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GENERALIZATION OF PASCAL'S RULE AND LEIBNIZ'S RULE FOR DIFFERENTIATION

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Abstract. We generalize the combinatorial identity for binomial coefficients underlying the construction of Pascal's Triangle to multinomial coefficients underlying the construction of Pascal's Simplex. Using this identity, we present a new proof of the formula for calculating the n^{th} derivative of the product of k functions, a generalization of Leibniz's Rule for differentiation.

Acknowledgements: I took a freshman sequence in Advanced Calculus at the University of Connecticut using Volume 1 of Calculus by Apostol (1967) as the textbook in 2013-14 with Professor William Abikoff. Without Professor Abikoff's continuous encouragement to push the envelope and untiring patience in answering each and every question, I would not have developed the fortitude to undertake this investigation. While I started the work in the summer of 2014, the upper divisional Honors Probability course I took with the late Professor Evarist Giné in Fall 2014 was extremely influential in helping me formulate the extension of Pascal's Rule, a key step in my proof of the generalization of Leibniz's Rule. I would like to dedicate this paper to my fond memories of Professor Giné.

1 Introduction

For a real-valued function y defined on an open interval $I \subseteq \Re$, and any nonnegative integer k, let $y^{(k)}$ denote the k^{th} derivative of y with the convention that $y^{(0)} = y$. Let f, g be two real-valued functions defined on an open interval $I \subseteq \Re$ such that $f^{(n)}$ and $g^{(n)}$ exist for some nonnegative integer n. For $h(x) = f(x) g(x)$, Leibniz's Rule asserts

$$h^{(n)}(x) = \sum_{k=0}^{n} \binom{n}{k} f^{(k)}(x)\, g^{(n-k)}(x). \tag{1}$$

See, for example, Exercise 5.11.4 of Apostol's Calculus, Volume 1 [1]. For $n = 1$, (1) reduces to the product rule for differentiation. The formula in (1) is proved by induction on n using Pascal's Rule

$$\binom{q}{j-1} + \binom{q}{j} = \binom{q+1}{j}, \tag{2}$$

where q and j are non-negative integers, $0 \leq j \leq q$. Note that

$$\binom{q}{-1} = 0$$

under the convention that $(r!)^{-1} = 0$ if r is a negative integer.

A formula for calculating the derivative of the product of k differentiable functions is outlined in Exercise 4.6.24 of Apostol's Calculus, Volume 1 [1]. Let $\{f_1, \ldots, f_k\}$ be k real-valued differentiable functions on an open interval $I \subseteq \Re$ and let

$$g = \prod_{i=1}^{k} f_i; \tag{3}$$

then

$$g^{(1)} = \sum_{i=1}^{k} f_i^{(1)} \prod_{\{j \neq i\}} f_j. \tag{4}$$

The equality in (4) is vacuously true for $k = 1$, is the product rule for $k = 2$, and follows easily by induction on k using the product rule.

Theorem 1 of this paper presents a generalization of the formula in (4) for higher order derivatives. We need to define a multi-index to state the theorem.

Definition 1. A k-dimensional multi-index

$$\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_k)$$

is a k-tuple of non-negative integers, with

$$|\boldsymbol{\alpha}| = \sum_{i=1}^{k} \alpha_i \text{ and } \boldsymbol{\alpha}! = \prod_{i=1}^{k} \alpha_i!.$$

Theorem 1. *For $n \geq 1$, let $\{f_1, \ldots, f_k\}$ be real-valued functions on an open interval $I \subseteq \Re$ such that $f_i^{(n)}$ exists for all $1 \leq i \leq k$. Let g be as in (3); then*

$$g^{(n)} = \sum_{\{\boldsymbol{\alpha}:|\boldsymbol{\alpha}|=n\}} \frac{n!}{\boldsymbol{\alpha}!} \prod_{i=1}^{k} f_i^{(\alpha_i)}, \tag{5}$$

where $\boldsymbol{\alpha}$ is a k-dimensional multi-index.

Remark 1. It should be noted here that the coefficient of the product in the right-hand side of (5),

$$\frac{n!}{\boldsymbol{\alpha}!} = \frac{n!}{\alpha_1! \ldots \alpha_k!} = \binom{n}{\alpha_1 \ldots \alpha_k},$$

is nothing but the multinomial coefficient.

