a function

$$x(t) = \mathrm{sinc}^2\left(c\pi\frac{t}{t_0}\right), \quad \text{where coefficient}$$
$$c = 0.95 \text{ and } t_o \text{ stands for an arbitrary time unit}, \tag{13}$$

within intervals (a) $-5t_o \leqslant t \leqslant 5t_o$, (b) $-0.5t_o \leqslant t \leqslant 0.5t_o$ and (c) $-0.2t_o \leqslant t \leqslant 0.2t_o$ and impaired with computer-simulated white normally distributed noise. The filter width was set to just over the band width $\Omega_o = 4c\pi/t_o$ of the filtered function.

A discrete FT of the samples in Fig. 2a using the Fast Fourier Transformation (FFT) algorithm gives a rather well resolved ($\delta\omega = 0.053\Omega_o$) spectrum (empty squares in Fig. 2d) that corresponds well with the continuous FT of the function $x(t)$, i.e.

$$\tilde{x}(\omega) = \frac{1}{c}\left(1-\frac{2\omega}{\Omega_0}\right) \quad \text{when} \quad |\omega| \leqslant \frac{\Omega_0}{2} \tag{14}$$

and zero elsewhere. Applying the filter to these samples results in a significantly cleaner signal (continuous line in Fig. 2a) that preserves all the features of the original data set. Theoretically (see Eq. (7)), signal-to-noise ratio could increase by a factor of 2.53. An FT of the truncated signal in Fig. 2b results in a distorted and poorly resolved spectrum (empty squares in Fig. 2e), as the spectral resolution ($\delta\omega = 0.53\Omega_o$) is now insufficient to discriminate among frequencies within the spectral width of the function $x(t)$. Applied to these samples, the filter gives a cleaner signal (continuous line in Fig. 2b) that differs, however, markedly from the original data set. Applying the same filter to the even more truncated signal (empty squares in Fig. 2c) with, thus, even poorer spectral resolution ($\delta\omega = 1.32\Omega_o$) gives a clean, albeit completely disfigured signal (continuous line in Fig. 2c). Convolution filters with more sophisticated kernels, e.g. Gaussian or Lanczos, proved hardly better (not shown here). Nor can zero-filling solve the problem (not shown here either). The filter based on using truncated cardinal series, contrariwise, proves (see Fig. 3) suitable for processing truncated signals.

The cardinal series filter can be useful not only for filtering white Gaussian electronic noise, but also for eliminating other type of noise, generated by auxiliary electric devices. Fig. 4a shows raw samples of the real part of a data set recorded in one of the 32 individual data sets of a pulsed gradient spin echo (PGSE) experiment. The experiment consisted in forcing a yield-stress emulsion (blend of water and oil; see details in Section 5) to flow through a porous medium (randomly packed glass beads), by means of a piston

