

APPLICATION-ORIENTED APPROACH TO MATHEMATICAL MODELLING OF MEASUREMENT PROCESSES

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Abstract: The need for broader use of concepts of modelling in the development of a conceptual basis for measurement science is ascertained. A brief review of basic concepts of mathematical modelling is provided, and a class of models, most frequently used in measurement science, is characterised. A meta-model of measuring systems, unifying many existing methodologies of mathematical modelling in measurement science, is proposed. Its applicability is illustrated with a set of diversified examples.

Keywords: measurement, modelling, calibration

1. INTRODUCTION

The history of the *International vocabulary of basic and general terms in metrology* (compare its consecutive versions VIM1 [1], VIM2 [2] and VIM3 [3]), and especially the discussions related to its recent version, have demonstrated the growing importance of the concepts of modelling – in particular of mathematical modelling – for the development of a conceptual basis of measurement science.

The need for a general model of measurement – called hereinafter "measurement meta-model", to emphasise that it should be able to encompass the models of specific measurement processes and systems – is widely recognised. Various attempts, aimed at designing such a meta-model, have been undertaken since the second half of the XIXth century – for their review see [4].

The measurement meta-model should be general enough to encompass all or at least vast majority of measuring systems, met in practice, and specific enough to have higher explanatory power with respect to those systems than any general methodology of abstract modelling of material objects. It should describe the structure and behaviour of a generic measuring system, together with the procedure necessary for its proper operation. It is also reasonable to expect the measurement meta-model be compatible with the conceptual basis of VIM3. In this paper, an attempt has been made to develop a meta-model satisfying all those requirements, but only at the application level, which means that its transformation to a fundamental-level meta-model (*cf.* [4]) has not been undertaken here.

The paper is structured as follows: first, in Section 2, a general introduction to mathematical modelling and model validation is given; next, in Sections 3 and 4, the proposed meta-model is outlined; finally, in Section 5, several examples of measuring systems are described in terms of that meta-model.

2. BASIC CONCEPTS OF MATHEMATICAL MODELLING

Let's assume that an entity to be modelled – for brevity, called "system" hereinafter – is an object, or a phenomenon, or an event, or... of physical, or chemical, or biological, or psychological, or sociological, or economical, or..., or mixed nature. Its mathematical model is its description – composed of entities such as numbers, variables, sets, equations, functions, relations,... – which enables one to infer about its properties and/or behaviour under various conditions. The identification of the system itself, *i.e.*, the distinction between the system and the surrounding environment, is not objectively given, but is already part of the modelling process. It's possible that even in trivial situations, a mathematical model does not carry full information on the modelled system. So, a general criterion to evaluate the quality of a mathematical model is based on the trade-off between simplicity and informativeness: a mathematical model should be as simple as possible, but sufficiently informative for its target application. The process of mathematical modelling typically starts with an informal description of the system in terms of its features which are considered to be important for the given application. Next, this description is translated into a more formal language of quantities which are idealised features of the system, obtained by means of abstraction. Here, the proper definition of a mathematical model begins, being generally an iterative procedure, composed of two fundamental operations:

- *structural identification*, *i.e.*, the selection of a structure for the model (most frequently, a type of function or equation, *e.g.*, a linear algebraic equation);
- *parametric identification*, *i.e.*, the estimation of the model parameters (*e.g.*, the coefficients of the linear algebraic equation).

The first operation hardly can be algorithmised: the choice of the model structure is usually based on some intuitive premises, anterior experience, and trial-and-error actions. On the other hand, the second operation is subject of advanced algorithmisation.

Both model structure and parameters are affected by the mentioned trade-off between simplicity and informativeness. Consequently, a model provides only an approximate description of the properties and behaviour of the modelled system:

- structural inadequacies derive from the limitations of the available knowledge on the modelled object, implied by omission of some factors in the choice of the quantities (input, output and influence quantities) modelling the system, the inappropriate specification of such quantities, the inappropriate choice of the equation modelling the relationships among those quantities;
- inaccuracies in the parameter estimates are due to accuracy limitations of the parameter identification method, errors of its technical implementation, errors in the data used for identification.

The assessment of such inadequacies and inaccuracies is highly problematic in practice, since they may be estimated only by means of a so-called extended model of the system, *i.e.*, a model that is structurally richer and/or more exact in its parameter values than the model under consideration. The extended model differs from the initial model in that it may have more input, output, influence quantities, and/or parameters, or because its parameter values are deemed to be obtained more accurately. Some other model validation strategies can also be envisaged (in particular based on sameness of results obtained from empirically independent models and effectiveness of model-based decision processes [5]), but all of them emphasise that model quality is not an absolute characteristic, and must be assessed relatively to an external and independent reference.

3. CLASS OF MODELS TO BE USED IN THE PROPOSED APPROACH

The proposed application-oriented approach is based on a particular class of mathematical models which may be called *input-output models* since they refer to the classification of the quantities, describing a modelled object or phenomenon into input and output quantities. The input quantities are further subdivided into desirable and undesirable input quantities; among the latter ones controllable input quantities (called *influence quantities*) and uncontrollable input quantities (called *disturbances*) are distinguished. It should be stressed that the input-output models cover the bulk majority of needs related to mathematical modelling in engineering and empirical sciences. They are adequate tools for describing both causal and correlation-type relationships. Depending on the origin and quantity of information used for modelling they may be of black-box type, white-box type or grey-box type. Let's

illustrate their usefulness in measurement science and technology with some examples of modelling from metrological literature. They will be presented in groups referring to the same mathematical structure used for modelling (after [6]).

