Modelling adequacy of calibration curves and dynamic characteristics of measuring instruments

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Abstract. Calibration curves and dynamic characteristics are widely used as metrological models of measuring instruments properties; but the initial concepts and formal representations have not been clearly formulated so far. This paper focuses on the construction of a formal framework, which should enable introduction and estimation of adequacy as a characteristic of the model quality. The formal system is constructed, that is similar to the representative theory formalization. So, an initial model for calibration curve is a complex \{U, C_0, \Phi\}, containing a set of dependences U, a space of continuous monotonous functions C_0, and monotonic homomorphism \Phi: U \rightarrow C_0. Construction of calibration curve is started from an initial table of experimental data, and transfer to the analytical form of calibration curve is analysed. It is demonstrated that adequacy parameters should be expressed by functionals of both measurement accuracy and frequency range. The analogy of measurement and modelling of metrological characteristics should be extended up to the construction of system ensuring the traceability of calibration curves and dynamic characteristics. This system can be created using the experience in constructing a system ensuring the measurement traceability.

1. Introduction
Metrological characteristics of measuring instruments – such as calibration curves and dynamic characteristics – are widely used as examples in metrological publications devoted to modelling problems. Moreover, these characteristics usually influence deeply on the quality of measurements. However, the modelling problem in this area has not been clearly formulated so far, thus not allowing correct definition or estimation of the result adequacy.

This paper focuses on the construction of a system of initial representations, which should enable correct introduction and estimation of adequacy as a characteristic of quality of the modelling procedure and its results.

It seems appropriate to construct a formal system which is similar to the system of measurement formalization provided by the representative measurement theory. It may be based on the formal scheme of representative theory, and on the main stages of measurement, and also on the adequacy analysis as applied to measurement modelling.

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2 General Formalization

2.1 Formalization of Measurement Procedure
As is known, in representative theory the measurement is interpreted as a complex (ordered triple) [1]:

\[ \{ X, R, \Phi \} \]

containing: \( X \) – set of object physical characteristics (empirical system with relations),
\( R \) – complete numerical set with relations,
\( \Phi : X \to R \) – homomorphic mapping of the empirical system into numerical set.

As applied to a certain measurement, this general complex may be defined concretely, and it is rational to realize in compliance with the main stages of measurement [2]. Therefore, at the stage of a measurement problem statement this complex is realized as the triple

\[ \{ X_0, R, \Phi_0 \} \]

where \( X_0 \) - the considered characteristic of the object under study;
\( \Phi_0 \) - operation of comparison with the corresponding unit.

After the preparation measurement stage the complex takes the form:

\[ \{ X_1, R, \Phi_1 \} \]

where \( X_1 \) is the measurand,
\( \Phi_1 \) is the measurement method.

The complex, corresponding to the stage of measurement experiment, is of the form:

\[ \{ x_1, R, \varphi_1 \} \]

where \( x_1 \) is the input signal,
\( \varphi_1 \) is the measurement procedure.

Finally, the measurement result may be presented in the form

\[ r = \varphi_1 (x_1) \]  

The error (or uncertainty) of this result can be expressed as follows:

\[ \Delta (r) = \varepsilon (\Phi_1, \varphi_1) (X_1) \]

As the error as expressed by (6) is estimated by experimental data, the expression

\[ \Delta_1 (r) = \varepsilon (\Phi_1, \varphi_1) x_1 \]

can serve as an estimate of error (uncertainty) \( \Delta (r) \).

2.2 Formalization of Calibration Curve
While proceeding from the measurement to modelling of metrological characteristics, particularly, the calibration curve, we may construct a formal scheme, which is similar to (1) – (4). First of all, we have an initial general complex (triple) of the form:

\[ \{ U, C_0, \Phi \} \]

where \( U \) - a set of all monotonic dependences (between two physical quantities),
\( C_0 \) - a space of continuous monotonous functions,
\( \Phi : U \to C_0 \) - a order preserving function (homomorphism).

