High speed and exception-free interval arithmetic, from closed and bounded real intervals to connected sets of real numbers

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Abstract

This paper gives a brief sketch of the development of interval arithmetic. Early books consider interval arithmetic for closed and bounded real intervals. It was then extended to unbounded real intervals. Considering $-\infty$ and $+\infty$ only as bounds but not as elements of unbounded real intervals leads to an exception-free calculus.

Formulas for computing the lower and the upper bound of the interval operations including the dot product are independent of each other. On the computer high speed can and should be obtained by computing both bounds in parallel and simultaneously. Another increase of speed and accuracy can be obtained by computing dot products exactly.

Arithmetic for closed real intervals even can be extended to open and half-open real intervals, to connected sets of real numbers. Also this leads to a calculus that is free of exceptions.

1 Remarks on the History of Interval Arithmetic

In early books on Interval Arithmetic by R. E. Moore, [30], G. Alefeld and J. Herzberger [7, 8], E. Hansen [15], and others interval arithmetic is defined and studied for closed and bounded real intervals. Frequent attempts to extend it to unbounded intervals [19, 20, 37] led to inconsistencies again and again. If $-\infty$ and $+\infty$ are considered as elements of a real interval, unsatisfactory operations like $\infty - \infty$, $0 \cdot \infty$, ∞/∞ occur and are to be dealt with.

The books [25, 27] eliminated these problems. Here interval arithmetic just deals with closed and connected sets of real numbers. Since $-\infty$ and $+\infty$ are not real numbers, they can not be elements of a real interval. They only serve as bounds for the description of real intervals. In real analysis a set of real numbers is called closed, if its complement is open. So intervals like $(-\infty, a]$ or $[b, +\infty)$ with real numbers a and b nevertheless are closed real intervals.

Formulas for the operations for unbounded real intervals can now be obtained from those for bounded real intervals by continuity considerations. Obscure operations as mentioned above do not occur in the operations for unbounded real intervals. For a proof of this assertion see section 4.10 in [27]. This result also remains valid for floating-point interval arithmetic. For details and proof see section 4.12 in [27]. Fortunately this understanding of arithmetic for unbounded real and floating-point intervals was accepted by IEEE 1788.

Early books on interval arithmetic as mentioned in the first paragraph just make use of the four basic arithmetic operations add, subtract, multiply, and divide $(+, -, \cdot, /)$ for real and floating-point intervals. The latter are provided with maximum accuracy. Later books [16, 17, 18, 19, 20, 25, 27] in addition provide and make use of an exact dot product.

2 High Speed Interval Arithmetic by Exact Evaluation of Dot Products

Since 1989 major scientific communities like GAMM and the IFIP Working Group on Numerical Software repeatedly required [1, 2, 5, 6] exact evaluation of dot products of two floating-point vectors on computers. The exact dot product (EDP) brings speed and accuracy to floating-point and interval arithmetic.

Solution of a system of linear equations is a central task of Numerical Analysis. A guaranteed solution can be obtained in two steps. The first step computes an approximate solution by some kind of Gaussian elimination in conventional floating-point arithmetic. A second step, the verification step, then computes a highly accurate enclosure of the solution.

By an early estimate of S. M. Rump [36] the verification step can be done with less than 6 times the number of elementary floating-point operations needed for computing an approximation in the first step.

The verification step just consists of dot products. For details see Section 9.5 on Verified Solution of Systems of Linear Equations, pp. 333-340 in [27]. Hardware implementations of the EDP at Karlsruhe in 1993 [9, 10] and at Berkeley in 2013 [11] show that it can be computed in about 1/6th of the time needed for computing a possibly wrong result in conventional floating-point arithmetic! So the EDP reduces the computing time needed for the verification step to the one needed for computing an approximate solution by Gaussian elimination. In other words: A guaranteed solution of a system of linear equations can be computed in twice the time needed for computing an approximation in conventional floating-point arithmetic.

The time needed for solving a system of linear equations can additionally be reduced if the EDP is already applied during Gaussian elimination in the first step. The inner loop here just consists of dot products. The EDP would reduce the computing time and additionally increase the accuracy of the approximate solution.

Using a software routine for a correctly rounded dot product as an alterna-

tive for a hardware implemented EDP leads to a comparatively slow process. A correctly rounded dot product is built upon a computation of the dot product in conventional floating-point arithmetic. This is already 5 to 6 times slower than an EDP. High accuracy then is obtained by clever and sophisticated mathematical considerations which all together make it slower than the EDP by more than one magnitude. High speed and accuracy, however, are essential for acceptance and success of interval arithmetic.

The simplest and fastest way computing a dot product is to compute it exactly. The unrounded products are accumulated into a modest fixed-point register on the arithmetic unit with no memory involvement. By pipelining this can be done in the time the processor needs to read the data, i.e., no other method can be faster, pp. 267-268 in [27], and [28].

A frequent argument against computing dot products exactly is that it needs an accumulator of about 4 thousand bits. This, however, is not well taken. The 4 thousand bits are a consequence of the huge exponent range of the IEEE 754 arithmetic standard. It aims for reducing the number of under- and overflows in a floating-point computation. There is no under- and overflow, however, in interval arithmetic. Interval arithmetic does not need an extreme exponent range of $10^{\pm 308}$ or $2^{\pm 1023}$. If in an interval computation a bound becomes $-\infty$ or $+\infty$ the other bound still is a finite floating-point number. In a following operation this interval can become finite again.

