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Some results on derangement polynomials

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Abstract. We study moments of the difference $D_n(x) - x^n n!\, \mathrm{e}^{-1/x}$ concerning derangement polynomials $D_n(x)$. For the first moment, we obtain an explicit formula in terms of the exponential integral function and we show that it is always negative for $x > 0$. For the higher moments, we obtain a multiple integral representation of the order of the moment under computation.

Keywords: derangement; permutation; integration

Classification: 05A05, 05A16, 26A06

1. Introduction

A derangement of a list is a permutation of the entries such that no entry remains in the original position. We denote the number of derangements on a set of cardinality n by D_n. The derangement polynomials are natural extensions of the derangement numbers, and are defined in several different ways in literature, see [4], [5], [6], [15], [14] and the references given there. The most common definition of derangement polynomials are those considered by C. Radoux in [15], [14], where he studied a Hankel determinant constructed on derangement polynomials $D_n(x)$ defined by

$$D_n(x) = n! \sum_{j=0}^{n} \frac{(-1)^j}{j!}\, x^{n-j}.$$

These polynomials are associated with the number of derangements on a set of cardinality n by $D_n = D_n(1)$. Recently, the first author in [10, Theorem 2] computed the kth moments of the difference $D_n - \mathrm{e}^{-1} n!$ for each integer $k \geqslant 1$. The aim of this note is to compute the kth moments of the difference

$$D_n(x) - \frac{x^n n!}{\mathrm{e}^{1/x}}. \tag{1.1}$$

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The first moment can be computed in terms of the exponential integral function, Ei, which is defined by the Cauchy principal value of the integral

$$\mathrm{Ei}(x) = -\int_{-x}^{\infty} \frac{\mathrm{e}^{-z}}{z}\,\mathrm{d}z.$$

Theorem 1.1. *Let $x > 0$. We have*

$$\sum_{n=1}^{\infty}\Big(D_n(x) - \frac{x^n n!}{\mathrm{e}^{1/x}}\Big) = -1 + \frac{1}{\mathrm{e}^{1/x}} + \frac{1}{x\,\mathrm{e}^{2/x}}\Big(\mathrm{Ei}\Big(\frac{2}{x}\Big) - \mathrm{Ei}\Big(\frac{1}{x}\Big)\Big). \tag{1.2}$$

Moreover, the above first moment is always negative for $x > 0$.

For the higher moments of the difference (1.1), we obtain a multiple integral representation of the order of the moment under computation, but we are able to simplify the second moment following an argument due to W. J. LeVeque, see [13], which has been described by M. Aigner and G. M. Ziegler in [1, Chapter 9].

Theorem 1.2. *Let $x > 0$. For each integer $k \geqslant 1$ the following multiple integral representation holds*

$$\begin{aligned}\sum_{n=1}^{\infty}\Big(D_n(x) - \frac{x^n n!}{\mathrm{e}^{1/x}}\Big)^k = &- \frac{(\mathrm{e}^{1/x}-1)^k}{\mathrm{e}^{k/x}} \\ &+ \frac{1}{\mathrm{e}^{k/x}}\int_0^{1/x}\cdots\int_0^{1/x}\frac{\mathrm{e}^{z_1+\cdots+z_k}}{1-(-x)^k z_1\cdots z_k}\,\mathrm{d}\mathbf{Z},\end{aligned} \tag{1.3}$$

where $\mathbf{Z}$ represents the k-tuple $(z_1,\ldots,z_k)$. More precisely, for the case $k=2$ we have

$$\sum_{n=1}^{\infty}\Big(D_n(x) - \frac{x^n n!}{\mathrm{e}^{1/x}}\Big)^2 = -\frac{(\mathrm{e}^{1/x}-1)^2}{\mathrm{e}^{2/x}} + \frac{4}{\mathrm{e}^{2/x}}\int_0^{1/2x} h(z)\,\mathrm{d}z, \tag{1.4}$$

where

$$h(z) = \frac{\mathrm{e}^{2z}}{x\sqrt{1-x^2z^2}}\arctan\frac{xz}{\sqrt{1-x^2z^2}} + \frac{\mathrm{e}^{2/x-2z}}{x\sqrt{xz(2-xz)}}\arctan\frac{xz}{\sqrt{xz(2-xz)}}.$$

We provide the proofs of the above theorems in next section. Before the proofs, we give a remark on the values of derangement polynomials at negative arguments.