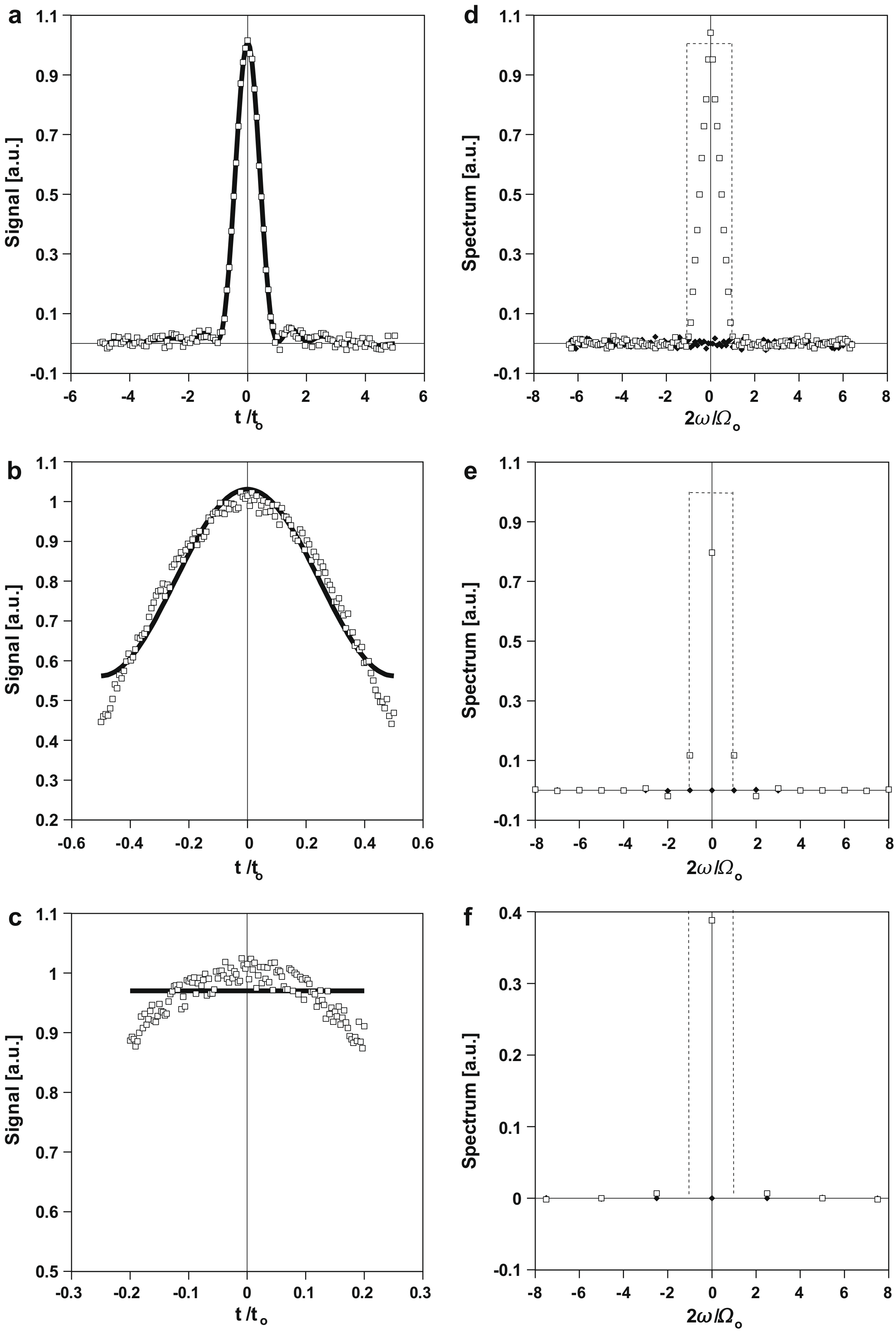

Fig. 2. Signals modelled as a $\mathrm{sinc}^2(c\pi t/t_o)$, where $c = 0.95$, function defined for (a) $-5 \leqslant t/t_o \leqslant 5$, (b) $-0.5 \leqslant t/t_o \leqslant 0.5$ and (c) $-0.2 \leqslant t/t_o \leqslant 0.2$ and impaired with real computer-simulated normally distributed noise before (empty squares) and after (continuous lines) an application of a sinc convolution filter with rectangular-shaped spectrum of unit hight (dotted squares in d–f). The filter width was set to just over the band width $\Omega_o = 4c\pi/t_o$ of the filtered function. The real (empty) and imaginary (filled squares) parts of the spectra in (d)–(f) of the signals in (a)–(c), respectively, were obtained by the Fast Fourier Transform (FFT) algorithm.

