

Towards Interval Techniques for Model Validation

Jaime Nava · Vladik Kreinovich

Received: date / Accepted: date

Abstract In many practical situations, the values of the known measured quantity depend on the values of the desired quantities, on the values of known auxiliary quantities (e.g., measurement parameters that we ourselves set up), and on the values of the unknown auxiliary quantities.

For example, when we observe a distant quasar by using Very Large Base Interferometry, the measured time delay depends both on the actual coordinates of this quasar and on the parameters that describe the radiointerferometer itself: e.g., on the distance and direction between the antennas, and on the time shift between the clocks located at these antennas.

In practice, we often only have an approximate model for the dependence. In this case, a natural idea is to find the values of the unknowns for which the largest of model inaccuracies is minimal.

In the linearizable case, finding such values becomes a linear programming problem.

In the paper, we describe the application of the resulting techniques to a benchmark thermal problem presented at the Sandia Validation Challenge Workshop (Albuquerque, New Mexico, May 2006).

Keywords interval computations · Model validation · Linear programming

This work was presented at the 14th GAMM-IMACS International Symposium on Scientific Computing, Computer Arithmetic and Validated Numerics SCAN'2010 (Lyon, France, September 27–30, 2010).

This research was supported in part by the National Science Foundation grants HRD-0734825 and DUE-0926721, by Grant 1 T36 GM078000-01 from the National Institutes of Health, by Grant MSM 6198898701 from MŠMT of Czech Republic, and by Grant 5015 “Application of fuzzy logic with operators in the knowledge based systems” from the Science and Technology Centre in Ukraine (STCU), funded by European Union.

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 Measurement Under Exact Model: Example

To illustrate the class of problem that we will solve in this paper, let us start with an example. Suppose that for some 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 . From the simple geometric arguments, we can conclude that

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

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 the ideal case, if we knew \mathbf{b}_i and Δt_i with high accuracy, the above equation becomes linear in terms of the unknown components of \mathbf{e}_k . By solving this system of equations, we could then easily find \mathbf{e}_k .

In practice, we only know \mathbf{b}_i and Δt_i approximately, and moreover, we know these values with much lower (relative) accuracy than the measured time delays $\tau_{i,j,k}$.

2 Measurement Under Exact Model

General case: description. In general (see, e.g., [12]),

- we have the measured values z_1, \dots, z_n ($\tau_{i,j,k}$ in the VLBI example), and
- we need to find the desired values x_1, \dots, x_m (\mathbf{e}_k in the VLBI example).

The values z_j depend not only on x_1, \dots, x_n , they also depend:

- on the values s_1, \dots, s_p of known auxiliary quantities (e.g., time of the experiment), and
- on the values y_1, \dots, y_q of the auxiliary quantities which are only approximately known (in the VLBI example, values \mathbf{b}_j and Δt_i).

VLBI example. In the VLBI example, we know the exact dependence $z = f(x, y, s)$, i.e.,

$$z_j = f_j(x_1, \dots, x_m, y_1, \dots, y_q, s_1, \dots, s_p).$$

In such situations, we can determine all the unknowns (i.e., x_1, \dots, x_m and y_1, \dots, y_q) if we perform measurements for each of several (M) different objects $x^{(\alpha)} = (x_1^{(\alpha)}, \dots, x_m^{(\alpha)})$, $1 \leq \alpha \leq M$ in

- several (Q) different settings $y^{(\beta)} = (y_1^{(\beta)}, \dots, y_q^{(\beta)})$, $1 \leq \beta \leq Q$, and
- several (P) different settings $s^{(\gamma)} = (s_1^{(\gamma)}, \dots, s_p^{(\gamma)})$, $1 \leq \gamma \leq P$.

