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EXPLICIT FORMULAS FOR DERANGEMENT NUMBERS AND THEIR GENERATING FUNCTION

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Abstract. In the paper, by deriving a formula for special values of the Bell polynomials of the second kind, with the help of the Faà di Bruno formula for computing higher order derivatives of composite functions, the authors establish explicit formulas for derangement numbers and their generating function in terms of the Stirling numbers of the second kind.

Keywords. Bell polynomial of the second kind; Derangement number; Faà di Bruno formula; Generating function; Tridiagonal determinant

1. Introduction

In combinatorial mathematics, a derangement is a permutation of the elements of a set, such that no element appears in its original position. The number of derangements of a set of size n is called a derangement number and usually denoted by $!n$. The problem of counting derangements was first considered in 1708 and solved in 1713 both by Pierre Raymond de Montmort, as did Nicholas Bernoulli at about the same time. The first eleven derangement numbers $!n$ for $0 \le n \le 10$ are

$$1, \quad 0, \quad 1, \quad 2, \quad 9, \quad 44, \quad 265, \quad 1854, \quad 14833, \quad 133496, \quad 1334961.$$

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A simple formula for computing derangement numbers $!n$ is

$$!n = n! \sum_{\ell=0}^{n} \frac{(-1)^{\ell}}{\ell!}. \tag{1}$$

Derangement numbers $!n$ can be generated by the generating function

$$D(x) = \frac{e^{-x}}{1-x} = \frac{1}{e^{x}(1-x)} = \sum_{n=0}^{\infty} !n \frac{x^n}{n!}.$$

For more and detailed information on derangement numbers $!n$ and their generating function, please refer to [1, 2, 23, 24] and plenty of references therein.

In the papers [11, 19], by studying the generating function $D(\pm x)$ and making use of other techniques, a result in [7, 8] was corrected and another result in [9] was recovered as follows: derangement numbers $!n$ for $n \ge 0$ can be represented by a tridiagonal $(n+1)\times(n+1)$ determinant

$$!n = -\begin{vmatrix}
-1 & 1 & 0 & 0 & 0 & \dots & 0 & 0 & 0\\
0 & 0 & 1 & 0 & 0 & \dots & 0 & 0 & 0\\
0 & -1 & 1 & 1 & 0 & \dots & 0 & 0 & 0\\
0 & 0 & -2 & 2 & 1 & \dots & 0 & 0 & 0\\
0 & 0 & 0 & -3 & 3 & \dots & 0 & 0 & 0\\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots\\
0 & 0 & 0 & 0 & 0 & \dots & n-3 & 1 & 0\\
0 & 0 & 0 & 0 & 0 & \dots & -(n-2) & n-2 & 1\\
0 & 0 & 0 & 0 & 0 & \dots & 0 & -(n-1) & n-1
\end{vmatrix}.$$

In a forthcoming paper by the authors, also by studying the generating function $D(x)$, it was obtained that derangement numbers $!n$ for $n \ge 0$ can be expressed in terms of the Hessenberg determinant by

$$!n=\begin{vmatrix}
1 & -1 & 0 & \dots & 0 & 0 & 0\\
0 & 0 & -1 & \dots & 0 & 0 & 0\\
0 & \binom{2}{0} & 0 & \dots & 0 & 0 & 0\\
0 & \binom{3}{0}2 & \binom{3}{1} & \dots & 0 & 0 & 0\\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots\\
0 & \binom{n-3}{0}(n-4) & \binom{n-3}{1}(n-5) & \dots & -1 & 0 & 0\\
0 & \binom{n-2}{0}(n-3) & \binom{n-2}{1}(n-4) & \dots & 0 & -1 & 0\\
0 & \binom{n-1}{0}(n-2) & \binom{n-1}{1}(n-3) & \dots & \binom{n-1}{n-3} & 0 & -1\\
0 & \binom{n}{0}(n-1) & \binom{n}{1}(n-2) & \dots & \binom{n}{n-3}2 & \binom{n}{n-2} & 0
\end{vmatrix}$$

and that the nth derivative of the generating function $D(x)$ can be computed by

$$\frac{\mathrm{d}^n}{\mathrm{d}x^n}\left(\frac{e^{-x}}{1-x}\right)=\frac{e^{-x}}{(1-x)^{n+1}}\sum_{i=0}^{n}\langle n\rangle_i[!(n-i)]\frac{x^i}{i!}, \tag{2}$$

where

$$\langle x\rangle_n=\prod_{k=0}^{n-1}(x-k)=\begin{cases}x(x-1)\cdots(x-n+1), & n\ge 1,\\ 1, & n=0\end{cases}$$

stands for the nth falling factorial of x.

