

INTERVAL MATHEMATICS AS A POTENTIAL WEAPON AGAINST UNCERTAINTY

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SUMMARY

This chapter is devoted to introducing the *theories of interval algebra* to people who are interested in applying the interval methods to *uncertainty analysis* in science and engineering. In view of this purpose, we shall introduce the key concepts of the algebraic theories of intervals that form the foundations of the interval techniques as they are now practised, provide a historical and epistemological background of interval mathematics and uncertainty in science and technology, and finally describe some typical applications that clarify the need for interval computations to cope with uncertainty in a wide variety of scientific disciplines.

Keywords • Interval mathematics, Uncertainty, Quantitative Knowledge, Reliability, Complex interval arithmetic, Machine interval arithmetic, Interval automatic differentiation, Computer graphics, Ray tracing, Interval root isolation.

MSC: 65G30, 03E20, 26E25

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1 INTRODUCTION: CAN WE KNOW ABOUT THE WORLD?

Are we imprisoned in *Descartes' dualism*? That is, are we stuck between two worlds: the world of physical reality and the world of mental reasoning? The answer may be: “*Yes, we are*”. Moreover, does the way, in which we learn about the physical world, meet our persistent seeking for deterministic scientific knowledge? With the fact that the machinery we employ to acquire our knowledge about the world is not absolute, the answer to this question may be negative. So, how can we get certain knowledge about the world? Heidegger¹ adds another version of this dilemma by claiming that the question should not be only about how we acquire knowledge about the world, but also we should ask: “*How does the world reveal itself to us through our encounters with it?*” [HEIDEGGER, 1962].

In many cases, we can definitely achieve *qualitative* knowledge with absolute certainty, but *quantitative* knowledge, about the present and future of the physical world, is completely different: quantitative knowledge is acquired through intuition, experiments, measurements, and proposed hypotheses². That is, quantitative inquiries can be regarded as the main source of uncertainty, and therefore our whole

¹ Martin Heidegger (1889–1976) was a German philosopher known for his work in phenomenology and existentialism.

² The terms “*hypothesis*” and “*theory*” are used here to mean “*scientific hypothesis*” and “*scientific theory*”, respectively. Each of the two terms is used in a different sense in mathematical logic.

knowledge cannot be completely certain. Pascal³, within this dilemma, says, in [PASCAL, 1995]: “*We sail within a vast sphere, ever drifting in uncertainty, driven from end to end*”. At this point, a crucial question should be posed: Is uncertainty *anti-knowledge* or *pro-knowledge*? Hoppe⁴, in his article “*On Certainty and Uncertainty*” [HOPPE, 1997], gives us a way out from this dilemma by a brilliant mental experiment. He begins his article by saying:

“It is possible to imagine a world characterized by complete certainty. All future events and changes would be known in advance and could be predicted precisely. There would be no errors and no surprises. We would know all of our future actions and their future outcomes. In such a world, nothing could be learned, and accordingly, nothing would be *worth knowing*. Indeed, the possession of consciousness and knowledge would be *useless*. For why would anyone want to know anything if all future actions and events were completely predetermined and it would not make any difference for the future course of events whether or not one possessed this or any knowledge? Our actions would be like those of an automaton, and an automaton has no need of any knowledge. Thus, rather than representing a state of *perfect knowledge*, complete certainty actually *eliminates* the value of all knowledge.”

Thus uncertainty is *pro-knowledge*, not *anti-knowledge*. Obviously, our scientific knowledge is not perfect and we commit errors. But, indeed, we can grasp, measure, and correct our errors, and develop ways to deal with uncertainty. All of these add to our knowledge and make it valuable. Knowledge is not the absolute certainty. Knowledge, however, is the tools we develop to purposely get better and better outcomes through our learning about the world. In other words, uncertainty should always exist; for us to develop the weapons against it. This understanding of “*what knowledge is*” coincides with our understanding of “*what science is*”. Popper⁵, in [POPPER, 2002], uses the notion of *falsification* as a *criterion of demarcation* to distinguish between those theories that are scientific and those that are unscientific, that is, “*a theory is scientific if, and only if, it is falsifiable*”.

Scientific knowledge is thus not perfect exactitude: it is learning with uncertainty, not eliminating it. There are many approaches that enable us to deal with uncertainty and get reliable knowledge about the world. As examples of these approaches, we can mention: *probabilization*, *fuzzification*, *anglification*, and *intervalization*. For the great degree of reliability it provides, intervalization is usually a part of all other methods that deal with uncertainty. Whenever *uncertainty* exists, there is always a need for *interval computations*. Intervals arise naturally in a wide variety of disciplines that deal with uncertain data, including physical measurements, expert estimations, numerical approximations, tolerance problems, economical predictions, quality control techniques, sensitivity analysis, robustness measures of robotic systems, and many others. Thus, because of these, and because of its great importance in many practical applications, this chapter is devoted to introduce how to cope with uncertainty through interval mathematics.

The eight sections of the chapter are organized as follows. This introductory section has provided a philosophical perspective on the dilemma of knowledge and uncertainty. Section 2 describes briefly the ways to acquire knowledge about real-world systems, how error and uncertainty threaten our inquiries about the world, and finally how to get reliable knowledge about the world through interval mathematics. Section 3 gives a historical perspective of the field of interval mathematics. Section 4 is devoted to introducing the key concepts of the *classical interval theory* and the fundamental properties of its algebraic system. In section 5, we provide a bit of perspective on the algebraic system of *machine interval arithmetic* and some of its fundamental properties. In section 6, we give

³ Blaise Pascal (1623-1662) was a French mathematician, physicist, and philosopher.

⁴ Hans-Hermann Hoppe is an Austrian economist and libertarian anarcho-capitalist philosopher.

⁵ Karl Raimund Popper (1902-1994) was an Austro-British philosopher. He is regarded as one of the greatest philosophers of science of the 20th century.

a formulation of the notion of *interval dependency*, and then briefly mention some *alternate interval theories*. Section 7 describes three typical applications that clarify the need for interval computations to cope with uncertainty in science and engineering: *interval estimates of the image of real functions*, *interval automatic differentiation*, and *interval methods in computer graphics*. Finally, the chapter closes with section 8, which provides a view to the future of the interval theory, a concluding look ahead, and further information resources.

2 INTERVALS, ERRORS, AND UNCERTAINTIES

Scientists are, all the time, in a struggle with *error* and *uncertainty*. Uncertainty is the quantitative estimation of errors present in measured data; all measurements contain some uncertainty generated through many types of error. Error (“*mistaken result*”, or “*mistaken outcome*”) is common in all scientific practice, and is always a serious threat to the search for a trustworthy scientific knowledge and to reliable epistemic foundations of science. This section is intended to provide a bit of motivation and perspective about the field of interval arithmetic, and how it is a potential weapon against uncertainty in science and technology (For further background, the reader may consult, e.g., [ALLCHIN, 2000A], [ALLCHIN, 2000B], [DAWOOD, 2011], [DAWOOD, 2012], and [KREINOVICH, 2008]).

2.1

Is Our Scientific Knowledge in Jeopardy?

In 1597, Sir Francis Bacon defined science as “*the process used everyday to logically complete thoughts through inference of facts determined by calculated experiments*”. The epistemology of scientific knowledge, that is the study of how scientific knowledge is acquired, tells us that in all scientific and engineering disciplines, our knowledge of real-world systems (which can be physical, chemical, biological, economical, social, and so forth) is acquired through *observing*, *experimenting*, *measuring identifiable features*, and *formulating hypotheses* with the aid of formal reasoning. In their way to acquire this knowledge, scientists and engineers always perform one or both of the following two inquiries:

- **Present-State Inquiry.** To quantify an identifiable property ρ that provides some information about the present state of the real-world system.
- **Future-State Inquiry.** To quantify an identifiable property τ that provides some information about a future state of the real-world system.

In most practical problems, the properties ρ and τ are not directly identifiable, that is, they are not quantifiable by direct measurements or expert estimations. However, we usually know a *present-state function* (or *algorithm*) p that relates the present property ρ to some quantifiable auxiliary properties x_1, \dots, x_m , and a *future-state function* (or *algorithm*) f that relates the future property τ to some quantifiable auxiliary properties y_1, \dots, y_n . So, to quantify the properties ρ and τ , we *measure* or *estimate* the related quantifiable auxiliary properties, and then apply the known present-state and future-state functions

$$\begin{aligned}\rho &= p(x_1, \dots, x_m), \\ \tau &= f(y_1, \dots, y_n).\end{aligned}$$

At this point the crucial question is: *Do measurements or expert estimations provide reliable information about the quantifiable properties?* The answer is: “*Unfortunately, no*”. In practical situations, uncertainty naturally arises when processing values which come from *measurements* or from *expert estimations*. From both the *epistemological* and *physical* viewpoints, neither measurements nor expert estimations can be exact for the following reasons:

- The actual value of the measured quantity is a real number; so, in general, we need *infinitely* many bits to describe the exact value, while after every measurement, we gain only a *finite* number of bits of information (e.g., a finite number of binary digits in the binary expansion of the number).
- There is always some difficult-to-delete noise which is mixed with the measurement results.
- Expert estimates cannot be absolutely exact, because an expert generates only a finite amount of information.
- Experts are usually even less accurate than are measuring instruments.

In addition to measurement and expert estimation errors, there are types of error that arise when doing computations with the measured or estimated values. There are usually three sources of error while performing numerical computations with real numbers:

- **Input Errors.** Input errors usually arise from human mistakes. An input error is committed when a human inputs to a machine a wrong value for the measured or estimated quantity.
- **Truncation Errors.** Truncation errors arise when replacing a continuous or infinite operation by a computable discrete operation.
- **Rounding Errors.** Rounding errors arise when doing arithmetic on a machine. This error is the difference between the result obtained using exact arithmetic and the result computed using finite precision arithmetic.

All of these uncertainties, generated through many types of error, threaten our inquiries about the world, and a mistaken outcome is always a concern in scientific research. That is, our scientific knowledge and its epistemic foundations may be in jeopardy.

2.2

Scientific Reliability with Intervals

Interval arithmetic (also known as “*interval mathematics*”, “*interval analysis*”, and “*interval computation*”) is an arithmetic defined on sets of real intervals, rather than sets of real numbers. It specifies a precise method for performing arithmetic operations on closed intervals (*interval numbers*). The concept is simple: in the interval number system, each interval number represents some fixed real number between the *lower* and *upper endpoints* of the closed interval. So, an interval arithmetic operation produces two values for each result. The two values correspond to the lower and upper endpoints of the resulting interval such that the true result certainly lies within this interval, and the *accuracy* of the result is indicated by the *width* of the resulting interval.

As a result of error, we all the time have to face situations in which scientific measurements give *uncertain values*. Let x be a real number whose value is uncertain, and assume a measurement gives adequate information about an acceptable range, $\underline{x} \leq x \leq \bar{x}$, in which the true value of x is estimated to lie. The closed interval (interval number),

$$[\underline{x}, \bar{x}] = \{x \in \mathbb{R} | \underline{x} \leq x \leq \bar{x}\},$$

is called the “*interval of certainty*” (or the “*interval of confidence*”) about the value of x . That is, we are certain that the true value of x lies within the interval $[\underline{x}, \bar{x}]$.

If it is the case that $\vec{x}_n = \langle x_1, x_2, \dots, x_n \rangle$ is a *multidimensional quantity (real-valued vector)* such that for each x_i there is an interval of certainty $X_i = [\underline{x}_i, \bar{x}_i]$, then the quantity \vec{x}_n has an “*n-dimensional parallelootope of certainty*”, \mathcal{X}_n , which is the Cartesian product of the intervals X_1, X_2, \dots, X_n .

Figure 1 illustrates the case $n = 2$; with $\vec{x}_2 = \langle x_1, x_2 \rangle$, $x_1 \in [\underline{x}_1, \bar{x}_1]$, $x_2 \in [\underline{x}_2, \bar{x}_2]$, and \mathcal{X}_2 is a rectangle of certainty.

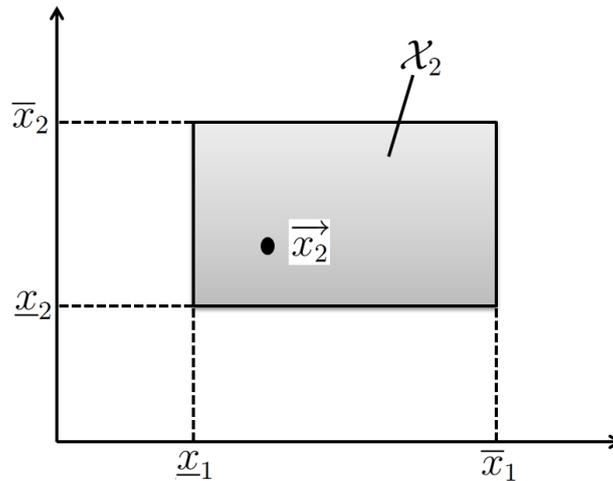


FIGURE 1. A 2-dimensional parallelotope of certainty.

Thus, interval arithmetic keeps track of all error types simultaneously, because an interval arithmetic operation produces an *interval of certainty* within which the true *real-valued* result is guaranteed to lie. To illustrate this, we give two numerical examples.

EXAMPLE 2.1.

The Archimedes's constant, π , is an irrational number, which means that its value cannot be expressed exactly as a fraction. Consequently, it has no certain decimal representation because its decimal representation never ends or repeats. Since $314 \times 10^{-2} \leq \pi \leq 315 \times 10^{-2}$, the number π can be represented as the interval number

$$[\underline{\pi}, \bar{\pi}] = [314 \times 10^{-2}, 315 \times 10^{-2}].$$

That is, we are certain that the true value of π lies within the interval $[\underline{\pi}, \bar{\pi}]$ whose width indicates the maximum possible error,

$$\begin{aligned} \text{Error} &= \text{width}([\underline{\pi}, \bar{\pi}]) \\ &= \bar{\pi} - \underline{\pi} \\ &= 315 \times 10^{-2} - 314 \times 10^{-2} \\ &= 10^{-2}. \end{aligned}$$

EXAMPLE 2.2.

Suppose two independent scientific measurements give different uncertain results for the same quantity q . One measurement gives $q = 1.4 \pm 0.2$. The other gives $q = 1.5 \pm 0.2$. These uncertain values of q can be represented as the interval numbers $X = [1.2, 1.6]$ and $Y = [1.3, 1.7]$, respectively. Since q lies in both, it certainly lies in their intersection $X \cap Y = [1.3, 1.6]$. So, if $X \cap Y \neq \emptyset$, we can get a better (tighter) “interval of certainty”. If not, we can be certain that at least one of the two measurements is wrong.

