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A RANDOM PERMUTATION MODEL ARISING IN CHEMISTRY

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Abstract

We study a model arising in chemistry where *n* elements numbered 1, 2, ..., n are randomly permuted and if *i* is immediately to the left of i + 1 then they become stuck together to form a cluster. The resulting clusters are then numbered and considered as elements, and this process keeps repeating until only a single cluster is remaining. In this article we study properties of the distribution of the number of permutations required.

Keywords: Random permutation; hat-check problem

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1. Introduction

For the classic hat-check problem first proposed in 1708 by Montmort [2], the following variation appears in [6, p. 93]. Each member of a group of n individuals throws his or her hat in a pile. The hats are shuffled, each person chooses a random hat, and the people who receive their own hat depart. Then the process repeats with the remaining people until everybody has departed; let N be the number of shuffles required. With X_i representing the total number of people who have departed after shuffle number i, it is easy to show that $X_i - i$ is a martingale and, thus, by the optional sampling theorem we elegantly see that E[N] = n.

Someone getting their own hat can also be thought of as corresponding to a cycle of length one in a random permutation. Properties of cycles of various lengths in random permutations have been studied extensively; see [1] and [3] for entry points to this literature. A variation of this problem was presented in [5], where it was given as a model for a chemical bonding process. Below we discuss this variation and study its properties. We quote the following description of the chemistry application from [5], where a recursive formula was given to numerically compute the mean.

There are 10 molecules in some hierarchical order operating in a system. A catalyst is added to the system and a chemical reaction sets in. The molecules line up. In the line-up from left to right molecules in consecutive increasing hierarchical order bond together and become one. A new hierarchical order sets among the fused molecules. The catalyst is added again

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to the system and the whole process starts all over again. The question raised is how many times catalysts are expected to be added in order to get a single lump of all molecules.

This variation presented in [5] can be abstractly stated as follows. Suppose that we have n elements numbered 1, 2, ..., n. These elements are randomly permuted, and if i is immediately to the left of i + 1 then i and i + 1 become stuck together to form (possibly with other adjacently numbered elements) a cluster. These clusters are then randomly permuted and if a cluster ending with i immediately precedes one starting with i + 1 then those two clusters join together to form a new cluster. This continues until there is only one cluster, and we are interested in N(n), the number of permutations that are needed. For instance, suppose that n = 7 and that the first permutation is

which results in the clusters {3, 4, 5}, {1, 2}, {6}, and {7}. If a random permutation of these four clusters gives the ordering

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

then the new sets of clusters are $\{6, 7\}$, $\{3, 4, 5\}$, and $\{1, 2\}$. If a random permutation of these three clusters gives the ordering

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

then the new sets of clusters are $\{3, 4, 5, 6, 7\}$ and $\{1, 2\}$. If a random permutation of these two clusters gives the ordering

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

then there is now a single cluster $\{1, 2, 3, 4, 5, 6, 7\}$ and N(7) = 4.

The random variable N(n) can be analyzed as a first passage time from state n to state 1 of a Markov chain whose state is the current number of clusters. When the state of this chain is i, we will designate the clusters as $1, \ldots, i$, with 1 being the cluster whose elements are smallest, 2 being the cluster whose elements are the next smallest, and so on. For instance, in the preceding n = 7 case, the state after the first transition is 4, with 1 being the cluster $\{1, 2\}, 2$ being the cluster $\{3, 4, 5\}, 3$ being the cluster $\{6\},$ and 4 being the cluster $\{7\}$. With this convention, the transitions from state i are exactly the same as if the problem began with the i elements, $1, \ldots, i$.

In Section 2 we compute the transition probabilities of this Markov chain and use them to obtain some stochastic inequalities. In Section 3 we obtain upper and lower bounds on E[N(n)], as well as bounds on its distribution. In Section 4 we give results for a circular version of the problem.

2. The transition probabilities

With the above definitions, let D_n be the decrease in the number of clusters starting from state n. Then we have the following proposition.

