Graded Automatic Differentiation

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Abstract

Based on a class of associative algebras with zero-divisors which are called real-like algebras by us, we introduce the concept of the graded automatic differentiation induced a real-like algebra and present a new way of doing automatic differentiation to compute the first, the second and the third derivatives of a function exactly and simultaneously.

Automatic differentiation is indispensable to perform many optimization algorithms for large-scale machine learning problems. Computer scientists in machine learning community describe automatic differentiation as the computing techniques to evaluate accurately the numerical values of a derivative up to machine precision without using the explicit formula for the derivative, and emphasize that automatic differentiation is neither numerical differentiation nor symbolic differentiation. These popular description and emphasis about automatic differentiation are informative, but they do not indicate which kinds of mathematical objects we should search to find the techniques of doing automatic differentiation. Hence, an interesting problem is how to conceptualize automatic differentiation mathematically so that we know exactly which kinds of mathematical objects are sufficient for getting a procedure of executing automatic differentiation.

In addition to machine learning, many applications in scientific computation require to compute higher-order derivatives precisely. It is well-known that even a differential function is given explicitly by a mathematical formula, the explicit expression of its higher-order derivatives is usually too complicated to evaluate the higher-order derivatives precisely. Hence, in order to compute higher-order derivatives at machine precision, automatic differentiation seems to be unavoidable. The success of first-order automatic differentiation in scientific computation comes from its nice property given in the section 3.1.1 of [5]: the derivative is obtained exactly by computing the value of a function from the
dual numbers to the dual numbers just once, where the dual numbers were introduced by C. L. Clifford in [1]. Therefore, another interesting problem is how to find a new way of doing automatic differentiation so that the higher-order derivatives up to an arbitrary order can be obtained exactly by computing the value of a function from an algebra to the algebra just once.

The goal of this paper is to give our answer to these two problems by using a class of associative algebras called real-like algebras. Based on our observation, the automatic differentiation techniques appearing in machine learning community are always related to some real-like algebras which generalize the dual numbers. In section 1 of this paper, we define real-like algebras and discuss their basic properties. In section 2, we will introduce the concept of the graded automatic differentiation induced by a real-like algebra \( A \) and present a new technique of automatic differentiation to compute higher-order derivatives. To simplify our presentation, we will just explain how to use the graded automatic differentiation induced by a real-like algebra to get the first, the second and the third derivatives of a function exactly and simultaneously by computing the value of a function from the real-like algebra to the real-like algebra just once. In the last section of this paper, we will do an example by using the new technique of automatic differentiation.

Throughout this paper, we use the following notations and assumptions:

- \( \mathbb{R} \) is the real number field;
- An algebra means an associative algebra with the identity;
- \( S^n := \{ (x_1, x_2, \ldots, x_n) | x_1, x_2, \ldots, x_n \in S \} \) is the set of all \( n \)-tuples of elements in a set \( S \);
- \( F(S^n, S) := \{ f | f : S^n \to S \text{ is a function} \} \);
- \( D^k(\mathbb{R}, \mathbb{R}) := \{ f | f : \mathbb{R} \to \mathbb{R} \text{ has the } k\text{-th derivative} \} \).

1 Real-like Algebras

Let \( n \) be non-negative integer. We say that a vector space \( A \) over the real number field \( \mathbb{R} \) is the direct sum of its non-zero subspaces \( A_0, A_1, \ldots, A_n \) and we write \( A = \bigoplus_{i=0}^{n} A_i \) if each \( x \) in \( A \) can be represented uniquely in the form \( x = \sum_{i=0}^{n} x_i \) for \( x_i \in A_i \) for \( 0 \leq i \leq n \). The subspaces \( A_0, A_1, \ldots, A_n \) are called the homogeneous subspaces of \( A \). The elements of \( A_i \) are said to be homogeneous of degree \( i \) for \( 0 \leq i \leq n \). After expressing an element \( a \) in \( A \) as a sum of non-zero homogeneous elements of distinct degrees, these non-zero
homogeneous elements are called the **homogeneous components** of \( a \) and the homogeneous components of \( a \) of least degree is called the **initial component** of \( a \).

We now define real-like algebras which are the kind of real associative algebras we need in the study of automatic differentiation.

**Definition 1.1** A commutative associative algebra \( A \overline{\otimes} \mathbb{R} \) is called a **real-like algebra** if \( A \) is the direct sum \( A = \bigoplus_{i=0}^{n} A_i \) of its non-zero subspaces \( A_0, A_1, \ldots, A_n \) satisfying \( A_0 = \mathbb{R} \) and \( A_i A_j \subseteq A_{i+j} \) for \( 0 \leq i, j \leq n \), where \( A_{i+j} := 0 \) for \( i + j > n \).

The real-like algebras we will used in this paper is the **real-like** \( n \)-algebra \( \mathbb{R}^{(n)} \), where

\[
\mathbb{R}^{(n)} := \mathbb{R}[X] / \langle \{ X^k | k \geq n \} \rangle
\]

is the quotient associative algebra of the polynomial ring \( \mathbb{R}[X] \) with respect to the ideal \( \langle \{ X^k | k \geq n \} \rangle \) generated by the subset \( \{ X^k | k \geq n \} \) of \( \mathbb{R}[X] \). Clearly, \( \mathbb{R}^{(n)} \) is a real-like algebra. In fact, if \( \epsilon := X + \langle \{ X^k | k \geq n \} \rangle \in \mathbb{R}^{(n)} \), then we have

\[
\mathbb{R}^{(n)} = \bigoplus_{i=0}^{n-1} \mathbb{R} \varepsilon^i, \quad \mathbb{R} \varepsilon^0 = \mathbb{R}, \quad (\mathbb{R} \varepsilon^i)(\mathbb{R} \varepsilon^j) = \begin{cases} \mathbb{R} \varepsilon^{i+j} & \text{if } i + j < n \\ 0 & \text{if } i + j \geq n \end{cases},
\]

where \( 0 \leq i, j \leq n - 1 \). The real-like \( n \)-algebra \( \mathbb{R}^{(n)} \) has appeared in automatic differentiation for a long time (see Section 13.2 in [4]). To the best of our knowledge, although \( \mathbb{R}^{(n)} \) is a \( \ell_1 \)-normed algebra by [4], a \( \ell_2 \)-normed algebraic structure has not been introduced on the real-like \( n \)-algebra \( \mathbb{R}^{(n)} \). Since \( \ell_2 \)-norm is generally preferred in neural networks and more computational efficient than \( \ell_1 \)-norm, it is advantageous to have a \( \ell_2 \)-normed algebraic structure on the algebras appearing in the study of automatic differentiation. At the end of this section, we give many ways of introducing a \( \ell_2 \)-norm on the real-like \( n \)-algebra \( \mathbb{R}^{(n)} \). For convenience, we use \( \mathbb{R}^{(n)} \)-**numbers** to name the elements of the real-like \( n \)-algebra \( \mathbb{R}^{(n)} \). Clearly, \( \mathbb{R}^{(2)} \)-number are the dual numbers introduced by C. L. Clifford in [1]. Based on our research about the applications of the dual numbers, we strongly feel that if there exists a class of new numbers which can be used to extend the known mathematics based on real numbers in a satisfyingly way, then \( \mathbb{R}^{(n)} \)-numbers should be the best candidate for this class of new numbers.

The following proposition gives the basic properties of real-like algebras.

**Proposition 1.1** Let \( A = \bigoplus_{i=0}^{n} A_i \) be a real-like algebra and let \( a = \sum_{i=0}^{n} a_i \) be an element of \( A \) with \( a_i \in A_i \) for \( 0 \leq i \leq n \).
(i) \(a\) is a zero-divisor if and only if \(a_0 = 0\).