It is also rational to proceed in compliance with the main stages of modelling procedure [3]. So, at the stage of the modelling problem setting the complex becomes as follows

\[ \{ U_0, C_0, \Phi_0 \} \]
where $U_0$ - the required dependence,

$\Phi_0$ - two-dimensional comparison with the units of two quantities (mapping onto coordinate plane).

Further, a modelling preparation step stage yields the complex

$$\{U_1, C_0, \Phi_1\},$$

where $U_1$ is the modelled dependence, $\Phi_1$ is the modelling method.

After obtaining the initial experimental data, i.e., the basic data table

$$u_1 = \{(x_i, y_i), i=1...n\},$$

we get the complex

$$\{u_1, C_0, \varphi_1\},$$

where $\varphi_1$ is the table generation procedure.

Based on the introduced representations, the modelling adequacy and its estimate can be defined by analogy with (6) – (7), and these may be presented as follows

$$\alpha = \delta(\Phi_1, \varphi_1)(U_1), \quad \alpha_1 = \delta(\Phi_1, \varphi_1)(u_1),$$

where $\delta(\Phi_1, \varphi_1)$ denotes the discrepancy between operations $\Phi_1$ and $\varphi_1$.

3 Analysis of Calibration Curve Adequacy

3.1 Factors of Calibration Curve Adequacy

Definition of adequacy concept makes it possible to analyze it as a qualitative characteristic of modelling results of calibration curves and dynamic characteristics.

We start with the calibration curve by saying that it can be represented in tabular, graphic, or analytical form. So the table (11) is an initial form, which is quite suitable for practical application. However, the issue of proceeding to other representation form, i.e., to continue modelling, is relevant. Therefore, adequacy analysis is inseparably connected with the validation of the curve form.

If Table (11) is used in itself, the objective meaning contained in experimental data is saved in complete and non-changed form. To construct a table, the primary data are processed for each point, and estimates of errors (uncertainties) are also obtained. Thus, we have an extended table:

$$u_e = \{(x_i, \Delta x_i; y_i, \Delta y_i), i = 1...m\}.$$ (14)

The expected way of adequacy analysis is to realize the modelling adequacy estimates (13) as applied to Table (11), which is a model of the required input-output dependence. At the same time, we come to recognize that adequacy of the table as a model of dependence is not merely conditioned by the measurement accuracy $\Delta$, but it is also determined by the level of the table detailing. Here the accuracy $\Delta$ is expressed by data error set $\{(\Delta x_i; \Delta y_i), i = 1...m\}$, and the level of detailing $H$ is expressed by the number of point $m$ or, in other words, the frequency range of the model.

Therefore the measurement accuracy $\Delta$ and frequency range $H$ are the two factors (two coordinates) of adequacy, whose increase, if assumed independent, should result in higher model adequacy. The factors can be changed independently; however, the effect on the model adequacy depends on the level of the other factor. For instance, with fixed sampling interval $h$ (sample size $m$) the increasing accuracy enhances the adequacy in limited range only depending on $h$. On the other side, with the fixed accuracy $\Delta$, if $h$ grows from the low initial level, it will lead to adequacy increase, and above the certain level, to its decrease. Therefore adequacy parameters should be expressed by functionals of both $\Delta$ and $h$.

3.2 Analysis of Calibration Curve Representation

If one need to convert a calibration curve from the tabular (11) to the analytical form, such as

$$Y = f(X) = f(X, a_1, ..., a_k),$$ (15)
the additional a priori data are required. These may be obtained from analysis of physical principles of measuring instruments, or some previous experiments. On the other side, during the conversion some primary information is inevitably lost, and further it would be irretrievable. Additionally, revision of Table (11) may be needed irrespective of the form of calibration curve.

If particular importance in constructing the calibration curves is given to adequacy, then selection of the curve form becomes less significant, especially with modern IT capabilities.

However, obvious drawbacks of the tabular form should be mentioned as follows:

- complexity of obtaining and storage of calibration curves;
- possible uncertainty of curve usage.

