On a Theoretical Justification of The Choice of Epsilon-Inflation in PASCAL-XSC

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Abstract

In many interval computation methods, if we cannot guarantee a solution within a given interval, it often makes sense to "inflate" this interval a little bit. There exist many different "inflation" methods. The authors of PASCAL-XSC, after empirically comparing the behavior of different inflation methods, decided to implement the formula $[x^-,x^+]_\varepsilon = [(1+\varepsilon)x^- - \varepsilon\cdot x^+, (1+\varepsilon)x^+ - \varepsilon\cdot x^-]$. A natural question is: Is this choice really optimal (in some reasonable sense), or is it only an empirical approximation to the truly optimal choice?

In this paper, we show that this empirical choice can be theoretically justified. Namely, we will give two justifications:

- First, the inflation method used in PASCAL-XSC is the only inflation that is invariant w.r.t. some reasonable symmetries; and
- Second, that this inflation method is *optimal* in some reasonable sense.

1 Introduction

1.1 What is $\varepsilon-$inflation

In many interval computation methods, if we cannot guarantee a solution within a given interval, it often makes sense to "inflate" this interval a little bit. This "inflating a little bit" is called $\varepsilon-$*inflation.*

There exist many different $\varepsilon-$inflation methods (see the survey [3]): we can take $[x^-,x^+]_\varepsilon = [x^- - \varepsilon, x^+ + \varepsilon]$ $(= [x^-,x^+] + [-\varepsilon,\varepsilon])$, etc. The authors of PASCAL-XSC (see, e.g., [1]), after empirically comparing the behavior of different inflation methods, decided to implement the following formula:

$$[x^-,x^+]_\varepsilon = [(1+\varepsilon)x^- - \varepsilon\cdot x^+, (1+\varepsilon)x^+ - \varepsilon\cdot x^-] \quad (1)$$

This formula is sometimes reformulated in the equivalent form

$$[x^-,x^+]_\varepsilon = [x^-,x^+] + \varepsilon\cdot d([x^-,x^+])\cdot[-1,1], \quad (2)$$

where $d([x^-, x^+]) = x^+ - x^-$ denotes the diameter of the interval $[x^-, x^+]$.

Comment. We also need to describe what roundings we apply to the results of these operations; in PASCAL-XSC, a natural choice of roundings is made: the lower bound of the interval $[x^-, x^+]_\varepsilon$ is replaced by the nearest preceding machine number, and the upper bound by the nearest succeeding one.

1.2 The problem

Is this choice really optimal (in some reasonable sense), or is it only an empirical approximation to the truly optimal choice?

1.3 Our answer

We show that this empirical choice can be theoretically justified. Namely, we will give two justifications:

- First, the inflation (1) is the only inflation that is invariant w.r.t. some reasonable symmetries; and
- Second, that the inflation (1) is *optimal* in some reasonable sense.

2 Invariance: Motivations for the Following Definitions

2.1 Scale Invariance

Intervals often come from measurements. In this case, if we change the unit in which we measure the corresponding physical quantity (e.g., use centimeters instead of meters), all numerical values will be multiplied by a constant λ. It is natural to require that the result of the inflation operation should not depend on the choice of units.

How does replacing a unit change the inflation function $\mathbf{x} \to f(\mathbf{x})$? If we replace a unit by a one that is λ times smaller, then the quantity that was initially described by an interval $\mathbf{x}$ will be described by a new interval $\lambda \cdot \mathbf{x}$. When we inflate this interval using the original inflation f, we get the interval $f(\lambda \cdot \mathbf{x})$. This is the expression of this interval in the new units. In the old units, its expression is $\lambda^{-1} \cdot f(\lambda \cdot \mathbf{x})$. We will denote the resulting "re-scaled" inflation function $\mathbf{x} \to \lambda^{-1} \cdot f(\lambda \cdot \mathbf{x})$ by $S_\lambda(f)$.

In these terms, the inflation function f is scale invariant iff $S_\lambda(f) = f$ for all λ.

2.2 Shift Invariance and Reverse Invariance

There are two other natural symmetries:

- First, when we measure, e.g., time, we can also change the starting point; in this case, a constant will be added to all numerical values $x \to x + a$. This leads to a "shifted" inflation function $T_a(f) : \mathbf{x} \to f(\mathbf{x} + a) - a$.

