Interval Divided-Difference Arithmetic*

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Abstract

Divided difference arithmetic computes divided differences of functions defined by algorithms without the error-prone operation of subtraction called for by the standard definition. This arithmetic is reviewed, and certain intrinsic functions are redefined in terms of what are called cardinal functions, such as the well-known cardinal sine function $\operatorname{sinc}(x)$. The extension of divided difference arithmetic to interval values to obtain inclusions of divided differences is introduced. Since division by the increment is avoided, increments containing zero are permitted, and a zero increment simply results in inclusion of the function and its derivative values in interval differentiation arithmetic.

Keywords: divided differences, divided-difference arithmetic, interval arithmetic, differentiation arithmetic, cardinal functions
AMS subject classifications: 65G30, 65G40, 65Y04, 26A06, 33E99, 65D05

1 Computer Arithmetics

By a *computer arithmetic*, we mean a set of elements to which a computer can apply arithmetic operations and specified *intrinsic functions* to obtain results expressible in terms of the given elements. The simplest example of a computer arithmetic is *floating-point* arithmetic, whose elements are numbers of finite precision. The arithmetic operations and intrinsic functions applied to these produce finite precision approximations to the exact mathematical results; the goal is to be as accurate as possible. Other arithmetics using the set of floating-point numbers have been created, including the floating-point versions of complex, interval, differentiation and divided-difference arithmetics [4, 5, 8, 10, 11].

One way to implement these arithmetics is by *overloading*, available in programming languages such as C++ [2]. Here, one defines elements representing the new arithmetic and uses the same symbols for arithmetic operations and intrinsic functions as in floating-point arithmetic to form expressions. Thus, to evaluate

$$f(x) = x \tan x + \log \cos x - \frac{x^2}{2} \tag{1.1}$$

*Submitted: January 20, 2016; Revised: March 1, 2016; Accepted: March 10, 2016.

in one of these arithmetics, we use an expression such as

$$\texttt{f} = \texttt{x} * \texttt{tan(x)} + \texttt{log(cos(x))} - \texttt{sqr(x)/2}.$$

For example, in basic differentiation arithmetic, the elements are pairs $(f(x), f'(x))$ which represent the values of the function f and its derivative f' at x [7]. This applies to algorithms as well as single expressions and does not need a symbolic form for the derivative. The formulation of divided-difference arithmetic is similar. It should be mentioned that simple overloading puts the computation in forward mode in which the elements are dealt with in the same order as the calculation of the function value. For discussion of general algorithmic differentiation in reverse mode, see [3, 6].

Divided-difference arithmetic also generalizes to higher-order differences and divided differences of functions of several variables [4, 11]. These extensions depend on the formulas for overloading arithmetic operations and intrinsic functions presented below.

2 Review of Divided-Difference Arithmetic

Divided differences were a mainstay of classical numerical analysis. Computation of values of even the elementary functions of ordinary calculus was laborious, so tables of values of needed functions were constructed. Interpolation between tabulated results and construction of local polynomial approximations used divided differences. These techniques apply to functions observed from measurement as well as those defined by algorithms as considered here. Given the power of computers to evaluate algorithmicly defined functions at given points, why use divided-difference arithmetic at all? One reason is that the standard definition

$$[x_0, x_1]f = \frac{f(x_1) - f(x_0)}{x_1 - x_0},$$

or simply $[x_0, x_1]$ if the function f is understood, requires performing the subtraction $f(x_1) - f(x_0)$. If $\Delta x = x_1 - x_0$ is small, then this can remove most or all of the significant digits of the result, and the resulting error is multiplied by the large number $1/\Delta x$. On the other hand, a properly designed evaluation of $[x_0, x_0 + \Delta x]f$ in divided-difference arithmetic can retain many significant digits, and furthermore, the values of the divided difference will gracefully approach the value of the derivative $f'(x_0)$ as $\Delta x \to 0$. In addition, if one has an accurate value of the divided difference $[x_0, x_0 + \Delta x]f$, then the difference $\Delta f = f(x_0 + \Delta x) - f(x_0)$ can be calculated accurately as

$$\Delta f = f(x_1) - f(x_0) = \Delta x \cdot [x_0, x_0 + \Delta x]f \tag{2.1}$$

by multiplication instead of subtraction.