How to solve the problem. As a result of each measurement, we get n different values $z_1^{(\alpha,\beta,\gamma)}, \dots, z_n^{(\alpha,\beta,\gamma)}$. Thus, as a result of the measurements, we thus get $n \cdot M \cdot P \cdot Q$ equations

$$z_j^{(\alpha,\beta,\gamma)} = f_j \left(x_1^{(\alpha)}, \dots, x_m^{(\alpha)}, y_1^{(\beta)}, \dots, y_q^{(\beta)}, s_1^{(\gamma)}, \dots, s_p^{(\gamma)} \right),$$

$1 \leq j \leq n$, to determine $N \cdot m + Q \cdot q$ unknown (to be more exact, approximately known) values $x_1^{(\alpha)}, \dots, x_m^{(\alpha)}$ ($1 \leq \alpha \leq M$) and $y_1^{(\beta)}, \dots, y_q^{(\beta)}$ ($1 \leq \beta \leq Q$).

When the values M and Q are large, the number of equations $n \cdot M \cdot P \cdot Q$ exceeds the number of unknowns $N \cdot m + Q \cdot q$. Thus, in general, we can solve this system, and find the x values for all the objects and and y values for all the settings; see, e.g., [10].

Approximate values of x and y are usually known. Usually, we know approximate values $\tilde{x}_i^{(\alpha)}$ and $\tilde{y}_k^{(\beta)}$ of the quantities $x_i^{(\alpha)}$ and $y_k^{(\beta)}$, and we know the upper bounds $\Delta_{x,i}^{(\alpha)}$ and $\Delta_{y,k}^{(\beta)}$ on the approximation errors $\Delta x_i^{(\alpha)} \stackrel{\text{def}}{=} \tilde{x}_i^{(\alpha)} - x_i^{(\alpha)}$ and $\Delta y_k^{(\beta)} \stackrel{\text{def}}{=} \tilde{y}_k^{(\beta)} - y_k^{(\beta)}$: $|\Delta x_i^{(\alpha)}| \leq \Delta_{x,i}^{(\alpha)}$ and $|\Delta y_k^{(\beta)}| \leq \Delta_{y,k}^{(\beta)}$. see, e.g., [12]. In this case, we know that the actual values $x_i^{(\alpha)}$ and $y_k^{(\beta)}$ belong to the corresponding intervals $[\tilde{x}_i^{(\alpha)} - \Delta_{x,i}^{(\alpha)}, \tilde{x}_i^{(\alpha)} + \Delta_{x,i}^{(\alpha)}]$ and $[\tilde{y}_k^{(\beta)} - \Delta_{y,k}^{(\beta)}, \tilde{y}_k^{(\beta)} + \Delta_{y,k}^{(\beta)}]$.

Linearizable case. Often, the approximation errors are small, so we can safely ignore terms which are quadratic in these errors and linearize the corresponding system $z = f(x, s, y)$. In such situations, we need to solve the resulting system of linear equations in terms of the unknowns $\Delta x_i^{(\alpha)}$ and $\Delta y_j^{(\beta)}$:

$$z_j^{(\alpha,\beta,\gamma)} = f_j \left(\tilde{x}^{(\alpha)}, \tilde{y}^{(\beta)}, s^{(\gamma)} \right) + \sum_{i=1}^n \frac{\partial f}{\partial x_i} \cdot \Delta x_i^{(\alpha)} + \sum_{k=1}^q \frac{\partial f}{\partial y_j} \cdot \Delta y_j^{(\beta)}.$$

3 Case of Approximate Model: Model Validation

Need for model validation. In practice, we often only have an *approximate* model $f(x, s, y)$ for the dependence of z on x , s , and y . In such situations, it is desirable to *validate* this model, i.e., to supplement the expression $f(x, s, y)$ with a guaranteed accuracy $\varepsilon > 0$ of this approximate model.

