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Towards Interval Techniques for Model Validation

Jaime Nava · Vladik Kreinovich

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Abstract Most physical models are approximate. It is therefore important to find out how accurate are the predictions of a given model. This can be done by *validating* the model, i.e., by comparing its predictions with the experimental data. In some practical situations, it is difficult to directly compare the predictions with the experimental data, since models usually contain (physically meaningful) parameters, and the exact values of these parameters are often not known. One way to overcome this difficulty is to get a statistical distribution of the corresponding parameters. Once we substitute these distributions into a model, we get statistical predictions – and we can compare the resulting probability distribution with the actual distribution of measurement results. In this approach, we combine all the measurement results, and thus, we are ignoring the information that some of these results correspond to the same values of the parameters – e.g., they come from measuring the same specimen under different conditions. In this paper, we propose an interval approach that takes into account this important information. This approach is illustrated on the example of a benchmark thermal problem presented at the Sandia Validation Challenge Workshop (Albuquerque, New Mexico, May 2006).

Keywords interval computations · Model validation · Linear programming

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Jaime Nava and Vladik Kreinovich
Department of Computer Science
University of Texas at El Paso
500 W. University
El Paso, TX 79968, USA
E-mail: jenava@miners.utep.edu, vladik@utep.edu

1 Formulation of the Problem

Need for model validation. Most physical models are approximate. It is therefore necessary to estimate the model accuracy by comparing the model's predictions with the experimental data. This estimation of the model accuracy is known as *model validation*.

Case study: the thermal challenge problem. As the main case study, we consider a benchmark thermal problem presented at the 2006 Sandia Validation Challenge Workshop [2,5–7,9,11]. In this problem, we need to analyze temperature response $T(x,t)$ of a safety-critical device to a heat flux.

Specifically, a slab of metal (or other material) of a given thickness L is exposed to a given heat flux q. We know:

- the initial temperature $T_i = 25$ C, and
- an approximate model:

$$T(x,t) = T_i + \frac{q \cdot L}{k} \cdot \left[\frac{(k/\rho C_p) \cdot t}{L^2} + \frac{1}{3} - \frac{x}{L} + \frac{1}{2} \cdot \left(\frac{x}{L} \right)^2 - \right.$$

$$\left. \frac{2}{\pi^2} \cdot \sum_{n=1}^{6} \frac{1}{n^2} \cdot \exp\left(-n^2 \cdot \pi^2 \cdot \frac{(k/\rho C_p) \cdot t}{L^2} \right) \cdot \cos\left(n \cdot \pi \cdot \frac{x}{L} \right) \right].$$

We do not know a priori how accurate is the approximate model.

As for the thermal conductivity k and the volumetric heat capacity of the material ρC_p, we know their nominal values, and we have measured values of k and ρC_p for different specimens.

We also have the results of measuring temperature for several different specimens (which are, in general, different from the specimens for which we measure k and ρC_p). Specifically, for each specimen, we measure temperature at different moments of time.

Let us start with a simplified problem. To better describe our idea, let us start with a simplified version of this problem, in which we assume that for each specimen, the values of all parameters – including the thermal conductivity k and the volumetric heat capacity of the material ρC_p – are known exactly. We also assume that the actual temperatures are known exactly, i.e., that the temperature measurements are reasonably accurate – so that the measurement uncertainty can be safely ignored.

In this simplified situation, the predicted value $T(x,t)$ of the temperature is well defined for all x and t; the only reason why the measured values are different from the model's predictions is that the model itself is only approximate. So, to estimate the accuracy (or inaccuracy) in a model, we can simply compare these predictions $T(x,t)$ with the actual measurement results $\widetilde{T}(x,t)$.

The largest possible difference $\max\limits_{x,t} \left| \widetilde{T}(x,t) - T(x,t) \right|$ between the measured values and the theory's prediction can be used as a reasonable measure of the model's accuracy.

For example, if in all the measurements, the measured values differ from the theory's prediction by no more than 10 degrees, we conclude that the model's prediction are accurate with the accuracy ± 10 degrees.

How to take variability into account: the probabilistic approach. In real life, the values of the parameters k and ρC_p are only approximately known. It is known that these values differ from one specimen to another. How can we take this variability into account when we estimate the accuracy of the given model?

