Propagating Range (Uncertainty) and Continuity Information Through Computations: From Real-Valued Intervals to General Sets

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1. How to Describe Quantities: From Real Values to General Sets

- Usually, the values of physical quantities are described by real numbers.
- However, some physical quantities require a more complex description:
  - some quantities are characterized by a vector (e.g., force or velocity),
  - some by a function (e.g., a current value of a field) or by a geometric shape.
- In view of this possibility, we will assume that the set S of possible values of each quantity:
  - is not necessarily a set of real numbers,
  - it can be a general set.

2. Functional Dependencies are Ubiquitous and Can Be Complex

- In many practical situations, quantities are dependent on each other.
- Often, we know a function $y = f(x_1, \ldots, x_n)$ that relates quantities $x_1, \ldots, x_n$ with a quantity y.
- In simple cases, we have an explicit expression relating x_i and y.
- In more complex cases, we have a *sequence* of such expressions
  - we first determine some intermediate quantities z_j in terms of x_i,
  - then other intermediate quantities z_k in terms of z_j,
  - ...
  - finally, y in terms of the the intermediate quantities z_j (and maybe also in terms of x_i).

3. Definition

- Let n and N be natural numbers, and let $S_1, \ldots, S_n$ be sets.
- A *computation scheme* f of length N w/n inputs is a seq. of tuples t_{n+j} $(j = 1, \ldots, N)$ each of which has:
  - a set S_{n+j};
  - a finite sequence of positive integers

$$a(j,1) < \ldots < a(j,k(j)) < n+j; \text{ and}$$

  - a function $f_{n+j} : S_{a(j,1)} \times \ldots \times S_{a(j,k(j))} \to S_{n+j}$.
- Let us select a sequence $x_1 \in S_1, \ldots, x_n \in S_n$.
- Once the values $x_1, \ldots, x_{n+j-1}$ are defined, the next value x_{n+j} is defined as $f_{n+j}(x_{a(j,1)}, \ldots, x_{a(j,k(j))})$.
- The value x_{n+N} is called the *result* $f(x_1, \ldots, x_n)$ of applying f to x_i.

4. Example

- The expression $f(x_1) = x_1 \cdot (1 - x_1)$ can be described by the following computation scheme:
  - first, we compute $x_2 = 1 - x_1$,
  - then we compute $y = x_3 = x_1 \cdot x_2$.
- In this case:
  - $S_1 = S_2 = S_3 = \mathbb{R}$,
  - on the first intermediate step, we have a function of one variable $f_2(a) = 1 - a$;
  - on the second computation step, we have a function of two variables $f_3(a, b) = a \cdot b$.

5. Intermediate Results as Functions of the Inputs

- The result of each intermediate step is a function of the inputs: $x_{n+j} = g_{n+j}(x_1, \ldots, x_n)$.
- Then, $g_{n+N}(x_1, \ldots, x_n) = f(x_1, \ldots, x_n)$.
- The function g_{n+j} appears if we "truncate" the original computation scheme on the j-th step.
- The original values $x_1, \ldots, x_n$ can also be viewed as functions of the n input variables $x_1, \ldots, x_n$:

$$g_i(x_1, \ldots, x_{i-1}, x_i, x_{i+1}, \ldots, x_n) = x_i.$$

- In terms of these functions, each computation step takes the form

$$x_{n+j} = g_{n+j}(x_1, \ldots, x_n) =$$

$$f_{n+j}(g_{a(j,1)}(x_1, \ldots, x_n), \ldots, g_{a(j,k(j))}(x_1, \ldots, x_n)).$$

6. Need to Take Uncertainty into Account

- In practice, we only have partial information about the inputs x_i.
- For each i, there is a whole set X_i of values which are consistent with our knowledge.
- In general, different values $x_i \in X_i$ lead to different values $y = f(x_1, \ldots, x_n)$.
- It is therefore desirable to find the *range* of possible values, i.e., the set

$$f(X_1, \ldots, X_n) \stackrel{\text{def}}{=} \{f(x_1, \ldots, x_n) : x_1 \in X_1, \ldots, x_n \in X_n\}.$$

- If it is difficult to compute the range, we need at least an *enclosure* $Y \supseteq f(X_1, \ldots, X_n)$ for this range.

