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From intervals to domains: Towards a general description of validated uncertainty, with potential applications to geospatial and meteorological data

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Abstract

When physical quantities x_i are numbers, then the corresponding measurement accuracy can be usually represented in interval terms, and interval computations can be used to estimate the resulting uncertainty in $y = f(x_1, \ldots, x_n)$.

In some practical problems, we are interested in more complex structures such as functions, operators, etc. Examples: we may be interested in how the material strain depends on the applied stress, or in how a physical quantity such as temperature or velocity of sound depends on a 3-D point.

For many such structures, there are ways to represent uncertainty, but usually, for each new structure, we have to perform a lot of complex analysis from scratch. It is desirable to come up with a general methodology that would automatically produce a natural description of validated uncertainty for all physically interesting situations (or at least for as many such situations as possible). In this paper, we describe the foundations for such a methodology; it turns out that this problem naturally leads to the technique of *domains* first introduced by D. Scott in the 1970s.

In addition to general domain techniques, we also describe applications to geospatial and meteorological data.

Keywords: Interval computations; Domains; Geospatial data; Meteorological data

1. From intervals to domains

Formulation of the problem: Usually, physical quantities x_i are numbers. In this case, intervals provide a reasonable description of measurement accuracy. Sometimes, however, we are interested in more complex structures such as functions, operators, etc. For example, in meteorology, we are interested in knowing how the temperature depends on a 3-D point. At present, for each new structure, we have to invent a new representation of uncertainty. It is therefore desirable to come up with a general description of validated uncertainty.

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In this paper, we show that a natural approach leads to Scott's domains; see, e.g., [4–6,8]. We will also show how this general approach can be applied to meteorology.

Binary domains: In real-life measurements, a measurement result has to be represented in a computer. Thus, it has to be represented as a sequence of 0s and 1s, and the length of this sequence is bounded. There are only finitely many such sequences, so we have a finite set X of possible measurement results.

Measurement uncertainty means, in particular, that when measuring the value of the same quantity with the same measurement result, we may get different values. Thus, a natural way to describe uncertainty is to describe a binary relation $a \sim b$ on the set X, a relation in which $a \sim b$ if and only if the same object can lead to both a and b.

Definition 1. A *binary domain* is a pair $\langle X, \sim\rangle$, where X is a finite set, and $\sim$ is a symmetric reflexive relation on X.

Comment: Binary domains are also called *webs*, or *graphs.*

Examples. Let us first show how the standard interval uncertainty fits into this general picture. For example, suppose that we measure temperature with the accuracy 1°, and the scale consists of the values $X = \{0, 1, 2, 3 \ldots, T\}$. Here, e.g., $\tilde{t} = 0$ means that the actual temperature t is in the interval $[-1, 1]$; so, $a \sim b$ if the corresponding intervals $[a-1, a+1]$ and $[b-1, b+1]$ intersect, i.e., if $|a-b| \leqslant 2$.

An even simpler example comes from counting. Every actual counting device has a limitation of how many objects we can count, so here, $X = \{1, 2, \ldots, n, \text{many}\}$, where "many" means that we have exhausted this device, and there are still objects to count. Here, $a \sim b$ if and only if $a = b$.

Yet another example comes from "yes"–"no" questions; here, possible results are "false" (usually denoted by 0), "true" (usually denoted by 1), and "unknown" (we will denote it by U). Here, $X = \{0, 1, U\}$, and the relation $\sim$ has the form $0 \sim U$ and $U \sim 1$. Indeed, if we do not know the truth value (U), then, in reality, the answer may turn out to be "true" (hence $U \sim 1$) or "false" (hence, $U \sim 0$). However, once we know the answer "true", we cannot get the answer "false", hence $0 \not\sim 1$.

In general, a measuring instrument can be described by a binary domain $\langle X, \sim\rangle$.

Simplicial complexes: To get a better description of a measuring instrument, it is desirable to know not only which pairs are "compatible", but also which triples, etc., can come from the same object. If $a \sim b$, $b \sim c$, and $a \sim c$, then for some measuring instruments, all three values are possible outcomes for some object, while for others, no single object can lead to these three outcomes.

Informally, let us say that a set $S \subseteq X$ is *compatible* if for some object, all values from S are possible. Then, a measuring instrument can be represented as a pair $\langle X, \mathcal{S}\rangle$, where $X \subseteq \mathcal{S} \subseteq 2^X$ is the class of all compatible sets. Clearly, if a set S is compatible then each subset of S is compatible too. In mathematical terms, such a pair is called a *simplicial complex*: X is the set of vertices, and $\mathcal{S}$ is the set of faces.

