Lecture Notes in Computer Science

Edited by G. Goos and J. Hartmanis

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Interval Mathematics

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A GENERALIZED INTERVAL ARITHMETIC

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1. INTRODUCTION

Interval arithmetic suffers from an inherent shortcoming that causes it to produce results which are not sharp. Perhaps the simplest example is the fact that there is no additive inverse. If we subtract an interval $X = [a,b]$ from itself, we obtain

$$X - X = [a - b, b - a] .$$

That is, $X - X \neq [0,0]$ (unless $a = b$).

The difficulty is that in the arithmetic process, it is not recognized that the correct result is

$$X - X = \{x - x : x \in X\} = [0,0] .$$

Instead, we obtain

$$\{x_1 - x_2 : x_1 \in X, x_2 \in X\} .$$

That is, the real variables $x_1 \in X$ and $x_2 \in X$ are treated as if they were independent.

More generally, if a given interval X occurs more than once in a computation, the result may fail to be sharp.

In this paper, we shall introduce a generalized interval arithmetic (which we abbreviate as g.i.a.) which reduces this effect.

2. MOTIVATION

Suppose we want to evaluate a function $f(X)$ with interval argument X. This could be achieved by simply performing the arithmetic operations to evaluate $f(x)$ (x real) in interval arithmetic rather than real arithmetic.

If $f(x)$ has a continuous derivative $f'(x)$, we could use the mean value theorem and evaluate (see [1])

$$f(x) + (X - x)\, f'(X) \supset f(X) \tag{2.1}$$

for some $x \in X$. The real term $f(x)$ can be evaluated with arbitrarily high accuracy. The effect of the loss of sharpness in evaluating $f'(X)$ is reduced since it is multiplied by the quantity $X - x$ which is small if the width of X is small.

Our approach will be to use a procedure somewhat similar to that expressed by (2.1). However, we shall avoid the necessity of knowing the derivative $f'(x)$.

Note that a sharper relation than (2.1) involving higher derivatives could be used. For example,

$$f(X) \subset f(x) + (X - x) f'(x) + \frac{1}{2}(X - x)^2 f''(X) .$$

Our method can be made sharper also. However, we shall restrict this discussion to what might be called the first order case.

3. REPRESENTATION OF AN INTERVAL

For our purposes, it is convenient to represent an interval $X = [a,b]$ in the form $X = y + [-c,c]$ where $y - c = a$ and $y + c = b$. Thus an arbitrary point $x \in X$ is expressed as $x = y + \zeta$ where $\zeta \in [-c,c]$ and $c \geq 0$.

Assume we wish to evaluate a function depending on n input intervals X_i $(i = 1,\ldots,n)$. We represent each variable $x_i \in X_i$ as $x_i = y_i + \zeta_i$ where $\zeta_i \in [-c_i,c_i]$.

As we shall see, any computed interval X_i $(i > n)$ depending (implicitly perhaps) on these intervals can be expressed as

$$X_i = Y_i + \sum_{r=1}^{n} \zeta_r Z_{ir} \tag{3.1}$$

where Y_i and Z_{ir} $(i = 1,2,\ldots;\ r = 1,\ldots,n)$ are computed numerical intervals and $\zeta_r \in [-c_r,c_r]$. We shall call X_i expressed in the form (3.1) a <u>generalized interval</u>.

We have used the equality sign in (3.1). However, this is not strictly correct until we replace ζ_r by $[-c_r,c_r]$. When this is done, we shall say that the generalized interval has been <u>reduced</u> to an interval.

When we reduce the generalized interval in (3.1) to an ordinary interval, we obtain

$$X_i = Y_i + \sum_{r=1}^{n} [-c_r,c_r] Z_{ir}$$

$$= Y_i + [-1,1] \sum_{r=1}^{n} c_r z_{ir}$$

where $z_{ir} = |Z_{ir}|$. In general, the absolute value of an interval $A = [a,b]$ is defined to be $|A| = \max(|a|,|b|)$.

Note that (3.1) holds for $i \leq n$ since any $x_i \in X_i$ $(i \leq n)$ can be expressed as $x_i = y_i + \zeta_i$. Thus for $i \leq n$, $Y_i = [y_i, y_i]$, $Z_{ii} = [1,1]$, and $Z_{ir} = [0,0]$ for $r \neq i$.

