One ill-posed estimation problem of experimental process parameters. Interval approach

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Keywords: experimental process, measurements, bounded error, parameters, estimation, interval approach, approximate *a priori* data

Introduction and problem formulation

In a chemical experiment, the following dependency of a reagent activity is investigated:

$$P(T,a,b,c) = T^2\,a\,b/c,\;\; a>0,\;\; b>0, c>0, \tag{1}$$

where T is the temperature, the main variable, C°; $P(\cdot)$ is the reagent activity, dimensionless; a, b, and c are unknown constant parameters with dimensions, respectively, in moles, 1/mole, and $(\mathrm{C}^\circ)^2$.

After experiment, the sample (with length N) of the activity measurements P_n is given

$$\{T_n, P_n\},\;\; n=\overline{1,N}, \tag{2}$$

where the temperature values are known exactly, but the values P_n are noised with the bounded measuring errors

$$P_n = P_n^* + e_n,\;\; |e_n| \le e_{\max},\;\; n=\overline{2,N},\;\; n=1,\;\; T_1=0,\;\; P_1=0, \tag{3}$$

where P_n^* is an unknown true value under measuring; e_n is the error in the nth measurement; $e_{\max}$ is the bound (by modulus) on the maximal error value; $P_1=0$ is the *conditional exact* zero initial measurement.

Specifics of the experiment is in the following: the probabilistic characteristics of the noise are *absolutely unknown*, the sample is fatally short (usually, $N \sim 6-7$ measurements are only provided), and only rough approximate *a priori* intervals of the parameters in (1) can be given

$$\boldsymbol{a}^{\rm ap} = [\underline{\boldsymbol{a}}^{\rm ap},\ \overline{\boldsymbol{a}}^{\rm ap}],\ \boldsymbol{b}^{\rm ap} = [\underline{\boldsymbol{b}}^{\rm ap},\ \overline{\boldsymbol{b}}^{\rm ap}],\ \boldsymbol{c}^{\rm ap} = [\underline{\boldsymbol{c}}^{\rm ap},\ \overline{\boldsymbol{c}}^{\rm ap}],$$
$$0 < \underline{\boldsymbol{a}}^{\rm ap} < \overline{\boldsymbol{a}}^{\rm ap},\ 0 < \underline{\boldsymbol{b}}^{\rm ap} < \overline{\boldsymbol{b}}^{\rm ap},\ 0 < \underline{\boldsymbol{c}}^{\rm ap} < \overline{\boldsymbol{c}}^{\rm ap}. \quad (4)$$

Problem formulation: *Using data* (1)–(4)*, construct the informational set* (*set-membership*) *for admissible* (*consistent*) *values of parameters* (1).

The problem is ill-posed since of the "stuck"-character of parameters in (1) and since it is impossible to validate application of standard statistical approaches to estimating such a set. So, here, the approach on the basis of the interval analysis has been used. Theoretical aspects of the approach is highlighted in [1], special algorithms and software for solving practical problems of the mentioned type has been elaborated and described in [2].

Interval procedures for estimating the process parameters and the main results

The following procedure of the interval approach are implemented.

1) The standard [1, 2] uncertainty intervals $\boldsymbol{H}_n = [P_n - e_{\max}, P_n + e_{\max}]$ are constructed for each measurement P_n from (3) by the given bound $e_{\max}$ (Fig.1a); and, introducing the auxiliary "joined" parameter $g = ab/c$, its corresponding informational interval $\boldsymbol{g} = [\underline{\boldsymbol{g}},\ \overline{\boldsymbol{g}}]$ is calculated [2]. Additionally, it is worthy to calculate the *a priori* interval of the parameter g and compare it with the obtained interval $\boldsymbol{g}$ for analysis of *consistency* of the *a priori* data (4) on parameters a, b, and c with the given sample of measurements (3).

2) Having the interval equation $ad = \boldsymbol{g}$, where $d = b/c$, solve it w.r.t. the auxiliary parameter d as follows: $\boldsymbol{d} = \boldsymbol{g}/\boldsymbol{a}^{\rm ap}$. As a result in the plane $a \times d$, we obtain the informational set $I(a, d)$ with the curve (hyperbolic) lower $\underline{Fr}_d(a)$ and upper $\overline{Fr}_d(a)$ boundaries (Fig.1b) as a functions of the parameter a values from its *a priori* interval $\boldsymbol{a}^{\rm ap}$. In Figure 1b, a cross-section of the set $I(a, d)$ is shown for value $a = 1.89$ mole; it is the interval $\boldsymbol{d}(1.89)$. In Figure 1b (at the left) the *a priori* interval of the auxiliary parameter d is shown (the thick dash-dotted

vertical segment) calculated by the *a priori* intervals $\boldsymbol{b}^{\rm ap}$ and $\boldsymbol{c}^{\rm ap}$. Here, the thick vertical line in dashes marks the outer interval of $I(a,d)$ on d for the *a priori* interval $\boldsymbol{a}^{\rm ap}$. Comparison of these two intervals allows one to check out *consistency* of the *a priori* data (4) on parameters a, b, and c with the given sample of measurements (3).