Definition 2. A *simplicial complex* is a pair $\langle X, \mathcal{S}\rangle$, where $X \subseteq \mathcal{S} \subseteq 2^X$.

Example. For example, if $X = \{a, b, c\}$, $a \sim b$, $b \sim c$, $a \sim c$, and there is an object for which all three outcomes are possible, then the corresponding simplicial complex is a filled triangle $\mathcal{S} = \{\{a\}, \{b\}, \{c\}, \{a, b\}, \{b, c\}, \{a, c\}, \{a, b, c\}\}$. Alternatively, if no such object exists, then we have an empty triangle $\mathcal{S} = \{\{a\}, \{b\}, \{c\}, \{a, b\}, \{b, c\}, \{a, c\}\}$.

How to describe actual values of measured quantities: A single measurement only leads to an *approximate* value of the measured quantity. To describe the *actual* value of the measured quantity, we must consider a sequence of more and more accurate measuring instruments.

Let X_k describe results of first k measurements. Then, for every $k < l$, there exists a natural "forgetful functor" $\pi_{lk} : X_l \to X_k$ that simply erases the results of the last $l - k$ measurements. It is easy to see that this projection π satisfies the following properties:

(i) if $a' \sim' b'$, then $\pi(a') \sim \pi(b')$;
(ii) if $a \sim b$, then $\exists a', b'$ such that $\pi(a') = a$, $\pi(b') = b$, and $a' \sim' b'$.

Definition 3. Let $\langle X, \sim\rangle$ and $\langle X', \sim'\rangle$ be finite domains. A mapping $\pi : X' \to X$ is called a *projection* if it satisfies the properties (i)–(ii).

We thus arrive at the following definition.

Definition 4.

- By a *physical quantity*, we mean a sequence of binary domains $\langle X_i, \sim_i\rangle$ with projections: $X_1 \overset{\pi_{2,1}}{\leftarrow} X_2 \overset{\pi_{3,2}}{\leftarrow} X_3 \overset{\pi_{4,3}}{\leftarrow} \ldots$.
- By an *actual value of the quantity*, we mean a sequence $x = (x_1, x_2, \ldots)$, where $x_i \in X_i$ and $\pi_{lk}(x_l) = x_k$ for all $k < l$.
- The set X of all actual values is called a *projective limit* of the sequence X_i.
- Two values $a, b \in X$ are called *equivalent* if $a_i \sim_i b_i$ for all i.

On the set X of possible values of the quantity, we can naturally define neighborhoods and limits:

Definition 5.

- By a *neighborhood* of a value a we mean a set $N_n(a) \overset{\text{def}}{=} \{b \mid b \sim_n a\}$ for some integer n.
- If $a^{(k)}$ is a sequence of elements form X, then we say that $a^{(k)}$ *tends to a limit* a (denoted $a^{(k)} \to a$) if $\forall n\, \exists m\, \forall k > m\ (a_n^{(k)} \sim_n a)$.

Examples. It is easy to see that if we consider interval-related sets $X_i = \{-p_i/q_i, -(p_i-1)/q_i, \ldots, (p_i-1)/q_i, p_i/q_i\}$ (where $k/q_i \sim_i (k+1)/q_i$) with a better and better accuracy ($q_i \to \infty$) and broader and broader span ($p_i/q_i \to \infty$), then the corresponding set X is the set of all real numbers (+ two extra values $-\infty$ and $+\infty$) with a natural topology.

If we start with n-dimensional "boxes", we naturally end up with the set R^n.

For "yes"–"no" questions, if one measurement does not lead to a definite answer (i.e., if the answer is U), we can perform a more accurate measurement; as a result, we may get a definite answer, i.e., we may get a sequence of answers $U0$ or $U1$, or we may still get "unknown" — i.e., the sequence UU. So, after two measurements, we have five possible results: $X_2 = \{0, 1, U0, U1, UU\}$. In the set X_2, all "yes" answers (0 and $U0$) can happen in the same state, so $0 \sim U0$; it is also possible that in the same state, sometimes, the answer is "yes", and sometimes, the answer is still unknown, so $0 \sim UU$ and $U0 \sim UU$. The natural projection from X_2 to X_1 simply deleted the second answer: e.g., $\pi_{2,1}(U0) = U$. So, here:

- X_1: $0 \sim_1 U$, $U \sim_1 1$;
- X_2: $0 \sim_2 U0$, $0 \sim_2 UU$, $U0 \sim_2 UU$, $1 \sim_2 U1$, $1 \sim_2 UU$, $U1 \sim_2 UU$;

etc. Thus, the projective limit X consists of three different elements 0, 1, and U, with the relation $0 \sim U$ and $U \sim 1$.

