An intuitive presentation of Faà di Bruno's formula

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Suppose that $f, g : \mathbb{R} \to \mathbb{R}$ are functions admitting n derivatives:
Faà di Bruno's formula enumerates the terms in the expansion of the n-th derivative

$$\frac{d^n}{dx^n} f(g(x)) = (f \circ g)^{(n)}(x) \ .$$

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To compute these derivatives we use two precedent results in calculus.

- One is the *chain rule* for derivation of a composition of functions
$$\frac{d}{dx} f(g(x)) = f'(g(x))\, g'(x) \ .$$
As we see this produces a "monomial" that is the product of two functions.
- The other one is the *rule for products* for deriving the product of functions, that we present for the case of three functions $a, b, c : \mathbb{R} \to \mathbb{R}$:
$$\frac{d}{dx}\Big(a(x)b(x)c(x)\Big) = a'(x)b(x)c(x) + a(x)b'(x)c(x) + a(x)b(x)c'(x) \ .$$
We see that this formula produces a sum of "monomials", in each we derive one of the terms of the given product.

(Both formulas appear in works by Leibniz, circa 1680).

To compute the n-th derivative we will apply the above rules many many times. We can predict that the resulting expression will be long and complex, since the first rule increases the number of terms in a monomial, and the second increases the number of monomials

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Cases $n = 1, 2, 3$

We may start with a simple direct calculation. We compute the derivatives for $n = 1, 2, 3$. The first derivative is obtained by the chain rule.

$$(f \circ g)'(x) = f'(g(x))g'(x) \quad .$$

The second derivative is obtained by performing product differentiation and then chain rule.

$$\begin{aligned}(f \circ g)''(x) &= \Big(f'(g(x))g'(x)\Big)' = \\ &\stackrel{\text{product}}{=} \Big(f'(g(x))\Big)' g'(x) + f'(g(x))g''(x) = \\ &\stackrel{\text{chain}}{=} f''(g(x))g'(x)^2 + f'(g(x))g''(x) \quad .\end{aligned}$$

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\end{aligned}$$

Let's see in detail the computation of third derivative. We derive once more the second derivative

$$(f \circ g)''(x) = f''(g(x))g'(x)^2 + f'(g(x))g''(x) \quad .$$

Note that we have a **tree of derivations**.

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product / product+ +collect / product / product

$$\Big(f''(g(x))\Big)' g'(x)^2 + \quad 2f''(g(x))g'(x)g''(x) + \quad \Big(f'(g(x))\Big)' g''(x) + \quad f'(g(x))g'''(x)$$

chain / copy / chain / copy

$$f'''(g(x))g'(x)\, g'(x)^2 + \quad 2f''(g(x))g'(x)g''(x) + \quad f''(g(x))g'(x)g''(x) + \quad f'(g(x))g'''(x)$$

copy / collect / collect / copy

$$f'''(g(x))g'(x)\, g'(x)^2 + \quad 3f''(g(x))g'(x)g''(x) + \quad f'(g(x))g'''(x)$$

Note that we have a **tree of derivations**.

Summarizing the derivatives $n = 1, 2, 3, 4$ are:

$$\begin{aligned}
(f \circ g)'(x) &= f'(g(x))g'(x) \\
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(f \circ g)'''(x) &= f'''(g(x))g'(x)^3 + 3f''(g(x))g'(x)g''(x) + \\
&+ \; f'(g(x))g'''(x) \\
(f \circ g)''''(x) &= f''''(g(x))g'(x)^4 + 6f'''(g(x))g''(x)g'(x)^2 \\
&+ \; 3f''(g(x))g''(x)^2 + 4f''(g(x))g'''(x)g'(x) \\
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\end{aligned}$$

We see that the expansion of $\frac{d^n}{dx^n} f(g(x))$ is always the sum of many monomials of the form $a f^{(m)}(g(x)) g'(x)^{i_1} \dots g^{(n)}(x)^{i_n}$ with appropriate integer coefficients $a, n, m, i_1, \dots i_n$.

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Faà di Bruno's formula is a closed form formula to enumerate all such monomials.
The formula comes in many different formats.

