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ALGORITHMIC SUPPORT FOR PRE-PROCESSING DEVICES SPECTROMETRIC SIGNALS

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Abstract

In systems intended for preliminary processing of spectrometric information, when implementing spectrometric analytical methods, due to the complexity of processing tasks, they have a two or even three-level structure. At the lower level of the system for preliminary processing of spectrometric signals, there are means for converting analytical spectrometric signals and their preliminary processing (smoothing, filtering), at the upper level - computer tools for complex processing of analytical spectrometric information (linearization of the characteristics of analytical spectrometric instruments, approximation of discrete values of an analytical spectrometric signal , compression of analytical spectrometric data, determination of the intensities of analytical peaks at the output of spectrometric equipment, separation of combined peaks, identification of components of analytes, control of the process of analytical spectrometric measurements, etc.). To determine the tasks to be performed at each level, an algorithm of tasks to be performed is used. This article presents the algorithmic support of devices for pre-processing of spectrometric signals, on the basis of which each process can be distributed over certain levels.

Keywords: spectrometry, devices for preliminary processing of information, analog-digital converters.

The multiplicity and complexity of the tasks solved at the top level of the system for processing analytical spectrometric signals leads to an increase in the processing time of analytical spectrometric information and, accordingly, the time of analytical spectrometric measurement. In order to speed up the processing of analytical data, it is advisable to transfer part of the standard tasks of the upper level of the system for processing analytical spectrometric signals to the means of preliminary processing of analytical signals located at its lower level.
Such standard tasks include compression of spectrometric data in terms of range and time, filtering of the spectrometric signal, and linearization of the characteristics of spectrometric instruments.
In connection with the recent widespread use of relatively inexpensive but sufficiently powerful signal processors, it has become possible to solve problems such as separating the combined peaks and determining their intensities using the lower-level tools of the spectrometric information processing system.
In this regard, it is topical to develop methods for preliminary processing of spectrometric signals that allow solving the above problems when organizing the most common types of analytical measurements.
Analysis of the tasks of processing spectrometric signals allows us to group them depending on the complexity as follows:
1. Compression of spectrometric data by range, linearization of characteristics of spectrometric instruments;
2. Filtering of the spectrometric signal, time compression based on the approximation of its discrete values;
3. Detection (detection) of spectrometric peaks, separation of combined peaks, baseline correction.
To solve problems of the 1st group, it is advisable to use specialized ADCs with a functional characteristic and an uneven quantization scale (functional analog-to-digital converter), tasks of the 2nd group are solved by unified microprocessor devices for information preprocessing based on signal processors, tasks of the 3rd group are solved at the upper level of the structures of the spectrometric data preprocessing system using computer tools.
Analog-to-digital converters of spectrometric measurement signals with a linear characteristic in order to compress the measurement information must have a non-uniform quantization scale if the dynamic range of the signal change is large enough. In addition, some of the analyzer transducers (detectors) have non-linear characteristics (for example, spectrophotometric detectors). In this regard, it is expedient to set, in the general case, the task of developing functional analog-to-digital converters of spectrometric measuring signals in a system for processing spectrometric information.
Functional transformation of measuring signals in most cases is implemented either with the help of analog converters or with the help of microprocessor tools using tabular functional transformations, by implementing the expansion of a function in a power series, by using other methods of computational mathematics.
Analog functional converters are characterized by a significant instrumental error, and microprocessor tools require appropriate software. In addition, microprocessor tools that use standard algorithmic and, accordingly, software, in most cases do not have high performance.

To a certain extent, functional analog-to-digital converters are free from the noted shortcomings, in the construction of which standard methods of analog-to-digital conversion are used - bit-by-bit balancing, time-pulse and frequency conversion, integration.

Let us consider methods for constructing a functional analog-to-digital converter of bitwise balancing, which have a high speed compared to other known structures of analog-to-digital converters and, for this reason, are used to convert rapidly changing analytical signals. Functional analog-to-digital converters of this type implement the relation

$$N_y = F(x) = F\left(\frac{U_x}{U_0}\right); \qquad (1)$$

Here U_x - is the input voltage, U_0 - is the reference voltage,

N_y - binary code at the output of the converter:

$$N_y = \sum_{i=0}^{m} 2^i k_i,$$

where m - is the number of digits of the code, k_i - is the digit of the i-th digit.