Example 1. Algebraic equations have been used for modelling sensors in the following cases:

- a magnetostrictive sensor of strain [7] (the relationship between the spiky component of its voltage response and the measured stress is modelled by means of a single algebraic equation whose parameters are related to the selected working conditions of the sensor);
- a tin-oxide sensor of gas concentration [8] (the relationship between its static resistance y and the concentrations x_1 , x_2 , and x_3 of components of a gaseous analyte is modelled by means of the following algebraic equation:

$$y = \begin{bmatrix} p_1 \\ p_2 \\ p_3 \\ p_4 \\ p_5 \\ p_6 \\ p_7 \\ p_8 \end{bmatrix}^T \begin{bmatrix} 1 \\ \log(x_1) \\ \log(x_2) \\ \log(x_3) \\ \log(x_1)\log(x_2) \\ \log(x_1)\log(x_3) \\ \log(x_2)\log(x_3) \\ \log(x_1)\log(x_2)\log(x_3) \end{bmatrix} \quad (1)$$

where p_1, \dots, p_8 are the parameters of the model);

- a capacitive sensor of acceleration, based on a micromachined disc levitating between two electrodes [9] (the dependence of its capacitance on the 3D-space coordinates is modelled by means of a rational function). ♣

Example 2. Ordinary differential equations (ODEs) have been used for modelling sensors in the following cases:

- a capacitor-based sensor of soil moisture [10] (the relationship between its voltage response, depending on the measurand, and a current excitation is modelled by means of a linear first-order ODE, represented by an impedance block);
- a fibre-optic sensor of temperature [11] (the relationship between its voltage response and a square-wave excitation signal is modelled by means of a linear first-order ODE represented by an apparatus function whose time constant depends on the temperature);
- a ceramic sensor of gas concentration [12] (its impedance is modelled by means of a linear sixth-order ODE represented by an equivalent RC circuit);
- sensors for measuring the relative mass loss of fuel for applications in fire detectors [13] (the relationship between their response and the relative mass

loss is modelled by means of a linear ODE and, alternatively, corresponding discrete convolution-type equations);

- a thermal-flow sensor of sound particle velocity [14] (its voltage response to the velocity is modelled by means of a linear ODE represented by the following transfer function:

$$G(j\omega) = \int_0^\omega \frac{\Delta U_2(j\omega')}{C + \Delta U_1(j\omega')} d\omega' \quad (2)$$

where $\Delta U_1(j\omega')$ and $\Delta U_2(j\omega')$ are the amplitude spectra of two voltages measured during characterisation of the sensor, and C is a constant). ♣

Example 3. Some other mathematical structures have been used for modelling sensors in the following cases:

- The response of a quenched-luminescence sensor of oxygen concentration (a complex luminescence signal) is modelled by means of an integral of a function whose parameters depend not only on the measurand but also on two influence quantities, viz. distributions of dye and excitation in the sensor [15].
- The response of a resistive sensor of oxygen concentration is modelled by means of a linear first-order partial differential equation, nonlinear with respect to a variable modelling particle positions [16].

4. PROPOSED META-MODEL OF MEASUREMENT

The presentation of the most general meta-model of measurement will be accomplished here in three steps:

- First, a meta-model, aggregating functions which must appear in any so-called *canonical measuring system*, will be introduced.
- Then, its generalisation on functionally-richer canonical measuring systems will be carried out.
- Finally, the generalisation on non-canonical measuring systems will be proposed.

The class of canonical measuring systems, introduced above, encompasses the systems for measuring physical quantities by converting them into electrical digital signals and processing the latter by means of digital processors. The current importance of this class is implied by the possibility to solve a very broad class of measurement problems by means of commercially available elements such as sensors, analogue-to-digital converters, standard interfaces and computers.

4.1. Step 1

The minimum meta-model of measurement, performed by means of a canonical measuring system, is shown in Fig. 1. In this figure: the blue-grey shadow represents the sphere of physical reality and the white block diagram – the sphere of mathematical abstracts. The input interface is a plurality of technical means enabling the interaction between MS and SuM, necessary for measurement. The output interface is for providing communication with an external receiver of

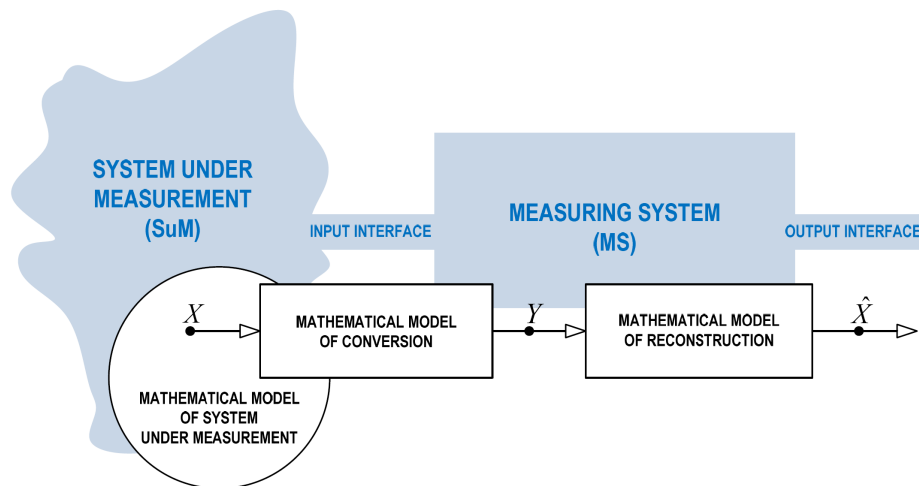


Fig. 1. Application-oriented meta-model of measurement.

- The relationship between the absorbance response and the concentration, in a spectrophotometric sensor for measuring the concentration of HCl vapours, is modelled by means of four linear second-order partial differential equations which describe the dynamic behaviour of the measurand and of three other concentrations of ions involved in the sensing process [17]. ♣

the result of measurement, i.e. with a person or a technical system MS is "working" for. The meta-model of measurement is composed of three interdependent parts:

- a mathematical model of SuM, including the measurand X ;
- a mathematical model of conversion, mapping the X into the raw result of measurement Y ;

- a mathematical model of reconstruction, mapping the raw result of measurement Y into the final result of measurement \hat{X} , *i.e.* an estimate of the measurand X .