4. GENERALIZED INTERVAL ARITHMETIC

Assume two intervals X_i and X_j are expressed in the form (3.1). We now consider the four arithmetic operations applied to these intervals. For addition or subtraction,

$$X_k = X_i \pm X_j$$
$$= Y_i \pm Y_j + \sum_{r=1}^{n} \zeta_r (Z_{ir} \pm Z_{jr}) \tag{4.1}$$

and we define

$$Y_k = Y_i \pm Y_j, \; Z_{kr} = Z_{ir} \pm Z_{jr} \tag{4.2}$$

where the arithmetic operations indicated in (4.2) are ordinary interval arithmetic (o.i.a.) operations.

Note that if (and only if)

$$x_i \in X_i = Y_i + \sum_{r=1}^{n} [-c_r, c_r] Z_{ir}$$

and

$$x_j \in X_j = Y_j + \sum_{r=1}^{n} [-c_r, c_r] Z_{jr} ,$$

then the sum or difference $x_i \pm x_j$ is contained in

$$X_k = Y_k + \sum_{r=1}^{n} [-c_r, c_r] Z_{kr} \tag{4.3}$$

provided Y_k and Z_{kr} are defined by (4.2).

We started with generalized intervals X_i and X_j of the form (3.1) and have obtained their sum or difference X_k in the same form.

To obtain a rule for multiplication of two generalized intervals, note that

$$X_k = X_i \, X_j$$
$$= Y_i \, Y_j + \sum_{r=1}^{n} \zeta_r (Y_i \, Z_{jr} + Y_j \, Z_{ir}) + \sum_{r=1}^{n} \sum_{s=1}^{n} \zeta_r \, \zeta_s \, Z_{ir} \, Z_{js} . \tag{4.4}$$

We shall choose to retain only linear terms in ζ_r $(r = 1,\ldots,n)$ although higher order terms could be kept. We can subsume the second order terms into the other terms in many ways. We choose the following procedure.

Note that the terms for $r = s$ involve ζ_r^2 which can be replaced by $[-c_r, c_r]^2 = [0, c_r^2]$. For $r \neq s$, we cannot take advantage of the special result that the square of an interval must be positive. We replace $\zeta_r \zeta_s$ by $\zeta_r[-c_s, c_s]$ since $\zeta_s \in [-c_s, c_s]$. Thus the right member of (4.4) is contained in

$$X_k = Y_k + \sum_{r=1}^{n} \zeta_r Z_{kr} \tag{4.5}$$

where

$$Y_k = Y_i Y_j + \sum_{r=1}^{n} [0, c_r^2] Z_{ir} Z_{jr} \tag{4.6}$$

and

$$\begin{aligned} Z_{kr} &= Y_i Z_{jr} + Y_j Z_{ir} + Z_{ir} \sum_{\substack{s=1 \\ s \neq r}}^{n} [-c_s, c_s] Z_{js} \\ &= Y_i Z_{jr} + Y_j Z_{ir} + [-1,1] z_{ir} \sum_{\substack{s=1 \\ s \neq r}}^{n} c_s z_{js} \end{aligned} \tag{4.7}$$

where as before $z_{ir} = |Z_{ir}|$ and $z_{jr} = |Z_{jr}|$. Thus we define the product of two generalized intervals X_i and X_j to be that given by (4.5) with Y_k defined by (4.6) and Z_{kr} defined by (4.7).

Division of two generalized intervals can also be done in many ways. We shall adopt a compromise between the simplest and more complex alternatives. Note that

$$\begin{aligned} X_k &= X_i / X_j \\ &= \frac{Y_i + \sum_{r=1}^{n} \zeta_r Z_{ir}}{Y_j + \sum_{s=1}^{n} \zeta_s Z_{js}} \qquad (4.8) \\ &= \frac{Y_i}{Y_j} + \frac{\sum_{r=1}^{n} \zeta_r (Y_j Z_{ir} - Y_i Z_{jr})}{Y_j \left(Y_j + \sum_{s=1}^{n} \zeta_s Z_{js}\right)} \end{aligned}$$