(ii) \(a\) is invertible if and only if \(a_0 \neq 0\), in which case, the inverse \(a^{-1}\) of \(a\) is given by \(a^{-1} = \sum_{i=0}^{n} \frac{\det M_i}{a_0^{n+1}}\), where \(M_i\) is the \((n+1) \times (n+1)\)-matrix obtained by replaying the \(i\)-th column of the \((n+1) \times (n+1)\)-matrix

\[
M := \begin{bmatrix}
a_0 & 0 & 0 & \cdots & 0 & 0 \\
a_1 & a_0 & 0 & \cdots & 0 & 0 \\
a_2 & a_1 & a_0 & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
a_{n-1} & a_{n-2} & a_{n-3} & \cdots & a_0 & 0 \\
a_n & a_{n-1} & a_{n-2} & \cdots & a_1 & a_0
\end{bmatrix}
\]

with the \((n+1) \times 1\)-matrix \[
\begin{bmatrix}
1 \\
\vdots \\
0
\end{bmatrix}
\]
and \(\det M_i\) is the determinant of the \((n+1) \times (n+1)\)-matrix \(M_i\).

**Proof** (i) If \(a\) is a zero-divisor, then \(ab = 0\) for some \(0 \neq b \in A\). Let \(p\) be the degree of the initial component of \(b\). Then we have \(b = \sum_{i=p}^{n} b_i\), where \(b_i \in A_i\) for \(p \leq i \leq n\) and \(b_p \neq 0\). Assume that \(a_0 \neq 0\). By the fact that \(a_0\) is in \(A_0 = \mathcal{R}\), the inverse \(a_0^{-1}\) of \(a_0\) exists. It follows that

\[
0 = a_0^{-1}ab = a_0^{-1} \left( \sum_{i=0}^{n} a_i \right) \left( \sum_{i=p}^{n} b_i \right) = b_p + \sum_{i=p+1}^{n} b_i + \left( \sum_{i=1}^{n} a_i \right) \left( \sum_{i=p}^{n} b_i \right).
\]

(1)

Since the degree of the initial component of \(\sum_{i=p+1}^{n} b_i + \left( \sum_{i=1}^{n} a_i \right) \left( \sum_{i=p}^{n} b_i \right)\) is at least \(p + 1\), we have to have \(b_p = 0\) by (1), which is impossible. This proves that \(a_0\) has to be 0.

Conversely, if \(a_0 = 0\), then \(a = \sum_{i=1}^{n} a_i\). After choosing \(0 \neq b_n \in A_n\), we get

\[
ab_n = \left( \sum_{i=1}^{n} a_i \right) b_n = 0.
\]
This proves that \(a\) is a zero-divisor.

(ii) \(a\) is invertible if and only if there exists \(x = \sum_{i=0}^{n} x_i\) with \(x_i \in A_i\) for
0 \leq i \leq n \text{ such that } \left( \sum_{i=0}^{n} a_i \right) \left( \sum_{i=0}^{n} x_i \right) = ax = 1, \text{ which is equivalent to }

1 = a_0 x_0 + (a_0 x_1 + a_1 x_0) + (a_2 x_0 + a_1 x_1 + a_0 x_2) + \cdots + (a_n x_0 + a_{n-1} x_1 + \cdots + a_0 x_n)

or

$$M = \begin{bmatrix}
  x_0 & a_0 & 0 & 0 & \cdots & 0 & 0 \\
  x_1 & a_1 & a_0 & 0 & \cdots & 0 & 0 \\
  x_2 & a_2 & a_1 & a_0 & \cdots & 0 & 0 \\
  \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
  x_{n-1} & a_{n-1} & a_{n-2} & a_{n-3} & \cdots & a_0 & 0 \\
  x_n & a_n & a_{n-1} & a_{n-2} & \cdots & a_1 & a_0
\end{bmatrix} = \begin{bmatrix}
  x_0 & 1 \\
  x_1 & 0 \\
  x_2 & 0 \\
  \vdots & \vdots \\
  x_{n-1} & 0 \\
  x_n & 0
\end{bmatrix}.$$

It follows from that \( x_i = \frac{\det M_i}{a_0^{n+1}} \) for \( 0 \leq i \leq n \). Thus (ii) holds. 

\[ \square \]

To study the norm algebraic structure of a real-like algebra, we introduce the concept of a homogeneous norm algebra in the following

**Definition 1.2** We say that a real-like algebra \( A = \bigoplus_{i=0}^{n} A_i \) has a homogeneous norm \( | \cdot | \) if \( | \cdot | : \bigcup_{i=0}^{n} A_i \to \mathcal{R} \) is a function on the set \( \bigcup_{i=0}^{n} A_i \) of homogeneous elements of \( A \) such that for \( r \in \mathcal{R}, x_i \in A_i, y_j \in A_j \) and \( 0 \leq i, j \leq n \):

(i) \( |x_i| \geq 0, \text{ and } |x_i| = 0 \text{ if and only if } x_i = 0 \),

(ii) \( |rx_i| = |r| \cdot |x_i| \),

(iii) \( |x_i + y_i| \leq |x_i| + |y_i| \),

(iv) \( |x_i y_j| \leq |x_i| \cdot |y_j| \).

Let \( A = \bigoplus_{i=0}^{n} A_i \) be a real-like algebra which has a homogeneous norm \( | \cdot | : \bigcup_{i=0}^{n} A_i \to \mathcal{R} \). Mimicking the definitions of the ordinary \( \ell_1 \)-norm and \( \ell_2 \)-norm on \( \mathcal{R}^n \), we have the following natural extensions \( || \cdot ||_1 : A \to \mathcal{R} \) and \( || \cdot ||_2 : A \to \mathcal{R} \) of the function \( | \cdot | : \bigcup_{i=0}^{n} A_i \to \mathcal{R} \):

\[ ||a||_1 := \sum_{i=0}^{n} |a_i| \] and \[ ||a||_2 := \left( \sum_{i=0}^{n} |a_i|^2 \right)^{\frac{1}{2}} \quad (2) \]
where $a = \sum_{i=0}^{n} a_i \in A$ with $a_i \in A_i$ for $0 \leq i \leq n$. The following proposition gives the basic properties of the two real-valued functions $|| \cdot ||_1$ and $|| \cdot ||_{2,*}$.

**Proposition 1.2** Let $A = \bigoplus_{i=0}^{n} A_i$ be a real-like algebra which has a homogeneous norm $| | _* : \bigcup_{i=0}^{n} A_i \to \mathcal{R}$, and let $|| \cdot ||_1$ and $|| \cdot ||_{2,*}$ be the real-valued functions defined by (2).

(i) $A$ is a normed algebra with respect to the norm $|| \cdot ||_1$.

(ii) If $| e |_* = 1$ for the identity $e$ of the algebra $A$, then $A$ can not be made into a normed algebra via the real-valued function $|| \cdot ||_{2,*}$.

(iii) $|| \cdot ||_{2,*}$ is a norm on $A$.

**Proof** Recall that a function $|| \cdot || : A \to \mathcal{R}$ is called a norm on $A$ if for $r \in \mathcal{R}$ and $x, y \in A$, we have

$$||rx|| = |r||x||, \quad ||x|| \geq 0, \quad \text{and} \quad ||x|| = 0 \text{ if and only if } x = 0$$ (3)

and

$$||x + y|| \leq ||x|| + ||y||.$$ (4)

Also, $A$ is called a normed algebra if there is a norm $|| \cdot ||$ on $A$ such that

$$||xy|| \leq ||x|| \cdot ||y||$$ for all $x, y \in A$.

