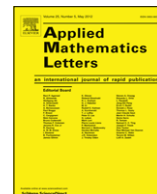




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# The expected value under the Yule model of the squared path-difference distance

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## ABSTRACT

The path-difference metric is one of the oldest and most popular distances for the comparison of phylogenetic trees, but its statistical properties are still quite unknown. In this work we compute the expected value under the Yule model of evolution of its square on the space of fully resolved rooted phylogenetic trees with  $n$  leaves. This complements previous work by Steel and Penny and by Mir and Rosselló, who computed this mean value for fully resolved unrooted and rooted phylogenetic trees, respectively, under the uniform distribution.

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## 1. Introduction

The definition and study of metrics for the comparison of rooted phylogenetic trees on the same set of taxa is a classical problem in phylogenetics [1, Chapter 30]. A classical and popular family of such metrics is based on the comparison, by different methods, of the vectors of lengths of the (undirected) paths connecting all pairs of taxa in the corresponding trees [2–5]. These metrics are generically called *nodal distances*, although some of them also have specific names. For instance, the metric defined through the euclidean distance between path-length vectors is called the *path-difference metric* [6], or the *cladistic difference* [2].

In contrast with those of other metrics, the statistical properties of these nodal distances are mostly unknown. Actually, the only statistical property that has been established so far for any one of them is the expected, or mean, value of the square of the path-difference metric for unrooted [6] and rooted [7] fully resolved phylogenetic trees under the uniform distribution (that is, when all phylogenetic trees with the same number of taxa are equiprobable). The knowledge of the expected value of a metric is useful, because it provides an indication about the significance of the similarity of two individuals measured through this metric [6].

But phylogeneticists consider also other probabilistic distributions on the space of phylogenetic trees on a fixed set of taxa, defined through stochastic models of evolution [1, Chapter 33]. The most popular such model is Yule's [8,9], defined by an evolutionary process where, at each step, each currently extant species can give rise, with the same probability, to two new species. Under this model, different phylogenetic trees with the same number of leaves may have different probabilities. Formal details of this model are given in the next section.

In this work we compute the expected value of the square of the path-difference metric for rooted fully resolved phylogenetic trees under the Yule model. Besides the aforementioned application of this value in the assessment of tree comparisons, the knowledge of formulas for this expected value under different models may allow the use of the path-difference metric to test stochastic models of tree growth, a popular line of research in the last few years which so far has been mostly based on shape indices [10].

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The proof of our formula for this expected value is based on several long algebraic computations. Since the space constraints prevent us from providing full detail in these computations, we give here only the overall idea of their thread, which enables the willing reader to reproduce them, and we have posted a version of this work containing all details on the arXiv preprint server [11].

## 2. Preliminaries

In this work, by a *phylogenetic tree* on a set  $S$  of taxa we mean a fully resolved, or binary, rooted tree with its leaves bijectively labeled in  $S$ . We understand such a rooted tree as a directed graph, with its arcs pointing away from the root. To simplify the language, we shall always identify a leaf of a phylogenetic tree with its label. We shall also use the term *phylogenetic tree with  $n$  leaves* to refer to a phylogenetic tree on the set  $\{1, \dots, n\}$ . We shall denote by  $\mathcal{T}(S)$  the space of all phylogenetic trees on  $S$  and by  $\mathcal{T}_n$  the space of all phylogenetic trees with  $n$  leaves.

Whenever there exists a directed path from  $u$  to  $v$  in a phylogenetic tree  $T$ , we shall say that  $v$  is a *descendant* of  $u$ . The *distance*  $d_T(u, v)$  between two nodes  $u, v$  in a phylogenetic tree  $T$  is the length (in numbers of arcs) of the unique undirected path connecting  $u$  and  $v$ . The *depth*  $\delta_T(v)$  of a node  $v$  in  $T$  is the distance from the root  $r$  of  $T$  to  $v$ . The *path-difference distance* [2,3] between a pair of trees  $T, T' \in \mathcal{T}_n$  is

