ONE ILL-POSED ESTIMATION PROBLEM OF EXPERIMENTAL PROCESS PARAMETERS. INTERVAL APPROACH

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The aim of this presentation is to demonstrate one interesting practical problem of estimation of experimental process parameters under uncertainty conditions when components of the parameter vector can be only estimated on the basis of the Interval Analysis approach and available a priori data

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Topics of presentation

Experimental process and its model.

Measured information and its uncertainty.

Interval approach and its peculiarities.

Problem formulation and how to solve it ?

Computation results.

Conclusions.

References.

Experimental process and its model

Description of a reagent activity vs the temperature (similarly to [10,12]) has the form

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

where T is the temperature (the argument), C°;

$P(\cdot)$ is the reagent activity, dimensionless value;

a, b, and c are parameters (to be estimated)

with dimensions: mole, 1/mole, and (C°)^2.

Measured information and its uncertainty

Results of the experiment are presented as the following collection (a sample with lenght N) of the reagent activity P measurements:

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

where values T_n are supposed to be know exactly, but the activity values P_n are measured with error (noise)

$$P_n = P_n^* + e_n,\ |e_n| \leq e_{\text{max}},\ n = \overline{2, N}, \text{and for } T_1 = 0,\ P_1 = 0, \tag{3}$$

where P_n is a noised measurement; P_n^* is unknown true value under measuring; e_n is the error value in the nth measurement; e_{max} is the bound onto the maximal (by modulus) value of the error. By physical reasoning, the *conditional exact initial measurement* at $T_1 = 0$ is given zero.

Conditions for estimation and a priori information

No probabilistic information on errors is known and the sample is dramatically short: $N \approx 5 \sim 7$ measurements only.

In (1), parameters a, b and c are merged (“stuck”) that hampers estimation of their own admissible intervals without some additional information.

From theoretical estimations and previous experience, the following rough *a priori* constraints on possible values of the coefficients are given:

$$\begin{aligned} &\boldsymbol{a}^{\mathrm{ap}} = [\underline{\boldsymbol{a}}^{\mathrm{ap}},\ \overline{\boldsymbol{a}}^{\mathrm{ap}}],\ \boldsymbol{b}^{\mathrm{ap}} = [\underline{\boldsymbol{b}}^{\mathrm{ap}},\ \overline{\boldsymbol{b}}^{\mathrm{ap}}],\ \boldsymbol{c}^{\mathrm{ap}} = [\underline{\boldsymbol{c}}^{\mathrm{ap}},\ \overline{\boldsymbol{c}}^{\mathrm{ap}}], \\ &0 < \underline{\boldsymbol{a}}^{\mathrm{ap}} < \overline{\boldsymbol{a}}^{\mathrm{ap}},\ 0 < \underline{\boldsymbol{b}}^{\mathrm{ap}} < \overline{\boldsymbol{b}}^{\mathrm{ap}},\ 0 < \underline{\boldsymbol{c}}^{\mathrm{ap}} < \overline{\boldsymbol{c}}^{\mathrm{ap}}. \end{aligned} \tag{4}$$

The LSQM-curve and pointwise estimation of parameters a, b, c and their practically meaningless “cloud-built” intervals are available by **only formal application** of standard statistical procedures [15–17].

Interval approach and its essence

Ideas and methods of the Interval Analysis Theory and Applications arose from the fundamental, pioneer work by L.V. Kantorovich [1]. Nowadays, very effective developments of the theory and computational methods were created by many researchers, *e.g*. [2–4] and in Russia [5–8].

Special interval algorithms have been elaborated for estimating parameters of experimental chemical processes [9–14].

Remind that essence of this branch of numerical methods theory and application consists in **estimation (or identification) of parameters under bounded errors (noises or perturbations) in the input information to be processed, and under complete absence of probabilistic characteristics of errors.**

The main definitions

Uncertainty set (interval) of each measurement (USM). It is the interval of values of measured process consistent with the measurement and the error bound

$$\boldsymbol{H}_n = [\underline{h_n}, \overline{h_n}] : \ \underline{h_n} = P_n - e_{\max}, \ \overline{h_n} = P_n + e_{\max}, \ n = \overline{2, N}, \tag{5}$$

and for $n = 1$, $\boldsymbol{H}_1 = \boldsymbol{H}(0) = [0]$, trivially.