- Second, if we, e.g., measure a spatial coordinate x (or an electric current), then we can reverse the direction of the axis ($x \to -x$) without changing the physical situation. This leads to the operation $R(f) : \mathbf{x} \to -f(-\mathbf{x})$.

It is natural to require that the inflation operation is invariant w.r.t. these symmetries as well, i.e., that $T_a(f) = R(f) = f$.

3 Invariance: Definitions and the Result

Definition 1.

- *By an* inflation function, *we mean a continuous function $f : I \to I$ from the set of all intervals to itself for which $\mathbf{x} \subseteq f(\mathbf{x})$ for all intervals $\mathbf{x}$, and for which $f(\mathbf{x}) \neq \mathbf{x}$ for at least one interval $\mathbf{x}$. The set of all possible inflation functions will be denoted by A.*

- *For every inflation function f, and for every $\lambda > 0$, by a* re-scaled *inflation function $S_\lambda(f)$, we mean an inflation function $\mathbf{x} \to \lambda^{-1} \cdot f(\lambda \cdot \mathbf{x})$*

- *For every inflation function f, and for every a, by a* shifted *inflation function $T_a(f)$, we mean $\mathbf{x} \to f(\mathbf{x} + a) - a$.*

- *For every inflation function f, we define a* reversed *inflation function $R(f)$ as $\mathbf{x} \to -f(-\mathbf{x})$.*

- *We say that the inflation function f is* scale-invariant *if for all λ, we have $S_\lambda(f) = f$.*

- *We say that the inflation function f is* shift-invariant *if for all a, we have $T_a(f) = f$.*

- *We say that the inflation function f is called* reverse-invariant *if we have $R(f) = f$.*

Theorem 1. *For an inflation function f, the following two conditions are equivalent to each other:*

- *f is scale-invariant, shift-invariant, and reverse-invariant;*

- *f is described by the expression* (1) *for some $\varepsilon > 0$.*

Comments.

- In other words, if the optimality criterion is invariant w.r.t. natural symmetries, then the optimal inflation function coincides with one of the functions (1).

- Due to this theorem, inflation operations that are different from (1) are thus not invariant. For example, the inflation $[x^-, x^+]_\varepsilon = [x^- - \varepsilon, x^+ + \varepsilon]$ mentioned in Section 1 is not scale-invariant.

- In this section, we have considered *exact* interval operations, i.e., operations that use intervals whose endpoints can be arbitrary real numbers (not necessarily representable in the computer). Since this paper is motivated by the implementation of $\varepsilon-$inflation in Pascal-XSC, it is worth mentioning that invariances do not hold for most *rounded* inflation operations.

  Indeed, if we only consider numbers that can be represented in a computer, then we have to consider numbers of the type $k \cdot 2^{-N}$ (where N is the maximal numbers of binary digits after a binary point that can be represented in the computer). Hence, the width $\mathrm{w}(\mathbf{x})$ of each rounded interval $\mathbf{x}$ is also a number of this type. Let f be a scale-invariant inflation function from rounded intervals to rounded intervals for which $f([0,1]) \neq [0,1]$. Then, the width $w_0 = \mathrm{w}(f([0,1]))$ of the resulting interval $f([0,1])$ is greater than 1. From scale invariance, it follows that the width w_0' of the interval $f([0, 1-2^{-N}]) = (1-2^{-N}) \cdot f([0,1])$ is equal to $w_0(1-2^{-N})$. Both widths w_0 and w_0' are multiples of 2^{-N} and thus, their difference $w_0 \cdot 2^{-N}$ must also be a multiple of 2^{-N}. Hence, the width $w_0 > 1$ must be an integer. Thus, $w_0 \geq 2$, i.e., after the operation f every interval becomes at least twice wider than before. However, as the very term "$\varepsilon-$inflation" indicates, this inflation is about increasing the widths of the intervals *a little bit*, and *not* about making every interval twice wider. Thus, scale-invariant operations on rounded intervals are *not* $\varepsilon-$inflations. We can reformulate this conclusion by saying that *$\varepsilon-$inflations are not invariant for rounded intervals.*

4 Optimality: Motivations for the Following Definitions

4.1 What is "Optimality Criterion"?

When we say that some *optimality criterion* is given, we mean that, given two different inflation functions, we can decide whether the first one is better, or that the second one is better, or that these functions are equivalent w.r.t. the given criterion. In mathematical terms, this means that we have a *pre-ordering relation* $\preceq$ on the set of all possible inflation functions.