$$d_v(T, T') = \sqrt{\sum_{1 \leq i < j \leq n} (d_T(i, j) - d_{T'}(i, j))^2}.$$

The *Yule*, or *equal-rate Markov*, model of evolution [8,9] is a stochastic model of phylogenetic trees' growth. It starts with a node, and at every step a leaf is chosen randomly and uniformly and it is split into two leaves. Finally, the labels are assigned randomly and uniformly to the leaves once the desired number of leaves is reached. Under this model, if  $T$  is a phylogenetic tree with  $n$  leaves and set of internal nodes  $V_{\text{int}}(T)$ , and if for every internal node  $v$  we denote by  $\ell_T(v)$  the number of its descendant leaves, then the probability of  $T$  is [12,13]

$$P_Y(T) = \frac{2^{n-1}}{n!} \prod_{v \in V_{\text{int}}(T)} \frac{1}{\ell_T(v) - 1}.$$

For every  $n \geq 1$ , let  $H_n = \sum_{i=1}^n 1/i$  and  $H_n^{(2)} = \sum_{i=1}^n 1/i^2$ . Let, moreover,  $H_0 = H_0^{(2)} = 0$ .  $H_n$  is called the  *$n$ th harmonic number*, and  $H_n^{(2)}$ , the  *$n$ th generalized harmonic number of power 2*.

## 3. The main results

Let  $N_n^2$  be the random variable that chooses independently a pair of trees  $T, T' \in \mathcal{T}_n$  and computes  $d_v(T, T')^2$ . In this section we establish the following result.

**Theorem 1.** *The expected value of  $N_n^2$  under the Yule model is*

$$E_Y(N_n^2) = \frac{2n}{n-1} (2(n^2 + 24n + 7)H_n + 13n^2 - 46n + 1 - 16(n+1)H_n^2 - 8(n^2 - 1)H_n^{(2)}).$$

To prove this theorem, we shall use the auxiliary random variables  $D_n$  and  $D_n^{(2)}$  that choose a tree  $T \in \mathcal{T}_n$  and compute  $D(T) = \sum_{1 \leq i < j \leq n} d_T(i, j)$  and  $D^{(2)}(T) = \sum_{1 \leq i < j \leq n} d_T(i, j)^2$ , respectively. The connection between  $E_Y(N_n^2)$  and the expected values under the Yule model of  $D_n$  and  $D_n^{(2)}$  is given by the following result.

**Proposition 2.**  $E_Y(N_n^2) = 2(E_Y(D_n^{(2)}) - E_Y(D_n)^2 / \binom{n}{2})$ .

**Proof.** By developing  $E_Y(N_n^2)$  from its raw definition, we obtain

$$\begin{aligned} E_Y(N_n^2) &= \sum_{T, T' \in \mathcal{T}_n} d_v(T, T')^2 p_Y(T) p_Y(T') = \sum_{T, T' \in \mathcal{T}_n} \left( \sum_{1 \leq i < j \leq n} (d_T(i, j) - d_{T'}(i, j))^2 \right) p_Y(T) p_Y(T') \\ &= 2 \sum_T \left( \sum_{1 \leq i < j \leq n} d_T(i, j)^2 \right) p_Y(T) - 2 \sum_{1 \leq i < j \leq n} \left( \sum_T d_T(i, j) p_Y(T) \right)^2 \\ &= 2E_Y(D_n^{(2)}) - 2 \binom{n}{2} \left( \sum_T d_T(1, 2) p_Y(T) \right)^2 \end{aligned}$$

and now

$$E_Y(D_n) = \sum_{T \in \mathcal{T}_n} \sum_{1 \leq i < j \leq n} d_T(i, j) p_Y(T) = \sum_{1 \leq i < j \leq n} \sum_T d_T(i, j) p_Y(T) = \binom{n}{2} \sum_T d_T(1, 2) p_Y(T)$$

which implies that  $(\sum_T d_T(1, 2) p_Y(T))^2 = E_Y(D_n)^2 / \binom{n}{2}^2$ , and the formula in the statement follows.  $\square$

It is known that the expected value under the Yule model of  $D_n$  is  $E_Y(D_n) = 2n(n + 1)H_n - 4n^2$  [14]. As regards  $E_Y(D_n^{(2)})$ , its value is given by the following result. We postpone the proof to the Appendix at the end of the work.