It is well known in combinatorics that the Stirling number of the second kind $S(n,k)$ is the number of ways of partitioning a set of n elements into k nonempty subsets and that $S(n,k)$ can be generated by

$$\frac{(e^x-1)^k}{k!}=\sum_{n=k}^{\infty}S(n,k)\frac{x^n}{n!},\quad k\in\{0\}\cup\mathbb{N}. \tag{3}$$

For more information, please refer to [4, 12] and closely-related references therein.

In combinatorial mathematics, the Bell polynomials of the second kind $\mathrm{B}_{n,k}$ are defined by

$$\mathrm{B}_{n,k}(x_1,x_2,\dots,x_{n-k+1})=\sum_{\substack{\ell_i\in\{0\}\cup\mathbb{N}\\ \sum_{i=1}^{n}i\ell_i=n\\ \sum_{i=1}^{n}\ell_i=k}}\frac{n!}{\prod_{i=1}^{n-k+1}\ell_i!}\prod_{i=1}^{n-k+1}\left(\frac{x_i}{i!}\right)^{\ell_i}$$

for $n\ge k\ge 0$. See [4, p. 134, Theorem A]. The well-known Faà di Bruno formula for computing higher order derivatives of composite functions can be described in terms of the Bell polynomials of the second kind $\mathrm{B}_{n,k}$ by

$$\frac{\mathrm{d}^n}{\mathrm{d}t^n}[f\circ h(t)]=\sum_{k=0}^{n} f^{(k)}(h(t))\mathrm{B}_{n,k}\bigl(h'(t),h''(t),\dots,h^{(n-k+1)}(t)\bigr). \tag{4}$$

See [4, p. 139, Theorem C].

In this paper, by deriving an explicit formula for the Bell polynomials of the second kind $\mathrm{B}_{n,k}(x,1+x,2+x,\dots,n-k+x)$, and with the help of the Faà di Bruno formula (4), we will establish explicit formulas for derangement numbers $!n$ and for their generating function $D(x)$ in terms of the Stirling numbers of the second kind $S(n,k)$.

Theorem 1. *For $n\in\mathbb{N}$, the nth derivative of the generating function $D(x)$ can be computed by*

$$D^{(n)}(x)=\frac{1}{e^x}\sum_{k=1}^{n}(-1)^{k+1}k!k^{n-k}\binom{n}{k}\sum_{\ell=0}^{k}\binom{k}{\ell}\sum_{q=0}^{n-k}\frac{(-1)^q}{k^q}\binom{n-k}{q}\frac{S(q+\ell,\ell)}{\binom{q+\ell}{\ell}}\frac{1}{(x-1)^{k-\ell+1}}. \tag{5}$$

Consequently, derangement numbers $!n$ for $n\in\mathbb{N}$ can be computed by

$$!n=\sum_{k=1}^{n}k!k^{n-k}\binom{n}{k}\sum_{\ell=0}^{k}(-1)^{\ell}\binom{k}{\ell}\sum_{q=0}^{n-k}\frac{(-1)^q}{k^q}\binom{n-k}{q}\frac{S(q+\ell,\ell)}{\binom{q+\ell}{\ell}}. \tag{6}$$

2. Lemmas

In order to prove Theorem 1, we need two lemmas below.

Lemma 1 ([4, p. 135])**.** *For $n\ge k\ge 0$,*

$$\mathrm{B}_{n,k}\bigl(abx_1,ab^2x_2,\dots,ab^{n-k+1}x_{n-k+1}\bigr)=a^kb^n\mathrm{B}_{n,k}(x_1,x_2,\dots,x_{n-k+1}), \tag{7}$$

where a and b are any complex numbers.