Model validation: precise formulation of the problem. In precise terms, we need to find the smallest possible $\varepsilon > 0$ for which there exist values

$$x_i^{(\alpha)} \in \left[\tilde{x}_i^{(\alpha)} - \Delta_{x,i}^{(\alpha)}, \tilde{x}_i^{(\alpha)} + \Delta_{x,i}^{(\alpha)} \right] \text{ and } y_k^{(\beta)} \in \left[\tilde{y}_k^{(\beta)} - \Delta_{y,k}^{(\beta)}, \tilde{y}_k^{(\beta)} + \Delta_{y,k}^{(\beta)} \right]$$

such that for every j , α , β , and γ , we have

$$z_j^{(\alpha,\beta,\gamma)} \in \left[f_j \left(x^{(\alpha)}, y^{(\beta)}, s^{(\gamma)} \right) - \varepsilon, f_j \left(x^{(\alpha)}, y^{(\beta)}, s^{(\gamma)} \right) + \varepsilon \right].$$

Linearizable case. In the linearizable case, when the expression $f_j(x^{(\alpha)}, y^{(\beta)}, s^{(\gamma)})$ can be approximated by the above formula linear in terms of $\Delta x_i^{(\alpha)}$ and $\Delta y_j^{(\beta)}$, this problem takes the following form:

Minimize ε under the constraints that

$$z_j^{(\alpha, \beta, \gamma)} - \varepsilon \leq f_j(\tilde{x}^{(\alpha)}, \tilde{y}^{(\beta)}, s^{(\gamma)}) + \sum_{i=1}^n \frac{\partial f}{\partial x_i} \cdot \Delta x_i^{(\alpha)} + \sum_{k=1}^q \frac{\partial f}{\partial y_j} \cdot \Delta y_j^{(\beta)} \leq z_j^{(\alpha, \beta, \gamma)} + \varepsilon;$$

$$-\Delta_{x,i}^{(\alpha)} \leq \Delta_i^{(\alpha)} \leq \Delta_{x,i}^{(\alpha)}; \quad -\Delta_{y,k}^{(\beta)} \leq \Delta_k^{(\beta)} \leq \Delta_{y,k}^{(\beta)}.$$

Both the objective function and the constraints (inequalities) are linear in terms of the unknown ε , $\Delta x_i^{(\alpha)}$, and $\Delta y_j^{(\beta)}$; so, this optimization problem is a particular case of the general class of linear programming problems – a class for which efficient algorithms are known; see, e.g., [14].

Linearizable case: making the result more adequate. The value ε obtained from solving this linear programming problem is based on linearization approximation. In critical situations, when we need to guarantee the accuracy for all measurements, we should take, as the model accuracy, the largest of the differences between the observed values and the values predicted by the original (non-linearized) approximate model with the newly determined parameters $x_i^{(\alpha)} = \tilde{x}_i^{(\alpha)} - \Delta x_i^{(\alpha)}$ and $y_j^{(\beta)} = \tilde{y}_j^{(\beta)} - \Delta y_j^{(\beta)}$, i.e., the value

$$\tilde{\varepsilon} \stackrel{\text{def}}{=} \max_{j, \alpha, \beta, \gamma} \left| z_j^{(\alpha, \beta, \gamma)} - f_j(x^{(\alpha)}, y^{(\beta)}, s^{(\gamma)}) \right|.$$

Need for general case. Linearization is based on the assumption that the measurement errors $\Delta x_i^{(\alpha)}$ and $\Delta y_j^{(\beta)}$ are small so that terms quadratic in these errors can be safely ignored. In practice, sometimes, these errors are not that small, so quadratic terms must be taken into account.

General case: idea. The idea for handling a general case comes from Newton's method for solving an equation $F(x) = 0$, method that is based on several linearizations. In Newton's method,

- we pick an initial approximation $x^{(0)}$;
- then, for $p = 0, 1, \dots$, once we have $x^{(p)}$, solve the linearized problem, with $x = x^{(p)} + \Delta x$:

$$F(x^{(p)}) + \frac{\partial F}{\partial x}(x^{(p)}) \cdot \Delta x = 0;$$

- we use the solution $x^{(p)} + \Delta x$ as the next approximation $x^{(p+1)}$.