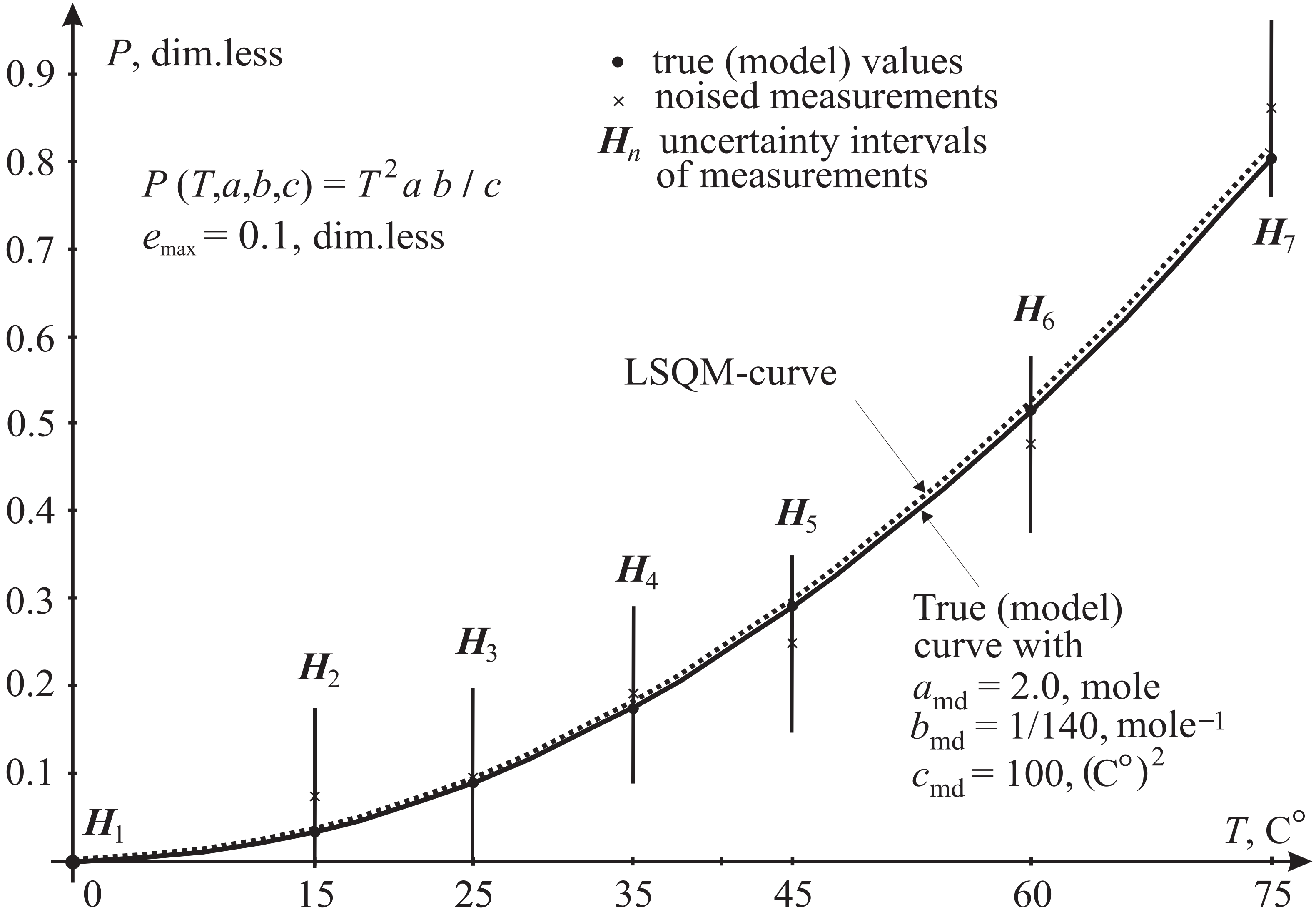
Admissible value of the parameter vector and corresponding admissible curve

$$(a, b, c) : \ P(T_n, a, b, c) \in \boldsymbol{H}_n, \ \text{for all } n = \overline{1, N}. \tag{6}$$

Informational Set (InfSet) is a totality of admissible values of the parameters vector satisfying the system of interval inequalities (6)

$$I(a, b, c) = \Big\{(a, b, c) : \ P(T_n, a, b, c) \in \boldsymbol{H}_n, \ \text{for all } n = \overline{1, N}\Big\}. \tag{7}$$

Measurements and their uncertainty sets (USM)



If the actual level of errors in the sample is lower the initially given *a priori* bound $e_{\max}$, the LSQM-curve and values of its parameters could be *admissible*.

Since of very short length of the measurements sample,
absence of probabilistic characteristics of the errors,
and measurements uncertainty,
it is impossible to use (with any good reasoning)
the standard statistical methods [15–17]).

It is necessary:
on the basis of the Interval Analysis methods to built
the Informational set $I(a, b, c)$ of admissible values
(or the Set-membership) of coefficients a, b, and c
consistent with the described data.

Applied procedures
Direct set-estimation approach

There are several approaches to solve system (6) of the interval inequalities
– classic linear programming methods [1, and many others],
– parallelotopes Fiedler M., *et al* [2], Hansen [3], Jaulin, *et al* [4], Shary [5],
– by the "stripes" method Shary&Sharaya [6], Sharaya [7], Zhilin [8].

More convenient and faster DIRECT method has been elaborated (see, Kumkov and with co-authors [9–14]) that gives *exact* estimation of the Informational set (7) on part of parameters for each node of the grid on other parameters. In the case under consideration, we represent the set $I(a, b, c)$ in the form of a collection of its cross-sections $\left\{I_a(b, c)\right\}$ for nodes of the grid on the parameter a on its minimal outer interval $\boldsymbol{a}^*$ of admissible values.

It is performed in contrast, for example, to outer approximation of informational sets in the parallelotope approaches.