Replacing ζ_s by $[-c_s, c_s]$ in the denominator we see that we can define

$$Y_k = Y_i / Y_j \tag{4.9}$$

and

$$Z_{kr} = \frac{Y_j Z_{ir} - Y_i Z_{jr}}{Y_j(Y_j + [-1,1] \sum_{s=1}^{n} c_s z_{js})} . \tag{4.10}$$

The denominator in (4.10) should not be written as

$$Y_j^2 + Y_j[-1,1] \sum_{s=1}^{n} c_s z_{js}$$

since this form will always yield a wider interval unless the width of Y_j is zero. No advantage can be gained by using the special definition of the square of an interval to compute Y_j^2 since $0 \notin Y_j$. For $0 \in Y_j$, we have $0 \in X_j$ and we cannot perform the division.

It is possible to derive a comparable result by using Taylor series with the remainder involving zero-th order and first derivative terms only. However, such a result is slightly less sharp.

Note that the algebra involved in deriving the above results is not necessarily valid when Y_i, Y_j, Z_{ir}, and Z_{jr} are intervals. However, the results are correct since we can derive them when these quantities are real. After such a derivation, note that the results hold for any $y_i \in Y_i$, etc. and hence are valid.

5. MULTIPLICATION

In this section, we shall consider multiplication for g.i.a. in detail and present some examples.

We first note that to obtain the square of a generalized interval, we can use a special definition as in the case for o.i.a.. For $X_j = X_i$, equation (4.6) becomes

$$\begin{aligned} Y_k &= Y_i^2 + \sum_{r=1}^{n} [0, c_r^2] Z_{ir}^2 \\ &= Y_i^2 + \sum_{r=1}^{n} [0, c_r^2] z_{ir}^2 . \end{aligned} \tag{5.1}$$

The term Y_i^2 should be computed using the special definition for the square for an ordinary interval. Equation (4.7) becomes

$$Z_{kr} = 2Y_i Z_{ir} + [-1,1] z_{ir} \sum_{\substack{s=1 \\ s \neq r}}^{n} c_s z_{is} . \tag{5.2}$$

Consider the square of a datum interval $X = Y + \zeta$ with $\zeta \in [-c,c]$. In this case, Y is a real number and (5.1) and (5.2) yield

$$X^2 = Y^2 + [0,c^2] + 2\zeta Y .$$

Reducing to an interval,

$$X^2 = [Y^2 - 2c|Y|, Y^2 + c^2 + 2c|Y|]$$
$$= [Y^2 - 2c|Y|, (|Y| + c)^2] .$$

The right endpoint is correct. However, the left endpoint should be

$$0 \quad \text{if} \quad 0 \in X,$$
$$(|Y| - c)^2 \quad \text{if} \quad 0 \notin X .$$

Hence we obtain an incorrect left endpoint for our result unless $Y = 0$.

The magnitude of the error is

$$|Y^2 - 2c|Y|| \qquad \text{if} \quad 0 \in X,$$
$$c^2 \qquad \text{if} \qquad 0 \notin X .$$

Thus if c is small, the error is small. In fact, the error is $O(c^2)$ since in case $0 \in X$, we must have $|Y| \leq c$. If c is much greater than 1, the error can be unacceptably large.

This lack of sharpness for multiplication occurs in general for g.i.a.. However, in a sequence of calculations, this shortcoming tends to have less effect (when c is small) than the inherent lack of sharpness of o.i.a.

As an example, consider $X = [-.3,.9]$. Using o.i.a., $X^2 = [0,.81]$ while g.i.a. yields $X^2 = (.3 + \zeta)^2 = [.09,.45] + .6\zeta$ with $\zeta \in [-.6,.6]$. The latter result reduces to $[-.27,.81]$ with an incorrect left endpoint.

However, let us evaluate $F = X^2 - X^4$. Using o.i.a., we find $F = [-.6561,.81]$. Squaring $X^2 = [.09,.45] + .6\zeta$ using g.i.a., we obtain $X^4 = [.0081,.3321] + [.108,.54]\zeta$ so that

$$F = [-.2421,.4419] + [.06,.492]\zeta$$

which reduces to $[-.5373,.7371]$. This is an improvement over the o.i.a. result. The correct result (the united extension of F) is $[-.1539,.25]$.