Proposition 1. For $0 \le k < n$,

$$\mathbf{P}(D_n = k) = \frac{n - k + 1}{nk!} \sum_{i=0}^{n-k+1} \frac{(-1)^i}{i!}.$$

Proof. Letting A_i be the event that *i* immediately precedes i + 1 in the random permutation, then D_n is the number of events A_1, \ldots, A_{n-1} that occur. Then, with

$$S_j = \sum_{0 < i_1 < \cdots < i_j < n} \mathbf{P}(A_{i_1} \cdots A_{i_j}),$$

the inclusion/exclusion identity (see [4, p. 106]) gives

$$P(D_n = k) = \sum_{j=k}^{n-1} S_j {j \choose k} (-1)^{j+k}.$$

Now consider $P(A_{i_1} \cdots A_{i_j})$. If we think of a permutation of *n* elements as having *n* degrees of freedom then, for each event A_i in the intersection, one degree of freedom in the permutation is dropped. For instance, suppose that we want $P(A_2A_3A_6)$. Then, in order for these three events to occur, 2, 3, and 4 must be consecutive values of the permutation, as must be 6 and 7. Because there are n - 5 other values, there are thus (n - 3)! such permutations. Similarly, for the event $A_2A_4A_6$ to occur, 2 and 3 must be consecutive values of the permutation, as must be 4, 5 and 6, 7. As there are n - 6 other values, there are (n - 3)! such permutations. Consequently, for $0 < i_1 < \cdots < i_j < n$,

$$\mathbf{P}(A_{i_1}\cdots A_{i_j})=\frac{(n-j)!}{n!}.$$

As a result,

$$S_j = \binom{n-1}{j} \frac{(n-j)!}{n!} = \frac{n-j}{nj!},$$

which yields

$$P(D_n = k) = \sum_{j=k}^{n-1} {j \choose k} (-1)^{j+k} \frac{n-j}{nj!}$$

= $\sum_{i=0}^{n-k-1} (-1)^i {k+i \choose k} \frac{n-k-i}{n(k+i)!}$
= $\sum_{i=0}^{n-k-1} (-1)^i \frac{n-k-i}{nk! \, i!}$
= $\frac{1}{nk!} \left((n-k) \sum_{i=0}^{n-k-1} \frac{(-1)^i}{i!} - \sum_{i=1}^{n-k-1} \frac{(-1)^i}{(i-1)!} \right)$
= $\frac{1}{nk!} \left((n-k+1) \sum_{i=1}^{n-k-2} \frac{(-1)^i}{i!} + (n-k) \frac{(-1)^{n-k-1}}{(n-k-1)!} \right).$

Thus, the result follows once we show that

$$(n-k)\frac{(-1)^{n-k-1}}{(n-k-1)!} = (n-k+1)\left(\frac{(-1)^{n-k-1}}{(n-k-1)!} + \frac{(-1)^{n-k}}{(n-k)!} + \frac{(-1)^{n-k+1}}{(n-k+1)!}\right)$$

or, equivalently, that

$$\frac{(-1)^{n-k}}{(n-k-1)!} = (n-k+1)\left(\frac{(-1)^{n-k}}{(n-k)!} + \frac{(-1)^{n-k+1}}{(n-k+1)!}\right)$$

or

$$1 = (n - k + 1) \left(\frac{1}{n - k} - \frac{1}{(n - k + 1)(n - k)} \right),$$

which is immediate.

Remark 1. A recursive expression for $P(D_n = k)$, though not in closed form, was given in [5].

From Proposition 1 we immediately conclude that D_n converges in distribution to a Poisson random variable with mean 1.

Corollary 1. We have $\lim_{n\to\infty} P(D_n = k) = e^{-1}/k!$.

We now present two results that will be used in the next section. Recall from [6, p. 133] that a discrete random variable X is said to be likelihood ratio smaller than Y if P(X = k)/P(Y = k) is nonincreasing in k.

Corollary 2. With the above definitions, D_n is likelihood ratio smaller than a Poisson random variable with mean 1.

Proof. We need to show that $k! P(D_n = k)$ is nonincreasing in k. But, with $B_k = nk! P(D_n = k)$ we have

$$B_{k-1} - B_k = \sum_{i=0}^{n-k+1} \frac{(-1)^i}{i!} + (n-k+2)\frac{(-1)^{n-k+2}}{(n-k+2)!}$$
$$= \sum_{i=0}^{n-k} \frac{(-1)^i}{i!}$$
$$> 0,$$

which proves the result.