We iterate until $|\Delta x|$ is small enough. For example, we can iterate until the maximum value of $|\Delta x|$ on the current iteration decreased by less than 10% in comparison with the previous iteration.

A similar idea can be applied to our case as well.

General case: algorithm.

- We start with the initial approximations $x_i^{(\alpha, 0)} = \tilde{x}_i^{(\alpha)}$ and $y_j^{(\beta, 0)} = \tilde{y}_j^{(\beta)}$.

- Then, for $p = 0, 1, \dots$, we solve the corresponding linear programming problem $\varepsilon \rightarrow \min$ under the constraints

$$z_j^{(\alpha, \beta, \gamma)} - \varepsilon \leq f_j \left(x^{(\alpha, p)}, y^{(\beta, p)}, s^{(\gamma)} \right) + \sum_{i=1}^n \frac{\partial f}{\partial x_i} \cdot \Delta x_i^{(\alpha)} + \sum_{k=1}^q \frac{\partial f}{\partial y_j} \cdot \Delta y_j^{(\beta)} \leq z_j^{(\alpha, \beta, \gamma)} + \varepsilon;$$

$$\tilde{x}_i^{(\alpha)} - \Delta_{x,i}^{(\alpha)} \leq x_i^{(\alpha, p)} + \Delta x_i^{(\alpha)} \leq \tilde{x}_i^{(\alpha)} + \Delta_{x,i}^{(\alpha)};$$

$$\tilde{y}_j^{(\beta)} - \Delta_{y,j}^{(\beta)} \leq y_j^{(\beta, p)} + \Delta y_j^{(\beta)} \leq \tilde{y}_j^{(\beta)} + \Delta_{y,j}^{(\beta)}.$$

We iterate until the values the values $\Delta x_i^{(\alpha)}$ and $\Delta y_j^{(\beta)}$ are small enough. For example, we can iterate until the maximum value of $|\Delta x_i^{(\alpha)}|$ and $|\Delta y_j^{(\beta)}|$ on the current iteration decreased by less than 10% in comparison with the previous iteration.

Then, we estimate the model's accuracy as

$$\tilde{\varepsilon} \stackrel{\text{def}}{=} \max_{j, \alpha, \beta, \gamma} \left| z_j^{(\alpha, \beta, \gamma)} - f_j \left(x^{(\alpha, p+1)}, y^{(\beta, p+1)}, s^{(\gamma)} \right) \right|.$$

4 Case Study: The Thermal Challenge Problem

In the paper, we illustrate the above ideas on the example of 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 thickness $L = 1.90$ cm is exposed to a heat flux $q = 3500$ W/m². We know:

- thermal conductivity k ,
- volumetric heat capacity of the material ρC_p ,
- the initial temperature $T_i = 25$ C, and
- an approximate model:

$$T(x, t) = T_i + \frac{q \cdot L}{k} \cdot \left[\frac{(k/\rho C_p) \cdot t}{L^2} + \frac{1}{3} - \frac{x}{L} + \frac{1}{2} \cdot \left(\frac{x}{L} \right)^2 - \frac{2}{\pi^2} \cdot \sum_{n=1}^6 \frac{1}{n^2} \cdot \exp \left(-n^2 \cdot \pi^2 \cdot \frac{(k/\rho C_p) \cdot t}{L^2} \right) \cdot \cos \left(n \cdot \pi \cdot \frac{x}{L} \right) \right].$$

We do not know how accurate is the approximate model. The main task is to estimate the model's accuracy ε .

A natural way to estimate this accuracy is to compare the model's predictions with the measurement results. As a result of this comparison, we conclude that the accuracy of the model is low: $\approx 25^\circ$. This low accuracy makes predictions based on this model inaccurate.