7. Types of Sets for Describing Uncertainty

- In interval computations, we usually assume:
  - that the set S_i is the set of real numbers, and
  - that the set X_i is an interval.
- However, it is also possible that the set X_i is more general.
- The set X_i may be a multi-interval: a union of finitely many intervals.
- When S_i is a multi-dimensional Euclidean space, the set X_i can be:
  - a box (rectangular parallelepiped),
  - an ellipsoid, or
  - a more general (convex or non-convex) set.

8. Propagating Range Through Computations: Idea

- We follow the computations of $f(x_1, \ldots, x_n)$ step-by-step:
  - we start with ranges $X_1, \ldots, X_n$ of the inputs,
  - we sequentially compute the enclosures X_{n+j} for the ranges of all intermediate results,
  - finally, on the last computation step, we get the desired enclosure $Y = X_{n+N}$.
- On each intermediate step, we have a procedure $G(Y_1, \ldots, Y_m)$ that transforms:
  - enclosures Y_i for the ranges $g_{a(j,k)}(X_1, \ldots, X_n)$
  - into an enclosure for the range of the result.
- Requirement: if $Y_i \supseteq Z_i$, then

$$G(Y_1, \ldots, Y_m) \supseteq g(Z_1, \ldots, X_n).$$

9. Propagating Range Through Computations: Interval Computations as an Example

- *Parsing:* inside the computer, every algorithm consists of elementary operations ($+$, $-$, $\cdot$, min, max, etc.).
- *Interval arithmetic:* for each elementary operation $f(a,b)$,
  - if we know the intervals $\mathbf{a}$ and $\mathbf{b}$,
  - we can compute the exact range $f(\mathbf{a},\mathbf{b})$:

$$[\underline{a},\overline{a}]+[\underline{b},\overline{b}]=[\underline{a}+\underline{b},\overline{a}+\overline{b}];\quad [\underline{a},\overline{a}]-[\underline{b},\overline{b}]=[\underline{a}-\overline{b},\overline{a}-\underline{b}];$$

$$[\underline{a},\overline{a}]\cdot[\underline{b},\overline{b}]=[\min(\underline{a}\cdot\underline{b},\underline{a}\cdot\overline{b},\overline{a}\cdot\underline{b},\overline{a}\cdot\overline{b}),\max(\underline{a}\cdot\underline{b},\underline{a}\cdot\overline{b},\overline{a}\cdot\underline{b},\overline{a}\cdot\overline{b})];$$

$$\frac{1}{[\underline{a},\overline{a}]}=\left[\frac{1}{\overline{a}},\frac{1}{\underline{a}}\right]\text{ if }0\notin[\underline{a},\overline{a}];\quad \frac{[\underline{a},\overline{a}]}{[\underline{b},\overline{b}]}=[\underline{a},\overline{a}]\cdot\frac{1}{[\underline{b},\overline{b}]}.$$

- *Main idea:* replace each elementary operation in f by the corresponding operation of interval arithmetic.
- *Known result:* we get an enclosure $\mathbf{Y}\supseteq\mathbf{y}$ for the desired range.

10. Interval Computations: toy example

- The expression $f(x_1) = x_1 \cdot (1 - x_1)$ can be described by the following computation scheme:
  - first, we compute $x_2 = 1 - x_1$,
  - then we compute $y = x_3 = x_1 \cdot x_2$.
- The range $\mathbf{y} = f(\mathbf{x}_1)$ of the function $f(x_1) = x_1 \cdot (1 - x_1)$ over the interval $\mathbf{x}_1 = [0, 1]$ is $\mathbf{y} = [0, 0.25]$.
- *Straightforward interval computations:*
  - compute

    $$\mathbf{x}_2 = 1 - [0, 1] = [1, 1] - [0, 1] = [1 - 1, 1 - 0] = [0, 1],$$
  - then compute