Corollary 3. The state of the Markov chain after a transition from state $n, n - D_n$, is likelihood ratio increasing in n.

Proof. From Proposition 1,

$$P(n - D_n = k) = \frac{k+1}{n(n-k)!} \sum_{i=0}^{k+1} \frac{(-1)^i}{i!}$$

Consequently,

$$\frac{P(n+1-D_{n+1}=k)}{P(n-D_n=k)} = \frac{n}{(n+1)(n+1-k)}$$

As the preceding is increasing in *k*, the result follows.

3. The random variable N(n)

Let X_i be the *i*th decrease in the number of clusters, so that

$$S_k \equiv n - \sum_{i=1}^k X_i$$

is the state of the Markov chain, starting in state *n*, after *k* transitions, $k \ge 1$.

Proposition 2. We have

$$P(N(n) > k) \ge \sum_{i=0}^{n-1} \frac{e^{-k}k^i}{i!}$$

Proof. Let the Y_i , i = 1, ..., k, be independent Poisson random variables, each with mean 1. Now, because likelihood ratio is a stronger ordering than stochastic order (see Proposition 4.20 of [6]), it follows by Corollary 2 that X_i , conditional on $X_1, ..., X_{i-1}$, is stochastically smaller than a Poisson random variable with mean 1. Consequently, the random vector $X_1, ..., X_k$ can be generated in such a manner that $X_i \leq Y_i$ for each i = 1, ..., k. But this implies that

$$P(N(n) > k) = P(X_1 + \dots + X_k < n)$$

$$\geq P(Y_1 + \dots + Y_k < n)$$

$$= \sum_{i=0}^{n-1} \frac{e^{-k}k^i}{i!}.$$

We now consider bounds on E[N(n)].

Proposition 3. We have

$$E[N(n)] \le n - 1 + \sum_{i=1}^{n-1} \frac{1}{i}.$$

Proof. First note that

$$E[D_n] = \sum_{i=1}^{n-1} P(i \text{ immediately precedes } i+1) = \frac{n-1}{n}.$$
 (1)

Because the Markov chain cannot make a transition from a state into a higher state and $E[D_n]$ is nondecreasing in *n*, it follows from Proposition 5.23 of [6] that

$$\mathbb{E}[N(n)] \le \sum_{i=2}^{n} \frac{1}{\mathbb{E}[D_i]} = n - 1 + \sum_{i=1}^{n-1} \frac{1}{i}.$$

Proposition 4. We have

$$E[N(n)] \ge n - 1 + \frac{e}{n(e-1)} + \frac{e}{(e-1)^2} \sum_{j=2}^{n-1} \frac{1}{j}.$$

Proof. To begin, note that

$$Z_k = \sum_{i=1}^k (X_i - \mathbb{E}[X_i \mid X_1, \dots, X_{i-1}]), \qquad k \ge 1,$$
(2)

is a zero-mean martingale. Hence, by the martingale stopping theorem,

$$E[Z_{N(n)}] = 0.$$
 (3)

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Now, because $E[X_i | X_1, ..., X_{i-1}]$ is the expected decrease from state S_{i-1} , it follows from (1) that

$$E[X_i | X_1, \dots, X_{i-1}] = E[X_i | S_{i-1}] = E[D_{S_{i-1}} | S_{i-1}] = 1 - \frac{1}{S_{i-1}}.$$

Using this, and the fact that $\sum_{i=1}^{N(n)} X_i = n - 1$, we obtain, from (2) and (3),

$$n - 1 - \mathbb{E}[N(n)] + \mathbb{E}\left[\sum_{i=1}^{N(n)} \frac{1}{S_{i-1}}\right] = 0.$$

Now (notationally suppressing its dependence on the initial state *n*), let T_j denote the amount of time that the Markov chain spends in state j, j > 1. Then

$$\sum_{i=1}^{N(n)} \frac{1}{S_{i-1}} = \sum_{j=2}^{n} \frac{T_j}{j}$$

Hence,

$$E[N(n)] = n - 1 + \sum_{j=2}^{n} \frac{1}{j} E[T_j] \ge n - 1 + \frac{e}{(e-1)^2} \sum_{j=2}^{n-1} \frac{1}{j} + \frac{e}{n(e-1)},$$

where, for the inequality, we made use of the following proposition.

