Evaluating the BCH formula

Serena Cicalò (*joint work with Willem de Graaf*)

We know that
$$e^x = 1 + x + \frac{1}{2!}x^2 + \frac{1}{3!}x^3 + \dots.$$

If x and y are two noncommuting variables we have that $e^x e^y = e^z$, where z is a formal series in x and y with rational coefficients.

If u is such that
$$e^z = 1 + z + \frac{1}{2!}z^2 + \frac{1}{3!}z^3 + \dots = 1 + u$$
we have that
$$z = \ln(1+u) = u - \frac{u^2}{2} + \frac{u^3}{3} - \frac{u^4}{4} + \dots.$$

Let $s_m(r)$ be the sum of all elements of degree r obtained by multiplication of m factors of the form $\frac{1}{k_i!h_i!}x^{k_i}y^{h_i}$ that appear in e^z and that we call *blocks*.

Now, let w be a *word* in x and y, that is $w = w_1 \dots w_n$ where $w_i = x^{k_i}y^{h_i}$ with $k_i, h_i > 0$ all but $k_1, h_n \geq 0$. The main our purpose is to determine a formula to calculate the coefficient z_w of the word w in z.

For this, firstly, we determine the coefficient of $w_i = x^{k_i}y^{h_i}$ in $s_m(k_i + h_i)$. We denote this coefficient with $f_m(k_i, h_i)$ or $f_m(w_i)$.

Lemma 1. *For all $m \leq h + k$, $f_m(k, h)$ is the coefficient of $x^k y^h$ in $s_m(k + h)$ and we have*
$$f_{m-1}(k,h) = \frac{1}{k!h!}\sum_{j=0}^{m-2}(-1)^j \varphi_{m-j}(k,h)\binom{m}{j} \tag{1}$$
where
$$\varphi_m(k,h) = \sum_{p+q=m} p^k q^h.$$

Remark 1. We can easily see that $f_m(k, h) = 0$ for all $m > k + h$ because m counts the number of blocks in which we can divide $x^k y^h$ in $s_m(k+h)$. Then it not makes sense to divide $x^k y^h$ in a number of blocks greater than its degree, that is $k + h$.

We can now give the formula to calculate the coefficient z_w of a word w.

Theorem 1. *Let $w = w_1 \dots w_n$ where $w_i = x^{k_i}y^{h_i}$ with $k_i, h_i > 0$ all but $k_1, h_n \geq 0$ and let $N = \sum_{i=1}^{n}(k_i + h_i)$. Then the coefficient of w in z is*
$$z_w = \sum_{m=n}^{N} \frac{(-1)^{m-1}}{m} F_m(w) \tag{2}$$
where
$$F_m(w) = \sum_{m_1+\dots+m_n=m} f_{m_1}(w_1)\cdots f_{m_n}(w_n). \tag{3}$$

Now we present an equivalent formula for z_w using the *Stirling numbers of the second kind* denoted by $\left\{ {n \atop m} \right\}$. We say that $\left\{ {n \atop m} \right\}$ stands for the number of ways to partition a set of n things into m nonempty subsets.

For example, there seven ways to split a four-element set into two parts:

$$\begin{array}{llll} \{1,2,3\}\cup\{4\}, & \{1,2,4\}\cup\{3\}, & \{1,3,4\}\cup\{2\}, & \{2,3,4\}\cup\{1\}, \\ \{1,2\}\cup\{3,4\}, & \{1,3\}\cup\{2,4\}, & \{1,4\}\cup\{2,3\}. & \end{array}$$

Thus $\left\{ {4 \atop 2} \right\} = 7$.

Let again $w = w_1 \dots w_n$, where $w_i = x^{k_i} y^{h_i}$ with $k_i, h_i > 0$ all but $k_1, h_n \geq 0$. We put

$$G_m(w) = \frac{1}{P} \sum_{\sum_{i=1}^n (s_i+t_i)=m} \prod_{i=1}^n s_i! t_i! \left\{ {k_i \atop s_i} \right\} \left\{ {h_i \atop t_i} \right\}. \tag{4}$$

where $P = \prod_{i=1}^n k_i! h_i!$.

Remark 2. We can remark that $G_m(w)$ depends only by the exponents that appear really in w.

Example 1. Let $w = x^3 y^2 x^4$. We want to calculate $G_5(w)$.

We have $v = (3,2,4)$ and $P = 3!2!4! = 288$. Then

$$\begin{aligned} G_5(w) &= \frac{1}{288}\left[3!\left\{ {3 \atop 3} \right\} 1! \left\{ {2 \atop 1} \right\} 1! \left\{ {4 \atop 1} \right\} + 2! \left\{ {3 \atop 2} \right\} 2! \left\{ {2 \atop 2} \right\} 1! \left\{ {4 \atop 1} \right\} + 2! \left\{ {3 \atop 2} \right\} 1! \left\{ {2 \atop 1} \right\} 2! \left\{ {4 \atop 2} \right\}\right] \\ &+ \frac{1}{288}\left[1!\left\{ {3 \atop 1} \right\} 2! \left\{ {2 \atop 2} \right\} 2! \left\{ {4 \atop 2} \right\} + 1! \left\{ {3 \atop 1} \right\} 1! \left\{ {2 \atop 1} \right\} 3! \left\{ {4 \atop 3} \right\}\right] \\ &= \frac{1}{288}[6 + 12 + 84 + 28 + 36] \\ &= \frac{1}{288} \cdot 166. \end{aligned}$$

Let now d defined as

$$d = \begin{cases} n, & \text{if } k_1, h_n \neq 0; \\ n-1, & \text{if } k_1 = 0,\ h_n \neq 0 \text{ (or vice versa)}; \\ n-2, & \text{if } k_1 = h_n = 0. \end{cases}$$

We have showed that:

Theorem 2. *Let* $N = \sum_{i=1}^n (k_i + h_i)$, *we have that*

$$z_w = \frac{1}{d+1} \sum_{m=d+n}^{N} (-1)^{m-d-1} \frac{G_m(w)}{\binom{m}{d+1}}. \tag{5}$$

Example 2. Let $w = y^4 x y^2$. We have $n = 2$, $d = 1$ and $N = 7$ then

$$z_w = \frac{1}{2} \sum_{m=3}^{7} (-1)^{m-2} \frac{G_m(w)}{\binom{m}{2}}.$$

Also we have $P = 4!1!2! = 48$ then

m	$48 \cdot G_m(w)$
3	1
4	16
5	64
6	96
7	48

Hence

$$z_w = \frac{1}{2} \cdot \frac{1}{48} \left[-\frac{1}{\binom{3}{2}} + \frac{16}{\binom{4}{2}} - \frac{64}{\binom{5}{2}} + \frac{96}{\binom{6}{2}} - \frac{48}{\binom{7}{2}} \right] = \frac{1}{2016}.$$