In section 4, we shall present a more formal description of the mathematical foundations of interval arithmetic, along with more advanced examples being provided.

2.3

Rediscovering the World through Intervalization

Let us revisit the uncertainty problem that we discussed in section 2.1, that of acquiring knowledge about the real world. When applying traditional numerical methods to estimate the error in the measurable auxiliary properties x_1, \dots, x_m and y_1, \dots, y_n , we get approximate (*non-guaranteed*) bounds to the measurement errors that are, in many cases, *not sufficient*. Moreover, we sometimes face situations in which the probability distribution for the measurement errors cannot be determined, and consequently *probabilization* is not valid. Furthermore, in some practical situations, fuzzifying the problem suffers from many limitations, and therefore the efficacy of *fuzzification*, in such situations, is questionable.

Now, let us *intervalize* the problems of inquiring the present and future states of a real-world system. We can measure or estimate the *quantifiable* auxiliary properties x_1, \dots, x_m and y_1, \dots, y_n . With intervals at hand, we have *intervals of certainty* X_i and Y_k for the auxiliary properties x_i and y_k respectively. Knowing the present-state function p and the future-state function f that relate the *directly-unquantifiable* present property ρ and future property τ to their auxiliary properties x_i and y_k respectively, we need to compute the images of X_i and Y_k with respect to the functions p and f . These images are defined and denoted by

$$\begin{aligned} I_p(X_1, \dots, X_m) &= \{\rho \in \mathbb{R} \mid (\exists_{i=1}^m x_i \in X_i) (\rho = p(x_1, \dots, x_m))\}, \\ I_f(Y_1, \dots, Y_n) &= \{\tau \in \mathbb{R} \mid (\exists_{k=1}^n y_k \in Y_k) (\tau = f(y_1, \dots, y_n))\}. \end{aligned}$$

The functions p and f are usually continuous, and therefore the images are in turn real closed intervals. That is, there are intervals of certainty $[\underline{\rho}, \bar{\rho}]$ and $[\underline{\tau}, \bar{\tau}]$ within which the desirable values of the properties ρ and τ are guaranteed to lie respectively.

It is thus natural to think of extending the ordinary arithmetic on *real-valued* quantities to *interval-valued* quantities in such a way that we can do arithmetic on the intervals X_i and Y_k to get, respectively, the intervals $[\underline{\rho}, \bar{\rho}]$ and $[\underline{\tau}, \bar{\tau}]$ as results (This arithmetic of intervals is described in section 4). So, the uncertainty problem of inquiring about real-world systems is now the problem of *interval evaluation of the image of real-valued functions*, which is also the *main problem of interval computations*. There are many interval methods and algorithms that successfully compute useful narrow bounds to the accurate image (the desirable *interval of certainty*). In section 7.1, we shall discuss some of these techniques.

3 INTERVAL ARITHMETIC: A HISTORY AGAINST UNCERTAINTY

The term “*interval arithmetic*” is reasonably recent: it dates from the 1950s, when the works of Paul S. Dwyer, R. E. Moore, R. E. Boche, S. Shayer, and others made the term popular (see, [Dwyer, 1951], [Moore, 1959], [Boche, 1963], and [Shayer, 1965]). But the notion of calculating with intervals is not completely new in mathematics: in the course of history, it has been invented and re-invented several times, under different names, and never been abandoned or forgotten. The concept has been known since the third century BC, when Archimedes used guaranteed lower and upper bounds to compute his constant, π (see [Archimedes, 2002]).

Early in the twentieth century, the idea seemed to be rediscovered. A form of interval arithmetic perhaps first appeared in 1924 by J. C. Burkill in his paper “*Functions of Intervals*” ([Burkill, 1924]), and in 1931 by R. C. Young in her paper “*The Algebra of Many-Valued Quantities*” ([Young, 1931]) that gives rules for calculating with intervals and other sets of real numbers; then later in 1951 by P. S. Dwyer in his book “*Linear computations*” ([Dwyer, 1951]) that discusses, in a heuristic manner, certain methods for performing basic arithmetic operations on real intervals, and in 1958 by T. Sunaga in his book “*Theory of an Interval Algebra and its Application to Numerical Analysis*” ([Sunaga, 1958]).

However, it was not until 1959 that new formulations of interval arithmetic were presented. Modern developments of the interval theory began in 1959 with R. E. Moore's technical report "*Automatic Error Analysis in Digital Computation*" ([MOORE, 1959]) in which he developed a number system and an arithmetic dealing with closed real intervals. He called the numbers "*range numbers*" and the arithmetic "*range arithmetic*" to be the first synonyms of "*interval numbers*" and "*interval arithmetic*". Then later in 1962, Moore developed a theory for exact or infinite precision interval arithmetic in his very influential dissertation titled "*Interval Arithmetic and Automatic Error Analysis in Digital Computing*" ([MOORE, 1962]) in which he used a modified digital (*rounded*) interval arithmetic as the basis for automatic analysis of total error in a digital computation. Since then, thousands of research papers and numerous books have appeared on the subject.

Interval arithmetic is now a broad field in which rigorous mathematics is associated with scientific computing. The connection between computing and mathematics provided by intervals makes it possible to solve problems that cannot be efficiently solved using floating-point arithmetic and traditional numerical approximation methods. Today, the interval methods are becoming rapidly popular as a prospective weapon against uncertainties in measurements and errors of numerical computations. Nowadays, interval arithmetic is widely used and has numerous applications in scientific and engineering disciplines that deal intensely with *uncertain data* (or *range data*). Practical application areas include electrical engineering, structure engineering, control theory, remote sensing, quality control, experimental and computational physics, dynamical and chaotic systems, celestial mechanics, signal processing, computer graphics, robotics, and computer-assisted proofs (In section 7, we shall discuss, in some detail, a number of typical applications of the interval techniques).

4 THE CLASSICAL THEORY OF INTERVAL ALGEBRA

A very simple and natural idea is that of enclosing real numbers in real closed intervals. Based on this idea, interval mathematics is constructed. This section is devoted to introducing the key concepts of the *classical interval theory* and the fundamental properties of its algebraic system (For further details, the reader may consult, e.g., [DAWOOD, 2011], [DAWOOD, 2012], [JAULIN ET AL., 2001], [MOORE, 1962], [MOORE ET AL., 2009], and [SHAYER, 1965]). Hereafter and throughout this chapter, the machinery used, and assumed priori, is the *standard (classical)* predicate calculus and axiomatic set theory. Moreover, elementary facts about operations and relations on the *real numbers* are usually used without explicit reference.

Most of our *interval-theoretic* notation is standard, and notational conventions are characterized, in detail, on their first occurrence. However, for the purpose of legibility, we give here a consolidated list of some basic *logical* and *set-theoretic* symbols, that we shall use in formulating this section and the succeeding sections of this chapter. These symbols include \Leftrightarrow (*equivalence*), \Rightarrow (*implication*), \vee (*inclusive disjunction*), \wedge (*conjunction*), \neg (*negation*), \forall (*universal quantifier*), \exists (*existential quantifier*), $\wp(\mathcal{S})$ (*The powerset of a set \mathcal{S}*), and $\mathcal{S}^{(n)}$ (*The n -th Cartesian power of a set \mathcal{S}*).

4.1

Algebraic Operations for Interval Numbers

The basic algebraic operations for real numbers can be extended to interval numbers. Next, we shall formulate the basic algebraic operations for classical interval numbers.

We first define what a classical interval number is.

Definition 4.1 (Classical Interval Number).

Let $\underline{x}, \bar{x} \in \mathbb{R}$ such that $\underline{x} \leq_{\mathbb{R}} \bar{x}$. A classical interval number $[\underline{x}, \bar{x}]$ is a closed and bounded nonempty real interval, that is

$$[\underline{x}, \bar{x}] = \{x \in \mathbb{R} \mid \underline{x} \leq_{\mathbb{R}} x \leq_{\mathbb{R}} \bar{x}\},$$

where $\underline{x} = \min([\underline{x}, \bar{x}])$ and $\bar{x} = \max([\underline{x}, \bar{x}])$ are called, respectively, the lower and upper bounds (end-points) of $[\underline{x}, \bar{x}]$.

In order to proceed to the formulation of the interval operations, it is convenient to introduce the following notational conventions.

✓ NOTATION 4.1.

The set of classical interval numbers shall be denoted by $[\mathbb{R}]$. It is a proper subset of the powerset of \mathbb{R} , that is

$$[\mathbb{R}] = \{X \in \wp(\mathbb{R}) \mid (\exists \underline{x} \in \mathbb{R}) (\exists \bar{x} \in \mathbb{R}) (\underline{x} \leq_{\mathbb{R}} \bar{x} \wedge X = [\underline{x}, \bar{x}])\}.$$

For simplicity of the language, throughout this chapter, we shall usually use the expression “interval numbers” instead of the expression “classical interval numbers” and the expression “interval arithmetic” instead of the expression “classical interval arithmetic”.

✓ NOTATION 4.2.

The set of all singleton (point) interval numbers is denoted by $[\mathbb{R}]_p$, that is

$$\begin{aligned} [\mathbb{R}]_p &= \{X \in [\mathbb{R}] \mid (\exists x \in \mathbb{R})(X = [x, x])\} \\ &= \{X \in [\mathbb{R}] \mid \min(X) = \max(X)\}. \end{aligned}$$

The set $[\mathbb{R}]_p$ is an infinite proper subset of $[\mathbb{R}]$ and is *isomorphically equivalent* to the set \mathbb{R} of real numbers. That is, every element $[x, x] \in [\mathbb{R}]_p$ is an *isomorphic copy* of an element $x \in \mathbb{R}$. By convention, and being less pedantic, we agree to *identify* a point interval number $[x, x] = \{x\}$ with its *real isomorphic copy* x . So, if confusion is not likely to ensue; throughout the chapter, we may write x for $[x, x]$.

Hereafter, the upper-case Roman letters X, Y , and Z (with or without subscripts), or equivalently $[\underline{x}, \bar{x}]$, $[\underline{y}, \bar{y}]$, and $[\underline{z}, \bar{z}]$, shall be employed as variable symbols to denote elements of $[\mathbb{R}]$.

The following theorem, concerning the equality relation on $[\mathbb{R}]$, is an immediate consequence of the axiom of extensionality⁶ of axiomatic set theory.

Theorem 4.1 (Equality on $[\mathbb{R}]$).

The equality relation for interval numbers is formulated in terms of the intervals' endpoints as

$$[\underline{x}, \bar{x}] = [\underline{y}, \bar{y}] \Leftrightarrow \underline{x} = \underline{y} \wedge \bar{x} = \bar{y}.$$

Interval numbers are sets of real numbers. It is therefore not surprising that the first proposed ordering relation, for interval numbers, was the ordinary set inclusion, \subseteq , which presented by Young

⁶ The axiom of extensionality asserts that two sets are equal if, and only if they have precisely the same elements (see, e.g., [CAUSEY, 1994], [DEVLIN, 1993], and [KLEENE, 1952]), that is

$$(\forall S) (\forall T) (S = T \Leftrightarrow (\forall z) (z \in S \Leftrightarrow z \in T)).$$

in [YOUNG, 1931]. Another ordering relation, $<_M$, that extends the standard strict ordering $<_{\mathbb{R}}$ on the reals, was presented by Moore in [MOORE, 1966]. Both the inclusion relation \subseteq and Moore's relation $<_M$ are partial orderings⁷ on $[\mathbb{R}]$. This is made precise in the following two easily derivable theorems.

Theorem 4.2 (The Ordering \subseteq on $[\mathbb{R}]$).

Let \subseteq be a binary relation on $[\mathbb{R}]$ defined by

$$[\underline{x}, \bar{x}] \subseteq [\underline{y}, \bar{y}] \Leftrightarrow \underline{y} \leq_{\mathbb{R}} \underline{x} \wedge \bar{x} \leq_{\mathbb{R}} \bar{y}.$$

Then \subseteq is a non-strict partial ordering⁸ on $[\mathbb{R}]$.

Theorem 4.3 (Moore's Ordering on $[\mathbb{R}]$).

Let $<_M$ be a binary relation on $[\mathbb{R}]$ defined by

$$[\underline{x}, \bar{x}] <_M [\underline{y}, \bar{y}] \Leftrightarrow \bar{x} <_{\mathbb{R}} \underline{y}.$$

Then $<_M$ is a strict partial ordering⁹ on $[\mathbb{R}]$.

Unlike the case with $<_M$, the partial ordering by the set inclusion is *compatible*¹⁰ with the interval algebraic operations (see theorem 4.8); and this is the reason why it plays an important role in Moore's foremost work in interval analysis (see, e.g. [MOORE, 1966], [MOORE, 1979], and [MOORE ET AL., 2009]). The problem of ordering interval numbers is of great importance in both fundamental research and practical applications of the interval theory. For a formal account of the existing approaches for ordering interval numbers, along with discussing their *compatibility* with the interval algebraic operations, see chapter 6 of [DAWOOD, 2012].

EXAMPLE 4.1.

For four given interval numbers $A = [1, 2]$, $B = [1, 2]$, $C = [1, 3]$, and $D = [4, 7]$, we have $A = B <_M D$ and $A \subseteq B \subseteq C$.

We now proceed to define the basic algebraic operations for interval numbers: two binary operations, namely *addition* (“+”) and *multiplication* (“×”), and two unary operations, namely *negation* (“−”) and *reciprocal* (“^{−1}”).

According to the fact that interval numbers are *sets*, the binary and unary classical algebraic operations for interval numbers can be characterized, respectively, in the following two *set-theoretic* definitions.

⁷ If a relation \mathfrak{R} is a partial ordering on a set \mathcal{S} , then \mathcal{S} has at least one pair which is *non-comparable*, in symbols

$$(\exists x \in \mathcal{S}) (\exists y \in \mathcal{S}) (\neg (x \mathfrak{R} y) \wedge \neg (y \mathfrak{R} x)).$$

If a relation \mathfrak{R} is a total ordering on a set \mathcal{S} , then \mathcal{S} has *no non-comparable* pairs (see, e.g. [CAUSEY, 1994], [DEVLIN, 1993], and [GLEASON, 1992]), in symbols

$$(\forall x \in \mathcal{S}) (\forall y \in \mathcal{S}) (x \mathfrak{R} y \vee y \mathfrak{R} x).$$

⁸ A relation \mathfrak{R} is a *non-strict partial ordering* (often referred to as an *order* or *ordering*) on a set \mathcal{S} iff \mathfrak{R} is *reflexive*, *antisymmetric*, and *transitive* in \mathcal{S} .