Proposition 5. We have

$$E[T_n] = \frac{1}{P(D_n > 0)} \ge \frac{e}{e - 1},$$

$$E[T_j] = \frac{P(T_j > 0)}{P(D_j > 0)} \ge \frac{e}{(e - 1)^2}.$$

To prove Proposition 5, we will need a series of lemmas.

Lemma 1. Let W_j , $2 \le j < n$, denote the state of the Markov chain from which the first transition to a state less than or equal to j occurs. Then, for r > j,

$$P(T_j > 0 | W_j = r) \ge P(T_j > 0 | W_j = j + 1) = P(D_{j+1} = 1 | D_{j+1} \ge 1).$$

Proof. Let $Y_r = r - D_r$. Then,

$$P(T_{j} > 0 | W_{j} = r) = P(D_{r} = r - j | D_{r} \ge r - j)$$

$$= P(Y_{r} = j | Y_{r} \le j)$$

$$= \frac{P(Y_{r} = j)}{\sum_{i=1}^{j} P(Y_{r} = i)}$$

$$= \frac{1}{\sum_{i=1}^{j} P(Y_{r} = i) / P(Y_{r} = j)}.$$
 (4)

But, for $i \leq j$, it follows from Corollary 4 that

$$\frac{P(Y_{r+1} = j)}{P(Y_r = j)} \ge \frac{P(Y_{r+1} = i)}{P(Y_r = i)}$$

or, equivalently, that

$$\frac{P(Y_{r+1}=i)}{P(Y_{r+1}=j)} \le \frac{P(Y_r=i)}{P(Y_r=j)}.$$

Thus, by (4), $P(T_j > 0 | W_j = r)$ is nondecreasing in r.

Lemma 2. For all $j \ge 2$,

$$P(D_{j+1} = 1 | D_{j+1} \ge 1) \ge \frac{e^{-1}}{1 - e^{-1}}.$$

Proof. Let $M_k = \sum_{i=0}^k (-1)^i / i!$. By Proposition 1 we need to show that

$$\frac{M_{j+1}}{1-(j+2)M_{j+2}/(j+1)} \ge \frac{\mathrm{e}^{-1}}{1-\mathrm{e}^{-1}}.$$

That is, we need to show that, for all $n \ge 3$,

$$M_n(1-e^{-1})-e^{-1}\left(1-\frac{n+1}{n}M_{n+1}\right)\geq 0.$$

Case 1. Suppose that *n* is even and that n > 2. Then,

$$\begin{split} M_n(1 - e^{-1}) &- e^{-1} \left(1 - \frac{n+1}{n} M_{n+1} \right) \\ &= M_n(1 - e^{-1}) - e^{-1} \left[1 - \frac{n+1}{n} \left(M_n - \frac{1}{(n+1)!} \right) \right] \\ &= M_n \left(1 + \frac{e^{-1}}{n} \right) - e^{-1} \left(1 + \frac{1}{nn!} \right) \\ &\ge e^{-1} \left(1 + \frac{e^{-1}}{n} \right) - e^{-1} \left(1 + \frac{1}{nn!} \right) \\ &= \frac{e^{-1}}{n} \left(e^{-1} - \frac{1}{n!} \right) \\ &> 0, \end{split}$$

where we used the fact that $M_n > e^{-1}$.

Case 2. Suppose that n is odd. In this case,

$$M_n(1 - e^{-1}) - e^{-1} \left(1 - \frac{n+1}{n} M_{n+1} \right)$$

= $\left(M_{n+1} - \frac{1}{(n+1)!} \right) (1 - e^{-1}) - e^{-1} \left(1 - \frac{n+1}{n} M_{n+1} \right)$
= $M_{n+1} \left(1 + \frac{e^{-1}}{n} \right) - \frac{1 - e^{-1}}{(n+1)!} - e^{-1}$
 $\ge e^{-1} \left(1 + \frac{e^{-1}}{n} \right) - \frac{1 - e^{-1}}{(n+1)!} - e^{-1}$
= $e^{-1} \left(\frac{e^{-1}}{n} + \frac{1}{(n+1)!} \right) - \frac{1}{(n+1)!},$

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which will be nonnegative provided that

$$e^{-2} \ge \frac{n}{(n+1)!}(1-e^{-1})$$

or, equivalently, that

$$\mathbf{e}(\mathbf{e}-1) \le \frac{(n+1)!}{n},$$

which is easily seen to be true when $n \ge 3$. This completes the proof of Lemma 2.