5 Thermal Challenge Problem: Interval-Related Approach

Idea. In the computations that lead to low (25 degrees) accuracy, it is assumed that the given values of k and ρC_p are exact. In practice, these values are only approximately known; they may change from sample to sample. So, a natural idea is not to assume any specific value of these quantities, just assume that for each sample, there are some values.

How this problem fits our general framework? In this case:

- we have only one measured quantity z : the temperature $z = T$; we know the measured values $z^{(k)}$ corresponding to different moments of time;
- we have one exactly known auxiliary quantity: time $s_1 = t$; we know the moments of time $s^{(k)}$ at which measurements were performed;
- unknown auxiliary quantities are $y_1 = k$ and $y_2 = \rho C_p$; we know the approximate values \tilde{y}_1 and \tilde{y}_2 ;
- we also know the approximate dependence $z_1 \approx f(y_1, y_2, s_1)$.

In this case, we know the value $z^{(k)} = T$ for different moments $t = s^{(k)}$. We need to find the values y_1 and y_2 for which $\varepsilon \rightarrow \min$, where:

$$\left| z^{(k)} - f\left(y_1, y_2, s_1^{(k)}\right) \right| \leq \varepsilon \text{ for all } k.$$

Comment. In this case, the accuracies of measuring y_1 and y_2 are not known, so we do not need the corresponding constraints.

Resulting algorithm.

- We start with the first approximation $y_1^{(0)} = \tilde{y}_1$ and $y_2^{(0)} = \tilde{y}_2$.
- Then, for $p = 0, 1, \dots$, we find Δy_1 and Δy_2 by solving the following linear programming problem: $\varepsilon \rightarrow \min$ under the constraints

$$-\varepsilon \leq z^{(k)} - f\left(y_1^{(p)}, y_2^{(p)}, s^{(k)}\right) - \frac{\partial f}{\partial y_1}\left(y_1^{(p)}, y_2^{(p)}\right) \cdot \Delta y_1 - \frac{\partial f}{\partial y_2}\left(y_1^{(p)}, y_2^{(p)}\right) \cdot \Delta y_2 \leq \varepsilon,$$

and take $y_1^{(p+1)} = y_1^{(p)} + \Delta y_1$ and $y_2^{(p+1)} = y_2^{(p)} + \Delta y_2$.

We iterate until the maximum value of $|\Delta y_1|$ and $|\Delta y_2|$ on the current iteration decreased by less than 10% in comparison with the previous iteration.

After that, we estimate the model's accuracy as

$$\tilde{\varepsilon} = \max_k \left| z^{(k)} - f\left(y_1^{(p+1)}, y_2^{(p+1)}, s_1^{(k)}\right) \right|.$$

Comment. Instead of the original model, in our computations, we used its simplified equivalent form; see Appendix for details.

Results are given in Table 5; the resulting model accuracy has gone down from 25 to 5 degrees:

6 Conclusions and Future Work

Conclusion. The original approach assumed that the parameters k and ρC_p are known. This led to predictions with accuracy 25° .

The new approach takes into account that we only know the values k and ρC_p with uncertainty. This leads to predictions with a much higher accuracy 5° .

Future work: on the example of our case study. On the example of our case study, we illustrate three directions in which our results can be further improved. In all three cases, it is easy to see how the corresponding idea can be extended to the general case.