The usual definition of the divided difference given above (see [1]) presents a notational problem if intervals are also considered. Here, $[x_0, x_1]$ is viewed as an *operator* applied to f. It is possible that $x_1 < x_0$ which is at variance with the definition of an interval. Instead of using nonstandard notation, the meaning of symbols such as $[x_0, x_1] = [x_0, x_0 + \Delta x]$ will depend on context. Thus, for differentiable functions,

$$[x_0, x_0 + \Delta x]f = \begin{cases} \dfrac{f(x_0 + \Delta x) - f(x_0)}{\Delta x} \text{ if } \Delta x \neq 0, \\ f'(x_0) \text{ if } \Delta x = 0. \end{cases} \tag{2.2}$$

This "subtract and divide" method for computing divided differences will be compared with their evaluation by divided-difference arithmetic, which is similar to differentiation arithmetic.

As in single-variable differentiation arithmetic, basic divided-differentiation arithmetic acts on ordered pairs $f = (f(x_0), [x_0, x_1]f)$. In this arithmetic, $\Delta x = x_1 - x_0$ is a universal constant, and differentiation arithmetic is the case $\Delta x = 0$, $f = (f(x_0), f'(x_0))$.

2.1 The Chain Rule

As in the case of differentiation arithmetic, what makes divided-difference arithmetic work is the *chain rule* for composite functions $w(x) = u(v(x))$. For $\Delta x \Delta v \neq 0$,

$$\frac{w(x_1) - w(x_0)}{x_1 - x_0} = \frac{u(v(x_1)) - u(v(x_0))}{v(x_1) - v(x_0)} \frac{v(x_1) - v(x_0)}{x_1 - x_0},$$

or in general from (2.2),

$$[x_0, x_1]w = [v_0, v_1]u \cdot [x_0, x_1]v, \tag{2.3}$$

by (2.2) where $v_0 = v(x_0)$, $v_1 = v(x_1)$.

2.2 Arithmetic Operations

Throughout, the notation $\Delta x = x_1 - x_0$ will be used.

2.2.1 Linear Combinations

Linear combinations

$$u = \alpha v + \beta w \tag{2.4}$$

subsume addition, subtraction and multiplication by constants. It follows at once that

$$[x_0, x_1]u = \alpha[x_0, x_1]v + \beta[x_0, x_1]w. \tag{2.5}$$

2.2.2 Multiplication

One has

$$\Delta(vw) = (v + \Delta v)(w + \Delta w) - vw = v\Delta w + w\Delta v + \Delta v \Delta w. \tag{2.6}$$

Thus, for $u = vw$,

$$[x_0, x_1](vw) = v_0 \cdot [x_0, x_1]w + w_0 \cdot [x_0, x_1]v + \Delta x \cdot [x_0, x_1]v \cdot [x_0, x_1]w, \tag{2.7}$$

where $v_0 = v(x_0)$, $w_0 = w(x_0)$ as above.

2.2.3 Division

Again, from

$$\Delta(v/w) = \frac{v + \Delta v}{w + \Delta w} - \frac{v}{w} = \frac{\Delta v - (v/w)\Delta w}{w + \Delta w}, \tag{2.8}$$

so the divided difference of the quotient $u = (v/w)$ is

$$[x_0, x_1](v/w) = ([x_0, x_1]v - u_0 \cdot [x_0, x_1]w)/(w_0 + \Delta x \cdot [x_0, x_1]w). \tag{2.9}$$

If $v = c$ is a constant, then of course $[x_0, x_1]c = 0$, and (2.9) is

$$[x_0, x_1](c/w) = -\frac{c}{w_0(w_0 + \Delta x \cdot [x_0, x_1]w)} \cdot [x_0, x_1]w. \tag{2.10}$$