⁹ A relation \mathfrak{R} is a *strict partial ordering* on a set \mathcal{S} iff \mathfrak{R} is *asymmetric* and *transitive* in \mathcal{S} .

¹⁰ A *compatible* ordering relation is preserved, in all contexts, by the algebraic operations.

Definition 4.2 (Binary Operations in $[\mathbb{R}]$).

For any two interval numbers X and Y , the binary algebraic operations are defined by

$$X \circ_c Y = \{z \in \mathbb{R} \mid (\exists x \in X) (\exists y \in Y) (z = x \circ_{\mathbb{R}} y)\},$$

where $\circ \in \{+, \times\}$.

Definition 4.3 (Unary Operations in $[\mathbb{R}]$).

For any interval number X , the unary algebraic operations are defined by

$$\diamond_c X = \{z \in \mathbb{R} \mid (\exists x \in X) (z = \diamond_{\mathbb{R}} x)\},$$

where $\diamond \in \{-,^{-1}\}$ and $0 \notin X$ if \diamond is “ -1 ”.

Hereafter, if confusion is unlikely, the subscript “c”, which stands for “classical interval operation”, and the subscript “ \mathbb{R} ”, in the real relation and operation symbols, may be suppressed.

By means of the above set-theoretic definitions and from the fact that interval numbers are *ordered sets* of real numbers, the following four theorems are derivable (see [DAWOOD, 2012]).

Theorem 4.4 (Addition on $[\mathbb{R}]$).

For any two interval numbers $[\underline{x}, \bar{x}]$ and $[\underline{y}, \bar{y}]$, interval addition is formulated in terms of the intervals' endpoints as

$$[\underline{x}, \bar{x}] + [\underline{y}, \bar{y}] = [\underline{x} + \underline{y}, \bar{x} + \bar{y}].$$

That is, interval addition is a *total*¹¹ operation, and it corresponds to the additive real function $f_{\text{sum}}(x, y) = x + y$, with $x \in [\underline{x}, \bar{x}]$ and $y \in [\underline{y}, \bar{y}]$, which is *monotonically increasing* with respect to both the variables x and y (The notion of *monotonicity* is indispensable for the interval evaluation of the image of real-valued functions. This shall be discussed, in detail, in section 7.1).

Theorem 4.5 (Multiplication on $[\mathbb{R}]$).

For any two interval numbers $[\underline{x}, \bar{x}]$ and $[\underline{y}, \bar{y}]$, interval multiplication is formulated in terms of the intervals' endpoints as

$$[\underline{x}, \bar{x}] \times [\underline{y}, \bar{y}] = [\min\{\underline{x}\underline{y}, \underline{x}\bar{y}, \bar{x}\underline{y}, \bar{x}\bar{y}\}, \max\{\underline{x}\underline{y}, \underline{x}\bar{y}, \bar{x}\underline{y}, \bar{x}\bar{y}\}].$$

That is, interval multiplication is a *total* operation, and it corresponds to the multiplicative real function $f_{\text{prod}}(x, y) = xy$, with $x \in [\underline{x}, \bar{x}]$ and $y \in [\underline{y}, \bar{y}]$, whose monotonicity is *dependent* on the values of x and y .

Theorem 4.6 (Negation on $[\mathbb{R}]$).

For any interval number $[\underline{x}, \bar{x}]$, interval negation is formulated in terms of the interval endpoints as

$$-[\underline{x}, \bar{x}] = [-\bar{x}, -\underline{x}].$$

That is, interval negation is a *total* operation, and it corresponds to the real function $f_{\text{neg}}(x) = -x$, with $x \in [\underline{x}, \bar{x}]$, which is *monotonically decreasing* with respect to the variable x .

¹¹ Let $\mathcal{S}^{(n)}$ be the n -th Cartesian power of a set \mathcal{S} . An n -ary (total) operation on \mathcal{S} is a total function $t_n : \mathcal{S}^{(n)} \mapsto \mathcal{S}$. An n -ary partial operation in \mathcal{S} is a partial function $p_n : \mathcal{U} \mapsto \mathcal{S}$, where $\mathcal{U} \subset \mathcal{S}^{(n)}$. The ordinal n is called the arity of t_n or p_n .

Theorem 4.7 (Reciprocal in \mathbb{R}).

For any zeroless interval number $[\underline{x}, \bar{x}]$ (that is, $0 \notin [\underline{x}, \bar{x}]$), interval reciprocal is formulated in terms of the interval endpoints as

$$[\underline{x}, \bar{x}]^{-1} = \left[\bar{x}^{-1}, \underline{x}^{-1} \right].$$

That is, interval reciprocal is a *partial* operation, and it corresponds to the real function $f_{\text{recip}}(x) = x^{-1}$, with $x \in [\underline{x}, \bar{x}]$, which is *monotonically decreasing* with respect to the variable x , with $0 \notin [\underline{x}, \bar{x}]$.

In accordance with the above theorems, we can now define the *total* operation of “*subtraction*”, and the *partial* operations of “*division*” and “*integer exponentiation*”, for classical interval numbers.

Definition 4.4 (Subtraction on \mathbb{R}).

For any two interval numbers X and Y , interval subtraction is defined by

$$X - Y = X + (-Y).$$

Definition 4.5 (Division in \mathbb{R}).

For any interval number X and any zeroless interval numbers Y (that is, $0 \notin Y$), interval division is defined by

$$X \div Y = X \times (Y^{-1}).$$

Definition 4.6 (Integer Exponentiation in \mathbb{R}).

For any interval number X and any integer n , the integer exponents of X are defined, in terms of multiplication and reciprocal in \mathbb{R} , by the following recursion scheme:

- (i) $X^0 = [1, 1]$,
- (ii) $0 < n \Rightarrow X^n = X^{n-1} \times X$,
- (iii) $0 \notin X \wedge 0 \leq n \Rightarrow X^{-n} = (X^{-1})^n$.

Since the interval operations are defined in terms of the corresponding real algebraic operations, and as long as division by zero is disallowed; it follows that the result of an interval operation is always an interval number.

Some numerical examples are shown below.

EXAMPLE 4.2.

For three given interval numbers $[1, 2]$, $[3, 4]$, and $[-2, 2]$, we have

- (i) $[1, 2] + [3, 4] = [4, 6]$,
- (ii) $[1, 2] \times [3, 4] = [3, 8]$,
- (iii) $[1, 2]^{-1} = [1/2, 1]$,
- (iv) $[-2, 2]^2 = [-2, 2] \times [-2, 2] = [-4, 4]$.

The result $[-4, 4]$ of $[-2, 2]^2$, in the above example, is not natural in the sense that a square is always nonnegative. Generally, for any *non-point* interval number $[\underline{x}, \bar{x}]$, with $0 \in [\underline{x}, \bar{x}]$, the square of

$[\underline{x}, \bar{x}]$ is given by

$$\begin{aligned} [\underline{x}, \bar{x}]^2 &= [\underline{x}, \bar{x}] \times [\underline{x}, \bar{x}] \\ &= \left[\min\{\underline{x}^2, \underline{x}\bar{x}, \bar{x}^2\}, \max\{\underline{x}^2, \underline{x}\bar{x}, \bar{x}^2\} \right] \\ &= \left[\underline{x}\bar{x}, \max\{\underline{x}^2, \bar{x}^2\} \right], \end{aligned}$$

which is consistent with interval multiplication (theorem 4.5), but it is *not consistent* with the fact that a square is always nonnegative, for the case when $\underline{x}\bar{x} < 0$. However, if we changed it to be

$$\begin{aligned} [\underline{x}, \bar{x}]^2 &= \{z \in \mathbb{R} \mid (\exists x \in [\underline{x}, \bar{x}]) (z = x^2)\} \\ &= \left[0, \max\{\underline{x}^2, \bar{x}^2\} \right], \end{aligned}$$

then it would be inconsistent with interval multiplication. This is not a problem if interval arithmetic is regarded as a *numerical approximation method*, for real-valued problems, such that the result of an interval operation contains all possible solutions.

4.2

Point Operations for Interval Numbers

A *point* (or *scalar*) interval operation is an operation whose operands are interval numbers, and whose result is a *point* interval (or, equivalently, a real number). This is made precise in the following definition (see [DAWOOD, 2011] and [DAWOOD, 2012]).

Definition 4.7 (Point Interval Operations).

For an ordinal n , let $[\mathbb{R}]^{(n)}$ be the n -th Cartesian power of $[\mathbb{R}]$. An n -ary point interval operation, ω_n , is a function that maps elements of $[\mathbb{R}]^{(n)}$ to the set $[\mathbb{R}]_p$ of point interval numbers, that is

$$\omega_n : [\mathbb{R}]^{(n)} \mapsto [\mathbb{R}]_p.$$

Several point interval operations can be defined. Next we define some *unary* and *binary* point interval operations.

Definition 4.8 (Interval Infimum).

The *infimum* of an interval number $[\underline{x}, \bar{x}]$ is defined to be

$$\inf([\underline{x}, \bar{x}]) = \min([\underline{x}, \bar{x}]) = \underline{x}.$$

Definition 4.9 (Interval Supremum).

The *supremum* of an interval number $[\underline{x}, \bar{x}]$ is defined to be

$$\sup([\underline{x}, \bar{x}]) = \max([\underline{x}, \bar{x}]) = \bar{x}.$$

Definition 4.10 (Interval Width).

The *width* of an interval number $[\underline{x}, \bar{x}]$ is defined to be

$$w([\underline{x}, \bar{x}]) = \bar{x} - \underline{x}.$$

Thus, the width of a point interval number is *zero*, that is

$$(\forall x \in \mathbb{R}) (w([x, x]) = x - x = 0).$$

Definition 4.11 (Interval Radius).

The radius of an interval number $[\underline{x}, \bar{x}]$ is defined to be

$$r([\underline{x}, \bar{x}]) = \frac{w([\underline{x}, \bar{x}])}{2} = \frac{(\bar{x} - \underline{x})}{2}.$$

Definition 4.12 (Interval Midpoint).

The midpoint (or mean) of an interval number $[\underline{x}, \bar{x}]$ is defined to be

$$m([\underline{x}, \bar{x}]) = \frac{(\underline{x} + \bar{x})}{2}.$$

Hence, the midpoint of a point interval number is its *real isomorphic copy*, that is

$$(\forall x \in \mathbb{R}) \left(m([x, x]) = \frac{(x + x)}{2} = x \right).$$

We observe that any interval number X can be expressed, in terms of its width and its midpoint, as the sum of its midpoint and a corresponding symmetric interval, that is

$$X = m(X) + \left[-\frac{w(X)}{2}, \frac{w(X)}{2} \right],$$

where, by convention, $m(X) = [m(X), m(X)]$.

Definition 4.13 (Interval Absolute Value).

The absolute value of an interval number $[\underline{x}, \bar{x}]$ is defined, in terms of the absolute values of its real endpoints, to be

$$|[\underline{x}, \bar{x}]| = \max\{|\underline{x}|, |\bar{x}|\}.$$

Thus, the absolute value of a point interval number is the usual absolute value of its *real isomorphic copy*, that is

$$(\forall x \in \mathbb{R}) (|[x, x]| = \max\{|x|, |x|\} = |x|).$$

All the above point interval operations are unary operations. An important definition of a binary point interval operation is that of the *interval distance* (*interval metric*, or *Moore's metric*¹²).

Definition 4.14 (Interval Distance).

The distance (or metric) between two interval numbers $[\underline{x}, \bar{x}]$ and $[\underline{y}, \bar{y}]$ is defined to be

$$d([\underline{x}, \bar{x}], [\underline{y}, \bar{y}]) = \max\{|\underline{x} - \underline{y}|, |\bar{x} - \bar{y}|\}.$$

¹² *Moore's metric* is named after the American mathematician Ramon Edgar Moore, who was the first to characterize the interval metricity and proved that it induces an interval metric space (see [MOORE, 1959]).

The importance of this definition is that starting from the distance function for interval numbers, we can verify that it induces a *metric space*¹³ for interval numbers which is a generalization of the usual metric space of real numbers. Thus, the notions of a sequence, convergence, continuity, and a limit can be defined for interval numbers in the standard way. These notions give rise to what we may call a “*measure theory for interval numbers*”. In section 7.1, the interval metric is used to measure the *overestimation* when estimating the image of real-valued functions using interval arithmetic.

EXAMPLE 4.3.

For three given interval numbers $[1, 2]$, $[3, 4]$, and $[-5, 3]$, we have

- (i) $w([1, 2]) = w([3, 4]) = 1$,
- (ii) $m([1, 2]) = 3/2$, $m([3, 4]) = 7/2$,
- (iii) $||[-5, 3]|| = \max\{|-5|, |3|\} = 5$,
- (iv) $d([1, 2], [3, 4]) = \max\{|1 - 3|, |2 - 4|\} = 2$.

4.3

Algebraic Properties of Interval Arithmetic

The algebraic properties of interval arithmetic are different than those of ordinary real arithmetic. In this section, with the help of the notions prescribed so far, we shall inquire into some fundamental algebraic properties of interval arithmetic (for *formal* proofs of the results of this section, see [DAWOOD, 2012]). A first important theorem that follows directly from definition 4.2 is the *inclusion monotonicity* theorem for classical interval arithmetic, which asserts that the partial ordering by the set inclusion relation is *compatible* with the algebraic operations on the set $[\mathbb{R}]$ of interval numbers.

Theorem 4.8 (Inclusion Monotonicity in $[\mathbb{R}]$).

Let X_1, X_2, Y_1 , and Y_2 be interval numbers such that $X_1 \subseteq Y_1$ and $X_2 \subseteq Y_2$. Then for any classical interval operation $\circ \in \{+, \times\}$, we have

$$X_1 \circ X_2 \subseteq Y_1 \circ Y_2.$$

In consequence of this theorem, and from the fact that $[x, x] \subseteq X \Leftrightarrow x \in X$, we have the following important special case.

Corollary 4.1.

Let X and Y be interval numbers with $x \in X$ and $y \in Y$. Then for any unary operation $\diamond \in \{-, ^{-1}\}$ and any binary operation $\circ \in \{+, \times\}$, we have

¹³ A *metric space* is an ordered pair (S, d) , where S is a set and d is a metric on S , that is

$$d : S^{(2)} \mapsto \mathbb{R},$$

such that for any $x, y, z \in S$, the following holds (see [BRYANT, 1985]):

- $x = y \Leftrightarrow d(x, y) = 0$,
- $d(x, y) = d(y, x)$,
- $d(x, z) \leq d(x, y) + d(y, z)$.