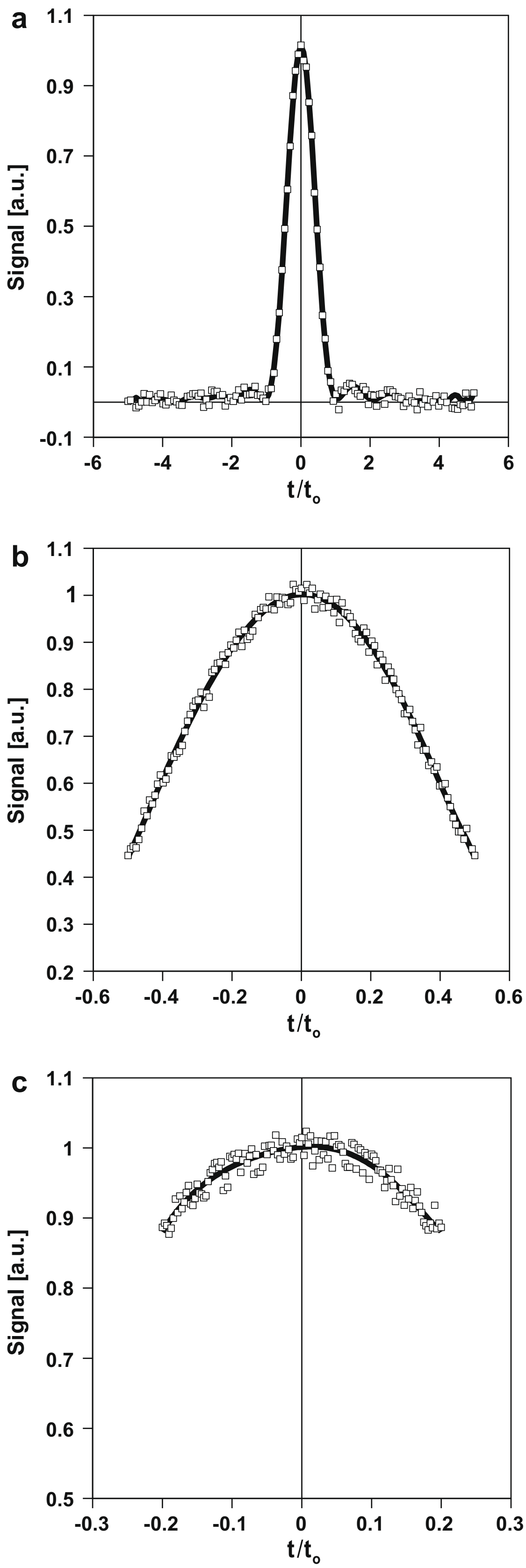

Fig. 3. Signals of Fig. 2a–c before (empty squares) and after (continuous lines) an application of the low pass cardinal series filter. The filter passband width was set to just over that of the signal to filter.