Remark 2. The generalized Leibniz's Rule presented in (5) is not a new result. As pointed out by Thaheem and Laradji [2], this generalization is overlooked by most calculus textbooks, and those that mention it typically do so without a proof. Thaheem and Laradji [2] presented this generalization in their Theorem 2; they proved the formula in (5) by fixing the order of the derivative, which is n in our notation, and using induction on the number of factors, which is k in our notation. They assumed Leibniz's Rule stated in (1). Also see Mazkewitsch [3]. In the next section, we establish the formula in (5) by fixing k and using induction on n. The key ingredients of our proof are the equalities in (4) and (9) of Lemma 1 below. Note that (9) is a generalization of Pascal's Rule stated in (2).

2 Proof of Theorem 1

To prove Theorem 1, we first need to state and prove Lemma 1. The formulation of Lemma 1 requires the following definition.

Definition 2. Given a k-dimensional multi-index $\boldsymbol{\alpha}$ and $i \in \{1, 2, \ldots k\}$, let ${}^{+}\boldsymbol{\alpha}^{(i)}$ be the k-dimensional multi-index with the j^{th} component given by

$${}^{+}\alpha_j^{(i)} = \begin{cases} \alpha_j & \text{if } j \neq i \\ \alpha_i + 1 & \text{if } j = i; \end{cases} \tag{6}$$

if $\alpha_i > 0$, let ${}_{-}\boldsymbol{\alpha}^{(i)}$ be the k-dimensional multi-index with the j^{th} component given by

$${}_{-}\alpha_j^{(i)} = \begin{cases} \alpha_j & \text{if } j \neq i \\ \alpha_i - 1 & \text{if } j = i. \end{cases} \tag{7}$$

Given a k-dimensional multi-index $\boldsymbol{\alpha}$, for $1 \leq i \leq k$, let

$$\gamma_i(\boldsymbol{\alpha}) = \begin{cases} 0 & \text{if } \alpha_i = 0 \\ \frac{(|\boldsymbol{\alpha}|-1)!}{{}_{-}\boldsymbol{\alpha}^{(i)}!} & \text{if } \alpha_i > 0. \end{cases} \tag{8}$$

Remark 3. Note that the definition of γ_i is an extension of the convention that $(r!)^{-1} = 0$ if r is a negative integer. Before proceeding further, let us explicitly compute for a couple of multi-indices the quantities defined in (6), (7), and (8). Let $k = 3$ and $\boldsymbol{\alpha} = (1, 4, 2)$. Then

$$\begin{aligned}
&{}^{+}\boldsymbol{\alpha}^{(1)} = (2,4,2)\,,\ {}^{+}\boldsymbol{\alpha}^{(2)} = (1,5,2)\,,\ {}^{+}\boldsymbol{\alpha}^{(3)} = (1,4,3)\\
&{}_{-}\boldsymbol{\alpha}^{(1)} = (0,4,2)\,,\ {}_{-}\boldsymbol{\alpha}^{(2)} = (1,3,2)\,,\ {}_{-}\boldsymbol{\alpha}^{(3)} = (1,4,1)\\
&\gamma_1(\boldsymbol{\alpha}) = 15,\ \gamma_2(\boldsymbol{\alpha}) = 60,\ \gamma_3(\boldsymbol{\alpha}) = 30.
\end{aligned}$$

Let $k = 3$ and $\boldsymbol{\alpha} = (3, 0, 5)$. Then

$$\begin{aligned}
&{}^{+}\boldsymbol{\alpha}^{(1)} = (4,0,5)\,,\ {}^{+}\boldsymbol{\alpha}^{(2)} = (3,1,5)\,,\ {}^{+}\boldsymbol{\alpha}^{(3)} = (3,0,6)\\
&{}_{-}\boldsymbol{\alpha}^{(1)} = (2,0,5)\,,\ {}_{-}\boldsymbol{\alpha}^{(2)} \text{ is undefined},\ {}_{-}\boldsymbol{\alpha}^{(3)} = (3,0,4)\\
&\gamma_1(\boldsymbol{\alpha}) = 21,\ \gamma_2(\boldsymbol{\alpha}) = 0,\ \gamma_3(\boldsymbol{\alpha}) = 35.
\end{aligned}$$

In both examples

$$\gamma_1(\boldsymbol{\alpha}) + \gamma_2(\boldsymbol{\alpha}) + \gamma_3(\boldsymbol{\alpha}) = \frac{|\boldsymbol{\alpha}|!}{\boldsymbol{\alpha}!},$$

a fact that is true in general and is the assertion of Lemma 1.