Proposition 1. (compactness). *For every projective limit X, every sequence $a^{(k)}$ has a convergent subsequence.*

Proof. Since the set X_1 is finite, and there are infinitely many elements $a^{(k)}$ in the sequence, there exist at least one value $x \in X_1$ for which infinitely many elements $a^{(k)}$ have $a_1^{(k)} = x$. We can therefore consider a subsequence consisting of such elements. Let us fix the first element in this new subsequence. There are infinitely many elements in the remaining part of the subsequence, and only finitely many elements in X_2. Thus, we can select a sub-subsequence in which all elements but one have the same value of a_2, etc. As a result, we get a convergent subsequence. □

Discussion: For example, for real numbers, instead of the set R, we have a compactification $R \cup \{-\infty, +\infty\}$.

Compactness is important for solving *inverse problems*; see, e.g., [7]. The main reason why we have measurements is that we want to reconstruct the actual values of the measured quantities. In general, we observe $f(x)$ for some continuous $f : X \to Y$, and we want to reconstruct x. For example, we want to reconstruct an image x, but what we

observe is an image $f(x)$ distorted by the inaccuracies of the lens. The problem is that even in the presence of noise, when the mapping f is 1–1, the function f^{-1} is often discontinuous, so a small measurement error y can lead to a large error in reconstructing x. A known solution is to restrict ourselves to compact sets X because for compact sets, the inverse f^{-1} to a continuous mapping is continuous as well.

The problem is that, e.g., the set X of all images is not compact under standard mathematical metrics such as L^2 or L^∞. Our result shows that this set is compact if we consider a topology that naturally comes from measurements.

Functions: Once we have a description of the set A and of the set B, how can we describe, in these terms, the set of all functions from A to B? For example, if we know how to describe time t and how to describe spatial coordinate x, how can we then describe a trajectory $x(t)$, i.e., a function that maps t into x?

In physical terms, a function $f : A \to B$ means that, once we know an approximation a_n to a, we can find some approximation b_m to b. Thus, we arrive at the following definition:

Definition 6. Let A and B be two projective limits. By a function $f : A \to B$, we mean a mapping from $\cup A_n$ to $\cup B_n$ such that:

- $a \sim a'$ implies $f(a) \sim f(a')$;
- if $a = \pi(a')$, then $f(a) = \pi(f(a'))$.

Comment: It is worth mentioning that functions may be partial, so the results do not converge: e.g., due to Heisenberg inequality, we cannot determine both $x(t)$ and $v(t)$ with arbitrary accuracy.

Definition 7. We say that a function f is continuous if

$$\forall n\, \exists m\, ((x_m \sim_m x'_m) \to f(x_m) \sim_n f(x'_m)).$$

Proposition 2. *If a function $f : X \to R$ is everywhere defined, then f is continuous.*

Proof. By using compactness and reduction to a contradiction. □

Let us show how this general vision can be applied to practical problems.

2. Towards meteorological and geophysical applications

Data compression: formulation of the problem: At present, a large amount of data are coming from measuring instruments. It is often necessary to compress this data before storing and processing. We can gain some storage space by using *lossless* compression. However, often, the gain available via lossless compression is not sufficient. So, we must use *lossy* compression as well.

For image compression, the JPEG2000 standard uses wavelet transform (and other efficient compression techniques) to provide a very efficient compression of 2-D images $I(x, y)$. Its important characteristic is bitrate b, i.e., number of bits per pixel that is required, on average, for the compressed image. Within JPEG2000, we can select different bitrates. The highest possible bitrate B leads to lossless compression, when image is reconstructed precisely, i.e., when the reconstructed image $\widetilde{I}^{[b]}(x, y)$ is identical to the original image $I(x, y)$. When we decrease the bitrate b, we get a lossy compression, for which $\widetilde{I}^{[b]}(x, y) \neq I(x, y)$; the smaller the bitrate b, the more the compressed/decompressed image $\widetilde{I}^{[b]}(x, y)$ will differ from the original image $I(x, y)$.

Known methods of data compression: In principle, it is possible to use JPEG2000 compression techniques to compress 2-D measurement data as well. In some cases, we have 3-D data: e.g., meteorological measurements taken in different places (x, y) at different heights z. To compress 3-D data, in principle, we can simply apply the 2-D JPEG2000 compression to each horizontal layer $f(x, y, z_0)$. However, a better compression is achieved if we use KLT transform:

We compute the average value $\bar{f}(z) = N^{-1} \cdot \sum_{x,y} f(x, y, z)$ of the analyzed quantity at a given height z, where N is the overall number of horizontal points (x, y).