- A combinatorial form. This is the simplest to understand, but is also the *more redundant* one, since the monomials are simply repeated (that is, the coefficients are 1).
- Factorial forms, that collect together monomials in the combinatorial form.

Factorial

Positive integer numbers are $1, 2, 3, 4, 5, \ldots$.
Given n positive integer, the product of the first n numbers is called **factorial** and is denoted by $\boxed{n! = 1 \cdot 2 \cdot 3 \cdots n.}$
$n!$ is the number of different ways of lining up n different objects.
(Conventionally when $n = 0$ then $n! = 1$).

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Cardinality

Given a set A, then $|A|$ is the number of elements in A. (In mathematical parlance $|A|$ is the **cardinality** of A)
Example. If $A = \{1, 44, 4, 133\}$ then $|A| = 4$. If n is a positive integer number and $A = \{1, 2, \ldots, n\}$ is the set of the first n numbers then $|A| = n$.

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Partitions

Consider the set $A = \{1, 2, \dots, n\}$ of the first n numbers. A **partition** of this set is a family of non empty subsets, each one containing one element of A, so that no element is left behind.

Example. Given $A = \{1, 2, 3, 4\}$ then $\{\{2\}, \{4\}, \{3, 1\}\}$ is a partition.

We will call P_n the set of all partitions of $\{1, 2, \dots, n\}$. It is a set of sets of sets of numbers!

Example. There are 5 partitions of $\{1, 2, 3\}$, namely

$$P_3 = \{ \quad \{\{1,2,3\}\}, \quad \{\{1,2\},\{3\}\}, \quad \{\{1\},\{2,3\}\}, \quad \{\{1,3\},\{2\}\}, \quad \{\{1\},\{2\},\{3\}\}, \quad \}$$

Note that $|P_3| = 5$.

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Note that $|P_3| = 5$.

Combinatorial form

The Faà di Bruno's formula has a "combinatorial" form:

$$(f \circ g)^{(n)}(x) = \sum_{\pi \in P_n} f^{(|\pi|)}(g(x)) \prod_{B \in \pi} g^{(|B|)}(x) \tag{1}$$

where

- $\sum_{\pi \in P_n}$ means *we sum what follows varying* π *between all partitions* P_n *of* $\{1, ..., n\}$,
- $\prod_{B \in \pi}$ means *we multiply what follows varying* B *between all the parts of the partition* π ; and moreover
- $|\pi|$ is the number of parts in the partition P_n and $|B|$ is the size of the part B.

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We now present an example to help understand why any possible way of deriving $f(g(x))$ for n times is associated to a partition.

First we note that any partition may be uniquely represented by ordering the numbers in each part, and the parts by the minimum element. E.g. $(n = 8)$

$$\{\{5,7\},\{2\},\{6\},\{3,1,8,4\}\} \rightarrow \{\{1,3,4,8\},\{2\},\{5,7\},\{6\}\}$$
$$\{\{8\},\{3\},\{7,1\},\{4\},\{2,5\},\{6\}\} \rightarrow \{\{1,7\},\{2,5\},\{3\},\{4\},\{6\},\{8\}\}$$

We now derive $f(g(x))$ for 8 times, following the scheme $\{\{1,3,4,8\},\{2\},\{5,7\},\{6\}\}$ down the tree of derivations.

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- The first step is obliged:

$$f(g(x)) \qquad \to \quad g'(x)f'(g(x))$$

and associate it to

$$\{\{1, \ldots$$
$$\ldots$$
$$\ldots$$
$$\ldots .$$

- We have now two terms, we decide to derive the second:

$$g'(x)f'(g(x)) \quad \rightarrow \quad g'(x)g'(x)f''(g(x))$$

and we associate it to

$$\{\{1, \dots$$
$$\{2, \dots$$
$$\dots$$
$$\dots$$

- We have now three terms, we decide to derive the first:

$$g'(x)g'(x)f''(g(x)) \quad \rightarrow \quad g''(x)g'(x)f''(g(x))$$

and we associate it to

$$\begin{array}{l} \{\{1, 3, \ldots \\ \;\{2, \ldots \\ \;\ldots \\ \;\ldots \end{array}$$