A probabilistic approach to solving this problem is described in [5]. This approach is motivated by the fact that while we do not know the *individual* values of the parameters k and ρC_p corresponding to different specimens, we do have a *sample* of values k and ρC_p corresponding to different specimens. Thus, we can estimate the probability distribution of k and ρC_p among the given class of specimens.

In the resulting description, k and ρC_p are random variables with known distributions. Since the model's parameters k and ρC_p are random, for each x and t, the resulting temperature $T(x,t)$ also becomes a random variable. By running simulations, we can find, for each x and t, the probability distribution of this random value $T(x,t)$ – the probability distribution that would be observed if the model $T(x,t)$ was absolutely accurate.

Since the model is only approximately true, for every x and t, the actual (empirical) probability distribution of the measured temperatures $\widetilde{T}(x,t)$ is, in general, different from the simulated distribution of the model's predictions. The difference between these two probability distributions – the distribution predicted by the model and the distribution observed in measurements – can be thus viewed as a measure of how accurate is our model.

Limitation of the probabilistic approach: description and need to overcome these limitations. In the probabilistic approach, to describe an empirical distribution, we, in effect, combine ("pool") the temperatures measured for all the specimens into a single sample. As a result, we ignore an important part of the available information about the measurement results – namely, the information that some measurements correspond to the same specimen and some measurements correspond to different specimens. To get more convincing estimates of the model, it is therefore desirable to take this additional information into account.

In this paper, we describe how this additional information can be used. We illustrate our approach on the example of the main case study. After that, we describe this approach in general terms, and provide another application example – Very Large Baseline Interferometry (VLBI).

Comment. In this paper, we gauge the model's accuracy by coming up with a guaranteed upper bound for the difference between the model's prediction and actual values. This approach is similar to using overall error bound Δ as a description of the measurement inaccuracy – i.e., the difference between the measurement result $\widetilde{x}$ and the actual value x; see, e.g., [12]. In measurements, once we have the measurement result $\widetilde{x}$ and the bound Δ for which $|\widetilde{x} - x| \le \Delta$, the only information that we have about the actual (unknown) values x is that x belongs to the interval $[\widetilde{x} - \Delta, \widetilde{x} + \Delta]$; see, e.g., [8]. Because of this similarity, we will call our approach *interval approach*.

2 Interval Techniques for Model Validation: Main Idea

What we know about each specimen: an example. Instead of pooling all the measured temperature values corresponding to different specimens into a single

sample, we would like to consider each specimen individually. For each specimen, we have temperatures measured at different moments of time.

For example, according to [2], we have several specimens corresponding to Configuration 1, in which the thickness L is equal to 1.27 cm (half an inch), and the heat flux is equal to $q = 1000$ W/m^2. We have the measurement results for four specimens corresponding to this configuration. These measurement results correspond to $x = 0$. The results of measuring the temperature $T(x,t) = T(0,t)$ for specimen i are known as Experiment i. In particular, the measurement results corresponding to specimen 1 (i.e., to Experiment 1) are as follows:

time (in sec)	measured temperature
100	105.5
200	139.3
300	165.5
400	188.7
500	210.6
600	231.9
700	253.0
800	273.9
900	294.9
1000	315.8

Table 1 Measurement results

Ideal case: exact model, exactly known parameters k and ρC_p. For each specimen, if the model was absolutely accurate (and if the measurement inaccuracy was negligible), the measured values $\widetilde{T}(x,t)$ would take the form $\widetilde{T}(x,t) = T(x,t,k,\rho C_p)$ for an appropriate values k and ρC_p; here, $T(x,t,k,\rho C_p)$ means that we explicitly take into account the dependence on the parameters k and ρC_p in the above formula.

In this ideal situation, if we know the exact values of k and ρC_p, to check the model's correctness, we can simply compare the measured values $\widetilde{T}(x,t)$ with the predicted values $T(x,t,k,\rho C_p)$. In this case, the largest possible difference between the measured and predicted values is 0: $\max\limits_{t}\left|\widetilde{T}(x,t) - T(x,t,k,\rho C_p)\right| = 0$. Vice versa, if this largest difference is equal to 0, this means that all the differences are equal to 0, i.e., that the model is indeed absolute accurate.