A measurand X is defined by a mathematical model of SuM as a parameter or a function explicitly appearing in this SuM, or a function of such parameters or functions, or a functional of such parameters or functions.

The mathematical model of conversion is describing the transfer of information carried by the measurand to the signals which are easy to process (today: electrical and digital signals). Thus, it represents all the conversions of the physical nature of the signals (*e.g.* optical to electrical) and of the type of signals (*e.g.* analogue to digital). The blocks representative of the model of conversion and of the model of SuM are overlapping in Fig. 1 because the "conversion" of the measurand into the raw result of measurement may partially take place in SuM and partially in MS. To illustrate this idea, let's consider an example, *viz.* MS for measuring frequency of the signal provided by a generator of sinusoidal voltage.

Example 4: In this case, the model of SuM may have the form:

$$u(t) = U \sin(2\pi ft + \varphi) + u_{\perp}(t) \text{ for } t \in [0, T] \quad (3)$$

where f denotes the measurand (X), *i.e.* the frequency to be measured; t denotes time; $u(t)$ stands for the voltage signal accessible for MS; U and φ are known or unknown model parameters (depending on the formulation of the measurement task); and $u_{\perp}(t)$ is a component of $u(t)$ satisfying the orthogonality condition:

$$\int_0^T \sin(2\pi ft + \varphi) u_{\perp}(t) dt = 0 \text{ for } t \in [0, T] \quad (4)$$

and the inequality:

$$\|u_{\perp}(t)\| \ll U \quad (5)$$

The corresponding model of conversion may have the form:

$$\tilde{u}_n = U \sin(2\pi ft_n + \varphi) + u_{\perp}(t) + \eta_n \text{ for } t_n \in [0, T] \text{ and } n = 1, \dots, N \quad (6)$$

where the sequence $\{\tilde{u}_n \mid n = 1, \dots, N\}$, containing the results of sampling the voltage $u(t)$ at the time instants t_n , is the raw result of measurement (Y); η_n is a random component of \tilde{u}_n , representative of all the uncontrollable factors influencing SuM and MS (it may also absorb $u_{\perp}(t)$ if no *a priori* information on this signal is available). ♣

A mathematical model of reconstruction is describing all the operations aimed at determination of the final result of measurement, *i.e.* an estimate \hat{X} of X , on the basis of the raw result of measurement Y , the mathematical model of conversion, and *a priori* information on the measurand (if it is not included in the model of conversion). The parameters of the forward or (pseudo)inverse model of conversion, necessary for measurand reconstruction, are obtained during *calibration* on the basis of the known (assumed) structure of the model and raw results of measurements, corresponding to some reference values of the measurand. In a canonical measuring system, the estimate \hat{X} is determined by a digital processor; so, the difference "between the model and reality" may be limited to the errors caused by the finite representation of numbers in that processor.

The final result of measurement, \hat{X} , is subject to uncertainty whose sources may be classified into two groups:

- the discrepancy between the mathematical models (white blocks in Fig. 1) and physical reality (blue-grey blocks in Fig. 1);
- the discrepancy between \hat{X} and X resulting from the properties of the mathematical models.

The evaluation of the first-group uncertainties is based on the assessment of the discrepancy between two mathematical models of the measurement channel: the principal model and the corresponding extended model.

Let's have a closer look at the mathematical description of the scheme from Fig. 1. All the symbols used there may denote scalars, vectors, matrices, functions or more complex operators. In particular, a symbol denoting the measurand (X) can represent:

- a scalar quantity x ; *e.g.* temperature, voltage or concentration of an analyte;
- a vector quantity $\mathbf{x} = [x_1 \ x_2 \ \dots]^T$; *e.g.* a vector of temperatures in an interior or a vector of mixed quantities (temperature, pressure and concentrations of analytes);
- a scalar or vector function of a scalar variable t or of a vector variable \mathbf{t} – $x(t)$, $\mathbf{x}(t)$, $x(\mathbf{t})$ or $\mathbf{x}(\mathbf{t})$; *e.g.* an optical spectrum being a function modelling the dependence of light intensity on wavelength or a vector of functions modelling the dependence of the voltages (in an electronic circuit) on time.

Further description of the model in Fig. 1 will be restricted to the most typical measurement situations when $X \equiv \mathbf{x}(\mathbf{t})$ and $Y \equiv \{\mathbf{y}_n\}$, but it will take into account disturbances which may influence both SuM and MS. The disturbed versions of the quantities will be indicated with tildes over corresponding symbols, and their exact versions with dots; in particular: $\dot{\mathbf{x}}(\mathbf{t})$ will be the exact version of $\mathbf{x}(\mathbf{t})$ and $\{\tilde{\mathbf{y}}_n\}$ – a sequence of disturbed values of vectors \mathbf{y}_n .

According to the scheme presented in Fig. 1, the final result of measurement is determined on the basis of the raw result of measurement $\{\tilde{y}_n\}$:

$$\hat{\mathbf{x}}(\mathbf{t}) = \mathcal{R}[\{\tilde{y}_n\}; \mathbf{p}_{\mathcal{R}}] \quad (7)$$

where \mathcal{R} is an operator, called *operator of measurement and reconstruction*, and $\mathbf{p}_{\mathcal{R}}$ is the vector of its parameters. The operator \mathcal{R} is an inverse, approximate inverse or pseudoinverse of the forward model of conversion:

$$\{\dot{y}_n\} = \mathcal{C}[\dot{\mathbf{x}}(\mathbf{t}); \mathbf{p}_{\mathcal{C}}] \quad (8)$$

where $\{\dot{y}_n\}$ denotes the "exact" raw result of measurement, as it might be recorded in the absence of disturbing factors, and $\mathbf{p}_{\mathcal{C}}$ is the vector of parameters. On the whole $\mathbf{p}_{\mathcal{R}} \neq \mathbf{p}_{\mathcal{C}}$, but if the operator \mathcal{R} is derived from the operator \mathcal{C} , the equality $\mathbf{p}_{\mathcal{R}} = \mathbf{p}_{\mathcal{C}}$ is not excluded.