- (i) $\diamond x \in \diamond X$,
- (ii) $x \circ y \in X \circ Y$.

The algebraic properties of the classical interval operations are prescribed by the following series of theorems.

Theorem 4.9 (Identity Elements in $[\mathbb{R}]$).

The interval numbers $[0, 0]$ and $[1, 1]$ are identity elements for interval addition and multiplication respectively, that is

- (i) $(\forall X \in [\mathbb{R}]) ([0, 0] + X = X + [0, 0] = X)$,
- (ii) $(\forall X \in [\mathbb{R}]) ([1, 1] \times X = X \times [1, 1] = X)$.

Theorem 4.10 (Commutativity in $[\mathbb{R}]$).

Both interval addition and multiplication are commutative, that is

- (i) $(\forall X, Y \in [\mathbb{R}]) (X + Y = Y + X)$,
- (ii) $(\forall X, Y \in [\mathbb{R}]) (X \times Y = Y \times X)$.

Theorem 4.11 (Associativity in $[\mathbb{R}]$).

Both interval addition and multiplication are associative, that is

- (i) $(\forall X, Y, Z \in [\mathbb{R}]) (X + (Y + Z) = (X + Y) + Z)$,
- (ii) $(\forall X, Y, Z \in [\mathbb{R}]) (X \times (Y \times Z) = (X \times Y) \times Z)$.

Theorem 4.12 (Cancellativity of Addition in $[\mathbb{R}]$).

Interval addition is cancellative, that is

$$(\forall X, Y, Z \in [\mathbb{R}]) (X + Z = Y + Z \Rightarrow X = Y).$$

In contrast to the case for addition, the following theorem asserts that multiplication is not always cancellative in $[\mathbb{R}]$.

Theorem 4.13 (Cancellativity of Multiplication in $[\mathbb{R}]$).

An interval number is cancellable for multiplication if, and only if, it is a zeroless interval, that is

$$(\forall X, Y, Z \in [\mathbb{R}]) ((X \times Z = Y \times Z \Rightarrow X = Y) \Leftrightarrow 0 \notin Z).$$

An important property peculiar to the classical interval theory figures in the following theorem.

Theorem 4.14 (Inverses in $[\mathbb{R}]$).

An interval number is invertible if, and only if, it is a point interval, that is

- (i) $(\forall X, Y \in [\mathbb{R}]) (X + Y = [0, 0] \Leftrightarrow X \in [\mathbb{R}]_p \wedge Y = -X)$,
- (ii) $(\forall X, Y \in [\mathbb{R}]) (X \times Y = [1, 1] \Leftrightarrow X \in [\mathbb{R}]_p \wedge Y = X^{-1} \wedge 0 \notin X)$.

The result formulated in the following theorem is an important property of classical interval arithmetic.

Theorem 4.15 (Subdistributivity in $[\mathbb{R}]$).

The distributive law does not always hold in classical interval arithmetic. Precisely, for any three interval numbers X , Y , and Z

$$Z \times (X + Y) = Z \times X + Z \times Y,$$

if, and only if,

- (i) Z is a point interval number, or
- (ii) $X = Y = [0, 0]$, or
- (iii) $(\forall x \in X) (\forall y \in Y) (xy \geq 0)$.

In general, classical interval arithmetic has only the subdistributive law:

$$(\forall X, Y, Z \in [\mathbb{R}]) (Z \times (X + Y) \subseteq Z \times X + Z \times Y).$$

The previous results, particularly theorems 4.14 and 4.15, illustrate the difference between the classical interval algebra and the algebra of ordinary real numbers. Two important properties, peculiar to the classical theory of interval arithmetic, figure in the theorems of this section: additive and multiplicative inverses do not always exist for classical interval numbers, and there is no distributivity between classical addition and multiplication except for certain special cases. Then, we have to sacrifice some useful properties of ordinary arithmetic, if we want to use the interval weapon against uncertainty. Precisely speaking, it is proved, in [DAWOOD, 2012], that the algebraic system of classical interval arithmetic is a *nondistributive abelian semiring*¹⁴, while the algebra of ordinary real numbers is *totally ordered field*.

Finally, let us remark that interval arithmetic can be extended, via *complex interval numbers*, to determine regions of uncertainty in computing with *ordinary complex numbers*. As it is the case with computing with real numbers, computing with complex numbers involves *uncertain data*. So, given the fact that an interval number is a real closed interval and a complex number is an ordered pair of real numbers, there is no reason to limit the application of interval arithmetic to the measure of uncertainties in computations with real numbers (For a variety of complex interval algebras, the reader may consult, e.g., [ALEFELD AND HERZBERGER, 1983], [BOCHE, 1966], [DAWOOD, 2012], and [PETKOVIC ET AL., 1998]). However, *complex interval arithmetic* comes with many sacrifices: we have to sacrifice many useful properties of the *field* of ordinary complex numbers, and moreover we lose the *nondistributive abelian semiring* of the classical interval theory. In addition, interval arithmetic can be extended analogously to other *multidimensional algebras*, beyond the ordinary complex algebra, such as *quaternions* and *octonions*, but with the expense that we have to sacrifice other useful properties of ordinary arithmetic (see [DAWOOD, 2012]).

¹⁴ An *abelian semiring* is a semiring whose multiplication is commutative. A *nondistributive semiring* is a semiring whose multiplication does not distribute over addition (see, e.g., [BARNES AND MACK, 1975], [LEVI, 1961], [MENINI AND OYSTAEYEN, 2004], and [STEEN, 2008]).

5 MACHINE REALIZATION OF INTERVAL ARITHMETIC

There are numerous software implementations for classical interval arithmetic, which are usually provided as class libraries. Interval class libraries and language extensions are available for many *numeric* and *symbolic* programming languages such as C++, Java, Fortran, Mathematica, Maple, Lisp, Macsyma, and Coq (For further details, see, e.g., [FATEMAN, 2009], [HANSEN AND WALSTER, 2003], [JAULIN ET AL., 2001], and [KEENE, 1988]).

However, existing software packages for interval arithmetic, in which interval calculations is simulated with floating-point routines, are often too slow for numerically intensive calculations. Therefore, interval arithmetic is about *five times slower* than floating-point arithmetic, if no special hardware implementations are provided such that interval arithmetic is directly supported on the machine level. Fortunately, computers are getting faster and most existing *parallel processors* provide a tremendous computing power. So, with little extra hardware, it is very possible to make interval computations as fast as floating point computations (For further reading about the hardware support for interval arithmetic, see, e.g., [VON GUDENBERG, 1996], [KOLEV, 1993], [MULLER ET AL., 2009], and [NEUMAIER, 1991]).

In this section, we provide a bit of perspective on the algebraic system of *machine interval arithmetic* and some of its fundamental properties (For further details, the reader may consult, e.g., [DAWOOD, 2011], [DAWOOD, 2012], [KULISCH AND MIRANKER, 1981], [KULISCH, 2008B], [MOORE, 1959], and [MOORE, 1962]).

The arithmetic of intervals defined in the preceding sections may be called an *exact interval arithmetic*, in the sense that no rounding or approximation is involved. However, when interval arithmetic is realized on a computer, we get some loss of accuracy due to round-off errors. Therefore, due to the fact that there is only a *finite* subset $\mathbb{M} \subset \mathbb{R}$ of *machine-representable numbers*, special care has to be taken to guarantee a proper hardware implementation of interval arithmetic. Thus, we need a *machine interval arithmetic* in which interval numbers have to be rounded so that the interval result computed by a machine always contains the exact interval result.

5.1

Rounded-Outward Interval Arithmetic

The algebraic operations of the classical theory of interval arithmetic are defined in such a way that they satisfy the property of *inclusion monotonicity* (see theorem 4.8 of section 4.3). An important immediate consequence of the inclusion monotonicity is that given two interval numbers $[\underline{x}, \bar{x}]$ and $[\underline{y}, \bar{y}]$ with $x \in [\underline{x}, \bar{x}]$ and $y \in [\underline{y}, \bar{y}]$, then for any unary operation $\diamond \in \{-,^{-1}\}$ and any binary operation $\circ \in \{+, \times\}$, the real and interval results shall satisfy

$$\begin{aligned} \diamond x &\in \diamond [\underline{x}, \bar{x}], \\ x \circ y &\in [\underline{x}, \bar{x}] \circ [\underline{y}, \bar{y}]. \end{aligned}$$

That is, guaranteed enclosures of the real-valued results can be obtained easily by computing on interval numbers. The following membership formulas can be deduced immediately from the property of inclusion monotonicity.

$$\begin{aligned} -x &\in [-\bar{x}, -\underline{x}], \\ x^{-1} &\in \left[\bar{x}^{-1}, \underline{x}^{-1} \right], \quad \text{if } 0 \notin [\underline{x}, \bar{x}], \\ x + y &\in [\underline{x} + \underline{y}, \bar{x} + \bar{y}], \\ x \times y &\in [\min\{\underline{x}\underline{y}, \underline{x}\bar{y}, \bar{x}\underline{y}, \bar{x}\bar{y}\}, \max\{\underline{x}\underline{y}, \underline{x}\bar{y}, \bar{x}\underline{y}, \bar{x}\bar{y}\}]. \end{aligned}$$

The preceding formulas use the arithmetic of real numbers that are not machine-representable.

However, using *outward rounding* for interval numbers, we can obtain alternate formulas that use floating-point arithmetic, and still satisfy the property of inclusion monotonicity.

Two definitions we shall need are those of the *downward* and *upward* rounding operators.

Definition 5.1 (Downward Rounding).

Let x be any real number and let x_m denote a machine-representable real number. Then there exists a machine-representable real number ∇x such that

$$\nabla x = \sup\{x_m \in \mathbb{M} \mid x_m \leq x\},$$

where ∇ is called the downward rounding operator.

Definition 5.2 (Upward Rounding).

Let x be any real number and let x_m denote a machine-representable real number. Then there exists a machine-representable real number Δx such that

$$\Delta x = \inf\{x_m \in \mathbb{M} \mid x \leq x_m\},$$

where Δ is called the upward rounding operator.

On the basis of these definitions, we can obtain a finite set $[\mathbb{M}] \subset [\mathbb{R}]$ of machine interval numbers by rounding interval numbers *outward*.

Definition 5.3 (Outward Rounding).

Let $[\underline{x}, \bar{x}]$ be any interval number. Then there exists a machine-representable interval number $\diamond[\underline{x}, \bar{x}]$ such that

$$\diamond[\underline{x}, \bar{x}] = [\nabla \underline{x}, \Delta \bar{x}],$$

where \diamond is called the outward rounding operator.

With outward rounding, a *machine interval arithmetic* can be defined such that the result of a machine interval operation is a machine interval number which is guaranteed to contain the exact result of an interval operation. In this manner, the classical interval operations can be redefined, in the language of machine interval arithmetic, as follows.

Definition 5.4 (Machine Interval Operations).

Let $[\underline{x}, \bar{x}]$ and $[\underline{y}, \bar{y}]$ be interval numbers. The unary and binary machine interval operations are defined as

$$\begin{aligned} \diamond(-[\underline{x}, \bar{x}]) &= [\nabla(-\bar{x}), \Delta(-\underline{x})], \\ \diamond([\underline{x}, \bar{x}]^{-1}) &= \left[\nabla(\bar{x}^{-1}), \Delta(\underline{x}^{-1}) \right], \quad \text{if } 0 \notin [\underline{x}, \bar{x}], \\ \diamond([\underline{x}, \bar{x}] + [\underline{y}, \bar{y}]) &= [\nabla(\underline{x} + \underline{y}), \Delta(\bar{x} + \bar{y})], \\ \diamond([\underline{x}, \bar{x}] \times [\underline{y}, \bar{y}]) &= [\nabla(\min\{\underline{x}\underline{y}, \underline{x}\bar{y}, \bar{x}\underline{y}, \bar{x}\bar{y}\}), \Delta(\max\{\underline{x}\underline{y}, \underline{x}\bar{y}, \bar{x}\underline{y}, \bar{x}\bar{y}\})]. \end{aligned}$$

With the help of the above definitions, it is not difficult to prove the following two theorems and their corollary.

Theorem 5.1.

For any two real numbers x and y , we have

- (i) $x \leq y \Rightarrow \nabla x \leq \nabla y$,
- (ii) $x \leq y \Rightarrow \Delta x \leq \Delta y$.

Theorem 5.2.

For any two interval numbers X and Y , we have

- (i) $X \subseteq Y \Rightarrow \diamond X \subseteq \diamond Y$,
- (ii) $X \circ Y \subseteq \diamond(X \circ Y)$,
- (iii) $\diamond X \subseteq \diamond(\diamond X)$.

Corollary 5.1.

For any two interval numbers X and Y with $x \in X$ and $y \in Y$, we have

- (i) $\diamond x \in \diamond(\diamond X)$,
- (ii) $x \circ y \in \diamond(X \circ Y)$.

Thus, outward rounding provides an efficient implementation of interval arithmetic, with the property of inclusion monotonicity still satisfied.

To illustrate this, we give two numerical examples.

EXAMPLE 5.1.

Let \mathbb{M}_3 be the set of machine-representable real numbers with three significant digits.

(i) We have

$$\begin{aligned} \diamond_3([1, 2] \div [2, 3]) &= [\nabla_3(1/3), \Delta_3(1)] \\ &= [0.333, 1], \end{aligned}$$

and

$$([1, 2] \div [2, 3]) \subset [0.333, 1].$$

(ii) We have

$$\begin{aligned} \diamond_3([0, 1] + [2.7182, 3.3841]) &= [\nabla_3(2.7182), \Delta_3(4.3841)] \\ &= [2.718, 4.385], \end{aligned}$$

and

$$([0, 1] + [2.7182, 3.3841]) \subset [2.718, 4.385].$$

5.2

Rounded-Upward Interval Arithmetic

Outward rounding of interval numbers involves performing computations with *two rounding modes* (upward and downward). This can be much costlier than performing the computations with one single rounding direction.

If, as usual, we have

$$(\forall x_m) (x_m \in \mathbb{M} \Rightarrow (-x_m) \in \mathbb{M}),$$

then the relation

$$(\forall x \in \mathbb{R}) (\nabla(-x) = -\Delta(x)),$$

which then holds, makes it possible to use upward rounding as one single rounding mode.