Combining with probabilistic knowledge. The original problem, as formulated in [2,5–7,9,11], also included the probabilistic task: find z_0 such that for given s , y_1 , and y_2 , we have $z \leq z_0$ with probability $\geq 1 - p_0$ ($=0.99$). In our analysis, we found the accuracy $\tilde{\varepsilon}$ of the given approximate model, and we found the values $y_1 = k$ and $y_2 = \rho C_p$ for which this accuracy is attained. Since $|z - f(y_1, y_2, s)| \leq \tilde{\varepsilon}$, to guarantee that $z \leq z_0$, it is sufficient to guarantee that $f(y_1, y_2, s) \leq z_0 - \tilde{\varepsilon}$. So, the original probabilistic task can be now reformulated as follows: find y_0 for which

$$P_0 \stackrel{\text{def}}{=} \text{Prob}(f(y_1, y_2, s) \leq z_0 - \tilde{\varepsilon}) \geq 1 - p_0.$$

Following [2,5–7,9,11], we can assume that y_1 and y_2 are independent normally distributed random variables. We can thus find their means and standard deviations from given data. Then, for each z_0 , we can find the desired probability $\text{Prob}(f(y_1, y_2, s) \leq z_0 - \tilde{\varepsilon})$, e.g., by using linearization (since z is also normal) or by using Monte-Carlo simulations.

Towards a more accurate description of the model’s accuracy. In general, for some values of the parameters s , measurements are easier; for some, they are more difficult. In the thermal challenge problem, this parameter is the thermal flow $s_2 = q$. We have more data for easier-to-measure values, and thus, the model is more accurate for easier-to-measure values of the parameters.

To take this fact into account, instead of a single measure ε of the model’s accuracy ε , it is desirable to explicitly consider the dependence $\varepsilon(s_2, \dots)$.

time (in sec)	measured temperature	prediction: original approach	prediction: interval approach
100	105.5	97.3	105.5
200	139.3	127.4	138.8
300	165.5	150.9	165.2
400	188.7	172.1	188.7
500	210.6	192.2	211.1
600	231.9	211.9	233.1
700	253.0	231.4	254.9
800	273.9	250.8	276.6
900	294.9	270.3	298.3
1000	315.8	289.7	319.9

Table 1 Prediction quality: original approach vs. interval-related approach

In our case, which model for the dependence $\varepsilon(q)$ shall we choose? From the physical viewpoint, the problem is invariant w.r.t. changing measuring units $q \rightarrow \lambda \cdot q$ (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 re-scaling $q \rightarrow \lambda \cdot q$, the dependence has the same form if we appropriately change the units for measuring ε , i.e., that for every $\lambda > 0$, there exists a $C(\lambda)$ for which $\varepsilon(\lambda \cdot q) = C(\lambda) \cdot \varepsilon(q)$. It is known (see, e.g., [1]) that the only monotonic solutions to this functional equations have the form $\varepsilon(q) = \varepsilon_0 \cdot q^\alpha$ for some ε_0 and α .

So, for each experimentally tested q , based on all samples with given q , we find $\varepsilon(q)$, and then find ε_0 and α for which $\varepsilon(q) \approx \varepsilon_0 \cdot q^\alpha$, i.e., equivalently, $\ln(\varepsilon(q)) \approx \ln(\varepsilon_0) + \alpha \cdot \ln(q)$. This is a system of linear equations with unknowns $\ln(\varepsilon_0)$ 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 $\varepsilon(q) \approx \varepsilon_0 \cdot q^\alpha$.

From validating a model to improving a model. The formula assumes that $y_1 = k$ and $y_2 = \rho C_p$ are constants. However, by estimating these values based on samples with different temperatures t , we conclude that the average value \bar{k} of $y_1 = k$ grows with temperature T ; see Table 6. It is therefore natural to conclude that y_1 is a function of T . For example, a linear function $y_1 \approx a + b \cdot T$. Applying the Least Square method to this data, we get $a \approx 0.63$ and $b \approx 0.24 \cdot 10^{-3}$. We hope that this formula will lead to an even better fit.

T	20	250	500	750	1000
\bar{k}	0.49	0.59	0.63	0.69	0.75

Table 2 Dependence of \bar{k} on T

Acknowledgements The authors are very thankful to all the participants of the 14th GAMM-IMACS International Symposium on Scientific Computing, Computer Arithmetic and Validated Numerics SCAN'2010 (Lyon, France, September 27–30, 2010) for useful discussions.