We thus see that g.i.a. does not necessarily give good results when input intervals are wide. However, as pointed out above, the error is of second order in c and hence good results are obtained for small c.

As a final note on multiplication we consider multiplication of a generalized interval by a real number or by an interval which we choose not to represent as a generalized interval. Let A be such a number or interval and

$$X = Y + \sum_{i=1}^{n} \zeta_i Z_i .$$

Then

$$AX = Y' + \sum_{i=1}^{n} \zeta_i Z_i'$$

where

$$Y' = AY, \quad Z_i' = AZ_i .$$

6. DIVISION

For an interval $X = Y + \zeta Z$ depending on only one datum interval, if the quantities Y and Z are real numbers, then from (4.9) and (4.10) we find $X/X = 1$. This is never true for o.i.a. if the width of X is nonzero.

In general, a single division in g.i.a. introduces errors which are of second order in the interval widths. We now show this for an interval $X = Y + \zeta Z$ where again $Y > 0$ and $Z > 0$ are real numbers and $\zeta \in [-c,c]$. Consider $X' = 1/X$.

From (4.9) and (4.10),

$$X' = \frac{1}{Y} - \frac{Z}{Y(Y + [-1,1]cZ)}\zeta$$

which reduces to

$$X' = [\frac{1}{Y} - \frac{cZ}{Y(Y - cZ)}, \frac{1}{Y} + \frac{cZ}{Y(Y - cZ)}] .$$

The width of this interval is

$$w' = \frac{2cZ}{Y(Y - cZ)} .$$

The correct result is

$$[\frac{1}{Y + cZ}, \frac{1}{Y - cZ}]$$

which has width

$$w = \frac{2cZ}{Y^2 - c^2 Z^2} .$$

The width is thus in error by an amount

$$w' - w = \frac{2c^2 Z^2}{Y(Y^2 - c^2 Z^2)}$$

which is of second order in c.

To illustrate the process of division in g.i.a., consider the following example of Moore's ([1], page 45, et.seq.) with wide data intervals $X_1 = [1,2]$ and $X_2 = [5,10$

We shall compute

$$X = \frac{X_1 + X_2}{X_1 - X_2} .$$

We first rewrite

$$X_1 = 1.5 + \zeta_1, \; X_2 = 7.5 + \zeta_2$$

where $\zeta_1 \in [-.5,.5]$ and $\zeta_2 \in [-2.5,2.5]$.

Define $X_3 = X_1 + X_2$ and $X_4 = X_1 - X_2$ so that $X = X_3/X_4$.

Using (4.2), $X_3 = 9 + \zeta_1 + \zeta_2$ and $X_4 = -6 + \zeta_1 - \zeta_2$. Using (4.9) and (4.10),

$$X = -\frac{9}{6} + \zeta_1[-\frac{5}{6}, -\frac{5}{18}] + \zeta_2[\frac{1}{18}, \frac{1}{6}] .$$

Replacing ζ_1 by $[-.5,.5]$ and ζ_2 by $[-2.5,2.5]$,

$$X = [-\frac{7}{3}, -\frac{2}{3}] \subset [-2.334, -.6666] .$$

This is the same result Moore obtains ([1], page 47) using the centered form with o.i.a. and better than the result $[-\frac{67}{18}, \frac{13}{18}] \subset [-3.723,.7223]$ he obtains ([1], page 49) using the mean value theorem. Incidentally, his latter result can be sharpened to $[-\frac{1073}{392}, -\frac{103}{392}] \subset [-2.738,-.2627]$ using ideas given in [2].

Direct use of o.i.a. yields $[-4,-2/3]$.

Rewriting X as

$$X = 1 + \frac{2}{\dfrac{X_1}{X_2} - 1},$$

we obtain exact results using o.i.a. since each variable occurs only once. We find $X = [-\frac{7}{3}, -\frac{11}{9}] \subset [-2.334, -1.222]$. Thus the result using g.i.a. has a sharp left endpoint but not a sharp right endpoint.

If we apply g.i.a. to the centered form, we obtain the same result $[-\frac{7}{3}, -\frac{2}{3}]$.

7. EXAMPLE

We now consider an example combining multiplication and division and having realistically small intervals.