    $$\mathbf{Y} = \mathbf{x_3} = \mathbf{x}_1 \cdot \mathbf{x}_2 = [0, 1] \cdot [0, 1] =$$

    $$[\min(0 \cdot 0, 0 \cdot 1, 1 \cdot 0, 1 \cdot 1), \max(0 \cdot 0, 0 \cdot 1, 1 \cdot 0, 1 \cdot 1)] =$$

    $$[0, 1].$$

11. Importance of Continuity Information

- In some cases, it is important to check whether a function $f(x_1, \ldots, x_n)$ is continuous.
- For example, it is useful to determine when the system of equations has a solution.
- When each range S_i is an interval, then Brouwer's fixed point theorem says that:
  - if f is a continuous function and
  $$f(S_1 \times \ldots \times S_n) \subseteq S_1 \times \ldots \times S_n,$$
  - then there exists a point
  $x = (x_1, \ldots, x_n) \in S_1 \times \ldots \times S_n$ for which $x = f(x)$.
- In other cases, it may be beneficial to know that a function is *not* continuous.
- For example, in physical applications, discontinuity may be an indication of a phase transition.

12. Propagating Continuity Information

- It is known that a composition of continuous functions is always continuous.
- This fact allows us to propagate continuity info.
- For such a propagation, on each intermediate step j, we need to keep:
  - not only the enclosure X_j for the corresponding function $g_{n+j}(x_1, \ldots, x_n)$,
  - but also an information re whether this intermediate function is continuous (c) or not (d).
- Our knowledge may be partial:
  - we may know that g_{n+j} is continuous: $C = \{c\}$;
  - we may know that g_{n+j} is discontinuous: $C = \{d\}$;
  - we may not know whether g_{n+j} is continuous or not: $C = \{c, d\}$.

13. Continuity Propagator: Precise (Formal) Definition

- Let $T_1, \ldots, T_m, Y$ be topological spaces, and let
$$g : T_1 \times \ldots \times T_m \to Y.$$
- We say that a mapping
$$p : 2^{T_1}_{\mathcal{C}} \times \{c, d\} \times \ldots \times 2^{T_m}_{\mathcal{C}} \times \{c, d\} \to \{\{c\}, \{d\}, \{c, d\}\}$$
is a *continuity propagator* corresponding to g if
  – for every topological space Z and for all functions
$$h_1 : Z \to T_1, \ldots, h_m : Z \to T_m,$$
  – once sets X_1, ..., X_m are enclosures for $h_1(Z)$, ..., $h_m(Z)$, and c_i are continuities of the functions h_i,
  – then the continuity c_h of the function
$$h(z) \stackrel{\text{def}}{=} g(h_1(z), \ldots, h_m(z))$$
is contained in the set $p(X_1, c_1, \ldots, X_m, c_m)$.

14. Discussion

- If for every i, we have $X_i \supseteq h_i(Z)$, then

$$c_h \in p(X_1, c_1, \ldots, X_m, c_m).$$

- Sometimes we do not know the continuity c_i of some of the inputs.
- Then we have to consider all possible values of these continuities:
  - if we only know the sets C_i that contain the actual (unknown) values c_i,
  - then $c_h \in p(X_1, C_1, \ldots, X_m, C_m)$, where

$$p(X_1, C_1, \ldots, X_m, C_m) \stackrel{\text{def}}{=} \bigcup_{c_i \in C_i} p(X_1, c_1, \ldots, X_m, c_m),$$

    and the union is taken over all possible combinations $c_i \in C_i$.

15. Propagating Continuity Information via Computations

- For each computation scheme f and for all inputs sets $X_1, \ldots, X_n$,
  - once we know set enclosures F_{n+j} for all the functions f_{n+j},
  - we replace each computation $f_{n+j}(x_{a(j,1)}, \ldots, x_{a(j,k(j))})$ by the corresponding computation with sets,
  - and simultaneously we compute the set C_{n+j}.
- As a result:
  - we get not only the desired enclosure $\widetilde{Y}$ for the range $f(X_1, \ldots, X_n)$,
  - we also get the continuity information C_f about the function $f(x_1, \ldots, x_n)$ s.t. $c_f \in C_f$.