Case when the model is exact, but the parameters k and ρC_p are only approximately known. In reality, we do not know the exact values of k of ρC_p, so we can only conclude that this largest difference is equal to 0 for *some* values k and ρC_p. In other words, we conclude that the smallest possible value of this largest difference – smallest over all possible combinations of the parameters k and ρC_p – is equal to 0:

$$\min_{k,\rho C_p}\max_{t}\left|\widetilde{T}(x,t) - T(x,t,k,\rho C_p)\right| = 0.$$

Vice versa, if this smallest value is equal to 0, this means that for *some* k and ρC_p, the largest error $\max\limits_t \left|\widetilde{T}(x,t) - T(x,t,k,\rho C_p)\right|$ is equal to 0 and so, the model is absolutely accurate.

General case, when we take into account that the model is approximate. In practice, the model is approximate. This means that no matter which values k and ρC_p we use for this specimen, the measured values will be different from the model's prediction: $\max\limits_t \left|\widetilde{T}(x,t) - T(x,t,k,\rho C_p)\right| > 0$.

For example, if the model differs from the observations by some value $\varepsilon > 0$, then even for the actual values of k and ρC_p, we will get $\left|\widetilde{T}(x,t) - T(x,t,k,\rho C_p)\right| = \varepsilon > 0$ and therefore, $\max\limits_t \left|\widetilde{T}(x,t) - T(x,t,k,\rho C_p)\right| = \varepsilon > 0$. Moreover, even when the model differs from the actual values at a single moment t, we will still have

$$\left|\widetilde{T}(x,t) - T(x,t,k,\rho C_p)\right| = \varepsilon > 0$$

for this moment of time t and therefore, $\max\limits_t \left|\widetilde{T}(x,t) - T(x,t,k,\rho C_p)\right| = \varepsilon > 0$.

To gauge the accuracy of the model, it is therefore reasonable to use the difference corresponding to the best possible values k and ρC_p, i.e., the value

$$a \stackrel{\text{def}}{=} \min_{k,\rho C_p} \max_t \left|\widetilde{T}(x,t) - T(x,t,k,\rho C_p)\right|.$$

Comment. This difference a is observed when we use the exact values of the parameters k and ρC_p. If, for prediction, we use approximate values $\widetilde{k}$ and $\widetilde{\rho C_p}$, then, in addition to the inaccuracy ε of the model, we also have an additional inaccuracy caused by the inaccuracy in k and ρC_p. In this case, it is reasonable to expect that the worst-case difference between the observed and the predicted values will be even larger than a:

$$\max_t \left|\widetilde{T}(x,t) - T(x,t,\widetilde{k},\widetilde{\rho C_p})\right| > a.$$

Resulting estimation of the model's accuracy: from the analysis of a single specimen to the analysis of all measurement results. For each specimen s, based on the observed values $\widetilde{T}_s(x,t)$ corresponding to this specimen, we can estimate the model's accuracy a_s in describing this specimen as

$$a_s = \min_{k,\rho C_p} \max_t \left|\widetilde{T}_s(x,t) - T_s(x,t,k,\rho C_p)\right|.$$

A model may have different accuracy for different specimens: e.g., a model may be more accurate for smaller values of the thermal flux q and less accurate for larger values of q. We are interested in guaranteed estimates of the model's accuracy, estimates which are applicable to all the specimens. Thus, as a reasonable estimate for the model's accuracy, we can take the largest value of a_s corresponding to different specimens:

$$a = \max_s a_s = \max_s \min_{k,\rho C_p} \max_t \left|\widetilde{T}_s(x,t) - T_s(x,t,k,\rho C_p)\right|.$$

Comment. The resulting formula for model's accuracy looks somewhat complicated, this is why we provided a detailed explanation of why we believe that this formula is adequate for model validation.

3 Interval Techniques for Model Validation: Preliminary Results

Estimating a_s as a constrained optimization problem. The above formula for a_s means that we need to find the values k and ρC_p for which the difference $\left|\widetilde{T}_s(x,t) - T_s(x,t,k,\rho C_p)\right|$ is the smallest possible. In other words, for each specimen s, we want to minimize a_s under the constraints that

$$\widetilde{T}_s(x,t) - a_s \le T_s(x,t,k,\rho C_p) \le \widetilde{T}_s(x,t) + a_s$$

for all the measurement results $\widetilde{T}_s(x,t)$ obtained for this specimen.

