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How to Select a Representative Sample for a Family of Functions?

Leobardo Valera
The University of Texas at El Paso, leobardovalera@gmail.com

Martine Ceberio
The University of Texas at El Paso, mceberio@utep.edu

Vladik Kreinovich
The University of Texas at El Paso, vladik@utep.edu

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Abstract Predictions are rarely absolutely accurate. Often, the future values of quantities of interest depend on some parameters that we only know with some uncertainty. To make sure that all possible solutions satisfy desired constraints, it is necessary to generate a representative finite sample, so that if the constraints are satisfied for all the functions from this sample, then we can be sure that these constraints will be satisfied for the actual future behavior as well. At present, such a sample is selected based by Monte-Carlo simulations, but, as we show, such selection may underestimate the danger of violating the constraints. To avoid such an underestimation, we propose a different algorithms that uses interval computations.

1 Formulation of the Problem

Often, we only known a family of functions. One of the important objectives of science and engineering is to predict the behavior of different systems. Examples include predicting the trajectories of celestial bodies (including the trajectories of satellites), predicting weather, predicting how a building will react to a strong earthquake, etc. In many such situations, we know the differential equations that describe how the corresponding quantities change with time, and we can use these equations to make predictions.

Sometimes, we can make (almost) exact predictions: e.g., we can predict the trajectories of celestial bodies hundreds of years into the future. In such case, we

Leobardo Valera
Deparment of Mathematical Sciences, University of Texas at El Paso, 500 W. University
El Paso, TX 79968, USA, e-mail: leobardovalera@gmail.com

Martine Ceberio and Vladik Kreinovich
Department of Computer Science, University of Texas at El Paso, 500 W. University
El Paso, TX 79968, USA, e-mail: mceberio@utep.edu, vladik@utep.edu

predict how the values of the corresponding quantities x change with time t, i.e., we know the exact form of the dependence $x(t)$.

In many other situations, however, the future values $x(t)$ of these quantities are not uniquely determined by available information, they also depend on the values of some quantities $c_1, \ldots, c_n$ which are not known exactly. In such situations, we know an algorithm that, given the value of the parameters c_i, returns the corresponding function $x(t, c_1, \ldots, c_n)$.

We do not know the exact values of the parameters c_i, we only know the approximate values $\widetilde{c}_i$. Based on these approximate values, we can find the approximate function

$$\widetilde{x}(t) = x(t, \widetilde{c}_1, \ldots, \widetilde{c}_n). \tag{1}$$

Since the (unknown) actual values c_i^{act} of the corresponding parameters are, in general, different from the approximate values, the actual dependence

$$x^{\text{act}}(t) = x\left(t, c_1^{\text{act}}, \ldots, c_n^{\text{act}}\right) \tag{2}$$

is, in general, different from the approximate dependence $\widetilde{x}(t)$.

How different can these two dependencies be depends on the accuracy of the approximations $\widetilde{c}_i$. Usually, we know the accuracy of the corresponding approximation, i.e., we know the upper bounds Δ_i on the absolute value of the approximation errors $\Delta c_i \stackrel{\text{def}}{=} \widetilde{c}_i - c_i$, i.e., the bounds for which $|\Delta c_i| \le \Delta_i$. (If we did not know such bounds, then we could not make any conclusion at all.) In this case, the actual value of the quantity c_i can take any value from the interval $[\widetilde{x}_i - \Delta_i, \widetilde{c}_i + \Delta_i]$

For each combination of values c_i, we have, in general, a different dependence on time $x(t) = x(t, c_1, \ldots, c_n)$. In such situations, we do not know the exact dependence $x(t)$, we only know that the family of functions that contains the desired function:

$$F = \{t \mapsto x(t, c_1, \ldots, c_n) : |\widetilde{c}_i - c_i| \le \Delta_i \text{ for all } i\}. \tag{3}$$

Comment. A similar problem appears if we want to predict a *field*, i.e., the future values of a quantity at different moments of time and at different spatial locations. In this case, the formulas (and algorithms) are similar, the only difference is that in this case, t is not a single number but a tuple of numbers – e.g., the moment of time and the spatial coordinates.

