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General theory of experiment containing reproducible data: The reduction to an ideal experiment

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ABSTRACT

The authors suggest a general theory for consideration of *all* experiments associated with measurements of *reproducible* data in one unified scheme. The suggested algorithm does not contain unjustified suppositions and the final function that is extracted from these measurements can be compared with hypothesis that is suggested by the theory adopted for the explanation of the object/phenomenon studied. This true function is free from the influence of the apparatus (instrumental) function and when the "best fit", or the most acceptable hypothesis, is *absent*, can be presented as a segment of the Fourier series. The discrete set of the decomposition coefficients describes the final function quantitatively and can serve as an *intermediate model* that coincides with the amplitude-frequency response (AFR) of the object studied. It can be used by theoreticians also for comparison of the suggested theory with experimental observations. Two examples (Raman spectra of the distilled water and exchange by packets between two wireless sensor nodes) confirm the basic elements of this general theory. From this general theory the following important conclusions follow:

1. The Prony's decomposition should be used in detection of the quasi-periodic processes and for *quantitative* description of reproducible data.

2. The segment of the Fourier series should be used as the fitting function for description of observable data corresponding to an *ideal* experiment. The transition from the initial Prony's decomposition to the conventional Fourier transform implies also the elimination of the apparatus function that plays an important role in the reproducible data processing.

3. The suggested theory will be helpful for creation of the unified metrological standard (UMS) that should be used in comparison of similar data obtained from the same object studied but in *different* laboratories with the usage of different equipment.

4. Many cases when the conventional theory confirms the experimental data obtained from equipment (where the apparatus function was not taken into account) should be remeasured and some of the competitive theoretical hypothesis can be reconsidered, as well.

Abbreviations: AFR, amplitude–frequency response; AF, apparatus function; IM, intermediate model; HF, high-frequency fluctuations; LLSM, linear least square method; MR, magnetic resonance; QP, quasi-periodic; RS, Raman spectra; REMV, the reduced experiment to its mean value; SRA, the sequence of the ranged amplitudes; UMS, the unified metrological standard.

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5. New theory after the optimization of its basic algorithm can automatize the whole procedure of measurements used as a basic tool for collection and further comparison of reproducible data.

Two examples (Raman spectra of the distilled water and exchange by packets between two wireless sensor nodes) confirm the basic elements of this new theory.

1. Introduction and formulation of the problem

The measurements and different data processing form the foundation stone of all natural science and any attempt to push this stone over the hump seems *useless*. Many excellent books, reviews, pile of papers written by outstanding mathematicians, statisticians, experimentalists and theoreticians form a stable trend in the region of science as the data/signal treatment and processing. Here we want to remind the most popular books that form the foundation stone of this science [1–10]. All the cited works represent the great effort in the last decades in dealing with the data processing, fitting and forecasting in several application fields, based on different approaches and principles. The question that we want to formulate in this paper should sound unexpectedly and paradoxical for many researches: *Is it possible to create rather general and the unified theory/approach for all reproducible data processing?*

In this paper we want to find and justify the *positive* answer for this question posed. This theory should lead to reconsideration of the conventional point of view associated with treatment of reproducible data and create a new trend in the science known as the theory of reproducible measurements and the data/signal processing.

2. The basics of the general theory

Let us remind the definition of the *ideal* experiment that will be widely used in this paper. Let us suppose that we have a deterministic (control) variable x that interacts with the object studied and evokes the desired response $\Pr(x)$. If this response is reproduced *ideally* in each current measurement m from the interval $[1,M]$ then we can write

$$y_m(x) \cong \Pr(x + m \cdot T_x) = \Pr(x + (m-1) \cdot T_x), \quad m = 1, 2, \ldots, M. \tag{1}$$

Here x – is the external (control) variable, T_x is a "period" of experiment expressed in terms of the control variable x. In expression (1) we make *a supposition* that the properties of the object studied during the period of "time" T_x is *not* changed. As one can notice from (1) each current measurement in an "ideal" experiment is *independent* from the previous measurements and in this sense it does not have a memory. If $x = t$ coincides with temporal variable then $T_x = T$ coincides with the conventional definition of a period. The solution of this functional equation is well-known and (in case of discrete distribution of the given data points $x = x_j$, $(j = 1,2,\ldots,N)$ coincides with the segment of the Fourier series

$$\Pr(x) = A_0 + \sum_{k=1}^{K>>1}\left[Ac_k \cos\left(2\pi k \frac{x}{T_x}\right) + As_k \sin\left(2\pi k \frac{x}{T_x}\right)\right]. \tag{2}$$

We *deliberately* show only the segment of the Fourier series because in reality all data points are always *discrete* and the number of "modes" $k = 1,2,\ldots,K$ (coinciding with the coefficients of the Fourier decomposition) is limited. We define here and below by the capital letter K the *finite* number of modes. This value of K should be chosen from the condition that it is sufficient to fit experimental data with the given (or acceptable) accuracy. As we will see below the value of K can be calculated from the requirement that the relative error is located in the interval [1–10%]. This interval provides the desired fit of the measured function $y(x)$ to $\Pr(x)$ with initially chosen number of modes $k = 1,2,\ldots,K$ figuring in (2). From relationships (1), (2) one important conclusion follows. For an *ideally* reproducible experiment, which satisfies to condition (1) the F-transform (2) can be used as *intermediate model* (IM) and the number $2K + 2$ of decomposition coefficients (A_0, Ac_k, As_k) (we should calculate independently the unknown value of T_x as an additional nonlinear fitting parameter also) can be used as a set of the fitting parameters belonging to the IM. The meaning of these coefficients is well-known and actually this set defines the amplitude-"frequency" response (AFR) associated with the recorded "signal" $y(x) \approx \Pr(x)$ and coinciding with the measured function $y(x) \in y_m(x)$ $(m = 1,2,\ldots,M)$. Here we increase only the limits of interpretation of the conventional F-transform with respect to *any* deterministic variable x (including frequency also, if the control variable x coincides with some current ω) and show that the segment of this transformation (following to definition (1)) can be used for description of an *ideal* experiment. Let us consider another functional equation that generalizes expression (1)

$$F(x + T_x) = aF(x) + b, \tag{3}$$

This functional equation has been considered in the first time in paper [11] by the first author (RRN) and was defined later as a quasi-periodic (QP) process [12]. The solution of this equation is written in the following form [11]