- We have again three terms, we decide to derive the first again:

$$g''(x)g'(x)f''(g(x)) \quad \rightarrow \quad g'''(x)g'(x)f''(g(x))$$

and we associate it to

$$\{\{1, 3, 4, \dots$$
$$\{2, \dots$$
$$\dots$$
$$\dots$$

- We have still three terms, we decide to derive the third:

$$g'''(x)g'(x)f''(g(x)) \quad \rightarrow \quad g'''(x)g'(x)g'(x)f'''(g(x))$$

and we associate it to

$$\{\{1,3,4,\ldots$$
$$\{2,\ldots$$
$$\{5,\ldots$$
$$\ldots$$

- We have now four terms, we decide to derive the fourth:

$$g'''(x)g'(x)g'(x)f'''(g(x)) \quad \rightarrow \quad g'''(x)g'(x)g'(x)g'(x)f^{(4)}(g(x))$$

and we associate it to

$$\{\{1,3,4,\ldots$$
$$\{2,\ldots$$
$$\{5,\ldots$$
$$\{6,\ldots$$

- We have now five terms, we decide to derive the third:

$$g'''(x)g'(x){\color{red}g'(x)}g'(x)f^{(4)}(g(x)) \quad \rightarrow \quad g'''(x)g'(x){\color{red}g''(x)}g'(x)f^{(4)}(g(x))$$

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$$g'''(x)g'(x)g''(x)g'(x)f^{(4)}(g(x)) \;\rightarrow\; g^{(4)}(x)g'(x)g''(x)g'(x)f^{(4)}(g(x))$$

and we associate it to

$$\{\{1,3,4,8\ldots$$
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We have obtained the monomial

$$g^{(4)}(x)g'(x)g''(x)g'(x)f^{(4)}(g(x))$$

that is associated to the partition

$$\{\{1,3,4,8\},\\ \{2\},\\ \{5,7\},\\ \{6\}\}$$

Redundancy

We also see that this form is highly redundant. E.g. when $n = 4$ the monomial $g''(x)g''(x)f''(g(x)) = g''(x)^2 f''(g(x))$ appears 3 times, associated to the partitions

$\{\{1,2\},\{3,4\}\}$
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Similarly the monomial
$g^{(4)}(x)g'(x)g''(x)g'(x)f^{(4)}(g(x)) = f^{(4)}(g(x))g'(x)^2 g''(x)g^{(4)}(x)$
that we derived in the example before can be obtained by 420 different partitions in P_8. (We will prove this fact later on).

We will see in next section that *factorial forms* reduce the redundancy (at the price of a longer formula....).

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that we derived in the example before can be obtained by 420 different partitions in P_8. (We will prove this fact later on).

We will see in next section that *factorial forms* reduce the redundancy (at the price of a longer formula....).

Redundancy

We also see that this form is highly redundant. E.g. when $n = 4$ the monomial $g''(x)g''(x)f''(g(x)) = g''(x)^2 f''(g(x))$ appears 3 times, associated to the partitions
$\{\{1,2\},\{3,4\}\}$
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We now prove formally that the combinatorial form formula holds true, using induction. The case $n = 1$ is true, since P_1 contains only one partition, namely $\pi = \{\{1\}\}$, that is associated to $\frac{d}{dx} f(g(x)) = f'(g(x))g'(x)$.

We now assume that

$$(f \circ g)^{(n)}(x) = \sum_{\pi \in P_n} f^{(|\pi|)}(g(x)) \prod_{B \in \pi} g^{(|B|)}(x)$$

is true, and we derive it once more.

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This produces two terms

$$(f \circ g)^{(n+1)}(x) = \sum_{\pi \in P_n} f^{(|\pi|+1)}(g(x))g'(x) \prod_{B \in \pi} g^{(|B|)}(x) + \\ + \sum_{\pi \in P_n} f^{(|\pi|)}(g(x)) \sum_{\hat{B} \in \pi} \prod_{B \in \pi} g^{(|B|+\delta_{B,\hat{B}})}(x)$$

where $\delta_{B,\hat{B}}$ is the **Kronecker delta** [1]

$$\delta_{A,B} = \begin{cases} 1, & \text{if } A = B \\ 0, & \text{if } A \neq B \end{cases}$$

[1] http://en.wikipedia.org/wiki/Kronecker_delta

The question now is: how do we generate the partitions in $\tilde{\pi} \in P_{n+1}$ starting from the partitions in $\pi \in P_n$.