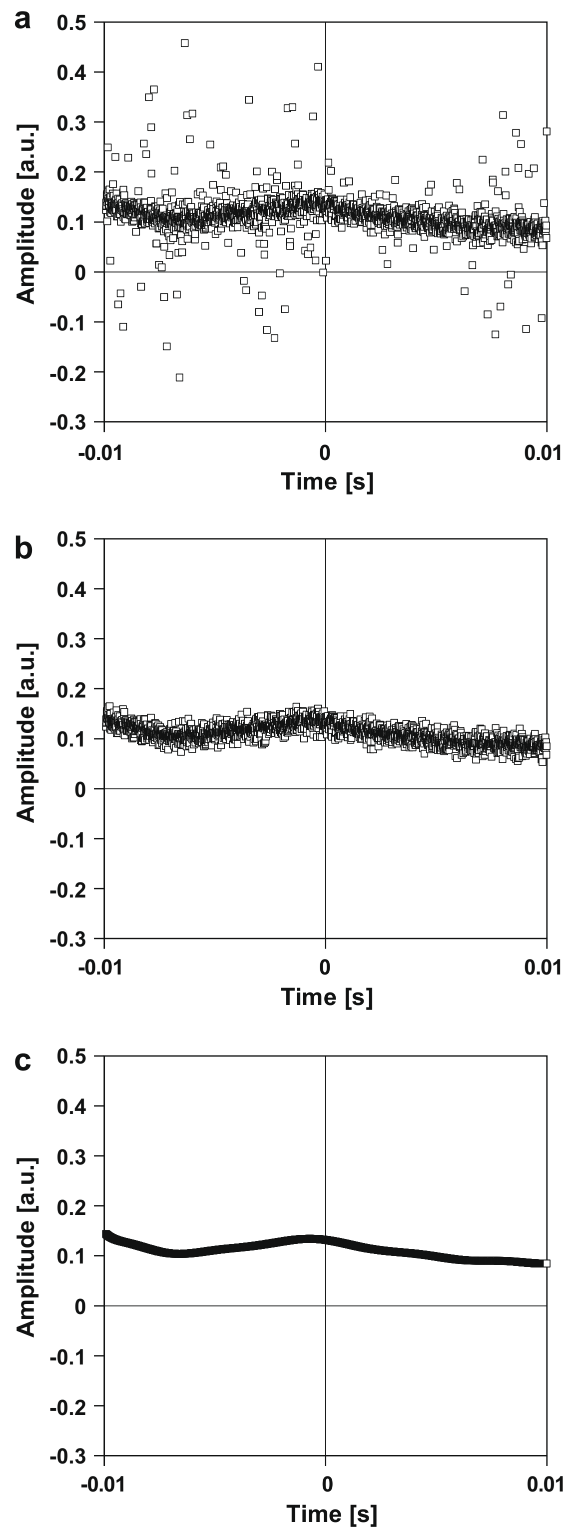

Fig. 4. Real part of the sampled (a) raw, (b) sieved and (c) sieved and then filtered signal acquired in a PGSE experiment, respectively.

syringe driven by an electric engine placed about one meter away from the magnet channel. Ten per cent of samples or so were greatly distorted by the non Gaussian noise and were sorted out and removed using the algorithm described above to give the restricted data set of Fig. 4b. The noise probability (black diamonds

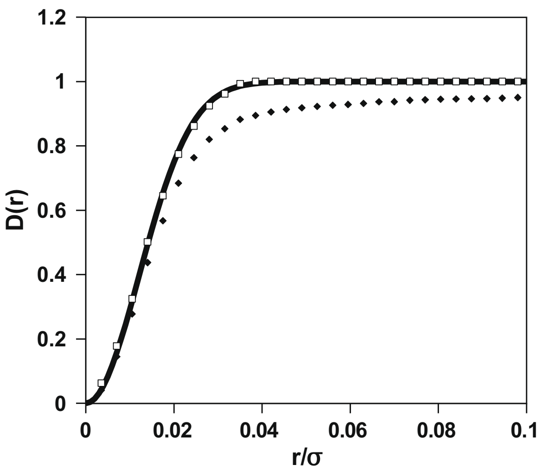

Fig. 5. Noise probability for the raw (black diamonds) and processed (empty squares) data, determined by comparison of the data in Fig. 4a and b with the data in Fig. 4c, as well as theoretical Gaussian probability function $D(r)$ (continuous line).

in Fig. 5) for the raw FID recording of Fig. 4a reaches a unity hight plateau more slowly than the theoretical Gaussian probability function $D(r)$ (solid line). This indicates that noise with other statistical distribution than Gaussian indeed interfered with the registered signal. On the contrary, the probability (empty squares in Fig. 5) for the restricted data set of Fig. 4b, processed as suggested above, corresponds to the Gaussian probability function, suggesting that defective samples of non Gaussian statistics have now been rejected. A cardinal series filter was then applied to this restricted data set to recalculate all the samples at the times t_n at which the raw data set was originally digitised by the analogue-to-digital converters (ADC) of the spectrometer. Thus calculated samples in Fig. 4c show further improvement in signal-to-noise ratio.