Lemma 2. *For $n\ge k\ge 1$, the Bell polynomials of the second kind $\mathrm{B}_{n,k}$ satisfy*

(8)

$$\mathrm{B}_{n,k}(x,1+x,2+x,\dots,n-k+x)=k^{n-k}\binom{n}{k}\sum_{\ell=0}^{k}\binom{k}{\ell}\left[\sum_{q=0}^{n-k}\frac{(-1)^q}{k^q}\binom{n-k}{q}\frac{S(q+\ell,\ell)}{\binom{q+\ell}{\ell}}\right](x-1)^{\ell}.$$

Consequently,

$$\mathrm{B}_{n,k}(0,1,2,\dots,n-k)=k^{n-k}\binom{n}{k}\sum_{\ell=0}^{k}(-1)^{\ell}\binom{k}{\ell}\sum_{q=0}^{n-k}\frac{(-1)^q}{k^q}\binom{n-k}{q}\frac{S(q+\ell,\ell)}{\binom{q+\ell}{\ell}}$$

and

$$\mathrm{B}_{n,k}(1,2,3,\dots,n-k+1)=k^{n-k}\binom{n}{k}. \tag{9}$$

Proof. In [4, p. 133], it was stated that

$$\frac{1}{k!}\left(\sum_{m=1}^{\infty} x_m \frac{t^m}{m!}\right)^k = \sum_{n=k}^{\infty} \mathrm{B}_{n,k}(x_1, x_2, \dots, x_{n-k+1}) \frac{t^n}{n!}, \quad k \ge 0. \tag{10}$$

Therefore, by (10), we have

$$\begin{aligned}
\sum_{n=k}^{\infty} \mathrm{B}_{n,k}(x, 1+x, 2+x, \dots, n-k+x) \frac{t^n}{n!} &= \frac{1}{k!}\left[\sum_{m=1}^{\infty} (m-1+x) \frac{t^m}{m!}\right]^k \\
&= \frac{1}{k!}\left[e^t t + (x-1)(e^t - 1)\right]^k = \frac{t^k e^{kt}}{k!}\left[1 + (x-1)\frac{1-e^{-t}}{t}\right]^k \\
&= \frac{t^k e^{kt}}{k!} \sum_{\ell=0}^{k} \binom{k}{\ell} (x-1)^\ell \left(\frac{1-e^{-t}}{t}\right)^\ell,
\end{aligned}$$

which is equivalent to

$$\sum_{\ell=0}^{\infty} \frac{\mathrm{B}_{k+\ell,k}(x, 1+x, 2+x, \dots, \ell+x)}{\binom{k+\ell}{\ell}} \frac{t^\ell}{\ell!} = e^{kt} \sum_{\ell=0}^{k} \binom{k}{\ell} (x-1)^\ell \left(\frac{1-e^{-t}}{t}\right)^\ell.$$

This implies that

$$\begin{aligned}
\frac{\mathrm{B}_{k+m,k}(x, 1+x, \dots, m+x)}{\binom{k+m}{m}} &= \sum_{\ell=0}^{k} (x-1)^\ell \binom{k}{\ell} \lim_{t\to 0} \frac{\mathrm{d}^m}{\mathrm{d} t^m}\left[e^{kt}\left(\frac{1-e^{-t}}{t}\right)^\ell\right] \\
&= \sum_{\ell=0}^{k} (x-1)^\ell \binom{k}{\ell} \lim_{t\to 0} \sum_{q=0}^{m} \binom{m}{q} k^{m-q} e^{kt} \frac{\mathrm{d}^q}{\mathrm{d} t^q}\left[\left(\frac{1-e^{-t}}{t}\right)^\ell\right] \\
&= \sum_{\ell=0}^{k} (x-1)^\ell \binom{k}{\ell} \sum_{q=0}^{m} \binom{m}{q} k^{m-q} \lim_{t\to 0} \frac{\mathrm{d}^q}{\mathrm{d} t^q}\left[\left(\frac{1-e^{-t}}{t}\right)^\ell\right].
\end{aligned} \tag{11}$$

The equation (3) can be rearranged as

$$\left(\frac{e^x-1}{x}\right)^k = \sum_{n=0}^{\infty} \frac{S(n+k,k)}{\binom{n+k}{k}} \frac{x^n}{n!}, \quad k \in \{0\} \cup \mathbb{N}.$$