**Proposition 3.**  $E_Y(D_n^{(2)}) = 8n(n + 1)(H_n^2 - H_n^{(2)}) - 2n(15n + 7)H_n + 45n^2 - n$ .

Then, replacing in the expression for  $E_Y(N_n^2)$  given in Proposition 2 the terms  $E_Y(D_n)$  and  $E_Y(D_n^{(2)})$  by their values, we obtain the formula for  $E_Y(N_n^2)$  given in Theorem 1.

### 4. Conclusions

In this work we have computed the expected value  $E_Y(N_n^2)$  of the square of the path-difference metric for rooted fully resolved phylogenetic trees under the Yule model. This complements the computation of this expected value under the uniform distribution carried out in [7].

The proof of the formula for  $E_Y(N_n^2)$  consists of several long algebraic manipulations of sums of sequences. Since it is not difficult to make some mistake in such long algebraic computations, to double check our result we have computed the exact value of  $E_Y(N_n^2)$  ( $n = 3, \dots, 7$ ), by generating all trees with up to seven leaves, as well as numerical approximations to  $E_Y(N_n^2)$  ( $n = 10, 20, \dots, 100$ ), by generating random trees until the numerical method stabilizes. These numerical experiments confirm that our formula gives the right figures. The Python scripts used in these computations, as well as a full account of the results obtained, are available on the Supplementary Material web page <http://bioinfo.uib.es/~recerca/phylo trees/nodal dist Yule/>.

The formulas for  $E_Y(N_n^2)$  and  $E_U(N_n^2)$  grow in different orders:  $E_Y(N_n^2)$  is in  $O(n^2 \ln(n))$ , while  $E_U(N_n^2)$  is in  $O(n^3)$  [7]. Therefore, they can be used to test the Yule and the uniform models as null stochastic models of evolution for collections of phylogenetic trees reconstructed by different methods. This kind of analysis has only been performed so far through shape indices of single trees, not by means of the comparison of pairs of trees. We shall report on it elsewhere.

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### Appendix

In this appendix we prove Proposition 3, as well as some preliminary lemmas. To begin with, the following identities on harmonic numbers will be systematically used in the subsequent proofs, usually without any further notice.

**Lemma.** For every  $n \geq 2$ :

$$\begin{aligned} (1) \sum_{k=1}^{n-1} H_k &= n(H_n - 1) & (2) \sum_{k=1}^{n-1} kH_k &= \frac{1}{4}n(n-1)(2H_n - 1) & (3) \sum_{k=1}^{n-1} H_k/(k+1) &= \frac{1}{2}(H_n^2 - H_n^{(2)}) \\ (4) \sum_{k=1}^{n-1} kH_k H_{n-k} &= \binom{n+1}{2} (H_{n+1}^2 - H_{n+1}^{(2)} - 2H_{n+1} + 2) & (5) \sum_{k=1}^{n-1} (H_k^2 - H_k^{(2)}) &= n(H_n^2 - H_n^{(2)}) - 2n(H_n - 1). \\ (6) \sum_{k=1}^{n-1} k(H_k^2 - H_k^{(2)}) &= \binom{n}{2} (H_n^2 - H_n^{(2)}) - \frac{1}{4}n(n-1)(2H_n - 1). \end{aligned}$$

**Proof.** Identities (1)–(3) are well known and easily proved by induction on  $n$ ; see, for instance, [15, Section 1.2.7]. Identity (4) is proved in [16, Theorem 2]. Identities (5) and (6) are easily proved using Abel’s lemma on summation by parts, as is done for other identities in [17].  $\square$

Let us consider now the random variables  $S_n$  and  $S_n^{(2)}$  that choose a tree  $T \in \mathcal{T}_n$  and compute their *Sackin indexes* [18]  $S(T) = \sum_{i=1}^n \delta_T(i)$  and  $S^{(2)}(T) = \sum_{1 \leq i < j \leq n} \delta_T(i)^2$ , respectively. It is known that the expected value under the Yule model of  $S_n$  is  $E_Y(S_n) = 2n(H_n - 1)$  [19]. We shall compute now the expected values under this model of  $S_n^{(2)}$  and  $D_n^{(2)}$ : the first will be used in the computation of the second.