From (1) we have:

$$\sum_{i=0}^{m} 2^i k_i = F\left(\frac{U_x}{U_0}\right). \qquad (2)$$

The maximum number represented by the N_y code is

$$N_{y\max} = 2^{m+1}.$$

Then the algorithm for generating the most significant digit has the form:

$$\left.\begin{aligned} k_m &= 0 \quad at \quad N_y < 2^m; \\ k_m &= 1 \quad at \quad N_y \geq 2^m. \end{aligned}\right\} \qquad (3)$$

Taking into account (2), for a function F satisfying the condition

$$\frac{dN_y}{dU_x} > 0,$$

we obtain the relations

$$\left.\begin{aligned} k_m &= 0 \quad at \quad \frac{U_x}{U_0} < F^{-1}(2^m); \\ k_h &= 1 \quad at \quad \frac{U_x}{U_0} \geq F^{-1}(2^m); \end{aligned}\right\} \qquad (4)$$

If the function F is such that the condition

$$\frac{dN_y}{dU_x} < 0,$$

then the signs of the inequalities in (4) are reversed.

Representing (2) in the form

$$\sum_{i=0}^{m-1} 2^i k_i = F\left(\frac{U_x}{U_0}\right) - 2^m k_m = F_1\left(\frac{U_x}{U_0}\right),$$

and also taking into account the relation (4), we determine the algorithm for the formation of the digit (*m-1*) - digit:

$$\left.\begin{aligned} k_m = 0 \quad at \quad \frac{U_x}{U_0} < F^{-1}(2^{m-1}); \\ k_m = 1 \quad at \quad \frac{U_x}{U_0} \geq F^{-1}(2^{m-1}); \end{aligned}\right\}$$

The formation algorithm is defined in the same way.
digits (*m-i*) - th digit:

$$\left.\begin{aligned} k_{m-i} = 0 \quad at \quad \frac{U_x}{U_0} < F_i^{-1}(2^{m-i}); \\ k_{m-i} = 1 \quad at \quad \frac{U_x}{U_0} \geq F_i^{-1}(2^{m-i}); \end{aligned}\right\} \quad (5)$$

Here the function F_i - is defined by the relation

$$F\left(\frac{U_x}{U_0}\right) = \sum_{j=0}^{m-i} 2^j k_j = F\left(\frac{U_x}{U_0}\right) - (2^m k_m + 2^{m-1} k_{m-1} + \ldots + 2^{m-(i-1)} k_{m-(i-1)}) = \\ = F\left(\frac{U_x}{U_0}\right) - \sum_{j=0}^{i-1} 2^{m-j} k_{m-j} \quad (6)$$

In particular, the algorithm for generating the digit (*m-1*) -th digit, defined taking into account (2) and (3), has the form

$$\left.\begin{aligned} k_{m-1} = 0 \quad at \quad 2^{m-1} > F_1\left(\frac{U_x}{U_0}\right) = F\left(\frac{U_x}{U_0}\right) - 2^m k_m; \\ k_{m-1} = 1 \quad at \quad 2^{m-1} \leq F_1\left(\frac{U_x}{U_0}\right) = F\left(\frac{U_x}{U_0}\right) - 2^m k_m); \end{aligned}\right\}$$

or

$$\left.\begin{aligned} k_{m-1} = 0 \quad at \quad \frac{U_x}{U_0} < F_i^{-1}(2^m k_m + 2^{m-1}); \\ k_{m-1} = 1 \quad at \quad \frac{U_x}{U_0} \geq F_i^{-1}(2^m k_m + 2^{m-1}); \end{aligned}\right\}$$

Similarly, based on (5) and (6), the algorithm is determined
digit formation (*m-i*) - th digit

$$\left.\begin{aligned} k_{m-i} = 0 \quad at \quad 2^{m-i} > F_i\left(\frac{U_x}{U_0}\right) = F\left(\frac{U_x}{U_0}\right) - \sum_{j=0}^{i-1} 2^{m-j} k_{m-j}; \\ k_{m-i} = 1 \quad at \quad 2^{m-i} \leq F_i\left(\frac{U_x}{U_0}\right) = F\left(\frac{U_x}{U_0}\right) - \sum_{j=0}^{i-1} 2^{m-j} k_{m-j}; \end{aligned}\right\}$$

which can be represented in the form

$$\left.\begin{array}{l} k_{m-i}=0 \quad at \quad \dfrac{U_x}{U_0}<F^{-1}(\sum_{j=0}^{i-1}2^{m-j}k_{m-j}+2^{m-1}); \\ k_{m-i}=1 \quad at \quad \dfrac{U_x}{U_0}\geq F_i^{-1}(\sum_{j=0}^{i-1}2^{m-j}k_{m-j}+2^{m-1}); \end{array}\right\} \qquad (7)$$

Expressions (7) are valid for i≥1.

The proposed algorithms are used in the developed functional analog-to-digital signal converters of spectrophotometric detectors, spectrometric detectors, as well as in wide-range analog-to-digital converters of analytical signals with compression of their conversion range.

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