2.2.4 Powers

The function $u = v^n$, n an integer, arises frequently in calculations. The general case can be derived from the identity

$$w^n - v^n = (w - v)(w^{n-1} + w^{n-2}v + \cdots + wv^{n-2} + v^{n-1}),$$

[4]. The simple case $n = 2$ is useful in interval arithmetic because $\boldsymbol{x}^2 = [\underline{x}, \overline{x}]^2 \neq \boldsymbol{x} \cdot \boldsymbol{x} = [\underline{x}, \overline{x}] \cdot [\underline{x}, \overline{x}]$ in general. Define $\text{sqr}(v) = v^2$, then

$$\Delta\text{sqr}(v) = (v + \Delta v)^2 - v^2 = 2v\Delta v + [\Delta v]^2,$$

and

$$[x_0, x_1]\text{sqr}(v) = 2v_0 \cdot [x_0, x_1]v + \Delta x \cdot ([x_0, x_1]v)^2. \tag{2.11}$$

2.3 Intrinsic Functions

Functions which are available to computer programs and yield results of high accuracy will be referred to as *intrinsic functions*. Here, a few examples of unary intrinsic functions will be considered: Square root, exponential and natural logarithm, trigonometric sine, cosine, tangent and arctangent. The methods for obtaining divided differences and derivatives of these functions are readily adaptable to others. The main technique is to replace additions and subtractions by multiplications and divisions to reduce relative errors. These formulas are numerically stable for small $|\Delta x|$, and many are found in elementary calculus books as part of the computation of derivatives of functions as $\Delta x \to 0$.

Use will be made of the *cardinal* function for various functions, such as the cardinal sine (or "sinc") function

$$\text{sinc}(0) = 1,\ \text{sinc}(x) = \frac{\sin x}{x},\ x \neq 0.$$

This function is useful in its own right in connection with Fourier transforms and signal processing.

If $f(x)$ is given by the convergent Taylor series expansion

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{1}{2!}f''(x_0)(x - x_0)^2 + \cdots,$$

at x_0, then its cardinal function $f_c(x, x_0)$ is given by

$$f_c(x, x_0) = f'(x_0) + \frac{1}{2!}f''(x_0)(x - x_0) + \frac{1}{3!}f'''(x_0)(x - x_0)^2 + \cdots. \tag{2.12}$$

It follows that

$$[x_0, x_1]f = f_c(x_1, x_0) = f_c(x_0 + \Delta x, x_0). \tag{2.13}$$

In the case $x_0 = 0$, the cardinal function for $f(x)$ will be denoted by $f_c(x) = f_c(x, 0)$. Some well-known identities will be used to derive formulas for divided differences in terms of $f_c(\Delta x)$. The use of cardinal functions avoids both subtraction and division by Δx, which will be helpful in formulation of the interval version of divided-difference arithmetic. In floating-point arithmetic, cardinal functions $f_c(x)$ can be implemented simply under the reasonable assumption that $f(x)$ is computed accurately for small x.

2.3.1 Square Root

For $u = \mathrm{sqrt}(v) = \sqrt{v}$, one has

$$\Delta u = \sqrt{v + \Delta v} - \sqrt{v} = \frac{\Delta v}{\sqrt{v + \Delta v} + \sqrt{v}}.$$

Thus,

$$[x_0, x_1]\mathrm{sqrt}(v) = \frac{[x_0, x_1]v}{\sqrt{v_0 + \Delta v} + \sqrt{v_0}}, \tag{2.14}$$

where of course $\Delta v = \Delta x \cdot [x_0, x_1]v$.

