Sampling in Relaxation Data Processing

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Abstract: - It is shown that the conventional sampling schemes are of limited use for conversion of monotonic long-time-interval and wide-frequency-band data of relaxation experiments, which can be measured over many decades of time or frequency. The problem of sampling is considered in combination with designing the discrete-time algorithms for relaxation data conversion has been generalized as a convolution on a logarithmic scale, for which implementation discrete-time filters with the logarithmic sampling are proposed. It is demonstrated that the sampling rate has a direct influence on the performance of the discrete-time filters to govern the potential accuracy and noise behaviour. A pragmatic approach is proposed for choosing sampling rate based on ensuring the maximum accurate output signal with the acceptable random error (noise). The optimum sampling is searched for an inverse filter executing the ill-posed inversion of an integral transform for determination of relaxation spectrum where sampling rate plays also a role of regularization.

Key-Words: - Relaxation data, integral transforms, logarithmic sampling, convolution, functional filters

1 Introduction

Material science and relaxation studies [1-3] especially face specific signals and problems have received little or no attention from the signal processing community yet. One of such problems is associated with conversion data of relaxation experiments yielding specific monotonic long-time-interval and wide-frequency-band signals (further named as relaxation signals (RSs)), which are typically measured on logarithmic scales where they can cover 10 – 12 and more decades. The specific monotonic behaviour and extension over many decades are reasons why many conventional sampling schemes are not effective for relaxation data.

In presented paper, a pragmatic approach is proposed for choosing sampling for conversion data of relaxation experiments based on ensuring the maximum accurate output signal with the acceptable random error (noise) to take into consideration the available range of input data.

2 Relaxation Signals and Their Spectra

The data of relaxation experiments are considered as time and frequency band unlimited signals [4] expressed mathematically through so-called relaxation spectrum (distribution of relaxation times) $F(\tau)$ by an integral relation

\[ x(u) = \int_0^\infty R(u, \tau) F(\tau) d\tau / \tau \]  

with aperiodic kernels $R(u, \tau)$ of the type

\[ 1 \quad \exp(-u / \tau) \quad \exp(-u / \tau) \quad 1 - \exp(-u / \tau) \quad 1/(1 + u^2 \tau^2) \quad u \tau / (1 + u^2 \tau^2) \quad u^2 \tau^2 / (1 + u^2 \tau^2) \]

where variable $u$ is time or frequency, and kernels $R(u, \tau)$ represent elementary (single-component) relaxation signals RSs.

RSs are usually considered and processed on a logarithmic scale [1-3] where they portray “good-perceiving” aperiodic signals (Fig.1). The Fourier transform of RS with logarithmically transformed independent variable

\[ u^* = \log_u u / u_0, \]  

(where $u_0$ is an arbitrary normalization constant) defines the spectrum of a signal on a logarithmic scale
\[ X(j\mu) = F[x(u')] = \int_{-\infty}^{\infty} x(u') \exp(-j\mu u') du' , \]

which is equal to the Mellin transform of the signal on linear scale

\[ X(j\mu) = M[x(u); -j\mu] = \int_{0}^{\infty} x(u)u^{-j\mu-1} du . \quad (4) \]

Further, we will name spectrum (4) as the Mellin spectrum, while parameter \( \mu \) described formally frequency in the logarithmic domain – as the Mellin frequency.

In Fig.2, the Mellin spectra \(|X(j\mu)|\) is shown for the elementary RSs depicted in Fig.1.

(i) the Fourier and related transforms for spectrum analysis and synthesis [5],
(ii) Kramers-Kronig (Hilbert) transforms – for conversion of the frequency functions [6], and
(iii) inversion of integral transforms of type (1) for determination of relaxation spectrum [4,7] from various input data.

All these tasks reduce mathematically to direct or inverse integral transforms with kernels depending on the ratio or product of arguments, which may be generalized in the form of the Mellin convolution type transform

\[ y(r) = x(r)M^* k(r) = \int_{0}^{\infty} x(u)k(r/u)du / u , \quad (5) \]

where * denotes the Mellin convolution.

For logarithmic arguments (3) transform (5) alters into the Fourier convolution type transform

\[ y(q^*) = x(q^*)F^* k(q^*) , \quad (6) \]

(sign * denotes the Fourier convolution) which can be identified as a linear system or linear filter operating on a logarithmic scale. Thus, relaxation data conversion can be generalized as a linear problem – convolution – on a logarithmic scale allowing one to use linear algorithms, e.g. discrete-time filters [4,8] for its implementation.

Function \( x(q^*) \) is usually an experimental signal measured at a limited sample set, while kernel or
Impulse response $k(q^r)$ is a band unlimited theoretical function, which may have the decreasing or increasing Mellin spectrum (frequency response) (Fig.3 and 4). The transforms with the decreasing frequency responses are specified as direct filters, while ones with the increasing responses – as inverse filters [4] having the kernels (impulse responses) existing in the class of non-integrable or generalized functions.