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$$\sum_{\pi \in P_n} f^{(|\pi|+1)}(g(x)) g'(x) \prod_{B \in \pi} g^{(|B|)}(x) = \\ = \sum_{\tilde{\pi} \in P_{n+1}, \{n+1\} \in \tilde{\pi}} f^{(|\tilde{\pi}|)}(g(x)) \prod_{\tilde{B} \in \tilde{\pi}} g^{(|\tilde{B}|)}(x) \quad (2)$$

indeed all such $\tilde{\pi}$ satisfy $\{n+1\} \in \tilde{\pi}$ and $|\tilde{\pi}| = |\pi| + 1$, and moreover the case $\tilde{B} = \{n+1\}$ generates the extra term $g'(x)$ that is in the left hand side.

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$$\sum_{\pi \in P_n} f^{(|\pi|)}(g(x)) \sum_{\hat{B} \in \pi} \prod_{B \in \pi} g^{(|B|+\delta_{B,\hat{B}})}(x) = $$
$$= \sum_{\tilde{\pi} \in P_{n+1}, \{n+1\} \notin \tilde{\pi}} f^{(|\tilde{\pi}|)}(g(x)) \prod_{\tilde{B} \in \tilde{\pi}} g^{(|\tilde{B}|)}(x) \qquad (3)$$

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Summing up the identities (2) and (3) we conclude that indeed

$$\begin{aligned}(f\circ g)^{(n+1)}(x) &= \sum_{\tilde{\pi}\in P_{n+1},\{n+1\}\in\tilde{\pi}} f^{(|\tilde{\pi}|)}(g(x))\prod_{\tilde{B}\in\tilde{\pi}} g^{(|\tilde{B}|)}(x)+\\ &\quad+\sum_{\tilde{\pi}\in P_{n+1},\{n+1\}\notin\tilde{\pi}} f^{(|\tilde{\pi}|)}(g(x))\prod_{\tilde{B}\in\tilde{\pi}} g^{(|\tilde{B}|)}(x)=\\ &=\sum_{\tilde{\pi}\in P_{n+1}} f^{(|\tilde{\pi}|)}(g(x))\prod_{\tilde{B}\in\tilde{\pi}} g^{(|\tilde{B}|)}(x)\end{aligned}$$

that is the formula for $n+1$. □

The factorial forms collect together monomials in the combinatorial form; the formula is more complex, but it is also more useful.

Factorial form

The monomials in the combinatorial form (1) may be collected, to give

$$\frac{d^n}{dx^n} f(g(x)) = \sum \frac{n!}{m_1!\,1!^{m_1}\,m_2!\,2!^{m_2}\,\cdots\,m_n!\,n!^{m_n}} \cdot \cdot f^{(m_1+\cdots+m_n)}(g(x)) \prod_{j=1}^{n} \left(g^{(j)}(x)\right)^{m_j} \tag{4}$$

where the sum is over all n-tuples of nonnegative integers $(m_1, \ldots, m_n)$ satisfying the constraint

$$1 \cdot m_1 + 2 \cdot m_2 + 3 \cdot m_3 + \cdots + n \cdot m_n = n.$$

The monomials

$$f^{(m_1+\cdots+m_n)}(g(x)) \cdot \prod_{j=1}^{n} \left(g^{(j)}(x)\right)^{m_j}$$

that appear in the formula (4) may be written as

$$f^{(m_1+\cdots+m_n)}(g(x)) \left(g'(x)\right)^{m_1} \left(g''(x)\right)^{m_2} \cdots \left(g^{(n)}(x)\right)^{m_n} \tag{5}$$

We clearly see that every derivative of g appears once, with varying exponential; then monomials are not repeated in this formula.

Hence the term

$$\frac{n!}{m_1!\,1!^{m_1}\,m_2!\,2!^{m_2}\,\cdots\,m_n!\,n!^{m_n}}$$

is the integer coefficient of the monomial.