In this manner, for instance, machine interval addition can be reformulated as

$$\diamond([\underline{x}, \bar{x}] + [\underline{y}, \bar{y}]) = [-\Delta((-x) - y), \Delta(\bar{x} + \bar{y})].$$

Similar optimal roundings can be applied to other interval operations so that we get more efficient implementations of interval arithmetic.

6 INTERVAL DEPENDENCY AND ALTERNATE INTERVAL THEORIES

As mentioned in section 4.3, it is proved, in [DAWOOD, 2012], that the algebraic system of classical interval arithmetic is a *nondistributive abelian semiring*, which is a primitive algebraic structure, if compared to the totally ordered field of real numbers. Another main drawback of the classical interval theory is that when estimating the image of real functions using the *naive* classical interval operations, we usually get overestimations that inevitably produce meaningless results, if the variables are *functionally dependent*. This persisting problem is known as the “*interval dependency problem*”.

The notion of dependency comes from the notion of a function. In the theory of real closed intervals, the notion of interval dependency naturally comes from the idea of *functional dependence* of real variables. Despite the fact that dependency is an essential and useful notion of real variables, interval dependency is the main unsolved problem of the classical theory of interval arithmetic and its modern generalizations. Our objective in this section is to formulate the notion of interval dependency, and then briefly mention some alternate interval theories (For a complete *systematic formalization* of the notion of interval dependency, by means of the notions of *Skolemization*¹⁵ and logical *quantification dependence*, see [DAWOOD, 2012]).

Before we proceed, it is convenient to introduce the following notational convention.

✓ NOTATION 6.1.

The left-superscripted letters ${}^{\mathbb{R}}f$, ${}^{\mathbb{R}}g$, ${}^{\mathbb{R}}h$ (with or without subscripts) shall be employed to denote real-valued functions, while the letters ${}^c f$, ${}^c g$, ${}^c h$ (with or without subscripts) shall be employed to denote classical interval-valued functions.

If the type of function is clear from its arguments, and if confusion is not likely to ensue, we shall usually drop the left superscripts “ \mathbb{R} ” and “ c ”. Thus, we may, for instance, write $f(x_1, \dots, x_n)$

¹⁵ *Skolemization* is named after the Norwegian logician Thoralf Skolem (1887–1963), who first presented the notion in [SKOLEM, 1920].

and $f(X_1, \dots, X_n)$ for, respectively, a real-valued function and an interval-valued function, which are both defined by the same rule. This convention shall be admitted, without explicit reference, in the succeeding sections of this chapter.

We begin by the following definition for the image set of real closed intervals.

Definition 6.1 (Image of Real Closed Intervals).

Let $f : \mathcal{D} \subseteq \mathbb{R}^{(n)} \mapsto \mathbb{R}$ be an n -ary function on \mathbb{R} . Let $(x_1, \dots, x_n) \in \mathcal{D}$, with each x_k is restricted to vary on a real closed interval X_k . Then, the image of the closed intervals X_k with respect to f , denoted I_f , is defined to be

$$I_f(X_1, \dots, X_n) = \{y \in \mathbb{R} \mid (\exists_{k=1}^n x_k \in X_k) (y = f(x_1, \dots, x_n))\} \subseteq \mathbb{R}.$$

An immediate consequence of definition 6.1, and the well-known *extreme value theorem*, is the following important property.

Theorem 6.1.

Let f be an n -ary real-valued function which is continuous in the real closed intervals X_k . The (accurate) image $I_f(X_1, \dots, X_n)$, of X_k , is in turn a real closed interval such that

$$I_f(X_1, \dots, X_n) = \left[\min_{x_k \in X_k} f(x_1, \dots, x_n), \max_{x_k \in X_k} f(x_1, \dots, x_n) \right].$$

The interval dependency problem can now be formulated in the following theorem (see [DAWOOD, 2012]).

Theorem 6.2 (Dependency Problem).

Let X_k be real closed intervals and let $f(x_1, \dots, x_n)$ be a continuous real-valued function with $x_k \in X_k$. Evaluating the accurate image of f for the interval numbers X_k , using naive classical interval arithmetic, is not always possible if some x_k are functionally dependent. That is,

$$(i) \quad (\exists f) (I_f(X_1, \dots, X_n) \neq f(X_1, \dots, X_n)).$$

In general,

$$(ii) \quad (\forall f) (I_f(X_1, \dots, X_n) \subseteq f(X_1, \dots, X_n)).$$

In order to clarify the matters, let f be a real-valued function defined by the rule $f(x) = x^2$ with $x \in [-a, a]$. According to theorem 6.1, the (accurate) image of $[-a, a]$ under the real-valued function f is

$$I_f([-a, a]) = \left[\min_{x \in [-a, a]} x^2, \max_{x \in [-a, a]} x^2 \right] = [0, a^2].$$

If we evaluate the image of $[-a, a]$ using classical interval arithmetic, by theorem 4.5, we obtain the interval-valued function,

$$\begin{aligned} f([-a, a]) &= [-a, a] \times [-a, a] \\ &= [-a^2, a^2]. \end{aligned}$$

Obviously, the result $[-a^2, a^2]$, obtained using classical interval arithmetic, has an overestimation of

$$|w([-a^2, a^2]) - w([0, a^2])| = a^2.$$

This overestimated result is due to the fact that the classical interval theory assumes *independence* of all interval variables, even when dependencies exist.

To illustrate this more clearly, we next give a numerical example.

EXAMPLE 6.1.

Consider the real-valued function

$$f(x) = x(x - 1),$$

with $x \in [0, 1]$.

The actual image of $[0, 1]$ under f is $[-1/4, 0]$. Evaluating the image using classical interval arithmetic, we get

$$f([0, 1]) = [0, 1] \times ([0, 1] - 1) = [-1, 0],$$

which has an overestimation of

$$|w([-1, 0]) - w([-1/4, 0])| = 3/4.$$

The problem of computing the image $I_f(X_1, \dots, X_n)$, using interval arithmetic, is the main problem of interval computations. This problem is, in general, NP-hard (see, e.g., [GAGANOV, 1985], [KREINOVICH, 2008], and [ROKNE AND RATSCHKE, 1984]). That is, for the classical interval theory, there is no efficient algorithm to make the identity

$$(\forall f) (I_f(X_1, \dots, X_n) = f(X_1, \dots, X_n)),$$

always hold unless $NP = P$, which is widely believed to be false. However, a considerable scientific effort is put into finding a way out from the interval dependency problem. There are many special methods and algorithms, based on the classical interval theory, that successfully compute useful narrow bounds to the desirable accurate image (see, e.g., [ALEFELD AND MAYER, 2000], [MOORE, 1966], [MOORE, 1979], [MOORE ET AL., 2009], and [HANSEN AND WALSTER, 2003]). As examples of these successful methods, we can mention: *generalized centered forms*, *circular complex centered forms*, *Hansen's method*, *remainder forms*, the *subdivision techniques*, and many others. In section 7.1, we shall discuss, some of these techniques.

Beyond the techniques based on the classical interval theory, various proposals for possible alternate theories of interval arithmetic were introduced to reduce the dependency effect or to enrich the algebraic structure of interval numbers. Among these alternate theories of intervals, we can mention as examples: *Hansen's generalized intervals* [HANSEN, 1975], *Kulisch's complete intervals* [KULISCH, 2008B], *modal intervals* [GARDENYES ET AL., 1985], *directed intervals* [MARKOV, 1995], *constraint intervals* [LODWICK, 1999], and *optimizational intervals* and *optimizational complex intervals* [DAWOOD, 2012].

7 INTERVAL METHODS FOR UNCERTAINTY IN SCIENCE AND TECHNOLOGY

Interval methods are becoming a mainstream. Interval arithmetic is still more accurate and reliable than floating-point arithmetic and traditional numerical approximation methods. Computational applications of interval arithmetic include estimations of the images of real functions, bounding definite integrals, bounding the error term in Taylor's Series and many others. Interval arithmetic techniques combined with automatic differentiation are also used mainly in global optimization methods, computer graphics and many other applications. Today, the interval theory has numerous applications in scientific and engineering disciplines that deal intensely with *uncertain data*. In *electrical engineering*, interval techniques are used in quality control in the *manufacturing* of radio-electronic devices.

Similar quality control techniques are used in other manufacturing applications. In *control* applications, interval techniques are used to analyze stability under uncertainty. In *remote sensing* and *geographical information systems (GIS)*, interval techniques are used to bound errors. In *economics*, interval techniques are used to model uncertainties in input parameters and prediction uncertainties. In *physics*, interval techniques help take care of bounds on systematic components of measurement errors and on modeling errors, and also in computation of physical constants. In *dynamic systems* (in particular, in *chaotic systems*), interval techniques enable us to verify the computation results and provide robustness of these results and of their visualization. In *computer graphics* and *computational geometry*, interval techniques provide robustness of the results, and are used heavily in some problems that arise in ray-tracing techniques, especially the problems of intersections between surfaces. The main purpose of this section is to briefly describe some typical applications that clarify the need for interval computations to cope with uncertainty in science and engineering (For further applications of interval arithmetic, the reader may consult, e.g., [HANSEN AND WALSTER, 2003], [JAULIN ET AL., 2001], [MOORE ET AL., 2009], [ALEFELD AND MAYER, 2000], [DAWOOD, 2011], and [DAWOOD, 2012]).

7.1

Interval Estimates of the Image of Real Functions

Unfortunately, in mathematics and computational sciences, the problem of evaluating the range of real functions is not, in general, an easy problem. In section 2.3, it was shown that the uncertainty problem of acquiring knowledge about the real world can lead to the problem of evaluating the image of real-valued functions for some *intervals of certainty*. So, it is necessary for this problem, and for many practical problems, to develop techniques for sufficiently estimating the image of real functions over some closed interval. Uses of such estimations include global optimization techniques, interval automatic differentiation, ray tracing algorithms, fixed point problems, initial value problems, checking for zeros of the function in some interval and many others. Although there are many numerical methods to approximate the image of real functions, none of them ensure the required accuracy of the result, and most of them suffer from difficulties imposed by long computational times.

Interval arithmetic offers simple and easy methods for estimating the image of continuous functions. This section is intended to discuss the naive method of interval arithmetic used in estimating the image of real continuous functions over some closed interval. Some improvements are performed on the naive method for more accurate estimations, an outline of such methods is presented at the end of this section (For further details on the naive method and other methods, see, e.g., [MOORE, 1966], [MOORE ET AL., 2009], [ALEFELD AND HERZBERGER, 1983], [KULISCH, 2008B], [ROKNE AND RATSCHKE, 1984], [DAWOOD, 2011], and [DAWOOD, 2012]).

A cornerstone result from theorem 6.1 of section 6, that should be stressed here, is that the *best* way to evaluate the *accurate* image of a continuous real-valued function is to apply *minimization* and *maximization* directly to determine the exact lower and upper endpoints of the image.

For the sake of simplicity, in what follows, we shall limit ourselves to the case of continuous functions in *one* real variable. In this case, the following theorem, which constructs an important result we shall employ, follows directly from theorem 6.1.

Theorem 7.1 (Image of Continuous Monotonic Functions).

Let $f : \mathcal{D} \subseteq \mathbb{R} \rightarrow \mathbb{R}$ be a continuous real-valued function which is monotonic in the real closed interval $X = [\underline{x}, \bar{x}] \subseteq \mathcal{D}$. The (accurate) image $I_f(X)$, of X , is a real closed interval given by

$$I_f(X) = [\min \{f(\underline{x}), f(\bar{x})\}, \max \{f(\underline{x}), f(\bar{x})\}].$$

With this theorem at hand, we have the following two corollaries.

Corollary 7.1.

Let $f : \mathcal{D} \subseteq \mathbb{R} \mapsto \mathbb{R}$ be a continuous real-valued function which is non-decreasing in the real closed interval $X = [\underline{x}, \bar{x}] \subseteq \mathcal{D}$. The (accurate) image $I_f(X)$, of X , is a real closed interval given by

$$I_f(X) = [f(\underline{x}), f(\bar{x})].$$

Corollary 7.2.

Let $f : \mathcal{D} \subseteq \mathbb{R} \mapsto \mathbb{R}$ be a continuous real-valued function which is non-increasing in the real closed interval $X = [\underline{x}, \bar{x}] \subseteq \mathcal{D}$. The (accurate) image $I_f(X)$, of X , is a real closed interval given by

$$I_f(X) = [f(\bar{x}), f(\underline{x})].$$

Here is an example.

EXAMPLE 7.1.

Consider the function $f(x) = e^x$ with $x \in X = [2, 3]$. This function is non-decreasing on X , so

$$I_f(X) = [f(2), f(3)] = [e^2, e^3].$$

For piecewise monotonic functions, we can divide the interval X as in the following example.

EXAMPLE 7.2.

Consider the function $f(x) = x^2$ with $x \in X = [-2, 2]$. This function is a non-increasing function in $[-2, 0]$ and a non-decreasing function in $[0, 2]$. So, the image of X under f is given by

$$\begin{aligned} I_f(X) &= [f(0), f(-2)] \cup [f(0), f(2)] \\ &= [0, 4] \cup [0, 4] \\ &= [0, 4]. \end{aligned}$$

The above examples illustrate that, with a knowledge of the monotonicity of some elementary functions on some interval number X , we could evaluate the accurate images of these functions. In fact, most elementary functions could be evaluated by this method. Also, the interval-valued function at X , $f(X)$, for some elementary function f is defined to be the exact image $I_f(X)$ of the function over X . For instance, $e^{[2,3]} = [e^2, e^3]$ and $[-2, 2]^2 = [0, 4]$.

For the more general continuous functions which are composed of the basic real elementary operations $+$, $-$, \times , and \div ; constants; variables; and elementary functions with known images on some closed interval X , we can estimate the image using the naive interval arithmetic techniques as follows.

Theorem 7.2.

Let $f : \mathcal{D} \subseteq \mathbb{R} \mapsto \mathbb{R}$ be a continuous real-valued function on the interval $X \subseteq \mathcal{D}$. Evaluating the interval-valued function f at X , $f(X)$, gives an enclosure of the exact image $I_f(X)$. That is

$$I_f(X) \subseteq f(X). \quad (7.1)$$

Theorem 7.2 indicates that the interval-valued function at X , $f(X)$, always contains the exact image of X under f . The accuracy of this estimation depends mainly on the expression of the real-valued function f . As we mentioned in section 6, more instances of the real variable x in the expression

of f means that dependency exists which results in an overestimation of the exact image. Also, the overestimation of the exact image decreases *linearly* with the size of the interval X , as illustrated by the following theorem.

Theorem 7.3.