4.2 We Want to Solve an Ambitious Problem: Enumerate all Inflation Functions that are Optimal Relative to some Natural Criteria

One way to approach the problem of choosing the "best" inflation function is to select *one* optimality criterion, and to find an inflation function that is the best with respect to this criterion. The main drawback of this approach is that there can be different optimality criteria, and they can lead to different optimal solutions. It is, therefore, desirable not only to describe an inflation function that is optimal relative to some criterion, but to describe *all* inflation functions that can be optimal relative to different natural criteria[1]. In this paper, we are planning to implement exactly this more ambitious task.

4.3 Examples of Optimality Criteria

Pre-ordering is the general formulation of optimization problems in general, not only of the problem of choosing an inflation function. In general optimization theory, in which we are comparing arbitrary *alternatives* a, b, ..., from a given set A, the most frequent case of such a pre-ordering is when a *numerical criterion* is used, i.e., when a function $J : A \to R$ is given for which $a \preceq b$ iff $J(a) \le J(b)$.

Several natural numerical criteria can be proposed for choosing the inflation functions: For example, $\varepsilon-$inflation is often used in an iterative algorithm that finds an interval vector $\mathbf{X}$ such that a given interval function $\mathbf{F}$ maps this interval vector $\mathbf{X}$ into itself (see, e.g., [2]). The faster we reach such an interval, the better. Therefore, as an optimality criterion, we can, e.g., choose the *average* number of iterations that lead to such "fixed point" vector $\mathbf{X}$ (average in the sense of some natural probability measure on the set of all problems).

Alternatively, we can fix a class of the problem, and take the largest number of iterations for problems of this class as the desired (numerical) optimality criterion.

Many other criteria of this type can be (and have actually been) proposed. For such "worst-case" optimality criteria, it often happens that there are several different alternatives that perform equally well in the worst case, but whose performance differ drastically in the average cases. In this case, it makes sense, among all the alternatives with the optimal worst-case behavior, to choose the one for which the average behavior is the best possible. This very natural idea leads to the optimality criterion that is not described by a numerical optimality

[1] In this phrase, the word "natural" is used informally. We basically want to say that from the purely mathematical viewpoint, there can be weird ("unnatural") optimality criteria. In our text, we will only consider criteria that satisfy some requirements that we would, from the common sense viewpoint, consider reasonable and natural.

criterion $J(a)$: in this case, we need *two* functions: $J_1(a)$ describes the worst-case behavior, $J_2(a)$ describes the average-case behavior, and $a \preceq b$ iff either $J_1(a) < J_2(b)$, or $J_1(a) = J_1(b)$ and $J_2(a) \leq J_2(b)$.

We could further specify the described optimality criterion and end up with *a* natural criterion. However, as we have already mentioned, the goal of this paper is not to find *an* inflation function that is optimal relative to some criterion, but to describe *all* inflation functions that are optimal relative to some natural optimality criteria. In view of this goal, in the following text, we will not specify the criterion, but, vice versa, we will describe a very general class of *natural* optimality criteria.

So, let us formulate what "natural" means.

Comment[2]. When we say that a criterion is natural, we use the word "natural" in its commonsense meaning. The fact that a criterion is "natural" in this sense does not necessarily means that the selected inflation function is any good. For example, at first glance, it may seem natural to select an inflation function for which the width of the inflated interval is the smallest possible. However, as one can easily see, this seemingly natural criterion leads to the trivial "inflation" function $f(\mathbf{x}) = \mathbf{x}$ that does not change the intervals at all.

4.4 What Optimality Criteria are Natural?

We have already mentioned that intervals often come from measurements, and that for such intervals, if we change the unit in which we measure the corresponding physical quantity (e.g., use centimeters instead of meters), all numerical values will be multiplied by a constant λ. It is natural to require that the relative quality of two inflation methods do not depend on the choice of units. In other words, we require that if f is better than g, then the "re-scaled" f (i.e., $S_\lambda(f)$) should be better than the "re-scaled" g (i.e., that $S_\lambda(g)$).

It is also natural to require that the optimality criterion is invariant w.r.t. shift- and reverse transformations. In other words, if f is better than g, then it is natural to require that $T_a(f)$ be better than $T_a(g)$, and that $R(f)$ be better than $R(g)$.