We then compute the covariances between different heights:

$$V(z_1, z_2) = \frac{1}{N} \cdot \sum_{x,y} (f(x, y, z_1) - \bar{f}(z_1)) \cdot (f(x, y, z_2) - \bar{f}(z_2)).$$

We find the eigenvectors λ_k and the eigenvectors $e_k(z)$ of the covariance matrix $V(z_1, z_2)$, and sort these eigenvalues into a sequence $e_1(z), e_2(z), \ldots$ so that $|\lambda_1| \geqslant |\lambda_2| \geqslant \cdots$.

Finally, we represent the original 3-D data values $f(x, y, z)$ as a linear combination of the eigenvectors $e_k(z)$: $f(x, y, z) = \bar{f}(z) + \sum_k a_k(x, y) \cdot e_k(z)$, and to each "slice" $a_k(x, y)$, we apply a 2-D JPEG2000 compression with the appropriate bit rate b_k. Based on the compressed data, we can reconstruct each slice as $\widetilde{a}_k^{[b_k]}(x, y)$, and then reconstruct the data as $\widetilde{f}(x, y, z) = \bar{f}(z) + \sum_k \widetilde{a}_k^{[b_k]}(x, y) \cdot e_k(z)$.

Specifics of data compression: There is a difference between image and data compression. In image compression, image quality is main objective, and the visual image quality is well described by the mean square difference (MSE) between the original image $I(x, y)$ and the compressed–decompressed image $\widetilde{I}(x, y)$.

In data compression, we want to reproduce each *measurement* result with a certain accuracy. For example, we want to know wind, temperature, pressure along the trajectory of a plane: if along this line, the values are not reconstructed accurately enough, the plane may crash, and the fact that on average, we get a good reconstruction, does not help.

Thus, we need a compression that guarantees the desired accuracy Δ, i.e.,

$$\|f - \widetilde{f}\|_{L^\infty} \stackrel{\text{def}}{=} \max_{x,y,z} |f(x, y, z) - \widetilde{f}(x, y, z)| \leqslant \Delta.$$

Among all such compressions, we must find the one for which the average bit rate $\overline{b} \stackrel{\text{def}}{=} (1/N_z) \cdot \sum_k b_k$ is the smallest possible, where N_z denotes the number of vertical layers (i.e., number of different heights).

In some cases, the bandwidth is limited by the capacity b_0 of the communication channel: $\overline{b} \leqslant b_0$. In such cases, among all compression schemes with $\overline{b} \leqslant b_0$, we must find a one for which the L^∞ compression/decompression error is the smallest possible. In this paper, we describe new efficient (suboptimal) techniques for data compression under such interval uncertainty.

2D case: We want to find the b for which $D(b) \leqslant \Delta$, where $D(b) \stackrel{\text{def}}{=} \max_{x,y} \left| \widetilde{f}^{[b]}(x, y) - f(x, y) \right|$. We know that $b_{\text{opt}} \in [b^-, b^+]$, where $b^- = 0$ and $b^+ = B$ (lossless), and that $D(b) \downarrow$ when $b \uparrow$. So, we can use the following bisection algorithm: on each iteration, we start with an interval $[b^-, b^+]$ that contains b_{opt}.

We take $b_{\text{mid}} \stackrel{\text{def}}{=} (b^- + b^+)/2$, apply JPEG2000 compression with $b = b_{\text{mid}}$, and compute $D(b_{\text{mid}})$. If $D(b_{\text{mid}}) \leqslant \Delta$, we replace the original interval $[b^-, b^+]$ with the half-size interval $[b^-, b_{\text{mid}}]$. Otherwise, we replace $[b^-, b^+]$ with $[b_{\text{mid}}, b^+]$.

After each iteration, the size of the interval halves. So, after k iterations, we get b_{opt} with accuracy 2^{-k}.

3-D case: *idea*: We want to find the bitrate allocation $b = (b_1, \ldots, b_{N_z})$ for which $\overline{b} \to \min$ among all b for which $D(b_1, b_2, \ldots) \leqslant \Delta$, where $D(b_1, \ldots) \stackrel{\text{def}}{=} \max_{x,y,z} \left| \widetilde{f}(x, y, z) - f(x, y, z) \right|$. Minimizing a function of many variables is difficult—running time grows exponentially with N_z.