The proof of Proposition 1.2 follows from direct computations. We now prove (ii) to explain the way of doing the computation. Let $0 \neq a_1 \in A_1$. Then

$$|a_1|_* > 0 \quad \text{and} \quad |a_1|^2_* = |a_1 \cdot a_1|_* \leq |a_1|_* \cdot |a_1|_* = |a_1|^2_*.$$ (6)

It follows from (2) and (6) that

$$|| (e + a_1) \cdot (e + a_1) ||^2_* = || e + 2a_1 + a_1^2 ||^2_* = |e|^2 + |2a_1|^2 + |a_1|^2$$

$$= |e|^2 + (2|a_1|_*)^2 + |a_1^2|_* = |e|^2 + 4|a_1|^2 + |a_1^2|_* > |e|^2 + 2|a_1|^2 + |a_1|^2$$

$$\geq |e|^2 + 2|a_1|_* + |a_1^2|_* = (|e|_* + |a_1^2|_*)^2$$

$$= (|e|_*^2 + |a_1^2|_*^2) = (|e + a_1|^2)_* = (|e + a_1|_{2,*})^2 = (|e + a_1|_{2,*} \cdot |e + a_1|_{2,*})^2$$

or

$$|| (e + a_1) \cdot (e + a_1) ||_{2,*} > |e + a_1|_{2,*} \cdot |e + a_1|_{2,*},$$

which proves that (5) fails for $x = y = e + a_1$. 

\[ \Box \]
Obviously, the map \( |\cdot|_\ast : \bigcup_{i=0}^{n-1} \mathcal{R}e^i \to \mathcal{R} \) defined by

\[
|x^i|_\ast := |x| \quad \text{for} \quad x \in \mathcal{R} \quad \text{and} \quad 0 \leq i \leq n - 1
\]
is a homogeneous norm on the real-like \( n \)-algebra \( \mathcal{R}^{(n)} \) which satisfies the assumption in Proposition 1.2 (ii), where \( |x| \) is the absolute value of the real number \( x \). Hence, the natural idea of extending the ordinary way of defining a \( \ell_2 \)-norm on \( \mathcal{R}^n \) can not give a \( \ell_2 \)-normed algebraic structure on the real-like \( n \)-algebra \( \mathcal{R}^{(n)} \) by Proposition 1.2 (ii). This is possibly why we have not seen the way of making the real-like \( n \)-algebra \( \mathcal{R}^{(n)} \) into a \( \ell_2 \)-normed algebra in automatic differentiation community even it has a \( \ell_2 \)-normed algebraic structure.

We now give many ways of introducing a \( \ell_2 \)-normed algebraic structure on the real-like \( n \)-algebra \( \mathcal{R}^{(n)} \).

**Proposition 1.3** Let \( \beta \) be a positive constant real numbers. If \( \| \cdot \|_\beta : \mathcal{R}^{(n+1)} \to \mathcal{R} \) is the non-negative real valued function defined by

\[
\left\| \sum_{k=0}^{n} x_k e^i \right\|_\beta := \sqrt{\sum_{k=0}^{n} (n + 1 - i) \beta^i x_k^2} \quad (7)
\]

for \( \sum_{k=0}^{n} x_k e^i \in \mathcal{R}^{(n+1)} \) with \( x_k \in \mathcal{R} \) for \( 0 \leq i \leq n \), then \( \| \cdot \|_\beta \) makes the real-like \( (n+1) \)-algebra \( \mathcal{R}^{(n+1)} \) into a normed algebra.

**Proof** For convenience, we set \( \alpha_i := (n + 1 - i) \beta^i \) for \( 0 \leq i \leq n \). Let \( |\cdot|_\ast : \bigcup_{i=0}^{n} \mathcal{R}e^i \to \mathcal{R} \) be a map defined by

\[
|x^i|_\ast := \sqrt{\alpha_i} |x_i| \quad \text{for} \quad x_i \in \mathcal{R} \quad \text{and} \quad 0 \leq i \leq n. \quad (8)
\]

For \( x_i, y_i, r \in \mathcal{R} \) and \( 0 \leq i \leq n \), we clearly have

\[
|x_i e^i|_\ast \geq 0, \quad \text{and} \quad |x_i e^i|_\ast = 0 \quad \text{if and only if} \quad x_i e^i = 0, \quad (9)
\]

\[
|r x_i e^i|_\ast = |r| |x_i e^i|_\ast \quad (10)
\]

and

\[
|x_i e^i + y_i e^i|_\ast = \sqrt{\alpha_i} |x_i + y_i| \leq \sqrt{\alpha_i} (|x_i| + |y_i|) \leq |x_i e^i|_\ast + |y_i e^i|_\ast. \quad (11)
\]

We now prove that

\[
|x_i e^i \cdot y_j e^j|_\ast \leq |x_i e^i|_\ast \cdot |y_j e^j|_\ast \quad \text{for} \quad 0 \leq i, j \leq n. \quad (12)
\]
Since
\[ |x_i \varepsilon^i \cdot y_j \varepsilon^j|_z = |(x_i y_j) \varepsilon^{i+j}|_z = \begin{cases} \sqrt{\alpha_{i+j}} |x_i y_j| & \text{if } i+j \leq n, \\ 0 & \text{if } i+j > n, \end{cases} \] (13)

(12) holds clearly if \( i+j > n \). In the case where \( i+j \leq n \), we have
\[
\alpha_i \alpha_j - \alpha_{i+j} = (n+1-i)\beta^i (n+1-j)\beta^j - (n+1-(i+j))\beta^{i+j}
\]
\[
= \beta^{i+j} \left( (n+1)^2 - (n+1)(i+j) + ij - (n+1-(i+j)) \right)
\]
\[
= \beta^{i+j} \left( (n+1)(n+1-(i+j)) + ij - (n+1-(i+j)) \right)
\]
\[
= \beta^{i+j} \left[ n(n+1-(i+j)) + ij \right] \geq 0 \text{ for } i+j \leq n
\]
or
\[
\alpha_{i+j} \leq \alpha_i \alpha_j \text{ for } 0 \leq i, j \leq n \text{ and } i+j \leq n. \tag{14}
\]

It follows from (13) and (14) that
\[
|x_i \varepsilon^i \cdot y_j \varepsilon^j|_z \leq \sqrt{\alpha_{i+j}} |x_i y_j| \leq \sqrt{\alpha_i} \sqrt{\alpha_j} |x_i| |y_j| = \sqrt{\alpha_i} |x_i| \cdot \sqrt{\alpha_j} |y_j|,
\]
which proves that (12) is also true if \( i+j \leq n \).

By (9), (10), (11) and (12), \( | \cdot |_z \) is a homogeneous norm on the real-like \( n \)-algebra \( R^{(n)} \). By (7) and (8), we have
\[
\left\| \sum_{i=0}^{n} x_i \varepsilon^i \right\|_\beta = \left( \sum_{i=0}^{n} (|\alpha_i x_i|_z)^2 \right)^{\frac{1}{2}} = \left\| \sum_{i=0}^{n} x_i \varepsilon^i \right\|_{2,\beta}. \tag{15}
\]

It follows from (15) and Proposition (12) (iii) that \( \| \cdot \|_\beta = \| \cdot \|_{2,\beta} \) is a norm on the real-like \( (n+1) \)-algebra \( R^{(n+1)} \).

In order to prove that the real-like \( (n+1) \)-algebra \( R^{(n+1)} \) is a normed algebra via the norm \( \| \cdot \|_\beta \), we need only to prove
\[
\|xy\|_\beta \leq \|x\|_\beta \|y\|_\beta \text{ for } x, y \in R^{(n+1)}. \tag{16}
\]

For \( x = \sum_{i=0}^{n} x_i \varepsilon^i \), we define
\[
\phi(x) = \begin{bmatrix}
x_0 \beta^0 & 0 & 0 & \cdots & 0 & 0 \\
x_1 \beta & x_0 \beta^0 & 0 & \cdots & 0 & 0 \\
x_2 \beta^2 & x_1 \beta & x_0 \beta^0 & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
x_{n-1} \beta^{n-1} & x_{n-2} \beta^{n-2} & x_{n-3} \beta^{n-3} & \cdots & x_0 \beta^0 & 0 \\
x_{n} \beta^{n} & x_{n-1} \beta^{n-1} & x_{n-2} \beta^{n-2} & \cdots & x_1 \beta & x_0 \beta^0 \end{bmatrix}. \tag{17}
\]

Then the map \( \phi : R^{(n+1)} \rightarrow M_{n+1}(R) \) defined by (17) is an injective algebra homomorphism. Using this algebra homomorphism \( \phi \) and the matrix norm which makes \( M_{n+1}(R) \) into a normed algebra, we get (16).
2 Automatic Differentiation induced by $R^{(4)}$

The following definition is our way of conceptualizing automatic differentiation mathematically.

**Definition 2.1** Let $A$ be a real-like algebra. A 3-tuple $(\Lambda, \Omega, \{\Gamma_i\}_{i=1}^k)$ consisting of an algebra homomorphism $\Lambda : D^k(R, R) \rightarrow F(A, A)$, a map $\Omega : R \rightarrow A$ and a family maps $\{\Gamma_i : A \rightarrow R | 1 \leq i \leq k\}$ is called the graded automatic differentiation induced by $A$ on $D^k(R, R)$ or the graded $A(\Lambda, \Omega, \{\Gamma_i\}_{i=1}^k)$-automatic differentiation if the following three conditions are satisfied:

(i) $\Lambda$ extends each function $f$ in $D^k(R, R)$, i.e., $\Lambda(f)(x) = f(x)$ for all $x \in R$;

(ii) $\Omega$ preserves the invertible real numbers, i.e., $\Omega(x)$ is an invertible element of $A$ for each non-zero real number $x$;

(iii) $\Lambda$ preserves the composition of two differentiable functions, i.e.,

$$\Lambda(f \circ g) = \Lambda(f) \circ \Lambda(g)$$  \hspace{1cm} (18)

and the map $\Gamma_i : A \rightarrow R$ for $i \in \{1, 2, \ldots, k\}$, which is called the $i$-th derivative map, has the following property:

$$\left(\Gamma_i \circ (\Lambda(f)) \circ \Omega\right)(c) = \frac{d^i f}{dx^i}(c),$$  \hspace{1cm} (19)

where $f = f(x), g = g(x) \in D^k(R, R)$ and $c \in R$.

Like the first-order automatic differentiation which depends on one parameter, which is denoted by $\dot{v}$ in the section 3.1.1 of [5], the higher-order automatic differentiation depends on many parameters. Different choices of these parameters give different ways of doing higher-order automatic differentiation.

We now explain how to get the graded automatic differentiation induced by $R^{(4)}$ on $D^3(R, R)$.

Let $\alpha \neq 0$, $\beta$ and $\gamma$ be three real constants. For $f(x) \in D^3(R, R)$, we define the maps $\Lambda : D^3(R, R) \rightarrow F(R^{(4)}, R^{(4)})$ and $\Omega_{\alpha,\beta,\gamma} : R \rightarrow R^{(4)}$ by

$$\Lambda(f)(x + a_1\varepsilon + a_2\varepsilon^2 + a_3\varepsilon^3) := f(x) + a_1 f'(x)\varepsilon + \left(a_2 f'(x) + \frac{1}{2}a_1^2 f''(x)\right)\varepsilon^2 + \left(a_3 f'(x) + a_1 a_2 f''(x) + \frac{1}{6} a_1^3 f'''(x)\right)\varepsilon^3$$  \hspace{1cm} (20)

and

$$\Omega_{\alpha,\beta,\gamma}(x) := x + \alpha \varepsilon + \beta \varepsilon^2 + \gamma \varepsilon^3$$  \hspace{1cm} (21)

where $x, a_1, a_2, a_3 \in R$.

The following theorem, which is the main theorem of this paper, presents the new technique of automatic differentiation to compute the first, the second and the third derivatives exactly and simultaneously.
Proposition 2.1 (The Main Theorem) Let $\alpha \neq 0$, $\beta$ and $\gamma$ be three real constants. If the maps $\Lambda : D^3(\mathcal{R}, \mathcal{R}) \rightarrow \mathbf{F}(\mathcal{R}^{(4)}, \mathcal{R}^{(4)})$ and $\Omega_{\alpha, \beta, \gamma} : \mathcal{R} \rightarrow \mathcal{R}^{(4)}$ are defined by (21) and (30), then the 3-tuple $(\Lambda, \Omega_{\alpha, \beta, \gamma}, \{\Gamma_i\}_{i=1}^3)$ is the graded $\mathcal{R}^{(4)}(\Lambda, \Omega_{\alpha, \beta, \gamma}, \{\Gamma_i\}_{i=1}^3)$-automatic differentiation, where the $i$-th derivative map $\Gamma_i : \mathcal{R}^{(4)} \rightarrow \mathcal{R}$ for each $i \in \{1, 2, 3\}$ is defined by

\[
\begin{align*}
\Gamma_1(y) & := \frac{1}{\alpha}y_1, \\
\Gamma_2(y) & := \frac{2}{\alpha^2}y_2 - \frac{2\beta}{\alpha^3}y_1, \\
\Gamma_3(y) & := \frac{6}{\alpha^3}y_3 - \frac{12\beta}{\alpha^4}y_2 + \left(\frac{12\beta^2}{\alpha^5} - \frac{6\gamma}{\alpha^4}\right)y_1
\end{align*}
\]

for $y = y_0 + y_1\,\varepsilon + y_2\,\varepsilon^2 + y_3\,\varepsilon^3 \in \mathcal{R}^{(4)}$ with $y_0, y_1, y_2, y_3 \in \mathcal{R}$.

**Proof** First, let $1_{D^3(\mathcal{R}, \mathcal{R})}$ and $1_{\mathbf{F}(\mathcal{R}^{(4)}, \mathcal{R}^{(4)})}$ be the identity of the algebra $D^3(\mathcal{R}, \mathcal{R})$ and the algebra $\mathbf{F}(\mathcal{R}^{(4)}, \mathcal{R}^{(4)})$, respectively. By (30), we have

\[
\Lambda\left(1_{D^3(\mathcal{R}, \mathcal{R})}\right) = 1_{\mathbf{F}(\mathcal{R}^{(4)}, \mathcal{R}^{(4)})}.
\]

Let $f, g \in D^3(\mathcal{R}, \mathcal{R})$. Clearly, we have

\[
\Lambda(f + g) = \Lambda(f) + \Lambda(g).
\]

Note that

\[
(fg)' = f'g + fg', \quad (fg)'' = f''g + 2f'g' + fg''
\]

and

\[
(fg)''' = f'''g + 3f''g' + 3f'g'' + fg'''.
\]

Let $x + a_1\varepsilon + a_2\varepsilon^2 + a_3\varepsilon^3 \in \mathcal{R}^{(4)}$, where $x, a_1, a_2$ and $a_3 \in \mathcal{R}$. By (30), (25) and (26), we have

\[
\Lambda(fg)(x + a_1\varepsilon + a_2\varepsilon^2 + a_3\varepsilon^3) = fg + a_1(fg)'\varepsilon +
\]

\[
+ \left[a_2(fg)' + \frac{1}{2}a_1^2(fg)''\right]\varepsilon^2 + \left[a_3(fg)' + a_1a_2(fg)'' + \frac{1}{6}a_1^3(fg)'''ight]\varepsilon^3
\]

\[
= fg + a_1(f'g + fg')\varepsilon + \left[a_2(f'g + fg') + \frac{1}{2}a_1^2(f''g + 2f'g' + fg'')\right]\varepsilon^2 +
\]

\[
+ \left[a_3(f'g + fg') + a_1a_2(f''g + 2f'g' + fg'') + \frac{1}{6}a_1^3(f'''g + 3f''g' + 3f'g'' + fg''')\right]\varepsilon^3
\]

and

\[
\left(\Lambda(f) \cdot \Lambda(g)\right)(x + a_1\varepsilon + a_2\varepsilon^2 + a_3\varepsilon^3)
\]
\[
\begin{align*}
&= \Lambda(f)(x + a_1\varepsilon + a_2\varepsilon^2 + a_3\varepsilon^3) \cdot \Lambda(g)(x + a_1\varepsilon + a_2\varepsilon^2 + a_3\varepsilon^3) \\
&= \left[ f + a_1f'\varepsilon + \left( a_2f' + \frac{1}{2}a_1^2f'' \right)\varepsilon^2 + \left( a_3f' + a_1a_2f'' + \frac{1}{6}a_1^3f''' \right)\varepsilon^3 \right] \cdot \\
&\quad \cdot \left[ g + a_1g'\varepsilon + \left( a_2g' + \frac{1}{2}a_1^2g'' \right)\varepsilon^2 + \left( a_3g' + a_1a_2g'' + \frac{1}{6}a_1^3g''' \right)\varepsilon^3 \right] \\
&= fg + (a_1f' \cdot g + f \cdot a_1g')\varepsilon + \\
&\quad + \left[ \left( a_2g' + \frac{1}{2}a_1^2g'' \right) + a_1f' + \left( a_2f' + \frac{1}{2}a_1^2f'' \right) \cdot g \right]\varepsilon^2 + \\
&\quad + \left[ a_3g' + a_1a_2g'' + \frac{1}{6}a_1^3g''' \right] + a_1f' \cdot \left( a_2g' + \frac{1}{2}a_1^2g'' \right) + \\
&\quad + \left( a_2f'(x) + \frac{1}{2}a_1^2f'' \right) \cdot a_1g' + \left( a_3f' + a_1a_2f'' + \frac{1}{6}a_1^3f''' \right) \cdot g \right]\varepsilon^3 \\
&= fg + a_1(f'g + fg')\varepsilon + \left[ a_2(f'g + fg') + \frac{1}{2}a_1^2(f''g + 2f'g' + fg'') \right]\varepsilon^2 + \\
&\quad + \left[ a_3(f'g + fg') + a_1a_2(f''g + 2f'g' + fg'') + \right. \\
&\quad \left. + \frac{1}{6}a_1^3(f''g + 3f'g' + 3f'g'' + fg''') \right]\varepsilon^3.
\end{align*}
\]

Using (27) and (28), we get

\[
\Lambda(f \cdot g) = \Lambda(f) \cdot \Lambda(g) \quad \text{for } f, g \in D^3(R, R). \quad (29)
\]

It follows from (23), (24) and (29) that the map \( \Lambda : D^3(R, R) \to F(R(4), R(4)) \) defined by (30) is an algebra homomorphism.

Next, by (30), the condition (i) is satisfied. By (21) and Proposition 1.1 (ii), the condition (ii) is satisfied. For \( f = f(x) \in D^3(R, R) \) and \( c \in R \), using (30) and (22), we have

\[
\left( (\Lambda(f) \circ \Omega_{a,\beta,\gamma})(c) = \Lambda(f)(c + \alpha\varepsilon + \beta\varepsilon^2 + \gamma\varepsilon^3) = f(c) + \alpha f'(c)\varepsilon + \\
+ \left( \beta f'(c) + \frac{1}{2}\alpha^2f''(c) \right)\varepsilon^2 + \left( \gamma f'(c) + \alpha\beta f''(c) + \frac{1}{6}\alpha^3f'''(c) \right)\varepsilon^3 \right)
\]

By (22) and (28), we get

\[
\left( \Gamma_1 \circ (\Lambda(f) \circ \Omega_{a,\beta,\gamma})(c) = \frac{1}{\alpha} \cdot \alpha f'(c) = f'(c),
\right)
\]

11
\[
\left( \Gamma_2 \circ (\Lambda(f)) \circ \Omega_{\alpha,\beta,\gamma} \right)(c) = \frac{2}{\alpha^2} \cdot \left( \beta f'(c) + \frac{1}{2} \alpha^2 f''(c) \right) - \frac{2\beta}{\alpha^3} \alpha f'(c) = f''(c)
\]
and
\[
\left( \Gamma_3 \circ (\Lambda(f)) \circ \Omega_{\alpha,\beta,\gamma} \right)(c) = \frac{6}{\alpha^3} \cdot \left( \gamma f'(c) + \alpha \beta f''(c) + \frac{1}{6} \alpha^3 f'''(c) \right) + \\
- \frac{12\beta}{\alpha^4} \left( \beta f'(c) + \frac{1}{2} \alpha^2 f''(c) \right) + \left( \frac{12\beta^2}{\alpha^5} - \frac{6\gamma}{\alpha^4} \right) \alpha f'(c) = f'''(c),
\]
which proves that (19) holds.

Finally, by [30], a direct computation gives
\[
\Lambda(f \circ g) = \Lambda(f) \circ \Lambda(g) \quad \text{for } f(x), g(x) \in D^3(\mathcal{R}, \mathcal{R}),
\]
i.e., \( \Lambda \) preserves the composition of two differentiable functions.

This completes the proof of the main theorem. \( \square \)

For \( f \in D^3(\mathcal{R}, \mathcal{R}) \), the function \( \Lambda(f) \in \mathcal{F}(\mathcal{R}^{(4)}, \mathcal{R}^{(4)}) \), which is also denoted by \( \overline{f} \), will be called the \( \mathcal{R}^{(4)} \)-extension of \( f \). The \( \mathcal{R}^{(4)} \)-extensions of some common elementary functions in \( D^3(\mathcal{R}, \mathcal{R}) \) are given as follows:

1. \[
\frac{1}{x + a_1 \varepsilon + a_2 \varepsilon^2 + a_3 \varepsilon^3} = \frac{1}{x} - \frac{a_1}{x^2} \varepsilon + \left( \frac{a_1^2}{x^4} - \frac{a_2}{x^3} \right) \varepsilon^2 + \left( -\frac{a_3}{x^4} + \frac{2a_1a_2}{x^3} - \frac{a_3}{x^2} \right) \varepsilon^3 \quad \text{for } 0 \neq x \in \mathcal{R}
\]
2. \[
\exp(x + a_1 \varepsilon + a_2 \varepsilon^2 + a_3 \varepsilon^3) = e^x + a_1 e^x \varepsilon + \left( \frac{a_2}{2} + a_2 \right) e^x \varepsilon^2 + \left( \frac{a_1}{6} + a_1 a_2 + a_3 \right) e^x \varepsilon^3
\]
3. \[
\sin(x + a_1 \varepsilon + a_2 \varepsilon^2 + a_3 \varepsilon^3) = \sin x + (a_1 \cos x) \varepsilon + \left( -\frac{a_2}{2} \sin x + a_2 \cos x \right) \varepsilon^2 + \left( -\frac{a_1}{6} \cos x - a_1 a_2 \sin x + a_3 \cos x \right) \varepsilon^3
\]
4. \[
\cos(x + a_1 \varepsilon + a_2 \varepsilon^2 + a_3 \varepsilon^3) = \cos x - (a_1 \sin x) \varepsilon + \left( -\frac{a_2}{2} \cos x - a_2 \sin x \right) \varepsilon^2 + \left( \frac{a_3}{6} \sin x - a_1 a_2 \cos x - a_3 \sin x \right) \varepsilon^3
\]
5. \[
\ln(x + a_1 \varepsilon + a_2 \varepsilon^2 + a_3 \varepsilon^3) = \ln x + a_1 \ln x \varepsilon + \left( -\frac{a_2}{2x^2} + a_2 \right) \varepsilon^2 + \left( \frac{a_3}{3x^3} - \frac{a_1 a_2}{x^2} + \frac{a_3}{x} \right) \varepsilon^3 \quad \text{for } 0 < x \in \mathcal{R}
\]
\[
\arctan (x + a_1 \varepsilon + a_2 \varepsilon^2 + a_3 \varepsilon^3) = \arctan x + \frac{a_1}{1 + x^2} \varepsilon + \\
\left( -\frac{a_1^2 x}{(1 + x^2)^2} + \frac{a_2}{1 + x^2} \right) \varepsilon^2 + \left( \frac{a_1^3 (3x^2 - 1)}{3(1 + x^2)^3} - \frac{2a_1 a_2 x}{(1 + x^2)^2} + \frac{a_3}{1 + x^2} \right) \varepsilon^3
\]

Since every function \( f(x) \in D^3(\mathcal{R}, \mathcal{R}) \) is formed in terms of some elementary functions in \( D^3(\mathcal{R}, \mathcal{R}) \), the first derivative \( f'(x) \), the second derivative \( f''(x) \) and the third derivative \( f'''(x) \) of \( f(x) \) can be obtained exactly and simultaneously by using the technique of the graded \( \mathcal{R}^{(4)}_{\alpha,\beta,\gamma} \)-automatic differentiation and the \( \mathcal{R}^{(4)} \)-extensions of those elementary functions which form the function \( f(x) \in D^3(\mathcal{R}, \mathcal{R}) \). We will do an example to explain this technique in the last section of this paper.

### 3 An Example

For convenience, the graded \( \mathcal{R}^{(4)}_{\Lambda, \Omega_1, \Omega_2, \Omega_3, \Gamma_i} \)-automatic differentiation introduce in Proposition 1.2 will be also denoted the graded \( \mathcal{R}^{(4)}_{\alpha,\beta,\gamma} \)-automatic differentiation. The different choices of the parameters \( \alpha \neq 0, \beta \) and \( \gamma \) give different ways of doing automatic differentiation to get the first, the second and the third derivatives of a function in \( D^3(\mathcal{R}, \mathcal{R}) \) exactly and simultaneously. In this section, we will choose \( (\alpha, \beta, \gamma) = (1, 0, 0) \) and \( (1, 1, 1) \) to do the graded \( \mathcal{R}^{(4)}_{\alpha,\beta,\gamma} \)-automatic differentiation.

After denoting a \( \mathcal{R}^{(4)} \)-number \( x + a_1 \varepsilon + a_2 \varepsilon^2 + a_3 \varepsilon^3 \in \mathcal{R}^{(4)} \) by a 4-tuple \((x, a_1, a_2, a_3)\) of real numbers, the algorithm, which compute the first derivative \( f'(c) \), the second derivative \( f''(c) \) and the third derivative \( f'''(c) \) of a function \( f(x) \in D^3(\mathcal{R}, \mathcal{R}) \) at a real number \( c \), can be written in a pseudocode as follows:

**Algorithm** \( \mathcal{R}^{(4)}_{\alpha,\beta,\gamma} \)-automatic differentiation

- **Input:** A real number \( c \) and a function \( f: \mathcal{R} \to \mathcal{R} \) which has the third derivative.
- **Output:** A 3-tuple \((z_1, z_2, z_3)\) of real numbers, where \( z_1 = f'(c), z_2 = f''(c) \) and \( z_3 = f'''(c) \).

1. Start
2. Get the \( \mathcal{R}^{(4)} \)-extension \( \mathcal{T}: \mathcal{R}^{(4)} \to \mathcal{R}^{(4)} \).
3. Compute the value of the function \( \mathcal{T} \) at \((c, \alpha, \beta, \gamma)\) to get the 4-tuple \((f(c), y_1, y_2, y_3)\) of real numbers.
4. Compute \( z_1 = \frac{1}{\alpha} y_1 \).

5. Compute \( z_2 = \frac{2}{\alpha^2} y_2 - \frac{2\beta}{\alpha^3} y_1 \).

6. Compute \( z_3 = \frac{6}{\alpha^3} y_3 - \frac{12\beta}{\alpha^4} y_2 + \left( \frac{12\beta^2}{\alpha^5} - \frac{6\gamma}{\alpha^4} \right) y_1 \).

7. Display \((z_1, z_2, z_3)\)

8. Stop

As an example, let \( f(x) \in D^3(\mathcal{R}, \mathcal{R}) \) be a function defined by

\[
f(x) = (\ln x) \cos \left( \frac{1}{x^2} \right),
\]

which is formed in terms of the elementary functions \( x^2, \frac{1}{x}, \ln x \) and \( \cos x \).

We now use both the graded \( \mathcal{R}^{(4)}_{1,0,0} \)-automatic differentiation and the graded \( \mathcal{R}^{(4)}_{1,1,1} \)-automatic differentiation to compute the first, the second and the third derivatives of the function \( f(x) \) defined by (31).

**The example of doing the graded \( \mathcal{R}^{(4)}_{1,0,0} \)-automatic differentiation.**

Using (21) and the \( \mathcal{R}^{(4)} \)-extensions of the elementary functions \( x^2, \frac{1}{x}, \ln x \) and \( \cos x \), we have

\[
(A(f)) \circ \Omega_{1,0,0}(x) = \mathcal{T}(\Omega_{1,0,0}(x)) = \mathcal{T}(x + \varepsilon)
\]

\[
= \ln(x + \varepsilon) \cdot \cos \left( \frac{1}{(x + \varepsilon)^2} \right) = \ln(x + \varepsilon) \cdot \cos \left( \frac{1}{x^2 + 2x\varepsilon + \varepsilon^2} \right)
\]

\[
= \ln(x + \varepsilon) \cdot \cos \left[ \frac{1}{x^2} - \frac{2x}{(x^2)^2} \varepsilon + \left( \frac{(2x)^2}{(x^2)^3} - \frac{1}{(x^2)^2} \right) \varepsilon^2 + \left( \frac{(2x)^3}{(x^2)^4} + \frac{2 \cdot 2x \cdot 1}{(x^2)^3} \right) \varepsilon^3 \right]
\]

\[
= \ln(x + \varepsilon) \cdot \cos \left( \frac{1}{x^2} - \frac{2}{x^3} \varepsilon + \frac{3}{x^4} \varepsilon^2 - \frac{4}{x^5} \varepsilon^3 \right)
\]

\[
= \left( \ln x + \frac{1}{x} \varepsilon + \frac{1}{2x^2} \varepsilon^2 + \frac{1}{3x^3} \varepsilon^3 \right) \cdot \left\{ \cos \left( \frac{1}{x^2} \right) - \left( -2 \frac{2}{x^3} \right) \sin \left( \frac{1}{x^2} \right) \varepsilon + \left[ -\frac{1}{2} \left( \frac{-2}{x^3} \right)^2 \cos \left( \frac{1}{x^2} \right) - \frac{3}{x^4} \sin \left( \frac{1}{x^2} \right) \right] \varepsilon^2 + \left[ \frac{1}{6} \left( \frac{-2}{x^3} \right)^3 \sin \left( \frac{1}{x^2} \right) - \left( -2 \frac{3}{x^4} \right) \cos \left( \frac{1}{x^2} \right) - \left( -4 \frac{4}{x^5} \right) \sin \left( \frac{1}{x^2} \right) \right] \varepsilon^3 \right\}
\]
\[
\begin{align*}
&= \left( \ln x + \frac{1}{x} \varepsilon + \frac{1}{2x^2} \varepsilon^2 + \frac{1}{3x^3} \varepsilon^3 \right) \cdot \left\{ \cos \left( \frac{1}{x^2} \right) + \frac{2}{x^3} \sin \left( \frac{1}{x^2} \right) \varepsilon + \\
&\quad + \left[ -\frac{2}{x^6} \cos \left( \frac{1}{x^2} \right) - \frac{3}{x^4} \sin \left( \frac{1}{x^2} \right) \right] \varepsilon^2 + \\
&\quad + \left[ -\frac{4}{3x^9} \sin \left( \frac{1}{x^2} \right) + \frac{6}{x^7} \cos \left( \frac{1}{x^2} \right) + \frac{4}{5x^5} \sin \left( \frac{1}{x^2} \right) \right] \varepsilon^3 \right\} \\
&= (\ln x) \cos \left( \frac{1}{x^2} \right) + \tilde{y}_1 \varepsilon + \tilde{y}_2 \varepsilon^2 + \tilde{y}_3 \varepsilon^3,
\end{align*}
\]

where
\[
\tilde{y}_1 = (\ln x) \cdot \frac{2}{x^3} \sin \left( \frac{1}{x^2} \right) + \frac{1}{x} \cos \left( \frac{1}{x^2} \right), \quad (32)
\]
\[
\tilde{y}_2 = (\ln x) \cdot \left[ -\frac{2}{x^6} \cos \left( \frac{1}{x^2} \right) - \frac{3}{x^4} \sin \left( \frac{1}{x^2} \right) \right] + \frac{1}{x} \cdot \frac{2}{x^3} \sin \left( \frac{1}{x^2} \right) + \\
\quad -\frac{1}{2x^2} \cdot \cos \left( \frac{1}{x^2} \right) \quad (33)
\]

and
\[
\tilde{y}_3 = (\ln x) \cdot \left[ -\frac{4}{3x^9} \sin \left( \frac{1}{x^2} \right) + \frac{6}{x^7} \cos \left( \frac{1}{x^2} \right) + \frac{4}{5x^5} \sin \left( \frac{1}{x^2} \right) \right] + \\
\quad + \frac{1}{x} \cdot \left[ -\frac{2}{x^6} \cos \left( \frac{1}{x^2} \right) - \frac{3}{x^4} \sin \left( \frac{1}{x^2} \right) \right] - \frac{1}{2x^2} \cdot \frac{2}{x^3} \sin \left( \frac{1}{x^2} \right) + \frac{1}{3x^3} \cdot \cos \left( \frac{1}{x^2} \right) \quad (34)
\]

Using the \(i\)-th derivative map \(\Gamma_i\) defined by (22) for \(i \in \{1, 2, 3\}\) and \((\alpha, \beta, \gamma) = (1, 0, 0)\), we get from \(32\), \(33\) and \(34\) that
\[
\Gamma_1(y) = y_1 = \frac{2}{x^3} (\ln x) \sin \left( \frac{1}{x^2} \right) + \frac{1}{x} \cos \left( \frac{1}{x^2} \right) = f'(x), \quad (35)
\]
\[
\Gamma_2(y) = 2y_2 = -\frac{4}{x^9} (\ln x) \cos \left( \frac{2}{x^2} \right) - \frac{6}{x^7} (\ln x) \sin \left( \frac{1}{x^2} \right) + \frac{4}{x^5} \sin \left( \frac{1}{x^2} \right) + \\
\quad -\frac{1}{x^2} \cos \left( \frac{1}{x^2} \right) = f''(x) \quad (36)
\]
\[
\Gamma_3(y) = 6y_3 = -\frac{8}{x^3} (\ln x) \sin \left(\frac{1}{x^2}\right) + \frac{36}{x^2} (\ln x) \cos \left(\frac{1}{x^2}\right) + \frac{24}{x^3} (\ln x) \sin \left(\frac{1}{x^2}\right) + \frac{12}{x^2} \cos \left(\frac{1}{x^2}\right) - \frac{24}{x^2} \sin \left(\frac{1}{x^2}\right) + \frac{2}{x^3} \cos \left(\frac{1}{x^2}\right) = f'''(x). \quad (37)
\]

By (35), (36) and (37), we get the first derivative \(f'(x)\), the second derivative \(f''(x)\) and the third derivative \(f'''(x)\) of \(f(x) = (\ln x) \cos \left(\frac{1}{x^2}\right)\) by doing the graded \(\mathcal{R}^{(4)}_{1,0,0}\)-automatic differentiation and without using any differentiation rule in calculus.

- **The example of doing the graded \(\mathcal{R}^{(4)}_{1,1,1}\)-automatic differentiation.**

Using (21) and the \(\mathcal{R}^{(4)}\)-extensions of the elementary functions \(x^2, \frac{1}{x}, \ln x\) and \(\cos x\), we have

\[
(\Lambda(f)) \circ \Omega_{1,1,1}(x) = \mathcal{T}(\Omega_{1,1,1}(x)) = \mathcal{T}(x + \varepsilon + \varepsilon^2 + \varepsilon^3)
\]

\[
= \ln \left(1 + (x + \varepsilon + \varepsilon^2 + \varepsilon^3) \cdot \frac{1}{x} \right) \cos \left(\frac{1}{x^2 + 2x\varepsilon + (2x + 1)\varepsilon^2 + (2x + 2)\varepsilon^3}\right)
\]

\[
= \ln \left(x + \frac{1}{x} \varepsilon + \left(\frac{1}{2x^2} + \frac{1}{x} \right) \varepsilon^2 + \left(\frac{1}{3x^3} - \frac{1}{x^2} + \frac{1}{x} \right) \varepsilon^3\right) \cos \left(\frac{1}{x^2} + \frac{2x}{x^2}\varepsilon\right)
\]

\[
+ \left(\frac{2x}{x^2}\varepsilon + \frac{2x + 1}{x^2}\varepsilon^2 + \left(\frac{2x}{x^2} + \frac{2(2x)(2x + 1)}{x^4} - \frac{2x + 2}{x^3}\varepsilon^3\right)\right)
\]

\[
+ \left(\frac{2x}{x^2} - \frac{2x + 1}{x^2}\varepsilon^2 + \left(-\frac{4}{x^3} + \frac{6}{x^4} - \frac{2}{x^5}\varepsilon^3\right)\right)
\]

\[
= \ln \left(x + \frac{1}{x} \varepsilon + \left(\frac{1}{2x^2} + \frac{1}{x} \right) \varepsilon^2 + \left(\frac{1}{3x^3} - \frac{1}{x^2} + \frac{1}{x} \right) \varepsilon^3\right) \cos \left(\frac{1}{x^2} + \frac{2x}{x^2}\varepsilon\right)
\]

\[
+ \left(-\frac{2}{x^3} \sin \left(\frac{1}{x^2}\right) \varepsilon + \left(-\frac{2}{x^3} - \frac{2}{x^3} \varepsilon^2 + \left(\frac{1}{3x^3} - \frac{1}{x^2} + \frac{1}{x} \right) \varepsilon^3\right)\right) \left\{ \cos \left(\frac{1}{x^2}\right) + \frac{2}{x^3} \sin \left(\frac{1}{x^2}\right) \varepsilon + \left[-\frac{2}{x^4} \cos \left(\frac{1}{x^2}\right) + \frac{2}{x^3} - \frac{3}{x^4} \sin \left(\frac{1}{x^2}\right) \right] \varepsilon^2 + \ldots \right\}
\]
\[
+ \left[ -\frac{4}{3x^3} \sin \left( \frac{1}{x^2} \right) + \left( \frac{6}{x^7} - \frac{4}{x^6} \right) \cos \left( \frac{1}{x^2} \right) + \left( \frac{4}{x^5} - \frac{6}{x^4} + \frac{2}{x^3} \right) \sin \left( \frac{1}{x^2} \right) \right] \varepsilon^3 \]

\[
= (\ln x) \cos \left( \frac{1}{x^2} \right) + y_1 \varepsilon + y_2 \varepsilon^2 + y_3 \varepsilon^3,
\]

where

\[
y_1 = \frac{2}{x^3} (\ln x) \sin \left( \frac{1}{x^2} \right) + \frac{1}{x} \cos \left( \frac{1}{x^2} \right), \tag{38}\]

\[
y_2 = (\ln x) \cdot \left[ -\frac{2}{x^6} \cos \left( \frac{1}{x^2} \right) + \left( \frac{2}{x^3} - \frac{3}{x^4} \right) \sin \left( \frac{1}{x^2} \right) \right] + \frac{1}{x} \cdot \left[ -\frac{2}{x^6} \cos \left( \frac{1}{x^2} \right) + \left( \frac{2}{x^3} - \frac{3}{x^4} \right) \sin \left( \frac{1}{x^2} \right) \right] + \left( -\frac{1}{2x^2} + \frac{1}{x} \right) \cdot \left[ \frac{2}{x^3} \sin \left( \frac{1}{x^2} \right) + \left( \frac{1}{3x^3} - \frac{1}{x^2} + \frac{1}{x} \right) \cdot \cos \left( \frac{1}{x^2} \right) \right]
\]

or

\[
y_3 = -\frac{4}{3x^9} (\ln x) \sin \left( \frac{1}{x^2} \right) + \left( \frac{6}{x^7} - \frac{4}{x^6} \right) (\ln x) \cos \left( \frac{1}{x^2} \right) + \left( \frac{4}{x^9} - \frac{6}{x^8} + \frac{2}{x^7} \right) (\ln x) \sin \left( \frac{1}{x^2} \right) - \frac{2}{x^7} \cos \left( \frac{1}{x^2} \right) + \left( \frac{2}{x^9} - \frac{3}{x^8} \right) \sin \left( \frac{1}{x^2} \right) + \left( -\frac{1}{2x^2} + \frac{2}{x^4} \right) \sin \left( \frac{1}{x^2} \right) + \left( \frac{1}{3x^3} - \frac{1}{x^2} + \frac{1}{x} \right) \cos \left( \frac{1}{x^2} \right). \tag{40}\]

Using the \(i\)-th derivative map \(\Gamma_i\) defined by (22) for \(i \in \{1, 2, 3\}\) and \((\alpha, \beta, \gamma) = (1, 1, 1)\), we get from (38), (39) and (40) that

\[
\Gamma_1(y) = y_1 = \frac{2}{x^3} (\ln x) \sin \left( \frac{1}{x^2} \right) + \frac{1}{x} \cos \left( \frac{1}{x^2} \right) = f'(x), \tag{41}\]

\[
\Gamma_2(y) = 2y_2 - 2y_1
\]

\[
= 2 \left[ \frac{2}{x^6} (\ln x) \cos \left( \frac{1}{x^2} \right) + \left( \frac{2}{x^3} - \frac{3}{x^4} \right) (\ln x) \sin \left( \frac{1}{x^2} \right) + \frac{2}{x^4} \sin \left( \frac{1}{x^2} \right) + \left( -\frac{1}{2x^2} + \frac{1}{x} \right) \cos \left( \frac{1}{x^2} \right) \right] +
\]
\[-2 \left[ \frac{2}{x^3} (\ln x) \sin \left(\frac{1}{x^2}\right) + \frac{1}{x} \cos \left(\frac{1}{x^2}\right) \right] \]
\[= -\frac{4}{x^6} (\ln x) \cos \left(\frac{1}{x^2}\right) + \left(\frac{4}{x^3} - \frac{6}{x^4}\right) (\ln x) \sin \left(\frac{1}{x^2}\right) + \frac{4}{x^4} \sin \left(\frac{1}{x^2}\right) + \]
\[+ \left(-\frac{1}{x^2} + \frac{2}{x^3}\right) \cos \left(\frac{1}{x^2}\right) - \frac{4}{x^3} (\ln x) \sin \left(\frac{1}{x^2}\right) - \frac{2}{x^2} \cos \left(\frac{1}{x^2}\right) \]
\[= -\frac{4}{x^6} (\ln x) \cos \left(\frac{1}{x^2}\right) - \frac{1}{x^2} \cos \left(\frac{1}{x^2}\right) - \frac{6}{x^4} (\ln x) \sin \left(\frac{1}{x^2}\right) + \frac{4}{x^4} \sin \left(\frac{1}{x^2}\right) + \]
\[+ \frac{4}{x^4} \sin \left(\frac{1}{x^2}\right) = f''(x) \]  \hspace{1cm} (42)

and
\[\Gamma_3(y) = 6y_3 - 12y_2 + 6y_1 \]
\[= 6 \left[ -\frac{4}{3x^9} (\ln x) \sin \left(\frac{1}{x^2}\right) + \left(\frac{6}{x^7} - \frac{4}{x^6}\right) (\ln x) \cos \left(\frac{1}{x^2}\right) + \right] \]
\[+ \left(\frac{4}{x^5} - \frac{6}{x^4} + \frac{2}{x^3}\right) (\ln x) \sin \left(\frac{1}{x^2}\right) - \frac{2}{x^7} \cos \left(\frac{1}{x^2}\right) + \left(\frac{2}{x^3} - \frac{3}{x^5}\right) \sin \left(\frac{1}{x^2}\right) + \]
\[+ \left(-\frac{1}{x^6} + \frac{2}{x^4}\right) \sin \left(\frac{1}{x^2}\right) + \left(\frac{1}{3x^3} - \frac{1}{x^2} + \frac{1}{x}\right) \cos \left(\frac{1}{x^2}\right) \]
\[+ \frac{12}{x^4} \sin \left(\frac{1}{x^2}\right) + \left(\frac{2}{x^3} - \frac{3}{x^4}\right) (\ln x) \sin \left(\frac{1}{x^2}\right) \]
\[+ \frac{2}{x^4} \sin \left(\frac{1}{x^2}\right) + \left(-\frac{1}{2x^2} + \frac{1}{x}\right) \cos \left(\frac{1}{x^2}\right) \right] + 6 \left[ \frac{2}{x^3} (\ln x) \sin \left(\frac{1}{x^2}\right) + \frac{1}{x} \cos \left(\frac{1}{x^2}\right) \right] \]
\[= -\frac{8}{x^7} (\ln x) \sin \left(\frac{1}{x^2}\right) + \left(\frac{36}{x^6} - \frac{24}{x^5}\right) (\ln x) \cos \left(\frac{1}{x^2}\right) + \]
\[+ \left(\frac{24}{x^5} - \frac{36}{x^4} + \frac{12}{x^3}\right) (\ln x) \sin \left(\frac{1}{x^2}\right) - \frac{12}{x^7} \cos \left(\frac{1}{x^2}\right) + \left(\frac{12}{x^4} - \frac{18}{x^5}\right) \sin \left(\frac{1}{x^2}\right) + \]
\[+ \left(-\frac{6}{x^3} + \frac{12}{x^4}\right) \sin \left(\frac{1}{x^2}\right) + \left(\frac{6}{x^5} - \frac{6}{x^2} \frac{6}{x^5}\right) + \frac{6}{x} \cos \left(\frac{1}{x^2}\right) + \]
\[+ \frac{24}{x^5} (\ln x) \cos \left(\frac{1}{x^2}\right) - \left(\frac{24}{x^4} - \frac{36}{x^5}\right) (\ln x) \sin \left(\frac{1}{x^2}\right) + \]

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\[-\frac{24}{x^4} \sin \left(\frac{1}{x^2}\right) + \left(\frac{12}{2x^2} - \frac{12}{x^6}\right) \cos \left(\frac{1}{x^2}\right) + \frac{12}{x^3} (\ln x \sin \left(\frac{1}{x^2}\right) + \frac{6}{x} \cos \left(\frac{1}{x^2}\right) \right) \]

\[= -\frac{8}{x^7} (\ln x) \sin \left(\frac{1}{x^2}\right) + \frac{36}{x^7} (\ln x) \cos \left(\frac{1}{x^2}\right) + \frac{24}{x^9} (\ln x) \sin \left(\frac{1}{x^2}\right) + \]

\[-\frac{12}{x^7} \cos \left(\frac{1}{x^2}\right) - \frac{24}{x^9} \sin \left(\frac{1}{x^2}\right) + \frac{2}{x^3} \cos \left(\frac{1}{x^2}\right) = f'''(x). \quad (43)\]

By (41), (42) and (43), we get the first derivative \(f'(x)\), the second derivative \(f''(x)\) and the third derivative \(f'''(x)\) of \(f(x) = (\ln x) \cos \left(\frac{1}{x^2}\right)\) by doing the graded \(\mathcal{R}_{1,1,1}^{(4)}\)-automatic differentiation and without using any differentiation rule in calculus.

We finish this paper by indicating that the technique of the graded \(\mathcal{R}_{1,1,1}^{(4)}(\Lambda, \Omega; \alpha, \beta, \gamma, \left\{\Gamma_i\right\}_{i=1}^3)\)-automatic differentiation can be generalized to get the technique of the graded \(\mathcal{R}_{1,1,1}^{(k+1)}(\Lambda, \Omega; \left\{\Gamma_i\right\}_{i=1}^k)\)-automatic differentiation which solves the problem of computing the first, the second, , , , , and the \(k\)-th derivatives of a function \(f \in \mathcal{D}^{(k+1)}(\mathcal{R}, \mathcal{R})\) exactly and simultaneously by computing the value of a function from \(\mathcal{R}_{1,1,1}^{(k+1)}\) to \(\mathcal{R}_{1,1,1}^{(k+1)}\) just once for any given positive integer \(k\).

References

[1] William K. Clifford, *Preliminary sketch of bi-quaternions*, Proceeding of the London Mathematical Society, 4, 381-385, 1873.

[2] J. A. Fike & J. J. Alonso, *The development of hyper-dual numbers for exact second-derivative calculations*. In AIAA paper 2011-886, 49th AIAA Aerospace Science Meeting, 2011.

[3] A. Griewank, *Automatic Differentiation*, Princeton Companion to Applied Mathematics, Nicolas Higham Ed., Princeton University Press, 2014.

[4] A. Griewank and A. Walther *Evaluating Derivatives: Principles and Techniques of Algorithmic Differentiation*, second edition, SIAM, Philadelphia, PA, 2008.

[5] A. G. Baydin, Barak A. Pearlmutter, Alexey Andreyevich Radul & Jeffrey Mark Siskind, *Automatic differentiation in machine learning: a survey*, arXiv: 1502.05767v4[cs.SC], 5 Feb 2018.

[6] Philipp H. W. Hoffmann, *A hitchhiker’s guide to automatic differentiation*, Numerical Algorithms 72(3), October 2015.