One of the operators, \mathcal{C} or \mathcal{R} , must be determined in advance, during calibration, on the basis of a set or sets of reference data:

$$\tilde{\mathcal{D}}^{cal} = \left\{ \tilde{\mathbf{x}}^{cal}(\mathbf{t}) \in \mathbb{X}(\mathbb{T}), \{\tilde{y}_n^{cal}\} \right\} \quad (9)$$

that cover the spaces of variation of $\mathbf{x}(\mathbf{t})$, denoted with the symbol $\mathbb{X}(\mathbb{T})$. The elements of the set $\tilde{\mathcal{D}}^{cal}$, although considered to be reference data, are subject to errors whose presence, unavoidably, makes uncertain the result of calibration.

4.2. Step 2

Let's move to the second step of the meta-model presentation, *i.e.* to its generalisation on measurement situations where neither influence quantities nor signals controlling the responses of SuM may be neglected. First, a generalised influence quantity V , which may have an impact on the behaviour of both SuM and MS, should be added. It is influencing the raw result of measurement, but – in contrast to disturbances – its value may be estimated and taken into account in the process of measurand reconstruction because it is measured or controlled. To produce an estimate \hat{X} of the measurand X , MS is acquiring two signals: a signal which is carrying information on the measurand X and a signal which is carrying information on the generalised influence quantity V . It is, moreover, generating two signals: a signal U_x , which is exciting SuM to provoke a desirable manifestation of the measurand X , and a signal U_v , which is controlling it to create a desirable state of the generalised influence quantity V .

The generalised formulation of the meta-model will be restricted to the most typical measurement situations when: $V \equiv \mathbf{v}$, $U_x \equiv \{\mathbf{u}_n\}$, and U_v is absent. The diacritical signs, hats, tildes and dots over the

corresponding signals – will be used in the same way as for $\mathbf{x}(\mathbf{t})$ and \mathbf{y}_n . Under such assumptions, the generalised model of reconstruction takes on the form:

$$\hat{\mathbf{x}}(\mathbf{t}) = \mathcal{R}[\{\tilde{y}_n\}; \hat{\mathbf{v}}, \{\hat{\mathbf{u}}_n\}; \mathbf{p}_{\mathcal{R}}] \quad (10)$$

where $\hat{\mathbf{v}}$ is the estimated (measured) value of the vector of influence quantities, and $\{\hat{\mathbf{u}}_n\}$ is the exact value of the control signal. The operator of measurand reconstruction \mathcal{R} is now an inverse, approximate inverse or pseudoinverse of the forward model of conversion:

$$\{\dot{y}_n\} = \mathcal{C}[\dot{\mathbf{x}}(\mathbf{t}), \dot{\mathbf{v}}, \{\dot{\mathbf{u}}_n\}; \mathbf{p}_{\mathcal{C}}] \quad (11)$$

One of the operators, \mathcal{C} or \mathcal{R} , must be determined in advance, during calibration, on the basis of an enhanced set of reference data:

$$\tilde{\mathcal{D}}^{cal} = \left\{ \tilde{\mathbf{x}}^{cal}(\mathbf{t}) \in \mathbb{X}(\mathbb{T}), \tilde{\mathbf{v}}_n^{cal} \in \mathbb{V}, \tilde{\mathbf{u}}_n^{cal} \in \mathbb{U} \right\} \quad (12)$$

covering the spaces of variation – $\mathbb{X}(\mathbb{T})$, \mathbb{V} and \mathbb{U} – of the quantities involved in the process of measurement – $\mathbf{x}(\mathbf{t})$, \mathbf{v} and \mathbf{u} – respectively. Again, the reference data $\tilde{\mathcal{D}}^{cal}$ are subject to errors whose presence makes uncertain the result of calibration.

There are two fundamentally different approaches of the calibration problem: the forward-model-based approach (FMA), and the inverse-model-based approach (IMA). The first, more traditional, approach, is based on the use of the forward model of conversion: the estimates of the parameters of the operator \mathcal{C} , obtained during calibration, are used in the reconstruction procedure, together with *a priori* information on the structure of this operator. This approach is founded on the following premises:

- The final result of measurement $\hat{\mathbf{x}}(\mathbf{t})$, generated by \mathcal{R} , should belong to the space $\mathbb{X}(\mathbb{T})$.
- Its image $\mathcal{C}[\hat{\mathbf{x}}(\mathbf{t}) \dots; \hat{\mathbf{p}}_{\mathcal{C}}]$, where $\hat{\mathbf{p}}_{\mathcal{C}}$ is an estimate of $\mathbf{p}_{\mathcal{C}}$ resulting from calibration, should be close to the vector of raw measurement data $\{\tilde{y}_n\}$ but not necessarily identical with it.
- Optionally, it should meet some additional requirements reflecting available *a priori* information about the properties of the measurand (such as non-negativity, bounded support or band-limited spectrum) known, *e.g.*, from the analysis of physical phenomena underlying the functioning of SuM.