16. How to Check Whether a Given Function is a Continuity Propagator?

- Our definition of a continuity propagator is that a certain property holds for all possible functions

$$h_i : Z \to X_i.$$

- Checking that some property holds for all possible functions may be difficult.
- It is therefore desirable to come up with a simpler equivalent definition.
- This equivalent definition is provided in this talk.
- To explain this new definition, we need to introduce several auxiliary notions.

17. First Auxiliary Notion: Dummy Variable

- For $g : X_1 \times \ldots \times X_m \to Y$, the i-th variable is *dummy* if the function does not depend on this variable.
- *In precise terms:* for all possible values $x_1 \in X_1, \ldots, x_{i-1} \in X_{i-1}, x_i, x'_i \in X_i, x_{i+1} \in X_{i+1}, \ldots, x_m \in X_m$, we have

$$g(x_1, \ldots, x_{i-1}, x_i, x_{i+1}, \ldots, x_m) =$$

$$g(x_1, \ldots, x_{i-1}, x'_i, x_{i+1}, \ldots, x_m).$$

- *Examples:*
  - for a constant function, all inputs are dummy variables;
  - for a function $g(x_1, x_2, x_3) = x_1^2 + x_2$, the variable x_3 is a dummy variable.
- A variable is called *essential* if it is not a dummy variable.

18. Second Auxiliary Notion: Continuously Reversible Functions

- We say that a function $g(x_1, \ldots, x_m)$ is *continuously reversible* from variables $x_{i_1}, \ldots, x_{i_k}$ to a variable x_j if:
  - given the value of $y = f(x_1, \ldots, x_n)$ and
  - given the values of these variables $x_{i_1}, \ldots, x_{i_k}$,
  - we can uniquely reconstruct the value of x_j:

$$x_j = H(y, x_{i_1}, \ldots, x_{i_k})$$

  - and the corresponding dependence H is continuous.
- *Example:* the function $f(x_1, x_2) = x_1 + x_2$ is continuously reversible with respect to each of the variables:

$$x_2 = y - x_1, \quad x_1 = y - x_2.$$

19. Main Result

- Let $g : T_1 \times \ldots \times T_m \to Y$ and
  $p : 2^{T_1}_{\mathcal{C}} \times \{c, d\} \times \ldots \times 2^{T_m}_{\mathcal{C}} \times \{c, d\} \to \{\{c\}, \{d\}, \{c, d\}\}$.
- p is a continuity propagator for g $\Leftrightarrow$ it satisfies the following 3 properties for all $X_i \subseteq T_i$ and $c_i \in \{c, d\}$:
  - if the function $g : X_1 \times \ldots \times X_m \to Y$ is continuous, then $c \in p(X_1, c, \ldots, X_m, c)$;
  - if g is cont. reversible from all the variables s.t. $c_i = c$ to one of the variables for which $c_j = d$, then
  $$d \in p(X_1, c_1, \ldots, X_m, c_m);$$
  - in all other cases, $p(X_1, c_1, \ldots, X_m, c_m) = \{c, d\}$.

20. How to Get the Narrowest Possible Enclosures for the Actual Continuity

If we want to get the narrowest possible enclosures for the actual continuity, we should take:

- if the function $g : X_1 \times \ldots \times X_m \to Y$ is continuous, then

$$p(X_1, c, \ldots, X_m, c) = \{c\};$$

- if the g is continuously reversible from all the variables for which $c_i = c$ to one of the variables for which $c_j = d$:

$$p(X_1, c_1, \ldots, X_m, c_m) = \{d\};$$

- in all other cases:

$$p(X_1, c_1, \ldots, X_m, c_m) = \{c, d\}.$$

21. Discussion

- On each computation step j, we compute

$$x_{n+j} = g_{n+j}(x_1, \ldots, x_n) =$$
$$f_{n+j}(g_{a(j,1)}(x_1, \ldots, x_n), \ldots, g_{a(j,k(j))}(x_1, \ldots, x_n)).$$