References

1. Aczel J (2006), Lectures on Functional Equations and Their Applications, Dover, New York
2. Dowding KJ, Pilch M, Hills RG (2008) Formulation of the thermal problem, Computer Methods in Applied Mechanics and Engineering 197(29–32):2385–2389
3. Dravskikh A, Finkelstein AM, Kreinovich V (1978) Astrometric and geodetic applications of VLBI 'arc method', Modern Astrometry, Proceedings of the IAU Colloquium No. 48, Vienna, 1978, pp. 143–153
4. Dravskikh AF, Kosheleva OM, Kreinovich V, Finkelstein AM (1979) The method of arcs and differential astrometry. Soviet Astronomy Letters, 5(3):160–162
5. Ferson S, Oberkampf WL, Ginzburg L (2008) Model validation and predictive capacity for the thermal challenge problem, Computer Methods in Applied Mechanics and Engineering 197(29–32):2408–2430
6. Hills RG, Dowding KJ, Swiler L (2008) Thermal challenge problem: summary. Computer Methods in Applied Mechanics and Engineering 197(29–32):2490–2495
7. Hills RG, Pilch M, Dowding KJ, Red-Horse J, Paez TL, Babuska I, Tempone R (2008) Validation Challenge Workshop, Computer Methods in Applied Mechanics and Engineering 197(29–32):2375–2380

8. Moore RE, Kearfott RB, Cloud MJ (2009) Introduction to Interval Analysis, SIAM Press, Philadelphia, Pennsylvania
9. Oberkampf WL, Roy CJ (2010) Verification and Validation in Scientific Computing, Cambridge University Press, Cambridge, UK
10. Osegueda R, Keller GR, Starks SA, Araiza R, Bizyaev D, Kreinovich V (2004) Towards a general methodology for designing sub-noise measurement procedures. Proceedings of the 10th IMEKO TC7 International Symposium on Advances of Measurement Science, St. Petersburg, Russia, June 30–July 2, 2004, Vol. 1, pp. 59–64
11. Pilch M (2008) Preface: Sandia National Laboratories Validation Challenge Workshop, Computer Methods in Applied Mechanics and Engineering 197(29–32):2373–2374
12. Rabinovich S (2005) Measurement Errors and Uncertainties: Theory and Practice. American Institute of Physics, New York
13. Thompson AR, Moran JM, Swenson Jr. GW (2001) Interferometry and Synthesis in Radio Astronomy, Wiley, New York
14. Vanderbei RJ (2008) Linear Programming: Foundations and Extensions, Springer Verlag, Berlin, New York
15. Verschuur GL, Kellerman KI (1988) Galactic and Extragalactic Radio Astronomy, Springer-Verlag, New York

A How to Simplify Computations

Our main formula has the form

$$T(x, t) = T_i + \frac{q \cdot L}{k} \cdot \left[\frac{(k/\rho C_p) \cdot t}{L^2} + \frac{1}{3} - \frac{x}{L} + \frac{1}{2} \cdot \left(\frac{x}{L} \right)^2 - \frac{2}{\pi^2} \cdot \sum_{n=1}^6 \frac{1}{n^2} \cdot \exp\left(-n^2 \cdot \pi^2 \cdot \frac{(k/\rho C_p) \cdot t}{L^2}\right) \cdot \cos\left(n \cdot \pi \cdot \frac{x}{L}\right) \right].$$

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

$$T(x, t) = T_i + Y_1 \cdot \left[Y_2 \cdot t + \frac{1}{3} - x_0 + \frac{1}{2} \cdot x_0^2 - \frac{2}{\pi^2} \cdot \sum_{n=1}^6 \frac{1}{n^2} \cdot \exp(-n^2 \cdot \pi^2 \cdot Y_2 \cdot t) \cdot \cos(n \cdot \pi \cdot x_0) \right],$$

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

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

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