The second, more modern, approach (IMA) consists in direct identification of the reconstruction operator \mathcal{R} – satisfying the above requirements – during calibration; the method of calibration is in this case at least partially determined by the chosen method of reconstruction. As a rule, this approach leads to more complicated procedures of calibration than the FMA; that is why it may be widely implemented only recent-

ly, due to the increase in performance of computing means. The main idea of this approach is to estimate the parameters $\mathbf{p}_{\mathcal{R}}$ in such a way as to control the error of reconstruction:

$$\mathcal{R}\left[\left\{\hat{\mathbf{y}}_n^{cal}\right\}, \hat{\mathbf{v}}^{cal}, \left\{\hat{\mathbf{u}}_n^{cal}\right\}, \mathbf{p}_{\mathcal{R}}\right] - \tilde{\mathbf{x}}^{cal}(\mathbf{t}) \quad (13)$$

rather than the error of simulation:

$$\mathcal{E}\left[\tilde{\mathbf{x}}^{cal}(\mathbf{t}), \hat{\mathbf{v}}^{cal}, \left\{\hat{\mathbf{u}}_n^{cal}\right\}, \mathbf{p}_{\mathcal{E}}\right] - \left\{\hat{\mathbf{y}}_n^{cal}\right\} \quad (14)$$

A justification for using the criteria of calibration defined in the domain of the measurand is given in numerous papers, e.g. [18], [19], [20], [21]. According to IMA, the operator of reconstruction may be globally optimised using the criteria of the quality of measurand reconstruction, defined in the space of vectors of measurand values. The attainable accuracy of measurand reconstruction is higher for IMA than for FMA since the latter is based on the optimisation of the forward model using the criteria of the quality of conversion simulation, defined in the space of vectors of data.

4.3. Step 3

The last step of the meta-model presentation is aimed at its generalisation on non-canonical measuring systems, in particular – on so-called analogue measuring systems (as opposed to digital measuring systems, being up to now considered in this section), and on systems for measuring non-physical (economic, social, psychological, *etc.*) quantities. Let's start with two simple examples: measurement of current by means of a d'Arsonval-Weston galvanometer and measurement of the intelligence quotient (IQ).

Example 5. The electromechanical core of a galvanometer is composed of a small pivoting coil of wire in the field of a permanent magnet. The coil is attached to a thin pointer that traverses a calibrated scale. A little torsion spring pulls the coil and pointer to the zero position. When a direct current (X) flows through the coil, then the coil generates a magnetic field which acts against the permanent magnet. The coil twists, pushing against the spring, and moves the pointer: the angular deflection (Y) of the pointer is approximately proportional to the current. By visual comparison of the position of the pointer with the calibrated scale, the user of the galvanometer is able to read the final result of measurement *i.e.* an approximate value (\hat{X}) of the measured current (X). This process may be viewed as a sequence of two transformations:

- the conversion of an electrical signal (current) whose value is to be measured into an optical signal (an image of the deflected pointer), performed by an electromagnetic core of the galvanometer;
- the reconstruction of the measurand on the basis of visual comparison of the image of the pointer with

the image of the scale, performed by the operator of the galvanometer.

Such a decomposition of the measurement process enables one to apply the developed meta-model to the analysis and design of a galvanometer. ♣

Example 6. IQ is an indicator of intellectual potential of a person, used in psychometrics. Due to the lack of a satisfactory definition of intelligence, it cannot be considered as its measure, but rather as a relatively independent quantity defined by the method for determining its values, *i.e.* by standardised tests developed for this purpose. IQ is used as a predictor of educational achievements of a person or of his/her job performance, due to its empirically confirmed correlation with some intellectual capacities. A standardised test, used for IQ measurements, is usually composed of multiple-choice or true-false questions; a point weight is attributed to each question. The test has a mean score of 100 points and a standard deviation of 15 points. It means that 68 % of the population score an IQ within the interval 85–115, and 95 % – within the interval 70–130. The IQ score of an individual is correlated with such factors as the social status of his/her parents; thus, those factors play the role of influence quantities. This process of IQ measurement may be viewed as a sequence of two transformations: the "conversion" of the intellectual abilities of an individual into a set of test scores, and the "reconstruction" of IQ value by numerical aggregation of those scores. Again, such a decomposition of the measurement process enables one to apply the presented meta-model to its analysis in terms mathematical tools used in measurements of physical quantities. ♣

Both above-outlined examples show the potential behind the presented meta-model (logical framework) to cover much broader class of measurements than those performed by canonical measuring systems. A key decision enabling the adaptation of the model developed for canonical measuring systems consists in the proper choice of the quantity considered to be the raw result of measurement. This quantity should belong to the domain of "easily interpretable phenomena" such as visual signals in the time of analogue measuring instruments or digital electrical signals today. Both examples show the importance of a "common denominator" of all measurements, *viz.* comparison with the standards, whose effectiveness depends on calibration.

5. SELECTED APPLICATIONS

5.1. Measurement of coin surface

Let's assume that the surface (x) of a golden coin (SuM) is to be measured by means of MS composed of a CCD line detector, followed by an analogue-to-digital converter, a digital interface, and a computer. Let's assume, moreover, that the coin is illuminated by a light source, and it is positioned by a coin holder,

both controlled by the computer. The measurement procedure comprises the following steps:

M1: The coin is fixed in the coin holder at its initial position (the surface of the coin parallel to the surface of the CCD detector, its centre on the projection of the CCD detector centre) and illuminated; the counter (n) in the computer is set to 1.

M2: The result of the analogue-to-digital conversion (\tilde{y}_n) of the output signal of the CCD line detector, assumed to be monotonically related to the coin diameter, is recorded in the computer memory.

M3: If $n < N$, then the coin is turned around by the angle $2\pi/N$, the counter is incremented by 1, and the procedure returns to the step M2.

M4: An estimate \hat{x} of the coin surface x is calculated in the computer on the basis of the raw results of measurement $\{\tilde{y}_n\}$ using an artificial neural network (ANN), appropriately trained during calibration (IMA).