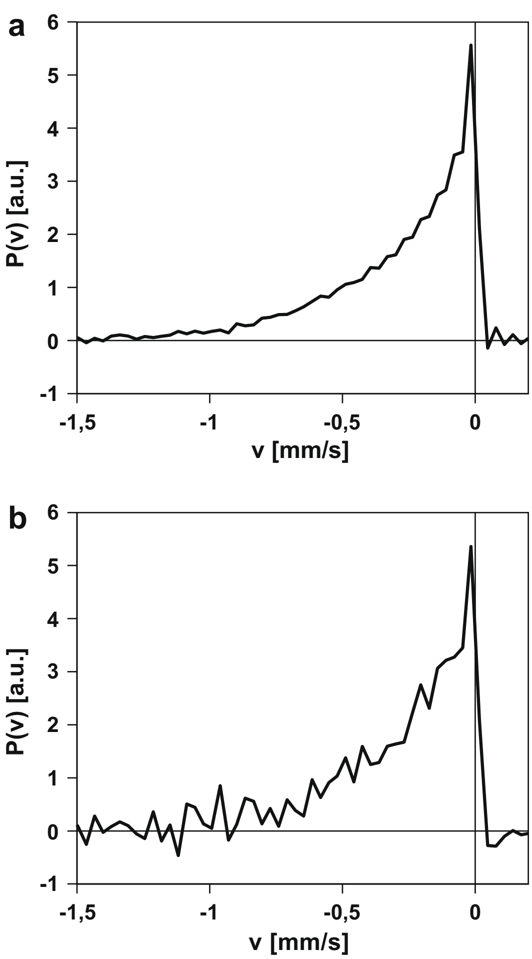

Fig. 6. Velocity distribution determined from a data acquired in a PGSE experiment (top) with and (bottom) without prior elimination of the defective samples and filtration.

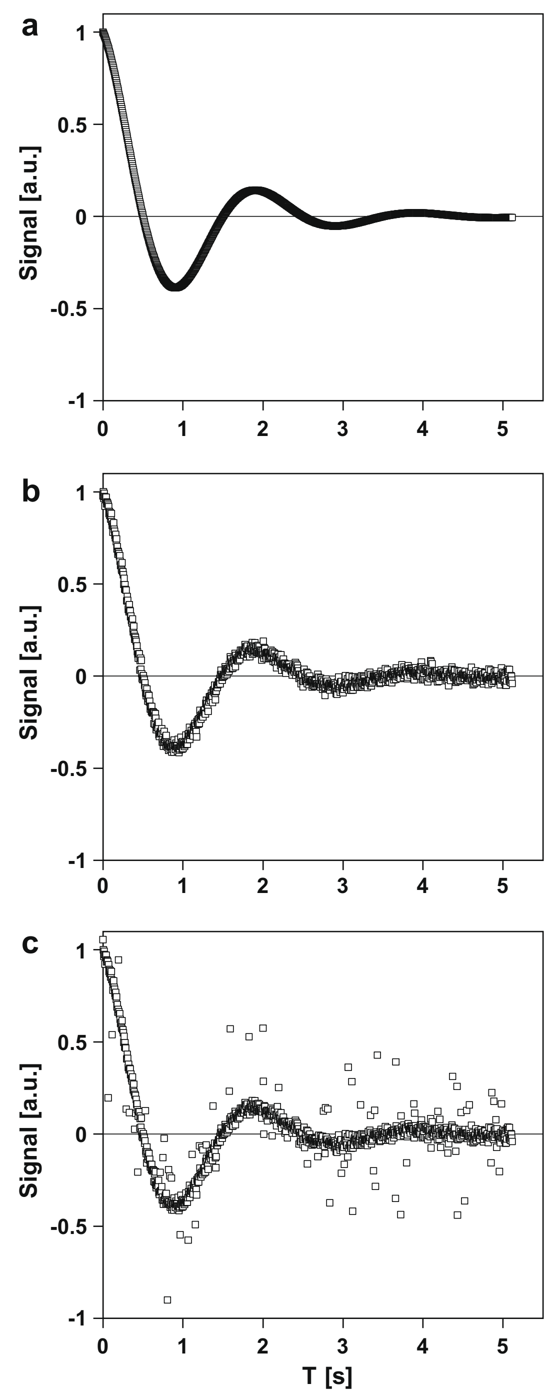

Fig. 7. (a) Data set modelled as 1024 equally-spaced noise-free samples of the function of Eq. (15). within an interval $t_1 \leqslant t = t_n \leqslant t_N$, $t_1 = 0$, $t_N = 5$ s and a sampling frequency of 200 Hz; (b) Data set of Fig. 7a impaired with noise (see Fig. 8 top) modelled as normally distributed random numbers of zero mean and standard deviation 0.02; (c) Data set of Fig. 7b of which ten per cent randomly selected samples impaired with defects (see Fig. 8 bottom) modelled as normally distributed random numbers of zero mean and standard deviation 0.2.