This means that

$$\lim_{t\to 0} \frac{\mathrm{d}^q}{\mathrm{d} t^q}\left[\left(\frac{1-e^{-x}}{x}\right)^k\right] = (-1)^q \frac{S(q+k,k)}{\binom{q+k}{k}}.$$

Substituting this into (11) and simplifying yield

$$\frac{\mathrm{B}_{k+m,k}(x, 1+x, 2+x, \dots, m+x)}{\binom{k+m}{m}} = \sum_{\ell=0}^{k} (x-1)^\ell \binom{k}{\ell} \sum_{q=0}^{m} \binom{m}{q} k^{m-q} (-1)^q \frac{S(q+\ell,\ell)}{\binom{q+\ell}{\ell}}$$

which can be rewritten as (8). The proof of Lemma 2 is complete. ∎

3. Proof of Theorem 1

We are now in a position to prove Theorem 1.

Applying the formula (4) to $f(u)=\frac{1}{u}$ and $u=h(x)=e^x(1-x)$ and making use of the identities (7) and (8) give

$$\begin{aligned}
\frac{\mathrm{d}^n}{\mathrm{d}x^n}\left(\frac{e^{-x}}{1-x}\right)&=\sum_{k=1}^{n}\left(\frac{1}{u}\right)^{(k)}\mathrm{B}_{n,k}\bigl(-e^xx,-e^x(1+x),\dots,-e^x(n-k+x)\bigr)\\
&=\sum_{k=1}^{n}(-1)^k\frac{k!}{u^{k+1}}(-e^x)^k\mathrm{B}_{n,k}\bigl(x,1+x,\dots,n-k+x\bigr)\\
&=\frac{1}{e^x}\sum_{k=1}^{n}\frac{k!}{(1-x)^{k+1}}k^{n-k}\binom{n}{k}\sum_{\ell=0}^{k}\binom{k}{\ell}\left[\sum_{q=0}^{n-k}\frac{(-1)^q}{k^q}\binom{n-k}{q}\frac{S(q+\ell,\ell)}{\binom{q+\ell}{\ell}}\right](x-1)^\ell\\
&\to\sum_{k=1}^{n}k!k^{n-k}\binom{n}{k}\sum_{\ell=0}^{k}(-1)^\ell\binom{k}{\ell}\sum_{q=0}^{n-k}\frac{(-1)^q}{k^q}\binom{n-k}{q}\frac{S(q+\ell,\ell)}{\binom{q+\ell}{\ell}}
\end{aligned}$$

as $x\to0$. The proof of Theorem 1 is complete.

4. Remarks

Finally we list several remarks about our main results and related ones.

Remark 1. The formula (6) connects derangement numbers $!n$ with the Stirling numbers of the second kind $S(n,k)$, although it is not easier than (1) to compute. Similarly, the formula (5) connects the nth derivative of the generating function $D(x)$ of derangement numbers $!n$ with the Stirling numbers of the second kind $S(n,k)$, although it is not easier than (2) to compute.

Remark 2. The number on the right hand side of the formula (9) is called an idempotent number in [4, pp. 91 and 134]. Hence, Lemma 2 generalizes [4, p. 135, Eq. [3i′]].

In recent years, some new formulas for special values of the Bell polynomials of the second kind were obtained and applied in [6, 20] and closely-related references therein.

Remark 3. Combining (2) and (5) with (12) results in a formula

$$\begin{vmatrix}
-x & 1-x & 0 & \dots & 0 & 0\\
-1 & -1-x & 1-x & \dots & 0 & 0\\
0 & -2 & -2-x & \dots & 0 & 0\\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots\\
0 & 0 & 0 & \dots & 1-x & 0\\
0 & 0 & 0 & \dots & 2-n-x & 1-x\\
0 & 0 & 0 & \dots & 1-n & 1-n-x
\end{vmatrix} = (-1)^n \sum_{i=0}^{n} \langle n\rangle_i [!(n-i)] \frac{x^i}{i!}$$

$$= \sum_{k=1}^{n} (-1)^k k! k^{n-k} \binom{n}{k} \sum_{\ell=0}^{k} \binom{k}{\ell} \sum_{q=0}^{n-k} \frac{(-1)^q}{k^q} \binom{n-k}{q} \frac{S(q+\ell,\ell)}{\binom{q+\ell}{\ell}} (x-1)^{n-k+\ell}$$

for $n \in \mathbb{N}$. This gives a formula of computing a special tridiagonal determinant. For more information on computation of general tridiagonal determintants, please refer to the paper [13] and closely-related references therein.