Let's assume that calibration is based on the use of K reference coins whose surfaces ($\hat{x}_k^{cal}, k = 1, \dots, K$) are known with the uncertainty at least 10 times lower than the target measurement uncertainty. Then, the calibration procedure comprises two steps:

C1: First, the raw results of measurement $\{\tilde{y}_{k,n}\}$, corresponding to all reference surfaces \hat{x}_k^{cal} ($k = 1, \dots, K$), are recorded.

C2: Next, the parameters of ANN are adjusted in such a way as to minimise the criterion $\sum_{k=1}^K (\hat{x}_k^{cal} - \hat{x}_k^{cal})^2$, where \hat{x}_k^{cal} is the ANN output corresponding to the input sequence $\{\tilde{y}_{k,n}\}$.

The above calibration procedure is consistent with the chosen method of measurand reconstruction (step M4), and must be modified if the latter is changed. Let's assume, for example, that instead of ANN the following formula of estimation is used:

$$\hat{x} = \sum_{n=1}^N (p_1 \tilde{y}_n + p_0)^2 \quad (15)$$

Then, during calibration, the parameters p_0 and p_1 should be determined via minimisation of the criterion

$$\sum_{k=1}^K (\hat{x}_k^{cal} - \hat{x}_k^{cal})^2, \text{ where:}$$

$$\hat{x}_k^{cal} = \sum_{n=1}^N (p_1 \tilde{y}_{k,n}^{cal} + p_0)^2 \quad (16)$$

If the step M2 of the measurement procedure were repeated N times without turning the coin around, then the reconstruction method based on the formula:

$$\hat{x} = \left(p_1 \sum_{n=1}^N \tilde{y}_n + p_0 \right)^2 \quad (17)$$

would be more appropriate. If the nonlinearity of the conversion were non-negligible, the reconstruction method:

$$\hat{x} = \sum_{n=1}^N (p_2 \tilde{y}_n^2 + p_1 \tilde{y}_n + p_0)^2 \quad (18)$$

could prove to be more accurate.

5.2. Measurement of optical spectrum [22]

The intensity spectrum, $x(\lambda)$, of an optical signal (light) is a scalar real-valued function representative of the distribution of optical power $x \in [x_{\min}, x_{\max}]$ in a given interval $[\lambda_{\min}, \lambda_{\max}]$ of wavelength λ . Thus, in the considered case SuM is a source of light, and MS is a spectrophotometer schematically depicted in Fig. 2. This spectrophotometer is composed of two principal blocks, viz.: a spectrophotometric transducer (ST) and a digital signal processor (DSP).

ST is converting an optical signal into a vector of data, $\tilde{y} \equiv [\tilde{y}_1 \dots \tilde{y}_N]^T$, representative of the spectrum $x(\lambda)$ of that signal. On the basis of that vector, containing integer numbers called counts, DSP is computing a vector \hat{x} whose elements are estimates of the spectrum values $x(\lambda_m)$, $m = 1, \dots, M$. The corresponding numerical procedure is referring to the information on the ST, acquired by means of reference measuring instruments, and preprocessed during the calibration, comprising acquisition of the reference data by means of reference instrumentation and their processing by means of an external computer (not by DSP of the spectrophotometer). The measurement procedure comprises the following steps:

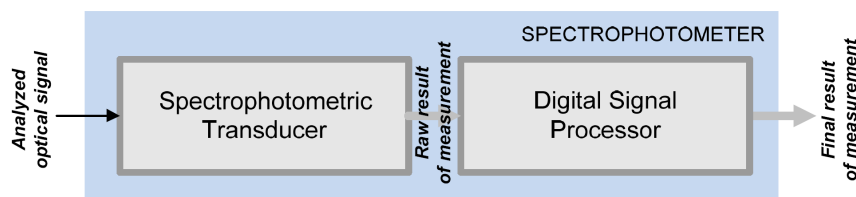


Fig. 2. The functional diagram of a spectrophotometer.

M1: The source of the optical signal, whose intensity spectrum is to be measured, is switched on and stabilised during one hour.

M2: The vector of raw measurement data \tilde{y} is recorded in the DSP memory and used for computing the function $\hat{y}(\lambda)$, interpolating the sequence of pairs $\langle \lambda_n^{cal}, \tilde{y}_n \rangle$, where λ_n^{cal} are elements of a vector of wavelength values λ^{cal} , obtained during calibration.

M3: The final result of measurement is determined according to the formula:

$$\hat{x}_m = p_2 \hat{y}(\lambda_m) + p_1 \hat{y}(\lambda_m) + p_0 \text{ for } m = 1, \dots, M \quad (19)$$

where p_0 , p_1 and p_2 are parameters determined during calibration.

A procedure of calibration, consistent with the above measurement procedure, is based on the use of a high-resolution tuneable source of monochromatic optical signal, calibrated with respect to wavelength and magnitude.

C1: First, this source is set to an average magnitude x_{avg}^{cal} and tuned from λ_{min} to λ_{max} ; in this way, the wavelength values λ_n^{cal} , corresponding to the maxima of the consecutive elements of the vector \tilde{y} , are identified.

C2: Next, the responses of ST to the monochromatic signal – whose wavelength value is set to λ_n^{cal}

It may turn out that the optical resolution of spectrum measurements, performed according to the above-described procedures of reconstruction and calibration, is insufficient. Then the following improvements can be introduced to the step M2 of the measurement procedure:

M2': The vector of raw measurement data \tilde{y} is recorded in the DSP memory and used for computing the function $\hat{y}(\lambda)$, approximately satisfying the following set of equations:

$$g(\lambda) * \hat{y}(\lambda) \Big|_{\lambda=\lambda_n^{cal}} = \tilde{y}_n \text{ for } n = 1, \dots, N \quad (21)$$

where $*$ is the operator of convolution; λ_n^{cal} are elements of the vector λ^{cal} , obtained during calibration, and $g(\lambda)$ is a so-called apparatus function determined during calibration.