Given two phylogenetic trees  $T, T'$  on disjoint sets of taxa  $S, S'$ , respectively, we shall denote by  $T \hat{\wedge} T'$  the phylogenetic tree on  $S \cup S'$  obtained by connecting the roots of  $T$  and  $T'$  to a (new) common root. Every phylogenetic tree on  $\{1, \dots, n\}$  is obtained as  $T_k \hat{\wedge} T'_{n-k}$ , for some  $1 \leq k \leq n - 1$ , some subset  $S_k \subseteq \{1, \dots, n\}$  with  $k$  elements, some tree  $T_k$  on  $S_k$  and some tree  $T'_{n-k}$  on  $S_k^c = \{1, \dots, n\} \setminus S_k$ . Actually, every phylogenetic tree on  $\{1, \dots, n\}$  is obtained in this way *twice*. The following easy lemma on the probability of  $T \hat{\wedge} T'$  under the Yule model is a direct consequence of the formula for the probability of a tree; see [20, Lemma 1].

**Lemma 4.** Let  $\emptyset \neq S_k \subsetneq \{1, \dots, n\}$  with  $|S_k| = k$ , and let  $T_k \in \mathcal{T}(S_k)$  and  $T'_{n-k} \in \mathcal{T}(S_k^c)$ . Then

$$P_Y(T_k \hat{\wedge} T'_{n-k}) = \frac{2}{(n-1) \binom{n}{k}} P_Y(T_k) P_Y(T'_{n-k}).$$

**Lemma.** Let  $T, T'$  be two phylogenetic trees on disjoint sets of taxa  $S, S'$ , with  $|S| = k$  and  $|S'| = n - k$ . Then:

- (1)  $S^{(2)}(T \hat{\wedge} T') = S^{(2)}(T) + S^{(2)}(T') + 2(S(T) + S(T')) + n$ .
- (2)  $D^{(2)}(T \hat{\wedge} T') = D^{(2)}(T) + D^{(2)}(T') + (n - k)(S^{(2)}(T) + 4S(T)) + k(S^{(2)}(T') + 4S(T')) + 2S(T)S(T') + 4k(n - k)$ .

**Proof.** Let us assume, without any loss of generality, that  $S = \{1, \dots, k\}$  and  $S' = \{k + 1, \dots, n\}$ . Then, these identities are a direct consequence of the equalities

$$\delta_{T \hat{\wedge} T'}(i)^2 = \begin{cases} (\delta_T(i) + 1)^2 & \text{if } 1 \leq i \leq k \\ (\delta_{T'}(i) + 1)^2 & \text{if } k + 1 \leq i \leq n \end{cases} \quad d_{T \hat{\wedge} T'}(i, j)^2 = \begin{cases} d_T(i, j)^2 & \text{if } 1 \leq i < j \leq k \\ d_{T'}(i, j)^2 & \text{if } k + 1 \leq i < j \leq n \\ (\delta_T(i) + \delta_{T'}(j) + 2)^2 & \text{if } 1 \leq i \leq k < j \leq n. \end{cases} \quad \square$$

Now we can compute explicit formulas for  $E_Y(S_n^{(2)})$  and  $E_Y(D_n^{(2)})$ .