To demonstrate the increase in the precision of indirectly measured physical quantities achievable with the benefit of our algorithm, we used the data acquired in the PGSE experiment to determine the statistical distribution of velocity along the main direction of the flow stream. After application of the present iterative filtering process, the signal processing first consists in measuring the intensity and phase of the NMR signal at the middle time of each of the 32 FID recordings. This middle time actually corresponded to the theoretical position of the top of a spin echo. Signal filtering in the time domain is particularly necessary in this case, because the relevant information for the experiment is a time domain information. The 32 collected echo values correspond to a sampling of the Fourier transform of the velocity distribution. The last processing then consisted in a Fourier transform to get the distributions displayed in Fig. 6. The distribution function in Fig. 6a was determined with most satisfactory precision from the data that were first freed from the samples corrupted with non Gaussian noise before being further filtered from the high frequency Gaussian noise. On the other hand, the distribution function in Fig. 6b lacked precision, when the data were analysed without prior application of the algorithm described above.

Finally, to convince ourselves and our readership that our method does not have any adverse effects on the exactitude of thus filtered data while enhancing their precision, we processed a numerically synthesised noise-impaired data set.

The Fig. 7a was modelled as 1024 equally-spaced noise-free samples of an FID-like function

$$x(t) = \exp\left(\frac{-t}{T_2}\right) \cdot \cos(\omega t), \qquad (15)$$

where we set $T_2 = 1$ s and $\omega = \pi$ rad/s, respectively. The sampling interval was $t_1 \leqslant t = t_n \leqslant t_N$, with $t_1 = 0$, $t_N = 5$ s and the sampling frequency was set to 200 Hz. These samples were then added one by one with 1024 samples of noise, shown in Fig. 8 (top), modelled as normally distributed random numbers of zero mean and standard deviation 0.02. The resultant noise-impaired samples are shown in Fig. 7b. Finally, 102, i.e. ten per cent, of the samples were selected at random (uniform randomness) and added one by one with 102 defective samples, shown in Fig. 8 (bottom), modelled as normally distributed random numbers of zero mean and standard deviation 0.2. The resultant noise-impaired and partially defective samples are shown in Fig. 7c. Fig. 9 (top) shows the result of processing the noise-impaired signal of Fig. 7c as described above. Fig. 9 (bottom) shows the difference between the noise-free data set of Fig. 7a and resultant data set of Fig. 9 (top). The residual standard deviation of the filtered data is $3.83 \cdot 10^{-3}$, which is about one fifth of that of the computer-synthesised noise-impaired data.

4. Conclusions

We devised a linear low pass filter based on the use of cardinal series and suitable for processing truncated oversampled NMR signals. We also proposed a procedure for freeing NMR data sets of samples severely impaired with noise brought about by electric devices put near the magnet of the spectrometer. Its algorithm relies on the cardinal series filter for estimating noise levels. We