2.3.2 Exponential and Natural Logarithm

For $u = \exp(v) = e^v$,

$$\Delta u = e^{v+\Delta v} - e^v = e^v(e^{\Delta v} - 1).$$

Thus, for $\mathrm{expc}(0) = 1$, $\mathrm{expc}(x) = (e^x - 1)/x$ for $x \neq 0$, or

$$\mathrm{expc}(x) = 1 + \frac{1}{2!}x + \frac{1}{3!}x^2 + \cdots. \tag{2.15}$$

one has

$$[x_0, x_1]\exp(v) = \exp(v_0) \cdot \mathrm{expc}(\Delta v) \cdot [x_0, x_1]v. \tag{2.16}$$

For $u = \log(v) = \log_e(v)$, one has

$$\Delta u = \log(v + \Delta v) - \log(v) = \log\left(\frac{v + \Delta v}{v}\right) = \log\left(1 + \frac{\Delta v}{v}\right).$$

Thus, for $\mathrm{lnc}(0) = 1$,

$$\mathrm{lnc}(x) = \frac{\log(1+x)}{x} = 1 - \frac{1}{2}x + \frac{1}{3}x^2 - \cdots, \ 0 < |x| < 1, \tag{2.17}$$

it follows that

$$[x_0, x_1]\log(v) = \frac{1}{v_0}\mathrm{lnc}\left(\frac{\Delta v}{v_0}\right) \cdot [x_0, x_1]v. \tag{2.18}$$

2.3.3 Trigonometric Sine and Cosine

Here, use will be made of the well-known identities

$$\sin(x) - \sin(y) = 2\sin[(x-y)/2]\cos[(x+y)/2],$$

$$\cos(x) - \cos(y) = -2\sin[(x+y)/2]\sin[(x-y)/2].$$

Hence, for $u = \sin(v)$, one has

$$\Delta u = \sin(v + \Delta v) - \sin(v) = 2\sin(\Delta v/2)\cos[(2v + \Delta v)/2].$$

and thus

$$[x_0, x_1]\sin(v) = \mathrm{sinc}(\Delta v/2)\cos(v_0 + \Delta v/2) \cdot [x_0, x_1]v. \tag{2.19}$$

Similarly, for $u = \cos(v)$,

$$[x_0, x_1]\cos(v) = -\mathrm{sinc}(\Delta v/2)\sin(v_0 + \Delta v/2) \cdot [x_0, x_1]v. \tag{2.20}$$

Derivation of divided-difference formulas for the hyperbolic sine and cosine follows the same pattern.

2.3.4 Tangent and Arctangent

It follows from the identity

$$\tan x - \tan y = \frac{\sin(x-y)}{\cos x \cdot \cos y}$$

for $u = \tan(v)$ that

$$\Delta u = \frac{\sin(\Delta v)}{\cos(v + \Delta v)\cos(v)},$$

so

$$[x_0, x_1]\tan(v) = \frac{\operatorname{sinc}(\Delta v)}{\cos(v_0 + \Delta v)\cos(v_0)} \cdot [x_0, x_1]v. \tag{2.21}$$

The divided difference formula for $u = \arctan(v)$ is based on the trigonometric identity

$$\tan(x-y) = \frac{\tan(x) - \tan(y)}{1 + \tan(x)\cdot\tan(y)}.$$

Let $x = \arctan(v + \Delta v)$, $y = \arctan(v)$. Then,

$$\tan(\arctan(v+\Delta v) - \arctan(v)) = \frac{\Delta v}{1 + v(v+\Delta v)},$$

hence, for $u = \arctan(v)$,

$$\Delta u = \arctan(v+\Delta v) - \arctan(v) = \arctan\left(\frac{\Delta v}{1 + v_0(v_0+\Delta v)}\right).$$

Thus, the divided difference formula is

$$[x_0, x_1]\arctan(v) = \frac{1}{1 + v_0(v_0+\Delta v)}\operatorname{atanc}\left(\frac{\Delta v}{1 + v(v+\Delta v)}\right)\cdot [x_0, x_1]v, \tag{2.22}$$

where $\operatorname{atanc}(0) = 1$,

$$\operatorname{atanc}(x) = \frac{\arctan(x)}{x} = 1 - \frac{1}{3}x^2 + \frac{1}{5}x^4 - \frac{1}{7}x^6 + \cdots,\ 0 < |x| < 1. \tag{2.23}$$