**Proposition.**  $E_Y(S_n^{(2)}) = 4n(H_n^2 - H_n^{(2)}) - 6n(H_n - 1)$ .

**Proof.** We compute  $E_Y(S_n^{(2)})$  using its definition:

$$\begin{aligned} E_Y(S_n^{(2)}) &= \sum_{T \in \mathcal{T}_n} S^{(2)}(T) \cdot P_Y(T) = \frac{1}{2} \sum_{k=1}^{n-1} \sum_{\substack{S_k \subseteq \{1, \dots, n\} \\ |S_k|=k}} \sum_{T_k \in \mathcal{T}(S_k)} \sum_{T'_{n-k} \in \mathcal{T}(S_k^c)} S^{(2)}(T_k \hat{\wedge} T'_{n-k}) \cdot P_Y(T_k \hat{\wedge} T'_{n-k}) \\ &= \frac{1}{2} \sum_{k=1}^{n-1} \binom{n}{k} \sum_{T_k \in \mathcal{T}_k} \sum_{T'_{n-k} \in \mathcal{T}_{n-k}} \left( S^{(2)}(T_k) + S^{(2)}(T'_{n-k}) + 2(S(T_k) + S(T'_{n-k})) + n \right) \cdot \frac{2}{(n-1) \binom{n}{k}} P_Y(T_k) P_Y(T'_{n-k}) \\ &= \frac{1}{n-1} \sum_{k=1}^{n-1} \left( \sum_{T_k} S^{(2)}(T_k) P_Y(T_k) + \sum_{T'_{n-k}} S^{(2)}(T'_{n-k}) P_Y(T'_{n-k}) + 2 \sum_{T_k} S(T_k) P_Y(T_k) \right. \\ &\quad \left. + 2 \sum_{T'_{n-k}} S(T'_{n-k}) P_Y(T'_{n-k}) + n \right) \\ &= \frac{1}{n-1} \sum_{k=1}^{n-1} \left( E_Y(S_k^{(2)}) + E_Y(S_{n-k}^{(2)}) + 2E_Y(S_k) + 2E_Y(S_{n-k}) + n \right) \\ &= \frac{2}{n-1} \sum_{k=1}^{n-1} E_Y(S_k^{(2)}) + \frac{4}{n-1} \sum_{k=1}^{n-1} E_Y(S_k) + n. \end{aligned}$$

And then

$$\begin{aligned} E_Y(S_n^{(2)}) &= \frac{n-2}{n-1} \cdot \frac{2}{n-2} \sum_{k=1}^{n-2} E_Y(S_k^{(2)}) + \frac{2}{n-1} E_Y(S_{n-1}^{(2)}) + \frac{n-2}{n-1} \cdot \frac{4}{n-2} \sum_{k=1}^{n-2} E_Y(S_k) \\ &\quad + \frac{4}{n-1} E_Y(S_{n-1}) + \frac{n-2}{n-1} \cdot (n-1) + 2 \\ &= \frac{n-2}{n-1} E_Y(S_{n-1}^{(2)}) + \frac{2}{n-1} E_Y(S_{n-1}^{(2)}) + \frac{4}{n-1} E_Y(S_{n-1}) + 2 = \frac{n}{n-1} E_Y(S_{n-1}^{(2)}) + 8H_{n-1} - 6. \end{aligned}$$

Setting  $x_n = E_Y(S_n^{(2)})/n$ , this recurrence becomes

$$x_n = x_{n-1} + \frac{8H_{n-1}}{n} - \frac{6}{n}.$$

Since  $S^{(2)}$  applied to a single node is 0,  $x_1 = E_Y(S_1^{(2)}) = 0$ , and the solution of this recursive equation with this initial condition is

$$x_n = \sum_{k=2}^n \left( \frac{8H_{k-1}}{k} - \frac{6}{k} \right) = 8 \sum_{k=1}^{n-1} \frac{H_k}{k+1} - 6 \sum_{k=2}^n \frac{1}{k} = 4(H_n^2 - H_n^{(2)}) - 6(H_n - 1)$$