Three successive auxiliary problems

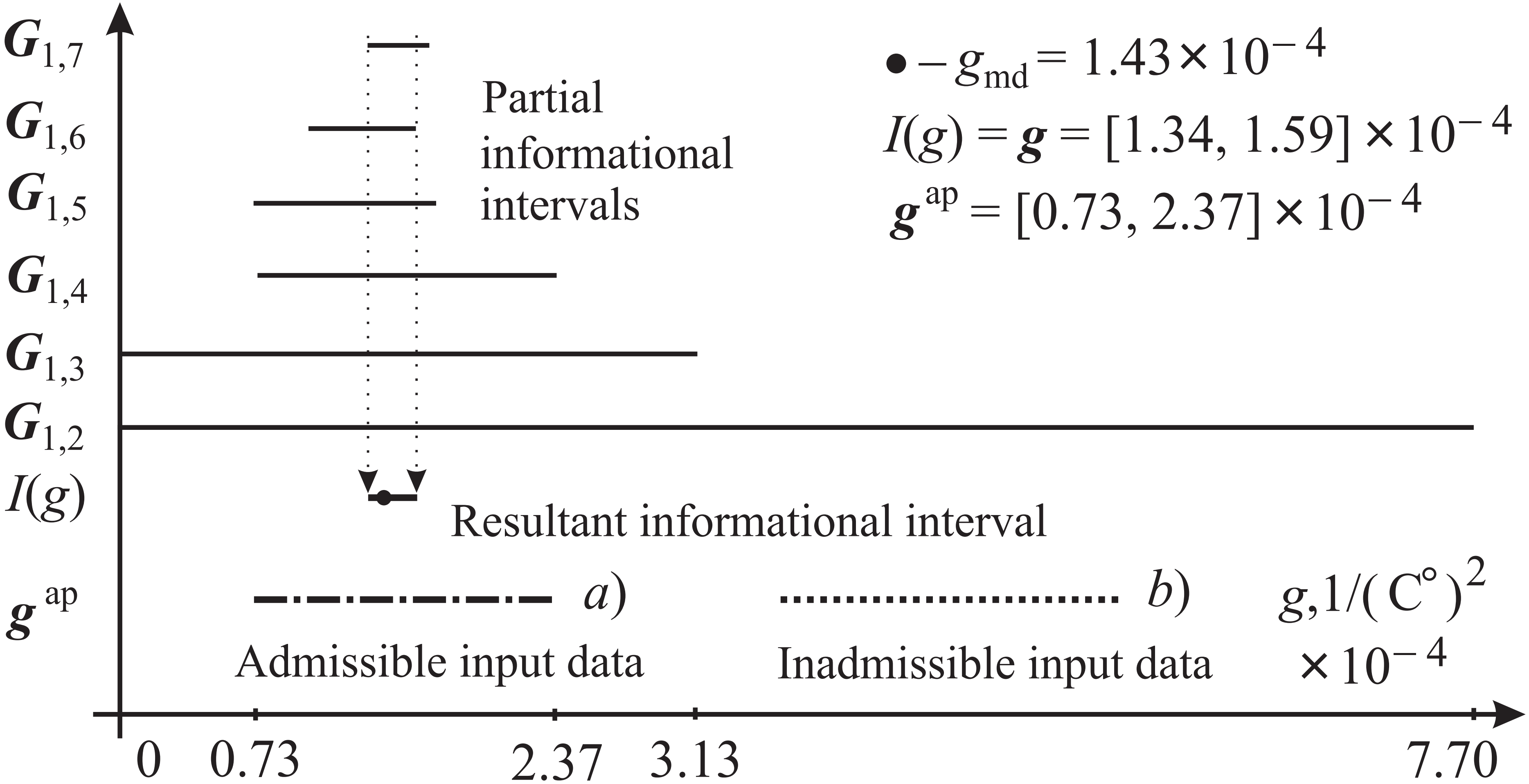
The following auxiliary problems are solved.

1) Introducing the auxiliary merged parameter $g = ab/c$ with $g > 0$, its corresponding informational interval $\boldsymbol{g} = [\underline{\boldsymbol{g}}, \overline{\boldsymbol{g}}]$ is calculated [10,12].

2) Having the interval equation $ad = \boldsymbol{g}$, where $d = b/c$, solve it w.r.t. the auxiliary parameter d as follows: $\boldsymbol{d} = \boldsymbol{g}/\boldsymbol{a}^{\mathrm{ap}}$. 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 as a functions of the parameter a values from its *a priori* interval $\boldsymbol{a}^{\mathrm{ap}}$.

3) For each value $a \in \boldsymbol{a}^{\mathrm{ap}}$ we have the interval $\boldsymbol{d}(a)$. So, it becomes possible to construct the informational set $I_a(b, c)$ of admissible values for parameters b, c for each admissible value of the parameter a.

