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A CONTRIBUTION TO THE ANALYSIS OF IN SITU PERMUTATION

P. Kirschenhofer, H. Prodinger and **R. F. Tichy,** Vienna, Austria

Abstract. There is a simple algorithm to replace $(x_1, \ldots, x_n)$ by $(x_{p(1)}, \ldots, x_{p(n)})$, where $\pi=(p(1), \ldots, p(n))$ is a permutation of $\{1, 2, \ldots, n\}$, essentially without further storage requirements. This paper continues some research work by D. E. Knuth about a characteristic parameter of this algorithm. Using generating function techniques alternative derivations for several results of Knuth as well as a number of new theorems are obtained.

1. Introduction

Let $\pi=\begin{pmatrix} 1, \ldots, n \\ p(1), \ldots, p(n) \end{pmatrix}$ be a permutation of the numbers $1, 2, \ldots, n$ and let us consider the following part of a program:

$$\begin{array}{l} \textit{for } j:=1 \textit{ to } n \textit{ do} \\ \quad \textit{begin } k:=p(j); \\ \quad \textit{while } k>j \textit{ do} \\ \qquad k:=p(k) \\ \textit{end}; \end{array} \tag{1.1}$$

These instructions can be used to check whether j is a *cycle leader*, i. e. the smallest number in its cycle. For this, one has to ask „$k=j$?“ after passing the while-loop.

The detection of the cycle leader is useful if one wants to permute an array $x[1], \ldots, x[n]$ along the permutation π essentially without further storage requirements (*in situ permutation*). For each cycle $(i_1, \ldots, i_k)$ the elements $x[i_1], \ldots, x[i_k]$ should be replaced by $x[p(i_1)], \ldots, x[p(i_k)]$. If we do that iff i_1 is the cycle leader, this will be done exactly once for each cycle. The complete algorithm was developed by Mac Leod [5] and analyzed by Knuth [4]:

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One of the three interesting parameters of this analysis is denoted by $a(\pi)$ and equals the number of times the instruction „$k:=p(k)$" is executed. Knuth [4] has shown that

$$0 \leqslant a(\pi) \leqslant \binom{n}{2}; \tag{1.2}$$

the *average* of $a(\pi)$ *is*

$$(n+1)H_n - 2n; \tag{1.3}$$

the *variance* of $a(\pi)$ is

$$2n^2 - (n+1)^2 H_n^{(2)} - (n+1)H_n + 4n \tag{1.4}$$

(where $H_n^{(s)} = \Sigma_{1 \leqslant k \leqslant n} k^{-s}$ denotes the n-th harmonic number of degree s, $H_n^{(1)} = H_n$).

In this paper we exploit a method which allows us to get these quantities by less computation. Furthermore, we are able to determine the *s-th factorial moment of* $a(\pi)$ asymptotically, viz.

$$n^s \log^s n + (\gamma - 2) s n^s \log^{s-1} n + \mathcal{O}(n^s \log^{s-2} n), \quad n \to \infty \tag{1.5}$$

where $\gamma = .57721\ldots$ is Euler's constant.

Since the *s-th moment* is just a linear combination of the *j-th factorial moments for* $j \leqslant s$, we obtain the same asymptotic expansion for the s-th moment.

To stress the method of our treatment in a few words, we introduce certain generating functions $G_n(z)$, obtain a recursion for them, which does *not* allow getting a simple explicit expression for $G_n(z)$; from this recursion we obtain differential equations for the generating functions of the *s-th* factorial moments, from which we can derive the above asymptotic expansion.

2. Generating functions

Assume that $\pi = q(n)$ is the canonical representation of the permutation π as a product of cycles in the way described in Knuth [3, p. 176]. In the following we always represent a permutation in this way; it is known that

$$a(\pi) = \text{card}\,\{(i,j): 1 \leqslant i < j \leqslant n,\ q(i) < q(k) \text{ for all } k \text{ with } i < k \leqslant j\}. \tag{2.1}$$

By a_{nk} we denote the number of permutations π of n elements such that $a(\pi) = k$ and by

$$G_n(z) = \sum_{k \geqslant 0} a_{nk} z^k / n!$$

the corresponding probability generating function.