Sometimes, to give it a memorable pattern, the formula (4) is written in this way :

$$\frac{d^n}{dx^n} f(g(x)) = \sum \frac{n!}{m_1!\, m_2!\, \cdots\, m_n!} \cdot f^{(m_1+\cdots+m_n)}(g(x)) \cdot \prod_{j=1}^{n} \left(\frac{g^{(j)}(x)}{j!} \right)^{m_j} .$$

This was original formula presented by Francesco Faà di Bruno in 1855 in *Annali di Scienze Matematiche e Fisiche*.

How can we reconnect this formula (4) with the previous combinatorial version (1)?

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Partition signature

Consider a partition $\pi \in P_n$. We define the integer m_j as number of parts in $A \in \pi$ such that $|A| = j$. We will say that the numbers $m_1, m_2, \dots m_n$ are the **signature** of the partition π.

Obviously for each partition, we have $|\pi| = (m_1 + \dots + m_n)$; moreover $1 \cdot m_1 + 2 \cdot m_2 + 3 \cdot m_3 + \dots + n \cdot m_n = n$ since π is a partition of $\{1, \dots, n\}$.

A partition with the signature $m_1, m_2, \dots m_n$ generates the monomial

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Partition signature

Consider a partition $\pi \in P_n$. We define the integer m_j as number of parts in $A \in \pi$ such that $|A| = j$. We will say that the numbers $m_1, m_2, \dots m_n$ are the **signature** of the partition π.

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Example signature

We once again follow up on the first example.
In the first example we computed one term of the 8-th derivative of $f(g(x))$ according to the partition $\pi = \{\{1,3,4,8\},\{2\},\{5,7\},\{6\}\}$, and we obtained the monomial

$$f^{(4)}(g(x))g'(x)^2 g''(x) g^{(4)}(x) \quad .$$

in this π we have
$m_1 = 2$ singletons, namely $\{2\},\{6\}$
$m_2 = 1$ pair, namely $\{5,7\}$
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Building a partition

Let us now fix a signature.
How can we build any partition with this same signature?
We use the signature from the example $m_1 = 2$, $m_2 = 1$, $m_3 = 0$, $m_4 = 1$, $m_5 = \ldots = m_8 = 0$ to show the mechanics.
We prepare the skeleton

$$\{\{\ \}, \{\ \}, \{\ ,\ \}, \{\ ,\ ,\ ,\ \}\}$$

Then we order the first $n = 8$ numbers and we insert this ordering in the skeleton.

$$\begin{array}{ccccccccc} & 6, & 2 & 5 & 7 & 8 & 4 & 1 & 3 \\ & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow \\ \{ & \{6\}, & \{2\}, & \{5, & 7\}, & \{8, & 4, & 1, & 3\} \quad \} \end{array}$$

This operation may be done in $n! = 8!$ different ways.

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This partition is not uniquely built.
We can indeed interchange partitions with the same number of elements.

$$\{\ \{6\},\ \{2\},\ \{5,7\},\ \{8,4,1,3\}\ \}$$

$$\{\ \{2\},\ \{6\},\ \{5,7\},\ \{8,4,1,3\}\ \}$$

This can be done in $m_1!m_2!\dots m_n!$ different ways.

We can moreover interchange numbers in the same partition.

$$\{\ \{6\},\ \{2\},\ \{5,7\},\ \{8,\ 4,\ 1,\ 3\}\ \}$$

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This can be done in

$$1!^{m_1}\ 2!^{m_2}\ \cdots\ n!^{m_n}$$

different ways. (Indeed for example in a triple the numbers can be reordered in $3! = 6$ different ways; if there are m_3 triples then there is a total of $(3!)^{m_3}$ reorderings inside the triples).