Remark 4. From the first proof of [19, Theorem 1], we can conclude that the nth derivative of the generating function $D(x)$ can be computed by

$$\frac{\mathrm{d}^n D(x)}{\mathrm{d} x^n} = \frac{(-1)^n e^{-x}}{(1-x)^{n+1}} \begin{vmatrix}
-x & 1-x & 0 & \dots & 0 & 0\\
-1 & -1-x & 1-x & \dots & 0 & 0\\
0 & -2 & -2-x & \dots & 0 & 0\\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots\\
0 & 0 & 0 & \dots & 1-x & 0\\
0 & 0 & 0 & \dots & 2-n-x & 1-x\\
0 & 0 & 0 & \dots & 1-n & 1-n-x
\end{vmatrix} \tag{12}$$

$$= \frac{(-1)^n e^{-x}}{(1-x)^{n+1}} |e_{ij}(x)|_{n\times n}$$

for $n \in \mathbb{N}$, where

$$e_{ij}(x) = \begin{cases} 1-x, & i-j=-1, \\ 1-i-x, & i-j=0, \\ 1-i, & i-j=1, \\ 0, & i-j \ne 0, \pm 1. \end{cases}$$

Combining this with absolute (complete) monotonicity obtained in the above remark reveals that the determinants

$$(-1)^n |e_{ij}(x)|_{n\times n} = (-1)^n \begin{vmatrix} -x & 1-x & 0 & \dots & 0 & 0 \\ -1 & -1-x & 1-x & \dots & 0 & 0 \\ 0 & -2 & -2-x & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 1-x & 0 \\ 0 & 0 & 0 & \dots & 2-n-x & 1-x \\ 0 & 0 & 0 & \dots & 1-n & 1-n-x \end{vmatrix} \ge 0$$

for $x \in [0,1)$ and $|e_{ij}(x)|_{n\times n} \le 0$ for $x \in (1,\infty)$.

Remark 5. Recall from [10, Chapter XIII], [21, Chapter 1], and [22, Chapter IV] that an infinitely differentiable function f is said to be completely (or absolutely, respectively) monotonic on an interval I if it satisfies

$$0 \le (-1)^k f^{(k)}(x) < \infty \quad \bigl(\text{or } 0 \le f^{(k)}(x) < \infty, \text{ respectively}\bigr)$$

on I for all $k \ge 0$ and that a function $f(x)$ is completely monotonic on I if and only if the function $f(-x)$ is absolutely monotonic on $-I$.

Recall from [14] that an infinitely differentiable and positive function f is said to be logarithmically completely monotonic on an interval I if $0 \le (-1)^k[\ln f(x)]^{(k)} < \infty$ hold on I for all $k \in \mathbb{N}$. It has been verified several times [3, 5, 14] that a logarithmically completely monotonic function must be completely monotonic.

It was defined in [5, Definition 1] that a positive function f is said to be logarithmically absolutely monotonic on an interval I if it has derivatives of all orders and $[\ln f(t)]^{(k)} \ge 0$ for

$t \in I$ and $k \in \mathbb{N}$. It was proved in [5, Theorem 1] that a logarithmically absolutely monotonic function on an interval I is also absolutely monotonic on I, but not conversely.

For more information on logarithmically absolutely (or completely, respectively) monotonic functions, please refer to [5, 14, 15, 16, 17, 18, 21] and closely-related references therein.

From the formula (2), it follows readily that the function $D(x)$ is absolutely monotonic on $[0,1)$ and the function $-D(x)$ is completely monotonic on $(1,\infty)$.

Since

$$\ln[-D(x)] = -x - \ln(x-1), \quad \{\ln[-D(x)]\}' = \frac{x}{1-x},$$

and

$$\{\ln[-D(x)]\}^{(k+1)} = (-1)^{k+1}\frac{k!}{(x-1)^{k+1}}, \quad k \in \mathbb{N},$$

the function $-D(x)$ is logarithmically completely monotonic, consequently completely monotonic, on $(1,\infty)$. Similarly, the generating function $D(x)$ is logarithmically absolutely monotonic, consequently absolutely monotonic, on $[0,1)$.

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