THEOREM 1. *For* $n \geqslant 1$

$$G_n(z) = n^{-1} \cdot \sum_{k=0}^{n-1} z^k G_k(z) G_{n-1-k}(z);$$

$$G_0(z) = 1.$$

Proof. In the following we write a permutation π of $\{1, \dots, n\}$ in the form $\pi = \rho 1 \sigma$, where ρ is a permutation of $n-1-k$ elements and σ a permutation of k elements. It is immediate that

$$a(\pi) = a(\rho) + a(\sigma) + k.$$

Summing up over all permutations π with $a(\pi) = s$ we obtain

$$a_{ns} = \sum_{k=0}^{n-1} \binom{n-1}{k} \sum_{i+j+k=s} a_{n-1-k,i}\, a_{k,j}.$$

Dividing by $n!$ and multiplying by z^s it follows that

$$a_{ns} z^s / n! = n^{-1} \cdot \sum_{k=0}^{n-1} z^k \sum_{i+j+k=s} a_{k,j} z^j \cdot a_{n-1-k,i} z^i / (k!(n-1-k)!).$$

Summing up over $s \geqslant 0$, Theorem 1 results immediately.

Let us now consider the double generating function $H(z, u)$ defined by

$$H(z, u) = \sum_{n \geqslant 0} G_n(z) u^n. \tag{2.3}$$

COROLLARY 1. $\dfrac{\partial}{\partial u} H(z, u) = H(z, u) \cdot H(z, zu);$

$$H(1, u) = (1-u)^{-1}.$$

Proof. We multiply the recursion in Theorem 1 by nu^{n-1} and sum up over all $n \geqslant 0$ to get the result. Since $G_n(1) = 1$, the identity for $H(1, u)$ follows.

In the following we consider the *s-th* factorial moments $\beta_s(n)$ of the random variable given by the probability generating function $G_n(z)$:

$$\beta_s(n) = \frac{d^s}{dz^s} G_n(z) \Big|_{z=1}. \tag{2.4}$$

Introducing the generating functions $f_s(u)$ of the s-th factorial moments by

$$f_s(u) = \sum_{n \geqslant 0} \beta_s(n) u^n, \tag{2.5}$$

we obtain by Taylor's formula and (2.4)

$$H(z, u) = \sum_{s \geqslant 0} f_s(u) (z-1)^s / s!. \tag{2.6}$$

THEOREM 2. *For* $s \geq 1$

$f'_s(u) - 2(1-u)^{-1} f_s(u) = h_s(u)$, *with*

$$h_s(u) = \sum_{i=1}^{s-1} \binom{s}{i} f_i(u) \sum_{r=0}^{s-i} \binom{s-i}{r} u^r f_{s-r-i}^{(r)}(u) + (1-u)^{-1} \sum_{r=1}^{s} \binom{s}{r} u^r f_{s-r}^{(r)}(u),$$

where $f^{(i)}(u)$ *denotes the i-th derivative of the function* $f(u)$;

$$f_0(u) = (1-u)^{-1},\ h_0(u) = -(1-u)^{-2} \text{ and } f_s(0) = 0 \text{ for } s \geq 1.$$

Proof. First note that

$$f_j(zu) = \sum_{k \geq 0} f_j^{(k)}(u)(z-1)^k u^k/k!$$

by Taylor's formula. Inserting (2.6) into the equation of Corollary 1 we get

$$\sum_{s \geq 0} f'_s(u)(z-1)^s/s! = \left[\sum_{i \geq 0} f_i(u)(z-1)^i/i!\right] \cdot \left[\sum_{j \geq 0} f_j(zu)(z-1)^j/j!\right] =$$

$$= \left[\sum_{i \geq 0} f_i(u)(z-1)^i/i!\right] \cdot \left[\sum_{j \geq 0} (z-1)^j/j! \left(\sum_{k \geq 0} f_j^{(k)}(u)(z-1)^k u^k/k!\right)\right] =$$