Lemma 1. *Given a k-dimensional multi-index $\boldsymbol{\beta}$,*

$$\frac{|\boldsymbol{\beta}|!}{\boldsymbol{\beta}!} = \sum_{i=1}^{k} \gamma_i(\boldsymbol{\beta})\,. \tag{9}$$

Proof. Since by definition

$$\gamma_i(\boldsymbol{\beta}) = \frac{|\boldsymbol{\beta}|!}{\boldsymbol{\beta}!} \times \frac{\beta_i}{|\boldsymbol{\beta}|} \text{ and } \sum_{i=1}^{k} \beta_i = |\boldsymbol{\beta}|,$$

the algebraic proof of (9) follows. □

Remark 4. The identity in (9) can (and should) be interpreted in terms of a selection problem. To get there, let us recall the following interpretation of (2). Clearly, the right-hand side of (2) is the number of samples of size j that can be chosen from a population of size $q + 1$. Let us mark an element of the population as E. The collection of samples of size j can be partitioned into two subcollections, where one subcollection consists of all the samples of size j that include E and the other subcollection consists of all the samples of size j that exclude E. This partition is mutually exclusive and exhaustive. Since the first term in the left-hand side of (2) is equal to the number of samples of size j that include E and the second term is equal to the number of samples of size j that exclude E, the assertion of (2) is immediate.

Now consider a population of size $q+1$, elements of which are to be partitioned into k mutually exclusive and exhaustive subsets of the population, say $\{G_1, \ldots, G_k\}$, where the size of G_i is β_i, $1 \leq i \leq k$; that is, $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_k)$ is a k-dimensional multi-index with

$$\left|\boldsymbol{\beta}\right| = \sum_{i=1}^{k} \beta_i = q+1.$$

Let $\mathcal{P}$ be the collection of all such partitions. Note that the left-hand side of (9) is the cardinality of $\mathcal{P}$. Let us once again mark an element of the population as E. For $i \in \{1, \ldots, k\}$, let $\mathcal{P}_i$ be the subcollection of all partitions that place E in G_i. The fact that the subsets G_i are mutually exclusive and exhaustive implies that $\{\mathcal{P}_1, \ldots, \mathcal{P}_k\}$ is a mutually exclusive and exhaustive partition of $\mathcal{P}$, so that

$$\text{left-hand side of (9)} = \sum_{i=1}^{k} \text{cardinality of } \mathcal{P}_i.$$

Note that

$$\text{cardinality of } \mathcal{P}_i = \begin{cases} 0 & \text{if } \beta_i = 0 \\ \frac{q!}{\left(\prod_{j \neq i} \beta_j!\right)(\beta_i - 1)!} & \text{if } \beta_i > 0; \end{cases} \tag{10}$$

since right-hand side of (10) $= \gamma_i\left(\boldsymbol{\beta}\right)$, (9) follows.

Proof of Theorem 1. We first observe that for $n=1$, the formula in (5) reduces to the formula in (4); that is, the formula in (5) holds for $n=1$. The number of k-dimensional multi-indices $\boldsymbol{\alpha}$ such that $\left|\boldsymbol{\alpha}\right| = 1$ is k; they can be enumerated as $\{\boldsymbol{e}_i : 1 \leq i \leq k\}$, where $\boldsymbol{e}_i$ has 1 in the i^{th} coordinate and 0 elsewhere. Since $\boldsymbol{e}_i! = 1$ and by convention $f_j^{(0)} = f_j$, the formula in (5) reduces to

$$g^{(1)} = \sum_{i=1}^{k} f_i^{(1)} \prod_{\{j \neq i\}} f_j,$$

which is precisely the formula in (4).

To prove the formula in (5) by induction on n, let us assume that (5) holds for $n=m$, that is,

$$g^{(m)} = \sum_{\{\boldsymbol{\alpha} : |\boldsymbol{\alpha}| = m\}} \frac{m!}{\boldsymbol{\alpha}!} \left(\prod_{i=1}^{k} f_i^{(\alpha_i)}\right). \tag{11}$$

From (11), by linearity of the operation of differentiation,

$$g^{(m+1)} = \sum_{\{\boldsymbol{\alpha} : |\boldsymbol{\alpha}| = m\}} \frac{m!}{\boldsymbol{\alpha}!} D \left(\prod_{i=1}^{k} f_i^{(\alpha_i)}\right), \tag{12}$$

where D denotes the differential operator. Using the formula for calculating the first derivative of the product of k functions, that is, the equality in (4), we obtain via (6)

$$D\left(\prod_{i=1}^{k} f_i^{(\alpha_i)}\right) = \sum_{i=1}^{k} f_i^{(\alpha_i+1)} \prod_{\{j\neq i\}} f_j^{(\alpha_j)} = \sum_{i=1}^{k}\left(\prod_{j=1}^{k} f_j^{\left({}^{+}\alpha_j^{(i)}\right)}\right). \tag{13}$$