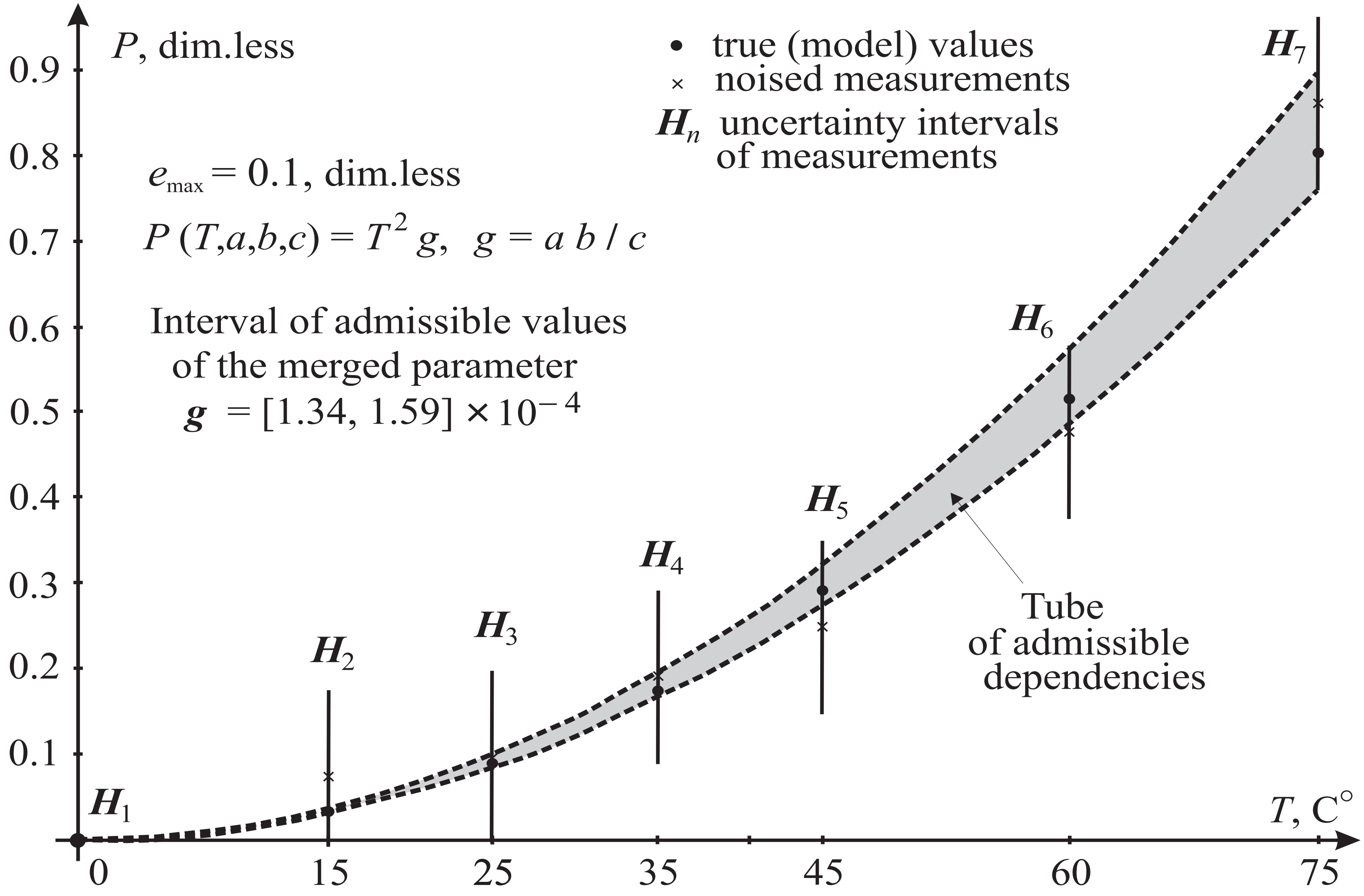
Solution of the auxiliary Problem 1. Informational set of the "merged" parameter $g = ab/c$