There is one more reasonable requirement for a criterion, that is related with the following idea: If the criterion does not select a single optimal inflation, i.e., if it considers several different inflation functions equally good, then we can always use some other criterion to help select between these "equally good" ones, thus designing a two-step criterion. If this new criterion still does not select a unique inflation, we can continue this process until we arrive at a combination multi-step criterion for which there is only one optimal inflation function. Therefore, we can always assume that our criterion is *final* in this sense.

[2]We are thankful to the anonymous referee for this comment.

5 Definitions and the Main Result

Definition 2. *By an optimality criterion, we mean a pre-ordering (i.e., a transitive reflexive relation) $\preceq$ on the set A. An optimality criterion $\preceq$ is called:*

- *scale-invariant if for all f, g, and λ, $f \preceq g$ implies $S_\lambda(f) \preceq S_\lambda(g)$.*
- *shift-invariant if for all f, g, and a, $f \preceq g$ implies $T_a(f) \preceq T_a(g)$.*
- *reverse-invariant if for all f and g, $f \preceq g$ implies $R(f) \preceq R(g)$.*
- *invariant if it is shift-invariant, scale-invariant, and reverse-invariant.*
- *final if there exists one and only one inflation function f that is preferable to all the others, i.e., for which $g \preceq f$ for all $g \neq f$.*

Theorem 2.

- *If an inflation function f is optimal w.r.t. some invariant and final optimality criterion, then for some $\varepsilon > 0$, the function f is described by a formula* (1)*.*
- *For every $\varepsilon > 0$, there exists an invariant and final optimality criterion for which the only optimal inflation function is the expression* (1) *that corresponds to this ε.*

Comment. In other words, if the optimality criterion satisfies the above-described natural properties, then the optimal inflation function coincides with one of the functions (1). (For different optimality criteria, optimal inflation functions may correspond to different values of ε.)

6 Proofs

6.1 Proof of Theorem 1

1. The fact that for every $\varepsilon > 0$, the formula (1) describes a scale-, shift-, and reverse-invariant inflation function, easily follows from its reformulation in the form (2).

2. Let us now show that every invariant inflation function f is of the form (1).

2.1. Let us first apply the property that f is *reverse* invariant to the interval $[-1, 1]$. For reverse invariance, $[R(f)](\mathbf{x}) = -f(-\mathbf{x})$. Therefore, the fact that f is reverse invariant means that

$$[R(f)]([-1,1])) = -f(-[-1,1]) = f([-1,1]).$$

Let us denote the interval $f([-1,1])$ by $\mathbf{a} = [a^-, a^+]$. We know that $-[-1,1] = [-1,1]$. Therefore, from the above equality, we conclude that

$$-f(-[-1,1]) = -f([-1,1]) = f([-1,1]),$$

or, in other words, that $-[a^-, a^+] = [a^-, a^+]$. This, in its turn, leads to $a^- = -a^+$; so, $f([-1, 1]) = [-a^+, a^+]$.

By definition of an inflation function, we must have $\mathbf{x} \subseteq f(\mathbf{x})$ for all $\mathbf{x}$. In particular, for $\mathbf{x} = [-1, 1]$, we have $[-1, 1] \subseteq [-a^+, a^+]$. This inclusion is equivalent to $a^+ \geq 1$. If we denote the half $(1/2)(a^+ - 1)$ of the difference $a^+ - 1$ by $\varepsilon \geq 0$, we will be able to conclude that $f([-1, 1]) = [-(1+2\varepsilon), 1+2\varepsilon]$. This formula can be easily reformulated as

$$f([-1, 1]) = [(1 + \varepsilon) \cdot (-1) - \varepsilon \cdot (+1), (1 + \varepsilon) \cdot (+1) - \varepsilon \cdot (-1)]. \qquad (3)$$

This formula is a particular case of the formula (1) for $x^- = -1$ and $x^+ = +1$.

2.2. Let us now show that for every $c > 0$, the interval $f([-c, c])$ can also be described by the formula (1).

To prove this fact, we will use *scale invariance* of the inflation function f. Scale invariance means that

$$[S_\lambda(f)](\mathbf{x}) = f(\mathbf{x})$$

for all $\lambda > 0$ and for all intervals $\mathbf{x}$. In other words,

$$\lambda^{-1} \cdot f(\lambda \cdot \mathbf{x}) = f(\mathbf{x}),$$

and, therefore,

$$f(\lambda \cdot \mathbf{x}) = \lambda \cdot f(\mathbf{x}).$$

Let us take $\mathbf{x} = [-1, 1]$ and $\lambda = c$. Then, $\lambda \cdot \mathbf{x} = c \cdot [-1, 1] = [-c, c]$, and we can conclude that $f([-c, c]) = c \cdot f([-1, 1])$. Substituting the above expression (3) for $f([-1, 1])$ into this formula, we conclude that