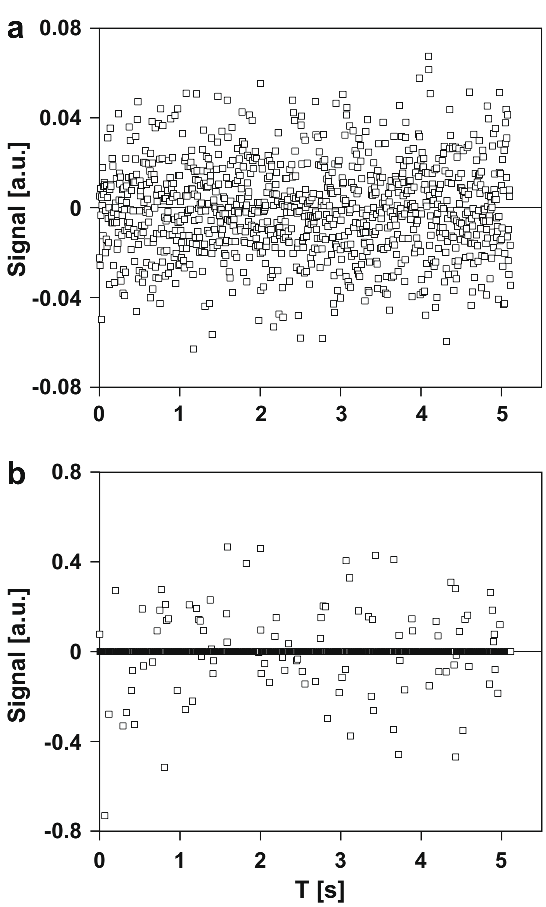

Fig. 8. (top) Noise modelled as normally distributed random numbers of zero mean and standard deviation 0.02; (bottom) Defects modelled as normally distributed random numbers of zero mean and standard deviation 0.2.

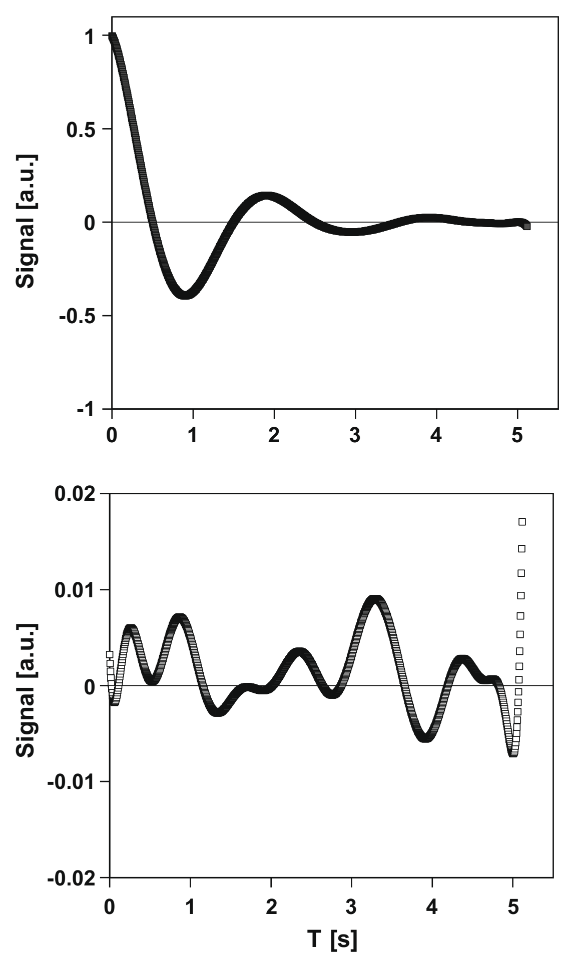

Fig. 9. (top) Result of processing the noise-impaired and partially defective data set of Fig. 7c with the benefit of the algorithm based using cardinal series; (bottom) Difference between the noise-free data set of Fig. 7a and resultant data set of Fig. 9 (top).

demonstrated the benefit of applying the procedure before any further data processing by using it to determine velocity distribution from data collected in a PGSE experiment.

5. Experimental

All numerical calculations, simulations and data processing algorithms were coded in Fortran 95 programming language [11,12]. Uniform and normally distributed random numbers were generated using Park–Miller with Bays–Durham shuffle and Box–Muller method, respectively. Where necessary, matrices were inverted using LDLT decomposition.

The water proton PGSE experiment was carried out on emulsion (a blend of CaOH, water and dodecane) extruded from a sample of sintered glass beads (diameter 2 mm) at a vertical wide-bore Bruker 24/80 Avance DBX MRI spectrometer equipped with a 20 cm birdcage RF coil and operating at 0.5 T.

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