$$= \sum_{m \geq 0} \sum_{i+j+k=m} u^k f_i(u) f_j^{(k)}(u)(z-1)^m/(i!j!k!).$$

Comparing the coefficients of $(z-1)^s/s!$ we obtain

$$f'_s(u) = \sum_{i+j+k=s} s! \cdot u^k f_i(u) f_j^{(k)}(u)/(i!j!k!)$$

$$= \sum_{i=0}^{s} \binom{s}{i} f_i(u) \sum_{r=0}^{s-i} \binom{s-i}{r} u^r f_{s-i-r}^{(r)}(u)$$

$$= 2(1-u)^{-1} f_s(u) + \sum_{i=1}^{s-1} \binom{s}{i} f_i(u) \sum_{r=0}^{s-i} \binom{s-i}{r} u^r f_{s-i-r}^{(r)}(u) +$$

$$+ (1-u)^{-1} \cdot \sum_{r=1}^{s} \binom{s}{r} u^r f_{s-r}^{(r)}(u),$$

because $\beta_0(n) = 1$ for all n and therefore $f_0(u) = (1-u)^{-1}$.

Since $G_0(z) = 1$ we have $\beta_s(0) = 0$ for $s \geq 1$ and therefore $f_s(0) = 0$ for $s \geq 1$, and the proof of Theorem 2 is complete.

Solving the first order linear differential equation of Theorem 2 we obtain

COROLLARY 2. *For* $s \geq 1$

$$f_s(u) = (1-u)^{-2} \int_0^u h_s(t)(1-t)^2\, dt,$$

where f_s *and* h_s *are as in Theorem 2.*

3. The first and second order factorial moments

In principle Corollary 2 allows to compute $f_s(u)$ (and thus $\beta_s(n)$) step by step for any s. To illustrate, we determine the first two moments.

THEOREM 3. *With* $L(u) := -\log(1-u)$ *we have*

$$f_1(u) = L(u)\cdot(1-u)^{-2} - (1-u)^{-2} + (1-u)^{-1},$$

$$f_2(u) = 2L^2(u)\cdot(1-u)^{-3} - 2L(u)\cdot(1-u)^{-3} + 2(1-u)^{-3} - \\ - L^2(u)\cdot(1-u)^{-2} - 2(1-u)^{-2};$$

$$\beta_1(n) = (n+1)H_n - 2n,$$

$$\beta_2(n) = (n+1)^2(H_n^2 - H_n^{(2)}) - (4n+2)(n+1)H_n + 6n(n+1).$$

Proof. Observing $h_1(u) = u(1-u)^{-3}$ the formula for $f_1(u)$ is immediate; a short computation yields

$$h_2(u) = 2L^2(u)(1-u)^{-4} + 2L(u)(1-u)^{-4} - 2L(u)(1-u)^{-3}$$

from which $f_2(u)$ follows by the formula indicated in Corollary 2.

Expanding $f_1(u)$ resp. $f_2(u)$ we use the following results (compare Greene/Knuth [2, p. 14]):

$$L(u)\cdot(1-u)^{-m-1} = \sum_{n\geq 0} (H_{n+m} - H_m)\binom{n+m}{m} u^n,$$

$$L^2(u)\cdot(1-u)^{-m-1} = \sum_{n\geq 0} ((H_{n+m} - H_m)^2 - (H_{n+m}^{(2)} - H_m^{(2)}))\binom{n+m}{m} u^n.$$

The following special instances are needed for our computations:

$$L(u)\cdot(1-u)^{-2} = \sum_{n\geq 0} [(n+1)H_n - n]u^n,$$

$$L^2(u)\cdot(1-u)^{-2} = \sum_{n\geq 0} [(n+1)(H_n^2 - H_n^{(2)}) - 2nH_n + 2n]u^n,$$

$$L(u)\cdot(1-u)^{-3} = \sum_{n\geq 0} \left[\binom{n+2}{2}H_n - (3/4)n^2 - (5/4)n\right]u^n,$$

$$L^2(u)\cdot(1-u)^{-3} = \sum_{n\geq 0} \left[\binom{n+2}{2}(H_n^2 - H_n^{(2)}) - (n/2)(5+3n)H_n + \right. \\ \left. + (7/4)n^2 + (9/4)n\right]u^n.$$

Inserting into the formulas for $f_1(u)$ and $f_2(u)$ and simplifying we get the announced results for $\beta_1(n)$ and $\beta_2(n)$.