$d(I_f(X), f(X)) \leq c.w(X)$, where $c \geq 0$ is a constant.

The following theorem illustrates that, the width of $f(X)$ also decreases *linearly* with the width of X .

Theorem 7.4.

$w(f(X)) \leq c_1.w(X)$, where $c_1 \geq 0$ is a constant.

So, less instances of the real variable x in the original real expression of f leads to better estimations. In fact, the following holds.

Theorem 7.5.

If the real variable x appears only once in the expression of f then $I_f(X) = f(X)$.

Examples are shown below.

EXAMPLE 7.3.

Consider the function $f(x) = x + 1$ with $x \in [-1, 3]$. Evaluating the interval-valued function at $[-1, 3]$ yields

$$\begin{aligned} f([-1, 3]) &= [-1, 3] + [1, 1] \\ &= [0, 4]. \end{aligned}$$

Hence, by theorem 7.2, we have $I_f([-1, 3]) \subseteq [0, 4]$. But we have the real variable x appears only once in the expression of f , then, by theorem 7.5, the image of $[-1, 3]$ is $[0, 4]$.

EXAMPLE 7.4.

Consider the function $f(x) = x^2 + x + 1$ with $x \in [-2, 2]$. Evaluating the interval-valued function at $[-2, 2]$ yields

$$\begin{aligned} f([-2, 2]) &= [-2, 2]^2 + [-2, 2] + [1, 1] \\ &= [0, 4] + [-1, 3] \\ &= [-1, 7]. \end{aligned}$$

Hence, by theorem 7.2, we have $I_f([-2, 2]) \subseteq [-1, 7]$.

Many techniques are used to improve the results obtained from the naive method by reducing the width of the resulting interval. Among these techniques *centered forms*, *generalized centered forms*, *circular complex centered forms*, *Hansen's method*, *remainder forms*, and many others (see, e.g., [ROKNE AND RATSCHKE, 1984]). Also, there are the *subdivision techniques* which work on subdividing the interval X and hence reduce the resulting overestimation (see, e.g., [MOORE, 1979], [ROKNE AND RATSCHKE, 1984], [KULISCH, 2008B], [ALEFELD AND HERZBERGER, 1983], and [ALEFELD AND MAYER, 2000]).

For instance, the subdivision method, which is due to Moore (see, e.g., [MOORE, 1966] and [MOORE, 1979]), can be described as follows. First, we subdivide the interval X into n subintervals X_i such that

$$X_i = [\underline{x} + (i-1)w(X)/n, \underline{x} + (i)w(X)/n],$$

where $w(X_i) = w(X)/n$, hence

$$X = \cup_{i=1}^n X_i.$$

Second, we evaluate the interval-valued function f for each subinterval X_i , $f(X_i)$. Hence, due to theorem 7.3, we get

$$I_f(X) \subseteq \cup_{i=1}^n f(X_i) \subseteq f(X). \quad (7.2)$$

That is, the subdivision method produces better approximations than the naive method. Moreover, the larger the number of subintervals n , the better the estimation of the image $I_f(X)$.

EXAMPLE 7.5.

Consider the function of example 7.4 given by

$$f(x) = x^2 + x + 1 \text{ with } x \in [-2, 2].$$

With the naive method we obtained the enclosure interval $[-1, 7]$. Here we shall try to improve this result using the subdivision method. We subdivide the interval $[-2, 2]$ to 3 subintervals $[-2, -2/3]$, $[-2/3, 2/3]$ and $[2/3, 2]$. Evaluating the interval-valued function f for $[-2, -2/3]$ yields

$$\begin{aligned} f([-2, -2/3]) &= [-2, -2/3]^2 + [-2, -2/3] + [1, 1] \\ &= [4/9, 4] + [-1, 1/3] \\ &= [-5/9, 13/3]. \end{aligned}$$

Evaluating the interval-valued function f for $[-2/3, 2/3]$ yields

$$\begin{aligned} f([-2/3, 2/3]) &= [-2/3, 2/3]^2 + [-2/3, 2/3] + [1, 1] \\ &= [0, 4/9] + [1/3, 5/3] \\ &= [1/3, 19/9]. \end{aligned}$$

Evaluating the interval-valued function f for $[2/3, 2]$ yields

$$\begin{aligned} f([2/3, 2]) &= [2/3, 2]^2 + [2/3, 2] + [1, 1] \\ &= [4/9, 4] + [5/3, 3] \\ &= [19/9, 7]. \end{aligned}$$

Hence, by equation 7.2, we have

$$I_f([-2, 2]) \subseteq f([-2, -2/3]) \cup f([-2/3, 2/3]) \cup f([2/3, 2]),$$

that is

$$I_f([-2, 2]) \subseteq [-5/9, 13/3] \cup [1/3, 19/9] \cup [19/9, 7] = [-5/9, 7].$$

The resulting interval is more narrow than the one obtained by the naive method and we have

$$I_f([-2, 2]) = [3/4, 7] \subseteq [-5/9, 7] \subseteq [-1, 7],$$

where $[3/4, 7]$ is the exact image of $[-2, 2]$.

We conclude from the above discussion that interval arithmetic techniques are very useful, reliable and simple for estimating the image of continuous functions over some closed interval. The naive method converges *linearly* to the exact image. Some improvements exist, like centered forms and

many others. With a centered form of f , the overestimation of the exact image decreases *quadratically* with the size of the interval X . Therefore, for intervals with small widths, this method gives better estimations than the naive method. Also, there are the subdivision methods which give very good estimations especially when the width of X is large. So, using interval arithmetic techniques ensures that we have the exact image included in the final result with the required accuracy.

7.2

Interval Automatic Differentiation

Many applications and algorithms in mathematics and scientific computing require the value of the derivative of a given function at some point. There are many ways to calculate the derivative at a point like symbolic or numerical differentiation methods. The usual symbolic method requires the expression of the function from which the expression of its derivative is derived, using some known rules, and then the value of the derivative is evaluated at the given point by substituting in this expression. It is obvious that this method is very inefficient especially with complex expressions and higher order derivatives and it is difficult to be computationally performed. The other numerical method which can be performed by a computer depends on approximating the derivative using finite differences. That is, for a differentiable function f ,

$$\text{first derivative} \cong \frac{f(x + dx) - f(x)}{dx},$$

for a small nonzero value of dx . As dx approaches zero, the derivative is better approximated. The drawback of this method is the difficulty in choosing the values for dx . Small values could enlarge the rounding errors on the computer and large values will lead to a bad approximation of the derivative. This method could be improved by using relatively small values of dx and fixing the round-off errors by using interval enclosures of the function f instead. However, with multivariate functions and higher derivatives, the complexity and round-off errors may inevitably increase. This section is devoted to provide some details on the basics of a technique called “*automatic differentiation*” and its arithmetic (For further reading about the techniques discussed here, see, e.g., [KULISCH, 2008B], [MOORE, 1966], [NEIDINGER, 2010], and [MITCHELL, 1991]).

Automatic differentiation (abbreviated “AD”; also called “*algorithmic differentiation*”, “*computational differentiation*”, or “*differentiation arithmetic*”) is an efficient technique that computes the value of the derivative concurrently with computing the value of the function at some point. Here, the formal expression of the derivative is not required, only the expression or the algorithm of the function is needed.

The concept perhaps first introduced in the works of Beda, Wengert, and Moore (see, e.g., [BEDA ET AL., 1959], [WENGERT, 1964], and [MOORE, 1966]). Modern developments of the subject appeared in [RALL, 1981] and [CORLISS AND RALL, 1996]. Moore in [MOORE, 1979] introduced a generalized notion under the title “*recursive evaluation of derivatives*” and used it to evaluate Taylor’s coefficients (A more detailed bibliography of AD can be found in [CORLISS, 1992]). Since then, many techniques and algorithms have used AD as a principal and accurate procedure for the evaluation of derivatives of first and higher order.

In what follows, we carefully construct the basics of differentiation arithmetic and deduce its fundamental properties. We shall use the notation $f^{(k)}$ to denote the k^{th} derivative of a k -times differentiable function f .

Let f and g be two differentiable functions. AD arithmetic is defined for ordered pairs of numbers, such as arithmetic on complex or interval numbers. This pair consists of the value of some function f at some point x_0 , $f(x_0)$, as its first component, and the value of the first derivative of the function f at the same point x_0 , $f^{(1)}(x_0)$, as its second component. We shall denote this pair by $(f, f^{(1)})_{x_0}$ and

call it *AD-pair*.

The differentiation arithmetic is then defined as follows.

$$\begin{aligned}
 (f, f^{(1)})_{x_0} +_{ad} (g, g^{(1)})_{x_0} &= (f + g, f^{(1)} + g^{(1)})_{x_0}, \\
 (f, f^{(1)})_{x_0} -_{ad} (g, g^{(1)})_{x_0} &= (f - g, f^{(1)} - g^{(1)})_{x_0}, \\
 (f, f^{(1)})_{x_0} \times_{ad} (g, g^{(1)})_{x_0} &= (fg, f^{(1)}g + fg^{(1)})_{x_0}, \\
 (f, f^{(1)})_{x_0} \div_{ad} (g, g^{(1)})_{x_0} &= (f/g, (f^{(1)}g - fg^{(1)})/g^2)_{x_0} \text{ and } g \neq 0.
 \end{aligned} \tag{7.3}$$

Where the operations on the left, with the subscript “*ad*”, are performed on AD-pairs, while the operations on the right are the usual operations on real numbers.

Hereafter, if confusion is not likely to ensue, the subscript “*ad*” may be suppressed. Also, for simplicity, we may write $(f, f^{(1)})_{x_0} (g, g^{(1)})_{x_0}$ for $(f, f^{(1)})_{x_0} \times (g, g^{(1)})_{x_0}$ and $(f, f^{(1)})_{x_0} / (g, g^{(1)})_{x_0}$ for $(f, f^{(1)})_{x_0} \div (g, g^{(1)})_{x_0}$.

The rules in 7.3 can be easily derived from the ordinary rules of differentiation. Differentiation arithmetic is easily performed by a computer. We start with the following seeds.

- (1) For a constant c , we have $(c, 0)_{x_0}$,
- (2) For the value of the independent variable x at x_0 , we have $(x_0, 1)_{x_0}$,
- (3) For the known elementary functions, we have the AD-pairs:

$$\begin{aligned}
 &(e^{x_0}, e^{x_0})_{x_0}, \\
 &(\log(x_0), 1/x_0)_{x_0}, \\
 &(\sin(x_0), \cos(x_0))_{x_0}, \\
 &(\cos(x_0), -\sin(x_0))_{x_0}, \\
 &(x_0^2, 2x_0)_{x_0}, \\
 &(\sqrt{x_0}, 1/(2\sqrt{x_0}))_{x_0}, \text{ and so on.}
 \end{aligned}$$

- (4) For elementary composite functions, we use the chain rule. For instance, if h is a differentiable function of x , we have the AD-pairs:

$$\begin{aligned}
 &(\sin(h), h^{(1)} \cos(h))_{x_0}, \\
 &(\sqrt{h}, h^{(1)} / (2\sqrt{h}))_{x_0}, \text{ and so on.}
 \end{aligned}$$

To calculate the AD-pair $(f, f^{(1)})_{x_0}$ for any real differentiable function f at the point x_0 , we apply 7.3 along with the seeds (1) through (4). Since the expression for f is composed of the basic real elementary operations $+$, $-$, \times , and \div , with operands composed of constants, variables, and differentiable elementary functions with well known derivatives, the technique of the computation is described by the following algorithm.

ALGORITHM 7.1

(COMPUTING THE REAL AD-PAIR $(f, f^{(1)})_{x_0}$)

Replace each operand occurring in the expression of f by the AD-pair with the corresponding first

component from the set of seeds (1) through (4), then apply the differentiation arithmetic defined by 7.3 on the AD-pairs to get finally the required AD-pair $(f, f^{(1)})_{x_0}$.

Some examples make things clear.

EXAMPLE 7.6.

Consider the function

$$f(x) = \frac{2(x+1)}{x+3} \text{ with } x \neq -3,$$

we want to compute the AD-pair $(f, f^{(1)})_3$. Applying algorithm 7.1 we get

$$\begin{aligned} (f, f^{(1)})_3 &= \frac{(2, 0)_3 ((3, 1)_3 + (1, 0)_3)}{(3, 1)_3 + (3, 0)_3} \\ &= \frac{(2, 0)_3 (4, 1)_3}{(6, 1)_3} \\ &= \frac{(8, 2)_3}{(6, 1)_3} \\ &= (8/6, 4/36)_3 \\ &= (4/3, 1/9)_3, \end{aligned}$$

hence the value of f at 3 is $4/3$ and the value of its first derivative $f^{(1)}$ at 3 is $1/9$.

EXAMPLE 7.7.

Consider the function

$$f(x) = \cos(\sqrt{x}) \text{ with } x \geq 0,$$

to compute the AD-pair $(f, f^{(1)})_4$, we apply algorithm 7.1 to get

$$\begin{aligned} (f, f^{(1)})_4 &= (\cos(\sqrt{4}), -\sin(\sqrt{4})/2\sqrt{4})_4 \\ &= (\cos(2), -\sin(2)/4)_4. \end{aligned}$$

In the above discussion we have considered only the computation of the first derivative. However, AD can be easily extended to include the computation of higher order derivatives. For instance, for computing the second derivative, we will have AD-triples instead of AD-pairs. The AD-triple for the value of a twice differentiable function f and its first and second derivatives' values at some point x_0 will be denoted by $\langle f, f^{(1)}, f^{(2)} \rangle_{x_0}$.

Now, the differentiation arithmetic in 7.3 would be extended to the arithmetic on AD-triples instead of AD-pairs. Thus, for twice differentiable functions f and g , the rules would be

$$\begin{aligned} \langle f, f^{(1)}, f^{(2)} \rangle_{x_0} \pm_{ad} \langle g, g^{(1)}, g^{(2)} \rangle_{x_0} &= \langle f \pm g, f^{(1)} \pm g^{(1)}, f^{(2)} \pm g^{(2)} \rangle_{x_0}, \\ \langle f, f^{(1)}, f^{(2)} \rangle_{x_0} \times_{ad} \langle g, g^{(1)}, g^{(2)} \rangle_{x_0} &= \langle fg, f^{(1)}g + fg^{(1)}, f^{(2)}g + 2f^{(1)}g^{(1)} + fg^{(2)} \rangle_{x_0}, \\ \langle f, f^{(1)}, f^{(2)} \rangle_{x_0} \div_{ad} \langle g, g^{(1)}, g^{(2)} \rangle_{x_0} &= \langle f/g, (f^{(1)}g - fg^{(1)})/g^2, h \rangle_{x_0} \text{ and } g \neq 0, \end{aligned} \quad (7.4)$$

where $h = \left((2g^{(1)2} - gg^{(2)})f + (f^{(2)}g - 2g^{(1)}f^{(1)})g \right) / g^3$.