Remark 1.3. Regarding to the summation identities of permutations, recently the first author [11, Theorem 1.3] showed that for any integer $n \geqslant 0$ and for each real $x \neq 0$ we have

$$S_n(x) := \sum_{j=0}^{n} P(n,j)\,x^j = (-1)^n x^n \mathrm{e}^{1/x} E_n\Big(-\frac{1}{x}\Big), \tag{1.5}$$

where

$$E_n(a) = \int_{-\infty}^{a} t^n \mathrm{e}^t \,\mathrm{d}t,$$

is defined for any fixed a and for any integer $n \geqslant 0$. Now, we observe that

$$D_n(-x) = (-1)^n n! \sum_{j=0}^{n} \frac{x^{n-j}}{j!} = (-1)^n \sum_{j=0}^{n} P(n,j)\, x^j. \tag{1.6}$$

Thus, for each real $x \neq 0$ we conclude from (1.5) that

$$D_n(-x) = x^n \mathrm{e}^{1/x} E_n\Big(-\frac{1}{x}\Big).$$

Replacing x by $-x$ in the last relation implies that

$$D_n(x) = (-1)^n x^n \mathrm{e}^{-1/x}\, E_n\Big(\frac{1}{x}\Big),$$

which is indeed equivalent with (2.3). Also, letting $x = 1$ in (1.6) we get

$$D_n(-1) = (-1)^n \sum_{j=0}^{n} P(n,j).$$

Note that

$$0 < \mathrm{e} - \sum_{k=0}^{n} \frac{1}{k!} = \sum_{k=1}^{\infty} \frac{1}{(n+k)!} = \frac{1}{n!} \sum_{k=1}^{\infty} \prod_{j=1}^{k} \frac{1}{n+j} < \frac{1}{n!} \sum_{k=1}^{\infty} \frac{1}{(n+1)^k} = \frac{1}{n \cdot n!}.$$

Thus, we obtain

$$D_n(-1) = (-1)^n \lfloor \mathrm{e}\, n! \rfloor.$$

This provides an analogue to a well-known identity concerning D_n due to the first author, see [8], [7], asserting that

$$D_n(1) = \lfloor \mathrm{e}^{-1}(n!+1) \rfloor.$$

Moreover, as the first author in [8], [9] shows, the quantity $(-1)^n D_n(-1)$ actually gives the number of all distinct paths between a specific pair vertices in a simple complete graph on $n+2$ vertices. Thus, the derangement polynomials may be meaningful also at negative arguments, too. Hence, we may ask about computing moments of the difference under study in this paper for $x < 0$.

2. Proofs

The key of the proof of Theorem 1.1 and Theorem 1.2 is an integral representation for the difference $D_n(x) - x^n n! \mathrm{e}^{-1/x}$, which itself is based on an integral representation for the alternating sum over $P(n,j)$, the number of j-permutations of n objects. Let $a \geqslant 1$ be a fixed real. For any positive integer n let

$$L_n(a) = \int_1^a \log^n t \,\mathrm{d}t. \tag{2.1}$$

The following relation is equivalent to one given by R. A. Askey and M. E. H. Ismail in [2] and P. M. Kayll in [12]. Recently, first author in [10, Theorem 1] reproved it in a different form. For any integer $n \geqslant 1$ and for $x \geqslant 0$ we have

$$\sum_{j=0}^{n}(-1)^j P(n,j)x^{n-j} = \frac{(-1)^n n! + L_n(\mathrm{e}^x)}{\mathrm{e}^x}. \tag{2.2}$$

To make a connection with derangement polynomials, we conclude from (1.6) that

$$D_n(x) = (-1)^n \sum_{j=0}^{n}(-1)^j P(n,j)x^j.$$

In the relation (2.2) we replace x by $1/x$. Thus, we obtain the following key relation

$$D_n(x) = \frac{x^n n!}{\mathrm{e}^{1/x}} + \frac{(-x)^n}{\mathrm{e}^{1/x}} L_n(\mathrm{e}^{1/x}). \tag{2.3}$$