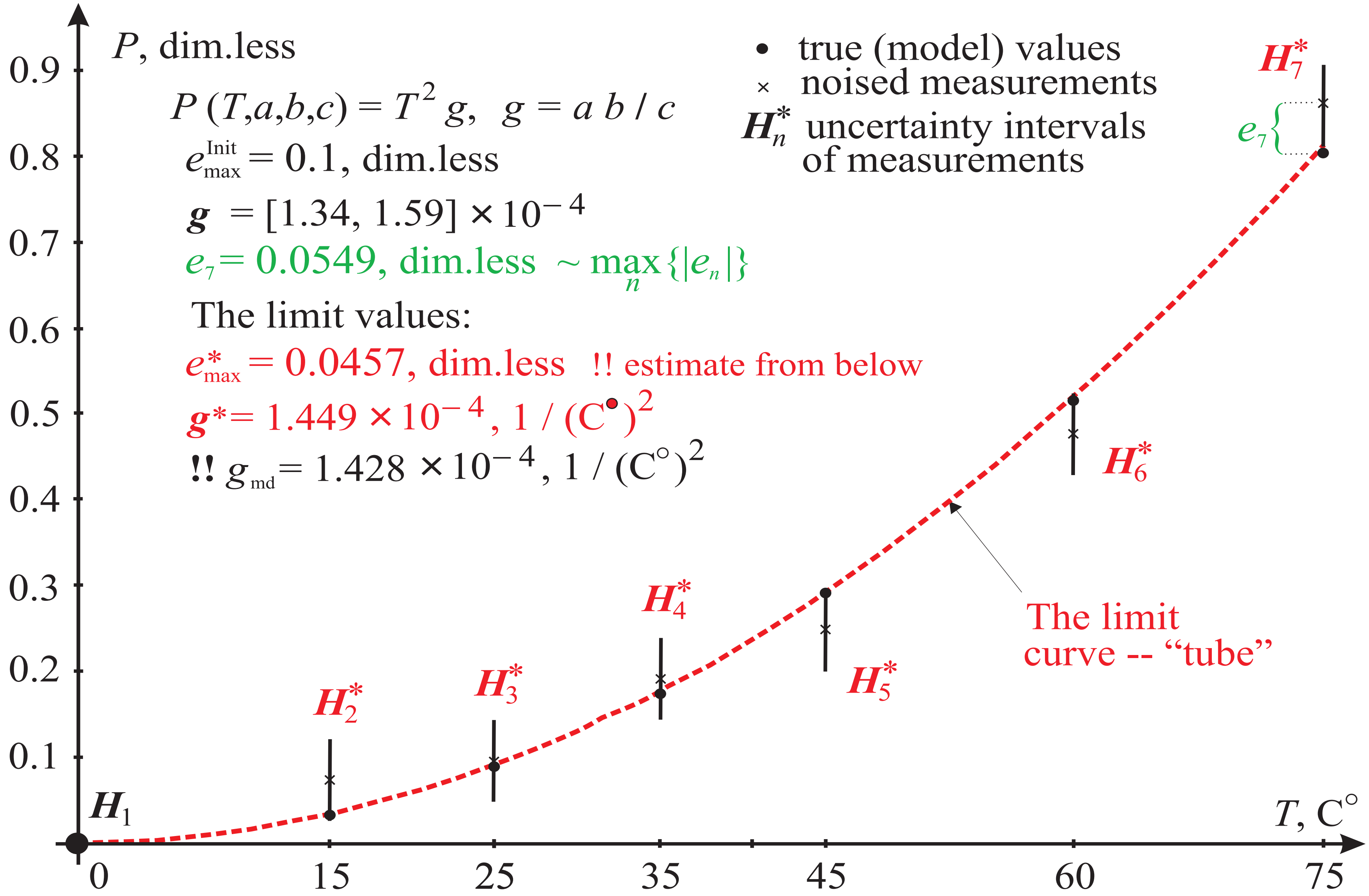
Analysis of consistency of a priori data with the measured ones

Note that it is worthy to calculate the *a priori* interval $\boldsymbol{g}^{\text{ap}}$ 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, c with the given sample of measurements (2),(3).

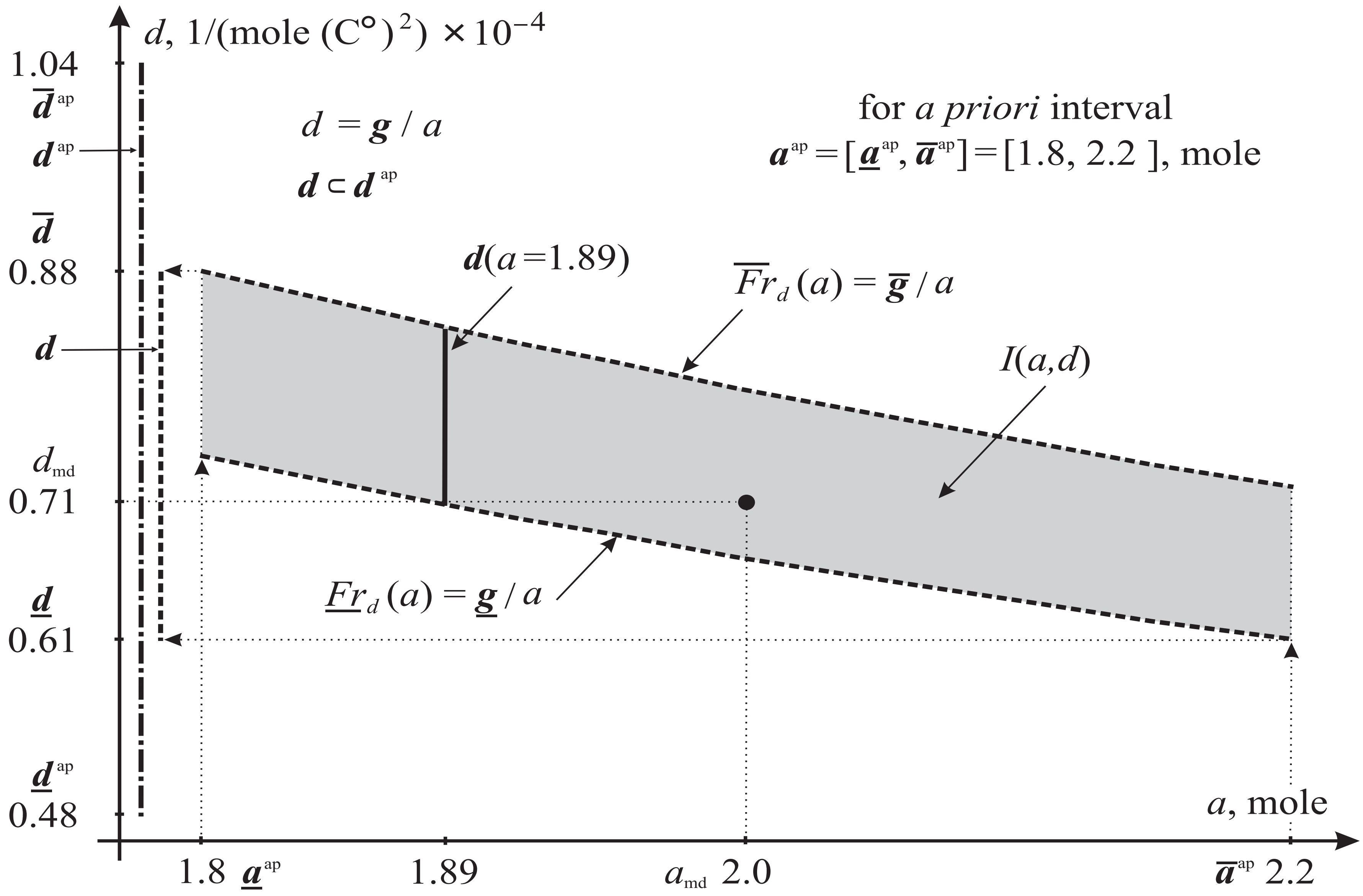
Solution of the auxiliary Problem 1. Tube of admissible dependencies