- If f_{n+j} and $g_{a(j,k)}$ (corr. to all essential variables) are continuous, then g_{n+j} is also continuous.
- If f_{n+j} is cont. reversible from the set of all cont. variables to one of the discont. variables, then g_{n+j} is discont.
- In all other cases, $C_{n+j} = \{c, d\}$: g_{n+j} can be continuous and can be discontinuous.
- *Comment:* the fact that the composition of continuous functions is continuous is well known.
- *What is new:* that in all other situations – except for cont. reversible f-s – no conclusion can be made.

22. Examples

- *Sample function:* $g(x_1, x_2) = x_1 + x_2$.
- *Example 1:* if $h_1(z)$ and $h_2(z)$ are continuous then $h(z) = g(x_1(z), x_2(z)) = h_1(z) + h_2(z)$ is continuous.
- *Proof:* straightforward.
- *Example 2:* if $h_1(z)$ is continuous and $h_2(z)$ is discontinuous, then $h(z) = h_1(z) + h_2(z)$ is discontinuous.
- *Proof:*
  - we can recover $h_2(z)$ as $h(z) - h_1(z)$;
  - this recovery function $a - b$ is continuous;
  - thus, if $h(z)$ was continuous, we could conclude that $h_2(z)$ is continuous as well – and it is not.

23. What If We Are Only Interested in Detecting Continuity?

- In many practical situations, we are only interested in knowing whether continuity can be confirmed or not.
- In such situations,
  - when the continuity cannot be confirmed,
  - we are not interested in spending time on confirming discontinuity.
- In terms of our symbols c and d, this means that we are interested only in two cases:
  - when the continuity is confirmed, i.e., when $C = \{c\}$; and
  - when the continuity has not been confirmed – but could still be, in which case $C = \{c, d\}$.
- This means that we are interested in continuity propagators whose possible values are $\{c\}$ or $\{c, d\}$.

24. Main Result: Simplified Version

- Let $g : T_1 \times \ldots \times T_m \to Y$ and

  $$p : 2^{T_1}_{\mathcal{C}} \times \{c, d\} \times \ldots \times 2^{T_m}_{\mathcal{C}} \times \{c, d\} \to \{\{c\}, \{c, d\}\}.$$

- p is a continuity propagator for $g \Leftrightarrow$ it satisfies the following 3 properties for all $X_i \subseteq T_i$ and $c_i \in \{c, d\}$:
  - if the function $g : X_1 \times \ldots \times X_m \to Y$ is continuous, then $c \in p(X_1, c, \ldots, X_m, c)$;
  - in all other cases, $p(X_1, c_1, \ldots, X_m, c_m) = \{c, d\}$.

25. How to Get the Narrowest Possible Enclosures for the Actual Continuity

If we want to get the narrowest possible enclosures for the actual continuity, we should take:

- if the function $g : X_1 \times \ldots \times X_m \to Y$ is continuous, then
$$p(X_1, c, \ldots, X_m, c) = \{c\};$$
- in all other cases:
$$p(X_1, c_1, \ldots, X_m, c_m) = \{c, d\}.$$

26. Discussion

- On each computation step j, we compute

$$x_{n+j} = g_{n+j}(x_1, \ldots, x_n) =$$

$$f_{n+j}(g_{a(j,1)}(x_1, \ldots, x_n), \ldots, g_{a(j,k(j))}(x_1, \ldots, x_n)).$$

- If f_{n+j} and $g_{a(j,k)}$ (corr. to all essential variables) are continuous, then g_{n+j} is also continuous.
- In all other cases, $C_{n+j} = \{c, d\}$: g_{n+j} can be continuous and can be discontinuous.
- *Comment:* the fact that the composition of continuous functions is continuous is well known.
- *What is new:* that in all other situations no conclusion can be made.

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