3) For each value $a \in \boldsymbol{a}^{\rm ap}$ we have the interval $\boldsymbol{d}(a)$ (Fig. 1b). So, it becomes possible to construct the informational set $I_a(b,c)$ (Fig.1c) of admissible values for parameters b, c for each value of the parameter a. It is seen (Fig.1c) that the set $I_a(b,c)$ is composed of intersection of the rectangle $\boldsymbol{b}^{\rm ap} \times \boldsymbol{c}^{\rm ap}$ with the cone between the lower $\underline{c}(b, 1/\overline{\boldsymbol{d}}(a)$ and upper $\overline{c}(b, 1/\underline{\boldsymbol{d}}(a)$ rays for $a \in \boldsymbol{a}^{\rm ap}$ and $b \in \boldsymbol{b}^{\rm ap}$. In Figure 1c, the set $I_a(b,c)$ (shadowed five-apex polygon) is shown for value $a = 1.89$ mole and corresponding interval $\boldsymbol{d}(1.89)$ from Fig.1b.

Conclusions

In the considered ill-posed estimation problem with the “stuck” parameters and under absence of probabilistic characteristics of the measuring errors, the elaborated interval approach allows one to analyze consistency of the given sample of measurements itself, to analyze consistency of the given sample of measurements and the given *a priori* data, and to construct the informational set of admissible values of the “stuck” parameters.

Acknowledgment

The work was supported by the RFBR Grant proj. 15-01-07909.

References

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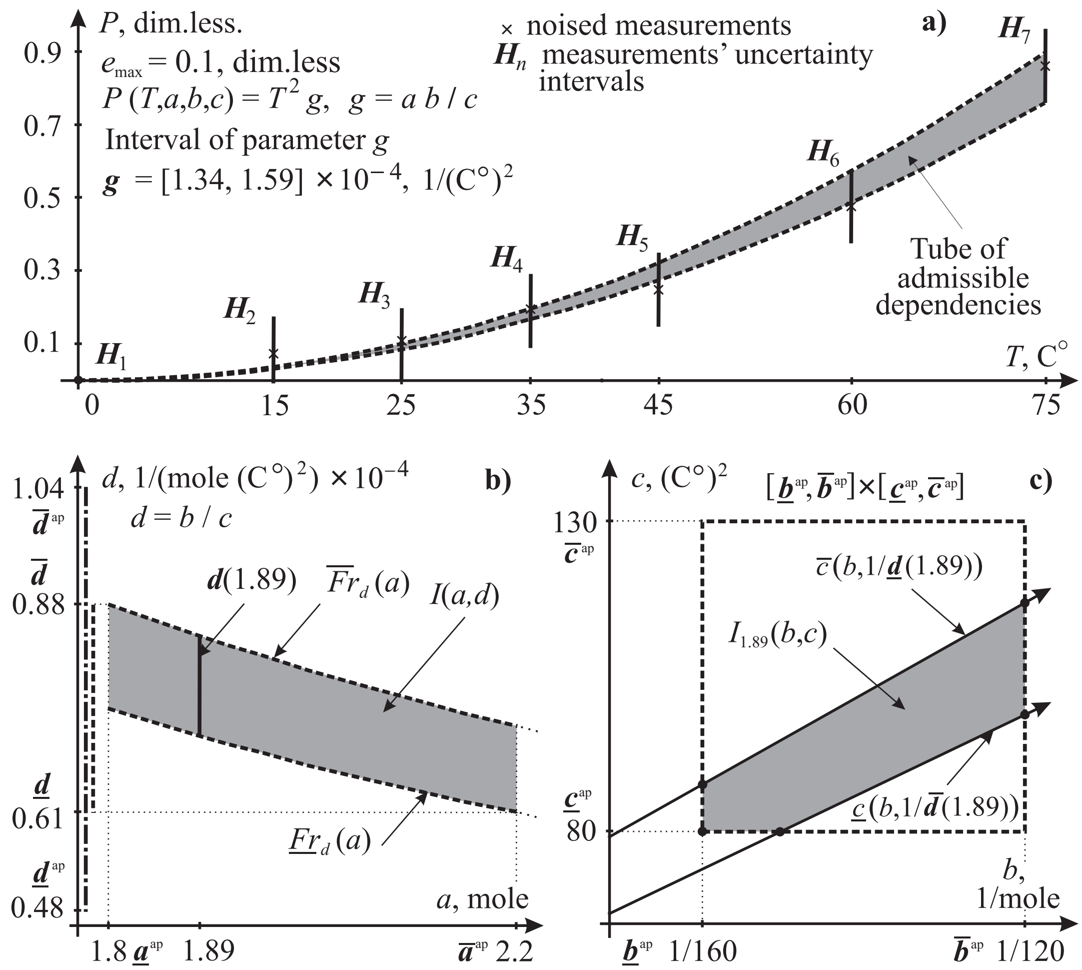

Figure 1: **a)** Input noised measurements (crosses); uncertainty intervals (thin vertical lines); tube of admissible dependencies (shadowed curve sector); the admissible interval of the parameter $\boldsymbol{g} = [1.34, 1.59] \times 10^{-4}$; the bound $e_{\max} = 0.1$ on the noise level; **b)** The set $I(a, d)$ of possible values for parameters a and d; the lower $\underline{Fr}_d(a)$ and upper $\overline{Fr}_d(a)$ boundaries; **c)** After taking into account *a priori* intervals $\boldsymbol{b}^{\text{ap}}$ of parameter b and $\boldsymbol{c}^{\text{ap}}$ of parameter c, the shadowed region is the informational set $I_{1.89}(a, d)$ of parameters b and c for the value of parameter $a = 1.89$ mole