Linearization as a first approximation to this constrained optimization problem. The dependence of the model prediction $T_s(x,t,k,\rho C_p)$ on the model prediction is non-linear. As a result, we get a difficult-to-solve non-linear optimization problem.

In practice, this problem can be simplified, because we know the nominal values $\widetilde{k}$ and $\widetilde{\rho C_p}$ of the parameters k and ρC_p, and we also know – from measurements – that the actual values of these parameters do not deviate too much from the nominal values: the differences $\Delta k = \widetilde{k} - k$ and $\Delta(\rho C_p) = \widetilde{\rho C_p} - \rho C_p$ are small. Thus, we can use the nominal values as the starting (0-th) approximations to k and ρC_p: $k^{(0)} = \widetilde{k}$ and $\rho C_p^{(0)} = \widetilde{\rho C_p}$.

In the first approximation, we can only keep terms which are linear in Δk and $\Delta(\rho C_p)$ in the expansion of the dependence

$$T_s(x,t,k,\rho C_p) = T_s\left(x,t,k^{(0)} - \Delta k, \rho C_p^{(0)} - \Delta(\rho C_p)\right):$$

$$T_s(x,t,k,\rho C_p) = T_s\left(x,t,k^{(0)},\rho C_p^{(0)}\right) - c_k^{(0)} \cdot \Delta k - c_{\rho C_p}^{(0)} \cdot \Delta(\rho C_p),$$

where

$$c_k^{(0)} \stackrel{\text{def}}{=} \frac{\partial T}{\partial k}, \quad c_{\rho C_p}^{(0)} \stackrel{\text{def}}{=} \frac{\partial T}{\partial(\rho C_p)},$$

and the derivatives are taken for $k = k^{(0)}$ and $\rho C_p = \rho C_p^{(0)}$. In this linear approximation, the above optimization problem takes the following form: minimize a_s under the constraints that

$$\widetilde{T}_s(x,t) - a_s \le T_s\left(x,t,k^{(0)},\rho C_p^{(0)}\right) - c_k^{(0)} \cdot \Delta k - c_{\rho C_p}^{(0)} \cdot \Delta(\rho C_p) \le \widetilde{T}_s(x,t) + a_s.$$

In this linearized problem, both the objective function and the constraints are linear in terms of unknowns, so we can use known (and efficient) algorithms of linear programming to solve this problem; see, e.g., [14].

Once we solve this problem, we get the values $\Delta k^{(1)}$ and $\Delta(\rho C_p)^{(1)}$ which are optimal in the first approximation. Based on these values, we can get a first approximation $k^{(1)}$ and $\rho C_p^{(1)}$ to the actual optimal values of k and ρC_p as $k^{(1)} = k^{(0)} - \Delta k^{(1)}$ and $\rho C_p^{(1)} = \rho C_p^{(0)} - \Delta(\rho C_p)^{(1)}$.

From a linearized solution to a general solution. To get a more accurate solution, we can use the "approximately optimal" values $\Delta k^{(1)}$ and $\Delta\rho C_p^{(1)}$ as a new first approximation, and use linearization around these values. As a result, we come up with the following iterative algorithm:

- we start with the values $k^{(0)} = \widetilde{k}$ and $\rho C_p^{(0)} = \widetilde{\rho C_p}$;
- on each iteration q, once we have the values $k^{(q-1)}$ and $\rho C_p^{(q-1)}$, we use linear programming to solve the following optimization problem: minimize a_s under the constraints that

$$\widetilde{T}_s(x,t) - a_s \le T_s\left(x,t,k^{(q-1)},\rho C_p^{(q-1)}\right) - c_k^{(q-1)}\cdot\Delta k - c_{\rho C_p}^{(q-1)}\cdot\Delta(\rho C_p) \le \widetilde{T}_s(x,t) + a_s,$$

  where

$$c_k^{(q-1)} \stackrel{\text{def}}{=} \frac{\partial T}{\partial k},\quad c_{\rho C_p}^{(q-1)} \stackrel{\text{def}}{=} \frac{\partial T}{\partial(\rho C_p)},$$

  and the derivatives are taken for $k = k^{(q-1)}$ and $\rho C_p = \rho C_p^{(q-1)}$;
- once we solve this linear programming problem and get the optimal values $\Delta k^{(q)}$ and $\Delta(\rho C_p)^{(q)}$, we compute the next approximations to parameters as $k^{(q)} = k^{(q-1)} - \Delta k^{(q)}$ and $\rho C_p^{(q)} = \rho C_p^{(q-1)} - \Delta(\rho C_p)^{(q)}$.