Estimating from below the maximal value of the actual error in the sample



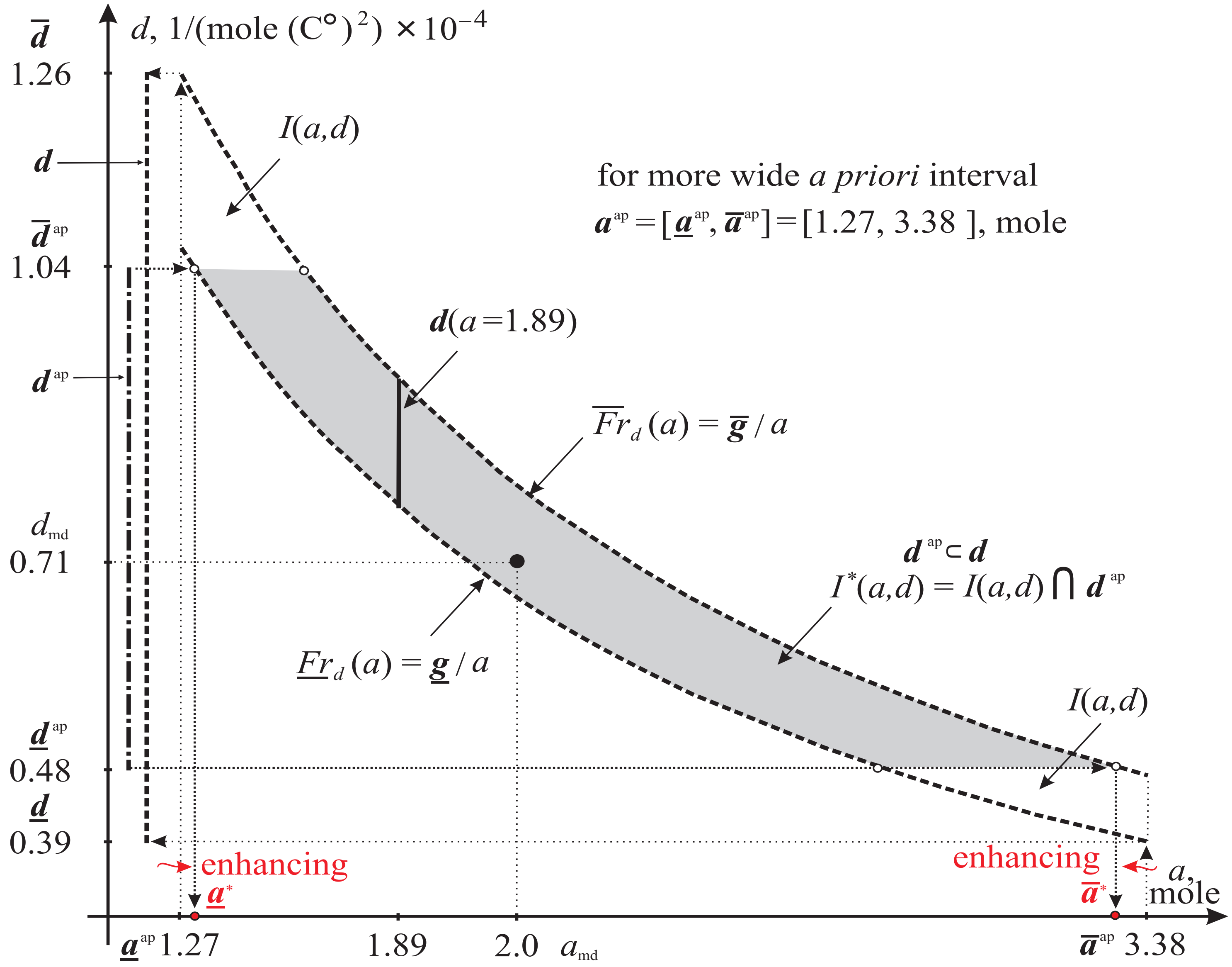
Solution of the auxiliary Problem 2. Informational set $I(a,d)$ of parameters a,d for $d = b/c$