(ii) the more unfavourable (in sampling sense) signal determines the needed sampling; the kernel frequently is this more unfavourable signal,

(iii) the sampling (Shannon) theorem is of limited use for signals $x(q^r)$ and $k(q^r)$ due to their band unlimitedness,

(iv) signal reconstruction approaches are not adaptable for the kernels described by generalized functions (for inverse filters).

On the other hand, searching sampling for the kernel is close associated with its discrete-time approximation or, in general, with the algorithm design for (6), therefore, the sampling problem must be solved often together with the implementation of convolution (6) on the whole.

### 3 Implementation of Convolution (6)

The simplest way is to implement convolution (6) directly in equispaced points on a logarithmic scale. First, this leads to logarithmic sampling [7,9], where distance between samples increases according to the geometric progression on the linear scale

$$r_n = r_0 q^n, \quad n = 0, \pm 1, \pm 2, \ldots,$$

which has been demonstrated [9] is in agreement with the monotonic behaviour of RSs. Thus, the sampling problem reduces to choose optimum progression ratio $q$ specifying the sampling rate.

Second, direct implementation of convolution (6) is actually a filtering problem leading to designing a discrete-time filter with the logarithmic sampling, which due to its specific application ideology [4,8] has been named as a functional filter (FF). Thus, a FF from a logarithmically sampled input sequence $x(r_0 q^n)$ produces a new logarithmically sampled output sequence

$$y(r_0 q^n) = \sum_{m=-\infty}^{\infty} h[n] x(r_0 q^{n-m}), \quad (7)$$

where $h[n]$ is impulse response, which, of course, have to be truncated to the finite length in practice. Filter (7) has a periodic frequency response [4,7]

$$H(e^{j\mu}) = \sum_{n=-\infty}^{\infty} h[n] \exp(-j\mu n),$$

in the Mellin transform domain, which approximates the frequency response of ideal filter (6) (and (5)) expressed by the Mellin transform of kernel $k(u)$.
Practice shows that there exist two noise-forming mechanisms of FFs designed by the identification method. The first one is inherent to a specific integral transform, which can be characterized by theoretical noise coefficient $S_{\text{ theor}}$ determined from ideal frequency response $H(j\mu)$ by Eq. (10). As seen from Eq. (10), increase of sampling rate (decrease of $q$) extends the band $[-\pi/\ln q, \pi/\ln q]$, in which a discrete-time filter operates, and, consequently, the area under the frequency response leading to variation of the noise coefficient. The most critical noise behaviour is observed for inverse FFs, i.e. transforms with the increasing frequency responses, for which the noise coefficient increases with increasing sampling rate and tends to $\infty$, when $q$ approaches 1. Such noise behaviour is a reason of the ill-posedness of these transforms [7].

Since the frequency response of a discrete-time filter differs from ideal one, there is a discrepancy between noise coefficients $S$ and $S_{\text{ theor}}$ depending on fitting quality in the frequency domain. The identification method, as a time domain method, does not control formation of the frequency response in direct way and, at high sampling rates, creates typically the additional noise coming from discrepancy of the frequency responses at high frequencies. This is the second noise-forming mechanism, which can be explained as follows: obviously, there is an optimum – depending on the ideal frequency response (kernel) and filter length – frequency band, which frequencies really act in generating the output signal. Decreasing $q$ increases the actual operating frequency band, and when it becomes broader that optimum one, the higher frequencies do not more act in generating the output signal. Then the identification method becomes insensitive to these frequencies (if no special precautions are taken [5]), which leads to uncontrolled variation of the frequency response at higher frequencies, and, consequently, to increase of noise coefficient.

5 Choice of Sampling Rate

The proposed method for choosing sampling rate is actually a further improvement of the regularization method [7] for the inverse ill-posed problems of relaxation data conversion based on choosing the sampling rate, which ensures the acceptable output error variance. In this study, the sampling rate estimation is made more accurate by employing the actual noise behaviour of trial filters designed for combinations of $q$ and $N - 1$ allowed by
the available dynamic range of argument of input signal portion used for computing an output sample
\[ d_x = q^{N-1}. \] (11)

Fig.6. Error \( E \) (a) and noise coefficient \( S \) (b) versus progression ratio \( q \) of filters for determining relaxation spectrum. The numbers above triangles in (b) are numbers \( N \) of filter coefficients. The thick dashed curve in (b) is theoretical noise coefficient \( S_{theo} \). Horizontal and vertical arrows show the values of error \( E \) and noise coefficient \( q_{min} \) corresponding to acceptable noise coefficient \( S_{acc} = 10 \).