4. Asymptotic results

Although, in principle, Corollary 2 allows to determine $f_s(u)$ explicitly for any s, terms get more and more complicated as s gets large. So we confine ourselves for general s to give the two leading terms of the asymptotic expansion of $f_s(u)$ about the singularity $u=1$. It turns out to be a crucial point in the derivation of the desired result that $f_s(u)$ is a linear combination of functions of the type $L^i(u)\cdot(1-u)^{-j-1}$ (with L from Theorem 3):

In the following we denote by $\mathcal{R}_{p,q}(u)$ an unspecified linear combination of terms of the form $L^i(u)(1-u)^{-j-1}$ where i, j are integers with either $j<q$ and i arbitrary, or $j=q$ and $i\leqslant p$. With this notation we have

THEOREM 4. *For* $s\geqslant 0$

$$f_s(u)=s!L^s(u)\cdot(1-u)^{-s-1}+\mathcal{R}_{s-1,s}(u).$$

Proof. We proceed by induction and start with $s=0$: $f_0(u)=(1-u)^{-1}$, and the theorem is valid in this case.

Assuming that the theorem is correct for all j with $0\leqslant j\leqslant s-1$, we prove that the same holds for s. We will frequently use the fact that for

$$g(u)=cq!L^p(u)\cdot(1-u)^{-q-1}+\mathcal{R}_{p-1,q}(u) \qquad (c \text{ a constant})$$

the derivatives $g^{(i)}(u)$ fulfill

$$g^{(i)}(u)=c(q+i)!L^p(u)\cdot(1-u)^{-q-i-1}+\mathcal{R}_{p-1,q+i}(u).$$

Especially we have for $j\leqslant s-1$

$$f_j^{(i)}(u)=(j+i)!L^j(u)\cdot(1-u)^{-j-i-1}+\mathcal{R}_{j-1,j+i}(u).$$

Inserting into the formula for $h_s(u)$ in Theorem 2 we get

$$h_s(u)=\sum_{i=1}^{s-1}\binom{s}{i}[i!L^i(u)\cdot(1-u)^{-i-1}+\mathcal{R}_{i-1,i}(u)]\sum_{r=0}^{s-i}\binom{s-i}{r}u^r\times$$

$$\times[(s-i)!L^{s-i-r}(u)\cdot(1-u)^{-s+i-1}+\mathcal{R}_{s-i-r-1,s-i}(u)]+$$

$$+(1-u)^{-1}\sum_{r=1}^{s}\binom{s}{r}u^r[s!L^{s-r}(u)\cdot(1-u)^{-s-1}+\mathcal{R}_{s-r-1,s}(u)].$$

It follows by a short consideration that all remainder terms $\mathcal{R}_{p,q}(u)$ as well as the second sum give a contribution of the form $\mathcal{R}_{s-1,s+1}(u)$. The other terms contribute

$$s!L^s(u)\cdot(1-u)^{-s-2}\cdot\sum_{i=1}^{s-1}(1+u/L(u))^{s-i}=s!(s-1)L^s(u)\cdot(1-u)^{-s-2}+$$
$$+\mathcal{R}_{s-1,s+1}(u),$$

hence $h_s(u)$ is of the same type.

Using Corollary 2 we get

$$f_s(u)=(1-u)^{-2}\cdot\int_0^u s!\,(s-1)\,L^s(t)\cdot(1-t)^{-s}\,dt+(1-u)^{-2}\cdot$$
$$\cdot\int_0^u \mathscr{R}_{s-1,s-1}(t)\,dt=$$
$$=s!L^s(u)\cdot(1-u)^{-s-1}+\mathscr{R}_{s-1,s}(u)$$

by integration by parts.