from where we deduce the identity in the statement.  $\square$

**Proposition 5.**  $E_Y(D_n^{(2)}) = 8n(n+1)(H_n^2 - H_n^{(2)}) - 2n(15n+7)H_n + 45n^2 - n$ .

**Proof.** If we compute  $E_Y(D_n^{(2)})$  as we did with  $E_Y(S_n^{(2)})$  in the last proposition, we obtain

$$\begin{aligned} E_Y(D_n^{(2)}) &= \sum_{T \in \mathcal{F}_n} D^{(2)}(T) \cdot p_Y(T) = \frac{1}{2} \sum_{k=1}^{n-1} \sum_{\substack{S_k \subseteq \{1, \dots, n\} \\ |S_k|=k}} \sum_{T_k \in \mathcal{F}(S_k)} \sum_{T'_{n-k} \in \mathcal{F}(S_k^c)} D^{(2)}(T_k \hat{\wedge} T'_{n-k}) \cdot p_Y(T_k \hat{\wedge} T'_{n-k}) \\ &= \frac{1}{n-1} \sum_{k=1}^{n-1} \left[ \sum_{T_k} D^{(2)}(T_k) P_Y(T_k) + \sum_{T'_{n-k}} D^{(2)}(T'_{n-k}) P_Y(T'_{n-k}) \right. \\ &\quad \left. + 2 \left( \sum_{T_k} S(T_k) P_Y(T_k) \right) \left( \sum_{T'_{n-k}} S(T'_{n-k}) P_Y(T'_{n-k}) \right) + (n-k) \sum_{T_k} S^{(2)}(T_k) P_Y(T_k) \right. \\ &\quad \left. + 4(n-k) \sum_{T_k} S(T_k) P_Y(T_k) + k \sum_{T'_{n-k}} S^{(2)}(T'_{n-k}) P_Y(T'_{n-k}) + 4k \sum_{T'_{n-k}} S(T'_{n-k}) P_Y(T'_{n-k}) + 4k(n-k) \right] \\ &= \frac{2}{n-1} \sum_{k=1}^{n-1} \left( E_Y(D_k^{(2)}) + E_Y(S_k) E_Y(S_{n-k}) + (n-k) E_Y(S_k^{(2)}) + 4(n-k) E_Y(S_k) \right) + \frac{2}{3} n(n+1) \end{aligned}$$

and therefore

$$\begin{aligned} E_Y(D_n^{(2)}) &= \frac{n-2}{n-1} \cdot \frac{2}{n-2} \sum_{k=1}^{n-2} E_Y(D_k^{(2)}) + \frac{2}{n-1} E_Y(D_{n-1}^{(2)}) \\ &\quad + \frac{n-2}{n-1} \cdot \frac{2}{n-2} \sum_{k=1}^{n-2} E_Y(S_k) E_Y(S_{n-1-k}) + \frac{2}{n-1} \left( \sum_{k=1}^{n-1} E_Y(S_k) E_Y(S_{n-k}) - \sum_{k=1}^{n-2} E_Y(S_k) E_Y(S_{n-1-k}) \right) \\ &\quad + \frac{n-2}{n-1} \cdot \frac{2}{n-2} \sum_{k=1}^{n-2} (n-1-k) E_Y(S_k^{(2)}) + \frac{2}{n-1} \left( \sum_{k=1}^{n-1} (n-k) E_Y(S_k^{(2)}) - \sum_{k=1}^{n-2} (n-1-k) E_Y(S_k^{(2)}) \right) \\ &\quad + \frac{n-2}{n-1} \cdot \frac{8}{n-2} \sum_{k=1}^{n-2} (n-1-k) E_Y(S_k) + \frac{8}{n-1} \left( \sum_{k=1}^{n-1} (n-k) E_Y(S_k) - \sum_{k=1}^{n-2} (n-1-k) E_Y(S_k) \right) \\ &\quad + \frac{n-2}{n-1} \cdot \frac{2}{3} n(n-1) + \frac{2}{3} n(n+1) - \frac{n-2}{n-1} \cdot \frac{2}{3} n(n-1) \\ &= \frac{n-2}{n-1} E_Y(D_{n-1}^{(2)}) + \frac{2}{n-1} E_Y(D_{n-1}^{(2)}) + \frac{2}{n-1} \sum_{k=1}^{n-2} E_Y(S_k) (E_Y(S_{n-k}) - E_Y(S_{n-k-1})) \\ &\quad + \frac{2}{n-1} \sum_{k=1}^{n-1} E_Y(S_k^{(2)}) + \frac{8}{n-1} \sum_{k=1}^{n-1} E_Y(S_k) + 2n \\ &= \frac{n}{n-1} E_Y(D_{n-1}^{(2)}) + 8n(H_n^2 - H_n^{(2)}) - 14nH_{n-1} + 15n - 14. \end{aligned}$$

Setting  $x_n = E_Y(D_n^{(2)})/n$ , this recurrence becomes

$$x_n = x_{n-1} + 8(H_n^2 - H_n^{(2)}) - 14H_{n-1} + 15 - \frac{14}{n}.$$

The solution of this recurrence with  $x_1 = E_Y(D_1^{(2)}) = 0$  is

$$\begin{aligned} x_n &= \sum_{k=2}^n \left( 8(H_k^2 - H_k^{(2)}) - 14H_{k-1} + 15 - \frac{14}{k} \right) \\ &= 8(n+1)(H_n^2 - H_n^{(2)}) - 2(15n+7)H_n + 45n - 1 \end{aligned}$$

from which we deduce the formula in the statement.  $\square$

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