The last issue has two main aspects, which are the formal one (poor conditioning of data processing task) and the technical one, that is required calibration accuracy depends on application conditions of measuring instruments.

For instance, if the measurements in calibration are accurate, but the measurements while using of calibration curve are inaccurate, then the considerable uncertainty in determination of input can occur. Vice versa, inaccurate calibration and accurate using of calibration curve can result in appearance of gaps, where the input cannot be determined.

Traditionally, the analytical form (15) is preferred, i.e., representation of calibration curve as a continuous function \( f \) which depends on a small number of estimated parameters \( a_1, \ldots, a_k \). However, this representation is not always possible or rational.

Advantages of analytical form include the following: easy use and tests of curve, compactness of representation, and possibility of estimating the results accuracy. This form is achieved first of all by applying physical principles, which should enhance the adequacy of calibration curves. There are, however, some drawbacks, since the objectivity of data contained in initial Table (11) is decreased.

Thus, the following requirements are placed upon the analytical model of calibration curve:

- optimization of resources during the curve construction and use;
- providing uncertainty during the use;
- possibility of estimating and validating the curve accuracy.

It follows from above that the decision on analytical modelling should be taken before the data are obtained, at the stage of experiment planning. Actually the data obtaining (initial table) should be planned and organized depending on the modelling problem. Generally speaking, the dimension of analytical model should be correlated at least with sampling interval \( h \) of initial Table (11): for example by transition from \( h \) to the upper frequency of model spectrum by sampling theorem.

3.3 Analysis of Analytical Form for Calibration Curve

The basic steps of analytical modelling are in general similar to the measurement stages. At the initial step, the model general structure is formed based on the physical principles of measuring instrument. Then, criteria to select the model order are formulated based on conditions of inversibility, i.e., effective use of calibration curves in practice.

Accuracy is interpreted in a specific way as applied to the analytical model of calibration curve. Unlike the general measurement problem, here the object under consideration is a function; therefore in the context of calibration curves it would be natural to use the notion of adequacy characteristic instead of error. The proposed notion can be interpreted in two ways: as uncertainty of the curve analytical form, or as inaccuracy of the curve parameters. The first type of uncertainty is surely more significant for the analysis of model adequacy.

Selection of the analytical form is illustrated as a stepwise search of embedded sequence using the stopping criteria [ 3 ]. The criteria should be based on physical principles of conversion implemented in the sensor or device, and on admissible deviations from them in real devices. Consequently the model adequacy should be coordinated with the practically required measurement accuracy.

On the whole, modelling of calibration curve is a cyclic process, which is conditioned by the above described principal uncertainty of the dependence inherent in the measuring instrument (device). Therefore, design of the calibration experiment and selection of criteria play the key role.
Mathematical design methods also gain some specific features in this context. Frequently optimal plans obtained using formal methods prove unpractical or physically unrealizable.

A simple example is a construction of linear calibration curve

$$Y = a + bx$$

on the specified interval \((x_{\text{min}}, x_{\text{max}})\). If the input values \(x_1, \ldots, x_m\) can be selected, and the curve is constructed using the least squares method (LSM), the formal optimal plan prescribes that the measurements are made at the extreme points, \(x_{\text{min}}\) and \(x_{\text{max}}\), with the equal number of observations. With the calibration curves, however, this plan is not rational, because in practice it is also important to determine nonlinearity of the curve, and also to investigate the middle part of interval in detail; besides, physical realization often requires time or space separation of the points. Frequently the uniform distribution of points \(x_i\) over the interval \((x_{\text{min}}, x_{\text{max}})\) proves practical; it is also convenient from the computational viewpoint.

Since the construction of calibration curve is a cyclic process, validation of transition from one model to the other, and selection of transition direction are of great importance. Initial requirements to the curve features are commonly minimal: continuity and monotonicity, and sometimes smoothness (for physical considerations). In most cases it is natural to start from a linear calibration curve (16).