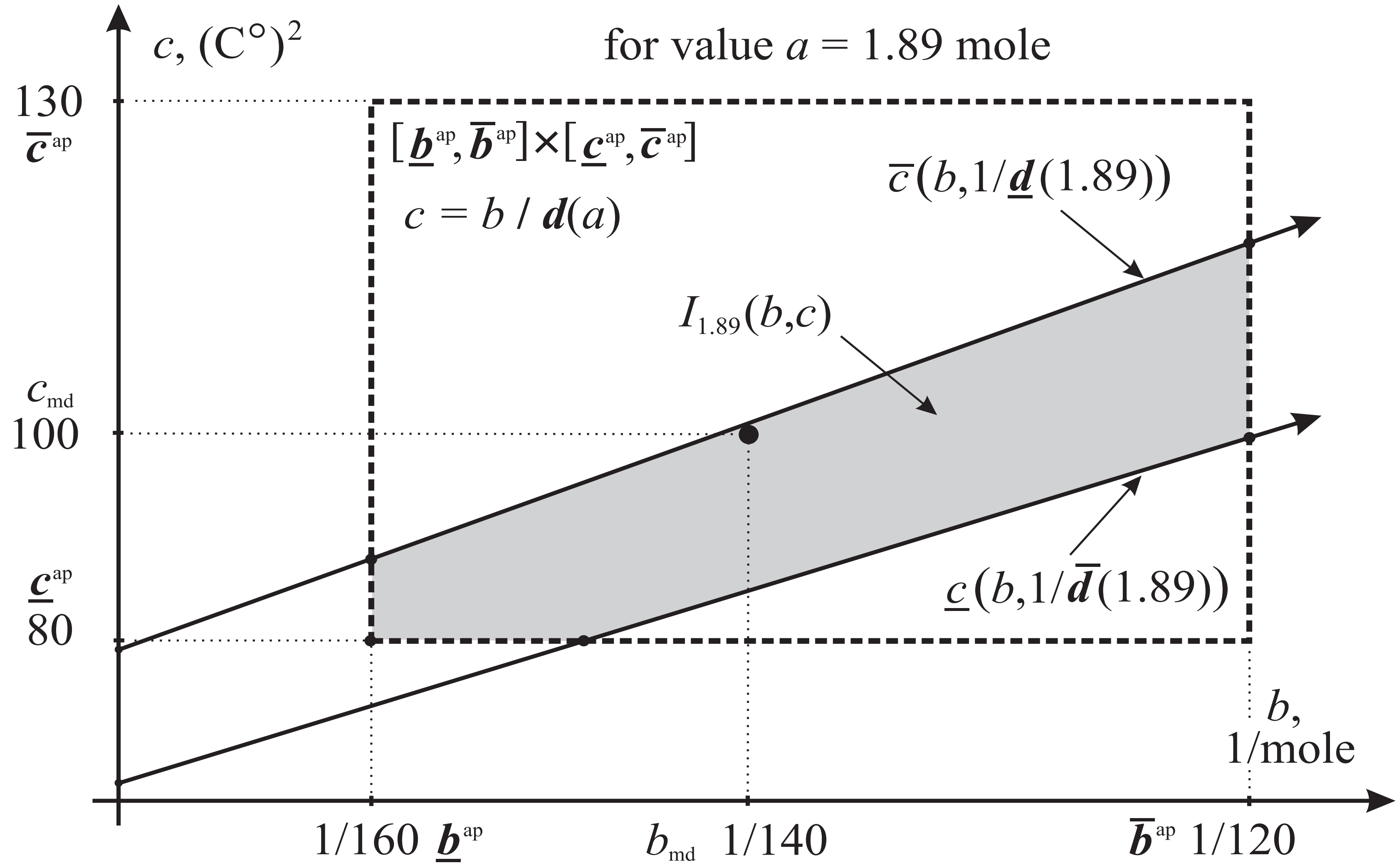
Analysis of consistency of a priori data with the measured ones

In figure the *a priori* interval $\boldsymbol{d}^{\text{ap}}$ of the auxiliary parameter d is shown (the thick dash-dotted vertical segment) calculated by the *a priori* intervals $\boldsymbol{b}^{\text{ap}}$ and $\boldsymbol{c}^{\text{ap}}$. The thick vertical line in dashes marks the outer interval in d of $I(a, d)$ for the *a priori* interval $\boldsymbol{a}^{\text{ap}}$. Comparison of these two intervals allows one to check out *consistency* of the *a priori* data (4) on parameters a, b, c with the given sample of measurements (2),(3).