Let $X = [-.001, .003]$. If we evaluate

$$f = \frac{1 + X + X^2}{1 + X + 2X^2} .$$

in o.i.a., we obtain a result which when rounded to six decimals is [.995994, 1.00402
The g.i.a. result is

$$[.999991, 1.00001] + \zeta[-.00200503, -.00198498]$$

which reduces to [.999986, 1.00001] . The united extension is $\bar{f}(x) = [.999991, .999999]$. Thus while the g.i.a. result is too wide by an amount .000016, the o.i.a. result is too wide by an amount .008018.

8. MULTIDIMENSIONAL PROBLEMS

In multidimensional problems, a region can be bounded in o.i.a. by a rectangular parallelopiped with sides parallel to the coordinate axes. Thus for example, the unit circle about the origin lies in the square bounded by the intervals $X = [-1,1]$ and $Y = [-1,1]$.

It was observed by Moore ([1], page 133) and subsequently by others, that the necessity to use such a parallelopiped can cause interval bounds to grow even when the region being bounded does not. For example, if the square $X = Y = [-1,1]$ is rotated through an angle $\pi/4$, it requires intervals which are $2^{1/2}$ times larger to bound the final region by a square with sides parallel to the axes.

We can express this numerically as follows: Given $X = Y = [-1,1]$, let

$$\begin{bmatrix} X' \\ Y' \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} X \\ Y \end{bmatrix}$$

We find $X' = Y' = \sqrt{2}\,[-1,1]$.

Let us now rotate back to the original position so that

$$\begin{bmatrix} X'' \\ Y'' \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} X' \\ Y' \end{bmatrix} .$$

We obtain $X'' = Y'' = [-2,2]$ so that the intervals are twice their original width.

Using g.i.a., we express $X = \zeta$ and $Y = \eta$ with $\zeta \in [-1,1]$ and $\eta \in [-1,1]$. The original rotation yields

$$X' = \frac{1}{\sqrt{2}} (\zeta - \eta), \quad Y' = \frac{1}{\sqrt{2}} (\zeta + \eta) .$$

Rotating back gives $X'' = \zeta$ and $Y'' = \eta$ which reduce to the original intervals and no enlargement of the region has occurred.

In general, a multidimensional region specified by generalized intervals will be smaller than the region obtained when the generalized intervals are reduced to ordinary intervals. This makes it useful, for example, in complex variables.

As an example, consider the region specified by

$$X = [0,1] + [1,2]\zeta + [2,3]\eta,$$

$$Y = [1,2] + [2,3]\zeta + [0,1]\eta,$$

where $\zeta \in [-1,1]$ and $\eta \in [-1,1]$.

Reducing to ordinary intervals, we obtain $X = [-5,6]$ and $[-3,6]$. The point $x = 4$ and $y = 0$ is an interior point of this final region. However there are no real numbers ζ and η satisfying $\zeta \in [-1,1]$ and $\eta \in [-1,1]$ such that when the generalized intervals are reduced to ordinary intervals, yields intervals containing the point $(4,0)$. That is, the set

$$\{x,y : x \in [0,1] + [1,2]\zeta + [2,3]\eta,\ y \in [1,2] + [2,3]\zeta + [0,1]\eta,\ \zeta \in [-1,1],\ \eta \in [-1,1]\}$$

is strictly contained in the set

$$\{x,y : x \in [-5,6],\ y \in [-3,6]\}\ .$$

9. ROOT FINDING

We now consider use of g.i.a. for root finding.

When Newton's method is implemented in interval form (see [1]), we iteratively obtain a new interval bound X' on a root of a function $f(x)$ from an old bound X as

$$X' = x - \frac{f(x)}{f'(X)} \qquad (9.1)$$

where $x \in X$. Only slight improvement can be obtained using g.i.a. in place of o.i.a. in this algorithm since only f' is evaluated for an interval (non-real) argument and a sharp result for $f'(X)$ is not important. Bounding the roundoff errors in the evaluation of $f(x)$ might just as well be done in o.i.a..

However, root finding procedures such as that of Dargel, Loscalzo, and Witt [3] and others require evaluation of f over an interval of nonzero width. In this case, g.i.a. is of value since a sharper "value" of f is obtained.