Similarly, the seeds could be extended to include the second derivative. For instance, the AD-triple for the constant would be $\langle c, 0, 0 \rangle_{x_0}$ and for the independent variable $\langle x_0, 1, 0 \rangle_{x_0}$. The elementary functions are extended by the same manner.

To compute the AD-triple $\langle f, f^{(1)}, f^{(2)} \rangle_{x_0}$, for a twice differentiable function f , we apply an extension of algorithm 7.1 by replacing AD-pairs with AD-triples and performing differentiation arithmetic on AD-triples defined by 7.4. To illustrate this, we next give an example.

EXAMPLE 7.8.

Consider the function

$$f(x) = x + 3,$$

to compute the AD-triple $\langle f, f^{(1)}, f^{(2)} \rangle_2$, we apply the extended rules above to obtain

$$\begin{aligned} \langle f, f^{(1)}, f^{(2)} \rangle_2 &= \langle 2, 1, 0 \rangle_2 + \langle 3, 0, 0 \rangle_2 \\ &= \langle 5, 1, 0 \rangle_2. \end{aligned}$$

The techniques described above could be generalized to compute more higher order derivatives. For multivariate differentiable functions, the values of the partial derivatives could be computed using AD with only the formal expression of the function. For instance, consider the function $f(x, y) = x + y$, one can compute the partial derivative with respect to x at some point (x_0, y_0) , denoted by $f_x^{(1)}(x_0, y_0)$, by starting with the AD-pairs $\langle c, 0 \rangle_{(x_0, y_0)}$, for a constant c , $\langle x_0, 1 \rangle_{(x_0, y_0)}$ for the independent variable x , and $\langle y_0, 0 \rangle_{(x_0, y_0)}$ for the independent variable y . That is, the other variable y is considered as a constant. This also can be generalized for higher order partial derivatives.

There are various interval algorithms and other applications which require evaluation of the derivative at a given interval or range of values. For these, combination of interval arithmetic and AD has been used. By the same concept as computing with real numbers, the interval value of the function and the interval value of the derivative over some given interval are computed together using interval arithmetic combined with differentiation arithmetic. This combination, which we shall call “*interval automatic differentiation*”, has proved accuracy and efficiency in many scientific computations like enclosures of Taylor coefficients, gradients, integrals, bounding boxes in ray tracing, and solutions of ordinary differential equations, it is also very efficient and robust in global optimization techniques.

Interval automatic differentiation can be simply described as follows. Let $f : \mathcal{D} \subseteq \mathbb{R} \mapsto \mathbb{R}$ be a continuously differentiable real-valued function and assume that we are given the formal expression for f . Let $X = [\underline{x}, \bar{x}]$ be an interval number such that $X \subseteq \mathcal{D}$. Then $f(X)$ is the expression for the interval-valued function defined by the same rule as f .

The interval AD-pair shall be denoted by $(f, f^{(1)})_{X_0}$. The first component of the pair represents the value of the interval-valued function f at X_0 , $f(X_0)$, and the second component represents the value of the interval-valued derivative $f^{(1)}$ at X_0 , $f^{(1)}(X_0)$.

Computing the interval AD-pair $(f, f^{(1)})_{X_0}$, for a continuously differentiable function f , follows the same technique as computing real AD-pairs. Thus, in algorithm 7.1, if we replace real numbers with interval numbers, real arithmetic with interval arithmetic, and real AD-pairs with interval AD-pairs, we finally get the required interval AD-pair $(f, f^{(1)})_{X_0}$.

The following example makes this clear.

EXAMPLE 7.9.

Consider again the function in example 7.7 given by

$$f(x) = \cos(\sqrt{x}) \text{ with } x \geq 0,$$

computing the interval AD-pair $(f, f^{(1)})_{[1,4]}$ yields

$$\begin{aligned} (f, f^{(1)})_{[1,4]} &= \left(\cos(\sqrt{[1,4]}), -\left(\sin(\sqrt{[1,4]})\right) / 2\sqrt{[1,4]} \right)_{[1,4]} \\ &= \left(\cos([\sqrt{1}, \sqrt{4}]), -\left(\sin([\sqrt{1}, \sqrt{4}])\right) / 2[\sqrt{1}, \sqrt{4}] \right)_{[1,4]} \\ &= (\cos([1, 2]), -(\sin([1, 2])) / 2[1, 2])_{[1,4]} \\ &= ([\cos(2), \cos(1)], -[\sin(1), 1] / [2, 4])_{[1,4]} \\ &= ([\cos(2), \cos(1)], [-1/2, -1/4][\sin(1), 1])_{[1,4]} \\ &= ([\cos(2), \cos(1)], [-1/2, (-1/4)\sin(1)])_{[1,4]}. \end{aligned}$$

In the last example, we computed the interval AD-pair $(f, f^{(1)})_{[1,4]}$ for the function in example 7.7 at the interval number $[1, 4]$. The first component of the resulting pair, $[\cos(2), \cos(1)]$, is an estimation of the image of f over the interval $[1, 4]$, while the second component, $[-1/2, (-1/4)\sin(1)]$, is an estimation of the image of $f^{(1)}$ over the same interval. That is

$$\begin{aligned} f(4) &= \cos(2) \in [\cos(2), \cos(1)] = f([1, 4]), \\ f^{(1)}(4) &= -\sin(2)/4 \in [-1/2, (-1/4)\sin(1)] = f^{(1)}([1, 4]). \end{aligned}$$

The resulting AD-pairs of examples 7.7 and 7.9 could be represented on the machine by floating-point numbers and outward or upward rounded interval numbers (see section 5), respectively.

Interval AD, like real AD, could be generalized for higher order derivatives and multivariate functions. The information we can get from the interval AD-pair $(f, f^{(1)})_{X_0}$ is very important and reliable. For instance, if $0 \notin f(X_0)$, then the interval X_0 cannot contain any solutions for the equation $f(x) = 0$ and this is very useful in solving systems of nonlinear equations. Many real and interval algorithms require the estimation of the image of $f^{(1)}$ over the interval X_0 to conclude some important properties about the function f and the interval X_0 . For example, if $0 \notin f^{(1)}(X_0)$, then f must be monotonic over X_0 and the image of f could be easily computed (see section 7.1), also this property is of extensive use in root-isolation algorithms such as “the interval root-isolation algorithm” used in ray tracing in computer graphics (A bit of perspective on the use of interval arithmetic in computer graphics shall be provided in section 7.3).

Finally, the above discussion showed that, real and interval automatic differentiation methods are very robust and efficient for computing the values of the function and its derivatives at some point simultaneously without the need to derive the expressions for the derivatives. Since AD operations deal with numbers, either real or interval, there are many software packages that easily perform AD operations for floating-point numbers or rounded interval numbers. Ideas of implementation vary, including object-oriented programming (OOP) and operator overloading. This implementation defines an object for the AD-tuple and overloads the usual floating-point operations with operations on the

AD-tuples. Examples of AD software include “INTLAB”¹⁶, “FADBAD++”¹⁷, “GlobSol”¹⁸, and many others¹⁹.

7.3

Interval Methods in Computer Graphics

Interval arithmetic plays an important role in computer graphics and its applications. In computer graphics, ray tracing is a technique that generates many special effects and hence can generate more realistic images. Among these effects are lighting, shading, hidden surface elimination, transparency, and many other effects. The basic idea of ray tracing algorithms is to follow the paths of light rays and detect intersections between these rays and the various objects in the scene. The main drawback of ray tracing is that it is computationally too costly; rendering may take days (For further details on ray tracing, see, e.g., [AGOSTON, 2005], [BUSS, 2003] and [BAKER ET AL., 2010]).

Testing of intersections is a main part of ray tracing algorithms. In fact, the long computational time of ray tracing is due to this test. Test of intersections has a wide range in other applications like test of collisions, and any motion-related applications.

In intersection testing, three criteria should be met: accuracy, robustness, and speed. For these, interval arithmetic techniques are used. In what follows we study the use of interval arithmetic in ray tracing implicit surfaces, in particular, in the ray-surface intersection problems (For further reading about using interval arithmetic in ray tracing, see, e.g., [MITCHELL, 1991], [SANJUAN-ESTRADA ET AL., 2003], [MITCHELL, 1990], [XIA AND ZHANG, 2003], and [ABBOTT, 2012]).

The principal problem in ray tracing is the problem of ray-surface intersections. For simplicity of rendering, each object in the scene is represented by an implicit surface.

Let \mathcal{S} be an implicit surface, then \mathcal{S} is given by

$$\mathcal{S} = \left\{ s = (x, y, z) \in \mathbb{R}^{(3)} \mid f(s) = 0 \right\}, \quad (7.5)$$

where $f : \mathcal{D} \subseteq \mathbb{R}^{(3)} \mapsto \mathbb{R}$ is a real-valued function. Now consider the parametric representation of a ray (see Figure 2) given by

$$\mathbf{r} = \mathbf{o} + t\mathbf{d}, \quad (7.6)$$

where

$\mathbf{o} = (\mathbf{o}_x, \mathbf{o}_y, \mathbf{o}_z)$ is the initial position,

$\mathbf{d} = (\mathbf{d}_x, \mathbf{d}_y, \mathbf{d}_z)$ is a unit vector that defines the direction of the ray,

$t \geq 0$ is the parameter that represents the distance of any point \mathbf{r} along the ray from \mathbf{o} .

Then, we can write the ray as the set of points

$$\begin{aligned} \mathcal{R} &= \left\{ \mathbf{r}(t) \in \mathbb{R}^{(3)} \mid t \geq 0 \right\} \\ &= \left\{ (\mathbf{o}_x + t\mathbf{d}_x, \mathbf{o}_y + t\mathbf{d}_y, \mathbf{o}_z + t\mathbf{d}_z) \in \mathbb{R}^{(3)} \mid t \geq 0 \right\}. \end{aligned}$$

¹⁶ <http://www.ti3.tu-harburg.de/rump/intlab/>

¹⁷ <http://www.fadbad.com/fadbad.html>

¹⁸ http://interval.louisiana.edu/GlobSol/download_GlobSol.html

¹⁹ <http://www.autodiff.org/?module=Tools>

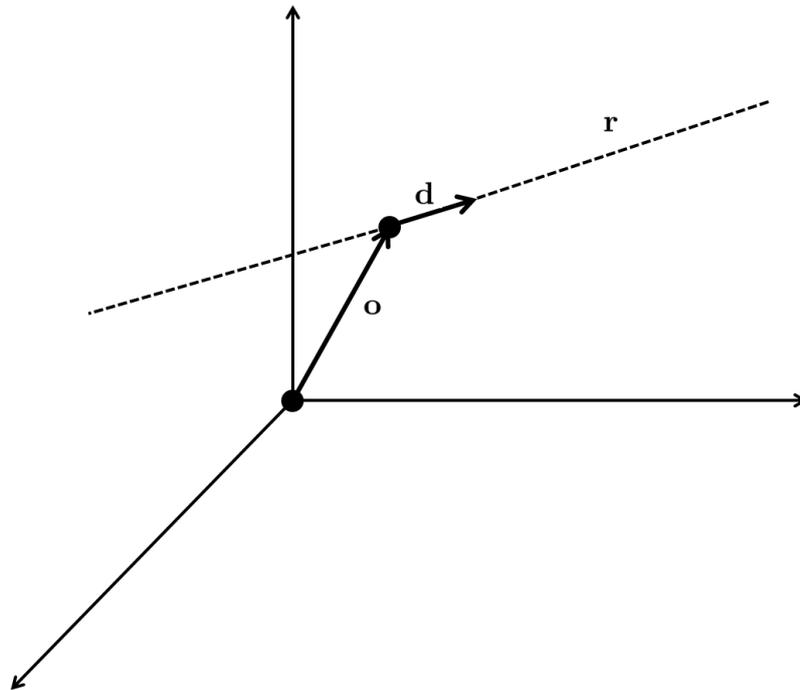


FIGURE 2. An illustration of the ray \mathcal{r} .

To find the intersection points (see Figure 3) between \mathcal{R} and \mathcal{S} , we solve the surface equation in 7.5 for \mathbf{r} in 7.6 which reduces the problem to just finding the roots of a function g of one variable t . That is

$$f(\mathbf{r}) = f(\mathbf{o} + t\mathbf{d}) = g(t) = 0. \quad (7.7)$$

Solving 7.7 locates values for the parameter t which are the distances from \mathbf{o} to the points of intersection on the surface \mathcal{S} along the ray \mathcal{R} .

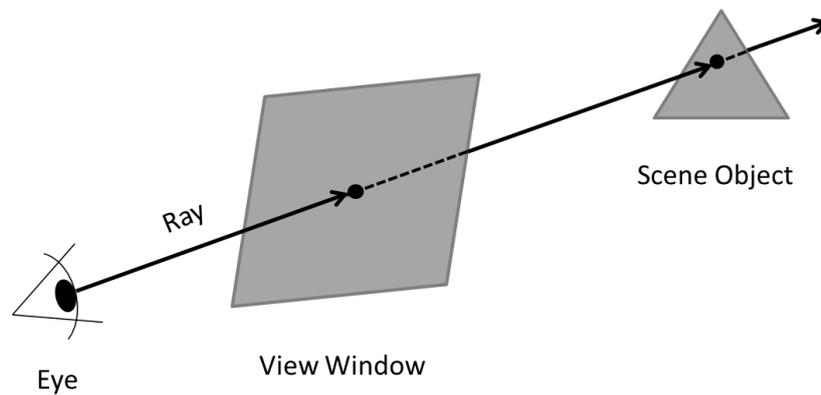


FIGURE 3. A diagrammatic representation of ray intersection.

To illustrate the matters, consider the following example.

EXAMPLE 7.10.