Proof of Theorem 1.1: We conclude from (2.3) that

$$\begin{aligned}\sum_{n=1}^{\infty}\Big(D_n(x) - \frac{x^n n!}{\mathrm{e}^{1/x}}\Big) &= \sum_{n=1}^{\infty}\frac{(-x)^n}{\mathrm{e}^{1/x}} L_n(\mathrm{e}^{1/x}) = \frac{1}{\mathrm{e}^{1/x}}\lim_{N\to\infty}\sum_{n=1}^{N}(-x)^n L_n(\mathrm{e}^{1/x}) \\ &= \frac{1}{\mathrm{e}^{1/x}}\lim_{N\to\infty}\sum_{n=1}^{N}(-x)^n \int_1^{\mathrm{e}^{1/x}} \log^n t \,\mathrm{d}t \\ &= \frac{1}{\mathrm{e}^{1/x}}\lim_{N\to\infty}\int_1^{\mathrm{e}^{1/x}} \sum_{n=1}^{N}(-x\log t)^n \,\mathrm{d}t.\end{aligned}$$

We use the following finite geometric series computation

$$\sum_{n=1}^{N} y^n = \frac{y}{1-y}(1-y^N).$$

Hence,

$$\sum_{n=1}^{\infty}\Big(D_n(x) - \frac{x^n n!}{\mathrm{e}^{1/x}}\Big) = -\frac{x}{\mathrm{e}^{1/x}}\lim_{N\to\infty}\int_1^{\mathrm{e}^{1/x}} \frac{\log t}{1+x\log t}\big(1-(-x\log t)^N\big)\,\mathrm{d}t.$$

Note that for $1 < t < \mathrm{e}^{1/x}$, with $x > 0$, we have $0 < x \log t < 1$. Thus we may use the bounded convergence theorem [3, Theorem 3.26] to interchange the limit and integral in the last relation. Consequently,

$$\begin{aligned}\sum_{n=1}^{\infty}\Big(D_n(x) - \frac{x^n n!}{\mathrm{e}^{1/x}}\Big) &= -\frac{x}{\mathrm{e}^{1/x}}\int_1^{\mathrm{e}^{1/x}} \lim_{N\to\infty}\frac{\log t}{1+x\log t}\big(1-(-x\log t)^N\big)\,\mathrm{d}t\\ &= -\frac{x}{\mathrm{e}^{1/x}}\int_1^{\mathrm{e}^{1/x}} \frac{\log t}{1+x\log t}\big(1-\lim_{N\to\infty}(-x\log t)^N\big)\,\mathrm{d}t\\ &= -\frac{x}{\mathrm{e}^{1/x}}\int_1^{\mathrm{e}^{1/x}} \frac{\log t}{1+x\log t}\,\mathrm{d}t.\end{aligned}$$

We apply the change of variable $w = 1 + x\log t$ to evaluate the last integral. Thus,

$$\begin{aligned}\sum_{n=1}^{\infty}\Big(D_n(x) - \frac{x^n n!}{\mathrm{e}^{1/x}}\Big) &= -\frac{1}{x\mathrm{e}^{2/x}}\int_1^2 \Big(1-\frac{1}{w}\Big)\mathrm{e}^{w/x}\,\mathrm{d}w\\ &= -1 + \frac{1}{\mathrm{e}^{1/x}} + \frac{1}{x\mathrm{e}^{2/x}}\int_1^2 \frac{\mathrm{e}^{w/x}}{w}\,\mathrm{d}w.\end{aligned}$$

Also, to evaluate the last integral we apply the change of variable $w/x = -z$. This implies that

$$\int_1^2 \frac{\mathrm{e}^{w/x}}{w}\,\mathrm{d}w = \int_{-1/x}^{-2/x}\frac{\mathrm{e}^{-z}}{-xz}(-x\,\mathrm{d}z) = -\int_{-2/x}^{-1/x}\frac{\mathrm{e}^{-z}}{z}\,\mathrm{d}z = \mathrm{Ei}\Big(\frac{2}{x}\Big) - \mathrm{Ei}\Big(\frac{1}{x}\Big).$$

This gives (1.2). Finally, let $M(x)$ be the function at the right hand side of (1.2). We observe that $\lim_{x\to 0^+} M(x) = -1/2$ and $\lim_{x\to\infty} M(x) = 0$. Also,

$$\frac{\mathrm{d}}{\mathrm{d}x}M(x) = \frac{1}{x^3\mathrm{e}^{2/x}}\Big(2x\mathrm{e}^{1/x} - x\,\mathrm{e}^{2/x} + (2-x)\Big(\mathrm{Ei}\Big(\frac{2}{x}\Big) - \mathrm{Ei}\Big(\frac{1}{x}\Big)\Big)\Big).$$