Iterations continue until the process converges – or until we exhaust the computation time that was allocated for these computations. We then take the latest values of k and ρC_p and estimate the model's accuracy as $\max\limits_g \widetilde{a}_g$, where

$$\widetilde{a}_g = \max_{x,t}\left|\widetilde{T}_s(x,t) - T_s(x,t,k,\rho C_p)\right|.$$

Numerical results. For the above specimen 1, the iterative process converges after the 1st iteration (i.e., the 2nd iteration leads to very small changes). The resulting values of k and ρC_p lead to the predictions listed in the following Table:

time (in sec)	measured temperature	prediction: interval approach
100	105.5	105.5
200	139.3	138.8
300	165.5	165.2
400	188.7	188.7
500	210.6	211.1
600	231.9	233.1
700	253.0	254.9
800	273.9	276.6
900	294.9	298.3
1000	315.8	319.9

Table 2 Prediction accuracy: interval approach

The largest difference between the measured and predicted values is about 5 degrees. For other specimens, we got a similar difference of ≤ 5 degrees, so we conclude that the original model is accurate with accuracy ± 5 degrees.

Computational comment. To simplify computations, we used an equivalent reformulation of the original thermal model; see Appendix.

Comments: how to get better accuracy estimates. The above model assumes that for each specimen, the values k and ρC_p remain the same. Measurement results show, however, that these values slightly change with temperature. This can be seen, e.g., if we plot the average value $k_{\rm av}$ of k measured for a given temperature as a function of temperature T; see Table 3.

T	20	250	500	750	1000
$k_{\rm av}$	0.49	0.59	0.63	0.69	0.75

Table 3 Dependence of $k_{\rm av}$ on T

In the probabilistic approach, this dependence is taken into account by allowing correlation between the model and k; see, e.g., [5]. Linear correlation means, in effect, that instead of considering k as an independent random variables, we consider a dependence $k = k_0 + k_1 \cdot T$, where k_0 is independent on T and k_1 is a parameter to be determined. In the interval approach, for each specimen, we can similarly "plug in" the expressions $k = k_0 + k_1 \cdot T$ and $\rho C_p = \rho C_{p,0} + \rho C_{p,1} \cdot T$ into the above model and use the parameters k_0, k_1, $\rho C_{p,0}$, and $\rho C_{p,1}$ as the new unknowns in the similar constrained optimization approach.

Another possible improvement is related to the fact that we get slightly different values a_s depending on the thermal flow q: the higher q, the larger a_s. The objective is to predict how the system will react to thermal flows which may be even higher than in any of the experiments. So instead of taking the value $a(q_0)$ that corresponds to the current thermal flows q_0, we can estimate the dependence of $a(q)$ on q and extrapolate this dependence to the desired high thermal flow.

In our case, which model for the dependence $a(q)$ shall we choose? From the physical viewpoint, the problem is invariant w.r.t. changing measuring units $q \to \lambda \cdot q$ (i.e., in mathematical terms, scale-invariant). So it is reasonable to select a space-invariant dependence, i.e., a dependence for which, for each rescaling $q \to \lambda \cdot q$, the dependence has the same form if we appropriate change the units for measuring a, i.e., that for every $\lambda > 0$, there exists a $C(\lambda)$ for which $a(\lambda \cdot q) = C(\lambda) \cdot a(q)$. It is known (see, e.g., [1]) that the only monotonic solutions to this functional equations have the form $a(q) = a_0 \cdot q^\alpha$ for some a_0 and α.

So, for each experimentally tested q, based on all samples with given q, we find $a(q)$, and then find a_0 and α for which $a(q) \approx a_0 \cdot q^\alpha$, i.e., equivalently, $\ln(a(q)) \approx \ln(a_0) + \alpha \cdot \ln(q)$. This is a system of linear equations with unknowns $\ln(a_0)$ and α, so we can use the Least Squares method to solve it. Once we find the solution, we can predict the model's accuracy as $a(q) \approx a_0 \cdot q^\alpha$.