Assume that the surface \mathcal{S} is a cylinder with radius r and height h centered at the origin and whose axis is the z -axis. That is

$$\mathcal{S} = \{(x, y, z) \in \mathbb{R}^{(3)} \mid x^2 + y^2 - r^2 = 0 \wedge 0 \leq z \leq h\}.$$

Our objective is to find the points, if any, that satisfy both the ray equation 7.6 and the above cylinder equation. Solving for \mathbf{r} in 7.6, we get

$$(\mathbf{o}_x + t\mathbf{d}_x)^2 + (\mathbf{o}_y + t\mathbf{d}_y)^2 - r^2 = 0 \wedge 0 \leq \mathbf{o}_z + t\mathbf{d}_z \leq h \wedge t \geq 0.$$

Hence the problem is reduced to

$$g(t) = at^2 + bt + c = 0 \wedge 0 \leq \mathbf{o}_z + t\mathbf{d}_z \leq h \wedge t \geq 0,$$

where

$$\begin{aligned} a &= \mathbf{d}_x^2 + \mathbf{d}_y^2, \\ b &= 2\mathbf{o}_x\mathbf{d}_x + 2\mathbf{o}_y\mathbf{d}_y, \\ c &= \mathbf{o}_x^2 + \mathbf{o}_y^2 - r^2. \end{aligned}$$

We then have two cases.

Case 1. $a = 0$. Then the ray is parallel to the cylinder axis. We then have to check if the ray lies in the cylinder. That is $\mathbf{o}_x^2 + \mathbf{o}_y^2 = r^2$.

Case 2. $a \neq 0$. In this case we have to find the solutions to the quadratic equation $g(t) = 0$ along with the condition $0 \leq \mathbf{o}_z + t\mathbf{d}_z \leq h \wedge t \geq 0$.

If there were no intersection points between the ray and the sides of the cylinder and the cylinder is closed with a top or bottom or both, then the ray may intersect these parts instead. To find these points of intersection, if exist, we must solve the following equation for \mathbf{r}

$$x^2 + y^2 \leq r^2 \wedge (z = 0 \vee z = h).$$

The previous example shows that the intersection problem has been reduced to the problem of solving a quadratic equation $g(t) = at^2 + bt + c = 0$. Unfortunately, the problem of intersections is not, in general, that easy one, especially for scenes with many objects that lead to nonlinear equations. Therefore, we shall need suitable numerical methods for approximating the solutions of general nonlinear equations $g(t) = 0$.

Several methods were developed for solving these problems and to reduce the time spent on the testing of intersections. For the general types of nonlinear equations $g(t) = 0$, and starting with an initial interval $I = [\underline{a}, \bar{a}]$ (may be obtained by intersection with a simple bounding box) we usually perform two steps (see Figure 4) to find the roots.

Step 1 (root isolation). The roots are isolated by finding subintervals $I_i = [\underline{a}_i, \bar{a}_i]$ in I which are known to contain one and only one root of the function $g(t) = 0$.

Step 2 (root refinement). Each of the intervals, obtained from step 1, for each single root is refined by reducing its width until we reach the machine bounds to accurately isolate the root. Usually local search techniques are used in this step.

The root isolation step is the harder. Many root isolation algorithms were developed for finding the real roots for polynomials. For more general functions beyond the polynomials, few attempts have been made and mostly based on heuristic methods. On the other hand, many efficient algorithms exist for the root refinement step including techniques based on the use of interval arithmetic (see, e.g., [ABBOTT, 2012]).

Interval analysis techniques are used heavily to solve systems of nonlinear equations. For this

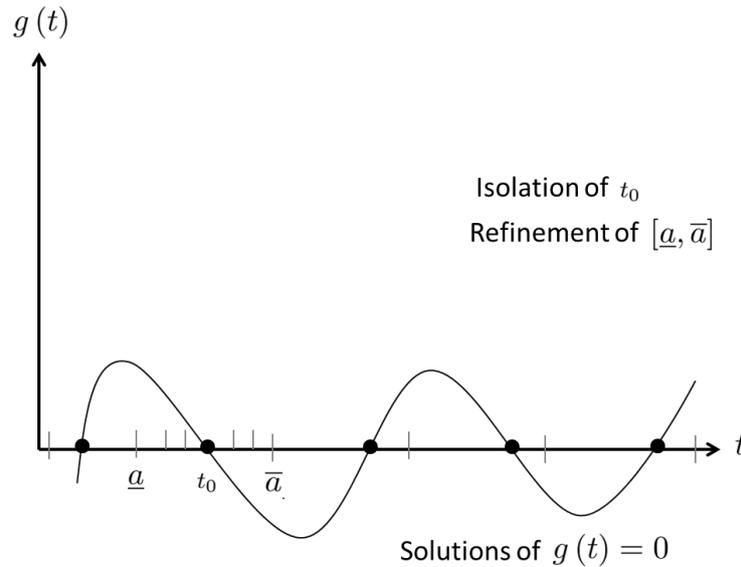


FIGURE 4. Root isolation and refinement.

reason, interval techniques play an important role in solving such problems and reducing their computational time. Moore in [MOORE, 1966] developed a root isolation algorithm based on interval arithmetic for a general class of functions involving rational and transcendental functions. Moore's algorithm is based on the power of interval arithmetic in estimating the image of real functions (see section 7.1).

Starting with the initial interval $I = [a, \bar{a}]$ and a continuously differentiable function g of one variable t , the recursive interval root-isolation algorithm developed by Moore to isolate the roots of the function g is described as follows.

ALGORITHM 7.2

(THE INTERVAL ROOT-ISOLATION ALGORITHM)

The algorithm is described by the following four steps.

- Step 1.** Evaluate $g(I)$. If $0 \notin g(I)$, then there are no roots in this interval and we are done with this interval.
- Step 2.** Evaluate the first derivative $g^{(1)}(I)$. If $0 \notin g^{(1)}(I)$, then g is monotonic in the interval. In this case, if $g(\underline{a})g(\bar{a}) \leq 0$, then there is one root in the interval which can be located accurately by some root refinement method. If $g(\underline{a})g(\bar{a}) > 0$, then there are no roots in the interval.
- Step 3.** If $g(I)$ and $g^{(1)}(I)$ both contain zero, then subdivide the interval I at its midpoint and recursively process $[\underline{a}, (\underline{a} + \bar{a})/2]$ and $[(\underline{a} + \bar{a})/2, \bar{a}]$.
- Step 4.** The process of subdivision should be stopped when the width of an interval approaches the machine bounds. For instance, if the subdivision, in step 3, at the midpoint reaches the machine endpoints or if the width of the interval reaches the allowed minimum value.

In some applications of computer graphics the first intersection point is only needed. This intersection point is the closest root of g to the initial position \mathbf{o} of the ray, that is, the smallest value of t satisfying $g(t) = 0$ with $t \geq 0$. Hence, for this purpose, the closest interval in step 3 is processed first and the algorithm can stop once the first root has been found in step 2 or 4.

The dependency problem of the classical interval theory, see section 6, could appear when we

deal with more complex surfaces. Because of this problem the speed of the algorithm may depend on the form of the expression of the function. Some improvements could be made like subdivision techniques which produce more narrow intervals and thus give more accurate results (For more details on subdivision techniques see section 7.1).

Interval AD could improve the efficiency of the algorithm. With this technique, the values of the interval AD-pair $(g, g^{(1)})_I$ can be computed concurrently and without the need to know the expression of $g^{(1)}$ (Refer to section 7.2 for more details on AD).

Sometimes the problem of deriving an explicit closed-form expression for g from the ray and surface equations is not easily solved. However, with the help of automatic differentiation, we can find the AD-pair $(g, g^{(1)})_{t_0}$, for some point t_0 , by the following two-step technique.

(1) Start with a point (x, y, z) in \mathcal{R} and generate the following AD-pairs

$$\begin{aligned} (x, x^{(1)})_{t_0} &= (\mathbf{o}_x + t_0 \mathbf{d}_x, \mathbf{d}_x)_{t_0}, \\ (y, y^{(1)})_{t_0} &= (\mathbf{o}_y + t_0 \mathbf{d}_y, \mathbf{d}_y)_{t_0}, \\ (z, z^{(1)})_{t_0} &= (\mathbf{o}_z + t_0 \mathbf{d}_z, \mathbf{d}_z)_{t_0}. \end{aligned}$$

(2) Substitute for (1) in the surface equation 7.5, and use differentiation arithmetic to finally get the required AD-pair $(g, g^{(1)})_{t_0}$.

For instance, assume that the surface is a simple unit circle given by

$$x^2 + y^2 - 1 = 0.$$

Substituting from (1) above and applying differentiation arithmetic we get

$$(\mathbf{o}_x + t_0 \mathbf{d}_x, \mathbf{d}_x)_{t_0}^2 + (\mathbf{o}_y + t_0 \mathbf{d}_y, \mathbf{d}_y)_{t_0}^2 - (1, 0)_{t_0} = (0, 0)_{t_0},$$

hence

$$\left((\mathbf{o}_x + t_0 \mathbf{d}_x)^2, 2\mathbf{d}_x (\mathbf{o}_x + t_0 \mathbf{d}_x) \right)_{t_0} + \left((\mathbf{o}_y + t_0 \mathbf{d}_y)^2, 2\mathbf{d}_y (\mathbf{o}_y + t_0 \mathbf{d}_y) \right)_{t_0} - (1, 0)_{t_0} = (0, 0)_{t_0},$$

which yields

$$\left((\mathbf{o}_x^2 + \mathbf{o}_y^2 - 1) + (2\mathbf{o}_x \mathbf{d}_x + 2\mathbf{o}_y \mathbf{d}_y) t_0 + (\mathbf{d}_x^2 + \mathbf{d}_y^2) t_0^2, 2\mathbf{d}_x (\mathbf{o}_x + t_0 \mathbf{d}_x) + 2\mathbf{d}_y (\mathbf{o}_y + t_0 \mathbf{d}_y) \right)_{t_0} = (0, 0)_{t_0},$$

and with some simplification the result is

$$(g, g^{(1)})_{t_0} = (\alpha, \beta)_{t_0} = (0, 0)_{t_0},$$

where

$$\begin{aligned} \alpha &= (\mathbf{o}_x^2 + \mathbf{o}_y^2 - 1) + (2\mathbf{o}_x \mathbf{d}_x + 2\mathbf{o}_y \mathbf{d}_y) t_0 + (\mathbf{d}_x^2 + \mathbf{d}_y^2) t_0^2, \\ \beta &= (2\mathbf{o}_x \mathbf{d}_x + 2\mathbf{o}_y \mathbf{d}_y) + (2\mathbf{d}_x^2 + 2\mathbf{d}_y^2) t_0. \end{aligned}$$

Finally, we should mention that it is a hard problem to find a reliable technique that is robust, accurate, and fast for better rendering scenes with many complex objects. Interval arithmetic techniques described above are very successful and viable and have been used in ray tracing with various algebraic and non-algebraic surfaces.

8 INTERVALS, AND MORE INTERVALS: A VIEW TO THE FUTURE

What is the future of interval computations? The answer may be brief: “*Whenever uncertainty exists, there shall be always intervalizations*”. Fortunately, computers are getting faster and most existing *parallel processors* provide a tremendous computing power. So, with little extra hardware, it is very possible to make interval computations as fast as floating-point computations. The interval theory is likely to have more widespread applications in the future, for many reasons:

- Interval algorithms are *naturally parallel*, because they progress by deleting regions where solutions are proved not to exist. Intervals provide the *only known* general algorithms that achieve *linear* speedup, as the number of processors increases in parallel computing systems.
- Interval arithmetic is, arguably, the *best* and *most efficient* way to safely translate ever-increasing computer speed into mission-critical problem solutions that are otherwise impractical or impossible to obtain.
- By using interval algorithms to solve nonlinear problems, more accurate mathematical models of physical phenomena become practical.
- With interval arithmetic, it is possible to automatically perform rigorous error analysis, and solve nonlinear problems that were previously thought to be impossible to solve.
- Speed is not all-important anymore. We can get worthwhile accurate results by sacrificing some speed.

In the early stages, classical interval arithmetic was preoccupied with the effect of rounding errors on the accuracy of expression evaluation. Later, it was realized that the interval theory has the potential of going beyond expression evaluation and on to solving problems that are inaccessible to conventional approaches. For example, interval analysis has been used, by Thomas Hales of the university of Michigan, in computational parts of a proof of *Kepler’s conjecture* on the densest packing of spheres. Making use of classical interval mathematics, Hales introduced a *definitive proof* of a conjecture that perplexed mathematicians for nearly 400 years (see, e.g., [HALES, 2005] and [MOORE ET AL., 2009]). Another long-standing problem, *Smale’s fourteenth conjecture*, was solved by Warwick Tucker, by showing, using interval arithmetic, that a strange attractor ensues from Lorenz equations (see, e.g., [SMALE, 1998], [TUCKER, 2002], and [LODWICK, 2008]).

Current and future research efforts in interval mathematics can be classified mainly into three categories; *interval standardizations*, *interval implementations*, and *generalizations* of the mathematical theory of intervals. Now, the subject of interval mathematics concerns numerous scientific journals and publishers. The journal “*Interval Computations*” started as a joint Soviet-Western enterprise in 1991, and continues as the journal “*Reliable Computing*”. Besides that, “*Computing*” commonly publishes material related to interval computations, as well as the journal “*Global Optimization*”. Traditional numerical analysis journals such as “*BIT*”, the “*SIAM Journal on Numerical Analysis*”, the “*SIAM Journal on Scientific and Statistical Computing*”, and the “*ACM Transactions on Mathematical Software*” contain articles on interval computations (For further resources, see, e.g., [HANSEN AND WALSTER, 2003], [JAULIN ET AL., 2001], [KEARFOTT, 1996], and [MOORE ET AL., 2009]).

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10 KEY TERMS AND DEFINITIONS

Quantitative Knowledge: Knowledge acquired through intuition, experiments, measurements, and proposed hypotheses.

Uncertainty: The quantitative estimation of errors present in measured data.

Interval Arithmetic: An arithmetic defined on sets of real intervals (*interval numbers*), rather than sets of real numbers.

Nondistributive Abelian Semiring: An abelian semiring whose multiplication does not distribute over addition.

Complex Interval Arithmetic: An arithmetic defined on sets of complex intervals (*complex interval numbers*).

Machine Interval Arithmetic: A machine realization of interval arithmetic defined such that the result of a machine interval operation is guaranteed to contain the exact result of an interval operation.

Interval Dependency Problem: The persisting problem of getting overestimations when estimating the image of real functions, some of whose variables are *functionally dependent*, using naive interval computations.

Automatic Differentiation: A technique that computes the value of the derivative concurrently with computing the value of the function at some point, without the need to know the formal expression of the derivative.

Ray Tracing: A technique in computer graphics that generates many special effects such as lighting, shading, hidden surface elimination and many others; and hence can generate more realistic images.

Interval Root Isolation: Using interval arithmetic to isolate the roots for a general class of functions involving rational and transcendental functions.

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