The corresponding procedure of calibration must include a step of $g(\lambda)$ determination, e.g. by recording and centring the ST response \tilde{y}_g to a signal generated by the monochromator tuned to the wavelength value $\lambda_g = (\lambda_{min} + \lambda_{max})/2$.

5.3. Spectrophotometric analysis of liquids [23]

A spectrophotometric analyser is an instrument for measuring physical and/or chemical parameters – such as concentrations c_1, \dots, c_J – of selected compounds of a liquid sample, representative of a pre-defined class of chemical or biochemical substances. The spectrophotometer, described in the previous example,

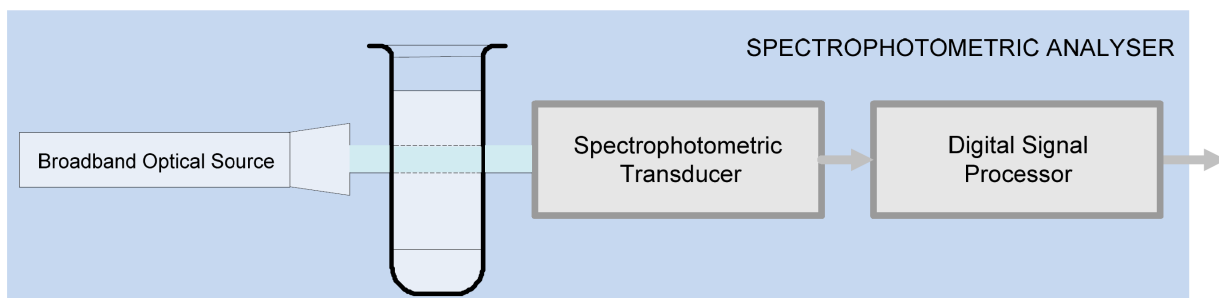


Fig. 3. A spectrophotometric analyser – the principle of functioning.

and magnitude to $x_{min}^{cal} \cong x_{min}$ and $x_{max}^{cal} \cong x_{max}$ – are recorded.

C3: Finally, the maximum values of those responses – $y_{min,n}^{cal}$ and $y_{max,n}^{cal}$ ($n = 1, \dots, N$) – are used for estimation of the parameters p_0 , p_1 and p_2 by minimising the following criterion:

$$\sum_{n=1}^N \left[x_{min}^{cal} - p_2 (x_{min,n}^{cal})^2 - p_1 x_{min,n}^{cal} - p_0 \right]^2 + \sum_{n=1}^N \left[x_{max}^{cal} - p_2 (y_{max,n}^{cal})^2 - p_1 y_{max,n}^{cal} - p_0 \right]^2 \quad (20)$$

is the heart of such an analyser (Fig. 3).

The measurement procedure comprises the following steps:

M1: The source optical signal is converted into the data \tilde{y}_0 representative of its intensity spectrum $x_0(\lambda)$.

M2: The same source optical signal is passed through a cuvette, containing a sample of the substance to be analysed, and converted into the data \tilde{y}_1 representative of its intensity spectrum, modified by a sample, $x_1(\lambda)$.

M3: The intensity data \tilde{y}_0 and \tilde{y}_1 are processed by a digital signal processor in order to obtain estimates of the concentrations c_1, \dots, c_J .

The latter step is based on the transformation of the intensity spectra $x_0(\lambda)$ and $x_1(\lambda)$ into the transmittance spectrum defined as:

$$x^{Tr}(\lambda) = \frac{x_1(\lambda)}{x_0(\lambda)} \quad (22)$$

and the corresponding transformation of the data \tilde{y}_0 and \tilde{y}_1 into the transmittance data, representative of $x^{Tr}(\lambda)$, according to the formula:

$$\tilde{y}_n^{Tr} = \frac{\tilde{y}_{1,n} - b_n}{\tilde{y}_{0,n} - b_n} \text{ for } n = 1, \dots, N \quad (23)$$

where $\mathbf{b} = [b_1 \dots b_N]^T$ is the ST response to the zero-intensity optical signal. The transmittance data are further transformed into the corresponding absorbance data:

$$\tilde{y}_n^{Ab} = -\log_{10}(\tilde{y}_n^{Tr}) \text{ for } n = 1, \dots, N \quad (24)$$

representative of the absorbance spectrum:

$$x^{Ab}(\lambda) = -\log_{10}(x^{Tr}(\lambda)) \quad (25)$$

An example of transmittance and absorbance data is shown in Fig. 4. The absorbance data emphasise the most informative parts of the spectrum, *viz.* absorption peaks whose parameters, positions and magnitudes, are determined by the qualitative and quantitative composition of the sample under study. The graphical image of those data is a finger-print enabling the identification of the sample. Thus, the coordinates of the maxima of absorption peaks:

$$\langle n_1, \tilde{y}_{n_1}^{Ab} \rangle, \langle n_2, \tilde{y}_{n_2}^{Ab} \rangle, \dots \quad (26)$$

may be used for estimation of c_1, \dots, c_J , for example, by means of an artificial neural network.

A procedure of calibration, consistent with the above-described measurement procedure, is based on

the use of a set of reference samples of the analysed liquid (*e.g.* red wine) whose composition (the values of c_1, \dots, c_J) is known with an uncertainty significantly smaller than expected uncertainty of the analyser under development:

- C1: For each reference sample, the peak parameters – $\langle n_1, \tilde{y}_{n_1}^{Ab} \rangle, \langle n_2, \tilde{y}_{n_2}^{Ab} \rangle, \dots$ – are determined in the same way as during measurement.
- C2: They are used, together with the reference values of concentrations, for training the neural network.