It should be remarked that from Theorem 4 the leading term of $\beta_s(n)$ for $n\to\infty$ is

$$\beta_s(n)\sim n^s\cdot\log^s n, \tag{4.1}$$

either by observing that $L^s(u)$ varies slowly at infinity and applying Hardy-Littlewood-Karamata's Tauberian Theorem (e.g. [1]) or by the explicit knowledge of the coefficients of functions of the following type (compare Zave [6]):

$$L^p(u)\cdot(1-u)^{-q-1}=\sum_{n\geq 0}\cdot P_p(H^{(1)}_{n+q}-H^{(1)}_q,\dots,H^{(p)}_{n+q}-H^{(p)}_q)\cdot\binom{n+q}{q}u^n, \tag{4.2}$$

where $P_p(s_1,\dots,s_p)$ is defined by $P_0=1$ and

$$P_p(s_1,\dots,s_p)=(-1)^p\,Y_p(-s_1,-s_2,-2s_3,\dots,-(p-1)!s_p)$$

with Y_p the p-th Bell polynomial.

With the information on the structure of the remainder term in Theorem 4 it is possible to determine the second term in the expansion of $f_s(u)$ about $u=1$ explicitly:

THEOREM 5. *For* $s\geq 0$

$$f_s(u)=s!L^s(u)\cdot(1-u)^{-s-1}+s!s\,(H_s-2)\,L^{s-1}(u)\cdot(1-u)^{-s-1}+\mathscr{R}_{s-2,s}(u).$$

Proof. From Theorem 4 we know that $f_i(u)$ is of the form

$$f_i(u)=i!L^i(u)\cdot(1-u)^{-i-1}+a_i i!L^{i-1}(u)\cdot(1-u)^{-i-1}+\mathscr{R}_{i-2,i}(u)$$

with some constant a_i. Observing that

$$f_i'(u)=(i+1)!L^i(u)\,(1-u)^{-i-2}+(i+a_i\,(i+1))\,i!L^{i-1}(u)\,(1-u)^{-i-2}+$$
$$+\mathscr{R}_{i-2,i+1}(u),$$
$$f_i^{(j)}(u)=(i+j)!L^i(u)\,(1-u)^{-i-j-1}+\mathscr{R}_{i-1,i+j}(u). \qquad (j\geq 2)$$

and inserting these formulas in the definition of $h_s(u)$ (Theorem 2) we obtain

$$h_s(u)=\sum_{i=1}^{s-1}\binom{s}{i}[i!L^i(u)(1-u)^{-i-1}+a_i i!L^{i-1}(u)(1-u)^{-i-1}+\mathscr{R}_{i-2,i}(u)]\times$$

$$\times[(s-i)!L^{s-i}(u)(1-u)^{-s+i-1}+a_{s-i}(s-i)!L^{s-i-1}(u)(1-u)^{-s+i-1}+$$

$$+(s-i)(s-i)!L^{s-i-1}(u)(1-u)^{-s+i-1}+\mathscr{R}_{s-i-2,s-i}(u)]+$$

$$+(1-u)^{-1}\sum_{r=1}^{s}\binom{s}{r}[s!L^{s-r}(u)(1-u)^{-s-1}+\mathscr{R}_{s-r-1,s+1}(u)]=$$

$$=s!(s-1)L^s(u)(1-u)^{-s-2}+s!L^{s-1}(u)(1-u)^{-s-2}\times$$

$$\times\left[s+\sum_{i=1}^{s-1}(a_i+a_{s-i}+s-i)\right]+\mathscr{R}_{s-2,s+1}(u).$$

On the other hand we have

$$f_s'(u)-2(1-u)^{-1}f_s(u)=(s+1)!L^s(u)(1-u)^{-s-2}+$$

$$+(s+a_s(s+1))s!L^{s-1}(u)(1-u)^{-s-2}-$$

$$-2s!L^s(u)(1-u)^{-s-2}-2a_s s!L^{s-1}(u)(1-u)^{-s-2}+\mathscr{R}_{s-2,s+1}(u)=$$

$$=s!(s-1)L^s(u)(1-u)^{-s-2}+(s+a_s(s-1))s!L^{s-1}(u)(1-u)^{-s-2}+$$

$$+\mathscr{R}_{s-2,s+1}(u).$$

Comparing the coefficients of $s!L^{s-1}(1-u)^{-s-2}$ we obtain the recurrence relation

$$(s-1)a_s=\binom{s}{2}+2\cdot\sum_{i=1}^{s-1}a_i.$$

Subtracting this equation from

$$sa_{s+1}=\binom{s+1}{2}+2\cdot\sum_{i=1}^{s}a_i$$

we derive

$$sa_{s+1}=(s-1)a_s+2a_s+s,$$

or

$$a_{s+1}/(s+1)=a_s/s+1/(s+1),\qquad a_1=-1.$$

Summing up we get

$$a_s/s=-1+\sum_{i=1}^{s-1}(i+1)^{-1}=H_s-2,$$

hence

$$a_s = s\,(H_s - 2)$$

and the proof is complete.