4 Interval Approach to Model Validation: General Description

Problem: general description. In general, we have a model $z = f(x_1, \ldots, x_n, y_1, \ldots, y_m)$ that predicts the value z of the desired quantity as a function of known quantities $x_1, \ldots, x_n$ and unknown quantities $y_1, \ldots, y_m$; see, e.g., [10]. To be more precise, we usually know some crude approximate values $\widetilde{y}_i$, but

the accuracy of these approximate values is orders of magnitude lower than the accuracy with which we know the measured values x_i and z.

Measurements are divided into groups with each of which we know that the values y_j are the same; the values y_j may differ from group to group.

Comment. In the thermal problem example, $n = 2$, $x_1 = x$, $x_2 = t$, $m = 2$, $y_1 = k$, and $y_2 = \rho C_p$. Groups correspond to specimens.

How to estimate the model's accuracy: general definition. In the general case, as an estimate for the model's accuracy, we propose to use the value

$$a = \max_g \min_{y_1,\ldots,y_m} \max_{x_1,\ldots,x_m} \left| \widetilde{f}_g(x_1,\ldots,x_n) - f_g(x_1,\ldots,x_n,y_1,\ldots,y_m) \right|,$$

where g indicates different groups, and $\widetilde{f}_g$ are measurement results corresponding to the g-th group.

In other words, as a desired value a, we take $\max\limits_g a_g$, where each a_g is the solution to the following optimization problem: minimize a_g under the constraints that

$$\widetilde{f}_g(x_1,\ldots,x_n) - a_g \le f_g(x_1,\ldots,x_n,y_1,\ldots,y_m) \le \widetilde{f}_g(x_1,\ldots,x_n) + a_g.$$

How to estimate the model's accuracy: general algorithm. By applying a similar linearization approach, we get the following algorithm:

- we start with the values $z_i^{(0)} = \widetilde{z}_i$;
- on each iteration q, once we have the values $z_i^{(q-1)}$, we use linear programming to solve the following optimization problem: minimize a_g under the constraints that

$$\widetilde{f}_g(x_1,\ldots,x_n) - a_s \le f_g\left(x_1,\ldots,x_n,y_1^{(q-1)},y_m^{(q-1)}\right) - \sum_{j=1}^{m} c_j^{(q-1)} \cdot \Delta y_j \le$$

$$\widetilde{f}_g(x_1,\ldots,x_n) - a_s,$$

  where $c_j^{(q-1)} \stackrel{\text{def}}{=} \dfrac{\partial f}{\partial j}$, and the derivatives are taken for $y_j = y_j^{(q-1)}$;
- once we solve this linear programming problem and get the optimal values $\Delta y_j^{(q)}$, we compute the next approximations to parameters as

$$y_j^{(q)} = y_j^{(q-1)} - \Delta y_j^{(q)}.$$

Iterations continue until the process converges – or until we exhaust the computation time that was allocated for these computations. We then take the latest values of y_j and estimate the model's accuracy as $\max\limits_g \widetilde{a}_g$, where

$$\widetilde{a}_g = \max_{x_1,\ldots,x_n} \left| \widetilde{f}_g(x_1,\ldots,x_n) - f_g(x_1,\ldots,x_n,y_1,\ldots,y_m) \right|.$$

Very Large Baseline Interferometry (VLBI): another example of the general approach. To get a better idea of the general problem, let us give another example of the general approach. For each distant astronomical radio-source, we want to find the exact direction from which the corresponding radio waves are coming. In precise terms, we need to find a unit vector $\mathbf{e}_k$ in the direction to the source.

One of the most accurate methods of finding the unit vector $\mathbf{e}_k$ in the direction to a distant astronomical radio-source is Very Large Baseline Interferometry (VLBI); see, e.g., [3,4,13,15]. In VLBI, we measure the time delay $\tau_{i,j,k}$ between the signal observed by antennas i and j. The corresponding model comes the simple geometric arguments, according to which

$$\tau_{i,j,k} = c^{-1} \cdot (\mathbf{b}_i - \mathbf{b}_j) \cdot \mathbf{e}_k + \Delta t_i - \Delta t_j,$$

where:

- $\mathbf{b}_i$ is the location of the i-th antenna, and
- Δt_i is its clock bias on the i-th antenna, i.e., the difference between the reading of this clock and the actual (unknown) time on this antenna.

In this model, the locations $\mathbf{b}_i$ and the clock biases are unknown (to be more precise, we know approximate values of the locations and biases, but these approximate values are orders of magnitude less accurate that the time delays).