3 An Example

The results of computing divided differences of the function (1.1) by divided-difference arithmetic and by the subtract and divide method (2.2) are shown in Table 1. Here, $x_0 = 0.99$, and the computation is carried out for various values of Δx. The column labeled $[x_0, x_1]f$ has the values obtained by divided-difference arithmetic, and the one headed $\Delta f/\Delta x$ those from (2.2). For $\Delta x = 0$, the value of $f'(x_0)$ in the second column used divided-difference arithmetic to obtain $f'(x_0) = [x_0, x_0]f$, while the third column used the formula

$$f'(x) = x\tan^2(x). \tag{3.1}$$

Δx	$[x_0, x_1]f$	$\Delta f/\Delta x$
10^{-02}	2.3613194732913079	2.3613194732913345
10^{-04}	2.2989921456495019	2.2989921456489926
10^{-06}	2.2983810742356123	2.2983810744614530
10^{-08}	2.2983749647199057	2.2983749847771406
10^{-10}	2.2983749036248682	2.2983759340178267
10^{-12}	2.2983749030139178	2.2982726832765366
10^{-14}	2.2983749030078071	2.3092638912203256
10^{-16}	2.2983749030077467	5.5511151231257827
10^{-18}	2.2983749030077467	0
10^{-20}	2.2983749030077467	0
0	2.2983749030077467	2.2983749030077458

Table 1 Divided-difference arithmetic vs. the subtract and divide method for $f(x) = x \tan x + \log \cos x - \frac{x^2}{2}$

This shows the subtract and divide method breaks down for small Δx, while divided difference arithmetic gives a close approximation to the derivative. Similarly, the differences Δf obtained as $\Delta f = \Delta x \cdot [x_1, x_0]f$ by divided-difference arithmetic and $\Delta f = f(x_1) - f(x_0)$ by direct subtraction are shown in Table 2.

Δx	$\Delta x \cdot [x_0, x_1]f$	$f(x_1) - f(x_0)$
10^{-02}	$2.3613194732913078e-02$	$2.3613194732913345e-02$
10^{-04}	$2.2989921456495021e-04$	$2.2989921456489926e-04$
10^{-06}	$2.2983810742356124e-06$	$2.2983810744614530e-06$
10^{-08}	$2.2983749647199057e-08$	$2.2983749847771406e-08$
10^{-10}	$2.2983749036248682e-10$	$2.2983759340178267e-10$
10^{-12}	$2.2983749030139178e-12$	$2.2982726832765366e-12$
10^{-14}	$2.2983749030078071e-14$	$2.3092638912203256e-14$
10^{-16}	$2.2983749030077468e-16$	$5.5511151231257827e-16$
10^{-18}	$2.2983749030077470e-18$	0
10^{-20}	$2.2983749030077470e-20$	0

Table 2 Differences from divided-difference arithmetic vs. direct subtraction

Table 2 gives values of the definite integral

$$\int_{x_0}^{x_1} x \tan^2(x) dx = \left[x \tan x + \log \cos x - \frac{x^2}{2} \right|_{x_0}^{x_1},$$

where $x_0 = 0.99$, $x_1 = 0.99 + \Delta x$.

4 Interval Divided-Differences

The definition of the divided difference given by (2.2) is inherently unsuited to interval arithmetic. For intervals $\boldsymbol{a}$, and $\boldsymbol{b}$, $\mathrm{diam}(\boldsymbol{a} - \boldsymbol{b}) = \mathrm{diam}(\boldsymbol{a}) + \mathrm{diam}(\boldsymbol{b})$, which increases the diameter of both the numerator and denominator. Furthermore, $\Delta \boldsymbol{x} = \boldsymbol{x}_1 - \boldsymbol{x}_0$ cannot contain zero, which excludes derivatives.