Combining Theorem 5 with formula (4.2) we reach our final result

THEOREM 6. *For* $s \geqslant 0$

$$\beta_s(n) = n^s \cdot \log^s n + s\,(\gamma - 2)\, n^s \cdot \log^{s-1} n + \mathcal{O}\,(n^s \cdot \log^{s-2} n),$$

where $\gamma = .57721 \ldots$ *denotes Euler's constant.*

Proof. From Theorem 5 and (4.2)

$$\beta_s(n) = s!P_s\,(H^{(1)}_{n+s} - H^{(1)}_s, \ldots, H^{(s)}_{n+s} - H^{(s)}_s)\binom{n+s}{s} +$$

$$+ s\,(H^s - 2)\, s!P_{s-1}\,(H^{(1)}_{n+s} - H^{(1)}_s, \ldots, H^{(s-1)}_{n+s} - H^{(s-1)}_s)\binom{n+s}{s} +$$

$$+ \mathcal{O}\,(n^s \cdot \log^{s-2} n),$$

since

$$P_p\,(H^{(1)}_{n+s} - H^{(1)}_s, \ldots, H^{(p)}_{n+s} - H^{(p)}_s) = \mathcal{O}\,(n^s \cdot H^p_n) = \mathcal{O}\,(n^s \cdot \log^p n).$$

Regarding

$$P_p\,(s_1, \ldots, s_p) = s_1^p - \binom{p}{2} s_1^{p-2} s_2 + \ldots$$

we have

$$\beta_s(n) = \binom{n+s}{s}\left[s!\,(H_{n+s} - H_s)^s + s!s\,(H_s - 2)\,(H_{n+s} - H_s)^{s-1}\right] +$$

$$+ \mathcal{O}\,(n^s \cdot \log^{s-2} n) = n^s\left[H^s_{n+s} - sH^{s-1}_{n+s} H_s + s\,(H_s - 2)\, H^{s-1}_{n+s}\right] +$$

$$+ \mathcal{O}\,(n^s \cdot \log^{s-2} n) = n^2\left[(\log(n+s) + \gamma)^s - 2s\,(\log(n+s) + \gamma)^{s-1}\right] +$$

$$+ \mathcal{O}\,(n^s \cdot \log^{s-2} n) = n^s\left[\log^s n + s\,(\gamma - 2)\log^{s-1} n\right] + \mathcal{O}\,(n^s \cdot \log^{s-2} n).$$

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P. Kirschenhofer and H. Prodinger
Inst. f. Algebra u. Diskrete Mathematik
R. F. Tichy
Inst. f. Analysis, Technische Mathematik u. Versicherungsmathematik
Technical University of Vienna
Wiedner Hauptstr. 8–10
A-1040 *Vienna, Austria*

PRILOG ANALIZI (IN SITU) PERMUTACIJA

P. Kirschenhofer, H. Prodinger i *R. F. Tichy*, Beč, Austrija

Sadržaj

Postoji jednostavni algoritam koji zamjenjuje (prevodi) $(x_1, \ldots, x_n)$ sa $(x_{p(1)}, \ldots, x_{p(n)})$ gdje je $\pi = (p(1), \ldots, p(n))$ permutacija od $1, 2, \ldots, n$, koji u biti ne zahtijeva dodatno korištenje memorije.

U ovom redu se nastavljaju istraživanja D. E. Knutha o jednom karakterističnom parametru tog algoritma. Korištenjem tehnika funkcija izvodnica dobiveno je osim alternativnih izvoda nekoliko rezultata Knutha i nekoliko novih rezultata.