Fig.6 (a, b). Error \( E \) (a) and noise coefficient \( S \) (b) versus progression ratio \( q \) of filters for determining relaxation spectrum. The numbers above triangles in (b) are numbers \( N \) of filter coefficients. The thick dashed curve in (b) is theoretical noise coefficient \( S_{theo} \). Horizontal and vertical arrows show the values of error \( E \) and noise coefficient \( q_{min} \) corresponding to acceptable noise coefficient \( S_{acc} = 10 \).

The method includes the following steps:

(i) determination of relationship of experimental noise coefficient \( S \) as a function of progression ratio \( q \) by designing and testing trial FFs for combinations of \( q \) and \( N-1 \) allowed by Eq. (11),

(ii) estimation of acceptable noise coefficient \( S_{acc} \) from the input and output error variances according to Eq. (9),

(iii) fixing minimum progression ratio \( q_{min} \) (and filter length \( N-1 \)) ensuring the acceptable noise coefficient \( S_{acc} \) from the relationship determined at step (i),

(iv) final filter design of chosen length for \( q \geq q_{min} \).

Fig.7. Magnitude responses of ideal (solid line) and discrete-time (discontinuous lines) filters for determination of relaxation spectrum. The vertical dotted lines show the frequency bands \([−\pi/\ln q, \pi/\ln q]\) corresponding to two sampling rates.

6 Simulation Results
The bellow, an example of choice of sampling rate is considered for a FF for determination of relaxation spectrum by inversion of integral transform (1) with kernel (2d) having frequency response shown in Fig.4 (curve d).

Let us assume that: (i) discrete-time filter with even number of coefficients have to be designed, (ii) available input signal argument range for computing an output sample is three decades \( (d_x = 10^3) \), and (iii) noise coefficient shall not exceed 10 \( (S_{acc} = 10) \).

In Fig.6 (a, b), error \( E \) and noise coefficient \( S \) is shown for combinations of \( q \) and \( N-1 \) allowed by Eq. (11) for \( d_x = 10^3 \). In this case, there is an optimum sampling rate at \( q \approx 1,87 \) with the minimum error, however, this sampling rate is not applicable in practice due to unrealistic high noise coefficient \( (S \approx 600) \). The noise coefficient can be decreased by increasing \( q \) thus, progression ratio \( q_{min} = 3,6 \) ensures the acceptable noise coefficient \( S_{acc} = 10 \).

In Fig.7, the magnitude responses are shown for FFs operating at \( q_1 = 1,874 \ (N = 12) \) having maximum accuracy (the point marked by the circle and arrow with 1 in Fig.6) and \( q_2 = 3,981 \ (N = 6) \) (the point marked by the circle and arrow with 2 in Fig.6) being the closest one to \( q_{min} = 3,6 \). As seen, to
achieve the maximum accuracy filter must operate in the frequency band [–5, 5], while to ensure $S \leq 10$, the frequency band must be restricted to approximately [–2,3, 2,3] (the shaded area in Fig.7).

It is well known [7,11] that inversion of integral transforms of type (1) represents an inherently ill-posed problem. Therefore, the proposed approach for searching optimum sampling rate plays also a role of regularization method employing the progression ratio (sampling rate) as a regularization parameter. It can be noted that other regularization methods [11], e.g. the Tikhonov method, for the similar convolution problems, also limits the area under the frequency response by artificial introducing special functionals distorting the frequency response. The approach proposed here gives the better results, because it employs a natural inherent regularization capability of a discrete-time algorithm, and, thus, does not distort a shape of the frequency response. Besides, the proposed method allows determining directly the regularization parameter $q$, while there is no strong criterion for the determination value of regularization parameter for the Tikhonov and other regularizations.

Thus, the sampling is very significant for discrete-time functional filters where it carries out not only its basic function – generation of a discrete-time signal from a continuous-time signal, but also governs the potential performance of an algorithm.

7 Conclusions
1. The conventional sampling schemes are of limited use for conversion of monotonic long-time-interval and wide-frequency-band data of relaxation experiments.
2. The problem of relaxation data conversion is generalized as a convolution on a logarithmic scale where one signal to be convolved (kernel) may be a generalized function.
3. Discrete-time filters with the logarithmic sampling are proposed for implementing the convolution on a logarithmic scale.
4. The sampling rate has a direct influence on the performance of the discrete-time filters to govern the potential accuracy and random error (noise) of an output signal.
5. The problem of sampling is considered in combination with designing a discrete-time algorithm and a pragmatic approach is proposed for choosing sampling rate based on ensuring the maximum accurate output signal with the acceptable random error (noise) to take into consideration the available range of input data.
6. It is shown that the proposed approach carries out an inherent to discrete-time algorithm regularization for inverse problems.
7. As an example, an optimum sampling is searched for an inverse filter executing the ill-posed inversion of an integral transform for determination of relaxation spectrum where sampling rate plays a role of regularization.

References: