Science Publications

American Journal of Applied Sciences 4 (10): 792-794, 2007 ISSN 1546-9239 © 2007 Science Publications

A Recurrence Formula for Computing the Derivative of Composition of Functions

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Abstract: A new recursion formula for computing the n-th derivative of the composition of two functions has been introduced in this contribution. The importance of this new formula is associated with its counterpart; Leibniz rule for finding the n-th derivative of the product of two functions. Furthermore the process of computing this formula has been presented in algorithmic format herein.

Key Words: Leibniz rule, differentiation formula, composite functions, mathematical methods.

INTRODUCTION

The object of this research is trying to introduce a formula to find the n-th derivative of the composition of two functions, like the Leibniz rule of differentiation the product of two functions^[3]. This is one of the basic theorems in applied mathematics, and the most useful formula in differentiation^[1, 2, 3]. The Leibniz rule to find the n-th derivative of the product of two functions u(x), v(x) is given by formula :

$$\frac{d^n}{dx^n}[u(x)v(x)] = \sum_{i=0}^n \binom{n}{i} \frac{d^i}{dx^i}u(x) \frac{d^{n-i}}{dx^{n-i}}v(x)$$

A generalization of this formula to three functions u(x), v(x), h(x), is given by:

$$\frac{d^n}{dx^n}([u(x)v(x)]h(x)) = \sum_{i=0}^n \binom{n}{i}$$
$$\frac{d^i}{dx^i}[u(x)v(x)] \frac{d^{n-i}}{dx^{n-i}}h(x)$$
$$= \sum_{i=0}^n \binom{n}{i} \sum_{r=0}^i \binom{i}{r} \frac{d^r}{dx^r}u(x) \frac{d^{i-r}}{dx^{i-r}}v(x) \frac{d^{n-i}}{dx^{n-i}}h(x)$$

The proof of the Leibniz rule follows from the binomial theorem

$$(a+b)^n = \sum_{i=0}^n \binom{n}{i} a^i b^{n-i}$$
,

and by assuming an operator:

$$\frac{d}{dx} =: D = D_u + D_v,$$

where D_u acts only on u and D_v acts only on v.

Then
$$\frac{d}{dx^n}[u(x)v(x)] = (D_u + D_v)^n[u(x)v(x)].$$

The operator $D_u + D_v$ can be expanded by the binomial theorem to give the Leibniz rule.

Now, we will try in the next section to find a general formula like that in the Leibniz rule, to find the n-th derivative of the composition of two functions given by $y = (u \circ v)(x) = u(v(x))$. An algorithm for computer programming to find the formula derived in section 2, will be presented in section 3.

RESULTS AND DISCUSSION

Description of the Formula: To have an idea about a possible formula for the derivative $\frac{d^n y}{dx^n}$ of the function y = u(v(x)), let us write the derivative when n = 1,2,3,4. We will use the dots to represent differentiation with respect to x and the primes represent differentiation with respect to v

$$\dot{y} = u'\dot{v}$$
$$\ddot{y} = u''\dot{v}^{2} + u'\ddot{v}$$
$$y_{3} = u'''\dot{v}^{3} + 3u''\dot{v}\ddot{v} + u'v_{3}$$

 $y_4 = u_4 v_1^{-1} + 6u_3 v_1^{-2} v_2 + 3u_2 v_2^{-2} + 4u_2 v_1 v_3 + u_1 v_4$, where u_i is the i-th derivative of u with respect to v and v_i , y_i are the i-th derivatives of v, y with respect to x, respectively. The n-th derivative of y = u(v(x)) is founded by differentiating the $(n-1)^{st}$ derivative of u(v(x)).

The $(n-1)^{st}$ derivative of y = u(v(x)) has the form:

$$y_{n-1} = \sum_{i=1}^{n-1} a(i, p_1, ..., p_i) u_i v_{p_1} ... v_{p_i},$$

$$p_1 + ... + p_i = n - 1,$$
 (2.1)

where $a(i, p_1, ..., p_i)$ is a strictly positive integer depends on $i, p_1, ..., p_i$. The above formula can be proved by induction on n-1. And thus

$$\frac{d}{dx}y_{n-1} = y_n = \frac{d}{dx} \left[\sum_{i=1}^{n-1} a(i, p_1, \dots, p_i)u_i v_{p_1} \dots v_{p_i}\right],$$

$$p_1 + \dots + p_i = n - 1$$
(2.2)

The coefficient $a(i, p_1, ..., p_i)$ depends also on n-1, but the n-1 is dropped because also $p_1, ..., p_i$ depend on n-1. The equation (2.2) can also be written in the form:

$$y_n = \frac{d}{dx} \left[\sum_{i=1}^{n-1} a(i, (p_1, r_1), ..., (p_s, r_s)) u_i v_{p_1}^{r_1} ... v_{p_i}^{r_s} \right], \qquad (2.3)$$

under the conditions $r_1 p_1 + \ldots + r_s p_s = n-1$ and $r_1 + \ldots + r_s = i$,

where $s, r_1, ..., r_s, p_1, ..., p_s$ are all strictly positive integers.

The above equation can be rewritten in the form:

$$y_n = \sum_{i=1}^n b(i, (q_1, t_1), \dots, (q_v, t_v)) u_i v_{q_1}^{t_1} \dots v_{q_v}^{t_v}$$
(2.4)

under the conditions $t_1q_1 + ... + t_{\nu}q_{\nu} = n$ and $t_1 + ... + t_v = i$, where $v, t_1, ..., t_v$ $q_1, ..., q_v$ are all strictly positive integers. Thus this derivative is determining completed by the coefficients $b(i, (q_1, t_1), \dots, (q_v, t_v))$ associated with $u_i v_{q_1}^{t_1} \dots v_{q_v}^{t_v}$ under the mentioned conditions $1 \le i \le n$. $t_1 q_1 + \dots + t_v q_v = n$ and, $t_1 + \ldots + t_v = i$. In order to find a possible recursion

formula for these coefficients; that is writing the coefficients of the n-th derivative in terms of the

coefficients of the $(n-1)^{st}$ derivatives, the following remarks must be noted:

- In differentiating (2.3), the rule of differentiating the product of functions is used, u_i is first differentiated to give u_{i+1}v₁; which causes only a multiple of v₁.
- 2. The other factors in the product are also differentiated; i.e. $v_{p_1}^{r_1} \dots v_{p_s}^{r_s}$, which gives:

$$r_1 v_{p_1}^{r_1 - 1} v_{p_1 + 1} v_{p_2}^{r_2} \dots v_{p_s}^{r_s} + \dots + r_s v_{p_1}^{r_1} \dots v_{p_s}^{r_s - 1} v_{p_s + 1}$$

Recursion formula: Thus, by the above argument, the n-th derivative y_n of y with respect to x has the form:

$$y_{n} = \sum_{i=1}^{n-1} a(i,(p_{1},r_{1}),...,(p_{s},r_{s})) \times [u_{i+1}v_{p_{1}}^{r_{1}}...v_{p_{i}}^{r_{s}} + u_{i}(r_{1}v_{p_{1}}^{r_{1}-1}v_{p_{1}+1}...v_{p_{s}}^{r_{s}} + ...+r_{s}v_{p_{1}}^{r_{1}}...v_{p_{s}}^{r_{s}-1}v_{p_{s}+1})]$$

$$=:\sum_{i=1}^{n} b(i,(q_{1},t_{1}),...,(q_{v},t_{v}))u_{i}v_{q_{1}}^{t_{1}}...v_{q_{v}}^{t_{v}} ,$$

$$r_{1}p_{1} + ...+r_{s}p_{s} = n-1 \text{ and } r_{1} + ...+r_{s} = i$$

 $t_1q_1 + \ldots + t_vq_v = n$ and $t_1 + \ldots + t_v = i$. Specifically, we have:

$$b(1, (p_s + 1 = n, 1)) = 1 = \text{ coefficient of } u_1 v^{n_1}.$$

 $b(n, (1, n)) = 1 = \text{ coefficient of } u_n v_1^n$.