Program packages for interval arithmetic for the IBM /370 architecture developed by different commercial companies like IBM, Siemens and others in the 1980ies provide and make use of an exact dot product [38, 39, 40, 41]. See also [42].

3 A Floating-point Number Format Appropriate for Interval Arithmetic

Floating-point and interval arithmetic are distinct calculi. Floating-point arithmetic as specified by IEEE 754 is full of complicated constructs, data and events like rounding to nearest, overflow, underflow, $+\infty$, $-\infty$, +0, -0 as numbers, or operations like $\infty - \infty$, ∞/∞ , $0 \cdot \infty$. All these constructs do not occur in interval arithmetic. In contrast to this, reasonably defined interval arithmetic leads to an exception-free calculus. It is thus only reasonable to keep the two calculi strictly separate.

For interval arithmetic an exponent range between -77 and +77 seems to be reasonable. This is a huge range of numbers.¹ It is 1/4th of the exponent range of the IEEE 754 floating-point format double precision. Then 9 bits suffice for the representation of the exponent. So in comparison with the 11 bits of the IEEE 754 number representation two bits are left for other purposes. We use one of these bits for extending the number of fraction bits by one from 53 to 54 and the other bit to indicate whether the interval bracket is open or closed.

 $^{^{1}}$ The number of atoms in the universe is less than 10^{80} .



Figure 1: The floating-point number format.

In accordance with [14] we call this bit the ubit, u for short. A ubit u = 0 represents a closed and a ubit u = 1 an open interval bracket.

Figure 1 shows the format of a floating-point number.

So the ubit u allows to distinguish between open and closed interval bounds. A bound of the result of an interval operation only can be closed, if both operands are closed interval bounds. So in the majority of cases the bound in the result will be open.

We now consider a general floating-point number system S = S(b, f, emin, emax), with base b, f bits of the fraction, least and greatest exponent emin and emax, respectively. Then a register of

$$L = k + 2emax + 2f + 2|emin|$$

bits suffices for computing dot products exactly. Here k denotes a number of guard digits for counting intermediate overflows of the register. It is important to note that the size of this register only depends on the data format. In particular it is independent of the number n of components of the two vectors to be multiplied.

In case of a 64-bit interval bound, one bit is used for the sign s, 9 bits are used for the exponent, 53 bits for the fraction and one bit for the ubit u. As usual the leading bit of the fraction of a normalized binary floating-point number is not stored, so the fraction actually consists of 54 bits. For the exponent emin subnormal numbers with a denormalized mantissa are permitted.

For this data format with f = 54, emax = |emin| = 256, and k = 20, we get for L = 20 + 512 + 108 + 512 = 1152 bits. This register can be represented by 18 words of 64 bits.

As justification for the exponent range of emax = |emin| = 256 we just mention that the data format long of the IBM /370 architecture covers a range of about 10^{-75} to 10^{75} . This architecture dominated the market for more than 25 years and most problems could conviniently be solved with machines of this architecture within this range of numbers. We mention once more that there is no under- and overflow in interval arithmetic.

A reduction of the exponent range to 8 bits with emax = |emin| = 128 would allow an extension of the fraction by one more bit to f = 55 bits. This leads to a register of L = k + 2emax + 2f + 2|emin| = k + 256 + 110 + 256 = k + 622 bits and with k = 18 to 10 words of 64 bits.

For the data format single precision with a word length of 32 bits the size L of the register for computing dot products exactly even shrinks to 9 words of 64 bits: 1 bit is used for the sign, 8 bits are used for the exponent, 23 bits for the fraction, one bit is used for the ubit u, emax = 128, and emin = -128. So

with k = 18 we get L = k + 2emax + 2f + 2|emin| = 18 + 256 + 46 + 256 = 576 bits. This register can be represented by 9 words of 64 bits.

The formulas for computing the lower and the upper bound of an interval operation are independent of each other. This also holds for the EDP. So on the computer the lower and the upper bound of the result of an interval operation can and should be computed simultaneously in parallel. This allows performing any interval operation at the speed of the corresponding floating-point operation. For details see Section 7.3 in [27], or [29]. High speed is essential for acceptance and success of interval arithmetic.

4 From Closed Real Intervals to Connected Sets of real Numbers

For about 40 years interval arithmetic was defined for the set of closed and bounded real intervals. The books [25, 27] extended it to unbounded real intervals. The book The End of Error by John Gustafson [14] finally shows that it even can be extended to just connected sets of real numbers. These can be closed, open, half open, bounded or unbounded. The book shows that arithmetic for this expanded set is closed under addition, subtraction, multiplication, division, also square root, powers, logarithm, exponential, and many other elementary functions needed for technical computing, i.e., arithmetic operations for connected sets of real numbers always lead to a connected set of real numbers. The calculus is free of exceptions. It remains free of exceptions if the bounds are restricted to a floating-point screen. John Gustafson shows in his book that this extension of interval arithmetic opens new areas of applications.

A detailed description and analysis of this expanded interval arithmetic for connected sets of real numbers including an exact dot product is given in [29].

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