There are many options to extend the linear curve form, such as:

a) polynomial curves of low degree;

b) nonlinear curves linearized by transformation of variables;

c) linear-fractional curves;

d) nonlinear curves as presented by linear combinations of the known functions;

e) piecewise-linear curves obtained by several linear segments.

Each of extension options has its advantages and disadvantages. Polynomial extension, for instance, allows the use of LSM, and LSM-based analysis. On the other hand, a fortunate transformation of variables (option b) can significantly enhance the calibration adequacy, and provide more physically illustrative curve.

Modelling of calibration curves involves two closely connected aspects: physical principles and computation aids. Two formal languages corresponding to these aspects are transformation or group-oriented, and functional-computational language.

The most important classes of calibration curves are the most narrow, linear class, and the widest, containing all the continuous monotonic functions; both are the transformation groups. It means that these classes of functions \(\Omega\) have the following properties:

a) **closed composition**: if all functions \(f_i(x), i = 1 \ldots n\), belong to class \(\Omega\), then their composition \(f(x) = f_n(f_{n-1}( \ldots f_2(f_1(x)) \ldots ))\) also belongs to \(\Omega\);

b) **inversibility**: if function \(f(x) \in \Omega\) then the inverse function \(f^{-1}(x)\) belongs to \(\Omega\) as well.

The group of linear-fractional transformations meets these conditions, too; it specifies a class of calibration curves suitable for the measurements, which are physically realizable. The linear-fractional curves group is much broader than the linear group, and it is the only extension of the linear group, which does not coincide with the widest group of all monotonic curves.

The group structure of calibration curve classes is convenient for application problems, including description of transformation sequences or their inversions. Therefore, linear-fractional calibration curves are very promising for metrology.

### 4 Analysis of Dynamic Characteristics

As to the dynamic characteristics, everything described above about the calibration curves applies to them as well. For dynamic measurements (including determination of dynamic characteristics) the complex, by analogy with (8), becomes as follows

$$\{D, B, \Phi\},$$

(17)
where \( D \) - set of dependences (between input and output quantities), \( B \) - space of continuous operators, representing dynamic properties, \( \Phi : D \rightarrow B \) - corresponding homomorphism.

Nevertheless, this complex does essentially differ from the analogous sets for static case, such as (1) and (8). Namely, in the case of calibration curves, a structure of the set of dependences \( U \) is solely determined by the continuous scale of property under investigation. So the elements of the set are not interrelated in formal or physical ways, and the sequence of values \( x_1, \ldots, x_m \) is only determined by practical considerations. As opposed to this, in the case of dynamic measurements, the sequence of input values for dependences \( D \) is strictly ordered by fundamental time parameter. Thus, the dynamic measurements of the form

\[
\{ D_1, B_1, \Phi_1 \},
\]

may be only carried out according the rate of the physical process. In its turn, the set of dynamic characteristics \( B_1 = \{ \beta_i \} \) determine the accuracy of the process representation or measurement. So it is rational to determine the characteristics while the more rapid process, than the measurement process. Thus there are clear distinctions between calibration and dynamic measurements, which can be easily presented as relations in temporal and spectral domain.

Also, there exists a more strict and unambiguous classification of dynamic models based on physical properties of material systems. For modelling purposes, the dynamic characteristics are classified into linear and nonlinear, minimum and nonminimum phase, lumped and distributed parameter. Further, in linear class the dynamic characteristics are represented by typical functional models: rational transfer functions, transient and impulse response in the form of exponential series of various orders, etc.

Limitations of the spectrum of desired dynamic models have clear physical foundations, as contrary to their formal nature with respect to the calibration curves. These specific features do not make the modeling of dynamic characteristics more complicated, but allow a clearer formulation of the modeling problem.

### 5 Conclusions

Two significant conclusions can be drawn.

First, the adequacy is not reduced to the error (uncertainty), and it is a more complicated (two-dimensional, at least) attribute of the model.

Second, analogy of the modelling of metrological characteristics and the measurement should be extended up to the construction of system ensuring the traceability of calibration curves or dynamic characteristics. This system can be created using the experience in constructing a system ensuring the measurement traceability.

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