Proof

This line of reasoning in the example proves that the Faà di Bruno's formula (4) follows from the combinatorial form (1).
We saw that, given a signature $m_1, m_2, \ldots m_m$, we can fill the skeleton in $n!$ ways, but we obtain the same partition multiple times,hence we divide $n!$ by

$$m_1! m_2! \ldots m_n! \cdot 1!^{m_1}\ 2!^{m_2}\ \cdots\ n!^{m_n} \quad .$$

We so proved that there are exactly

$$\frac{n!}{m_1!\, 1!^{m_1}\ m_2!\, 2!^{m_2}\ \cdots\ m_n!\, n!^{m_n}}$$

partitions $\pi \in P_n$ with signature

$$m_1, m_2, \ldots m_m \quad .$$

All partitions with the same signature generate the same monomial

$$f^{(m_1+\cdots+m_n)}(g(x))\,\left(g'(x)\right)^{m_1}\,\left(g''(x)\right)^{m_2}\cdots\left(g^{(n)}(x)\right)^{m_n}.$$

Eventually if we callect together all the monomials in the combinatorial forms, the integer coefficient of the above monomial will be exactly

$$\frac{n!}{m_1!\,1!^{m_1}\,m_2!\,2!^{m_2}\,\cdots\,m_n!\,n!^{m_n}} \qquad \square$$

Coefficient in the example

The signature in the example is $m_1 = 2$, $m_2 = 1$, $m_3 = 0$, $m_4 = 1$, $m_5 = \ldots = m_8 = 0$.
So there are

$$\frac{n!}{m_1!\,1!^{m_1}\;m_2!\,2!^{m_2}\cdots m_n!\,n!^{m_n}} = \frac{8!}{2!\,1!^2\;1!\,2!^1\;0!\,3!^0\;1!\,4!^1} = 420$$

different partitions in P_8 that generate the monomial $f^{(4)}(g(x))g'(x)^2 g''(x) g^{(4)}(x)$.
This means that the coefficient of the monomial is 420.
We now appreciate the Faà di Bruno's formula, that provides the coefficient in monomials in a "computable form".

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Second factorial form

The monomials in the combinatorial form may be partially collected, to give

$$\frac{d^n}{dx^n} f(g(x)) = \sum_{m=1}^{n} \frac{f^{(m)}(g(x))}{m!} \sum \binom{n}{j_1, j_2, \ldots, j_m} \prod_{i=1}^{m} g^{(j_i)}(x)$$

where the second sum is over all m-tuples of positive integers $(j_1, \ldots, j_m)$ satisfying the constraint

$$j_1 + \cdots + j_m = n.$$

Proof

This formula is obtained from the combinatorial formula by two collecting operations.

First we collect together all partitions π with $|\pi| = m$; then we fix a vector of positive integer numbers $j_1, \dots j_m$ satisfying $j_1 + \cdots + j_m = n$; we write $\pi = \{B_1, \dots B_m\}$ we count how many partitions there are with $|B_1| = j_1 \dots |B_m| = j_m$.

This is a well known combinatorial problem [2] solved by the **multinomial coefficient**

$$\binom{n}{j_1, j_2, \dots, j_m} = \frac{n!}{j_1!\, j_2! \cdots j_m!} \ .$$

We eventually divide it by $m!$ to disregard the ordering of the parts. □

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Coefficient in the example

The monomial in the example was $f^{(4)}(g(x))g'(x)g'(x)g''(x)g^{(4)}(x)$. This is obtained by setting $n = 8, m = 4$ and considering all the quadruples j_1, j_2, j_3, j_4 where the numbers $1, 1, 2, 4$ appear (note that $j_1 + j_2 + j_3 + j_4 = n = 8$). There are 12 such quadruples, as seen on the right; hence the monomial is generated 12 times in the formula. There follows that the coefficient of the monomial is

$$12 \frac{1}{m!} \binom{n}{j_1, j_2, \ldots, j_m} = 12 \frac{1}{4!} \frac{8!}{1!\,1!\,2!\,4!} = 420 \quad .$$

j_1	j_2	j_3	j_4
1	1	2	4
1	2	1	4
2	1	1	4
1	2	4	1
2	1	4	1
2	4	1	1
1	1	4	2
1	4	1	2
4	1	1	2
1	4	2	1
4	1	2	1
4	2	1	1

These notes are available in English and in Italian, both in the *slide* format (that you are reading) and in the *article* format .

Credits

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http://calvino.polito.it/~nicola/convegnofaa/faadibruno

Some formulas and ideas were copy/pasted from

http://en.wikipedia.org/wiki/Faa_di_Bruno_formula

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