We need one additional lemma.

Lemma 3. As
$$n \to \infty$$
, $P(D_n = 0) \downarrow e^{-1}$.

Proof. By Proposition 1,

$$\mathbf{P}(D_n=0)=\frac{n+1}{n}M_{n+1},$$

yielding $\lim_{n} P(D_n = 0) = e^{-1}$. To show that the convergence is monotone, note that

$$\frac{n+1}{n}M_{n+1} - \frac{n+2}{n+1}M_{n+2} = \frac{n+1}{n}M_{n+1} - \frac{n+2}{n+1}\left(M_{n+1} + \frac{(-1)^n}{(n+2)!}\right)$$
$$= \frac{M_{n+1}}{n(n+1)} + \frac{(-1)^{n+1}}{(n+1)(n+1)!}.$$

When *n* is odd, the preceding is clearly positive. When *n* is even, $M_{n+1} = M_n - 1/(n+1)!$, and, thus, we must show that

$$M_n - \frac{1}{(n+1)!} \ge \frac{1}{(n+1)(n-1)!}$$

or, equivalently, that

$$M_n \geq \frac{1}{n!},$$

which follows since, for n even,

$$M_n = M_{n-1} + \frac{1}{n!} \ge \frac{1}{n!}.$$

Proof of Proposition 5. Given that state *j* is entered, the time spent in that state will have a geometric distribution with parameter $P(D_j > 0)$. Hence,

$$\operatorname{E}[T_j] = \frac{\operatorname{P}(T_j > 0)}{\operatorname{P}(D_j > 0)}.$$

Now, $P(T_n > 0) = 1$, and, by Lemma 3, $P(D_n > 0) \le 1 - e^{-1}$, which verifies the first part of Proposition 5. Also, for $2 \le j < n$, Lemmas 1 and 2 yield

$$P(T_j > 0) \ge P(D_{j+1} = 1 | D_{j+1} \ge 1) \ge \frac{e^{-1}}{1 - e^{-1}}.$$

Hence, by Lemma 3,

$$E[T_j] \ge \frac{e^{-1}}{(1-e^{-1})^2} = \frac{e}{(e-1)^2},$$

which completes the proof of Proposition 5.

Corollary 4. We have

$$n-1+\frac{e}{n(e-1)}+\frac{e}{(e-1)^2}\ln\left(\frac{n}{2}\right) \le E[N(n)] \le n+\ln\left(\frac{2n-1}{3}\right).$$

Proof. Let X be uniformly distributed between $j - \frac{1}{2}$ and $j + \frac{1}{2}$. Then,

$$\ln\left(\frac{j+1/2}{j-1/2}\right) = \int_{j-1/2}^{j+1/2} \frac{1}{x} \, \mathrm{d}x = \mathrm{E}\left[\frac{1}{X}\right] \ge \frac{1}{\mathrm{E}[X]} = \frac{1}{j},$$

where the inequality used Jensen's inequality. Hence,

$$\sum_{j=2}^{n-1} \frac{1}{j} \le \ln\left(\frac{n-1/2}{3/2}\right) = \ln\left(\frac{2n-1}{3}\right),$$

and the upper bound follows from Proposition 3. To obtain the lower bound, we use Proposition 4 along with the inequality

$$\ln\left(\frac{j+1}{j}\right) = \int_{j}^{j+1} \frac{1}{x} \, \mathrm{d}x \le \frac{1}{j}.$$

Remarks. 1. Corollary 4 yields the results given in Table 1.

2. It follows from Corollary 3, using a coupling argument, that N(n) is stochastically increasing in n.

4. The circular case

Whereas we have previously assumed that at each stage the clusters are randomly arranged in a linear order, in this section we suppose that they are randomly arranged around a circle, again with all possibilities being equally likely. We suppose that if a cluster ending with *i* is immediately counterclockwise to a cluster beginning with i + 1 then these clusters merge. Let $N^*(n)$ denote the number of stages needed until all *n* elements are in a single cluster, and let D_n^* denote the decrease in the number of clusters from state *n*.