An additional virtue of g.i.a. is that a set of results (depending on ζ) is obtained rather than a single interval. We now illustrate this fact by considering a root finding algorithm which uses this property of g.i.a..

Suppose we evaluate a function $f(X)$ using g.i.a. where $X = [y - c, y + c]$ so that we let $x = y + \zeta$. Let the result be $F + G\zeta$ where F and G are intervals. If there is an interval $A = [a,b] \subset [-c,c]$ such that

$$0 \notin F + GA,$$

then $f(x) \neq 0$ for $x \in [y - a, y + b]$. Hence any zero of f in X must occur outside this interval and we can restrict our attention to a smaller set of values of x. In some cases, two intervals in X can be simultaneously excluded.

As an example, consider the polynomial

$$f = (x-2)(x-1)(x+1)(x+2)(x+3)$$
$$= x^5 - 3x^4 - 5x^3 + 15x^2 + 4x - 12 .$$

Let $X = [.97, 1.01]$. Evaluating f in nested form for $x = .99 + \zeta$ with $\zeta \in [-.02, .02]$ and using five decimal digit arithmetic, we obtain

$$f = [-.125, -.11993] + [12.153, 12.16]\zeta .$$

If we replace ζ by $[-.02, .0098626]$, we find $f < 0$ and hence no value of ζ in this interval can give a value of x which is a root of f. If we replace ζ by $[.010286, .02]$, we find $f > 0$. Hence a root of f must lie in the interval

$$.99 + [.0098626, .010286] \subset [.99986, 1.0003] .$$

Note that this conclusion does not rely on a priori knowledge that X contains a root.

We can repeat the procedure using this new interval. It can be shown that asymptotically the convergence of the method is quadratic for a simple root. Convergency also seems to occur for multiple roots but it can only be linear convergence. Note that Newton's method cannot be used to bound multiple roots since $0 \in f'(X)$ and the ratio $f(x)/f'(X)$ in (9.1) is undefined. Our method does not suffer from this difficulty.

If we perform a step of the Newton method for this example using o.i.a. with the same starting interval $X = [.97, 1.01]$, we find $X' = [.99923, 1.0007]$ which is not quite as good a result.

10. SPECIAL FUNCTIONS

Special functions can be evaluated in g.i.a. by making use of Taylor series. As pointed out above when discussing division, we can sometimes derive particular relations which are better than what can be obtained using Taylor series. However, we shall not attempt to do so for any special functions.

If we use only first derivative terms, a function $f(x_1, \ldots, x_n)$ with

$$x_i = Y_i + \sum_{r=1}^{n} \zeta_r Z_{ir}$$

can be expanded as

$$f(x_1, \ldots, x_n) = f(Y_1, \ldots, Y_n) + \sum_{s=1}^{n} \zeta_s \sum_{r=1}^{n} Z_{rs} \frac{\partial}{\partial x_s} f(X_1, \ldots, X_n)$$

where

$$X_i = Y_i + \sum_{r=1}^{n} [-c_r, c_r] Z_{ir} .$$

As an example, consider $f(x) = e^x$ with $x = Y + \zeta_1 Z_1 + \zeta_2 Z_2$ where $\zeta_i = [-c_i, c_i]$ for $i = 1,2$. We obtain

$$e^x = e^Y + \zeta_1 Z_1 e^X + \zeta_2 Z_2 e^X$$

where $X = Y + [-c_1, c_1]Z_1 + [-c_2, c_2]Z_2$. The intervals e^Y and e^X can be obtained using o.i.a.. Note that

$$e^{[a,b]} = [e^a, e^b] .$$

A sharper result can be obtained using the sequential Taylor expansion discussed in [2] .

11. CONCLUSION

We have introduced and illustrated a generalized interval analysis which reduces the inherent lack of sharpness of o.i.a. to a second order effect. Our method may not be useful if second order quantities are not truly negligible. Moreover, our method is of little value if the original data for a problem is real rather than intervals of non-zero width.

However, it is substantially better than o.i.a. for many problems. Moreover, it provides a more powerful tool in some cases such as in bounding multiple roots.

The rules for multiplication and division should be regarded as tentative. Further study may reveal that alternative rules are preferable.

As a final comment, we note that it is easily shown that g.i.a. is subdistributive.

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