Since $\frac{\mathrm{d}}{\mathrm{d}x}M(x) > 0$ for $x > 0$, we deduce that $M(x)$ is negative and strictly increasing for $x > 0$. This completes the proof. □

Proof of Theorem 1.2: We follow an argument due to W. J. LeVeque, see [13], which has been described by M. Aigner and G. M. Ziegler in [1, Chapter 9]. By use of (2.1), we obtain

$$\begin{aligned}L_n(\mathrm{e}^{1/x})^2 &= \Big(\int_0^{1/x} z_1^n\mathrm{e}^{z_1}\,\mathrm{d}z_1\Big)\Big(\int_0^{1/x} z_2^n\mathrm{e}^{z_2}\,\mathrm{d}z_2\Big)\\ &= \int_0^{1/x}\int_0^{1/x}(z_1z_2)^n\mathrm{e}^{z_1+z_2}\,\mathrm{d}A_{z_1,z_2}.\end{aligned}$$

Hence, we conclude from (2.3) that

$$\sum_{n=1}^{\infty}\Big(D_n(x)-\frac{x^n n!}{\mathrm{e}^{1/x}}\Big)^2=-\frac{L_0(\mathrm{e}^{1/x})^2}{\mathrm{e}^{2/x}}+\frac{1}{\mathrm{e}^{2/x}}\sum_{n=0}^{\infty}x^{2n}L_n(\mathrm{e}^{1/x})^2.$$

Note that $L_0(\mathrm{e}^{1/x})=\mathrm{e}^{1/x}-1$, and

$$\sum_{n=0}^{\infty}x^{2n}L_n(\mathrm{e}^{1/x})^2=\sum_{n=0}^{\infty}\int_0^{1/x}\int_0^{1/x}(x^2z_1z_2)^n\mathrm{e}^{z_1+z_2}\,\mathrm{d}A_{z_1,z_2}.$$

Since the function $\mathrm{e}^{z_1+z_2}$ is bounded on the region $[0,1/x]\times[0,1/x]$, uniform convergence of the geometric series allows us to change the order of sum and integrals. Accordingly,

$$\sum_{n=1}^{\infty}\Big(D_n(x)-\frac{x^n n!}{\mathrm{e}^{1/x}}\Big)^2=-\frac{(\mathrm{e}^{1/x}-1)^2}{\mathrm{e}^{2/x}}+\frac{1}{\mathrm{e}^{2/x}}\,I,$$

where

$$I=\int_0^{1/x}\int_0^{1/x}\frac{\mathrm{e}^{z_1+z_2}}{1-x^2z_1z_2}\,\mathrm{d}A_{z_1,z_2}.$$

The same reasoning applies to the case of other moments. Thus, meanwhile we obtain (1.3). Let us compute I. For this purpose, we apply the change of coordinates. Let $2u=z_1+z_2$ and $2v=z_1-z_2$. We get the new domain of integration from old domain by first rotating it by -45° and then shrinking it by a factor of $\sqrt{2}$. This new domain of integration and the function to be integrated are symmetric with respect to the u-axis. Also, $\mathrm{d}A_{z_1,z_2}=2\,\mathrm{d}A_{u,v}$. Therefore,

$$I=4\int_0^{1/(2x)}\int_0^{u}\frac{\mathrm{e}^{2u}}{1-x^2u^2+x^2v^2}\,\mathrm{d}v\,\mathrm{d}u+4\int_{1/(2x)}^{1/x}\int_0^{1/x-u}\frac{\mathrm{e}^{2u}}{1-x^2u^2+x^2v^2}\,\mathrm{d}v\,\mathrm{d}u.$$

Computing the inner integrals, we get

$$I=4\int_0^{1/(2x)}\frac{\mathrm{e}^{2u}}{x\sqrt{1-x^2u^2}}\arctan\frac{xu}{\sqrt{1-x^2u^2}}\,\mathrm{d}u+4\int_{1/(2x)}^{1/x}\frac{\mathrm{e}^{2u}}{x\sqrt{1-x^2u^2}}\arctan\frac{1-xu}{\sqrt{1-x^2u^2}}\,\mathrm{d}u.$$

Substituting $u=1/x-z$ in the last integral and simplifying yields (1.4). □

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