To overcome this difficulty, we borrow the idea from interval computations. There, the problem is, given a function $f(x_1, \ldots, x_n)$ and intervals $\mathbf{x}_i$, to compute the range $\mathbf{y} \stackrel{\text{def}}{=} \{f(x_1, \ldots, x_n) \,|\, x_1 \in \mathbf{x}_1 \,\&\, \ldots \,\&\, x_n \in \mathbf{x}_n\}$, and the difficulty is that computing this range exactly is NP-hard—crudely speaking, no algorithm always computes $\mathbf{y}$ in reasonable time. The solution is that since we cannot find the exact range $\mathbf{y}$, we compute an *enclosure* $\mathbf{Y} \supseteq \mathbf{y}$.

Similarly, in our case, since it is difficult to minimize $D(b_1, \ldots)$, we find easier-to-optimize upper estimate $\widetilde{D}(b_1, b_2, \ldots) \geqslant D(b_1, b_2, \ldots)$, and then find the values b_i that minimize $\widetilde{D}(b_1, \ldots)$. As a result, we find b_i for which $\widetilde{D}(b_1, \ldots) \leqslant \widetilde{D}_{\min}$ hence $D(b_1, \ldots) \leqslant \widetilde{D}_{\min}$.

Since, in general, $D(b_1,\ldots)\leqslant\widetilde{D}(b_1,\ldots)$, the resulting allocation is only *suboptimal* with respect to $D(b_1,\ldots)$.

Explicit formulas: Once we know the L^∞-norms

$$D_k(b_k)\stackrel{\text{def}}{=}\max_{x,y}|a_k(x,y)-\widetilde{a}_k^{[b_k]}(x,y)|$$

of the compression/decompression errors of each slice, we can conclude that $|a_k(x,y)-\widetilde{a}_k^{[b_k]}(x,y)|\leqslant D_k(b_k)$. Hence,

$$|(a_k(x,y)-\widetilde{a}_k^{[b_k]}(x,y))\cdot e_k(z)|\leqslant D_k(b_k)\cdot E_k,$$

where $E_k\stackrel{\text{def}}{=}\max_z|e_k(z)|$. Thus, the desired L^∞ error is bounded by $\widetilde{D}(b_1,\ldots)\stackrel{\text{def}}{=}\sum_k D_k(b_k)\cdot E_k$.

To minimize $\widetilde{D}(b_1,\ldots)=\sum_k D_k(b_k)\cdot E_k$ under the condition $\sum_k b_k=N_z\cdot b_0$, we can use the Lagrange multiplier approach [1,3]. As a result, we arrive at the following algorithm:

Algorithm. Once we know how $D_k(b)$ depends on the bitrate b, it is sufficient to find the Lagrange multiplier λ; then, $|D_k'(b_k)|=\lambda/E_k$. We find λ for which the average bitrate is b_0 by bisection.

How can we find $D_k(b)$? We can try, for each layer k, *all* possible bitrates b. Alternatively, we have shown that $B_k(b)=A_1\cdot(b-b_0)^\alpha$ for $b\leqslant b_0$ and $B_k(b)=A_2\cdot 2^{-b}$ for $b\geqslant b_0$; thus, we need to try a *few* b to find A_i, b_0, and α.

Results. We tested our algorithm on 3-D meteorological data: temperature T, pressure P, the components U, V, and W of the wind speed vector, and the waver vapor ratio WV. These data describe the values of the six meteorological variables at $N_z=64$ different heights. The height is measured with respect to the terrain, so that the points on the surface correspond to $z=0$. Within each height z, the values are given at $N=129\times 129$ different points (x,y).

For meteorological data, the resulting compression indeed leads to a much smaller L^∞ error bound Δ_{new} than the L^∞ error bound Δ_{MSE} corresponding to the bitrate allocation that optimizes MSE error:

- For $b_0=0.1$, we have $\Delta_{\text{MSE}}\approx 6\%$ and $\Delta_{\text{new}}\approx 4\%$, so $\Delta_{\text{new}}/\Delta_{\text{MSE}}\approx 0.7$.
- For $b_0=0.5$, we have $\Delta_{\text{MSE}}\approx 2\%$ and $\Delta_{\text{new}}\approx 1\%$, so $\Delta_{\text{new}}/\Delta_{\text{MSE}}\approx 0.5$.
- For $b_0\geqslant 1$, we have $\Delta_{\text{MSE}}\approx 1\%$ and $\Delta_{\text{new}}\leqslant 0.1\%$, so $\Delta_{\text{new}}/\Delta_{\text{MSE}}\leqslant 0.1$.

For details, see [1–3].

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