Lemma 4. For $n \ge 2$,

$$E[D_n^*] = var(D_n^*) = 1.$$

Proof. If B_i is the event that *i* is the counterclockwise neighbor of i + 1 then

$$D_n^* = \sum_{i=1}^{n-1} \mathbf{1}_{B_i}$$

Now,

$$P(B_i) = \frac{(n-2)!}{(n-1)!} = \frac{1}{n-1}, \qquad i = 1, \dots, n-1,$$

and, for $i \neq j$,

$$P(B_i B_j) = \frac{(n-3)!}{(n-1)!}.$$

Hence,

$$E[D_n^*] = \sum_{i=1}^{n-1} \frac{1}{n-1} = 1$$

and

$$\operatorname{var}(D_n^*) = \sum_{i=1}^{n-1} \frac{1}{n-1} \left(1 - \frac{1}{n-1} \right) + 2 \binom{n-1}{2} \left(\frac{(n-3)!}{(n-1)!} - \frac{1}{(n-1)^2} \right)$$
$$= \frac{n-2}{n-1} + 1 - \frac{n-2}{n-1}$$
$$= 1.$$

Proposition 6. We have

$$\mathrm{E}[N^*(n)] = n - 1.$$

Proof. The proof is by induction on *n*. Because $P(N^*(2) = 1) = 1$, it is true when n = 2, and so assume that $E[N_k^*] = k - 1$ for all k = 2, ..., n - 1. Then,

$$E[N^*(n) \mid D_n^*] = 1 + E[N^*(n - D_n^*) \mid D_n^*],$$
(5)

yielding

$$E[N^*(n)] = 1 + \sum_{i=0}^{n-1} E[N^*(n-i)] P(D_n^* = i)$$

= 1 + E[N^*(n)] P(D_n^* = 0) + $\sum_{i=1}^{n-1} E[N^*(n-i)] P(D_n^* = i)$
= 1 + E[N^*(n)] P(D_n^* = 0) + $\sum_{i=1}^{n-1} (n-i-1) P(D_n^* = i)$
= 1 + E[N^*(n)] P(D_n^* = 0) + (n-1)(1 - P(D_n^* = 0)) - E[D_n^*]
= 1 + E[N^*(n)] P(D_n^* = 0) + (n-1)(1 - P(D_n^* = 0)) - 1,

which proves the result.

Remark. Proposition 6 could also have been proved by using a martingale stopping argument, as in the proof of Proposition 4.

Proposition 7. For n > 2,

$$\operatorname{var}(N^*(n)) = n - 1.$$

Proof. Let $V(n) = var(N^*(n))$. The proof is by induction on n. As it is true for n = 3, since $N^*(3)$ is geometric with parameter $\frac{1}{2}$, assume it is true for all values between 2 and n. Now,

$$\operatorname{var}(N^*(n) \mid D_n^*) = \operatorname{var}(N^*(n - D_n^*) \mid D_n^*)$$

and, from (5) and Proposition 6,

$$E[N^*(n) \mid D_n^*] = n - D_n^*.$$

Hence, by the conditional variance formula,

$$V(n) = \sum_{i=0}^{n-1} V(n-i) P(D_n^* = i) + \operatorname{var}(D_n^*)$$

= $V(n) P(D_n^* = 0) + \sum_{i=1}^{n-1} V(n-i) P(D_n^* = i) + 1.$ (6)

Now, because $P(D_n^* = n - 2) = 0$ and V(1) = 0, the induction hypothesis yields

$$\sum_{i=1}^{n-1} V(n-i) \operatorname{P}(D_n^* = i) = \sum_{i=1}^{n-1} (n-i-1) \operatorname{P}(D_n^* = i).$$

Hence, from (6),

$$V(n) = V(n) P(D_n^* = 0) + (n - 1)(1 - P(D_n^* = 0)) - E[D_n^*] + 1$$

= V(n) P(D_n^* = 0) + (n - 1)(1 - P(D_n^* = 0)),

which proves the result.

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