$$f([-c, c]) = c \cdot [(1 + \varepsilon) \cdot (-1) - \varepsilon \cdot (+1), (1 + \varepsilon) \cdot (+1) - \varepsilon \cdot (-1)] =$$

$$[(1 + \varepsilon) \cdot (-c) - \varepsilon \cdot (+c), (1 + \varepsilon) \cdot (+c) - \varepsilon \cdot (-c)]. \qquad (4)$$

The formula (1) is thus proven for symmetric intervals $[-c, c]$.

2.3. Finally, let us prove that the formula (1) is true for an *arbitrary* interval $[x^-, x^+]$.

To prove this statement, we will use *shift-invariance* of the inflation function f. This shift-invariance means that for every real number a, we have

$$[T_a(f)](\mathbf{x}) = f(\mathbf{x})$$

for all a and for all intervals $\mathbf{x}$. In other words,

$$f(\mathbf{x} + a) - a = f(\mathbf{x}).$$

Let us take $a = -(x^- + x^+)/2$. Then, $\mathbf{x} + a = [-(x^+ - x^-)/2, (x^+ - x^-)/2]$ is a symmetric interval, with $c = (x^+ - x^-)/2$, and therefore, according to (4),

$$f(\mathbf{x} + a) = f([-c, c]) = [(1 + \varepsilon) \cdot (-c) - \varepsilon \cdot (+c), (1 + \varepsilon) \cdot (+c) - \varepsilon \cdot (-c)].$$

Hence,

$$f(\mathbf{x}) = f(\mathbf{x}+a) - a = [(1+\varepsilon)\cdot(-c) - \varepsilon\cdot(+c) - a, (1+\varepsilon)\cdot(+c) - \varepsilon\cdot(-c) - a].$$

Substituting $a = -(x^- + x^+)/2$ and $c = (x^+ - x^-)/2$ into this formula, we can easily get the desired expression (1). Q.E.D.

Comment. In this theorem, we, crudely speaking, described all scale-, shift-, and reverse-invariant functions from intervals into intervals. A similar description has already been obtained (in slightly different terms) in [4, 5].

6.2 Proof of Theorem 2

1. To prove the first part of Theorem 2, we will show that the optimal inflation function $f_{\rm opt}$ is scale-invariant, shift-invariant, and reverse-invariant, i.e., that $S_\lambda(f_{\rm opt}) = T_a(f_{\rm opt}) = R(f_{\rm opt}) = f_{\rm opt}$ for all λ and a. Then, the result will follow from Theorem 1.

Indeed, let X be one of these transformations. Let us first show that each of these transformations is invertible, i.e., that the inverse transformation X^{-1} exists. Indeed:

- if $X = S_\lambda$, then $X^{-1} = S_{1/\lambda}$;
- if $X = T_a$, then $X^{-1} = T_{-a}$;
- if $X = R$, then $X^{-1} = X = R$.

Now, from the optimality of $f_{\rm opt}$, we conclude that for every $g \in A$, $X^{-1}(g) \preceq f_{\rm opt}$. From the invariance of the optimality criterion, we can now conclude that $g \preceq X(f_{\rm opt})$. This is true for all $g \in A$ and therefore, the inflation function $X(f_{\rm opt})$ is optimal. But since the criterion is final, there is only one optimal inflation function; hence, $X(f_{\rm opt}) = f_{\rm opt}$. In other words, $[X(f_{\rm opt})](\mathbf{x}) = f_{\rm opt}(\mathbf{x})$ for every interval $\mathbf{x}$. So, the optimal inflation function is indeed invariant and hence, due to Theorem 1, it coincides with one of the expressions (1). The first part is proven.

2. Let us now prove the second part of Theorem 2. Let $\varepsilon > 0$ be fixed, and let f_ε be the inflation operation (1). We will then define the optimality criterion as follows: $f \preceq g$ iff g is equal to this f_ε.

Since the inflation function f_ε is scale-invariant, shift-invariant, and reverse-invariant, thus defined optimality criterion is also scale-invariant, shift-invariant, and reverse-invariant. It is also clearly final. The inflation function f_ε is clearly optimal w.r.t. this invariant and final optimality criterion. Q.E.D.

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