In essence, interval divided-difference arithmetic is obtained from the point divided-difference discussed above by extending the arithmetic operations and intrinsic functions involved to those for interval arithmetic as done for differentiation arithmetic [9]. This avoids the subtraction and division in (2.2). The formulation of intrinsic functions in §2 requires trustworthy interval implementation of the corresponding cardinal functions. The function

$$g(x) = \frac{\sqrt{3x^2 - 2x}}{x}, \tag{4.1}$$

which requires only arithmetic operations and the algebraic functions sqr and sqrt will be used to illustrate the interval extension of divided-difference arithmetic. The basic element of interval divided-difference arithmetic is $x = (\boldsymbol{x}, 1)$, where $\boldsymbol{x} = [\underline{x}, \overline{x}]$ is a given interval. Application of the operations and functions of interval divided-difference arithmetic will then produce an interval inclusions $g(x) = (\boldsymbol{g}(\boldsymbol{x}), [\boldsymbol{x}, \boldsymbol{x} + \Delta\boldsymbol{x}]\boldsymbol{g})$ of the function values $g(x_0)$ and the divided differences $[x_0, x_1]g$ for $x_0 \in \boldsymbol{x}$, $x_1 \in (\boldsymbol{x} + \Delta\boldsymbol{x})$.

For example, take $\boldsymbol{x} = [0.99, 1, 00]$ and $\Delta\boldsymbol{x} = [0.399, 0.401]$. Then, the subtract-divide formula (2.2) gives

$$\frac{\Delta\boldsymbol{f}}{\Delta\boldsymbol{x}} = [0.5317, 0.7520], \tag{4.2}$$

an interval with diameter 0.2201. Evaluation of (4.1) in interval divided-difference arithmetic gives

$$g(x) = ([0.9696, 1.0202], [0.5943, 0.6899]),$$

that is, $\boldsymbol{g}(\boldsymbol{x}) = [0.9696, 1.0202]$ and

$$[\boldsymbol{x}, \boldsymbol{x} + \Delta\boldsymbol{x}]\boldsymbol{g} = [0.5943, 0.6899]. \tag{4.3}$$

This interval divided difference has diameter 0.0955, a considerable improvement over (4.2). The function value obtained for $\boldsymbol{g}(\boldsymbol{x})$ is the same as direct evaluation of (4.1) in interval arithmetic.

With regard to differences, subtraction yields

$$\Delta\boldsymbol{g} = \boldsymbol{g}(\boldsymbol{x} + \Delta\boldsymbol{x}) - \boldsymbol{g}(\boldsymbol{x}) = [0.2132, 0.3001],$$

while the divided-difference approach gives

$$\Delta\boldsymbol{g} = \Delta\boldsymbol{x} \cdot [\boldsymbol{x}, \boldsymbol{x} + \Delta\boldsymbol{x}]\boldsymbol{g} = [0.2371, 0.2767],$$

again an improvement for the divided-difference approach.

Of course, the subtract-divide formula cannot be applied if $\Delta\boldsymbol{x}$ contains zero. In interval divided-difference arithmetic, this just means that the result will contain values of the derivative of the function if differentiable. For example, if $\Delta\boldsymbol{x} = [-0.0011, 0.1001]$, then

$$g(x) = ([0.9696, 1.0202], [0.6890, 1.2640]).$$

Finally, for $\Delta\boldsymbol{x} = 0$,

$$g(x) = ([0.9696, 1.0202], [0.9304, 1.1039]),$$

which gives the inclusion $[0.9304, 1.1039]$ for $\boldsymbol{g}'(\boldsymbol{x})$ by interval differentiation arithmetic. Direct evaluation of

$$g'(x) = \frac{1}{x\sqrt{3x^2 - 2x}} \tag{4.4}$$

in interval arithmetic gives $\boldsymbol{g}'(\boldsymbol{x}) = [0.9901, 1.0417]$. The difference between these two methods is because differentiation arithmetic uses the original expression (4.1) for $f(x)$ and not the unnecessary symbolic derivative (4.4) [8].

Acknowledgments

First and foremost, Ramon E. Moore brought the concepts of interval computation and algorithmic differentiation to the attention of the Author. Later, Thomas W. Reps pointed out that the resulting methods of differentiation arithmetic extended to divided differences. The numerical computations in §§3–4 were carried out in MATLAB_R2015a™ with the interval toolbox INTLAB_V8 [12]. Comments provided by a reviewer resulted in increased clarity.

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