What we want. One of the reasons we want to make a prediction is to study how possible future conditions can affect our system. For example, we want to study how seismic waves from possible future earthquakes will affect the building that we are currently designing. For a chemical plant, we want to make sure that the concentration of the pollutants in the atmosphere does not exceed the tolerable micro-level, etc.

In all these cases, we want to check whether an appropriate numerical characteristic $q(x(t))$ of the solution $x(t)$ stays within the desired bounds – or goes beyond the desired bounds, into the danger zone.

Usually, there are several such characteristics q. For example, for a building, we want stress in all critical locations not to exceed the desired threshold. For a chemical plant, we want the level of all possible pollutants not to exceed the desired level, etc.

It is desirable to have a representative sample. Usually, we have a simulator that can describe the effect of each possible function $x(t)$, i.e., that estimates the corresponding values $q(x(t))$.

The problem is that in situations with uncertainty, there are infinitely many possible values of each quantity c_i and thus, infinitely many possible function $x(t)$. We cannot test them all, we need to select a representative sample.

In other words, we want to select a finite list of functions $x_1(t)$, ..., $x_L(t)$ – each of which is either themselves possible solutions or which are close to possible solutions – so that once we compute the value of the quantity $q(x_\ell(t)))$ on all these functions, the range

$$[\min q(x_\ell(t)), \max q(x_\ell(t))] \tag{4}$$

will give us a good approximation for the actual range

$$\{Q(c_1,\ldots,c_n) : c_i \in [\widetilde{c}_i - \Delta_i, \widetilde{c}_i + \Delta_i]\}, \tag{5}$$

where we denoted

$$Q(c_1,\ldots,c_n) \stackrel{\text{def}}{=} q(x(t,c_1,\ldots,c_n)).$$

Comment. We want to make sure that we do not underestimate the danger, that all possible deviations of the actual range (5) from the desired bounds are captured by the sample-based estimate (4) for this range. In other words, we want to make sure that the sample-based estimate (4) contains the actual range (5).

How this sample is usually selected: description and limitations. The usual way of selecting the sample is to choose, several times, random values of the parameters c_i from the corresponding intervals – e.g., values uniformly distributed on this interval. The problem with this method is that it often underestimates the effect.

Indeed, we want to check, e.g., whether the designed building will remain stable for all possible values of the quantities c_i describing the earthquake, i.e., whether a certain quantity q depending of the function $x(t)$ (and, thus, on the values of c_i) does not exceed a danger threshold. Usually, the deviations Δc_i are relatively small, so in the first approximation, we can expand the dependence of Q on $c_i = \widetilde{c}_i - \Delta c_i$ in Taylor series and only keep linear terms in this expansion:

$$Q(c_1,\ldots,c_n) = Q(\widetilde{c}_1 - \Delta c_1,\ldots,\widetilde{c}_i - \Delta c_n) = \widetilde{Q} - \sum_{i=1}^{n} Q_i \cdot \Delta c_i, \tag{6}$$

where we denoted $\widetilde{Q} \stackrel{\text{def}}{=} Q(\widetilde{c}_1,\ldots,\widetilde{c}_n)$ and

$$Q_i \stackrel{\text{def}}{=} \frac{\partial Q}{\partial c_i}_{|c_1=\widetilde{c}_1,\ldots,c_n=\widetilde{c}_n}.$$

The expression (6) is monotonic in Δc_i, so its largest possible value when $\Delta c_i \in [-\Delta_i, \Delta_i]$ is attained:

- when $\Delta c_i = \Delta_i$ for indices i for which $Q_i \geq 0$ and
- when $\Delta c_i = -\Delta_i$ for indices i for which $Q_i \leq 0$.

The resulting largest difference Δ between $\widetilde{Q}$ and Q is thus equal to

$$\Delta = \sum_{i=1}^{n} |Q_i| \cdot \Delta_i. \tag{7}$$

On other hand, if we use independent random values Δc_i, then, due to the Central Limit Theorem (see, e.g., [4]), for large n, the distribution of the sum (2) is close to Gaussian. For independent random variables, the mean is the sum of the means, and the variance is the sum of the variances. Each mean is 0, so the overall mean a is equal to 0 too. The variance of the uniform distribution on the interval $[-\Delta_i, \Delta_i]$ is equal to $(1/3) \cdot \Delta_i^2$. Thus, the overall variance is equal to

$$V = \frac{1}{3} \cdot \sum_{i=1}^{n} Q_i^2 \cdot \Delta_i^2,$$

with the standard deviation σ equal to

$$\sigma = \sqrt{V} = \sqrt{\frac{1}{3} \cdot \sum_{i=1}^{n} Q_i^2 \cdot \Delta_i^2}. \tag{8}$$