Solution of Problem 2. Informational set $I(a, d)$ of parameters a, d for more wide interval $\mathbf{a}^{ap}$



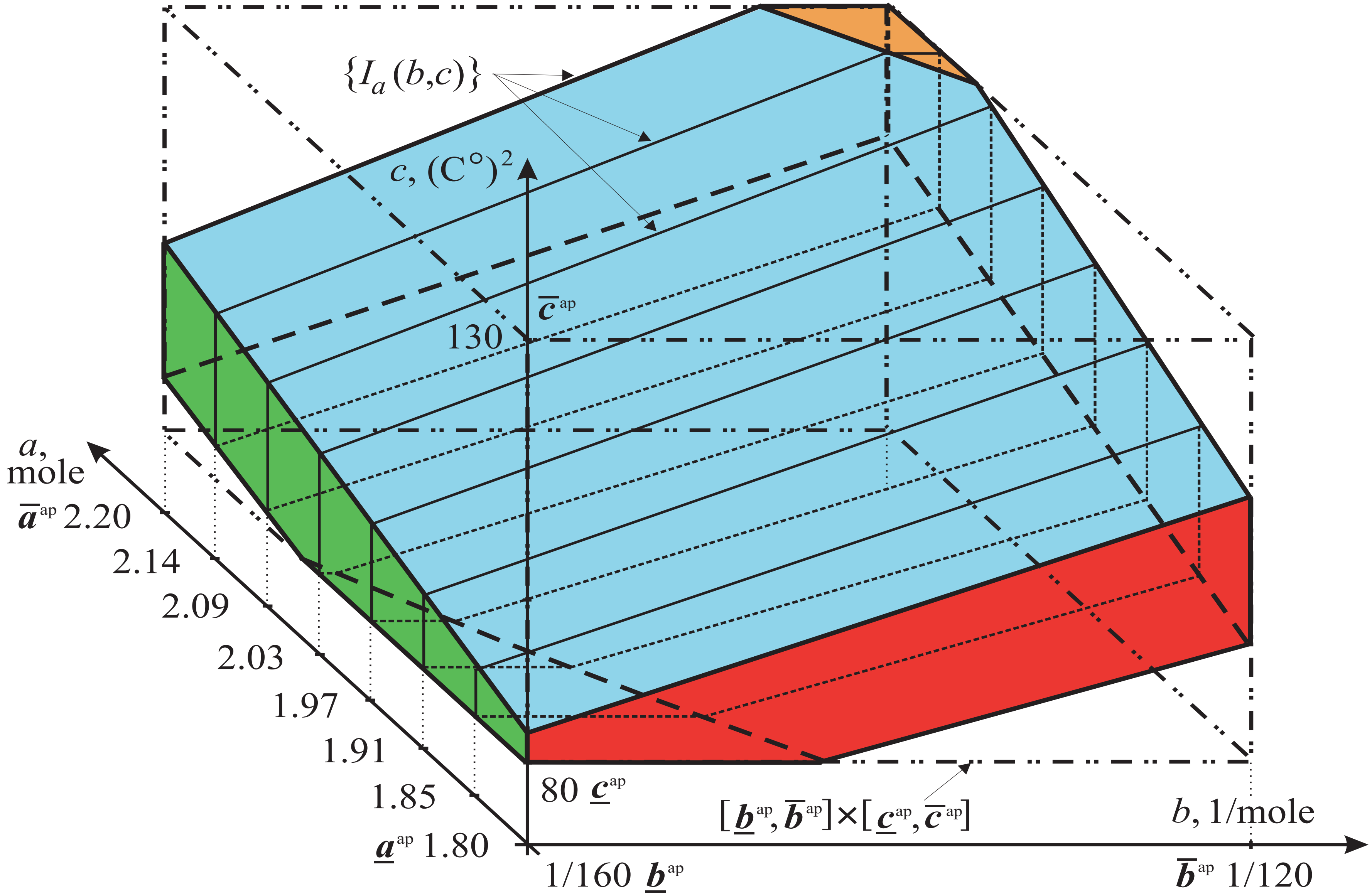
Solution of Problem 3. Informational set $I_a(b,c)$ of parameters b,c for fixed value $a = 1.89$, mole



Constructing the collection $\{I_a(b,c)\}$ of cross-sections of the informational set $I(a,b,c)$

It is seen that the set $I_a(b,c)$ is built by intersection of the rectangle $\boldsymbol{b}^{\text{ap}} \times \boldsymbol{c}^{\text{ap}}$ 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 $a \in \boldsymbol{a}^{\text{ap}}$ (or from the enhanced one $\boldsymbol{a}^{*}$) and $b \in \boldsymbol{b}^{\text{ap}}$. Here, the set $I_a(b,c)$ (shadowed five-apex polygon) is shown for value $a = 1.89$, mole and corresponding interval $\boldsymbol{d}(1.89)$ by solution of Problem 2.

Informational set $I(a,b,c)$ as a collection of its cross-sections $\{I_a(b,c)\}$



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 parameters.

Algorithms elaborated are simple in numeric implementation. In special cases, they can give exact estimations of the informational set and are faster than usual interval approaches on the basis of parallelotopes.

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Thanks for attention