5.4. Expanded-model-based evaluation of measurement uncertainty

Let's return to a methodology for measuring the surface of a golden coin, described in the sub-section 5.1.; let's assume that:

- The mathematical model of the coin, defined in the radial system of coordinates, has the form:

$$r = \frac{d_0}{2} \text{ for } \varphi \in [0, 2\pi] \quad (27)$$

where r is radius, φ is angle and d_0 is the average diameter of the coin.

- The measurement reconstruction is based on the mathematical model defined by (15).

The first of the above assumptions means that the coin is perfectly round and perfectly positioned; the second – that the nonlinearity of conversion is neglected. The evaluation of measurement uncertainty could be based in this case on the extended model of the coin and extended model of measurand reconstruction. The first of them might have the form:

$$r(\varphi) = \frac{d_0}{2} + \frac{d_1}{2} \sin\left(\frac{100}{2\pi} \varphi\right) + \Delta\rho(\varphi) \text{ for } \varphi \in [0, 2\pi] \quad (28)$$

where d_1 is the depth of 100 engravings on the edge of the coin, and $\Delta\rho(\varphi)$ is a realisation of a stochastic process modelling imperfections of the coin positioning, *i.e.* a non-random function of a random three-dimensional vector characterising the undesirable deviation of the actual coin position from its nominal position. The formula (18) could be used as an ex-

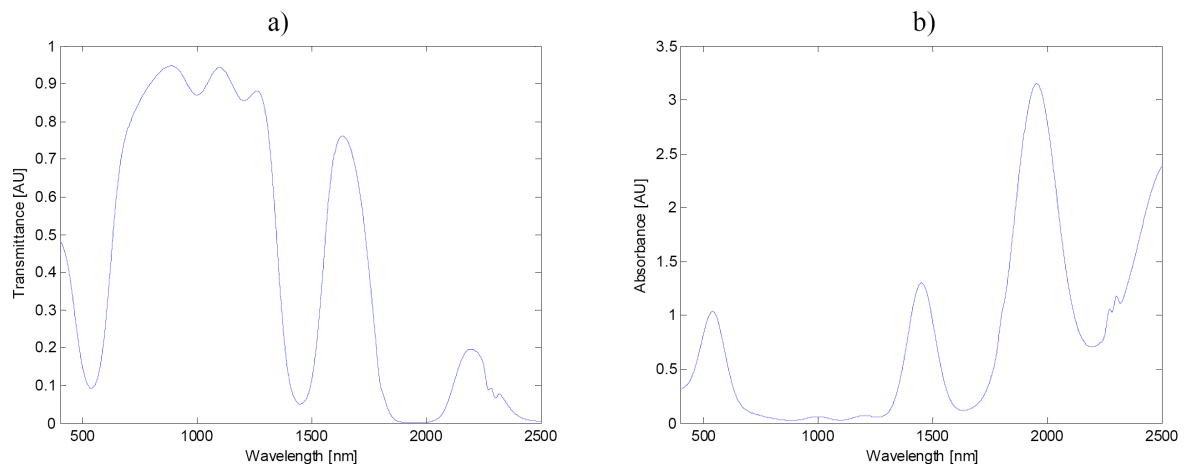


Fig. 4. The transmittance data (a) and the absorbance data (b), representative of the spectrum of red wine.

tended model of measurand reconstruction. The components of measurement error, assessed by means of those two extended models, have the form:

$$\Delta\hat{x}_1 = \int_0^{2\pi} \frac{d_0}{2} d\varphi - \int_0^{2\pi} \left[\frac{d_0}{2} + \frac{d_1}{2} \sin\left(\frac{100}{2\pi}\varphi\right) + \Delta\rho(\varphi) \right] d\varphi$$

$$= \int_0^{2\pi} \Delta\rho(\varphi) d\varphi \quad (29)$$

$$\Delta\hat{x}_2 = \sum_{n=1}^N (p'_1 \tilde{y}_n + p'_0)^2 - \sum_{n=1}^N (p_2 \tilde{y}_n^2 + p_1 \tilde{y}_n + p_0)^2 \quad (30)$$

where p'_0 and p'_1 are parameters obtained during calibration referring to the model defined by (15), while p_0 , p_1 and p_2 are parameters obtained during calibration referring to the model defined by (18). Under an assumption that the error components $\Delta\hat{x}_1$ and $\Delta\hat{x}_2$ are small enough, the following formula:

$$\Delta\hat{x} = \sup|\Delta\hat{x}_1| + \sup|\Delta\hat{x}_2| \quad (31)$$

might be used for evaluation of the worst-case measurement uncertainty. In the above formula, the operation "sup" is performed over:

- the range of the possible variation of d_0 ;
- the range of variation of all neglected influence quantities,
- the set of admissible realisations $\Delta\rho(\varphi)$,
- the set of possible realisations of calibration data.

6. CONCLUSION

The presented application-oriented approach to mathematical modelling of measurement processes is the product of the author's attempts – undertaken during last 20 years [24], [25], [26], [6] – to integrate and unify practical methodologies applied by theoreticians and practitioners in various domains of measurement science. Although it is far from being fully accomplished, it seems to provide useful and consistent answers to the questions about the role of mathematical modelling in defining measurands, in calibration of measuring systems and in evaluation of measurement uncertainty. It seems also to be at least consistent with the ways of thinking, developed in metrology of non-physical quantities. It is relatively "insensitive" to various ontic and epistemic assumptions used by various versions of the philosophy of measurement. It is quite friendly or affirmative with respect to various theoretical frameworks of measurement, such as probabilistic, fuzzy or morphological approaches.

ACKNOWLEDGMENT

The preparation of this paper has been supported by the Ministry of Science and Higher Education in Poland (grant No. N N505 464832). The author is also indebted to Dr. Luca Mari, Professor of Università

Carlo Cattaneo – LIUC (Italy), whose opinions significantly influenced the final shape of this paper.

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