For the Gaussian (normal) distribution with mean a and standard deviation σ, with high confidence, all the random values are within the 3-sigma interval $[a-3\sigma, a+3\sigma]$. So, with high confidence, all the values q generated by random simulations do not exceed 3σ. Herein lies a problem: in the simplest case when all the values Q_i are equal to 1 and $\Delta_1 = \ldots = \Delta_n$:

- the formula (7) leads to $\Delta = n \cdot \Delta_c$ (where we denoted by Δ_c the common value of all the Δ_i), while,
- according to the formula (9), we have $V = (1/3) \cdot n \cdot \Delta_c^2$ and thus,

$$3\sigma = 3 \cdot \sqrt{V} = \sqrt{3} \cdot \sqrt{n} \cdot \Delta_c.$$

For large n, we have $\sqrt{n} \ll n$, so this method indeed underestimates possible dangers.

Resulting problem. How to select a representative sample that would not underestimate possible dangers?

2 Analysis of the Problem

Analysis of the problem. In the linearized case (6), as we have mentioned, the largest and the smallest values of Q are attained when each parameter c_i is either equal to its largest possible value $\overline{c}_i = \widetilde{c}_i + \Delta_i$ or to its smallest possible value

$$\underline{c}_i = \widetilde{c}_i - \Delta_i.$$

The same property holds if we take into account that the linear expression (6) is an approximation – in a generic point $(\widetilde{c}_1, \ldots, \widetilde{c}_n)$ all partial derivatives are different from 0 and thus, they are different from 0 also in a small vicinity of this point.

First idea. Thus, in principle, as the desired sample, we can take functions $x(t, c_1, \ldots, c_n)$ corresponding to all possible combinations of these values

$$c_i = \widetilde{c}_i \pm \Delta_i.$$

Limitations of the first idea. For each parameter c_i, we need to select one of the two possible values, and we need to consider all possible combinations of n such selections – and there are 2^n such combinations.

The above first idea can be implemented for small n, but in realistic situations when n is large, the number of combinations becomes astronomic and not realistic.

Second idea. Since we cannot consider extreme values of all n parameters c_i, a natural next idea is to select $k < n$ most important parameters – i.e., parameters c_i for which the dependence on c_i as expressed, e.g., by the mean square value

$$D_i \stackrel{\text{def}}{=} \int \left(x(t, \widetilde{c}_1, \ldots, \widetilde{c}_{i-1}, \widetilde{c}_i + \Delta_i, \widetilde{c}_{i+1}, \ldots, \widetilde{c}_n) - \widetilde{x}(t)\right)^2 dt, \tag{9}$$

is the largest.

In other words, we compute the values D_i for all i, sort them in non-increasing order

$$D_1 \geq D_2 \ldots \geq D_k \geq \ldots \geq D_n, \tag{10}$$

and select the parameters c_i corresponding to the first k terms in this order (10).

Without losing generality, we can assume that the parameters c_i are already sorted in the inverse order of the corresponding D_i values. This way, we will only need to use 2^k combinations of the values $c_i = \widetilde{c}_i \pm \Delta_i$ corresponding to $i = 1, \ldots, k$.

For each of the remaining parameters c_{k+1}, …, c_n, we have to use a fixed value, e.g., the value $c_j = \widetilde{c}_j$.

Limitations of the second idea. By using the formula (6), we can conclude that by using this sample, the largest possible difference between the sample-based values Q and the nominal value $\widetilde{Q}$ is equal to

$$\Delta^{(k)} = \sum_{i=1}^{k} |Q_i| \cdot \Delta_i. \tag{11}$$

In general, this value is smaller that the largest possible value (7), since we ignore the terms corresponding to $i = k+1, \ldots, n$.

Thus, this idea shares the same limitation as the traditional method – it underestimates the possible difference between the actual (unknown) value q and the nominal value $\widetilde{q}$ and thus, underestimates the danger.