Substituting (13) in (12),

$$g^{(m+1)} = \sum_{\{\boldsymbol{\alpha}:|\boldsymbol{\alpha}|=m\}} \frac{m!}{\boldsymbol{\alpha}!} \sum_{i=1}^{k}\left(\prod_{j=1}^{k} f_j^{\left({}^{+}\alpha_j^{(i)}\right)}\right). \tag{14}$$

Interchanging the orders of (finite) summation over i and $\boldsymbol{\alpha}$ in (14),

$$g^{(m+1)} = \sum_{i=1}^{k} \sum_{\{\boldsymbol{\alpha}:|\boldsymbol{\alpha}|=m\}} \frac{m!}{\boldsymbol{\alpha}!}\left(\prod_{j=1}^{k} f_j^{\left({}^{+}\alpha_j^{(i)}\right)}\right) = \sum_{i=1}^{k} T_i, \tag{15}$$

where

$$T_i = \sum_{\{\boldsymbol{\alpha}:|\boldsymbol{\alpha}|=m\}} \frac{m!}{\boldsymbol{\alpha}!}\left(\prod_{j=1}^{k} f_j^{\left({}^{+}\alpha_j^{(i)}\right)}\right). \tag{16}$$

Now let us fix $i \in \{1, 2, \dots k\}$. Note that for every k-dimensional multi-index $\boldsymbol{\alpha}$ such that $|\boldsymbol{\alpha}| = m$, ${}^{+}\boldsymbol{\alpha}^{(i)}$ is a k-dimensional multi-index such that $\left|{}^{+}\boldsymbol{\alpha}^{(i)}\right| = m+1$. Conversely, for every k-dimensional multi-index $\boldsymbol{\beta}$ such that $\left|\boldsymbol{\beta}\right| = m+1$ and $\beta_i > 0$, there exists a k-dimensional multi-index $\boldsymbol{\alpha}$ $\left(= {}_{-}\boldsymbol{\beta}^{(i)}\right)$ such that $|\boldsymbol{\alpha}| = m$ and $\boldsymbol{\beta} = {}^{+}\boldsymbol{\alpha}^{(i)}$. Therefore, by a change of variable in the summation in the right-hand side of (16),

$$\begin{aligned} T_i &= \sum_{\{\boldsymbol{\beta}:|\boldsymbol{\beta}|=m+1,\ \beta_i>0\}} \frac{m!}{{}_{-}\boldsymbol{\beta}^{(i)}!}\left(\prod_{j=1}^{k} f_j^{(\beta_j)}\right) \\ &= \sum_{\{\boldsymbol{\beta}:|\boldsymbol{\beta}|=m+1\}} \gamma_i\left(\boldsymbol{\beta}\right)\left(\prod_{j=1}^{k} f_j^{(\beta_j)}\right), \end{aligned} \tag{17}$$

where the second equality follows from the definition of γ_i in (8). Substituting in (15) the expression for T_i obtained in (17),

$$g^{(m+1)} = \sum_{i=1}^{k} \sum_{\{\boldsymbol{\beta}:|\boldsymbol{\beta}|=m+1\}} \gamma_i\left(\boldsymbol{\beta}\right)\left(\prod_{j=1}^{k} f_j^{(\beta_j)}\right). \tag{18}$$

Interchanging the orders of (finite) summation over $\boldsymbol{\beta}$ and i in (18),

$$g^{(m+1)} = \sum_{\{\boldsymbol{\beta}:|\boldsymbol{\beta}|=m+1\}} \sum_{i=1}^{k} \gamma_i\left(\boldsymbol{\beta}\right)\left(\prod_{j=1}^{k} f_j^{(\beta_j)}\right). \tag{19}$$

Since $\prod_{j=1}^{k} f_j^{(\beta_j)}$ does not depend on i, it follows from (19) and (9) that

$$g^{(m+1)} = \sum_{\{\boldsymbol{\beta}:|\boldsymbol{\beta}|=m+1\}} \left(\prod_{j=1}^{k} f_j^{(\beta_j)}\right) \sum_{i=1}^{k} \gamma_i(\boldsymbol{\beta}) = \sum_{\{\boldsymbol{\beta}:|\boldsymbol{\beta}|=m+1\}} \frac{(m+1)!}{\boldsymbol{\beta}!} \left(\prod_{j=1}^{k} f_j^{(\beta_j)}\right),$$

thereby completing the proof of the theorem. $\square$

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[3] D. Mazkewitsch (1963): The n^{th} Derivative of a Product, The American Mathematical Monthly, 70:7, 739-742.