We assume that the directions $\mathbf{e}_k$ do not change during the measurements; this assumption make sense since the sources are distant ones, and even if they move with a speed v close to the speed of light, their angular speed v/R, where R is the distance, can be safely ignored. We also assume that the biases and the antenna locations do not change during one short group of measurements. In this case, z is the time delay, and $y_1, \ldots, y_m$ are directions $\mathbf{e}_k$, locations $\mathbf{b}_i$, and clock biases Δt_i. When we performed sufficiently many measurements in each group g, we have more measured values than the unknowns y_j and thus, we can meaningfully estimate the model's accuracy; for details, see [3,4].

An even more accurate description emerges when take into account that the Earth-bound antennas rotate with the Earth; to take rotation into account, we must take into account time between different consequent measurements within the same group, and this time can be measured very accurately – thus serving as x_i.

5 Closing Remarks

A model of real-life phenomena needs to be validated: we must compare the model's predictions with the experimental data and, based on this comparison, conclude how accurate is the model. This comparison becomes difficult if the model contains, as parameters, values of some auxiliary physical quantities – quantities which are usually not measured in the corresponding experiments. In such situations, we can use the results of previous measurements of these quantities in similar situations, results based on which we can determine the probabilities of different values of these auxiliary quantities. In the traditional probabilistic approach to model validation, we plug in the resulting random auxiliary variables into the model, and compare the distribution of the results with the observed distribution of the experimental data. In this approach, however, we do use the important

information that some measurement results correspond to the same specimen – and thus, correspond to the same values of the auxiliary quantities. To take this information into account, we propose a new approach, in which, for each specimen, we, in effect, first estimate the values of the auxiliary quantities based on the measurement results, then plug these estimated values back into the model – and use the resulting formula to gauge how accuracy the original model is on this specimen. We illustrate this approach on the example of a benchmark thermal problem.

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A How to Simplify Computations

Our main formula has the form

$$T(x,t) = T_i + \frac{q \cdot L}{k} \cdot \left[\frac{(k/\rho C_p) \cdot t}{L^2} + \frac{1}{3} - \frac{x}{L} + \frac{1}{2} \cdot \left(\frac{x}{L} \right)^2 - \right.$$

$$\frac{2}{\pi^2}\cdot\sum_{n=1}^{6}\frac{1}{n^2}\cdot\exp\left(-n^2\cdot\pi^2\cdot\frac{(k/\rho C_p)\cdot t}{L^2}\right)\cdot\cos\left(n\cdot\pi\cdot\frac{x}{L}\right)\Bigg].$$

In this formula, the parameter ρC_p always appears in a ratio $\dfrac{k/\rho C_p}{L^2}$. It is therefore reasonable, instead of the original variables $y_1 = k$ and $y_2 = \rho C_p$, to use new auxiliary variables $Y_1 = \dfrac{q\cdot L}{k}$ and $Y_2 = \dfrac{k/\rho C_p}{L^2}$. As a result, we get the following simplified formula:

$$T(x,t) = T_i + Y_1\cdot\Bigg[Y_2\cdot t + \frac{1}{3} - x_0 + \frac{1}{2}\cdot x_0^2 -$$

$$\frac{2}{\pi^2}\cdot\sum_{n=1}^{6}\frac{1}{n^2}\cdot\exp(-n^2\cdot\pi^2\cdot Y_2\cdot t)\cdot\cos(n\cdot\pi\cdot x_0)\Bigg],$$

where $x_0 \stackrel{\text{def}}{=} \dfrac{x}{L}$. In this case,

$$\frac{\partial T}{\partial Y_1} = Y_2\cdot t + \frac{1}{3} - x_0 + \frac{1}{2}\cdot x_0^2 - \frac{2}{\pi^2}\cdot\sum_{n=1}^{6}\frac{1}{n^2}\cdot\exp(-n^2\cdot\pi^2\cdot Y_2\cdot t)\cdot\cos(n\cdot\pi\cdot x_0);$$

$$\frac{\partial T}{\partial Y_2} = t\cdot\left[Y_1 - 2\cdot\sum_{n=1}^{6}\cdot\exp(-n^2\cdot\pi^2\cdot Y_2\cdot t)\cdot\cos(n\cdot\pi\cdot x_0)\right].$$