Towards the final idea. To avoid underestimation, for each combination of the parameter values $c_1 = \widetilde{c}_1 \pm \Delta_1$, ..., $c_k = \widetilde{c}_k \pm \Delta_k$, we need to provide bounds on the values of the function $x(t, c_1, \ldots, c_k, c_{k+1}, \ldots, c_n)$ corresponding to all possible values of

$$c_{k+1} \in [\widetilde{c}_{k+1} - \Delta_{k+1}, \widetilde{c}_{k+1} + \Delta_{k+1}], \ldots, c_n \in [\widetilde{c}_n - \Delta_n, \widetilde{c}_n + \Delta_n].$$

Techniques for providing such bounds are known as techniques of *interval computations*; see, e.g., [1, 2, 3]. Thus, we arrive at the following algorithm for selecting a representative sample.

3 Resulting Algorithm

What is given:

- an algorithm that, given n values c_i, returns a function $x(t, c_1, \ldots, c_n)$.
- approximate values $\widetilde{c}_1, \ldots, \widetilde{c}_n$, and
- upper bounds $\Delta_1, \ldots, \Delta_n$ on the corresponding approximation errors.

Based on the approximate values $\widetilde{c}_i$, we compute the approximate function

$$\widetilde{x}(t) = x(t, \widetilde{c}_1, \ldots, \widetilde{c}_n).$$

What we want. We want to generate a finite list of functions $x_1(t)$, ..., $x_L(t)$ with the following properties:

- that each of these functions is close to one of the possible solutions $x(t, c_1, \ldots, c_n)$ for some $c_i \in [\widetilde{c}_i - \Delta_i, \widetilde{c}_i + \Delta_i]$, and
- that for each characteristic q, the sample-based range (4) of the values of this characteristic contains the actual range (5) – and is close to the actual range.

Preliminary step. For each i, we use the given algorithm to compute the function

$$x_{+i}(t) \stackrel{\text{def}}{=} x(t, \widetilde{c}_1, \ldots, \widetilde{c}_{i-1}, \widetilde{c}_i + \Delta_i, \widetilde{c}_{i+1}, \ldots, \widetilde{c}_n)$$

and then compute the value

$$D_i = \int (x_{+i}(t) - \widetilde{x}(t))^2\, dt.$$

We then sort n parameters c_i in the non-increasing order of the values D_i. Without losing generality, we assume that

$$D_1 \geq D_2 \geq \ldots \geq D_n.$$

Main step. We select some value k so that we will be able to generate $2 \cdot 2^k$ functions. Then, for each of 2^k combinations of signs $\varepsilon = (\varepsilon_1, \ldots, \varepsilon_k)$, where $\varepsilon_i \in \{-, +\}$, we apply interval computations to find an estimate $\left[\underline{X_\varepsilon}(t), \overline{X}_\varepsilon(t)\right]$ for the range of the function

$$x(t, \widetilde{c}_1 + \varepsilon_1 \cdot \Delta_1, \ldots, \widetilde{c}_k + \varepsilon_k \cdot \Delta_k, c_{k+1}, \ldots, c_n)$$

when

$$c_{k+1} \in [\widetilde{c}_{k+1} - \Delta_{k+1}, \widetilde{c}_{k+1} + \Delta_{k+1}], \ldots, c_n \in [\widetilde{c}_n - \Delta_n, \widetilde{c}_n + \Delta_n].$$

The resulting $2 \cdot 2^k$ functions $\underline{X_\varepsilon}(t)$ and $\overline{X}_\varepsilon(t)$ form the desired list.

Comment. Since we use interval computations to take care of all possible values of $c_{k+1}, \ldots, c_n$, we expect that the sample-based range will indeed contain the actual range (5) of each quantity q.

For a sufficient large k, the effect of the quantities $c_{k+1}, \ldots, c_n$ is small, so:

- each selected function $\underline{X_\varepsilon}(t)$ or $\overline{X}_\varepsilon(t)$ is close to the corresponding actual solutions
$$x(t, \widetilde{c}_1 + \varepsilon_1 \cdot \Delta_1, \ldots, \widetilde{c}_k + \varepsilon_k \cdot \Delta_k, \widetilde{c}_{k+1}, \ldots, \widetilde{c}_n),$$
- and thus, the sample-based range should not differ too much from the actual range (5).

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