So, for possible factorization of the form $t_1q_1 + ... + t_vq_v = n$, where $t_1 + ... + t_v = i$ the coefficient $b(i, (q_1, t_1), ..., (q_v, t_v))$ associated with $u_i v_{q_1}^{t_1} ... v_{q_v}^{t_v}$, are to be founded, where q_i 's are distinct and $q_{l_2} > q_{l_1}$ whenever $l_2 > l_1$. These terms come from:

I. For all q_l , $1 \le l \le v$. It comes from the derivative of a term of the form:

$$a(i, (q_1, t_1), ..., (q_{k-1}, t_k + 1), (q_k, t_k - 1), ..., (q_v, t_v)) u_i v_{q_1}^{t_1} ... v_{q_k}^{t_k + 1} v_{k+1}^{t_{k+1} - 1} ... v_{q_v}^{t_k}$$

under the conditions

$$S_1 := \sum_{l=1}^{\nu} t_l = i ,$$

and

$$S_2 := t_1 q_1 + \dots + (t_k + 1)q_{k-1} + (t_k - 1)q_k + \dots + t_v q_v = n - 1$$

II. If $q_1 = 1$. A term is also added from the derivative of

$$a(i-1,(1,t_1-1),(q_2,t_2),...,(q_v,t_v))$$

$$u_{i-1}v_{q_1}^{t_1-1}v_{q_2}^{t_2}...v_{q_v}^{t_v}.$$

Combining these together gives the coefficients

$$b(i, (q_1, t_1), ..., (q_v, t_v))$$

by the formula

$$\begin{split} &\sum_{k=1}^{\nu} (t_{k}+1) \times a(i,(q_{1},t_{1}),...,(q_{k-1},t_{k}+1),(q_{k},t_{k}-1),...,(q_{\nu},t_{\nu})) \\ &+ (\text{if } q_{l}=1) a(i-1,(1,t_{1}-1),(q_{2},t_{2})...,(q_{\nu},t_{\nu})), \end{split}$$

where the sum is taken under the conditions S_1 and S_2 , which proves the following theorem:

Theorem 2.1: The n^{th} derivative of composite function y = u(v(x)) is given by the formula:

$$\sum_{i=1}^{n} \sum_{k=1}^{i} (t_{k} + 1) \times a(i, (q_{1}, t_{1}), ..., (q_{k-1}, t_{k} + 1), (q_{k}, t_{k} - 1), ..., (q_{v}, t_{v})).$$

(if $q_{1} = 1$) $a(i - 1, (1, t_{1} - 1), (q_{2}, t_{2})..., (q_{v}, t_{v}))$
 $u_{i}v_{q_{1}}^{t_{-11}}v_{q_{2}}^{t_{2}}...v_{q_{v}}^{t_{v}},$

where the second sum is taken under the conditions in S_1 and S_2 and the first sum is taken under the conditions in S_1 and S_3 , where,

$$S_3 \coloneqq t_1 q_1 + \ldots + t_v q_v = n$$

and the *a*'s are the coefficients of the $(n-1)^{st}$ differentiation of $(u \circ v)(x)$

3. Algorithm: The following algorithm can help to find computer programming to compute the composition rule.

For fixed *n*

- 1. b(1,(n,1)) = b(1,(1,n)) = 1.
- 2. For $2 \le i \le n-1$, we find all possible distinct pairs (p_j, r_j) , where $1 \le j \le s$ which satisfy $r_1p_1 + ... + r_sp_s = n$ and $r_1 + ... + r_s = i$
- 3. For possible factorization $(p_1, r_1), ..., (p_{s_0}, r_{s_0})$ associated with $u_i v_{p_1}^{r_1} v_{p_2}^{r_2} ... v_{p_{s_0}}^{r_{s_0}}$

the coefficient $b(i, (q_1, t_1), ..., (q_{s_0}, t_{s_0}))$ is a sum of the form

$$\sum_{k=1}^{s_0} (r_k + 1) \times a(i, (p_1, r_1), \dots, (p_{k-1}, r_k + 1), (p_k, r_k - 1), \dots, (p_{s_0}, r_{s_0}))$$

+(if $p_l = 1$) $a(i - 1, (1, r_1 - 1), (p_2, r_2), \dots, (p_{s_0}, r_{s_0}))$

where the a's are the coefficients of differentiating n-1 times.

CONCLUSION

A new recursion formula for computing the nth derivative of two functions has been introduced in this paper. Furthermore, an algorithm for the formula has been constructed. This algorithmic approach enables us to write a program to compute the required result. The obtained formula is important in many application areas of applied mathematics such as physics, engineering and computer science. Further work that can be done on this contribution is automating the introduced algorithm using one of the high-level programming languages. Our newly-introduced formula is considered as important as the well-known Leibniz Rule with respect to computing the nth derivative of two functions.

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